



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:10 PM EDT

PDB ID : 3AIC / pdb_00003aic
Title : Crystal Structure of Glucansucrase from Streptococcus mutans
Authors : Ito, K.; Ito, S.; Shimamura, T.; Iwata, S.
Deposited on : 2010-05-12
Resolution : 3.11 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

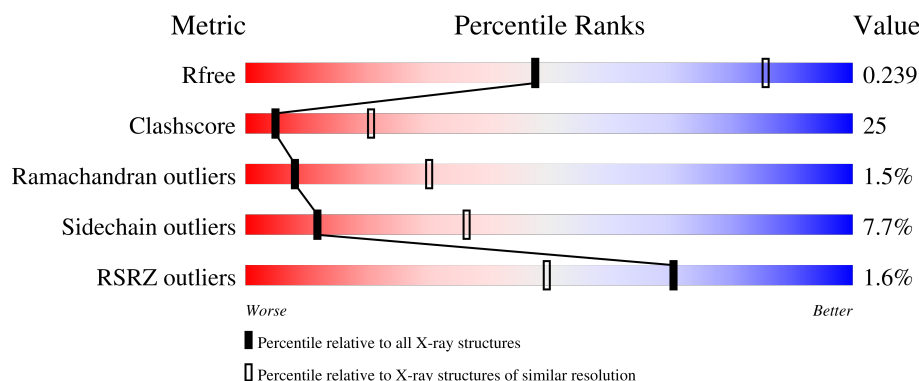
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

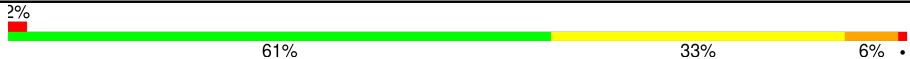
The reported resolution of this entry is 3.11 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



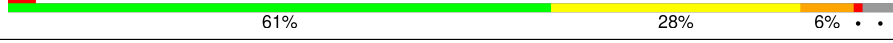
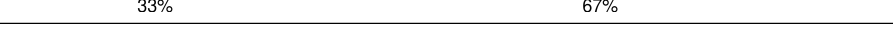
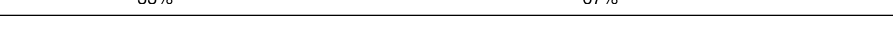
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	844	
1	B	844	
1	C	844	
1	D	844	
1	E	844	

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Mol	Chain	Length	Quality of chain
1	F	844	% 
1	G	844	% 
1	H	844	3% 
2	I	3	
2	J	3	
2	K	3	
2	L	3	
2	M	3	
2	N	3	
2	O	3	
2	P	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AC1	I	3	-	-	X	-
2	AC1	K	3	-	-	X	-
2	AC1	M	3	-	-	X	-
4	MES	B	5001	-	X	-	-
4	MES	F	5001	-	X	-	-
4	MES	G	5001	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 52865 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glucosyltransferase-SI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	842	Total	C	N	O	S	0	0	0
			6643	4184	1141	1302	16			
1	B	747	Total	C	N	O	S	0	0	0
			5854	3684	1005	1151	14			
1	C	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	D	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	E	843	Total	C	N	O	S	0	0	0
			6654	4193	1142	1303	16			
1	F	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	G	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	H	807	Total	C	N	O	S	0	0	0
			6372	4019	1093	1244	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	597	ASP	ASN	SEE REMARK 999	UNP P13470
A	600	LYS	ARG	SEE REMARK 999	UNP P13470
A	727	ILE	THR	SEE REMARK 999	UNP P13470
A	734	VAL	ALA	SEE REMARK 999	UNP P13470
B	597	ASP	ASN	SEE REMARK 999	UNP P13470
B	600	LYS	ARG	SEE REMARK 999	UNP P13470
B	727	ILE	THR	SEE REMARK 999	UNP P13470
B	734	VAL	ALA	SEE REMARK 999	UNP P13470
C	597	ASP	ASN	SEE REMARK 999	UNP P13470
C	600	LYS	ARG	SEE REMARK 999	UNP P13470
C	727	ILE	THR	SEE REMARK 999	UNP P13470
C	734	VAL	ALA	SEE REMARK 999	UNP P13470
D	597	ASP	ASN	SEE REMARK 999	UNP P13470

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Chain	Residue	Modelled	Actual	Comment	Reference
D	600	LYS	ARG	SEE REMARK 999	UNP P13470
D	727	ILE	THR	SEE REMARK 999	UNP P13470
D	734	VAL	ALA	SEE REMARK 999	UNP P13470
E	597	ASP	ASN	SEE REMARK 999	UNP P13470
E	600	LYS	ARG	SEE REMARK 999	UNP P13470
E	727	ILE	THR	SEE REMARK 999	UNP P13470
E	734	VAL	ALA	SEE REMARK 999	UNP P13470
F	597	ASP	ASN	SEE REMARK 999	UNP P13470
F	600	LYS	ARG	SEE REMARK 999	UNP P13470
F	727	ILE	THR	SEE REMARK 999	UNP P13470
F	734	VAL	ALA	SEE REMARK 999	UNP P13470
G	597	ASP	ASN	SEE REMARK 999	UNP P13470
G	600	LYS	ARG	SEE REMARK 999	UNP P13470
G	727	ILE	THR	SEE REMARK 999	UNP P13470
G	734	VAL	ALA	SEE REMARK 999	UNP P13470
H	597	ASP	ASN	SEE REMARK 999	UNP P13470
H	600	LYS	ARG	SEE REMARK 999	UNP P13470
H	727	ILE	THR	SEE REMARK 999	UNP P13470
H	734	VAL	ALA	SEE REMARK 999	UNP P13470

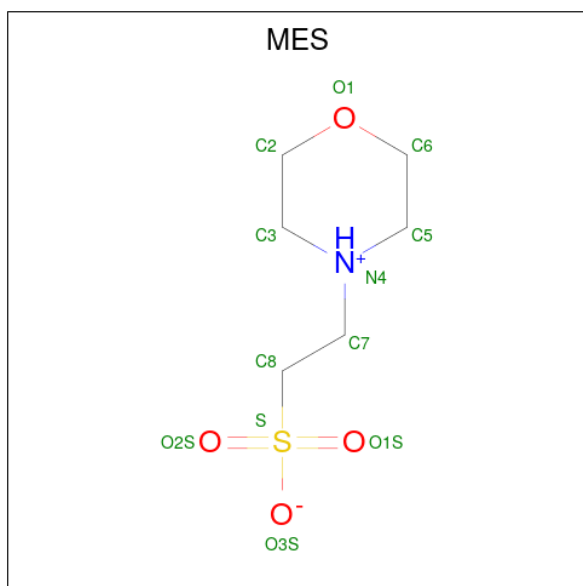
- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	J	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	K	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	L	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	M	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	N	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	O	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	P	3	Total	C	N	O	0	0	0
			44	25	1	18			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0
3	G	1	Total Ca 1 1	0	0
3	H	1	Total Ca 1 1	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 12 6 1 4 1	0	0
4	B	1	Total C N O S 12 6 1 4 1	0	0
4	C	1	Total C N O S 12 6 1 4 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

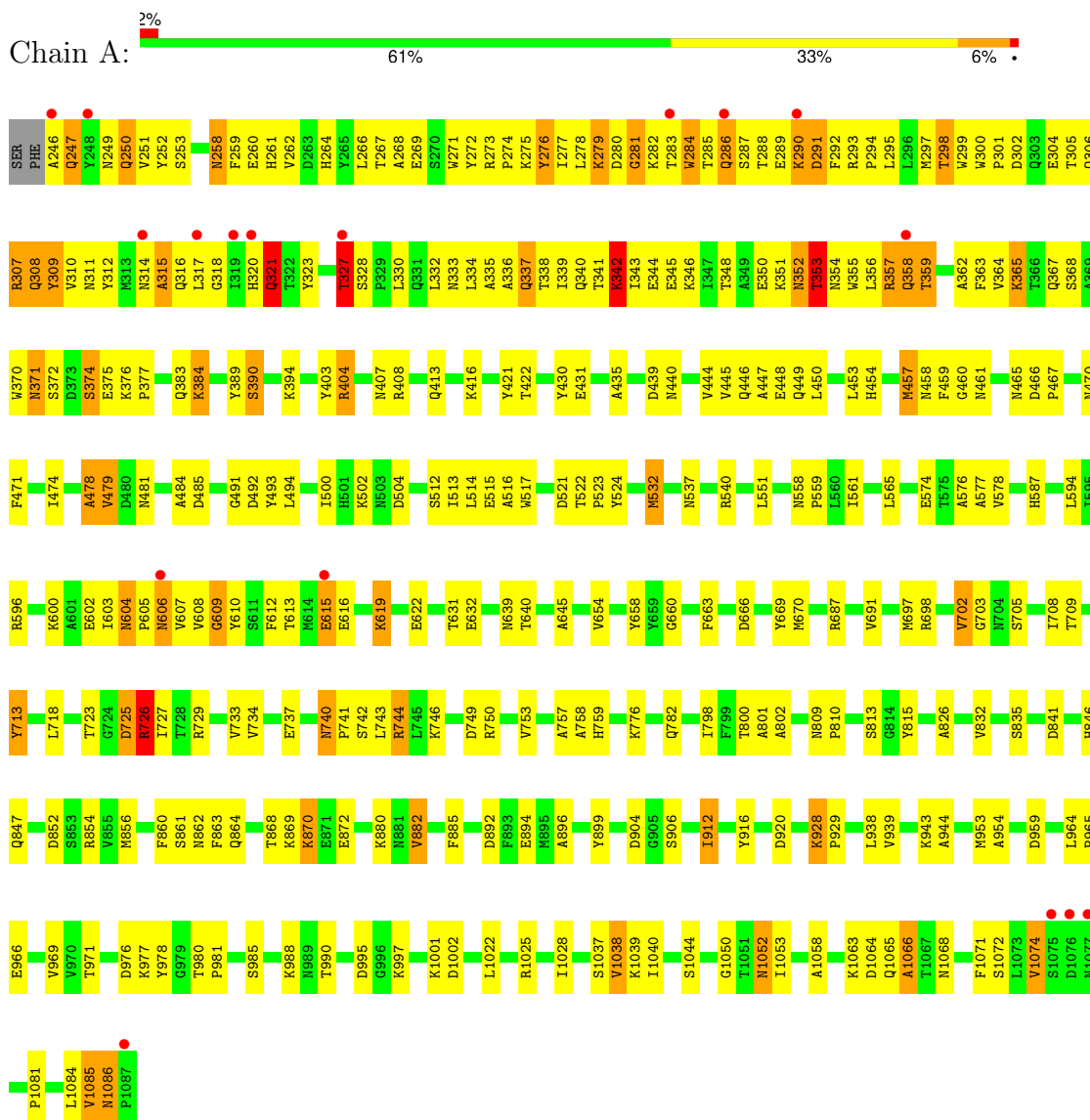
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	33	Total	O	0	0
			33	33		
5	B	20	Total	O	0	0
			20	20		
5	C	32	Total	O	0	0
			32	32		
5	D	40	Total	O	0	0
			40	40		
5	E	48	Total	O	0	0
			48	48		
5	F	15	Total	O	0	0
			15	15		
5	G	34	Total	O	0	0
			34	34		
5	H	24	Total	O	0	0
			24	24		

3 Residue-property plots

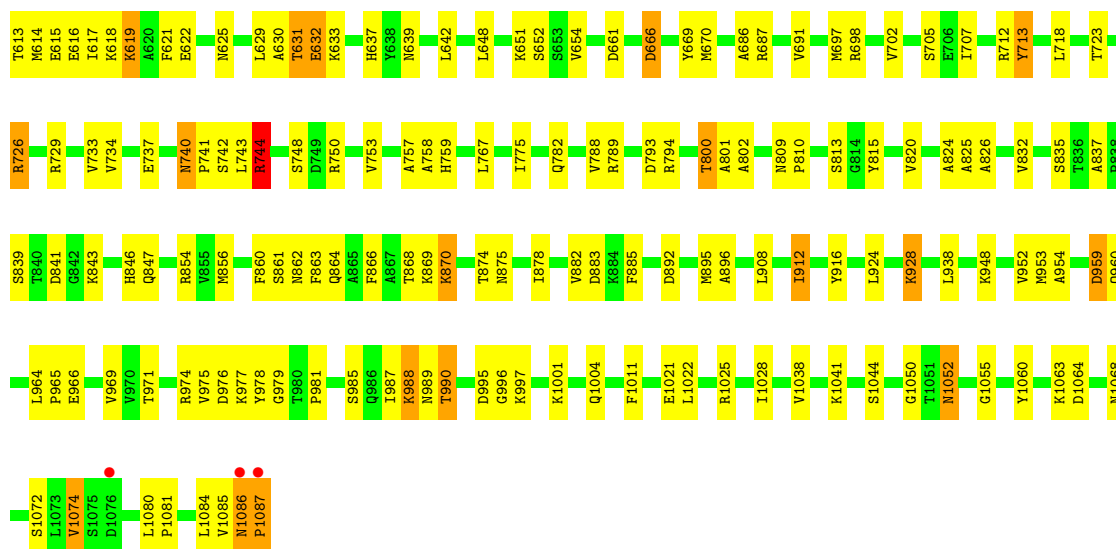
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Glucosyltransferase-SI

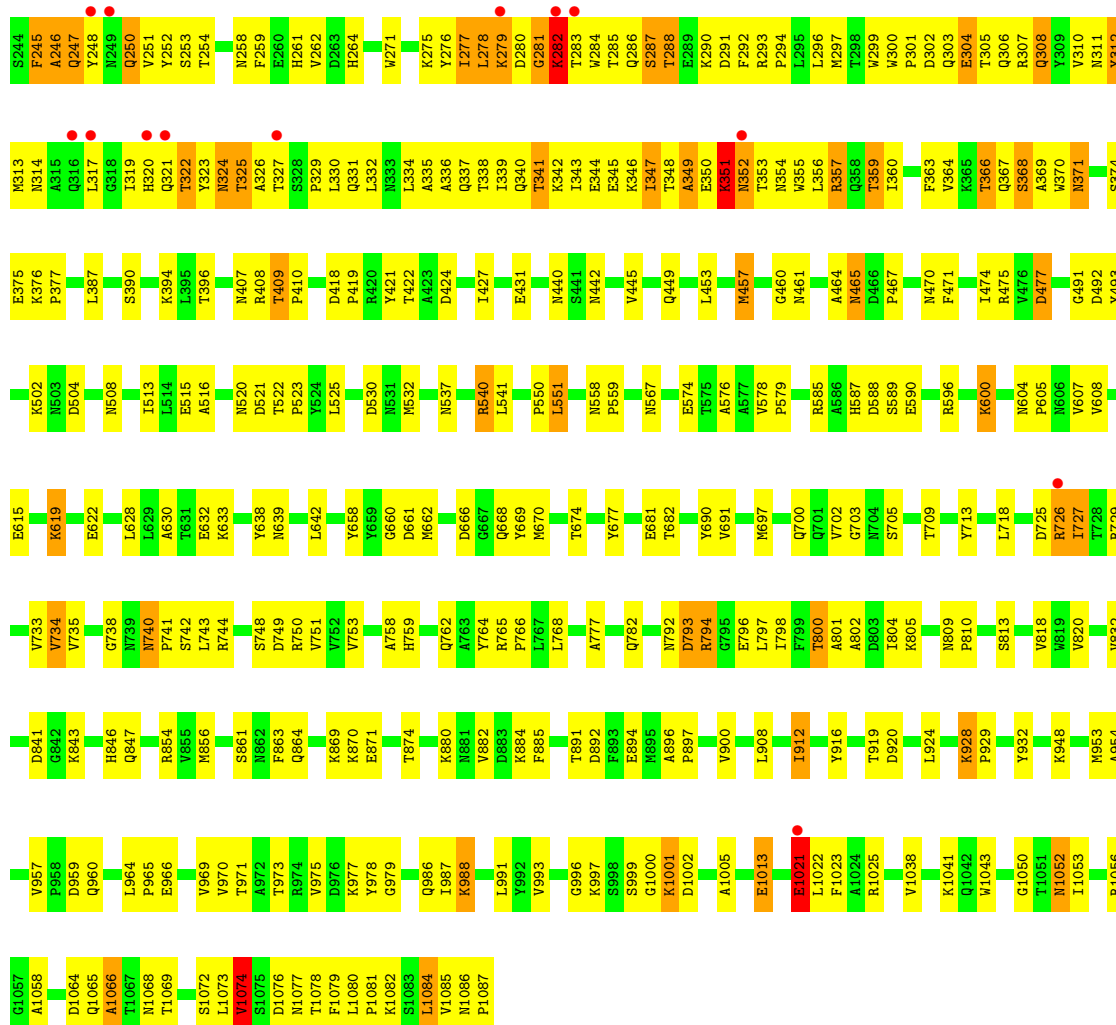


• Molecule 1: Glucosyltransferase-SI

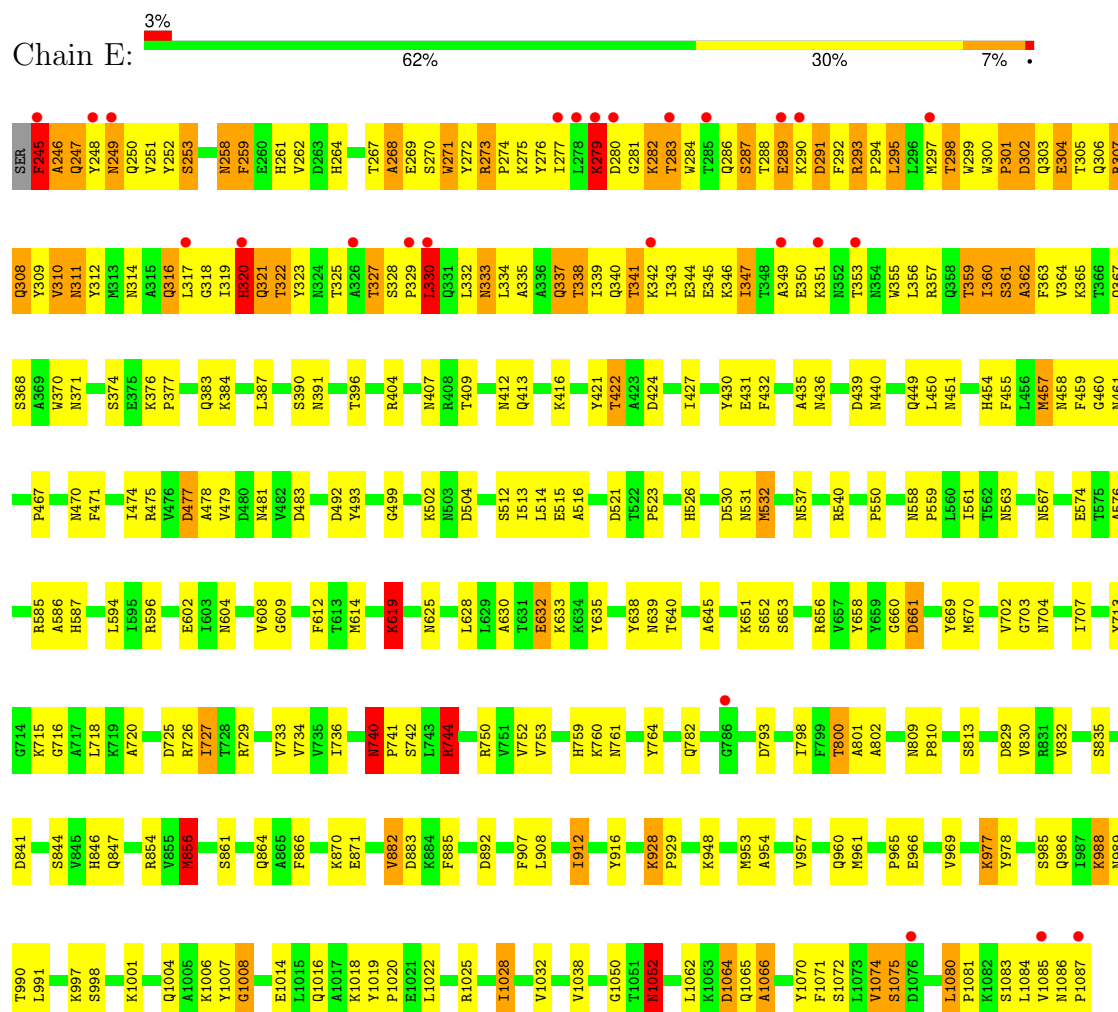


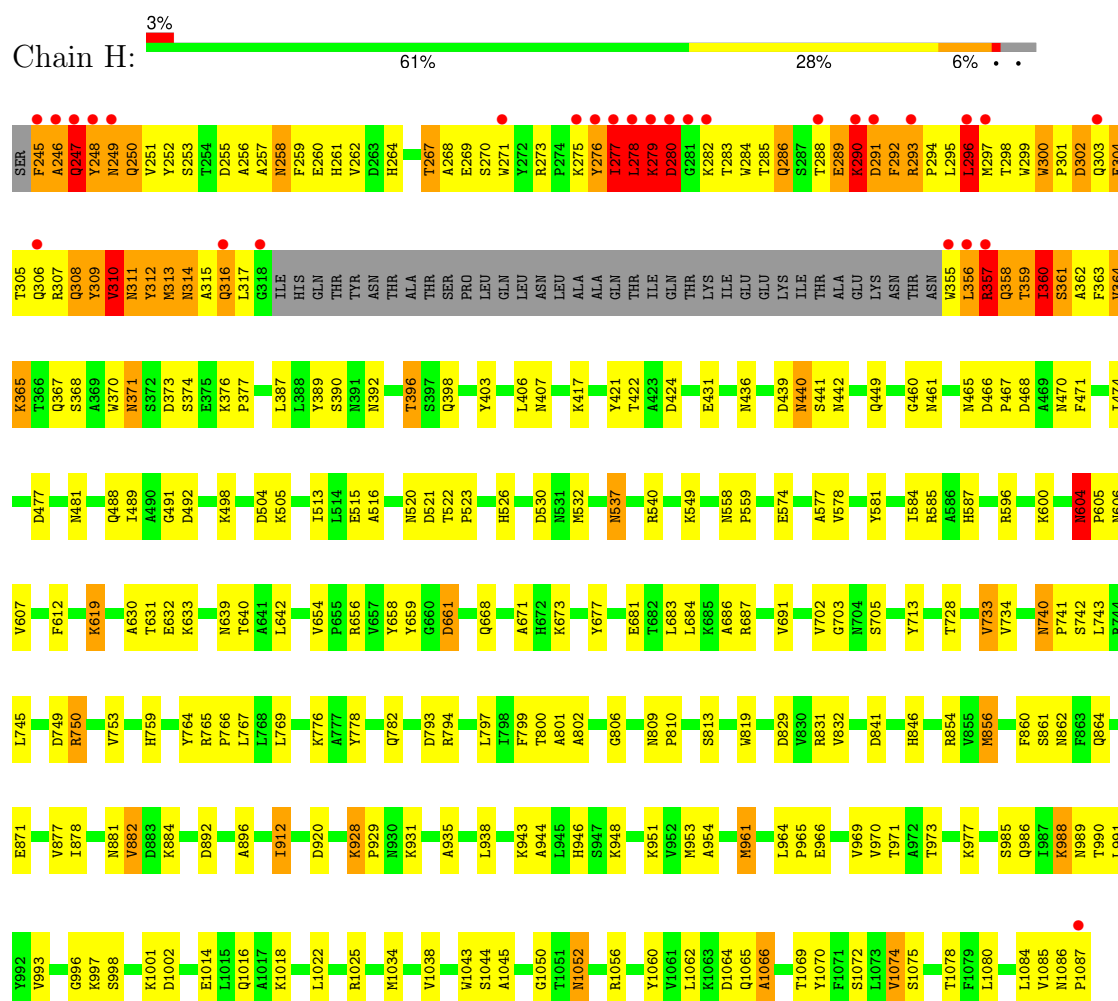


• Molecule 1: Glucosyltransferase-SI



• Molecule 1: Glucosyltransferase-SI





- Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose





- Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:



- Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain M:



- Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain N:



- Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain O:



- Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain P:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	295.52Å 214.41Å 220.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.77 – 3.11 61.77 – 3.11	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.77-3.11) 95.2 (61.77-3.11)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.211 , 0.244 0.208 , 0.239	Depositor DCC
R_{free} test set	12026 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	52865	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9554e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, CA, AC1, MES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.28	17/6784 (0.3%)	1.26	29/9213 (0.3%)
1	B	1.07	13/5976 (0.2%)	1.22	37/8113 (0.5%)
1	C	1.18	7/6802 (0.1%)	1.24	27/9237 (0.3%)
1	D	1.17	7/6802 (0.1%)	1.23	24/9237 (0.3%)
1	E	1.26	21/6796 (0.3%)	1.26	37/9229 (0.4%)
1	F	1.00	5/6802 (0.1%)	1.16	17/9237 (0.2%)
1	G	1.19	5/6802 (0.1%)	1.27	32/9237 (0.3%)
1	H	1.12	9/6510 (0.1%)	1.20	24/8837 (0.3%)
All	All	1.16	84/53274 (0.2%)	1.23	227/72340 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	H	0	1
All	All	0	2

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	HIS	CE1-NE2	33.41	1.66	1.32
1	E	245	PHE	N-CA	12.75	1.70	1.46
1	H	249	ASN	CG-OD1	11.93	1.46	1.23
1	A	320	HIS	CG-CD2	11.82	1.48	1.35
1	B	250	GLN	CD-NE2	11.48	1.57	1.33
1	B	1084	LEU	C-O	11.03	1.37	1.24
1	A	320	HIS	CG-ND1	10.89	1.50	1.38
1	E	273	ARG	CZ-NH1	10.06	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1086	ASN	CA-C	9.60	1.62	1.52
1	B	912	ILE	CA-CB	-8.91	1.43	1.54
1	E	320	HIS	CG-ND1	8.64	1.47	1.38
1	A	654	VAL	CA-C	-8.51	1.46	1.53
1	E	333	ASN	C-O	-8.06	1.14	1.24
1	E	279	LYS	CE-NZ	7.91	1.73	1.49
1	B	729	ARG	CZ-NH1	-7.86	1.21	1.32
1	A	290	LYS	CE-NZ	7.45	1.71	1.49
1	B	249	ASN	CB-CG	7.07	1.69	1.52
1	F	396	THR	CA-CB	7.03	1.58	1.53
1	E	245	PHE	CG-CD1	7.00	1.53	1.38
1	G	912	ILE	CA-CB	-6.97	1.46	1.54
1	E	320	HIS	CE1-NE2	6.73	1.39	1.32
1	B	271	TRP	CZ2-CH2	6.73	1.50	1.37
1	E	720	ALA	CA-CB	-6.70	1.41	1.53
1	B	257	ALA	CA-CB	6.68	1.64	1.53
1	B	1087	PRO	N-CD	6.66	1.57	1.47
1	B	271	TRP	CD2-CE3	6.59	1.50	1.40
1	H	403	TYR	N-CA	-6.57	1.42	1.46
1	D	1074	VAL	CA-CB	6.56	1.61	1.54
1	E	245	PHE	CE2-CZ	6.53	1.58	1.38
1	C	856	MET	CA-C	-6.47	1.45	1.52
1	A	654	VAL	CA-CB	-6.37	1.47	1.53
1	D	282	LYS	CD-CE	6.35	1.71	1.52
1	A	478	ALA	CA-CB	-6.30	1.44	1.53
1	A	1086	ASN	CA-C	6.29	1.60	1.52
1	H	733	VAL	CA-CB	-6.16	1.51	1.55
1	E	632	GLU	CA-CB	-6.13	1.45	1.53
1	A	421	TYR	CA-C	-6.11	1.45	1.52
1	C	1087	PRO	N-CD	-6.10	1.39	1.47
1	D	751	VAL	CA-CB	-5.98	1.46	1.53
1	D	1013	GLU	CA-CB	-5.96	1.43	1.53
1	E	273	ARG	CD-NE	5.94	1.54	1.46
1	A	337	GLN	CA-C	5.80	1.60	1.52
1	F	912	ILE	CA-CB	-5.79	1.47	1.54
1	E	330	LEU	C-O	5.69	1.31	1.24
1	A	479	VAL	CA-CB	-5.66	1.47	1.54
1	H	277	ILE	CA-C	5.61	1.59	1.52
1	H	280	ASP	C-N	5.60	1.41	1.33
1	H	245	PHE	CD2-CE2	-5.59	1.21	1.38
1	E	750	ARG	CA-C	-5.55	1.45	1.52
1	B	403	TYR	N-CA	-5.54	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1013	GLU	CD-OE1	5.54	1.35	1.25
1	E	726	ARG	CZ-NH1	5.53	1.40	1.32
1	B	249	ASN	C-O	-5.53	1.16	1.24
1	D	324	ASN	C-N	5.50	1.41	1.33
1	G	753	VAL	CA-CB	-5.47	1.47	1.54
1	A	606	ASN	N-CA	5.44	1.53	1.46
1	H	357	ARG	NE-CZ	-5.42	1.27	1.33
1	B	271	TRP	NE1-CE2	5.41	1.43	1.37
1	D	1082	LYS	CB-CG	5.41	1.68	1.52
1	B	249	ASN	CG-OD1	5.38	1.33	1.23
1	E	645	ALA	CA-CB	-5.37	1.45	1.53
1	G	279	LYS	CD-CE	5.37	1.68	1.52
1	E	282	LYS	C-N	5.36	1.40	1.33
1	C	952	VAL	CA-CB	-5.35	1.48	1.54
1	H	245	PHE	CD1-CE1	-5.32	1.22	1.38
1	E	736	ILE	CA-CB	-5.28	1.48	1.54
1	H	290	LYS	CA-CB	5.27	1.60	1.53
1	C	436	ASN	CA-C	-5.23	1.46	1.52
1	E	563	ASN	CA-C	-5.23	1.46	1.53
1	G	615	GLU	CA-C	-5.21	1.46	1.53
1	D	371	ASN	CA-C	-5.20	1.46	1.52
1	E	271	TRP	CD2-CE2	-5.20	1.32	1.41
1	A	284	TRP	NE1-CE2	5.18	1.43	1.37
1	E	561	ILE	CA-CB	-5.15	1.48	1.54
1	A	798	ILE	CA-CB	-5.15	1.47	1.54
1	F	1014	GLU	N-CA	-5.14	1.40	1.46
1	F	354	ASN	CA-C	-5.12	1.46	1.52
1	G	946	HIS	CA-C	-5.11	1.46	1.52
1	A	645	ALA	C-O	-5.10	1.18	1.24
1	C	1028	ILE	CA-CB	-5.07	1.48	1.54
1	A	327	THR	N-CA	5.04	1.52	1.46
1	C	837	ALA	CA-CB	-5.04	1.46	1.53
1	E	283	THR	N-CA	5.02	1.52	1.45
1	A	1040	ILE	CA-CB	-5.01	1.47	1.53

All (227) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	GLN	OE1-CD-NE2	15.61	138.21	122.60
1	E	744	ARG	CB-CA-C	-9.96	95.71	110.24
1	C	744	ARG	CB-CA-C	-9.54	96.31	110.24
1	B	250	GLN	CG-CD-NE2	-9.51	102.14	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	283	THR	N-CA-C	8.85	124.02	109.24
1	H	289	GLU	N-CA-C	-8.84	102.40	113.01
1	B	653	SER	CA-C-N	-8.59	116.40	122.59
1	B	653	SER	C-N-CA	-8.59	116.40	122.59
1	G	245	PHE	N-CA-C	-8.38	101.67	112.23
1	F	306	GLN	N-CA-C	-8.03	102.53	111.28
1	D	793	ASP	CB-CA-C	-8.03	93.38	110.32
1	G	912	ILE	CB-CA-C	-7.87	96.69	110.94
1	D	1021	GLU	CB-CG-CD	-7.67	99.56	112.60
1	D	321	GLN	N-CA-C	7.60	120.69	110.35
1	E	653	SER	CA-C-N	-7.60	117.12	122.59
1	E	653	SER	C-N-CA	-7.60	117.12	122.59
1	A	1085	VAL	CB-CA-C	-7.58	102.86	111.80
1	A	358	GLN	N-CA-C	7.58	122.83	112.90
1	H	604	ASN	CA-C-N	7.31	128.97	119.84
1	H	604	ASN	C-N-CA	7.31	128.97	119.84
1	B	960	GLN	N-CA-C	7.21	119.83	108.79
1	A	713	TYR	N-CA-C	7.08	119.86	111.71
1	H	245	PHE	CG-CD2-CE2	-7.02	108.77	120.70
1	F	933	GLY	N-CA-C	6.99	120.89	110.97
1	A	320	HIS	ND1-CG-CD2	6.97	113.07	106.10
1	G	466	ASP	CA-C-N	6.95	126.63	119.82
1	G	466	ASP	C-N-CA	6.95	126.63	119.82
1	D	896	ALA	CA-C-N	-6.93	112.62	119.76
1	D	896	ALA	C-N-CA	-6.93	112.62	119.76
1	D	1021	GLU	N-CA-C	6.87	125.43	110.80
1	D	409	THR	CA-C-N	-6.86	112.11	119.24
1	D	409	THR	C-N-CA	-6.86	112.11	119.24
1	A	826	ALA	N-CA-C	-6.76	103.91	111.28
1	E	283	THR	N-CA-C	6.75	120.15	109.81
1	C	631	THR	N-CA-C	-6.75	103.39	111.69
1	E	301	PRO	N-CA-C	-6.74	105.92	114.35
1	B	594	LEU	N-CA-C	-6.73	103.41	111.69
1	H	245	PHE	CD1-CG-CD2	6.68	128.63	118.60
1	C	578	VAL	CA-C-N	-6.66	113.78	120.31
1	C	578	VAL	C-N-CA	-6.66	113.78	120.31
1	A	291	ASP	N-CA-C	6.64	121.75	112.72
1	B	733	VAL	CB-CA-C	-6.61	105.53	111.74
1	D	798	ILE	CB-CA-C	-6.59	101.41	110.77
1	A	1028	ILE	N-CA-C	6.58	117.33	110.62
1	F	1013	GLU	CB-CA-C	-6.55	100.55	110.90
1	H	291	ASP	N-CA-C	6.54	118.28	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1028	ILE	N-CA-C	6.53	116.69	110.42
1	D	427	ILE	N-CA-C	-6.50	106.40	112.83
1	B	1085	VAL	CA-C-N	-6.49	115.62	122.89
1	B	1085	VAL	C-N-CA	-6.49	115.62	122.89
1	C	574	GLU	N-CA-C	-6.48	105.20	113.23
1	C	245	PHE	N-CA-C	-6.38	105.48	113.20
1	H	989	ASN	CB-CA-C	-6.38	102.84	111.89
1	H	753	VAL	CB-CA-C	-6.33	103.21	111.25
1	C	793	ASP	CB-CA-C	-6.32	98.20	110.46
1	H	392	ASN	CA-C-N	-6.29	113.90	122.77
1	H	392	ASN	C-N-CA	-6.29	113.90	122.77
1	E	432	PHE	N-CA-C	6.27	118.51	108.41
1	A	959	ASP	N-CA-C	6.25	117.89	111.14
1	H	276	TYR	N-CA-C	6.25	120.25	107.69
1	E	422	THR	CB-CA-C	6.22	118.69	109.29
1	E	1028	ILE	N-CA-C	6.22	116.39	110.42
1	B	753	VAL	N-CA-C	6.21	116.77	107.51
1	B	569	THR	N-CA-C	-6.11	104.31	110.97
1	B	1085	VAL	CB-CA-C	-6.10	104.60	111.80
1	E	1080	LEU	CA-C-N	6.09	126.04	119.76
1	E	1080	LEU	C-N-CA	6.09	126.04	119.76
1	B	912	ILE	CB-CA-C	-6.09	99.92	110.94
1	A	594	LEU	N-CA-C	-6.07	104.22	111.69
1	A	358	GLN	N-CA-CB	-6.07	101.23	110.33
1	F	691	VAL	N-CA-C	6.06	115.98	107.37
1	G	367	GLN	N-CA-C	6.03	118.36	108.52
1	C	409	THR	CA-C-N	-6.00	112.68	119.28
1	C	409	THR	C-N-CA	-6.00	112.68	119.28
1	E	740	ASN	CA-C-N	5.96	125.64	119.56
1	E	740	ASN	C-N-CA	5.96	125.64	119.56
1	G	1021	GLU	CB-CG-CD	-5.95	102.49	112.60
1	A	308	GLN	N-CA-C	-5.94	104.14	111.75
1	C	637	HIS	N-CA-C	5.92	118.81	110.23
1	E	333	ASN	O-C-N	5.92	129.92	122.23
1	E	989	ASN	CB-CA-C	-5.91	102.78	112.06
1	H	944	ALA	N-CA-C	-5.90	104.54	110.97
1	E	328	SER	CA-C-N	-5.88	113.70	119.64
1	E	328	SER	C-N-CA	-5.88	113.70	119.64
1	G	313	MET	N-CA-C	5.87	119.27	111.75
1	A	1039	LYS	CA-C-N	-5.87	115.14	122.48
1	A	1039	LYS	C-N-CA	-5.87	115.14	122.48
1	G	912	ILE	CB-CG1-CD1	-5.85	101.51	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	GLN	CB-CG-CD	-5.85	102.66	112.60
1	F	870	LYS	N-CA-C	5.84	118.11	111.11
1	B	427	ILE	N-CA-C	-5.82	106.73	111.91
1	G	409	THR	CA-C-N	-5.82	112.69	119.32
1	G	409	THR	C-N-CA	-5.82	112.69	119.32
1	B	1086	ASN	N-CA-C	5.82	119.10	109.79
1	G	899	TYR	CA-CB-CG	-5.81	103.44	113.90
1	E	334	LEU	N-CA-C	5.79	117.27	111.07
1	H	292	PHE	N-CA-C	5.79	118.67	110.50
1	B	753	VAL	CB-CA-C	-5.76	103.24	111.31
1	E	1032	VAL	CA-C-N	5.75	125.95	120.31
1	E	1032	VAL	C-N-CA	5.75	125.95	120.31
1	F	431	GLU	N-CA-C	5.74	118.75	111.69
1	G	549	LYS	N-CA-C	5.74	118.34	110.01
1	C	713	TYR	N-CA-C	5.74	118.48	111.82
1	E	1075	SER	N-CA-C	5.74	117.21	111.07
1	G	753	VAL	CB-CA-C	-5.70	103.09	110.84
1	G	1084	LEU	N-CA-C	5.70	118.43	111.82
1	G	1020	PRO	N-CA-C	-5.69	105.97	113.65
1	E	727	ILE	CG1-CB-CG2	-5.69	93.64	110.70
1	B	1021	GLU	N-CA-C	5.68	117.93	111.11
1	G	982	VAL	CB-CA-C	-5.67	102.87	111.33
1	A	357	ARG	N-CA-C	-5.66	98.75	110.80
1	A	725	ASP	N-CA-C	5.64	115.56	108.45
1	B	403	TYR	N-CA-C	5.64	116.63	108.34
1	G	793	ASP	CB-CA-C	-5.64	100.20	110.63
1	H	537	ASN	N-CA-C	5.63	117.50	111.36
1	F	1021	GLU	CB-CG-CD	-5.63	103.03	112.60
1	B	911	VAL	N-CA-C	-5.62	105.62	111.58
1	G	247	GLN	N-CA-C	5.62	118.60	111.69
1	F	497	ALA	N-CA-C	5.61	118.59	111.69
1	B	652	SER	N-CA-C	5.60	119.41	112.58
1	B	248	TYR	N-CA-CB	5.59	120.00	110.50
1	C	748	SER	N-CA-C	5.58	119.80	113.15
1	G	714	GLY	CA-C-O	-5.57	118.60	122.22
1	E	753	VAL	N-CA-C	5.56	116.11	107.99
1	A	744	ARG	CB-CA-C	-5.56	101.58	110.14
1	B	666	ASP	CA-C-N	-5.55	117.23	122.17
1	B	666	ASP	C-N-CA	-5.55	117.23	122.17
1	G	306	GLN	N-CA-C	-5.53	105.35	111.71
1	B	403	TYR	N-CA-CB	-5.53	106.45	111.59
1	B	744	ARG	N-CA-C	5.53	117.11	107.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	ASN	N-CA-C	5.52	118.23	111.82
1	B	250	GLN	CB-CA-C	-5.52	99.44	110.42
1	G	1021	GLU	N-CA-C	5.48	122.48	110.80
1	H	661	ASP	N-CA-C	-5.48	106.43	113.23
1	D	891	THR	N-CA-C	-5.47	107.15	113.88
1	C	666	ASP	CA-C-N	-5.46	114.06	122.69
1	C	666	ASP	C-N-CA	-5.46	114.06	122.69
1	B	1021	GLU	CB-CA-C	-5.45	102.09	110.81
1	H	371	ASN	CB-CA-C	-5.45	100.49	111.17
1	E	856	MET	CA-C-N	-5.44	115.33	123.00
1	E	856	MET	C-N-CA	-5.44	115.33	123.00
1	E	594	LEU	N-CA-C	-5.44	105.00	111.69
1	A	726	ARG	CB-CA-C	-5.43	101.72	110.74
1	F	928	LYS	CA-C-N	-5.42	114.37	119.85
1	F	928	LYS	C-N-CA	-5.42	114.37	119.85
1	H	403	TYR	N-CA-C	5.41	116.29	108.34
1	E	371	ASN	CB-CA-C	-5.40	100.58	111.17
1	E	293	ARG	N-CA-C	5.40	118.36	110.10
1	G	1085	VAL	CA-C-N	-5.40	116.38	123.34
1	G	1085	VAL	C-N-CA	-5.40	116.38	123.34
1	H	1075	SER	N-CA-C	5.39	118.08	111.82
1	D	313	MET	N-CA-C	5.39	118.07	111.82
1	C	726	ARG	CB-CA-C	-5.38	101.85	110.79
1	G	533	ILE	N-CA-C	5.38	117.07	108.89
1	A	753	VAL	CB-CA-C	-5.37	104.25	110.91
1	D	1013	GLU	CB-CG-CD	-5.36	103.49	112.60
1	D	615	GLU	CB-CA-C	-5.35	102.72	110.96
1	D	738	GLY	N-CA-C	-5.35	100.50	113.18
1	H	293	ARG	CA-C-N	5.35	126.53	119.84
1	H	293	ARG	C-N-CA	5.35	126.53	119.84
1	D	753	VAL	CB-CA-C	-5.31	104.53	110.96
1	E	282	LYS	CA-C-N	-5.31	113.53	123.03
1	E	282	LYS	C-N-CA	-5.31	113.53	123.03
1	G	584	ILE	N-CA-C	-5.31	107.66	112.12
1	E	960	GLN	N-CA-C	5.30	116.86	108.96
1	E	1052	ASN	N-CA-C	-5.30	103.54	110.53
1	B	1082	LYS	N-CA-C	5.29	117.47	111.02
1	B	1076	ASP	N-CA-C	-5.27	105.70	111.82
1	C	824	ALA	N-CA-C	-5.27	101.11	109.96
1	E	249	ASN	CA-CB-CG	5.26	117.86	112.60
1	E	661	ASP	N-CA-C	-5.25	106.87	113.28
1	C	959	ASP	N-CA-C	5.24	118.14	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	245	PHE	N-CA-C	-5.24	106.88	113.28
1	F	657	VAL	CB-CA-C	-5.24	103.90	111.34
1	C	617	ILE	N-CA-C	5.23	115.38	110.30
1	F	989	ASN	CB-CA-C	-5.23	104.46	111.89
1	G	1071	PHE	N-CA-C	-5.22	101.95	110.20
1	G	1086	ASN	N-CA-C	5.22	118.47	108.97
1	A	899	TYR	CA-CB-CG	-5.20	104.54	113.90
1	D	279	LYS	N-CA-C	5.20	117.71	109.96
1	B	583	PHE	CA-C-N	-5.19	117.62	122.66
1	B	583	PHE	C-N-CA	-5.19	117.62	122.66
1	A	390	SER	N-CA-C	5.18	117.86	110.24
1	H	309	TYR	N-CA-C	-5.18	106.65	112.87
1	D	608	VAL	N-CA-C	5.17	115.72	108.89
1	G	1085	VAL	CB-CA-C	-5.17	105.70	111.80
1	C	726	ARG	N-CA-CB	5.17	117.71	110.12
1	A	404	ARG	N-CA-C	-5.16	104.27	111.39
1	F	1028	ILE	N-CA-C	5.16	115.89	110.62
1	G	790	TYR	N-CA-C	5.16	117.98	109.72
1	A	332	LEU	N-CA-C	-5.16	105.66	111.28
1	G	661	ASP	N-CA-C	-5.16	107.03	113.38
1	H	441	SER	N-CA-C	-5.15	106.40	113.30
1	A	446	GLN	N-CA-C	-5.15	105.56	111.07
1	E	409	THR	CA-C-N	-5.15	113.34	119.05
1	E	409	THR	C-N-CA	-5.15	113.34	119.05
1	A	448	GLU	N-CA-C	5.15	116.89	111.28
1	E	246	ALA	N-CA-C	-5.14	102.93	111.37
1	C	750	ARG	CA-CB-CG	-5.14	103.81	114.10
1	C	1041	LYS	N-CA-C	-5.14	107.14	113.41
1	H	296	LEU	N-CA-C	-5.14	106.96	113.18
1	C	753	VAL	N-CA-C	5.14	115.49	107.99
1	F	617	ILE	N-CA-C	5.13	115.75	110.36
1	F	793	ASP	CB-CA-C	-5.13	102.22	110.74
1	D	691	VAL	N-CA-C	5.13	115.73	107.73
1	B	989	ASN	CB-CA-C	-5.13	104.66	111.63
1	A	247	GLN	N-CA-C	5.13	121.72	110.80
1	B	1028	ILE	N-CA-C	5.11	115.83	110.62
1	A	517	TRP	N-CA-C	5.11	118.67	112.23
1	G	360	ILE	N-CA-C	5.11	115.83	110.62
1	A	753	VAL	N-CA-C	5.09	115.91	108.58
1	C	820	VAL	CA-C-N	-5.09	114.71	119.85
1	C	820	VAL	C-N-CA	-5.09	114.71	119.85
1	F	753	VAL	CB-CA-C	-5.09	104.01	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	270	SER	N-CA-C	5.08	117.60	110.23
1	D	622	GLU	N-CA-C	-5.08	105.44	111.69
1	D	794	ARG	N-CA-C	-5.07	106.51	113.30
1	B	1039	LYS	CA-C-N	-5.05	116.17	122.48
1	B	1039	LYS	C-N-CA	-5.05	116.17	122.48
1	C	928	LYS	CA-C-N	-5.04	115.04	120.03
1	C	928	LYS	C-N-CA	-5.04	115.04	120.03
1	B	899	TYR	CA-CB-CG	-5.03	104.84	113.90
1	E	619	LYS	N-CA-C	-5.02	105.88	111.36
1	D	1013	GLU	N-CA-C	5.02	117.53	111.40
1	F	396	THR	CB-CA-C	-5.02	103.81	112.44
1	A	321	GLN	N-CA-C	-5.01	101.75	109.52
1	G	960	GLN	N-CA-C	5.00	116.42	108.96

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	370	TRP	Peptide
1	H	245	PHE	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6643	0	6475	357	0
1	B	5854	0	5691	262	0
1	C	6660	0	6489	270	0
1	D	6660	0	6489	342	0
1	E	6654	0	6484	370	0
1	F	6660	0	6489	338	0
1	G	6660	0	6489	299	0
1	H	6372	0	6196	349	0
2	I	44	0	30	10	0
2	J	44	0	30	8	0
2	K	44	0	30	9	0
2	L	44	0	30	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	44	0	30	10	0
2	N	44	0	30	6	0
2	O	44	0	30	7	0
2	P	44	0	30	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	12	0	12	2	0
4	B	12	0	12	0	0
4	C	12	0	12	2	0
4	D	12	0	12	2	0
4	E	12	0	12	1	0
4	F	12	0	12	0	0
4	G	12	0	12	1	0
4	H	12	0	12	0	0
5	A	33	0	0	5	0
5	B	20	0	0	6	0
5	C	32	0	0	2	0
5	D	40	0	0	2	0
5	E	48	0	0	2	0
5	F	15	0	0	10	0
5	G	34	0	0	2	0
5	H	24	0	0	4	0
All	All	52865	0	51138	2618	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (2618) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:245:PHE:N	1:E:245:PHE:CA	1.70	1.54
1:E:277:ILE:CD1	1:E:291:ASP:HB3	1.38	1.54
1:A:290:LYS:NZ	1:A:290:LYS:CE	1.71	1.53
1:E:279:LYS:NZ	1:E:279:LYS:CE	1.73	1.51
1:E:273:ARG:CD	1:E:287:SER:HB2	1.40	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:ARG:HD2	1:E:287:SER:CB	1.43	1.44
1:B:939:VAL:CG1	1:B:943:LYS:NZ	1.87	1.35
1:D:281:GLY:HA3	1:D:341:THR:CG2	1.56	1.33
1:E:271:TRP:NE1	1:E:294:PRO:HB3	1.46	1.28
1:G:355:TRP:O	1:G:359:THR:HG22	1.33	1.28
1:H:299:TRP:C	1:H:300:TRP:CE3	2.12	1.26
1:H:277:ILE:HD11	1:H:291:ASP:CB	1.63	1.26
2:L:2:GLC:H61	2:L:3:AC1:O5	1.36	1.25
2:K:2:GLC:H61	2:K:3:AC1:O5	1.36	1.24
2:P:2:GLC:H61	2:P:3:AC1:O5	1.36	1.24
1:E:280:ASP:O	1:E:282:LYS:HG3	1.38	1.23
1:E:300:TRP:CG	1:E:306:GLN:HB2	1.75	1.22
1:B:939:VAL:HG13	1:B:943:LYS:NZ	1.55	1.21
2:N:2:GLC:H61	2:N:3:AC1:O5	1.36	1.20
2:O:2:GLC:H61	2:O:3:AC1:O5	1.36	1.20
1:H:309:TYR:CD2	1:H:309:TYR:O	1.94	1.20
2:M:2:GLC:H61	2:M:3:AC1:O5	1.36	1.20
2:J:2:GLC:H61	2:J:3:AC1:O5	1.36	1.19
1:B:743:LEU:C	1:B:744:ARG:HG2	1.64	1.18
1:B:800:THR:HG22	1:B:802:ALA:N	1.59	1.18
1:A:300:TRP:CD2	1:A:306:GLN:HG3	1.78	1.17
1:D:281:GLY:CA	1:D:341:THR:HG23	1.75	1.17
1:F:1021:GLU:CA	1:F:1021:GLU:OE1	1.92	1.16
1:H:277:ILE:CD1	1:H:291:ASP:HB3	1.75	1.16
1:B:743:LEU:O	1:B:744:ARG:HG2	1.43	1.16
1:E:346:LYS:HE2	1:E:350:GLU:OE2	1.46	1.15
1:H:466:ASP:OD2	1:H:943:LYS:HE2	1.44	1.15
1:E:277:ILE:HD11	1:E:291:ASP:CB	1.75	1.15
1:D:339:ILE:O	1:D:343:ILE:HG13	1.46	1.14
1:B:1083:SER:O	1:B:1087:PRO:HG3	1.46	1.14
1:H:862:ASN:O	1:H:912:ILE:HD13	1.46	1.14
1:G:800:THR:HG22	1:G:802:ALA:H	1.10	1.13
1:H:278:LEU:HA	1:H:284:TRP:HA	1.27	1.13
1:A:278:LEU:HG	1:A:281:GLY:HA2	1.21	1.13
1:F:250:GLN:HE21	1:F:275:LYS:CE	1.61	1.13
1:D:281:GLY:CA	1:D:341:THR:CG2	2.25	1.12
1:H:310:VAL:HG12	1:H:311:ASN:H	1.03	1.12
1:A:271:TRP:CZ2	1:A:357:ARG:HA	1.85	1.11
1:F:357:ARG:HH11	1:F:357:ARG:CG	1.60	1.11
1:E:277:ILE:HD12	1:E:291:ASP:HB3	1.16	1.10
1:G:339:ILE:O	1:G:343:ILE:HG13	1.51	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:GLU:OE1	1:E:304:GLU:HA	1.36	1.10
1:G:316:GLN:NE2	1:G:316:GLN:HA	1.51	1.10
1:A:271:TRP:HZ2	1:A:357:ARG:HA	1.09	1.10
1:A:346:LYS:O	1:A:350:GLU:HG2	1.48	1.10
1:E:277:ILE:CD1	1:E:291:ASP:CB	2.29	1.10
1:E:271:TRP:CD1	1:E:294:PRO:HA	1.87	1.09
1:F:357:ARG:HH11	1:F:357:ARG:HG2	1.10	1.09
1:H:248:TYR:HB3	1:H:276:TYR:HB2	1.33	1.08
1:H:277:ILE:HD12	1:H:291:ASP:OD2	1.51	1.08
1:C:800:THR:HG22	1:C:802:ALA:H	1.13	1.08
1:F:782:GLN:HE21	1:F:782:GLN:HA	0.99	1.08
1:H:252:TYR:HB3	1:H:258:ASN:HD21	1.12	1.08
1:F:250:GLN:HE21	1:F:275:LYS:HE3	1.05	1.07
1:D:800:THR:HG22	1:D:802:ALA:H	1.12	1.07
1:F:800:THR:HG22	1:F:802:ALA:H	1.17	1.06
1:E:246:ALA:HB3	1:E:247:GLN:HE21	1.21	1.06
1:F:862:ASN:O	1:F:912:ILE:HG21	1.56	1.06
1:E:300:TRP:CD1	1:E:306:GLN:HB2	1.89	1.06
1:B:1073:LEU:HD21	1:B:1080:LEU:HD21	1.37	1.05
1:D:281:GLY:HA3	1:D:341:THR:HG22	1.10	1.05
1:D:1021:GLU:OE1	1:D:1021:GLU:HA	1.28	1.05
1:H:288:THR:CG2	1:H:289:GLU:H	1.70	1.04
1:E:277:ILE:HD11	1:E:291:ASP:HB3	1.11	1.04
1:A:281:GLY:HA3	1:A:341:THR:HG23	1.08	1.04
1:A:800:THR:HG22	1:A:802:ALA:H	1.22	1.04
1:E:245:PHE:CA	1:E:248:TYR:HD2	1.70	1.04
1:H:300:TRP:CE3	1:H:300:TRP:N	2.26	1.04
1:F:713:TYR:O	1:F:759:HIS:HE1	1.40	1.03
1:A:339:ILE:O	1:A:343:ILE:HG13	1.56	1.03
1:E:800:THR:HG22	1:E:802:ALA:H	1.22	1.03
1:D:310:VAL:HG13	1:D:339:ILE:HD11	1.39	1.03
1:F:670:MET:HE1	1:F:885:PHE:HZ	1.23	1.03
1:E:966:GLU:HB2	1:E:997:LYS:HB2	1.41	1.02
1:H:294:PRO:HD2	1:H:297:MET:CE	1.88	1.02
1:H:310:VAL:HG12	1:H:311:ASN:N	1.60	1.02
1:A:604:ASN:HD21	1:A:607:VAL:CA	1.73	1.01
1:A:604:ASN:ND2	1:A:607:VAL:HB	1.74	1.01
1:B:800:THR:CG2	1:B:802:ALA:H	1.73	1.01
1:D:280:ASP:OD1	1:D:345:GLU:HA	1.59	1.01
1:H:294:PRO:HD2	1:H:297:MET:HE2	1.42	1.01
1:D:1021:GLU:OE1	1:D:1021:GLU:CA	2.08	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1085:VAL:HG23	1:H:1086:ASN:H	1.25	1.01
1:C:639:ASN:HD21	1:C:813:SER:H	1.09	1.00
1:F:1021:GLU:OE1	1:F:1021:GLU:HA	1.21	1.00
1:C:252:TYR:HB3	1:C:258:ASN:HD21	1.23	1.00
1:H:288:THR:HG22	1:H:289:GLU:H	1.22	1.00
1:H:288:THR:HG22	1:H:289:GLU:N	1.74	1.00
1:D:323:TYR:HB3	1:D:327:THR:OG1	1.60	1.00
1:F:250:GLN:HB2	1:F:1084:LEU:O	1.62	1.00
1:F:782:GLN:HA	1:F:782:GLN:NE2	1.73	1.00
1:H:440:ASN:HD21	1:H:449:GLN:HE21	1.04	1.00
1:A:281:GLY:CA	1:A:341:THR:HG23	1.91	0.99
1:A:639:ASN:HD21	1:A:813:SER:H	1.05	0.99
1:D:740:ASN:ND2	1:D:742:SER:H	1.59	0.99
1:E:321:GLN:HG3	1:E:322:THR:H	1.26	0.99
1:E:639:ASN:HD21	1:E:813:SER:H	1.00	0.99
1:D:281:GLY:HA2	1:D:341:THR:HG23	1.38	0.99
1:C:1063:LYS:HE2	1:C:1068:ASN:ND2	1.78	0.99
1:E:440:ASN:HD21	1:E:449:GLN:HE21	1.06	0.98
1:E:861:SER:H	1:E:864:GLN:HE21	1.00	0.98
1:E:587:HIS:NE2	2:M:3:AC1:O3B	1.95	0.98
1:B:491:GLY:HA3	5:B:31:HOH:O	1.62	0.98
1:H:316:GLN:HG2	1:H:359:THR:HG21	1.42	0.98
1:F:252:TYR:HB3	1:F:258:ASN:HD21	1.24	0.98
1:F:261:HIS:HD2	1:F:264:HIS:H	0.99	0.98
1:F:311:ASN:HD21	1:F:323:TYR:H	1.10	0.98
1:H:861:SER:H	1:H:864:GLN:NE2	1.62	0.98
1:B:262:VAL:HG12	1:B:969:VAL:HG23	1.43	0.97
1:G:252:TYR:HA	1:G:275:LYS:HG2	1.45	0.97
1:G:316:GLN:NE2	1:G:316:GLN:CA	2.23	0.97
1:D:271:TRP:CD1	1:D:294:PRO:HA	1.99	0.97
1:G:252:TYR:HB3	1:G:258:ASN:HD21	1.27	0.97
1:G:316:GLN:HA	1:G:316:GLN:HE21	1.06	0.97
1:B:687:ARG:HA	1:B:691:VAL:CG2	1.94	0.97
1:E:245:PHE:HA	1:E:248:TYR:HD2	1.27	0.97
1:A:966:GLU:HB2	1:A:997:LYS:HB2	1.44	0.96
1:A:861:SER:H	1:A:864:GLN:HE21	1.12	0.96
1:F:360:ILE:O	1:F:364:VAL:HG23	1.65	0.96
1:H:311:ASN:O	1:H:314:ASN:HB2	1.65	0.96
1:H:639:ASN:HD21	1:H:813:SER:H	1.07	0.96
1:F:262:VAL:HG12	1:F:969:VAL:HG23	1.46	0.96
1:F:1085:VAL:HG23	1:F:1086:ASN:H	1.31	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:ASN:HD22	1:A:740:ASN:C	1.73	0.95
1:B:861:SER:H	1:B:864:GLN:HE21	1.01	0.95
1:A:440:ASN:HD21	1:A:449:GLN:NE2	1.64	0.95
1:G:440:ASN:HD21	1:G:449:GLN:HE21	1.11	0.95
1:G:912:ILE:HG22	1:G:912:ILE:O	1.66	0.95
1:A:271:TRP:HZ2	1:A:357:ARG:CA	1.78	0.95
1:C:460:GLY:H	1:C:470:ASN:HD22	1.11	0.95
1:D:740:ASN:HD22	1:D:742:SER:H	1.12	0.95
1:A:281:GLY:HA3	1:A:341:THR:CG2	1.96	0.95
1:E:252:TYR:CE2	1:E:273:ARG:NH2	2.34	0.95
1:B:670:MET:HE1	1:B:885:PHE:CZ	2.01	0.95
1:D:276:TYR:HD1	1:D:285:THR:O	1.48	0.95
1:E:271:TRP:CE2	1:E:294:PRO:HB3	2.01	0.95
1:G:1052:ASN:H	1:G:1052:ASN:ND2	1.61	0.95
1:G:310:VAL:HG11	1:G:335:ALA:HB1	1.49	0.94
1:F:250:GLN:NE2	1:F:275:LYS:HE3	1.82	0.94
1:F:782:GLN:HE21	1:F:782:GLN:CA	1.71	0.94
1:E:346:LYS:O	1:E:350:GLU:HG3	1.67	0.94
1:H:300:TRP:N	1:H:300:TRP:HE3	1.64	0.94
1:A:278:LEU:CG	1:A:281:GLY:HA2	1.97	0.94
1:D:300:TRP:CD2	1:D:306:GLN:HG3	2.02	0.94
1:E:245:PHE:HA	1:E:248:TYR:CD2	2.03	0.94
1:H:800:THR:HG22	1:H:802:ALA:H	1.33	0.94
1:A:440:ASN:ND2	1:A:449:GLN:HE21	1.66	0.94
1:H:1052:ASN:HD22	1:H:1052:ASN:H	1.00	0.94
1:A:301:PRO:HG2	1:A:302:ASP:H	1.33	0.94
1:C:1052:ASN:HD22	1:C:1052:ASN:H	1.05	0.94
1:B:939:VAL:HG12	1:B:943:LYS:NZ	1.80	0.93
1:G:861:SER:H	1:G:864:GLN:HE21	1.05	0.93
1:D:297:MET:SD	1:D:340:GLN:HG3	2.08	0.93
1:F:800:THR:HG22	1:F:802:ALA:N	1.83	0.93
1:G:304:GLU:OE1	1:G:304:GLU:HA	1.64	0.93
1:B:939:VAL:HG13	1:B:943:LYS:HZ2	1.17	0.93
1:D:440:ASN:HD21	1:D:449:GLN:HE21	1.14	0.93
1:D:1052:ASN:H	1:D:1052:ASN:HD22	0.97	0.93
1:F:440:ASN:HD21	1:F:449:GLN:HE21	1.08	0.93
1:E:288:THR:HG22	1:E:289:GLU:H	1.30	0.93
1:H:246:ALA:O	1:H:247:GLN:C	2.10	0.93
1:D:293:ARG:HB3	1:D:297:MET:HE2	1.49	0.92
1:D:1052:ASN:HD22	1:D:1052:ASN:N	1.66	0.92
1:G:862:ASN:O	1:G:912:ILE:HG21	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:306:GLN:O	1:E:309:TYR:HB3	1.69	0.92
1:C:440:ASN:HD21	1:C:449:GLN:HE21	1.11	0.92
1:H:260:GLU:OE1	1:H:271:TRP:HB2	1.69	0.92
1:B:939:VAL:CG1	1:B:943:LYS:HZ3	1.73	0.92
1:B:1052:ASN:H	1:B:1052:ASN:HD22	1.02	0.92
1:A:335:ALA:O	1:A:339:ILE:HG13	1.69	0.92
1:F:861:SER:H	1:F:864:GLN:HE21	1.00	0.92
1:E:271:TRP:NE1	1:E:294:PRO:CB	2.32	0.92
1:C:261:HIS:CD2	1:C:264:HIS:H	1.86	0.92
1:D:277:ILE:HG22	1:D:277:ILE:O	1.68	0.92
1:G:800:THR:HG22	1:G:802:ALA:N	1.83	0.92
1:D:492:ASP:HB3	1:D:1022:LEU:HD22	1.50	0.91
1:A:1052:ASN:H	1:A:1052:ASN:HD22	1.16	0.91
1:H:278:LEU:HB3	1:H:284:TRP:CE3	2.06	0.91
1:H:310:VAL:CG1	1:H:311:ASN:N	2.32	0.91
1:H:277:ILE:CD1	1:H:291:ASP:OD2	2.16	0.91
1:A:250:GLN:HB2	1:A:1084:LEU:O	1.71	0.91
1:H:1085:VAL:HG23	1:H:1086:ASN:N	1.82	0.91
1:D:861:SER:H	1:D:864:GLN:HE21	1.08	0.91
1:C:740:ASN:C	1:C:740:ASN:HD22	1.77	0.91
1:E:304:GLU:OE1	1:E:304:GLU:CA	2.19	0.91
1:F:861:SER:H	1:F:864:GLN:NE2	1.69	0.91
1:A:604:ASN:HD21	1:A:607:VAL:HA	1.34	0.91
1:H:360:ILE:HG22	1:H:361:SER:N	1.86	0.91
1:H:966:GLU:HB2	1:H:997:LYS:HB2	1.53	0.90
1:C:861:SER:H	1:C:864:GLN:NE2	1.68	0.90
1:C:861:SER:H	1:C:864:GLN:HE21	0.96	0.90
1:D:330:LEU:HD12	1:D:330:LEU:O	1.69	0.90
1:F:278:LEU:HD23	1:F:281:GLY:HA2	1.52	0.90
1:A:252:TYR:HB3	1:A:258:ASN:HD21	1.37	0.90
1:H:262:VAL:HG12	1:H:969:VAL:HG23	1.54	0.90
1:F:670:MET:HE1	1:F:885:PHE:CZ	2.05	0.90
1:B:687:ARG:HA	1:B:691:VAL:HG23	1.52	0.90
2:I:2:GLC:H61	2:I:3:AC1:O5	1.71	0.89
1:E:320:HIS:O	1:E:321:GLN:O	1.90	0.89
1:G:349:ALA:O	1:G:350:GLU:HG2	1.71	0.89
1:E:245:PHE:N	1:E:248:TYR:CD2	2.41	0.89
1:B:939:VAL:CG1	1:B:943:LYS:HZ2	1.64	0.89
1:C:861:SER:N	1:C:864:GLN:HE21	1.70	0.89
1:B:670:MET:HE1	1:B:885:PHE:HZ	1.36	0.89
1:G:1052:ASN:HD22	1:G:1052:ASN:N	1.70	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:LYS:O	1:E:279:LYS:HG2	1.71	0.89
1:B:252:TYR:HB3	1:B:258:ASN:ND2	1.88	0.88
1:D:276:TYR:CD1	1:D:285:THR:O	2.25	0.88
1:H:299:TRP:CA	1:H:300:TRP:CE3	2.56	0.88
1:C:261:HIS:HD2	1:C:264:HIS:N	1.71	0.88
1:E:347:ILE:HG12	1:E:353:THR:HB	1.54	0.88
1:E:740:ASN:C	1:E:740:ASN:HD22	1.77	0.88
1:F:669:TYR:CD2	1:F:670:MET:HG3	2.08	0.88
1:F:687:ARG:HA	1:F:691:VAL:CG2	2.02	0.88
1:F:350:GLU:HB3	1:F:352:ASN:ND2	1.88	0.88
1:E:346:LYS:CE	1:E:350:GLU:OE2	2.21	0.88
1:G:492:ASP:HB3	1:G:1022:LEU:HD22	1.55	0.88
1:A:251:VAL:HG21	1:A:259:PHE:CZ	2.09	0.87
1:C:261:HIS:HD2	1:C:264:HIS:H	0.93	0.87
1:D:639:ASN:HD21	1:D:813:SER:H	1.22	0.87
1:H:278:LEU:HD12	1:H:278:LEU:O	1.72	0.87
1:D:251:VAL:HG21	1:D:259:PHE:CZ	2.07	0.87
1:G:604:ASN:ND2	1:G:607:VAL:HB	1.90	0.87
1:F:261:HIS:HD2	1:F:264:HIS:N	1.73	0.87
1:H:740:ASN:C	1:H:740:ASN:HD22	1.82	0.87
1:A:316:GLN:HE21	1:A:359:THR:HG22	1.38	0.87
1:F:670:MET:CE	1:F:885:PHE:HZ	1.88	0.87
1:A:300:TRP:CE3	1:A:306:GLN:HG3	2.10	0.87
1:C:251:VAL:HG21	1:C:259:PHE:CZ	2.08	0.87
1:E:271:TRP:CD1	1:E:294:PRO:CA	2.58	0.87
1:H:861:SER:H	1:H:864:GLN:HE21	0.87	0.87
1:C:460:GLY:N	1:C:470:ASN:HD22	1.73	0.86
1:A:782:GLN:HE21	1:A:782:GLN:HA	1.40	0.86
1:F:248:TYR:HB3	1:F:276:TYR:HB2	1.57	0.86
1:F:250:GLN:OE1	1:F:1087:PRO:CG	2.24	0.86
1:G:740:ASN:ND2	1:G:742:SER:H	1.73	0.86
1:G:740:ASN:C	1:G:740:ASN:HD22	1.83	0.86
1:G:861:SER:N	1:G:864:GLN:HE21	1.72	0.86
1:A:440:ASN:HD21	1:A:449:GLN:HE21	0.88	0.86
1:H:309:TYR:O	1:H:309:TYR:CG	2.28	0.86
1:A:261:HIS:HD2	1:A:264:HIS:H	1.23	0.86
1:B:639:ASN:HD21	1:B:813:SER:H	1.22	0.86
1:A:376:LYS:HB3	1:A:377:PRO:HA	1.58	0.85
1:E:245:PHE:CA	1:E:248:TYR:CD2	2.59	0.85
1:A:604:ASN:ND2	1:A:607:VAL:CA	2.40	0.85
1:G:861:SER:H	1:G:864:GLN:NE2	1.73	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:TYR:CE2	1:B:660:GLY:HA3	2.12	0.85
1:A:302:ASP:OD1	1:A:304:GLU:HB3	1.76	0.85
1:D:587:HIS:NE2	2:L:3:AC1:O3B	2.09	0.85
1:G:794:ARG:NH1	1:G:794:ARG:HG2	1.91	0.85
1:C:376:LYS:HB3	1:C:377:PRO:HA	1.59	0.85
1:F:357:ARG:CG	1:F:357:ARG:NH1	2.34	0.85
1:D:271:TRP:CE2	1:D:294:PRO:HD3	2.12	0.85
1:F:687:ARG:HA	1:F:691:VAL:HG23	1.57	0.85
1:H:861:SER:N	1:H:864:GLN:HE21	1.72	0.85
1:E:245:PHE:N	1:E:245:PHE:HD1	1.75	0.85
1:D:352:ASN:OD1	1:D:354:ASN:HB2	1.76	0.85
1:D:800:THR:HG22	1:D:802:ALA:N	1.91	0.85
1:E:245:PHE:N	1:E:245:PHE:CD1	2.44	0.85
1:B:466:ASP:OD2	1:B:943:LYS:HE3	1.77	0.85
1:C:639:ASN:ND2	1:C:813:SER:H	1.75	0.85
1:H:300:TRP:CD1	1:H:306:GLN:HA	2.12	0.85
1:A:604:ASN:ND2	1:A:607:VAL:CB	2.39	0.84
1:D:271:TRP:CZ2	1:D:294:PRO:HD3	2.12	0.84
1:G:261:HIS:HD2	1:G:264:HIS:H	1.25	0.84
1:F:713:TYR:O	1:F:759:HIS:CE1	2.30	0.84
1:F:357:ARG:HG2	1:F:357:ARG:NH1	1.89	0.84
1:C:740:ASN:ND2	1:C:742:SER:H	1.75	0.84
1:E:639:ASN:ND2	1:E:813:SER:H	1.74	0.84
1:A:309:TYR:C	1:A:309:TYR:CD2	2.54	0.84
1:F:321:GLN:OE1	1:F:321:GLN:HA	1.76	0.84
1:A:278:LEU:HG	1:A:281:GLY:CA	2.05	0.84
1:A:639:ASN:ND2	1:A:813:SER:H	1.76	0.84
1:D:782:GLN:HA	1:D:782:GLN:HE21	1.43	0.83
1:H:440:ASN:HD21	1:H:449:GLN:NE2	1.74	0.83
1:D:245:PHE:O	1:D:247:GLN:N	2.10	0.83
1:F:460:GLY:H	1:F:470:ASN:ND2	1.74	0.83
1:F:261:HIS:CD2	1:F:264:HIS:H	1.91	0.83
1:D:460:GLY:H	1:D:470:ASN:HD22	1.25	0.83
1:G:966:GLU:HB2	1:G:997:LYS:HB2	1.61	0.83
1:G:303:GLN:OE1	1:G:329:PRO:HG3	1.79	0.83
1:A:861:SER:N	1:A:864:GLN:HE21	1.77	0.83
1:C:966:GLU:HB2	1:C:997:LYS:HB2	1.59	0.83
1:D:245:PHE:CE1	1:D:284:TRP:HZ2	1.97	0.83
1:E:246:ALA:HB3	1:E:247:GLN:NE2	1.93	0.83
1:F:964:LEU:HD12	1:F:996:GLY:HA2	1.61	0.83
2:K:2:GLC:H61	2:K:3:AC1:C1	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:2:GLC:H61	2:P:3:AC1:C1	2.09	0.83
1:B:440:ASN:HD21	1:B:449:GLN:HE21	1.27	0.83
1:E:271:TRP:HE1	1:E:294:PRO:HB3	1.41	0.83
1:E:587:HIS:HE2	2:M:3:AC1:HOB3	1.09	0.83
1:G:1052:ASN:H	1:G:1052:ASN:HD22	0.86	0.83
1:H:304:GLU:OE1	1:H:304:GLU:O	1.95	0.82
1:F:1052:ASN:HD22	1:F:1052:ASN:H	1.26	0.82
1:H:277:ILE:CD1	1:H:291:ASP:CB	2.46	0.82
2:M:2:GLC:H61	2:M:3:AC1:C1	2.09	0.82
2:O:2:GLC:H61	2:O:3:AC1:C1	2.09	0.82
1:A:321:GLN:OE1	1:A:321:GLN:HA	1.76	0.82
1:D:293:ARG:HB3	1:D:297:MET:CE	2.08	0.82
2:J:2:GLC:H61	2:J:3:AC1:C1	2.09	0.82
1:B:743:LEU:C	1:B:744:ARG:CG	2.52	0.82
1:F:669:TYR:CE2	1:F:670:MET:HG3	2.15	0.82
2:N:2:GLC:H61	2:N:3:AC1:C1	2.09	0.82
1:E:262:VAL:HG12	1:E:969:VAL:HG23	1.60	0.82
1:H:309:TYR:CD2	1:H:309:TYR:C	2.56	0.82
1:G:639:ASN:HD21	1:G:813:SER:H	1.27	0.82
1:G:355:TRP:O	1:G:359:THR:CG2	2.23	0.82
1:H:252:TYR:HB3	1:H:258:ASN:ND2	1.94	0.82
1:B:261:HIS:HD2	1:B:264:HIS:H	1.24	0.81
1:F:912:ILE:O	1:F:912:ILE:HG22	1.78	0.81
1:H:246:ALA:O	1:H:247:GLN:O	1.98	0.81
1:B:862:ASN:O	1:B:912:ILE:HG21	1.80	0.81
1:H:1085:VAL:CG2	1:H:1086:ASN:H	1.93	0.81
1:A:740:ASN:ND2	1:A:742:SER:H	1.77	0.81
1:D:1085:VAL:HG23	1:D:1086:ASN:H	1.43	0.81
1:E:261:HIS:HD2	1:E:264:HIS:H	1.26	0.81
2:L:2:GLC:H61	2:L:3:AC1:C1	2.09	0.81
1:G:251:VAL:HG21	1:G:259:PHE:CZ	2.15	0.81
1:H:278:LEU:CA	1:H:284:TRP:HA	2.09	0.81
1:H:360:ILE:HG22	1:H:361:SER:H	1.44	0.81
1:E:245:PHE:N	1:E:248:TYR:HD2	1.79	0.81
1:B:912:ILE:O	1:B:912:ILE:HG22	1.79	0.81
1:H:251:VAL:HG21	1:H:259:PHE:CZ	2.15	0.81
1:B:740:ASN:ND2	1:B:742:SER:H	1.77	0.81
1:D:334:LEU:O	1:D:335:ALA:C	2.20	0.81
1:H:1080:LEU:HB2	1:H:1085:VAL:HG11	1.59	0.81
1:A:604:ASN:HD22	1:A:607:VAL:HB	1.42	0.81
1:A:782:GLN:HA	1:A:782:GLN:NE2	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1052:ASN:HD22	1:E:1052:ASN:H	1.26	0.81
1:H:299:TRP:CA	1:H:300:TRP:CZ3	2.65	0.81
1:C:800:THR:HG22	1:C:802:ALA:N	1.93	0.80
1:B:740:ASN:HD22	1:B:742:SER:H	1.25	0.80
1:C:339:ILE:O	1:C:343:ILE:HG13	1.81	0.80
1:F:1085:VAL:HG23	1:F:1086:ASN:N	1.92	0.80
1:E:287:SER:HB3	1:E:291:ASP:HB2	1.64	0.80
1:C:407:ASN:HD21	1:C:431:GLU:H	1.30	0.80
1:D:920:ASP:OD2	1:D:1002:ASP:HB2	1.82	0.80
1:E:300:TRP:CD1	1:E:306:GLN:CB	2.65	0.80
1:H:277:ILE:CD1	1:H:291:ASP:CG	2.55	0.80
1:D:355:TRP:CE3	1:D:359:THR:HG21	2.16	0.80
1:D:250:GLN:HB2	1:D:1084:LEU:O	1.82	0.79
1:D:300:TRP:CE3	1:D:306:GLN:HG3	2.17	0.79
1:F:782:GLN:NE2	1:F:782:GLN:CA	2.36	0.79
1:E:861:SER:N	1:E:864:GLN:HE21	1.80	0.79
1:H:466:ASP:OD2	1:H:943:LYS:CE	2.27	0.79
1:B:1052:ASN:HD22	1:B:1052:ASN:N	1.80	0.79
1:A:271:TRP:CZ2	1:A:357:ARG:CA	2.59	0.79
1:C:407:ASN:ND2	1:C:431:GLU:H	1.80	0.79
1:H:278:LEU:O	1:H:278:LEU:CG	2.31	0.79
1:F:279:LYS:O	1:F:280:ASP:HB3	1.82	0.79
1:C:587:HIS:NE2	2:K:3:AC1:O3B	2.16	0.79
1:D:966:GLU:HB2	1:D:997:LYS:HB2	1.64	0.79
1:H:294:PRO:CD	1:H:297:MET:HE2	2.12	0.79
1:E:252:TYR:HB3	1:E:258:ASN:HD21	1.47	0.79
1:H:278:LEU:O	1:H:278:LEU:CD1	2.30	0.79
2:I:2:GLC:C6	2:I:3:AC1:O5	2.30	0.79
1:D:666:ASP:HA	1:D:863:PHE:O	1.83	0.78
1:F:966:GLU:HB3	5:F:205:HOH:O	1.82	0.78
1:D:1052:ASN:H	1:D:1052:ASN:ND2	1.74	0.78
1:H:273:ARG:CZ	1:H:288:THR:O	2.31	0.78
1:C:1052:ASN:HD22	1:C:1052:ASN:N	1.79	0.78
1:F:651:LYS:O	1:F:652:SER:HB2	1.80	0.78
1:D:310:VAL:HG13	1:D:339:ILE:CD1	2.13	0.78
1:A:615:GLU:HA	1:A:615:GLU:OE1	1.81	0.78
1:H:312:TYR:CE2	1:H:363:PHE:HB2	2.18	0.78
1:B:1052:ASN:H	1:B:1052:ASN:ND2	1.77	0.78
1:D:861:SER:N	1:D:864:GLN:HE21	1.81	0.78
1:H:740:ASN:ND2	1:H:742:SER:H	1.80	0.78
1:A:251:VAL:HG21	1:A:259:PHE:HZ	1.46	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:639:ASN:HD22	1:F:642:LEU:HD13	1.48	0.77
1:H:705:SER:HB3	1:H:743:LEU:HD13	1.66	0.77
1:F:460:GLY:N	1:F:470:ASN:ND2	2.31	0.77
1:H:249:ASN:O	1:H:250:GLN:O	2.02	0.77
1:H:1052:ASN:H	1:H:1052:ASN:ND2	1.76	0.77
1:E:277:ILE:HD12	1:E:291:ASP:CB	2.07	0.77
1:A:687:ARG:HA	1:A:691:VAL:HG23	1.64	0.77
1:D:312:TYR:C	1:D:312:TYR:CD2	2.63	0.77
1:D:639:ASN:ND2	1:D:813:SER:H	1.81	0.77
1:D:841:ASP:OD1	1:D:846:HIS:HE1	1.67	0.77
1:D:1085:VAL:O	1:D:1087:PRO:HD3	1.84	0.77
1:E:337:GLN:O	1:E:340:GLN:N	2.16	0.77
1:G:300:TRP:CD2	1:G:306:GLN:HG3	2.18	0.77
1:G:368:SER:O	1:G:371:ASN:HB2	1.84	0.77
1:C:407:ASN:ND2	1:C:431:GLU:N	2.33	0.77
1:A:861:SER:H	1:A:864:GLN:NE2	1.83	0.77
1:H:285:THR:O	1:H:286:GLN:O	2.01	0.77
1:H:759:HIS:CD2	1:H:764:TYR:OH	2.37	0.77
1:F:492:ASP:HB3	1:F:1022:LEU:HD22	1.64	0.77
1:G:639:ASN:ND2	1:G:813:SER:H	1.82	0.77
1:A:276:TYR:HB3	1:A:285:THR:O	1.85	0.77
1:E:1064:ASP:HB2	1:E:1071:PHE:CE1	2.20	0.77
1:E:861:SER:H	1:E:864:GLN:NE2	1.81	0.76
1:G:359:THR:O	1:G:362:ALA:HB3	1.84	0.76
1:A:277:ILE:HD11	1:A:291:ASP:HB3	1.67	0.76
1:F:460:GLY:H	1:F:470:ASN:HD22	1.31	0.76
1:D:740:ASN:HD22	1:D:740:ASN:C	1.93	0.76
1:D:861:SER:H	1:D:864:GLN:NE2	1.82	0.76
1:F:669:TYR:HE2	1:F:670:MET:HE3	1.49	0.76
1:H:277:ILE:HD11	1:H:291:ASP:HB3	0.82	0.76
1:D:276:TYR:HD1	1:D:285:THR:C	1.94	0.75
1:E:670:MET:HE1	1:E:885:PHE:HZ	1.51	0.75
1:D:252:TYR:HB3	1:D:258:ASN:HD21	1.49	0.75
1:B:687:ARG:HA	1:B:691:VAL:HG21	1.67	0.75
1:B:939:VAL:HG13	1:B:943:LYS:HZ1	1.50	0.75
1:F:293:ARG:HG2	1:F:293:ARG:HH11	1.52	0.75
1:A:252:TYR:HA	1:A:275:LYS:HG2	1.69	0.75
1:H:269:GLU:OE2	1:H:361:SER:HB3	1.85	0.75
1:A:287:SER:HA	1:A:291:ASP:OD2	1.86	0.75
1:G:1085:VAL:HG23	1:G:1086:ASN:N	2.00	0.75
1:H:376:LYS:HB3	1:H:377:PRO:HA	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:TRP:CG	1:E:294:PRO:HA	2.21	0.75
1:F:311:ASN:HD21	1:F:323:TYR:N	1.84	0.75
1:B:417:LYS:HE3	1:F:555:SER:HB3	1.67	0.74
1:H:294:PRO:HD2	1:H:297:MET:HE1	1.67	0.74
1:B:809:ASN:HB2	1:B:810:PRO:HD2	1.68	0.74
1:D:800:THR:CG2	1:D:801:ALA:N	2.50	0.74
1:E:321:GLN:HG3	1:E:322:THR:N	1.94	0.74
1:A:966:GLU:HB2	1:A:997:LYS:CB	2.16	0.74
1:A:1085:VAL:HG23	1:A:1086:ASN:N	2.00	0.74
1:F:965:PRO:HD2	1:F:997:LYS:O	1.86	0.74
1:E:716:GLY:HA2	5:E:33:HOH:O	1.87	0.74
1:C:1085:VAL:HG23	1:C:1086:ASN:N	2.02	0.74
1:E:329:PRO:HA	1:E:332:LEU:HD12	1.69	0.74
1:E:740:ASN:ND2	1:E:742:SER:H	1.85	0.74
1:F:587:HIS:NE2	2:N:3:AC1:O3B	2.19	0.74
1:H:298:THR:C	1:H:300:TRP:CZ3	2.66	0.74
1:C:350:GLU:O	1:C:352:ASN:N	2.21	0.73
1:E:321:GLN:CG	1:E:322:THR:N	2.51	0.73
1:F:966:GLU:HB2	1:F:997:LYS:HB2	1.69	0.73
1:B:252:TYR:HB3	1:B:258:ASN:HD21	1.51	0.73
1:B:966:GLU:HB2	1:B:997:LYS:HB2	1.69	0.73
1:H:311:ASN:O	1:H:314:ASN:CB	2.36	0.73
1:C:355:TRP:O	1:C:359:THR:HG22	1.88	0.73
1:B:861:SER:N	1:B:864:GLN:HE21	1.81	0.73
1:C:965:PRO:HD2	1:C:997:LYS:O	1.87	0.73
1:E:252:TYR:HD1	1:E:275:LYS:HG2	1.52	0.73
1:H:1085:VAL:CG2	1:H:1086:ASN:N	2.51	0.73
1:H:304:GLU:OE1	1:H:304:GLU:CA	2.36	0.73
1:D:334:LEU:O	1:D:336:ALA:N	2.21	0.73
1:F:251:VAL:HG21	1:F:259:PHE:CZ	2.24	0.73
1:H:304:GLU:OE1	1:H:304:GLU:C	2.32	0.73
1:H:587:HIS:NE2	2:P:3:AC1:O3B	2.21	0.73
1:F:352:ASN:HD22	1:F:352:ASN:H	1.36	0.73
1:E:299:TRP:CH2	1:E:301:PRO:HB3	2.24	0.73
1:F:740:ASN:HD22	1:F:741:PRO:N	1.87	0.73
1:C:670:MET:HE1	1:C:885:PHE:HZ	1.53	0.73
1:F:740:ASN:HD22	1:F:741:PRO:CD	2.02	0.73
1:B:800:THR:CG2	1:B:801:ALA:N	2.51	0.73
1:F:312:TYR:C	1:F:312:TYR:CD2	2.66	0.72
1:G:310:VAL:HG11	1:G:335:ALA:CB	2.19	0.72
1:C:460:GLY:N	1:C:470:ASN:ND2	2.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:658:TYR:CE2	1:G:660:GLY:HA3	2.23	0.72
1:H:1052:ASN:HD22	1:H:1052:ASN:N	1.81	0.72
1:E:271:TRP:CE2	1:E:294:PRO:CB	2.71	0.72
1:G:335:ALA:O	1:G:339:ILE:HG13	1.88	0.72
1:H:639:ASN:ND2	1:H:813:SER:H	1.85	0.72
1:A:330:LEU:HD12	1:A:330:LEU:O	1.90	0.72
1:D:347:ILE:HG12	1:D:353:THR:HG22	1.71	0.72
1:F:261:HIS:CD2	1:F:264:HIS:HA	2.24	0.72
1:G:346:LYS:HE3	1:G:355:TRP:CD2	2.24	0.72
1:E:752:VAL:HG22	1:E:798:ILE:HD13	1.72	0.72
1:F:861:SER:N	1:F:864:GLN:HE21	1.83	0.72
1:F:737:GLU:HA	1:F:815:TYR:O	1.90	0.72
1:E:330:LEU:O	1:E:333:ASN:HB2	1.89	0.71
1:F:669:TYR:CE1	1:F:874:THR:HG23	2.24	0.71
1:G:882:VAL:HG13	1:G:948:LYS:HG3	1.72	0.71
1:H:299:TRP:N	1:H:300:TRP:CZ3	2.58	0.71
1:E:280:ASP:O	1:E:282:LYS:CG	2.30	0.71
1:E:291:ASP:N	1:E:291:ASP:OD1	2.23	0.71
1:E:316:GLN:HG2	1:E:359:THR:CG2	2.20	0.71
1:H:278:LEU:O	1:H:278:LEU:HG	1.90	0.71
1:A:740:ASN:C	1:A:740:ASN:ND2	2.47	0.71
1:D:504:ASP:OD1	1:D:846:HIS:HD2	1.74	0.71
1:G:330:LEU:HD12	1:G:330:LEU:O	1.90	0.71
1:B:713:TYR:O	1:B:759:HIS:CE1	2.43	0.71
1:D:278:LEU:HB2	1:D:284:TRP:CH2	2.26	0.71
1:D:312:TYR:C	1:D:312:TYR:HD2	1.98	0.71
1:D:1085:VAL:HG23	1:D:1086:ASN:N	2.04	0.71
1:E:299:TRP:HH2	1:E:301:PRO:HB3	1.55	0.71
1:E:311:ASN:N	1:E:311:ASN:HD22	1.87	0.71
1:E:800:THR:HG22	1:E:802:ALA:N	2.02	0.71
1:C:614:MET:O	1:C:618:LYS:HG3	1.90	0.71
1:E:316:GLN:HG2	1:E:359:THR:HG21	1.72	0.71
1:A:352:ASN:O	1:A:353:THR:HG22	1.89	0.71
1:D:278:LEU:HG	1:D:278:LEU:O	1.90	0.71
1:E:276:TYR:HB3	1:E:284:TRP:CE3	2.26	0.71
1:E:347:ILE:CG1	1:E:353:THR:HB	2.21	0.71
1:H:740:ASN:HD22	1:H:742:SER:H	1.38	0.71
1:G:604:ASN:HD21	1:G:607:VAL:CA	2.04	0.71
1:H:299:TRP:C	1:H:300:TRP:CD2	2.69	0.71
1:D:245:PHE:C	1:D:247:GLN:N	2.44	0.70
1:D:809:ASN:HB2	1:D:810:PRO:CD	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:TRP:CZ2	1:E:301:PRO:HA	2.26	0.70
1:A:300:TRP:HB2	1:A:306:GLN:HB2	1.72	0.70
1:D:253:SER:H	1:D:258:ASN:ND2	1.89	0.70
1:D:303:GLN:HE22	1:D:329:PRO:HG3	1.56	0.70
1:E:440:ASN:HD21	1:E:449:GLN:NE2	1.84	0.70
1:G:259:PHE:N	1:G:259:PHE:CD2	2.59	0.70
1:B:939:VAL:CG1	1:B:943:LYS:HZ1	2.00	0.70
1:B:1063:LYS:HE2	1:B:1068:ASN:ND2	2.06	0.70
1:E:245:PHE:N	1:E:248:TYR:CE2	2.60	0.70
1:B:577:ALA:O	1:B:578:VAL:HG23	1.91	0.70
1:A:346:LYS:O	1:A:350:GLU:CG	2.37	0.70
1:G:1021:GLU:OE1	1:G:1021:GLU:CA	2.38	0.70
1:H:299:TRP:HA	1:H:300:TRP:CE3	2.27	0.70
1:C:587:HIS:HE2	2:K:3:AC1:HOB3	1.40	0.70
1:C:306:GLN:O	1:C:310:VAL:HG23	1.91	0.70
1:C:669:TYR:HE2	1:C:670:MET:HE3	1.56	0.70
1:A:307:ARG:HG2	1:A:307:ARG:NH1	2.05	0.70
1:F:612:PHE:CD2	1:F:612:PHE:N	2.57	0.70
1:H:504:ASP:OD1	1:H:846:HIS:HD2	1.74	0.70
1:F:250:GLN:OE1	1:F:1087:PRO:HG3	1.92	0.69
1:F:1085:VAL:CG2	1:F:1086:ASN:H	2.05	0.69
1:H:440:ASN:ND2	1:H:449:GLN:HE21	1.85	0.69
2:I:2:GLC:H61	2:I:3:AC1:C1	2.22	0.69
1:D:245:PHE:C	1:D:247:GLN:H	1.99	0.69
1:E:273:ARG:CG	1:E:287:SER:CB	2.71	0.69
1:D:251:VAL:HG21	1:D:259:PHE:HZ	1.56	0.69
1:E:883:ASP:OD1	1:E:948:LYS:HE3	1.93	0.69
1:G:271:TRP:CZ2	1:G:357:ARG:HD3	2.27	0.69
1:H:260:GLU:CD	1:H:271:TRP:HB2	2.17	0.69
1:B:964:LEU:HD12	1:B:996:GLY:HA2	1.74	0.69
1:E:300:TRP:CD1	1:E:306:GLN:HA	2.27	0.69
1:F:440:ASN:HD21	1:F:449:GLN:NE2	1.87	0.69
1:F:800:THR:CG2	1:F:802:ALA:H	2.01	0.69
1:D:299:TRP:CH2	1:D:301:PRO:HA	2.28	0.69
1:E:323:TYR:HB3	1:E:327:THR:OG1	1.93	0.69
1:E:474:ILE:O	1:E:953:MET:HE2	1.92	0.69
1:H:299:TRP:HA	1:H:300:TRP:CZ3	2.26	0.69
1:C:1052:ASN:H	1:C:1052:ASN:ND2	1.80	0.69
1:E:303:GLN:O	1:E:304:GLU:C	2.36	0.69
1:C:516:ALA:HB1	1:C:521:ASP:OD2	1.92	0.69
1:D:460:GLY:N	1:D:470:ASN:HD22	1.89	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:639:ASN:ND2	1:F:642:LEU:HD13	2.07	0.69
1:F:669:TYR:CD1	1:F:874:THR:HG23	2.27	0.69
1:H:293:ARG:HB3	1:H:294:PRO:HD2	1.73	0.69
1:A:663:PHE:CZ	1:A:670:MET:HG2	2.28	0.69
1:C:262:VAL:HG12	1:C:969:VAL:HG23	1.74	0.69
1:E:330:LEU:O	1:E:333:ASN:N	2.24	0.69
1:F:1061:VAL:HG12	1:F:1070:TYR:CD1	2.28	0.69
1:G:800:THR:CG2	1:G:802:ALA:H	1.98	0.69
1:H:261:HIS:HD2	1:H:264:HIS:HA	1.56	0.69
1:A:300:TRP:CG	1:A:306:GLN:HG3	2.28	0.69
1:E:273:ARG:HH11	1:E:288:THR:C	2.01	0.69
1:F:250:GLN:HE21	1:F:275:LYS:HE2	1.56	0.69
1:H:360:ILE:CG2	1:H:361:SER:N	2.55	0.69
1:A:705:SER:HB3	1:A:743:LEU:HD13	1.75	0.69
1:B:391:ASN:C	1:B:392:ASN:HD22	2.01	0.69
1:B:540:ARG:HB2	5:B:106:HOH:O	1.92	0.69
1:D:245:PHE:CD1	1:D:284:TRP:HZ2	2.10	0.69
1:D:356:LEU:HA	1:D:359:THR:CG2	2.23	0.69
1:G:261:HIS:CD2	1:G:264:HIS:HA	2.28	0.68
1:H:733:VAL:HG22	1:H:734:VAL:N	2.07	0.68
2:P:2:GLC:C6	2:P:3:AC1:O5	2.30	0.68
1:A:273:ARG:HH12	1:A:289:GLU:HG2	1.58	0.68
1:G:440:ASN:ND2	1:G:449:GLN:HE21	1.88	0.68
1:H:304:GLU:OE1	1:H:304:GLU:HA	1.92	0.68
1:C:346:LYS:HB3	1:C:355:TRP:CZ2	2.28	0.68
1:C:440:ASN:HD21	1:C:449:GLN:NE2	1.86	0.68
1:A:613:THR:OG1	1:A:615:GLU:HB2	1.93	0.68
1:C:1085:VAL:HG23	1:C:1086:ASN:H	1.57	0.68
1:E:740:ASN:HD22	1:E:741:PRO:N	1.92	0.68
1:H:261:HIS:CD2	1:H:264:HIS:HA	2.28	0.68
1:C:537:ASN:OD1	1:C:540:ARG:NH1	2.26	0.68
1:C:713:TYR:O	1:C:759:HIS:HE1	1.75	0.68
1:E:513:ILE:HG12	1:E:953:MET:HE1	1.75	0.68
1:A:299:TRP:CH2	1:A:301:PRO:HA	2.28	0.68
1:B:368:SER:HA	1:B:371:ASN:HD22	1.58	0.68
1:E:513:ILE:HG12	1:E:953:MET:CE	2.23	0.68
1:G:492:ASP:HB3	1:G:1022:LEU:CD2	2.23	0.68
1:G:602:GLU:O	1:G:603:ILE:HG13	1.94	0.68
1:H:310:VAL:HG12	1:H:311:ASN:HD22	1.57	0.68
1:A:596:ARG:HB2	1:A:612:PHE:HZ	1.59	0.68
1:A:687:ARG:HA	1:A:691:VAL:CG2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:PRO:HG2	1:A:302:ASP:N	2.07	0.68
1:A:457:MET:HE2	1:A:493:TYR:HE2	1.59	0.68
1:E:416:LYS:HD3	5:E:100:HOH:O	1.93	0.68
1:H:308:GLN:C	1:H:310:VAL:N	2.50	0.68
1:C:514:LEU:HD21	1:C:532:MET:HG3	1.76	0.68
1:C:1063:LYS:CE	1:C:1068:ASN:ND2	2.55	0.68
1:D:713:TYR:O	1:D:759:HIS:HE1	1.75	0.68
1:F:917:ALA:HA	1:F:962:TYR:CD1	2.29	0.68
1:H:1080:LEU:HB2	1:H:1085:VAL:CG1	2.24	0.68
1:B:526:HIS:HA	1:B:530:ASP:OD1	1.93	0.68
1:A:356:LEU:O	1:A:357:ARG:C	2.37	0.67
1:A:740:ASN:HD22	1:A:741:PRO:N	1.91	0.67
1:C:300:TRP:CD2	1:C:306:GLN:HG3	2.29	0.67
1:D:305:THR:HG23	1:D:367:GLN:HE21	1.59	0.67
1:C:740:ASN:HD22	1:C:742:SER:H	1.40	0.67
1:E:440:ASN:ND2	1:E:449:GLN:HE21	1.88	0.67
1:E:670:MET:HE1	1:E:885:PHE:CZ	2.30	0.67
1:D:356:LEU:HD11	1:D:360:ILE:HD11	1.74	0.67
1:D:993:VAL:O	1:D:1056:ARG:NH1	2.27	0.67
1:F:250:GLN:NE2	1:F:275:LYS:CE	2.47	0.67
1:F:740:ASN:ND2	1:F:741:PRO:HD2	2.08	0.67
1:F:1022:LEU:HD23	1:F:1022:LEU:N	2.10	0.67
1:H:800:THR:HG22	1:H:801:ALA:N	2.09	0.67
2:O:2:GLC:C6	2:O:3:AC1:O5	2.30	0.67
1:B:1085:VAL:HG23	1:B:1086:ASN:N	2.08	0.67
1:C:350:GLU:C	1:C:352:ASN:H	2.02	0.67
1:D:355:TRP:CG	1:D:356:LEU:H	2.12	0.67
1:H:585:ARG:HD3	1:H:661:ASP:OD1	1.94	0.67
1:B:988:LYS:O	1:B:989:ASN:HB2	1.94	0.67
1:G:293:ARG:HB3	1:G:297:MET:HE2	1.77	0.67
1:H:931:LYS:HA	5:H:17:HOH:O	1.93	0.67
1:B:713:TYR:O	1:B:759:HIS:HE1	1.77	0.67
1:B:742:SER:O	1:B:744:ARG:HG3	1.94	0.67
1:C:248:TYR:HB3	1:C:276:TYR:HB2	1.76	0.67
1:F:606:ASN:O	1:F:607:VAL:C	2.38	0.67
1:B:939:VAL:HG12	1:B:943:LYS:HZ3	1.45	0.67
1:C:515:GLU:OE1	2:K:3:AC1:O3	2.12	0.67
1:D:261:HIS:HD2	1:D:264:HIS:H	1.43	0.67
1:A:271:TRP:CE2	1:A:294:PRO:HG3	2.30	0.67
1:F:248:TYR:HB2	1:F:284:TRP:CZ3	2.29	0.67
1:G:1085:VAL:CG2	1:G:1086:ASN:N	2.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:322:THR:CG2	1:E:323:TYR:N	2.57	0.66
1:H:800:THR:CG2	1:H:801:ALA:N	2.57	0.66
1:F:350:GLU:HB3	1:F:352:ASN:HD21	1.60	0.66
1:F:669:TYR:HE2	1:F:670:MET:CE	2.06	0.66
1:G:1021:GLU:OE1	1:G:1021:GLU:HA	1.80	0.66
1:D:513:ILE:HG12	1:D:953:MET:CE	2.25	0.66
1:A:261:HIS:HD2	1:A:264:HIS:N	1.92	0.66
1:C:251:VAL:O	1:C:275:LYS:HE3	1.95	0.66
1:D:245:PHE:CE1	1:D:284:TRP:CZ2	2.84	0.66
1:F:658:TYR:CE2	1:F:660:GLY:HA3	2.31	0.66
1:B:743:LEU:O	1:B:744:ARG:CG	2.35	0.66
1:H:809:ASN:HB2	1:H:810:PRO:HD2	1.76	0.66
1:B:809:ASN:HB2	1:B:810:PRO:CD	2.25	0.66
1:F:368:SER:O	1:F:371:ASN:HB2	1.96	0.66
1:G:278:LEU:HG	1:G:281:GLY:HA2	1.78	0.66
1:G:376:LYS:HB3	1:G:377:PRO:HA	1.78	0.66
1:H:250:GLN:HB2	1:H:1084:LEU:O	1.96	0.66
1:A:279:LYS:N	1:A:283:THR:O	2.29	0.66
1:B:376:LYS:HB3	1:B:377:PRO:HA	1.77	0.66
1:G:310:VAL:CG1	1:G:335:ALA:HB1	2.24	0.66
1:A:250:GLN:HE21	1:A:275:LYS:HE3	1.60	0.66
1:G:740:ASN:HD22	1:G:741:PRO:N	1.93	0.66
1:A:342:LYS:O	1:A:346:LYS:HB2	1.95	0.66
1:B:759:HIS:CD2	1:B:764:TYR:OH	2.48	0.66
1:C:365:LYS:HE3	1:C:1055:GLY:O	1.96	0.66
1:C:800:THR:CG2	1:C:801:ALA:N	2.59	0.66
1:D:334:LEU:C	1:D:336:ALA:N	2.46	0.66
1:E:809:ASN:HB2	1:E:810:PRO:CD	2.25	0.65
1:H:277:ILE:HD11	1:H:291:ASP:CG	2.17	0.65
1:A:670:MET:HE1	1:A:885:PHE:CZ	2.31	0.65
1:C:245:PHE:CE2	1:C:337:GLN:HB3	2.31	0.65
1:E:740:ASN:HD22	1:E:742:SER:H	1.44	0.65
1:F:740:ASN:HD22	1:F:741:PRO:HD2	1.61	0.65
1:F:329:PRO:O	1:F:333:ASN:ND2	2.29	0.65
1:A:293:ARG:HB3	1:A:297:MET:HE2	1.77	0.65
1:A:317:LEU:HD13	1:A:342:LYS:HB3	1.76	0.65
1:B:261:HIS:HD2	1:B:264:HIS:N	1.95	0.65
1:D:440:ASN:HD21	1:D:449:GLN:NE2	1.91	0.65
1:G:297:MET:SD	1:G:340:GLN:HG3	2.37	0.65
1:A:309:TYR:HD2	1:A:310:VAL:N	1.94	0.65
1:B:639:ASN:ND2	1:B:813:SER:H	1.93	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1085:VAL:O	1:F:1087:PRO:HD3	1.96	0.65
1:H:310:VAL:O	1:H:311:ASN:C	2.39	0.65
1:E:800:THR:CG2	1:E:801:ALA:N	2.59	0.65
1:E:988:LYS:O	1:E:990:THR:HG23	1.97	0.65
1:F:860:PHE:HB2	1:F:864:GLN:HE22	1.61	0.65
1:H:276:TYR:HB3	1:H:284:TRP:HB3	1.78	0.65
1:A:327:THR:HG22	1:A:328:SER:O	1.97	0.65
1:B:466:ASP:OD2	1:B:943:LYS:CE	2.45	0.65
1:C:280:ASP:HB2	1:C:348:THR:OG1	1.97	0.65
1:D:277:ILE:O	1:D:277:ILE:CG2	2.37	0.65
1:H:294:PRO:HG2	1:H:297:MET:HB2	1.78	0.65
1:C:261:HIS:CD2	1:C:264:HIS:HA	2.31	0.65
1:C:705:SER:HB3	1:C:743:LEU:HD13	1.78	0.65
1:D:551:LEU:HD21	1:D:741:PRO:HG2	1.79	0.65
1:D:782:GLN:HA	1:D:782:GLN:NE2	2.11	0.65
1:E:271:TRP:CD2	1:E:357:ARG:NH1	2.64	0.65
1:E:297:MET:HG2	1:E:297:MET:O	1.96	0.65
1:F:750:ARG:HB2	5:F:55:HOH:O	1.96	0.65
1:G:809:ASN:HB2	1:G:810:PRO:CD	2.27	0.65
1:H:312:TYR:O	1:H:314:ASN:N	2.30	0.65
1:C:514:LEU:CD2	1:C:532:MET:HG3	2.27	0.65
1:G:917:ALA:HA	1:G:962:TYR:CD1	2.32	0.65
1:E:504:ASP:OD1	1:E:846:HIS:HD2	1.80	0.65
1:F:516:ALA:HB1	1:F:521:ASP:OD2	1.97	0.65
1:G:252:TYR:HB3	1:G:258:ASN:ND2	2.06	0.65
1:B:551:LEU:HD12	1:B:551:LEU:O	1.97	0.64
1:C:311:ASN:HD21	1:C:323:TYR:H	1.43	0.64
2:M:2:GLC:C6	2:M:3:AC1:O5	2.30	0.64
1:B:587:HIS:NE2	2:J:3:AC1:O3B	2.29	0.64
1:F:537:ASN:OD1	1:F:540:ARG:NH1	2.29	0.64
1:C:245:PHE:N	1:C:245:PHE:CD1	2.63	0.64
1:E:279:LYS:NZ	1:E:279:LYS:HG3	2.11	0.64
1:G:740:ASN:HD22	1:G:742:SER:H	1.41	0.64
1:H:288:THR:HB	1:H:291:ASP:OD1	1.96	0.64
1:H:398:GLN:HG2	1:H:398:GLN:O	1.98	0.64
1:B:513:ILE:HG12	1:B:953:MET:CE	2.26	0.64
1:B:587:HIS:HE2	2:J:3:AC1:HOB3	1.46	0.64
1:F:492:ASP:HB3	1:F:1022:LEU:CD2	2.27	0.64
1:E:299:TRP:CH2	1:E:301:PRO:CA	2.80	0.64
1:B:939:VAL:O	1:B:943:LYS:HG3	1.97	0.64
1:F:300:TRP:HB3	1:F:301:PRO:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1052:ASN:HD22	1:F:1052:ASN:N	1.96	0.64
1:B:752:VAL:HG22	1:B:798:ILE:HG12	1.79	0.64
1:E:273:ARG:NH1	1:E:288:THR:C	2.56	0.64
1:H:854:ARG:NH1	1:H:892:ASP:OD2	2.30	0.64
1:B:250:GLN:HA	1:B:1084:LEU:O	1.98	0.64
1:C:669:TYR:CE2	1:C:670:MET:HE3	2.31	0.64
1:E:294:PRO:HG3	1:E:356:LEU:HD21	1.78	0.64
1:G:504:ASP:OD1	1:G:846:HIS:HD2	1.80	0.64
2:L:2:GLC:C6	2:L:3:AC1:O5	2.30	0.64
1:D:355:TRP:CG	1:D:356:LEU:N	2.66	0.64
1:G:371:ASN:HB3	1:G:373:ASP:H	1.63	0.64
1:C:407:ASN:ND2	1:C:431:GLU:HB2	2.13	0.64
1:D:1052:ASN:N	1:D:1052:ASN:ND2	2.35	0.64
1:F:357:ARG:HH11	1:F:357:ARG:HG3	1.57	0.64
1:F:749:ASP:O	1:F:750:ARG:HG2	1.98	0.64
1:C:359:THR:HG23	1:C:360:ILE:H	1.63	0.63
1:G:350:GLU:O	1:G:352:ASN:ND2	2.22	0.63
1:A:928:LYS:HB2	1:A:929:PRO:HD2	1.79	0.63
1:B:406:LEU:HD22	1:B:431:GLU:HG2	1.80	0.63
1:C:364:VAL:HG13	1:C:370:TRP:CE3	2.33	0.63
1:C:687:ARG:HA	1:C:691:VAL:HG23	1.80	0.63
1:D:537:ASN:OD1	1:D:540:ARG:NH1	2.31	0.63
1:H:316:GLN:HG2	1:H:359:THR:CG2	2.22	0.63
1:A:290:LYS:NZ	1:A:290:LYS:CD	2.61	0.63
1:A:1052:ASN:H	1:A:1052:ASN:ND2	1.90	0.63
1:E:279:LYS:NZ	1:E:279:LYS:CD	2.60	0.63
1:B:733:VAL:HG22	1:B:734:VAL:N	2.13	0.63
1:E:306:GLN:O	1:E:309:TYR:N	2.31	0.63
1:E:346:LYS:HA	1:E:349:ALA:HB3	1.79	0.63
1:F:513:ILE:HG12	1:F:953:MET:CE	2.29	0.63
1:F:687:ARG:HA	1:F:691:VAL:HG21	1.79	0.63
1:G:912:ILE:O	1:G:912:ILE:CG2	2.45	0.63
1:G:1065:GLN:HG3	1:G:1066:ALA:N	2.13	0.63
1:H:299:TRP:CZ2	1:H:301:PRO:HA	2.34	0.63
1:D:1080:LEU:HB3	1:D:1081:PRO:CD	2.28	0.63
1:H:303:GLN:O	1:H:304:GLU:C	2.38	0.63
1:A:516:ALA:HB1	1:A:521:ASP:OD2	1.99	0.63
1:B:764:TYR:CE1	1:B:821:PRO:HD3	2.33	0.63
2:J:2:GLC:C6	2:J:3:AC1:O5	2.30	0.63
1:A:250:GLN:CB	1:A:1084:LEU:O	2.45	0.63
1:H:308:GLN:C	1:H:310:VAL:H	2.04	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:ASP:OD2	1:B:651:LYS:HG2	1.99	0.62
1:C:670:MET:HE1	1:C:885:PHE:CZ	2.33	0.62
1:D:1080:LEU:HB3	1:D:1081:PRO:HD2	1.80	0.62
1:E:713:TYR:O	1:E:759:HIS:HE1	1.82	0.62
1:E:871:GLU:H	1:E:871:GLU:CD	2.07	0.62
1:F:917:ALA:HA	1:F:962:TYR:CE1	2.34	0.62
1:A:252:TYR:HB3	1:A:258:ASN:ND2	2.12	0.62
1:H:713:TYR:O	1:H:759:HIS:HE1	1.81	0.62
1:E:471:PHE:CG	1:E:954:ALA:HB2	2.35	0.62
1:A:281:GLY:H	1:A:344:GLU:HB2	1.65	0.62
1:C:245:PHE:O	1:C:246:ALA:C	2.40	0.62
1:D:305:THR:O	1:D:308:GLN:HB2	2.00	0.62
1:G:669:TYR:CE1	1:G:874:THR:HG23	2.34	0.62
1:H:300:TRP:HD1	1:H:306:GLN:HA	1.63	0.62
2:K:2:GLC:C6	2:K:3:AC1:O5	2.30	0.62
1:A:294:PRO:O	1:A:297:MET:HB3	2.00	0.62
1:A:355:TRP:CE3	1:A:355:TRP:C	2.77	0.62
1:A:854:ARG:NH1	1:A:892:ASP:OD2	2.32	0.62
1:B:761:ASN:ND2	1:B:761:ASN:N	2.47	0.62
1:D:280:ASP:O	1:D:282:LYS:N	2.32	0.62
1:E:271:TRP:CD1	1:E:294:PRO:HB3	2.30	0.62
1:F:724:GLY:HA3	1:F:728:THR:OG1	2.00	0.62
1:H:284:TRP:O	1:H:285:THR:OG1	2.16	0.62
1:A:321:GLN:OE1	1:A:321:GLN:CA	2.48	0.62
1:E:279:LYS:NZ	1:E:279:LYS:CG	2.62	0.62
1:F:800:THR:CG2	1:F:801:ALA:N	2.63	0.62
1:A:261:HIS:CD2	1:A:264:HIS:HA	2.35	0.62
1:A:278:LEU:O	1:A:344:GLU:HG3	1.99	0.62
1:C:352:ASN:OD1	1:C:354:ASN:ND2	2.33	0.62
1:C:966:GLU:HB2	1:C:997:LYS:CB	2.27	0.62
1:B:259:PHE:N	1:B:259:PHE:CD2	2.68	0.62
1:B:861:SER:H	1:B:864:GLN:NE2	1.86	0.62
1:E:585:ARG:HD3	1:E:661:ASP:OD1	2.00	0.62
2:N:2:GLC:C6	2:N:3:AC1:O5	2.30	0.62
1:A:278:LEU:HD11	1:A:282:LYS:N	2.15	0.62
1:A:587:HIS:NE2	2:I:3:AC1:O3B	2.28	0.62
1:B:404:ARG:N	1:B:439:ASP:OD2	2.33	0.62
1:F:440:ASN:ND2	1:F:449:GLN:HE21	1.89	0.62
1:F:793:ASP:HB3	1:F:794:ARG:HG3	1.82	0.62
1:A:356:LEU:C	1:A:358:GLN:N	2.55	0.61
1:A:430:TYR:HB3	1:A:978:TYR:CE1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:PHE:CG	1:A:896:ALA:HB2	2.34	0.61
1:E:439:ASP:C	1:E:439:ASP:OD1	2.41	0.61
1:F:250:GLN:OE1	1:F:1087:PRO:HG2	2.00	0.61
1:A:841:ASP:OD1	1:A:846:HIS:HE1	1.82	0.61
1:B:670:MET:CE	1:B:885:PHE:HZ	2.12	0.61
1:C:440:ASN:ND2	1:C:449:GLN:HE21	1.93	0.61
1:F:723:THR:HG22	1:F:757:ALA:HB1	1.81	0.61
1:G:348:THR:HG22	1:G:349:ALA:N	2.14	0.61
1:A:293:ARG:HB3	1:A:297:MET:CE	2.30	0.61
1:D:551:LEU:CD2	1:D:741:PRO:HG2	2.30	0.61
1:E:454:HIS:CE1	1:E:458:ASN:ND2	2.67	0.61
1:H:882:VAL:HG13	1:H:948:LYS:HG3	1.81	0.61
1:A:280:ASP:OD1	1:A:348:THR:HB	2.01	0.61
1:A:334:LEU:O	1:A:335:ALA:C	2.43	0.61
1:D:245:PHE:O	1:D:246:ALA:C	2.42	0.61
1:A:307:ARG:HH11	1:A:307:ARG:CG	2.13	0.61
1:B:740:ASN:HD22	1:B:740:ASN:C	2.09	0.61
1:D:336:ALA:HA	1:D:339:ILE:HD12	1.83	0.61
1:G:604:ASN:ND2	1:G:607:VAL:CB	2.62	0.61
1:C:359:THR:HG23	1:C:360:ILE:N	2.15	0.61
1:C:874:THR:HG22	1:C:878:ILE:HD12	1.81	0.61
1:E:272:TYR:CD2	1:E:295:LEU:HD23	2.35	0.61
1:E:361:SER:O	1:E:362:ALA:C	2.43	0.61
1:H:363:PHE:O	1:H:364:VAL:C	2.44	0.61
1:H:800:THR:HG22	1:H:802:ALA:N	2.12	0.61
1:H:1034:MET:HE2	5:H:198:HOH:O	1.99	0.61
1:A:478:ALA:HB2	2:I:3:AC1:O3	2.01	0.61
1:D:471:PHE:CG	1:D:954:ALA:HB2	2.35	0.61
1:E:460:GLY:H	1:E:470:ASN:HD22	1.48	0.61
1:G:794:ARG:HG2	1:G:794:ARG:HH11	1.60	0.61
1:H:596:ARG:NH2	1:H:600:LYS:HD2	2.15	0.61
1:C:740:ASN:HD22	1:C:741:PRO:N	1.97	0.61
1:D:245:PHE:CD1	1:D:284:TRP:CZ2	2.88	0.61
1:D:252:TYR:HB3	1:D:258:ASN:ND2	2.16	0.61
1:E:359:THR:O	1:E:362:ALA:HB3	2.00	0.61
1:H:1072:SER:OG	1:H:1074:VAL:CG1	2.48	0.61
1:D:277:ILE:HD13	1:D:293:ARG:NH2	2.15	0.61
1:G:515:GLU:OE1	2:O:3:AC1:O3	2.17	0.61
1:D:278:LEU:HB2	1:D:284:TRP:CZ3	2.36	0.61
1:D:999:SER:O	1:D:1001:LYS:HG3	2.01	0.60
1:F:365:LYS:HE3	1:F:1055:GLY:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:ASN:HD22	1:A:742:SER:H	1.47	0.60
1:B:471:PHE:CG	1:B:954:ALA:HB2	2.35	0.60
1:D:639:ASN:HD21	1:D:813:SER:N	1.95	0.60
1:E:250:GLN:OE1	1:E:1087:PRO:CG	2.49	0.60
1:F:513:ILE:HG12	1:F:953:MET:HE1	1.83	0.60
1:G:965:PRO:HD2	1:G:997:LYS:O	2.01	0.60
1:H:261:HIS:HD2	1:H:264:HIS:CA	2.14	0.60
1:D:908:LEU:O	1:D:912:ILE:HG13	2.00	0.60
1:E:1052:ASN:H	1:E:1052:ASN:ND2	1.92	0.60
1:H:740:ASN:C	1:H:740:ASN:ND2	2.51	0.60
1:H:1072:SER:OG	1:H:1074:VAL:HG12	2.01	0.60
1:A:288:THR:OG1	1:A:290:LYS:HD2	2.02	0.60
1:A:782:GLN:NE2	1:A:782:GLN:CA	2.58	0.60
1:D:740:ASN:HD22	1:D:742:SER:N	1.90	0.60
1:G:861:SER:HB3	1:G:864:GLN:HG3	1.82	0.60
1:H:290:LYS:C	1:H:291:ASP:OD1	2.45	0.60
1:H:312:TYR:C	1:H:314:ASN:N	2.60	0.60
1:B:577:ALA:O	1:B:578:VAL:CG2	2.49	0.60
1:C:630:ALA:O	1:C:633:LYS:NZ	2.35	0.60
1:C:860:PHE:CG	1:C:896:ALA:HB2	2.36	0.60
1:D:297:MET:SD	1:D:340:GLN:CG	2.86	0.60
1:G:274:PRO:O	1:G:287:SER:OG	2.20	0.60
1:A:316:GLN:HE21	1:A:359:THR:CG2	2.12	0.60
1:A:800:THR:HG22	1:A:802:ALA:N	2.05	0.60
1:H:307:ARG:O	1:H:310:VAL:HB	2.00	0.60
1:H:312:TYR:C	1:H:314:ASN:H	2.10	0.60
1:C:513:ILE:HG23	1:C:953:MET:HE1	1.83	0.60
1:D:987:ILE:CG1	1:D:1058:ALA:HB2	2.32	0.60
1:G:261:HIS:HD2	1:G:264:HIS:N	1.96	0.60
1:H:993:VAL:O	1:H:1056:ARG:NH1	2.34	0.60
1:A:1052:ASN:HD22	1:A:1052:ASN:N	1.94	0.60
1:B:788:VAL:CG1	1:B:789:ARG:N	2.64	0.60
1:G:248:TYR:HB3	1:G:276:TYR:HB2	1.83	0.60
1:G:310:VAL:HG13	1:G:339:ILE:HD11	1.82	0.60
1:H:315:ALA:C	1:H:317:LEU:H	2.08	0.60
1:B:788:VAL:HG12	1:B:789:ARG:N	2.16	0.60
1:D:337:GLN:O	1:D:338:THR:C	2.44	0.60
1:E:245:PHE:N	1:E:245:PHE:CB	2.62	0.60
1:G:740:ASN:ND2	1:G:740:ASN:C	2.58	0.60
1:A:460:GLY:N	1:A:470:ASN:HD22	1.99	0.60
1:E:300:TRP:CD1	1:E:306:GLN:CA	2.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1085:VAL:CG2	1:A:1086:ASN:N	2.64	0.59
1:D:809:ASN:HB2	1:D:810:PRO:HD2	1.84	0.59
1:E:587:HIS:CD2	2:M:3:AC1:HOB3	2.19	0.59
1:E:1085:VAL:HG23	1:E:1086:ASN:N	2.17	0.59
1:H:513:ILE:HG23	1:H:953:MET:HE1	1.84	0.59
1:B:1040:ILE:HG12	1:B:1047:TYR:CE2	2.36	0.59
1:D:800:THR:HG22	1:D:801:ALA:N	2.16	0.59
1:E:306:GLN:O	1:E:309:TYR:CB	2.47	0.59
1:H:474:ILE:O	1:H:953:MET:HE2	2.02	0.59
1:H:856:MET:HG3	1:H:892:ASP:HB2	1.84	0.59
1:A:276:TYR:CB	1:A:285:THR:O	2.50	0.59
1:A:576:ALA:HB3	1:A:847:GLN:HB3	1.83	0.59
1:B:585:ARG:HD3	1:B:661:ASP:OD1	2.02	0.59
1:D:302:ASP:OD1	1:D:304:GLU:HB3	2.01	0.59
1:D:957:VAL:O	1:D:957:VAL:HG12	2.01	0.59
1:A:274:PRO:HG2	1:A:277:ILE:HD13	1.84	0.59
1:A:301:PRO:CG	1:A:302:ASP:H	2.12	0.59
1:F:639:ASN:HD21	1:F:813:SER:H	1.50	0.59
1:G:1081:PRO:HG2	1:G:1084:LEU:HB2	1.84	0.59
1:A:300:TRP:CD2	1:A:306:GLN:CG	2.72	0.59
1:D:352:ASN:C	1:D:352:ASN:ND2	2.61	0.59
1:D:460:GLY:N	1:D:470:ASN:ND2	2.51	0.59
1:H:809:ASN:HB2	1:H:810:PRO:CD	2.32	0.59
1:C:809:ASN:HB2	1:C:810:PRO:CD	2.32	0.59
1:D:322:THR:O	1:D:322:THR:HG22	2.03	0.59
1:D:697:MET:HA	1:D:709:THR:O	2.03	0.59
1:H:782:GLN:HA	1:H:782:GLN:NE2	2.18	0.59
1:A:280:ASP:O	1:A:281:GLY:C	2.45	0.59
1:B:800:THR:HG22	1:B:802:ALA:H	0.76	0.59
1:D:330:LEU:HD12	1:D:330:LEU:C	2.28	0.59
1:D:733:VAL:HG22	1:D:734:VAL:N	2.17	0.59
1:E:272:TYR:CE2	1:E:295:LEU:HD23	2.38	0.59
1:G:307:ARG:HA	1:G:332:LEU:CD2	2.33	0.59
1:A:390:SER:HB2	1:A:971:THR:HB	1.85	0.59
1:C:551:LEU:HD12	1:C:551:LEU:O	2.02	0.59
1:C:733:VAL:HG22	1:C:734:VAL:N	2.17	0.59
1:D:491:GLY:HA3	5:D:36:HOH:O	2.03	0.59
1:E:965:PRO:HD2	1:E:997:LYS:O	2.02	0.59
1:F:614:MET:O	1:F:618:LYS:HG3	2.03	0.59
1:H:360:ILE:O	1:H:363:PHE:N	2.33	0.59
1:E:1064:ASP:HB2	1:E:1071:PHE:CZ	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:262:VAL:CG1	1:H:969:VAL:HG23	2.30	0.59
1:H:298:THR:O	1:H:300:TRP:HZ3	1.85	0.59
1:A:604:ASN:HD21	1:A:607:VAL:N	2.01	0.59
1:B:516:ALA:HB1	1:B:521:ASP:OD2	2.02	0.59
1:B:939:VAL:HG11	1:B:943:LYS:NZ	2.06	0.59
1:D:278:LEU:O	1:D:278:LEU:CG	2.51	0.59
1:E:271:TRP:CD1	1:E:294:PRO:CB	2.84	0.59
1:G:476:VAL:HG22	1:G:956:TRP:HE3	1.68	0.59
1:G:669:TYR:CD1	1:G:874:THR:HG23	2.37	0.59
1:D:250:GLN:HE21	1:D:275:LYS:CE	2.16	0.58
1:D:277:ILE:O	1:D:279:LYS:N	2.36	0.58
1:D:293:ARG:CB	1:D:297:MET:CE	2.80	0.58
1:A:323:TYR:HB3	1:A:327:THR:OG1	2.03	0.58
1:A:457:MET:HE2	1:A:493:TYR:CE2	2.37	0.58
1:D:300:TRP:HB2	1:D:306:GLN:HB2	1.84	0.58
1:D:440:ASN:ND2	1:D:449:GLN:HE21	1.95	0.58
1:C:1063:LYS:HE2	1:C:1068:ASN:CG	2.28	0.58
1:G:430:TYR:CD1	1:G:977:LYS:HD2	2.38	0.58
1:G:602:GLU:C	1:G:603:ILE:HG13	2.29	0.58
1:H:526:HIS:HA	1:H:530:ASP:OD1	2.03	0.58
1:A:809:ASN:C	1:A:809:ASN:OD1	2.46	0.58
1:E:250:GLN:OE1	1:E:1087:PRO:HG2	2.03	0.58
1:E:271:TRP:CE2	1:E:294:PRO:HD3	2.38	0.58
1:E:271:TRP:CG	1:E:294:PRO:CA	2.83	0.58
1:F:780:SER:OG	1:F:782:GLN:HB3	2.04	0.58
1:F:1085:VAL:CG2	1:F:1086:ASN:N	2.64	0.58
1:H:277:ILE:HG12	1:H:293:ARG:HE	1.68	0.58
1:H:537:ASN:OD1	1:H:540:ARG:NH1	2.37	0.58
1:A:800:THR:CG2	1:A:801:ALA:N	2.67	0.58
1:E:261:HIS:HD2	1:E:264:HIS:N	1.99	0.58
1:E:279:LYS:HG3	1:E:279:LYS:HZ2	1.68	0.58
1:H:299:TRP:CH2	1:H:301:PRO:CA	2.87	0.58
1:H:299:TRP:CH2	1:H:301:PRO:HA	2.39	0.58
1:H:424:ASP:HB3	1:H:520:ASN:ND2	2.19	0.58
1:A:285:THR:HG22	1:A:286:GLN:O	2.03	0.58
1:B:577:ALA:C	1:B:578:VAL:HG23	2.29	0.58
1:B:800:THR:HG23	1:B:801:ALA:N	2.19	0.58
1:E:782:GLN:HA	1:E:782:GLN:NE2	2.18	0.58
1:F:705:SER:HB3	1:F:743:LEU:HD13	1.86	0.58
1:G:316:GLN:N	1:G:316:GLN:CD	2.61	0.58
1:G:794:ARG:HH11	1:G:794:ARG:CG	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:829:ASP:OD1	1:H:831:ARG:HB2	2.04	0.58
1:A:277:ILE:HG21	1:A:293:ARG:NH2	2.19	0.58
1:G:356:LEU:O	1:G:357:ARG:C	2.45	0.58
1:H:301:PRO:O	1:H:302:ASP:HB3	2.03	0.58
1:H:315:ALA:C	1:H:317:LEU:N	2.57	0.58
1:H:363:PHE:O	1:H:365:LYS:N	2.36	0.58
1:E:339:ILE:CG2	1:E:343:ILE:HD11	2.34	0.58
1:G:478:ALA:HB1	1:G:481:ASN:HD22	1.69	0.58
1:B:1016:GLN:HE21	1:G:748:SER:HA	1.69	0.57
1:C:729:ARG:HD2	1:C:758:ALA:O	2.03	0.57
1:F:311:ASN:ND2	1:F:323:TYR:H	1.91	0.57
1:G:251:VAL:HG21	1:G:259:PHE:HZ	1.66	0.57
1:H:288:THR:HG23	1:H:289:GLU:H	1.64	0.57
1:H:630:ALA:O	1:H:633:LYS:NZ	2.37	0.57
1:H:765:ARG:HB2	1:H:766:PRO:HD2	1.84	0.57
1:B:841:ASP:OD1	1:B:846:HIS:HE1	1.86	0.57
1:D:347:ILE:CG1	1:D:353:THR:HG22	2.34	0.57
1:D:854:ARG:NH1	1:D:892:ASP:OD2	2.33	0.57
1:E:271:TRP:CD2	1:E:294:PRO:HD3	2.38	0.57
1:E:457:MET:HE2	1:E:493:TYR:HE2	1.69	0.57
1:A:454:HIS:CE1	1:A:458:ASN:ND2	2.72	0.57
1:C:261:HIS:CD2	1:C:264:HIS:N	2.60	0.57
1:C:346:LYS:HE3	1:C:355:TRP:CE3	2.40	0.57
1:C:854:ARG:NH1	1:C:892:ASP:OD2	2.36	0.57
1:D:856:MET:HG3	1:D:892:ASP:HB2	1.86	0.57
1:D:874:THR:HB	1:D:932:TYR:HB3	1.85	0.57
1:G:269:GLU:HG3	1:G:364:VAL:HG21	1.85	0.57
1:A:596:ARG:HB2	1:A:612:PHE:CZ	2.38	0.57
1:B:709:THR:HG21	1:B:753:VAL:HG22	1.87	0.57
1:E:273:ARG:CG	1:E:287:SER:HB2	2.22	0.57
1:F:520:ASN:O	1:F:523:PRO:HG2	2.05	0.57
1:F:639:ASN:HB3	1:F:642:LEU:HB2	1.86	0.57
1:B:251:VAL:HG21	1:B:259:PHE:CZ	2.39	0.57
1:B:711:VAL:HG22	1:B:734:VAL:HG23	1.87	0.57
1:F:740:ASN:HD22	1:F:740:ASN:C	2.12	0.57
1:C:457:MET:HE2	1:C:493:TYR:HE2	1.69	0.57
1:F:252:TYR:HB3	1:F:258:ASN:ND2	2.08	0.57
1:F:874:THR:HG22	1:F:878:ILE:HD11	1.87	0.57
1:A:280:ASP:O	1:A:282:LYS:N	2.38	0.57
1:A:407:ASN:HD21	1:A:431:GLU:H	1.52	0.57
1:A:447:ALA:O	1:A:450:LEU:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:882:VAL:HG21	1:A:944:ALA:O	2.05	0.57
1:C:687:ARG:HA	1:C:691:VAL:CG2	2.34	0.57
1:D:308:GLN:HA	1:D:308:GLN:HE21	1.69	0.57
1:E:271:TRP:CZ2	1:E:294:PRO:HD3	2.40	0.57
1:E:457:MET:HE2	1:E:493:TYR:CE2	2.40	0.57
1:E:740:ASN:C	1:E:740:ASN:ND2	2.50	0.57
1:D:334:LEU:C	1:D:336:ALA:H	2.11	0.57
1:H:295:LEU:HD23	1:H:295:LEU:O	2.04	0.57
1:H:871:GLU:H	1:H:871:GLU:CD	2.13	0.57
1:D:793:ASP:HB2	1:D:794:ARG:HG3	1.86	0.57
1:E:430:TYR:HB3	1:E:978:TYR:CE1	2.40	0.57
1:G:245:PHE:O	1:G:246:ALA:C	2.48	0.57
1:A:383:GLN:O	1:A:384:LYS:HB2	2.05	0.57
1:D:492:ASP:HB3	1:D:1022:LEU:CD2	2.31	0.57
1:G:301:PRO:O	1:G:302:ASP:HB3	2.05	0.57
1:H:363:PHE:C	1:H:365:LYS:N	2.60	0.57
1:A:367:GLN:O	1:A:371:ASN:HB3	2.05	0.56
1:C:288:THR:OG1	1:C:290:LYS:HB2	2.04	0.56
1:C:371:ASN:HB3	1:C:373:ASP:H	1.69	0.56
1:C:632:GLU:HG2	5:C:18:HOH:O	2.04	0.56
1:D:987:ILE:HG12	1:D:1058:ALA:HB2	1.85	0.56
1:E:323:TYR:CD1	1:E:327:THR:HG21	2.40	0.56
1:G:663:PHE:CZ	1:G:670:MET:HG2	2.40	0.56
1:H:841:ASP:OD1	1:H:846:HIS:HE1	1.88	0.56
1:A:300:TRP:CB	1:A:306:GLN:HB2	2.35	0.56
1:C:347:ILE:HG22	1:C:348:THR:N	2.19	0.56
1:E:245:PHE:O	1:E:249:ASN:HB2	2.04	0.56
1:E:271:TRP:CH2	1:E:356:LEU:HD23	2.40	0.56
1:E:299:TRP:CH2	1:E:301:PRO:CB	2.87	0.56
1:E:651:LYS:O	1:E:652:SER:HB2	2.03	0.56
1:G:928:LYS:HB2	1:G:929:PRO:CD	2.33	0.56
1:H:311:ASN:H	1:H:311:ASN:ND2	2.03	0.56
1:A:280:ASP:H	1:A:344:GLU:HB3	1.69	0.56
1:A:309:TYR:CD2	1:A:310:VAL:N	2.73	0.56
1:A:310:VAL:O	1:A:311:ASN:C	2.48	0.56
1:B:531:ASN:ND2	1:B:844:SER:OG	2.38	0.56
1:B:742:SER:O	1:B:744:ARG:CG	2.53	0.56
1:B:869:LYS:O	1:B:870:LYS:C	2.48	0.56
1:C:619:LYS:O	1:C:622:GLU:HG3	2.05	0.56
1:D:356:LEU:HA	1:D:359:THR:HG23	1.86	0.56
1:D:363:PHE:O	1:D:366:THR:HG23	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:729:ARG:HD2	1:D:758:ALA:O	2.05	0.56
1:D:1085:VAL:CG2	1:D:1086:ASN:H	2.17	0.56
1:E:288:THR:HG22	1:E:289:GLU:N	2.11	0.56
1:E:335:ALA:O	1:E:339:ILE:HD12	2.05	0.56
1:F:376:LYS:HB3	1:F:377:PRO:HA	1.88	0.56
1:F:478:ALA:HB1	1:F:481:ASN:HD22	1.69	0.56
1:F:862:ASN:O	1:F:912:ILE:CG2	2.43	0.56
1:G:928:LYS:HB2	1:G:929:PRO:HD2	1.86	0.56
1:A:374:SER:HB2	1:A:1058:ALA:HB2	1.87	0.56
1:A:610:TYR:HA	1:A:612:PHE:CE2	2.40	0.56
1:B:1085:VAL:CG2	1:B:1086:ASN:N	2.68	0.56
1:C:1085:VAL:CG2	1:C:1086:ASN:N	2.69	0.56
1:D:271:TRP:CD1	1:D:294:PRO:CA	2.83	0.56
1:E:957:VAL:HG12	1:E:957:VAL:O	2.04	0.56
1:G:809:ASN:HB2	1:G:810:PRO:HD3	1.85	0.56
1:H:261:HIS:HD2	1:H:264:HIS:H	1.51	0.56
1:H:293:ARG:HB3	1:H:297:MET:HE1	1.88	0.56
1:A:352:ASN:C	1:A:353:THR:CG2	2.78	0.56
1:A:408:ARG:HD2	1:A:413:GLN:O	2.06	0.56
1:C:317:LEU:HD13	1:C:342:LYS:HB3	1.88	0.56
1:E:314:ASN:ND2	1:E:321:GLN:O	2.38	0.56
1:E:337:GLN:O	1:E:338:THR:C	2.49	0.56
1:E:856:MET:HG3	1:E:892:ASP:HB2	1.87	0.56
1:F:261:HIS:CD2	1:F:264:HIS:N	2.63	0.56
1:F:816:LEU:HD12	1:F:817:GLY:H	1.70	0.56
1:G:383:GLN:O	1:G:384:LYS:HB2	2.03	0.56
1:C:1052:ASN:N	1:C:1052:ASN:ND2	2.43	0.56
1:D:368:SER:HA	1:D:371:ASN:HD22	1.71	0.56
1:D:1072:SER:OG	1:D:1074:VAL:HG12	2.05	0.56
1:H:271:TRP:HZ2	1:H:357:ARG:HA	1.71	0.56
1:H:278:LEU:CB	1:H:284:TRP:CE3	2.86	0.56
1:H:313:MET:O	1:H:317:LEU:HG	2.04	0.56
1:C:245:PHE:N	1:C:245:PHE:HD1	2.04	0.56
1:C:247:GLN:NE2	1:C:247:GLN:HA	2.21	0.56
1:C:355:TRP:CG	1:C:356:LEU:N	2.73	0.56
1:C:561:ILE:HG12	1:C:697:MET:HB3	1.87	0.56
1:D:310:VAL:HG11	1:D:335:ALA:HB1	1.88	0.56
1:D:461:ASN:OD1	1:D:467:PRO:HA	2.04	0.56
1:E:669:TYR:HE2	1:E:670:MET:HE3	1.70	0.56
1:G:390:SER:HB2	1:G:971:THR:HB	1.86	0.56
1:H:311:ASN:N	1:H:311:ASN:HD22	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:740:ASN:HD22	1:D:741:PRO:N	2.03	0.56
1:E:656:ARG:HG3	1:E:856:MET:HB3	1.85	0.56
1:A:299:TRP:CD1	1:A:1081:PRO:HB3	2.41	0.56
1:A:856:MET:HG3	1:A:892:ASP:HB2	1.87	0.56
1:C:390:SER:HB2	1:C:971:THR:HB	1.88	0.56
1:D:355:TRP:CZ3	1:D:359:THR:HG21	2.41	0.56
1:E:343:ILE:HG23	1:E:355:TRP:CZ2	2.41	0.56
1:E:344:GLU:C	1:E:346:LYS:H	2.14	0.56
1:F:927:SER:OG	1:F:928:LYS:HG2	2.06	0.56
1:H:278:LEU:O	1:H:279:LYS:C	2.49	0.56
1:H:300:TRP:CD1	1:H:306:GLN:HG3	2.41	0.56
1:A:273:ARG:NH1	1:A:289:GLU:HG2	2.21	0.56
1:B:689:LYS:HD2	1:B:690:TYR:CE1	2.41	0.56
1:B:697:MET:HA	1:B:709:THR:O	2.05	0.56
1:C:555:SER:HB3	1:H:417:LYS:HE3	1.86	0.56
1:D:442:ASN:HB3	1:D:445:VAL:HG23	1.88	0.56
1:E:841:ASP:OD1	1:E:846:HIS:HE1	1.89	0.56
1:G:1052:ASN:ND2	1:G:1052:ASN:N	2.35	0.56
1:H:261:HIS:HD2	1:H:264:HIS:N	2.04	0.56
1:A:604:ASN:ND2	1:A:607:VAL:N	2.54	0.55
1:B:882:VAL:HG13	1:B:948:LYS:HG3	1.88	0.55
1:F:515:GLU:OE1	2:N:3:AC1:O3	2.25	0.55
1:H:733:VAL:CG2	1:H:734:VAL:N	2.70	0.55
1:B:537:ASN:OD1	1:B:540:ARG:NH1	2.36	0.55
1:D:288:THR:N	1:D:291:ASP:OD2	2.39	0.55
1:E:457:MET:CE	1:E:493:TYR:HE2	2.19	0.55
1:G:492:ASP:CB	1:G:1022:LEU:HD22	2.31	0.55
1:G:565:LEU:HD21	5:G:58:HOH:O	2.06	0.55
1:G:587:HIS:NE2	2:O:3:AC1:O3B	2.35	0.55
1:B:460:GLY:N	1:B:470:ASN:HD22	2.04	0.55
1:D:304:GLU:OE1	1:D:307:ARG:NH1	2.40	0.55
1:E:558:ASN:N	1:E:559:PRO:CD	2.70	0.55
1:F:843:LYS:HE2	5:F:84:HOH:O	2.05	0.55
1:B:1016:GLN:NE2	1:G:748:SER:HA	2.22	0.55
1:C:407:ASN:HD22	1:C:431:GLU:N	2.03	0.55
1:D:355:TRP:CD2	1:D:356:LEU:N	2.75	0.55
1:B:558:ASN:N	1:B:559:PRO:HD2	2.22	0.55
1:D:250:GLN:HE21	1:D:275:LYS:HD2	1.72	0.55
1:E:269:GLU:OE2	1:E:361:SER:HB3	2.07	0.55
1:F:245:PHE:O	1:F:247:GLN:N	2.40	0.55
1:C:740:ASN:C	1:C:740:ASN:ND2	2.51	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:LYS:HB3	1:D:377:PRO:HA	1.89	0.55
1:D:662:MET:C	1:D:674:THR:HG23	2.32	0.55
1:E:669:TYR:CE2	1:E:670:MET:HE3	2.42	0.55
1:G:369:ALA:O	1:G:370:TRP:HD1	1.90	0.55
1:G:440:ASN:HD21	1:G:449:GLN:NE2	1.91	0.55
1:H:267:THR:C	1:H:269:GLU:H	2.14	0.55
1:H:481:ASN:ND2	2:P:3:AC1:O2	2.39	0.55
1:A:355:TRP:C	1:A:355:TRP:CD2	2.84	0.55
1:D:251:VAL:CG2	1:D:259:PHE:CZ	2.87	0.55
1:E:670:MET:CE	1:E:885:PHE:HZ	2.18	0.55
1:A:310:VAL:HG22	1:A:339:ILE:CD1	2.37	0.55
1:B:481:ASN:ND2	2:J:3:AC1:O2	2.39	0.55
1:C:576:ALA:HB3	1:C:847:GLN:HB3	1.88	0.55
1:D:323:TYR:HB3	1:D:327:THR:HG1	1.71	0.55
1:D:347:ILE:HG22	1:D:348:THR:N	2.21	0.55
1:E:515:GLU:OE1	2:M:3:AC1:O3	2.25	0.55
1:E:988:LYS:C	1:E:990:THR:HG23	2.32	0.55
1:F:383:GLN:O	1:F:384:LYS:HB2	2.06	0.55
1:A:928:LYS:HB2	1:A:929:PRO:CD	2.37	0.55
1:B:740:ASN:ND2	1:B:741:PRO:HD2	2.22	0.55
1:E:306:GLN:O	1:E:307:ARG:C	2.49	0.55
1:F:302:ASP:C	1:F:302:ASP:OD1	2.50	0.55
1:F:321:GLN:OE1	1:F:321:GLN:CA	2.47	0.55
1:F:705:SER:HB3	1:F:743:LEU:CD1	2.36	0.55
1:F:848:ASN:OD1	1:F:850:ALA:HB3	2.06	0.55
1:F:1072:SER:OG	1:F:1074:VAL:CG1	2.55	0.55
1:A:666:ASP:HA	1:A:863:PHE:O	2.05	0.54
1:B:368:SER:O	1:B:371:ASN:HB2	2.07	0.54
1:D:245:PHE:CZ	1:D:284:TRP:HZ2	2.24	0.54
1:E:460:GLY:N	1:E:470:ASN:HD22	2.05	0.54
1:F:371:ASN:HB3	1:F:373:ASP:H	1.72	0.54
1:G:746:LYS:HB2	1:G:749:ASP:OD2	2.07	0.54
1:H:522:THR:N	1:H:523:PRO:HD2	2.20	0.54
1:A:460:GLY:H	1:A:470:ASN:HD22	1.53	0.54
1:D:1069:THR:HB	1:D:1079:PHE:HE2	1.71	0.54
1:F:988:LYS:H	1:F:990:THR:HG23	1.72	0.54
1:G:346:LYS:HE3	1:G:355:TRP:CE2	2.42	0.54
1:H:300:TRP:NE1	1:H:306:GLN:HG3	2.22	0.54
1:B:392:ASN:HD22	1:B:392:ASN:N	2.06	0.54
1:C:809:ASN:HB2	1:C:810:PRO:HD3	1.88	0.54
1:E:271:TRP:CH2	1:E:294:PRO:HD3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:863:PHE:CD2	1:G:912:ILE:HD11	2.42	0.54
1:H:273:ARG:NE	1:H:288:THR:O	2.40	0.54
1:H:293:ARG:HB3	1:H:294:PRO:CD	2.38	0.54
1:H:311:ASN:H	1:H:311:ASN:HD22	1.55	0.54
1:H:681:GLU:OE2	1:H:884:LYS:NZ	2.36	0.54
1:B:740:ASN:HD22	1:B:741:PRO:N	2.05	0.54
1:C:277:ILE:O	1:C:284:TRP:HA	2.07	0.54
1:D:342:LYS:O	1:D:346:LYS:HB2	2.08	0.54
1:E:277:ILE:HD13	1:E:293:ARG:NH2	2.23	0.54
1:G:299:TRP:CZ3	1:G:301:PRO:HD3	2.43	0.54
1:H:310:VAL:HG12	1:H:311:ASN:ND2	2.21	0.54
1:A:271:TRP:CH2	1:A:357:ARG:HG2	2.43	0.54
1:E:252:TYR:CD1	1:E:275:LYS:HG2	2.39	0.54
1:F:278:LEU:HD13	1:F:284:TRP:CE2	2.42	0.54
1:F:457:MET:HE3	1:F:493:TYR:HE2	1.71	0.54
1:F:461:ASN:OD1	1:F:467:PRO:HA	2.07	0.54
1:G:369:ALA:O	1:G:370:TRP:CD1	2.60	0.54
1:H:315:ALA:O	1:H:317:LEU:N	2.40	0.54
1:B:256:ALA:O	1:B:257:ALA:C	2.51	0.54
1:H:277:ILE:O	1:H:277:ILE:HG22	2.06	0.54
1:B:658:TYR:CE2	1:B:660:GLY:CA	2.87	0.54
1:E:299:TRP:CH2	1:E:301:PRO:HA	2.40	0.54
1:F:935:ALA:O	1:F:939:VAL:HG23	2.08	0.54
1:H:250:GLN:HG2	1:H:275:LYS:HG3	1.90	0.54
1:D:276:TYR:HA	1:D:285:THR:O	2.08	0.54
1:F:255:ASP:O	1:F:258:ASN:HB2	2.08	0.54
1:G:356:LEU:HA	1:G:359:THR:HG23	1.90	0.54
1:H:294:PRO:O	1:H:297:MET:N	2.29	0.54
1:H:966:GLU:HB2	1:H:997:LYS:CB	2.33	0.54
1:H:1069:THR:HG22	1:H:1070:TYR:O	2.08	0.54
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.71	0.54
1:A:310:VAL:HG22	1:A:339:ILE:HD12	1.88	0.54
1:A:407:ASN:ND2	1:A:431:GLU:N	2.55	0.54
1:A:920:ASP:OD2	1:A:1002:ASP:HB2	2.08	0.54
1:B:476:VAL:HB	1:B:514:LEU:HD22	1.90	0.54
1:B:492:ASP:HB3	1:B:1022:LEU:HD22	1.89	0.54
1:B:764:TYR:HE1	1:B:821:PRO:HD3	1.72	0.54
1:D:277:ILE:CD1	1:D:291:ASP:HB3	2.37	0.54
1:D:670:MET:HE1	1:D:885:PHE:HZ	1.73	0.54
1:G:759:HIS:CD2	1:G:764:TYR:OH	2.61	0.54
1:H:596:ARG:HB2	1:H:612:PHE:HZ	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ASN:HD22	1:A:311:ASN:N	2.06	0.54
1:A:461:ASN:H	1:A:470:ASN:HD21	1.53	0.54
1:A:916:TYR:HB3	2:I:3:AC1:HC61	1.89	0.54
1:B:809:ASN:OD1	1:B:812:VAL:N	2.33	0.54
1:C:1085:VAL:CG2	1:C:1086:ASN:H	2.21	0.54
1:D:513:ILE:HG12	1:D:953:MET:HE1	1.89	0.54
1:E:513:ILE:CG1	1:E:953:MET:HE1	2.37	0.54
1:H:251:VAL:HG21	1:H:259:PHE:HZ	1.69	0.54
1:A:307:ARG:C	1:A:309:TYR:N	2.60	0.53
1:B:266:LEU:HD21	1:B:1073:LEU:HD11	1.89	0.53
1:B:725:ASP:HB3	5:B:5:HOH:O	2.07	0.53
1:B:1063:LYS:HE2	1:B:1068:ASN:CG	2.33	0.53
1:B:1083:SER:O	1:B:1087:PRO:CG	2.37	0.53
1:C:359:THR:O	1:C:362:ALA:HB3	2.08	0.53
1:C:1072:SER:OG	1:C:1074:VAL:CG1	2.56	0.53
1:D:297:MET:O	1:D:297:MET:HG2	2.07	0.53
1:D:513:ILE:HG12	1:D:953:MET:HE2	1.89	0.53
1:D:516:ALA:HB1	1:D:521:ASP:OD2	2.08	0.53
1:F:863:PHE:CD2	1:F:912:ILE:HD11	2.43	0.53
1:G:300:TRP:CE3	1:G:306:GLN:HG3	2.43	0.53
1:G:471:PHE:CG	1:G:954:ALA:HB2	2.43	0.53
1:A:278:LEU:CD2	1:A:281:GLY:HA2	2.38	0.53
1:A:616:GLU:O	1:A:619:LYS:HB3	2.08	0.53
1:C:883:ASP:OD1	1:C:948:LYS:HE3	2.08	0.53
1:D:604:ASN:C	1:D:604:ASN:OD1	2.49	0.53
1:C:247:GLN:HA	1:C:247:GLN:HE21	1.73	0.53
1:D:271:TRP:CE2	1:D:294:PRO:CD	2.89	0.53
1:E:340:GLN:O	1:E:344:GLU:HG2	2.08	0.53
1:H:471:PHE:CG	1:H:954:ALA:HB2	2.44	0.53
1:A:697:MET:HA	1:A:709:THR:O	2.08	0.53
1:A:713:TYR:O	1:A:759:HIS:HE1	1.91	0.53
1:C:614:MET:HE1	1:C:866:PHE:HE2	1.73	0.53
1:C:670:MET:CE	1:C:885:PHE:HZ	2.22	0.53
1:C:707:ILE:C	1:C:707:ILE:HD12	2.33	0.53
1:E:782:GLN:HA	1:E:782:GLN:HE21	1.72	0.53
1:F:333:ASN:O	1:F:337:GLN:HG3	2.08	0.53
1:F:666:ASP:HA	1:F:863:PHE:O	2.08	0.53
1:F:1080:LEU:HB3	1:F:1081:PRO:HD2	1.90	0.53
1:G:316:GLN:NE2	1:G:316:GLN:N	2.56	0.53
1:G:608:VAL:O	1:G:609:GLY:C	2.50	0.53
1:H:316:GLN:CG	1:H:359:THR:HG21	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:390:SER:HB2	1:H:971:THR:HB	1.90	0.53
1:A:352:ASN:O	1:A:353:THR:CG2	2.56	0.53
1:C:250:GLN:HB2	1:C:1084:LEU:O	2.09	0.53
1:C:484:ALA:O	1:C:485:ASP:C	2.49	0.53
1:E:273:ARG:CD	1:E:287:SER:CB	2.28	0.53
1:F:471:PHE:CG	1:F:954:ALA:HB2	2.44	0.53
1:H:407:ASN:HD21	1:H:431:GLU:H	1.55	0.53
1:A:297:MET:HG2	1:A:298:THR:HG22	1.89	0.53
1:B:513:ILE:HG12	1:B:953:MET:HE2	1.89	0.53
1:F:1023:PHE:CD1	1:F:1036:PRO:HG3	2.43	0.53
1:H:277:ILE:HG22	1:H:279:LYS:HD3	1.90	0.53
1:D:346:LYS:O	1:D:350:GLU:HG2	2.08	0.53
1:E:630:ALA:O	1:E:633:LYS:NZ	2.42	0.53
1:F:610:TYR:HA	1:F:612:PHE:CE2	2.43	0.53
1:G:917:ALA:HA	1:G:962:TYR:CE1	2.43	0.53
1:E:346:LYS:HE2	1:E:350:GLU:CD	2.31	0.53
1:E:729:ARG:O	1:E:729:ARG:HG3	2.09	0.53
1:E:991:LEU:HG	1:E:1070:TYR:CE2	2.44	0.53
1:F:250:GLN:CB	1:F:1084:LEU:O	2.47	0.53
1:F:261:HIS:CD2	1:F:264:HIS:CA	2.91	0.53
1:F:689:LYS:HB3	1:F:690:TYR:CD1	2.44	0.53
1:F:988:LYS:O	1:F:990:THR:HG22	2.08	0.53
1:G:347:ILE:HG12	1:G:353:THR:HG22	1.90	0.53
1:H:389:TYR:CE1	1:H:1050:GLY:HA2	2.44	0.53
1:C:461:ASN:H	1:C:470:ASN:HD21	1.56	0.53
1:C:648:LEU:O	1:C:687:ARG:HG3	2.08	0.53
1:D:299:TRP:NE1	1:D:1081:PRO:HB3	2.24	0.53
1:D:356:LEU:O	1:D:357:ARG:C	2.52	0.53
1:E:311:ASN:N	1:E:311:ASN:ND2	2.55	0.53
1:G:800:THR:CG2	1:G:801:ALA:N	2.72	0.53
1:G:1065:GLN:HG3	1:G:1066:ALA:H	1.73	0.53
1:H:361:SER:O	1:H:362:ALA:C	2.50	0.53
1:H:406:LEU:HD22	1:H:431:GLU:HG2	1.91	0.53
1:B:581:TYR:HA	1:B:654:VAL:O	2.09	0.53
1:A:261:HIS:CD2	1:A:264:HIS:H	2.15	0.52
1:B:612:PHE:N	1:B:612:PHE:CD2	2.73	0.52
1:C:599:ILE:HG22	1:C:607:VAL:HG11	1.91	0.52
1:F:725:ASP:C	1:F:725:ASP:OD1	2.52	0.52
1:F:874:THR:HG22	1:F:878:ILE:CD1	2.40	0.52
1:G:973:THR:HG23	1:G:988:LYS:HA	1.90	0.52
1:H:1065:GLN:O	1:H:1066:ALA:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:GLY:N	1:A:470:ASN:ND2	2.56	0.52
1:C:478:ALA:HB1	1:C:481:ASN:HD22	1.73	0.52
1:C:639:ASN:HB3	1:C:642:LEU:HB2	1.91	0.52
1:D:964:LEU:HD12	1:D:996:GLY:HA2	1.91	0.52
1:E:279:LYS:HD2	1:E:283:THR:HG22	1.92	0.52
1:E:347:ILE:HG12	1:E:353:THR:CB	2.33	0.52
1:G:250:GLN:NE2	1:G:275:LYS:NZ	2.56	0.52
1:G:324:ASN:OD1	1:G:324:ASN:C	2.52	0.52
1:G:341:THR:O	1:G:342:LYS:C	2.53	0.52
1:G:466:ASP:OD2	1:G:943:LYS:HD2	2.09	0.52
1:H:558:ASN:N	1:H:559:PRO:CD	2.73	0.52
1:A:491:GLY:HA3	5:A:1:HOH:O	2.09	0.52
1:D:335:ALA:O	1:D:339:ILE:HG13	2.10	0.52
1:D:607:VAL:HG13	1:D:607:VAL:O	2.08	0.52
1:D:997:LYS:HA	1:D:1043:TRP:O	2.09	0.52
1:G:363:PHE:CE1	1:G:367:GLN:OE1	2.62	0.52
1:G:537:ASN:OD1	1:G:540:ARG:NH1	2.39	0.52
1:H:304:GLU:O	1:H:307:ARG:HB3	2.10	0.52
1:H:491:GLY:HA3	5:H:196:HOH:O	2.09	0.52
1:A:276:TYR:N	1:A:276:TYR:CD2	2.77	0.52
1:A:278:LEU:HD11	1:A:281:GLY:C	2.34	0.52
1:A:494:LEU:HB3	1:A:500:ILE:HD13	1.90	0.52
1:B:585:ARG:NH2	1:B:624:TYR:OH	2.42	0.52
1:D:304:GLU:OE1	1:D:304:GLU:HA	2.09	0.52
1:D:407:ASN:ND2	1:D:431:GLU:H	2.06	0.52
1:E:271:TRP:CE2	1:E:294:PRO:CD	2.92	0.52
1:E:387:LEU:O	1:E:1050:GLY:HA3	2.10	0.52
1:H:407:ASN:ND2	1:H:431:GLU:N	2.57	0.52
1:H:702:VAL:O	1:H:703:GLY:C	2.49	0.52
1:A:266:LEU:HD13	1:A:295:LEU:HD11	1.92	0.52
1:A:733:VAL:HG22	1:A:734:VAL:N	2.24	0.52
1:C:460:GLY:CA	1:C:470:ASN:ND2	2.72	0.52
1:C:551:LEU:HD22	1:C:741:PRO:HG2	1.91	0.52
1:E:360:ILE:O	1:E:363:PHE:N	2.41	0.52
1:G:250:GLN:NE2	1:G:275:LYS:HZ3	2.08	0.52
1:G:604:ASN:HD21	1:G:607:VAL:HA	1.74	0.52
1:C:346:LYS:HE3	1:C:355:TRP:CD2	2.44	0.52
1:E:430:TYR:CG	1:E:977:LYS:HD3	2.44	0.52
1:H:300:TRP:CD1	1:H:306:GLN:CA	2.90	0.52
1:A:603:ILE:CD1	1:A:619:LYS:HG3	2.40	0.52
1:B:504:ASP:OD1	1:B:846:HIS:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:VAL:CG2	1:B:734:VAL:N	2.72	0.52
1:E:271:TRP:CG	1:E:357:ARG:NH1	2.78	0.52
1:E:322:THR:HG23	1:E:323:TYR:N	2.24	0.52
1:G:293:ARG:HB3	1:G:297:MET:CE	2.39	0.52
1:H:604:ASN:OD1	1:H:604:ASN:C	2.53	0.52
1:A:606:ASN:O	1:A:607:VAL:C	2.52	0.52
1:B:272:TYR:CD1	1:B:273:ARG:N	2.78	0.52
1:B:610:TYR:HA	1:B:612:PHE:CE2	2.44	0.52
1:D:352:ASN:C	1:D:352:ASN:HD22	2.18	0.52
1:D:387:LEU:O	1:D:1050:GLY:HA3	2.10	0.52
1:E:271:TRP:CZ3	1:E:294:PRO:HD3	2.45	0.52
1:F:988:LYS:O	1:F:990:THR:CG2	2.57	0.52
1:H:363:PHE:C	1:H:365:LYS:H	2.18	0.52
1:A:289:GLU:HG3	5:A:201:HOH:O	2.09	0.52
1:B:924:LEU:HD12	1:B:924:LEU:N	2.24	0.52
1:D:308:GLN:HE21	1:D:308:GLN:CA	2.23	0.52
1:E:252:TYR:CD2	1:E:273:ARG:NH2	2.66	0.52
1:E:587:HIS:CD2	2:M:3:AC1:O3B	2.61	0.52
1:E:809:ASN:HB2	1:E:810:PRO:HD3	1.92	0.52
1:F:483:ASP:C	1:F:483:ASP:OD1	2.53	0.52
1:G:1076:ASP:OD2	1:G:1077:ASN:HB2	2.10	0.52
1:H:302:ASP:OD1	1:H:304:GLU:HB3	2.09	0.52
1:H:577:ALA:C	1:H:578:VAL:HG23	2.35	0.52
1:A:327:THR:CG2	1:A:328:SER:N	2.73	0.52
1:B:670:MET:CE	1:B:885:PHE:CZ	2.84	0.52
1:B:1052:ASN:N	1:B:1052:ASN:ND2	2.42	0.52
1:C:492:ASP:OD1	1:C:1025:ARG:NH1	2.43	0.52
1:D:297:MET:O	1:D:297:MET:CG	2.58	0.52
1:G:271:TRP:HZ2	1:G:357:ARG:HA	1.75	0.52
1:A:776:LYS:HE3	5:A:171:HOH:O	2.09	0.51
1:D:280:ASP:C	1:D:282:LYS:N	2.69	0.51
1:D:515:GLU:OE1	2:L:3:AC1:O3	2.28	0.51
1:D:928:LYS:HB2	1:D:929:PRO:CD	2.40	0.51
1:E:1085:VAL:CG2	1:E:1086:ASN:N	2.74	0.51
1:F:352:ASN:ND2	1:F:352:ASN:H	2.05	0.51
1:G:725:ASP:C	1:G:725:ASP:OD1	2.51	0.51
1:A:299:TRP:NE1	1:A:1081:PRO:HB3	2.26	0.51
1:A:504:ASP:OD1	1:A:846:HIS:HD2	1.93	0.51
1:A:603:ILE:HD13	1:A:619:LYS:HG3	1.91	0.51
1:D:735:VAL:HG22	1:D:818:VAL:HG22	1.91	0.51
1:E:882:VAL:HG13	1:E:948:LYS:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:TRP:C	1:F:300:TRP:CD2	2.88	0.51
1:H:673:LYS:HD3	1:H:677:TYR:CD2	2.45	0.51
1:A:271:TRP:HA	1:A:294:PRO:HA	1.92	0.51
1:A:725:ASP:O	1:A:726:ARG:C	2.53	0.51
1:C:551:LEU:CD2	1:C:741:PRO:HG2	2.40	0.51
1:D:639:ASN:HD22	1:D:642:LEU:HD13	1.75	0.51
1:E:250:GLN:HB2	1:E:1084:LEU:O	2.10	0.51
1:E:297:MET:O	1:E:298:THR:HG22	2.10	0.51
1:E:344:GLU:C	1:E:346:LYS:N	2.68	0.51
1:E:800:THR:HG22	1:E:801:ALA:N	2.26	0.51
1:F:860:PHE:HB2	1:F:864:GLN:NE2	2.26	0.51
1:F:912:ILE:O	1:F:912:ILE:CG2	2.53	0.51
1:H:271:TRP:CZ2	1:H:357:ARG:HA	2.45	0.51
1:H:293:ARG:HB3	1:H:297:MET:CE	2.41	0.51
1:A:301:PRO:CG	1:A:302:ASP:N	2.70	0.51
1:D:300:TRP:CB	1:D:306:GLN:HB2	2.40	0.51
1:E:273:ARG:HD3	1:E:288:THR:O	2.10	0.51
1:E:360:ILE:O	1:E:363:PHE:HB3	2.10	0.51
1:E:514:LEU:HD21	1:E:532:MET:HG3	1.93	0.51
1:G:368:SER:HA	1:G:371:ASN:HD22	1.75	0.51
1:G:687:ARG:HA	1:G:691:VAL:HG23	1.93	0.51
1:H:740:ASN:HD22	1:H:741:PRO:N	2.09	0.51
1:A:304:GLU:OE1	1:A:304:GLU:HA	2.09	0.51
1:A:307:ARG:NH1	1:A:308:GLN:OE1	2.42	0.51
1:B:261:HIS:CD2	1:B:264:HIS:H	2.15	0.51
1:B:492:ASP:HB3	1:B:1022:LEU:CD2	2.41	0.51
1:B:515:GLU:OE1	2:J:3:AC1:O3	2.27	0.51
1:D:1005:ALA:O	1:D:1041:LYS:HD2	2.11	0.51
1:F:357:ARG:NH1	1:F:357:ARG:HG3	2.19	0.51
1:H:308:GLN:O	1:H:310:VAL:N	2.44	0.51
1:H:860:PHE:CG	1:H:896:ALA:HB2	2.45	0.51
1:A:251:VAL:CG2	1:A:259:PHE:CZ	2.90	0.51
1:B:442:ASN:HB3	1:B:445:VAL:CG2	2.41	0.51
1:C:669:TYR:CD2	1:C:670:MET:HG3	2.46	0.51
1:E:916:TYR:HB3	2:M:3:AC1:HC61	1.93	0.51
1:F:568:ARG:HG3	1:F:568:ARG:HH11	1.75	0.51
1:F:750:ARG:CB	5:F:55:HOH:O	2.58	0.51
1:G:669:TYR:O	1:G:670:MET:HB2	2.10	0.51
1:H:356:LEU:O	1:H:356:LEU:HG	2.01	0.51
1:H:407:ASN:ND2	1:H:431:GLU:H	2.09	0.51
1:B:639:ASN:O	1:B:640:THR:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:MET:O	1:C:317:LEU:HG	2.11	0.51
1:F:719:LYS:NZ	5:F:202:HOH:O	2.43	0.51
1:G:246:ALA:HB1	1:G:1087:PRO:HB2	1.92	0.51
1:G:258:ASN:C	1:G:259:PHE:CD2	2.89	0.51
1:G:313:MET:HB2	1:G:339:ILE:HD13	1.93	0.51
1:G:658:TYR:CE2	1:G:660:GLY:CA	2.93	0.51
1:A:375:GLU:OE1	1:A:1053:ILE:HB	2.10	0.51
1:A:746:LYS:NZ	1:G:793:ASP:OD2	2.34	0.51
1:E:421:TYR:CD1	1:E:523:PRO:HB2	2.46	0.51
1:F:723:THR:HG22	1:F:757:ALA:CB	2.40	0.51
1:F:908:LEU:HD12	1:F:912:ILE:HG13	1.93	0.51
1:H:292:PHE:O	1:H:293:ARG:HG3	2.11	0.51
1:A:800:THR:HG22	1:A:801:ALA:N	2.24	0.51
1:B:1004:GLN:O	1:B:1004:GLN:HG3	2.11	0.51
1:C:585:ARG:HD3	1:C:661:ASP:OD1	2.11	0.51
1:E:271:TRP:CE3	1:E:294:PRO:HD3	2.46	0.51
1:E:347:ILE:CD1	1:E:353:THR:HB	2.40	0.51
1:F:278:LEU:CD1	1:F:284:TRP:CE2	2.94	0.51
1:F:300:TRP:CE3	1:F:300:TRP:N	2.79	0.51
1:H:300:TRP:CE2	1:H:306:GLN:HG3	2.46	0.51
1:A:278:LEU:HB2	1:A:284:TRP:CH2	2.46	0.51
1:A:613:THR:HG1	1:A:615:GLU:HB2	1.76	0.51
1:C:261:HIS:CD2	1:C:264:HIS:CA	2.94	0.51
1:C:299:TRP:CD1	1:C:1081:PRO:HB3	2.46	0.51
1:C:333:ASN:O	1:C:337:GLN:HG3	2.11	0.51
1:F:269:GLU:OE2	1:F:361:SER:HB3	2.10	0.51
1:H:271:TRP:HZ3	1:H:294:PRO:HD3	1.75	0.51
1:D:305:THR:HG23	1:D:367:GLN:NE2	2.25	0.50
1:E:1065:GLN:O	1:E:1066:ALA:C	2.54	0.50
1:F:568:ARG:HG3	1:F:568:ARG:NH1	2.26	0.50
1:G:277:ILE:O	1:G:284:TRP:HA	2.11	0.50
1:H:965:PRO:HD2	1:H:998:SER:HA	1.93	0.50
1:E:251:VAL:HG21	1:E:259:PHE:CZ	2.46	0.50
1:E:281:GLY:HA2	1:E:341:THR:CG2	2.42	0.50
1:E:361:SER:O	1:E:364:VAL:N	2.44	0.50
1:E:430:TYR:CE2	1:E:977:LYS:HE2	2.46	0.50
1:F:800:THR:HG23	1:F:801:ALA:N	2.27	0.50
1:G:250:GLN:HG3	1:G:251:VAL:N	2.25	0.50
1:G:988:LYS:H	1:G:990:THR:HG23	1.74	0.50
1:H:355:TRP:CD2	1:H:356:LEU:N	2.80	0.50
1:A:278:LEU:HG	1:A:278:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:668:GLN:OE1	1:D:668:GLN:HA	2.11	0.50
1:F:847:GLN:NE2	1:F:852:ASP:OD1	2.34	0.50
1:G:355:TRP:CE3	1:G:359:THR:HG21	2.46	0.50
1:G:576:ALA:HB3	1:G:847:GLN:HB3	1.92	0.50
1:H:389:TYR:CZ	1:H:1050:GLY:HA2	2.46	0.50
1:H:740:ASN:HD22	1:H:742:SER:N	2.07	0.50
1:D:407:ASN:ND2	1:D:431:GLU:N	2.59	0.50
1:E:310:VAL:HG22	1:E:339:ILE:HD11	1.94	0.50
1:F:348:THR:HB	5:F:59:HOH:O	2.10	0.50
1:F:670:MET:CE	1:F:885:PHE:CZ	2.79	0.50
1:G:666:ASP:HA	1:G:863:PHE:O	2.12	0.50
1:H:367:GLN:O	1:H:370:TRP:N	2.35	0.50
1:B:417:LYS:HE2	1:B:425:ARG:O	2.12	0.50
1:C:800:THR:HG22	1:C:801:ALA:N	2.26	0.50
1:D:457:MET:CE	1:D:493:TYR:HE2	2.24	0.50
1:D:585:ARG:HD3	1:D:661:ASP:OD1	2.12	0.50
1:D:740:ASN:ND2	1:D:740:ASN:C	2.61	0.50
1:D:928:LYS:HB2	1:D:929:PRO:HD2	1.93	0.50
1:E:988:LYS:H	1:E:990:THR:HG23	1.76	0.50
1:D:271:TRP:CH2	1:D:294:PRO:HD3	2.46	0.50
1:D:280:ASP:C	1:D:282:LYS:H	2.19	0.50
1:D:869:LYS:O	1:D:870:LYS:C	2.55	0.50
1:E:330:LEU:O	1:E:333:ASN:CB	2.57	0.50
1:F:409:THR:HG21	1:F:429:GLY:HA3	1.94	0.50
1:F:1052:ASN:H	1:F:1052:ASN:ND2	2.00	0.50
1:G:1065:GLN:CG	1:G:1066:ALA:N	2.74	0.50
1:B:725:ASP:C	1:B:725:ASP:OD1	2.55	0.50
1:C:360:ILE:O	1:C:364:VAL:HG23	2.11	0.50
1:F:604:ASN:C	1:F:604:ASN:OD1	2.55	0.50
1:G:312:TYR:OH	1:G:362:ALA:HB1	2.11	0.50
1:G:483:ASP:C	1:G:483:ASP:OD1	2.55	0.50
1:H:1064:ASP:N	1:H:1069:THR:O	2.41	0.50
1:A:280:ASP:OD1	1:A:348:THR:CB	2.59	0.50
1:B:561:ILE:HG12	1:B:697:MET:HB3	1.94	0.50
1:C:686:ALA:CB	1:C:767:LEU:HD21	2.42	0.50
1:D:782:GLN:NE2	1:D:782:GLN:CA	2.74	0.50
1:D:897:PRO:HG3	1:D:916:TYR:CE1	2.46	0.50
1:E:988:LYS:O	1:E:990:THR:CG2	2.59	0.50
1:F:436:ASN:HB2	1:F:961:MET:O	2.12	0.50
1:G:407:ASN:ND2	1:G:431:GLU:H	2.10	0.50
1:B:439:ASP:C	1:B:439:ASP:OD1	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:LEU:CD1	1:B:474:ILE:HG21	2.41	0.50
1:B:492:ASP:OD1	1:B:1025:ARG:NH1	2.45	0.50
1:C:975:VAL:HB	1:C:979:GLY:HA2	1.94	0.50
1:D:271:TRP:NE1	1:D:294:PRO:HB3	2.27	0.50
1:C:424:ASP:HB3	1:C:520:ASN:ND2	2.27	0.49
1:D:294:PRO:HG2	1:D:297:MET:HB2	1.94	0.49
1:E:457:MET:CE	1:E:493:TYR:CE2	2.95	0.49
1:H:439:ASP:OD1	1:H:439:ASP:C	2.51	0.49
1:B:689:LYS:HG2	1:B:690:TYR:CE1	2.47	0.49
1:C:250:GLN:OE1	1:C:1087:PRO:CG	2.60	0.49
1:C:346:LYS:O	1:C:349:ALA:HB3	2.13	0.49
1:F:407:ASN:ND2	1:F:431:GLU:H	2.10	0.49
1:F:581:TYR:HA	1:F:654:VAL:O	2.11	0.49
1:F:604:ASN:CG	1:F:604:ASN:O	2.55	0.49
1:H:249:ASN:O	1:H:250:GLN:C	2.55	0.49
1:B:390:SER:HB2	1:B:971:THR:HB	1.93	0.49
1:B:996:GLY:O	1:B:1044:SER:HA	2.12	0.49
1:C:312:TYR:C	1:C:312:TYR:CD2	2.90	0.49
1:E:367:GLN:O	1:E:370:TRP:N	2.37	0.49
1:F:572:ASN:OD1	1:F:718:LEU:O	2.30	0.49
1:F:762:GLN:N	1:F:791:THR:OG1	2.37	0.49
1:G:307:ARG:HA	1:G:332:LEU:HD22	1.94	0.49
1:H:279:LYS:O	1:H:280:ASP:C	2.55	0.49
1:B:262:VAL:CG1	1:B:969:VAL:HG23	2.31	0.49
1:B:614:MET:O	1:B:618:LYS:HG3	2.12	0.49
1:C:868:THR:O	1:C:869:LYS:HB3	2.12	0.49
1:E:271:TRP:CD2	1:E:294:PRO:CD	2.96	0.49
1:E:273:ARG:HG3	1:E:287:SER:CB	2.42	0.49
1:F:734:VAL:HB	1:F:755:MET:HE1	1.95	0.49
1:F:809:ASN:HB2	1:F:810:PRO:CD	2.42	0.49
1:H:769:LEU:HD21	1:H:819:TRP:CZ2	2.47	0.49
1:B:460:GLY:H	1:B:470:ASN:HD22	1.58	0.49
1:C:407:ASN:ND2	1:C:431:GLU:CB	2.76	0.49
1:E:310:VAL:CG2	1:E:339:ILE:CD1	2.90	0.49
1:E:513:ILE:HG12	1:E:953:MET:HE2	1.95	0.49
1:E:861:SER:HB3	1:E:864:GLN:HG3	1.94	0.49
1:G:912:ILE:HG22	1:G:931:LYS:HZ2	1.77	0.49
1:A:658:TYR:CE2	1:A:660:GLY:HA3	2.47	0.49
1:C:352:ASN:C	1:C:353:THR:CG2	2.86	0.49
1:C:492:ASP:HB3	1:C:1022:LEU:CD2	2.42	0.49
1:C:869:LYS:O	1:C:870:LYS:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:383:GLN:O	1:E:384:LYS:HB2	2.13	0.49
1:F:612:PHE:N	1:F:612:PHE:HD2	2.08	0.49
1:F:862:ASN:O	1:F:912:ILE:HD12	2.12	0.49
1:G:513:ILE:HG12	1:G:953:MET:CE	2.42	0.49
1:A:363:PHE:O	1:A:364:VAL:C	2.56	0.49
1:C:376:LYS:HA	1:C:377:PRO:C	2.38	0.49
1:D:285:THR:HG22	1:D:286:GLN:N	2.28	0.49
1:D:296:LEU:O	1:D:300:TRP:NE1	2.45	0.49
1:G:574:GLU:O	1:G:574:GLU:HG3	1.93	0.49
1:G:1064:ASP:HB2	1:G:1071:PHE:CE1	2.47	0.49
1:H:278:LEU:HA	1:H:284:TRP:CA	2.20	0.49
1:B:442:ASN:HB3	1:B:445:VAL:HG23	1.95	0.49
1:C:723:THR:HG22	1:C:757:ALA:HB1	1.94	0.49
1:E:407:ASN:HD21	1:E:431:GLU:H	1.59	0.49
1:F:271:TRP:CZ2	1:F:357:ARG:HG3	2.48	0.49
1:F:711:VAL:HG22	1:F:734:VAL:HG23	1.94	0.49
1:F:1072:SER:OG	1:F:1074:VAL:HG12	2.12	0.49
1:G:1065:GLN:CG	1:G:1066:ALA:H	2.26	0.49
2:I:3:AC1:O3	2:I:3:AC1:C1B	2.60	0.49
1:A:522:THR:N	1:A:523:PRO:HD2	2.28	0.49
1:A:577:ALA:C	1:A:578:VAL:HG23	2.38	0.49
1:D:800:THR:HG23	1:D:801:ALA:N	2.28	0.49
1:E:912:ILE:H	1:E:912:ILE:HG13	1.47	0.49
1:G:760:LYS:O	1:G:761:ASN:C	2.55	0.49
1:G:856:MET:HG3	1:G:892:ASP:HB2	1.95	0.49
1:H:249:ASN:ND2	1:H:298:THR:HG22	2.28	0.49
1:H:261:HIS:CD2	1:H:264:HIS:H	2.30	0.49
1:H:920:ASP:OD2	1:H:1002:ASP:HB2	2.12	0.49
1:A:862:ASN:O	1:A:912:ILE:HD13	2.13	0.49
1:C:462:ILE:HD13	1:C:1011:PHE:CZ	2.48	0.49
1:D:475:ARG:NH1	1:D:477:ASP:HB2	2.27	0.49
1:F:908:LEU:CD1	1:F:912:ILE:HG13	2.42	0.49
1:F:928:LYS:HB2	1:F:929:PRO:CD	2.43	0.49
1:B:689:LYS:HG2	1:B:690:TYR:CD1	2.48	0.48
1:C:504:ASP:OD1	1:C:846:HIS:HD2	1.96	0.48
1:D:285:THR:CG2	1:D:286:GLN:N	2.76	0.48
1:D:312:TYR:CD2	1:D:312:TYR:O	2.66	0.48
1:E:271:TRP:CD2	1:E:294:PRO:N	2.81	0.48
1:F:387:LEU:O	1:F:1050:GLY:HA3	2.13	0.48
1:F:603:ILE:CD1	1:F:619:LYS:HG3	2.43	0.48
1:G:530:ASP:HB2	1:G:843:LYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:588:ASP:OD1	1:G:588:ASP:N	2.44	0.48
1:G:988:LYS:N	1:G:990:THR:HG23	2.28	0.48
1:A:512:SER:O	1:A:532:MET:HB2	2.13	0.48
1:D:988:LYS:O	1:D:988:LYS:CG	2.60	0.48
1:E:537:ASN:OD1	1:E:540:ARG:NH1	2.38	0.48
1:F:669:TYR:O	1:F:670:MET:HB2	2.13	0.48
1:G:250:GLN:HB2	1:G:1084:LEU:O	2.13	0.48
1:G:976:ASP:OD1	1:G:976:ASP:C	2.56	0.48
1:G:997:LYS:HA	1:G:1043:TRP:O	2.14	0.48
1:H:686:ALA:HB2	1:H:767:LEU:HD21	1.96	0.48
1:F:663:PHE:CD1	1:F:670:MET:HA	2.49	0.48
1:F:703:GLY:HA3	1:F:744:ARG:O	2.13	0.48
1:F:930:ASN:O	1:F:932:TYR:N	2.46	0.48
1:G:344:GLU:OE1	1:G:344:GLU:HA	2.13	0.48
1:H:656:ARG:HG3	1:H:856:MET:HB3	1.96	0.48
1:H:793:ASP:HB3	1:H:794:ARG:HG3	1.96	0.48
1:A:277:ILE:HG21	1:A:293:ARG:HH21	1.77	0.48
1:A:292:PHE:O	1:A:293:ARG:HD3	2.14	0.48
1:A:965:PRO:HD2	1:A:997:LYS:O	2.12	0.48
1:C:376:LYS:HB3	1:C:377:PRO:CA	2.38	0.48
1:D:245:PHE:CZ	1:D:278:LEU:HD22	2.48	0.48
1:E:715:LYS:HD2	1:E:830:VAL:HB	1.95	0.48
1:G:387:LEU:O	1:G:1050:GLY:HA3	2.13	0.48
1:H:276:TYR:HD1	1:H:285:THR:N	2.12	0.48
1:A:1052:ASN:ND2	1:A:1052:ASN:N	2.55	0.48
1:B:723:THR:O	1:B:723:THR:OG1	2.29	0.48
1:C:251:VAL:HG21	1:C:259:PHE:HZ	1.72	0.48
1:D:323:TYR:CD1	1:D:327:THR:HG21	2.49	0.48
1:F:457:MET:HE3	1:F:493:TYR:CE2	2.48	0.48
1:F:1021:GLU:OE1	1:F:1021:GLU:N	2.45	0.48
1:G:409:THR:O	1:G:410:PRO:C	2.55	0.48
1:G:759:HIS:CD2	1:G:762:GLN:OE1	2.67	0.48
1:G:883:ASP:OD1	1:G:948:LYS:HE3	2.12	0.48
1:H:277:ILE:O	1:H:279:LYS:N	2.45	0.48
1:B:417:LYS:HE3	1:F:555:SER:CB	2.39	0.48
1:C:512:SER:O	1:C:532:MET:HB2	2.14	0.48
1:D:578:VAL:HG13	1:D:579:PRO:HD2	1.96	0.48
1:E:322:THR:HG22	1:E:323:TYR:N	2.29	0.48
1:F:504:ASP:HB3	1:F:834:ALA:HB1	1.96	0.48
1:F:745:LEU:N	1:F:745:LEU:HD12	2.28	0.48
1:G:355:TRP:CE3	1:G:355:TRP:C	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:871:GLU:CD	1:G:871:GLU:H	2.21	0.48
1:A:352:ASN:OD1	1:A:354:ASN:HB2	2.14	0.48
1:B:430:TYR:CE2	1:B:977:LYS:HE2	2.47	0.48
1:C:383:GLN:O	1:C:384:LYS:HB2	2.13	0.48
1:C:533:ILE:HA	5:C:181:HOH:O	2.13	0.48
1:C:615:GLU:OE1	1:C:615:GLU:HA	2.12	0.48
1:E:300:TRP:CD2	1:E:306:GLN:HB2	2.41	0.48
1:E:658:TYR:CE2	1:E:660:GLY:HA3	2.49	0.48
1:A:295:LEU:HD23	1:A:1084:LEU:HD11	1.96	0.48
1:A:602:GLU:C	1:A:603:ILE:HG13	2.39	0.48
1:A:703:GLY:HA3	1:A:744:ARG:O	2.13	0.48
1:B:454:HIS:ND1	1:B:1015:LEU:HD21	2.29	0.48
1:C:794:ARG:HG2	1:C:794:ARG:NH1	2.28	0.48
1:D:588:ASP:OD1	1:D:589:SER:N	2.43	0.48
1:E:245:PHE:CG	1:E:284:TRP:HZ2	2.31	0.48
1:E:483:ASP:C	1:E:483:ASP:OD1	2.57	0.48
1:E:516:ALA:HB1	1:E:521:ASP:OD2	2.13	0.48
1:H:687:ARG:HA	1:H:691:VAL:HG23	1.95	0.48
1:A:300:TRP:CD1	1:A:306:GLN:HA	2.48	0.48
1:E:965:PRO:HD2	1:E:998:SER:HA	1.95	0.48
1:H:247:GLN:O	1:H:249:ASN:N	2.47	0.48
1:H:359:THR:O	1:H:360:ILE:O	2.32	0.48
1:A:300:TRP:CG	1:A:306:GLN:CG	2.97	0.48
1:B:567:ASN:C	1:B:567:ASN:OD1	2.57	0.48
1:B:771:THR:O	1:B:772:ASP:C	2.56	0.48
1:C:841:ASP:OD1	1:C:846:HIS:HE1	1.96	0.48
1:D:292:PHE:C	1:D:293:ARG:HG2	2.39	0.48
1:F:749:ASP:C	1:F:750:ARG:CG	2.86	0.48
1:H:668:GLN:OE1	1:H:668:GLN:HA	2.14	0.48
1:A:278:LEU:HB2	1:A:284:TRP:CZ2	2.49	0.47
1:A:444:VAL:HG11	1:A:1038:VAL:HG22	1.96	0.47
1:A:723:THR:HG22	1:A:757:ALA:HB1	1.96	0.47
1:A:988:LYS:C	1:A:990:THR:HG23	2.39	0.47
1:B:919:THR:O	1:B:961:MET:CE	2.62	0.47
1:C:355:TRP:CG	1:C:356:LEU:H	2.32	0.47
1:C:524:TYR:C	1:C:524:TYR:CD2	2.91	0.47
1:E:252:TYR:HB3	1:E:258:ASN:ND2	2.23	0.47
1:E:356:LEU:O	1:E:357:ARG:C	2.56	0.47
1:F:675:ILE:O	1:F:811:GLN:NE2	2.47	0.47
1:F:974:ARG:HB2	1:F:985:SER:OG	2.14	0.47
1:G:365:LYS:HD3	1:G:365:LYS:HA	1.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:407:ASN:ND2	1:G:431:GLU:N	2.61	0.47
1:G:453:LEU:CD1	1:G:474:ILE:HG21	2.44	0.47
1:G:959:ASP:OD2	1:G:960:GLN:OE1	2.31	0.47
1:H:292:PHE:O	1:H:293:ARG:CG	2.62	0.47
1:H:581:TYR:HA	1:H:654:VAL:O	2.14	0.47
1:H:935:ALA:O	1:H:938:LEU:HB3	2.13	0.47
1:A:330:LEU:HD12	1:A:330:LEU:C	2.35	0.47
1:A:492:ASP:HB3	1:A:1022:LEU:HD22	1.95	0.47
1:E:271:TRP:CG	1:E:357:ARG:HH12	2.32	0.47
1:E:725:ASP:C	1:E:725:ASP:OD1	2.55	0.47
1:F:930:ASN:C	1:F:932:TYR:H	2.22	0.47
1:G:383:GLN:O	1:G:384:LYS:CB	2.62	0.47
1:G:975:VAL:HB	1:G:979:GLY:HA2	1.96	0.47
1:A:281:GLY:C	1:A:341:THR:HG23	2.37	0.47
1:A:327:THR:HG22	1:A:328:SER:N	2.29	0.47
1:A:809:ASN:HB2	1:A:810:PRO:CD	2.44	0.47
1:B:861:SER:O	1:B:864:GLN:HG3	2.14	0.47
1:E:245:PHE:O	1:E:249:ASN:CB	2.62	0.47
1:E:281:GLY:HA2	1:E:341:THR:HG22	1.96	0.47
1:E:297:MET:O	1:E:297:MET:CG	2.63	0.47
1:E:308:GLN:HE21	1:E:308:GLN:HB3	1.45	0.47
1:E:461:ASN:OD1	1:E:467:PRO:HA	2.13	0.47
1:E:475:ARG:NH1	1:E:477:ASP:HB2	2.29	0.47
1:H:389:TYR:CD1	1:H:389:TYR:N	2.80	0.47
1:H:687:ARG:HA	1:H:691:VAL:CG2	2.45	0.47
1:A:298:THR:HA	1:A:300:TRP:CH2	2.50	0.47
1:A:669:TYR:O	1:A:670:MET:HB2	2.12	0.47
1:D:567:ASN:C	1:D:567:ASN:OD1	2.56	0.47
1:E:458:ASN:O	1:E:459:PHE:C	2.56	0.47
1:G:339:ILE:O	1:G:343:ILE:CG1	2.42	0.47
1:H:991:LEU:HG	1:H:1070:TYR:CE2	2.50	0.47
2:O:2:GLC:H61	2:O:3:AC1:C5	2.39	0.47
1:A:374:SER:HB2	1:A:1058:ALA:CB	2.44	0.47
1:B:871:GLU:H	1:B:871:GLU:CD	2.21	0.47
1:C:455:PHE:C	1:C:455:PHE:CD2	2.92	0.47
1:C:614:MET:CE	1:C:866:PHE:HE2	2.27	0.47
1:C:875:ASN:OD1	1:C:895:MET:CE	2.63	0.47
1:C:988:LYS:O	1:C:989:ASN:HB2	2.15	0.47
1:E:1006:LYS:HD3	1:E:1007:TYR:CZ	2.50	0.47
1:F:603:ILE:HD11	1:F:619:LYS:HG3	1.96	0.47
1:G:303:GLN:O	1:G:304:GLU:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:642:LEU:HD12	1:G:642:LEU:N	2.29	0.47
1:H:267:THR:C	1:H:1062:LEU:HD11	2.39	0.47
1:H:271:TRP:CZ2	1:H:357:ARG:HG2	2.50	0.47
1:H:1052:ASN:ND2	1:H:1052:ASN:N	2.46	0.47
1:A:272:TYR:HE2	1:A:295:LEU:HA	1.80	0.47
1:C:445:VAL:O	1:C:449:GLN:HG2	2.15	0.47
1:C:686:ALA:HB2	1:C:767:LEU:HD21	1.96	0.47
1:C:988:LYS:H	1:C:990:THR:HG23	1.80	0.47
1:D:733:VAL:CG2	1:D:734:VAL:N	2.77	0.47
1:E:435:ALA:HA	1:E:1052:ASN:ND2	2.29	0.47
1:F:259:PHE:CD2	1:F:259:PHE:N	2.82	0.47
1:F:928:LYS:HB2	1:F:929:PRO:HD2	1.95	0.47
1:H:948:LYS:HD3	1:H:948:LYS:HA	1.67	0.47
1:A:737:GLU:HA	1:A:815:TYR:O	2.14	0.47
1:B:440:ASN:ND2	1:B:449:GLN:HE21	2.05	0.47
1:B:800:THR:C	1:B:802:ALA:N	2.72	0.47
1:C:356:LEU:HA	1:C:359:THR:CG2	2.45	0.47
1:C:561:ILE:HG12	1:C:697:MET:CB	2.44	0.47
1:C:976:ASP:C	1:C:976:ASP:OD1	2.57	0.47
1:D:250:GLN:HE21	1:D:275:LYS:CD	2.27	0.47
1:D:658:TYR:CE2	1:D:660:GLY:HA3	2.49	0.47
1:D:1064:ASP:O	1:D:1068:ASN:N	2.48	0.47
1:E:267:THR:C	1:E:269:GLU:H	2.23	0.47
1:E:288:THR:H	1:E:291:ASP:CG	2.22	0.47
1:E:316:GLN:C	1:E:318:GLY:H	2.23	0.47
1:E:407:ASN:ND2	1:E:430:TYR:HA	2.30	0.47
1:E:526:HIS:HA	1:E:530:ASP:OD1	2.14	0.47
1:F:690:TYR:HB3	1:F:732:GLY:O	2.15	0.47
1:G:293:ARG:CB	1:G:297:MET:HE2	2.44	0.47
1:G:307:ARG:HG3	1:G:332:LEU:HD21	1.95	0.47
4:G:5001:MES:H52	4:G:5001:MES:O3S	2.14	0.47
1:H:311:ASN:O	1:H:314:ASN:N	2.45	0.47
1:H:585:ARG:CD	1:H:661:ASP:OD1	2.62	0.47
1:A:246:ALA:O	1:A:249:ASN:HB2	2.15	0.47
1:A:868:THR:O	1:A:869:LYS:HB3	2.15	0.47
1:B:261:HIS:CD2	1:B:264:HIS:HA	2.50	0.47
1:B:765:ARG:HB2	1:B:766:PRO:HD2	1.97	0.47
1:B:1076:ASP:OD2	1:B:1077:ASN:HB2	2.15	0.47
1:C:492:ASP:HB3	1:C:1022:LEU:HD22	1.97	0.47
1:C:610:TYR:HA	1:C:612:PHE:CE2	2.50	0.47
1:D:551:LEU:CD2	1:D:741:PRO:CG	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:707:ILE:C	1:E:707:ILE:HD12	2.39	0.47
1:H:442:ASN:OD1	1:H:442:ASN:C	2.58	0.47
1:H:461:ASN:H	1:H:470:ASN:HD21	1.61	0.47
1:A:271:TRP:CD2	1:A:294:PRO:HG3	2.50	0.47
1:A:285:THR:CG2	1:A:286:GLN:N	2.78	0.47
1:A:1063:LYS:HE2	1:A:1068:ASN:ND2	2.29	0.47
1:B:658:TYR:O	1:B:659:TYR:C	2.58	0.47
1:B:920:ASP:HB3	1:B:923:ASP:HB2	1.97	0.47
1:C:492:ASP:CG	1:C:1025:ARG:HH11	2.22	0.47
1:D:294:PRO:HG2	1:D:297:MET:CB	2.45	0.47
1:D:421:TYR:CD1	1:D:523:PRO:HB2	2.50	0.47
1:E:277:ILE:HD11	1:E:291:ASP:CA	2.38	0.47
1:E:297:MET:C	1:E:298:THR:CG2	2.88	0.47
1:G:363:PHE:CZ	1:G:367:GLN:OE1	2.68	0.47
1:G:613:THR:N	1:G:616:GLU:OE1	2.37	0.47
1:H:312:TYR:O	1:H:313:MET:C	2.58	0.47
1:H:846:HIS:HA	5:H:11:HOH:O	2.14	0.47
1:A:293:ARG:CB	1:A:297:MET:HE2	2.44	0.47
1:A:515:GLU:O	1:A:515:GLU:HG2	2.15	0.47
1:D:442:ASN:HB3	1:D:445:VAL:CG2	2.45	0.47
1:E:514:LEU:CD2	1:E:532:MET:HG3	2.45	0.47
1:E:703:GLY:HA3	1:E:744:ARG:O	2.15	0.47
1:G:964:LEU:HD12	1:G:996:GLY:HA2	1.96	0.47
1:H:515:GLU:OE1	2:P:3:AC1:O3	2.34	0.47
1:A:341:THR:O	1:A:343:ILE:N	2.48	0.46
1:B:513:ILE:HG12	1:B:953:MET:HE1	1.95	0.46
1:C:276:TYR:HA	1:C:285:THR:O	2.15	0.46
1:C:471:PHE:CG	1:C:954:ALA:HB2	2.49	0.46
1:D:690:TYR:CE2	1:D:820:VAL:HB	2.50	0.46
1:D:965:PRO:HD2	1:D:997:LYS:O	2.15	0.46
1:D:987:ILE:HG12	1:D:1058:ALA:CB	2.45	0.46
1:F:639:ASN:ND2	1:F:813:SER:H	2.13	0.46
1:H:360:ILE:HD13	1:H:360:ILE:HA	1.75	0.46
1:C:718:LEU:HA	1:C:718:LEU:HD23	1.57	0.46
1:D:1073:LEU:HD21	1:D:1080:LEU:HD21	1.96	0.46
1:E:261:HIS:CD2	1:E:264:HIS:HA	2.49	0.46
1:E:427:ILE:N	4:E:5001:MES:O3S	2.47	0.46
1:F:854:ARG:NH1	1:F:892:ASP:OD2	2.44	0.46
1:G:627:ASP:OD2	1:G:636:THR:HG23	2.16	0.46
1:H:1069:THR:HG22	1:H:1070:TYR:N	2.30	0.46
1:A:267:THR:C	1:A:269:GLU:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ARG:O	1:A:308:GLN:C	2.57	0.46
1:A:355:TRP:CD2	1:A:356:LEU:N	2.83	0.46
1:B:424:ASP:C	1:B:424:ASP:OD1	2.58	0.46
1:D:804:ILE:O	1:D:805:LYS:HB3	2.14	0.46
1:D:1022:LEU:N	1:D:1022:LEU:HD23	2.29	0.46
1:E:793:ASP:O	1:E:793:ASP:OD1	2.33	0.46
1:F:816:LEU:HD12	1:F:817:GLY:N	2.29	0.46
1:G:912:ILE:HG22	1:G:931:LYS:NZ	2.30	0.46
1:H:294:PRO:O	1:H:296:LEU:N	2.49	0.46
1:A:729:ARG:HD2	1:A:758:ALA:O	2.15	0.46
1:A:976:ASP:C	1:A:976:ASP:OD1	2.58	0.46
1:B:824:ALA:N	5:B:195:HOH:O	2.48	0.46
1:C:697:MET:O	1:C:698:ARG:NH1	2.47	0.46
1:D:324:ASN:C	1:D:326:ALA:H	2.23	0.46
1:E:319:ILE:HD11	1:E:342:LYS:HD2	1.96	0.46
1:E:407:ASN:ND2	1:E:431:GLU:N	2.64	0.46
1:F:250:GLN:HB2	1:F:1084:LEU:C	2.38	0.46
1:F:457:MET:CE	1:F:493:TYR:HE2	2.29	0.46
1:F:734:VAL:HB	1:F:755:MET:SD	2.55	0.46
1:F:750:ARG:CA	5:F:55:HOH:O	2.64	0.46
1:H:359:THR:O	1:H:360:ILE:C	2.58	0.46
1:B:256:ALA:O	1:B:258:ASN:N	2.48	0.46
1:B:258:ASN:C	1:B:259:PHE:CD2	2.93	0.46
1:C:733:VAL:CG2	1:C:734:VAL:N	2.79	0.46
1:C:862:ASN:O	1:C:912:ILE:HD13	2.15	0.46
1:E:346:LYS:HD3	1:E:355:TRP:CZ2	2.51	0.46
1:E:512:SER:O	1:E:532:MET:HB2	2.15	0.46
1:F:912:ILE:HG22	1:F:931:LYS:NZ	2.30	0.46
1:G:355:TRP:CD2	1:G:356:LEU:N	2.83	0.46
1:G:604:ASN:HD21	1:G:607:VAL:CB	2.27	0.46
1:H:877:VAL:HG12	1:H:881:ASN:HD22	1.81	0.46
1:A:250:GLN:NE2	1:A:275:LYS:HE3	2.29	0.46
1:A:278:LEU:O	1:A:281:GLY:N	2.48	0.46
1:A:354:ASN:O	1:A:357:ARG:HB2	2.16	0.46
1:B:669:TYR:CE2	1:B:670:MET:HE3	2.50	0.46
1:B:1064:ASP:HB2	1:B:1071:PHE:CZ	2.51	0.46
1:C:874:THR:HG22	1:C:878:ILE:CD1	2.46	0.46
1:C:912:ILE:H	1:C:912:ILE:HG13	1.55	0.46
1:D:293:ARG:HB3	1:D:297:MET:HE1	1.96	0.46
1:D:726:ARG:HE	1:D:726:ARG:HB3	1.26	0.46
1:D:1065:GLN:HG3	1:D:1066:ALA:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1076:ASP:OD2	1:D:1077:ASN:HB2	2.15	0.46
1:E:280:ASP:C	1:E:282:LYS:N	2.73	0.46
1:E:454:HIS:CE1	1:E:458:ASN:HD21	2.33	0.46
1:F:630:ALA:O	1:F:633:LYS:NZ	2.48	0.46
1:F:800:THR:O	1:F:801:ALA:C	2.58	0.46
1:G:267:THR:O	1:G:268:ALA:C	2.58	0.46
1:G:920:ASP:OD2	1:G:923:ASP:HB2	2.16	0.46
1:B:987:ILE:HG13	1:B:1058:ALA:HB2	1.98	0.46
1:C:280:ASP:OD1	1:C:345:GLU:HA	2.15	0.46
1:C:297:MET:SD	1:C:340:GLN:HG3	2.56	0.46
1:C:1021:GLU:HG2	1:C:1022:LEU:N	2.29	0.46
1:E:298:THR:O	1:E:300:TRP:CZ3	2.68	0.46
1:F:352:ASN:OD1	1:F:354:ASN:ND2	2.48	0.46
1:G:309:TYR:O	1:G:310:VAL:C	2.58	0.46
1:H:733:VAL:HG23	1:H:819:TRP:O	2.16	0.46
2:I:3:AC1:O3	2:I:3:AC1:HCB1	2.15	0.46
1:B:604:ASN:HD21	1:B:607:VAL:HA	1.81	0.46
1:C:300:TRP:CE3	1:C:306:GLN:HG3	2.51	0.46
1:C:669:TYR:CE2	1:C:670:MET:CE	2.97	0.46
1:D:349:ALA:C	1:D:351:LYS:H	2.22	0.46
1:D:919:THR:O	1:D:919:THR:HG22	2.16	0.46
1:F:384:LYS:HA	5:F:149:HOH:O	2.16	0.46
1:G:252:TYR:CB	1:G:273:ARG:HG2	2.46	0.46
1:H:299:TRP:HH2	1:H:301:PRO:HB3	1.81	0.46
1:A:492:ASP:OD2	1:A:1025:ARG:NH1	2.42	0.46
1:A:608:VAL:O	1:A:609:GLY:C	2.59	0.46
1:C:387:LEU:O	1:C:1050:GLY:HA3	2.16	0.46
1:E:344:GLU:OE1	1:E:344:GLU:HA	2.16	0.46
1:F:551:LEU:HD22	1:F:741:PRO:HG2	1.97	0.46
1:G:396:THR:HG21	1:G:969:VAL:HG12	1.98	0.46
1:G:901:SER:OG	1:G:913:GLN:HA	2.16	0.46
1:H:299:TRP:O	1:H:300:TRP:CD2	2.69	0.46
1:H:305:THR:C	1:H:307:ARG:N	2.73	0.46
1:H:436:ASN:HB2	1:H:961:MET:O	2.16	0.46
1:B:457:MET:CE	1:B:493:TYR:HE2	2.28	0.46
1:B:669:TYR:HE2	1:B:670:MET:HE3	1.80	0.46
1:B:939:VAL:HG12	1:B:943:LYS:HZ2	1.53	0.46
1:C:334:LEU:O	1:C:335:ALA:C	2.57	0.46
1:D:407:ASN:HD21	1:D:431:GLU:H	1.63	0.46
1:E:250:GLN:HB3	1:E:1087:PRO:HG3	1.98	0.46
1:F:312:TYR:C	1:F:312:TYR:HD2	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:912:ILE:HG23	1:F:912:ILE:HD13	1.46	0.46
1:A:267:THR:C	1:A:269:GLU:N	2.74	0.45
1:A:841:ASP:OD1	1:A:846:HIS:CE1	2.67	0.45
1:B:267:THR:HB	1:B:1060:TYR:CE2	2.51	0.45
1:B:391:ASN:C	1:B:392:ASN:ND2	2.73	0.45
1:B:555:SER:HB3	1:F:417:LYS:HE3	1.98	0.45
1:C:365:LYS:HD3	1:C:365:LYS:HA	1.70	0.45
1:F:558:ASN:N	1:F:559:PRO:CD	2.79	0.45
1:F:836:THR:O	1:F:837:ALA:C	2.57	0.45
1:F:851:LEU:HD12	1:F:851:LEU:HA	1.81	0.45
1:F:951:LYS:HD3	1:F:951:LYS:HA	1.65	0.45
1:G:267:THR:O	1:G:269:GLU:N	2.49	0.45
1:B:625:ASN:O	1:B:628:LEU:HB2	2.16	0.45
1:B:1084:LEU:HD23	1:B:1084:LEU:N	2.29	0.45
1:C:1080:LEU:HB3	1:C:1081:PRO:HD2	1.97	0.45
1:D:245:PHE:O	1:D:248:TYR:N	2.48	0.45
1:D:356:LEU:HD12	1:D:360:ILE:HG12	1.98	0.45
1:F:809:ASN:HB2	1:F:810:PRO:HD2	1.97	0.45
1:G:376:LYS:HA	1:G:377:PRO:C	2.40	0.45
1:H:296:LEU:N	1:H:296:LEU:HD12	2.32	0.45
1:A:262:VAL:HG12	1:A:969:VAL:HG23	1.99	0.45
1:A:276:TYR:HA	1:A:285:THR:O	2.16	0.45
1:A:312:TYR:OH	1:A:362:ALA:HB3	2.16	0.45
1:C:615:GLU:OE1	1:C:615:GLU:CA	2.64	0.45
1:C:669:TYR:HE2	1:C:670:MET:CE	2.25	0.45
1:D:457:MET:HE2	1:D:493:TYR:HE2	1.80	0.45
1:D:948:LYS:NZ	5:D:226:HOH:O	2.49	0.45
1:E:337:GLN:O	1:E:339:ILE:N	2.49	0.45
1:F:278:LEU:HD13	1:F:284:TRP:CZ2	2.51	0.45
1:F:719:LYS:HE3	1:F:719:LYS:HB2	1.70	0.45
1:G:347:ILE:HA	1:G:355:TRP:HE1	1.82	0.45
1:G:513:ILE:HG12	1:G:953:MET:HE2	1.98	0.45
1:H:371:ASN:HB3	1:H:373:ASP:H	1.81	0.45
1:A:305:THR:C	1:A:307:ARG:H	2.23	0.45
1:D:504:ASP:OD1	1:D:846:HIS:CD2	2.62	0.45
1:D:1085:VAL:C	1:D:1087:PRO:HD3	2.42	0.45
1:F:407:ASN:ND2	1:F:431:GLU:N	2.64	0.45
1:F:613:THR:OG1	1:F:616:GLU:HG3	2.16	0.45
1:F:976:ASP:C	1:F:976:ASP:OD1	2.59	0.45
1:G:247:GLN:O	1:G:248:TYR:C	2.59	0.45
1:G:658:TYR:O	1:G:659:TYR:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:289:GLU:O	1:H:289:GLU:HG3	2.17	0.45
1:A:274:PRO:O	1:A:287:SER:HB3	2.16	0.45
1:A:376:LYS:CB	1:A:377:PRO:HA	2.31	0.45
1:C:1072:SER:OG	1:C:1074:VAL:HG13	2.16	0.45
1:D:330:LEU:C	1:D:330:LEU:CD1	2.89	0.45
1:F:627:ASP:O	1:F:628:LEU:C	2.54	0.45
1:F:1040:ILE:HG12	1:F:1047:TYR:CE2	2.52	0.45
1:G:439:ASP:OD1	1:G:439:ASP:C	2.59	0.45
2:J:2:GLC:H61	2:J:3:AC1:C5	2.39	0.45
1:A:355:TRP:CE3	1:A:355:TRP:O	2.69	0.45
1:A:613:THR:C	1:A:615:GLU:N	2.74	0.45
1:A:882:VAL:HG21	1:A:944:ALA:C	2.42	0.45
1:B:658:TYR:CZ	1:B:660:GLY:HA3	2.50	0.45
1:C:430:TYR:HB3	1:C:978:TYR:CE1	2.51	0.45
1:C:744:ARG:HA	1:C:744:ARG:HD3	1.37	0.45
1:D:576:ALA:HB3	1:D:847:GLN:HB3	1.98	0.45
1:D:619:LYS:HD2	1:D:619:LYS:HA	1.75	0.45
1:D:800:THR:HG23	1:D:801:ALA:H	1.82	0.45
1:F:293:ARG:HH11	1:F:293:ARG:CG	2.21	0.45
1:G:512:SER:O	1:G:532:MET:HB2	2.16	0.45
1:G:604:ASN:ND2	1:G:607:VAL:CA	2.77	0.45
1:G:841:ASP:OD1	1:G:846:HIS:HE1	2.00	0.45
1:G:1076:ASP:CG	1:G:1077:ASN:N	2.75	0.45
1:G:1080:LEU:HB3	1:G:1081:PRO:HD2	1.99	0.45
1:H:300:TRP:HE3	1:H:300:TRP:H	1.55	0.45
1:H:516:ALA:HB1	1:H:521:ASP:OD2	2.15	0.45
1:H:705:SER:HB3	1:H:743:LEU:CD1	2.43	0.45
1:A:537:ASN:OD1	1:A:540:ARG:NH1	2.49	0.45
1:A:1085:VAL:CG2	1:A:1086:ASN:H	2.30	0.45
1:B:510:HIS:CE1	5:B:197:HOH:O	2.68	0.45
1:C:315:ALA:O	1:C:317:LEU:N	2.50	0.45
1:E:829:ASP:C	1:E:829:ASP:OD1	2.58	0.45
1:F:585:ARG:HD3	1:F:661:ASP:OD1	2.17	0.45
1:F:690:TYR:CE2	1:F:820:VAL:HB	2.51	0.45
1:G:628:LEU:HD23	1:G:636:THR:HG21	1.98	0.45
1:G:809:ASN:CB	1:G:810:PRO:CD	2.93	0.45
1:G:882:VAL:HG21	1:G:944:ALA:C	2.42	0.45
1:A:299:TRP:C	1:A:300:TRP:CD2	2.95	0.45
1:A:312:TYR:O	1:A:315:ALA:HB3	2.17	0.45
1:B:409:THR:O	1:B:410:PRO:C	2.56	0.45
1:C:252:TYR:HB2	1:C:273:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:TYR:OH	1:C:362:ALA:HB1	2.17	0.45
1:C:666:ASP:HA	1:C:863:PHE:O	2.17	0.45
1:E:270:SER:O	1:E:295:LEU:HB2	2.16	0.45
1:E:301:PRO:O	1:E:302:ASP:HB3	2.17	0.45
1:E:531:ASN:ND2	1:E:844:SER:OG	2.50	0.45
1:F:278:LEU:HB3	1:F:344:GLU:HG3	1.98	0.45
1:F:279:LYS:O	1:F:280:ASP:CB	2.52	0.45
1:F:280:ASP:HA	1:F:348:THR:OG1	2.17	0.45
1:F:733:VAL:HG22	1:F:734:VAL:N	2.32	0.45
1:F:988:LYS:C	1:F:990:THR:HG23	2.42	0.45
1:G:263:ASP:OD2	1:G:968:GLU:HA	2.16	0.45
1:G:296:LEU:HA	1:G:296:LEU:HD23	1.62	0.45
1:G:567:ASN:C	1:G:567:ASN:OD1	2.59	0.45
1:G:705:SER:HB3	1:G:743:LEU:HD13	1.98	0.45
1:A:273:ARG:NH1	1:A:289:GLU:HA	2.32	0.45
1:A:481:ASN:ND2	2:I:3:AC1:O2	2.50	0.45
1:B:471:PHE:CD1	1:B:954:ALA:HB2	2.52	0.45
1:B:688:ILE:HD11	1:B:889:GLY:CA	2.47	0.45
1:B:761:ASN:N	1:B:761:ASN:HD22	2.15	0.45
1:C:988:LYS:O	1:C:988:LYS:CG	2.63	0.45
1:D:368:SER:O	1:D:371:ASN:HB2	2.17	0.45
1:E:293:ARG:HB3	1:E:294:PRO:HD2	1.98	0.45
1:F:740:ASN:ND2	1:F:742:SER:H	2.15	0.45
1:F:988:LYS:N	1:F:990:THR:HG23	2.30	0.45
1:G:448:GLU:OE2	1:G:922:TYR:OH	2.31	0.45
1:H:312:TYR:CD2	1:H:363:PHE:HB2	2.51	0.45
1:A:558:ASN:N	1:A:559:PRO:CD	2.79	0.45
1:A:561:ILE:HD13	1:A:561:ILE:HG21	1.71	0.45
1:C:457:MET:HE2	1:C:493:TYR:CE2	2.50	0.45
1:C:581:TYR:HA	1:C:654:VAL:O	2.17	0.45
4:C:5001:MES:H51	4:C:5001:MES:H81	1.48	0.45
1:D:339:ILE:HG22	1:D:343:ILE:HD11	1.99	0.45
1:D:700:GLN:HG2	1:D:702:VAL:HG13	1.99	0.45
1:E:1014:GLU:CG	1:E:1018:LYS:HE3	2.47	0.45
1:G:267:THR:C	1:G:269:GLU:N	2.73	0.45
1:G:759:HIS:HD2	1:G:762:GLN:OE1	2.00	0.45
1:A:292:PHE:C	1:A:293:ARG:HD3	2.42	0.44
1:A:847:GLN:NE2	1:A:852:ASP:OD1	2.39	0.44
1:B:1086:ASN:N	1:B:1087:PRO:HD3	2.32	0.44
1:C:314:ASN:HB3	1:C:319:ILE:O	2.17	0.44
1:D:703:GLY:HA3	1:D:744:ARG:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:705:SER:HB3	1:D:743:LEU:HD13	1.99	0.44
1:E:279:LYS:N	1:E:283:THR:O	2.50	0.44
1:E:407:ASN:ND2	1:E:431:GLU:H	2.14	0.44
1:E:576:ALA:HB3	1:E:847:GLN:HB3	1.98	0.44
1:F:566:VAL:HG21	1:F:652:SER:HB3	1.99	0.44
1:G:733:VAL:HG22	1:G:734:VAL:N	2.32	0.44
1:H:639:ASN:O	1:H:640:THR:C	2.56	0.44
2:K:2:GLC:H61	2:K:3:AC1:C5	2.39	0.44
1:A:281:GLY:N	1:A:344:GLU:HB2	2.31	0.44
1:A:340:GLN:O	1:A:341:THR:C	2.60	0.44
1:A:524:TYR:C	1:A:524:TYR:CD2	2.95	0.44
1:B:430:TYR:CD2	1:B:977:LYS:HE2	2.52	0.44
1:C:988:LYS:C	1:C:990:THR:HG23	2.43	0.44
1:E:928:LYS:HE3	1:E:928:LYS:HB2	1.63	0.44
1:F:300:TRP:CD2	1:F:300:TRP:N	2.86	0.44
1:H:421:TYR:CD1	1:H:523:PRO:HB2	2.52	0.44
1:H:686:ALA:CB	1:H:767:LEU:HD21	2.47	0.44
1:A:363:PHE:C	1:A:365:LYS:N	2.75	0.44
1:B:391:ASN:OD1	1:B:404:ARG:HD2	2.17	0.44
1:D:281:GLY:H	1:D:344:GLU:HB2	1.81	0.44
1:D:765:ARG:HB2	1:D:766:PRO:HD2	1.99	0.44
4:D:5001:MES:H82	4:D:5001:MES:H52	1.74	0.44
1:E:361:SER:C	1:E:363:PHE:N	2.75	0.44
1:E:391:ASN:OD1	1:E:404:ARG:HD2	2.18	0.44
1:F:615:GLU:O	1:F:616:GLU:C	2.61	0.44
1:G:713:TYR:O	1:G:759:HIS:HE1	2.00	0.44
1:G:860:PHE:HB2	1:G:864:GLN:HE22	1.81	0.44
1:G:862:ASN:O	1:G:912:ILE:HD12	2.16	0.44
1:H:299:TRP:CH2	1:H:301:PRO:HB3	2.52	0.44
1:A:551:LEU:HD22	1:A:741:PRO:HG2	1.98	0.44
1:B:697:MET:O	1:B:698:ARG:NH1	2.43	0.44
1:C:247:GLN:NE2	1:C:247:GLN:CA	2.81	0.44
1:E:303:GLN:O	1:E:307:ARG:N	2.47	0.44
1:E:513:ILE:CD1	1:E:953:MET:HE1	2.47	0.44
1:G:639:ASN:HD21	1:G:813:SER:N	2.05	0.44
1:A:310:VAL:CG1	1:A:314:ASN:ND2	2.81	0.44
1:A:776:LYS:CE	5:A:171:HOH:O	2.64	0.44
1:C:320:HIS:O	1:C:321:GLN:HB2	2.17	0.44
1:D:871:GLU:H	1:D:871:GLU:CD	2.25	0.44
1:D:978:TYR:CE1	4:D:5001:MES:H81	2.53	0.44
1:E:718:LEU:HD23	1:E:718:LEU:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:291:ASP:OD1	1:H:291:ASP:N	2.51	0.44
1:A:860:PHE:CD2	1:A:896:ALA:HB2	2.53	0.44
1:C:326:ALA:O	1:C:327:THR:C	2.59	0.44
1:E:287:SER:HA	1:E:291:ASP:OD2	2.18	0.44
1:E:345:GLU:O	1:E:349:ALA:HB2	2.16	0.44
1:E:1019:TYR:N	1:E:1020:PRO:CD	2.80	0.44
1:F:604:ASN:HA	1:F:605:PRO:HD2	1.77	0.44
1:F:606:ASN:HB3	5:F:228:HOH:O	2.17	0.44
1:G:357:ARG:HD3	1:G:357:ARG:HA	1.78	0.44
1:G:606:ASN:O	1:G:607:VAL:C	2.60	0.44
1:H:668:GLN:HB2	1:H:671:ALA:HB2	1.98	0.44
1:B:457:MET:HE2	1:B:493:TYR:HE2	1.83	0.44
1:C:908:LEU:O	1:C:912:ILE:HG13	2.18	0.44
1:D:669:TYR:CE2	1:D:670:MET:HE3	2.52	0.44
1:E:1004:GLN:O	1:E:1008:GLY:N	2.46	0.44
1:F:900:VAL:HG23	1:F:923:ASP:O	2.17	0.44
1:F:1052:ASN:N	1:F:1052:ASN:ND2	2.59	0.44
1:G:299:TRP:CD1	1:G:1081:PRO:HB2	2.53	0.44
1:G:311:ASN:HD21	1:G:323:TYR:H	1.66	0.44
1:G:630:ALA:O	1:G:633:LYS:NZ	2.51	0.44
1:H:741:PRO:O	1:H:806:GLY:HA3	2.17	0.44
1:H:951:LYS:HA	1:H:951:LYS:HD3	1.76	0.44
1:A:280:ASP:OD1	1:A:345:GLU:HA	2.18	0.44
1:A:513:ILE:HG12	1:A:953:MET:CE	2.47	0.44
1:C:615:GLU:HB2	1:C:616:GLU:H	1.37	0.44
1:C:916:TYR:HB3	2:K:3:AC1:HC61	1.98	0.44
1:D:390:SER:HB2	1:D:971:THR:HB	2.00	0.44
1:D:409:THR:O	1:D:410:PRO:C	2.57	0.44
1:D:973:THR:HG23	1:D:988:LYS:HA	1.98	0.44
1:G:294:PRO:O	1:G:297:MET:HB3	2.18	0.44
1:B:488:GLN:OE1	1:B:1028:ILE:HD12	2.18	0.44
1:B:951:LYS:HA	1:B:951:LYS:HD3	1.89	0.44
1:C:457:MET:CE	1:C:493:TYR:HE2	2.29	0.44
1:D:287:SER:HA	1:D:291:ASP:OD2	2.17	0.44
1:D:445:VAL:O	1:D:449:GLN:HG2	2.18	0.44
1:D:596:ARG:NH2	1:D:600:LYS:HD2	2.32	0.44
1:D:1065:GLN:HG3	1:D:1066:ALA:N	2.32	0.44
1:E:436:ASN:HB2	1:E:961:MET:O	2.18	0.44
1:G:280:ASP:O	1:G:282:LYS:N	2.51	0.44
1:A:371:ASN:OD1	1:A:372:SER:N	2.51	0.43
1:A:749:ASP:C	1:A:750:ARG:CG	2.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:912:ILE:H	1:A:912:ILE:HG13	1.54	0.43
1:C:466:ASP:HA	1:C:467:PRO:HD2	1.79	0.43
1:C:604:ASN:ND2	1:C:607:VAL:HB	2.32	0.43
1:C:621:PHE:O	1:C:625:ASN:ND2	2.51	0.43
1:C:988:LYS:O	1:C:988:LYS:HG2	2.17	0.43
1:D:541:LEU:HD23	1:D:541:LEU:HA	1.85	0.43
1:D:718:LEU:HA	1:D:718:LEU:HD23	1.73	0.43
1:D:894:GLU:HA	1:D:953:MET:HB3	1.99	0.43
1:E:245:PHE:HA	1:E:248:TYR:HB2	1.99	0.43
1:E:304:GLU:O	1:E:307:ARG:HB3	2.18	0.43
1:F:492:ASP:CB	1:F:1022:LEU:HD22	2.43	0.43
1:F:733:VAL:HG23	1:F:819:TRP:O	2.17	0.43
1:F:841:ASP:OD1	1:F:846:HIS:HE1	2.01	0.43
1:G:250:GLN:CG	1:G:251:VAL:N	2.73	0.43
1:H:356:LEU:C	1:H:358:GLN:N	2.75	0.43
1:A:278:LEU:CD1	1:A:282:LYS:N	2.81	0.43
1:B:460:GLY:N	1:B:470:ASN:ND2	2.66	0.43
1:D:530:ASP:HB2	1:D:843:LYS:HB3	2.00	0.43
1:E:300:TRP:C	1:E:302:ASP:N	2.75	0.43
1:E:733:VAL:HG22	1:E:734:VAL:N	2.33	0.43
1:F:299:TRP:C	1:F:300:TRP:CE3	2.96	0.43
1:F:421:TYR:CD1	1:F:523:PRO:HB2	2.53	0.43
1:H:278:LEU:HD22	1:H:284:TRP:CH2	2.53	0.43
1:A:279:LYS:HE2	1:A:279:LYS:HB3	1.58	0.43
1:A:310:VAL:HG13	1:A:339:ILE:HD11	2.00	0.43
1:A:458:ASN:O	1:A:459:PHE:C	2.60	0.43
1:A:551:LEU:CD2	1:A:741:PRO:HG2	2.48	0.43
1:B:670:MET:HE1	1:B:885:PHE:CE1	2.50	0.43
1:B:797:LEU:HA	1:B:797:LEU:HD23	1.85	0.43
1:C:612:PHE:CD2	1:C:612:PHE:N	2.84	0.43
1:C:825:ALA:O	1:C:826:ALA:C	2.60	0.43
1:D:262:VAL:HG12	1:D:969:VAL:HG23	1.99	0.43
1:E:608:VAL:O	1:E:609:GLY:C	2.61	0.43
1:E:1072:SER:OG	1:E:1074:VAL:HG12	2.17	0.43
1:G:280:ASP:O	1:G:281:GLY:C	2.60	0.43
1:H:315:ALA:O	1:H:316:GLN:C	2.60	0.43
1:A:604:ASN:ND2	1:A:607:VAL:HA	2.13	0.43
1:B:252:TYR:HD2	1:B:258:ASN:HD21	1.66	0.43
1:B:368:SER:HA	1:B:371:ASN:ND2	2.29	0.43
1:B:613:THR:C	1:B:615:GLU:N	2.74	0.43
1:B:825:ALA:O	1:B:826:ALA:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:LEU:HD13	1:C:284:TRP:CE2	2.53	0.43
1:C:389:TYR:CE1	1:C:1050:GLY:HA2	2.53	0.43
1:D:293:ARG:CB	1:D:297:MET:HE1	2.48	0.43
1:E:413:GLN:HG2	1:E:1028:ILE:HG22	1.99	0.43
1:G:314:ASN:ND2	1:G:319:ILE:HG22	2.33	0.43
1:G:371:ASN:HB3	1:G:373:ASP:HB2	2.00	0.43
1:G:522:THR:N	1:G:523:PRO:HD2	2.33	0.43
1:A:299:TRP:CZ2	1:A:301:PRO:HA	2.53	0.43
1:A:1065:GLN:HG3	1:A:1066:ALA:N	2.32	0.43
1:B:722:ASP:O	1:B:757:ALA:HB3	2.19	0.43
1:C:613:THR:OG1	1:C:615:GLU:HG2	2.18	0.43
1:D:317:LEU:HD13	1:D:342:LYS:HB3	2.00	0.43
1:D:350:GLU:C	1:D:352:ASN:H	2.26	0.43
1:D:749:ASP:C	1:D:750:ARG:CG	2.91	0.43
1:E:245:PHE:N	1:E:245:PHE:C	2.64	0.43
1:E:310:VAL:HG22	1:E:339:ILE:CD1	2.48	0.43
1:E:1080:LEU:HB2	1:E:1085:VAL:HG11	1.99	0.43
1:F:930:ASN:C	1:F:932:TYR:N	2.76	0.43
1:F:991:LEU:HG	1:F:1070:TYR:CE2	2.53	0.43
1:H:278:LEU:CB	1:H:284:TRP:HA	2.49	0.43
1:H:642:LEU:N	1:H:642:LEU:HD12	2.34	0.43
1:A:307:ARG:C	1:A:309:TYR:H	2.24	0.43
1:A:403:TYR:O	1:A:404:ARG:C	2.59	0.43
1:B:483:ASP:OD1	1:B:483:ASP:C	2.62	0.43
1:B:606:ASN:O	1:B:607:VAL:C	2.59	0.43
1:B:725:ASP:OD1	1:B:727:ILE:N	2.51	0.43
1:C:526:HIS:HA	1:C:530:ASP:OD1	2.18	0.43
1:C:924:LEU:HD12	1:C:924:LEU:N	2.33	0.43
1:D:669:TYR:HE2	1:D:670:MET:CE	2.31	0.43
1:D:884:LYS:HD3	1:D:884:LYS:HA	1.85	0.43
1:E:550:PRO:HA	1:E:638:TYR:CE2	2.53	0.43
1:E:760:LYS:O	1:E:761:ASN:C	2.62	0.43
1:F:313:MET:O	1:F:314:ASN:C	2.62	0.43
1:G:430:TYR:CG	1:G:977:LYS:HD2	2.53	0.43
1:A:272:TYR:CE2	1:A:295:LEU:HA	2.53	0.43
1:A:964:LEU:HB2	1:A:995:ASP:O	2.18	0.43
1:C:295:LEU:C	1:C:297:MET:H	2.26	0.43
1:D:999:SER:C	1:D:1001:LYS:H	2.25	0.43
1:E:299:TRP:C	1:E:300:TRP:CD2	2.97	0.43
1:E:478:ALA:HB1	1:E:481:ASN:HD22	1.83	0.43
1:E:499:GLY:O	1:E:502:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:273:ARG:NE	1:F:288:THR:O	2.51	0.43
1:F:278:LEU:CD2	1:F:281:GLY:HA2	2.35	0.43
1:F:340:GLN:O	1:F:344:GLU:HG2	2.18	0.43
1:F:341:THR:O	1:F:342:LYS:C	2.62	0.43
1:F:750:ARG:N	5:F:55:HOH:O	2.52	0.43
1:G:271:TRP:CZ2	1:G:357:ARG:HA	2.53	0.43
1:G:407:ASN:HD21	1:G:431:GLU:H	1.65	0.43
1:H:305:THR:C	1:H:307:ARG:H	2.27	0.43
1:A:453:LEU:CD1	1:A:474:ILE:HG21	2.49	0.43
1:A:461:ASN:OD1	1:A:467:PRO:HA	2.19	0.43
1:A:1085:VAL:HG23	1:A:1086:ASN:H	1.77	0.43
1:B:530:ASP:HB2	1:B:843:LYS:HB3	2.00	0.43
1:B:800:THR:HG22	1:B:801:ALA:N	2.24	0.43
1:B:874:THR:HB	1:B:932:TYR:HB3	2.00	0.43
1:C:380:ASP:O	1:C:381:HIS:C	2.61	0.43
1:C:809:ASN:C	1:C:809:ASN:OD1	2.62	0.43
1:D:259:PHE:CD2	1:D:259:PHE:N	2.85	0.43
1:D:271:TRP:CG	1:D:294:PRO:HA	2.50	0.43
1:D:669:TYR:CE2	1:D:670:MET:CE	3.01	0.43
1:D:700:GLN:HE21	1:D:702:VAL:CG1	2.32	0.43
1:D:759:HIS:HD2	1:D:762:GLN:OE1	2.01	0.43
1:E:310:VAL:HG21	1:E:335:ALA:HB1	2.01	0.43
1:E:424:ASP:OD1	1:E:424:ASP:C	2.60	0.43
1:F:253:SER:H	1:F:258:ASN:ND2	2.16	0.43
1:F:304:GLU:O	1:F:308:GLN:HG3	2.19	0.43
1:F:841:ASP:OD2	1:F:846:HIS:HE1	2.00	0.43
1:G:912:ILE:HG21	1:G:912:ILE:HD12	1.55	0.43
1:G:943:LYS:HB3	1:G:943:LYS:HE3	1.89	0.43
1:H:356:LEU:O	1:H:357:ARG:C	2.61	0.43
1:H:1022:LEU:N	1:H:1022:LEU:HD23	2.33	0.43
1:A:613:THR:OG1	1:A:616:GLU:HG3	2.18	0.43
1:A:938:LEU:O	1:A:939:VAL:C	2.61	0.43
1:B:709:THR:HG22	1:B:736:ILE:HG12	2.01	0.43
1:B:920:ASP:HB3	1:B:923:ASP:CB	2.49	0.43
1:D:639:ASN:ND2	1:D:642:LEU:HD13	2.34	0.43
1:E:277:ILE:CG2	1:E:293:ARG:HH21	2.31	0.43
1:E:586:ALA:O	1:E:587:HIS:C	2.60	0.43
1:E:759:HIS:CD2	1:E:764:TYR:OH	2.72	0.43
1:F:857:PHE:CE2	1:F:859:GLY:HA2	2.52	0.43
1:F:1063:LYS:HE2	1:F:1068:ASN:ND2	2.33	0.43
1:G:442:ASN:OD1	1:G:442:ASN:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:481:ASN:ND2	2:O:3:AC1:O2	2.47	0.43
1:G:639:ASN:HB3	1:G:642:LEU:HB2	2.00	0.43
1:H:492:ASP:OD2	1:H:1025:ARG:NH1	2.40	0.43
1:A:337:GLN:O	1:A:338:THR:C	2.59	0.43
1:B:565:LEU:HD23	1:B:565:LEU:HA	1.91	0.43
1:B:610:TYR:O	1:B:908:LEU:HB2	2.19	0.43
1:B:922:TYR:HB2	1:B:1003:GLN:HB3	1.99	0.43
1:C:996:GLY:O	1:C:1044:SER:HA	2.19	0.43
1:D:304:GLU:OE1	1:D:304:GLU:CA	2.67	0.43
1:D:314:ASN:O	1:D:319:ILE:N	2.52	0.43
1:E:273:ARG:HG2	1:E:274:PRO:O	2.19	0.43
1:E:322:THR:HG23	1:E:323:TYR:H	1.81	0.43
1:E:596:ARG:HB2	1:E:612:PHE:HZ	1.84	0.43
1:E:854:ARG:NH1	1:E:892:ASP:OD2	2.42	0.43
1:F:841:ASP:OD2	1:F:846:HIS:CE1	2.72	0.43
1:G:614:MET:O	1:G:618:LYS:HG3	2.19	0.43
1:H:288:THR:CG2	1:H:289:GLU:N	2.34	0.43
1:A:280:ASP:C	1:A:282:LYS:N	2.76	0.42
1:A:439:ASP:OD1	1:A:439:ASP:C	2.61	0.42
1:A:749:ASP:C	1:A:750:ARG:HG2	2.43	0.42
1:D:551:LEU:HD12	1:D:551:LEU:O	2.19	0.42
1:E:360:ILE:O	1:E:361:SER:C	2.62	0.42
1:E:454:HIS:O	1:E:455:PHE:C	2.62	0.42
1:E:1080:LEU:HB3	1:E:1081:PRO:HD2	2.01	0.42
1:F:988:LYS:H	1:F:990:THR:CG2	2.32	0.42
1:G:988:LYS:H	1:G:990:THR:CG2	2.32	0.42
1:H:488:GLN:O	1:H:489:ILE:C	2.60	0.42
1:H:683:LEU:O	1:H:684:LEU:C	2.62	0.42
2:L:2:GLC:H61	2:L:3:AC1:C5	2.39	0.42
1:A:376:LYS:HA	1:A:377:PRO:C	2.44	0.42
1:B:462:ILE:HD13	1:B:1011:PHE:CZ	2.54	0.42
1:B:558:ASN:N	1:B:559:PRO:CD	2.82	0.42
1:B:698:ARG:HA	1:B:698:ARG:HD3	1.86	0.42
1:C:712:ARG:HA	1:C:712:ARG:HD2	1.84	0.42
1:E:321:GLN:CG	1:E:322:THR:H	2.05	0.42
1:E:339:ILE:HG22	1:E:343:ILE:HD11	2.00	0.42
1:E:639:ASN:O	1:E:640:THR:C	2.60	0.42
1:E:734:VAL:O	1:E:734:VAL:HG13	2.19	0.42
1:F:875:ASN:OD1	1:F:895:MET:CE	2.67	0.42
1:G:873:TYR:CD1	1:G:933:GLY:HA2	2.54	0.42
1:G:966:GLU:HB2	1:G:997:LYS:CB	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:LYS:O	1:A:870:LYS:C	2.62	0.42
1:B:740:ASN:ND2	1:B:740:ASN:C	2.77	0.42
1:B:928:LYS:HE3	1:B:928:LYS:HB2	1.89	0.42
1:B:991:LEU:HD12	1:B:1061:VAL:HG11	2.01	0.42
1:C:567:ASN:OD1	1:C:567:ASN:C	2.62	0.42
1:D:725:ASP:C	1:D:725:ASP:OD1	2.62	0.42
1:E:268:ALA:HA	1:E:1062:LEU:HD11	2.02	0.42
1:E:280:ASP:C	1:E:282:LYS:H	2.26	0.42
1:E:619:LYS:HD2	1:E:619:LYS:HA	1.91	0.42
1:G:646:LEU:O	1:G:647:LEU:C	2.61	0.42
1:G:670:MET:HE1	1:G:885:PHE:CZ	2.54	0.42
1:G:697:MET:HA	1:G:709:THR:O	2.19	0.42
1:H:255:ASP:O	1:H:256:ALA:C	2.62	0.42
1:H:1014:GLU:O	1:H:1018:LYS:HG3	2.19	0.42
1:A:293:ARG:CB	1:A:297:MET:CE	2.97	0.42
1:A:471:PHE:CG	1:A:954:ALA:HB2	2.54	0.42
4:A:5001:MES:H51	4:A:5001:MES:H81	1.82	0.42
4:A:5001:MES:H51	4:A:5001:MES:O2S	2.20	0.42
1:B:741:PRO:HB3	1:B:807:TYR:O	2.20	0.42
1:C:533:ILE:HD13	1:C:533:ILE:HG21	1.83	0.42
1:C:964:LEU:HD12	1:C:996:GLY:HA2	2.02	0.42
1:C:1072:SER:OG	1:C:1074:VAL:HG12	2.18	0.42
1:D:324:ASN:C	1:D:326:ALA:N	2.77	0.42
1:D:352:ASN:OD1	1:D:354:ASN:CB	2.59	0.42
1:D:550:PRO:HA	1:D:638:TYR:CE2	2.54	0.42
1:D:628:LEU:HD23	1:D:628:LEU:HA	1.83	0.42
1:E:376:LYS:HB3	1:E:377:PRO:HA	1.99	0.42
1:E:604:ASN:OD1	1:E:604:ASN:C	2.61	0.42
1:F:304:GLU:OE2	1:F:307:ARG:NH1	2.52	0.42
1:F:397:SER:C	1:F:399:ALA:H	2.28	0.42
1:G:673:LYS:HD3	1:G:677:TYR:CD2	2.54	0.42
1:G:991:LEU:HD12	1:G:1061:VAL:HG11	2.00	0.42
1:H:251:VAL:O	1:H:251:VAL:HG13	2.20	0.42
1:H:294:PRO:O	1:H:295:LEU:C	2.60	0.42
1:H:604:ASN:OD1	1:H:606:ASN:N	2.50	0.42
1:H:782:GLN:HA	1:H:782:GLN:HE21	1.84	0.42
1:H:797:LEU:HD23	1:H:797:LEU:HA	1.77	0.42
2:I:2:GLC:C6	2:I:3:AC1:C1	2.93	0.42
1:A:312:TYR:CD2	1:A:312:TYR:C	2.97	0.42
1:A:389:TYR:CZ	1:A:1050:GLY:HA2	2.54	0.42
1:A:466:ASP:OD2	1:A:943:LYS:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:LEU:HD23	1:C:296:LEU:HA	1.72	0.42
1:C:299:TRP:NE1	1:C:1081:PRO:HB3	2.33	0.42
1:D:418:ASP:OD1	1:D:419:PRO:HD2	2.20	0.42
1:D:461:ASN:H	1:D:470:ASN:HD21	1.67	0.42
1:E:310:VAL:HG23	1:E:339:ILE:CD1	2.49	0.42
1:E:479:VAL:HG21	1:E:514:LEU:HB3	2.01	0.42
1:E:614:MET:CE	1:E:866:PHE:HE2	2.32	0.42
1:H:267:THR:HB	1:H:1060:TYR:CE2	2.55	0.42
1:H:612:PHE:CD2	1:H:612:PHE:N	2.85	0.42
1:A:299:TRP:CH2	1:A:301:PRO:CA	3.02	0.42
1:A:355:TRP:O	1:A:355:TRP:HE3	2.02	0.42
1:A:479:VAL:HG21	1:A:514:LEU:HB3	2.02	0.42
1:C:964:LEU:O	1:C:995:ASP:HB3	2.19	0.42
1:D:408:ARG:HA	1:D:408:ARG:HD3	1.74	0.42
1:D:797:LEU:HD23	1:D:797:LEU:HA	1.78	0.42
1:E:602:GLU:OE1	1:E:635:TYR:OH	2.32	0.42
1:F:364:VAL:HG13	1:F:370:TRP:CE3	2.54	0.42
1:F:797:LEU:HD23	1:F:797:LEU:HA	1.82	0.42
1:G:604:ASN:HD22	1:G:607:VAL:HB	1.81	0.42
1:G:738:GLY:O	1:G:814:GLY:HA3	2.19	0.42
1:H:355:TRP:CG	1:H:356:LEU:N	2.87	0.42
1:H:460:GLY:H	1:H:470:ASN:HD22	1.66	0.42
1:A:702:VAL:O	1:A:703:GLY:C	2.62	0.42
1:A:894:GLU:HA	1:A:953:MET:HB3	2.02	0.42
1:B:603:ILE:HG22	1:B:604:ASN:N	2.33	0.42
1:B:719:LYS:HB2	1:B:719:LYS:HE3	1.66	0.42
1:B:1012:LEU:HD23	1:B:1012:LEU:HA	1.83	0.42
1:C:304:GLU:OE1	1:C:304:GLU:HA	2.20	0.42
1:D:277:ILE:HD11	1:D:291:ASP:HB3	2.02	0.42
1:D:311:ASN:HD21	1:D:323:TYR:H	1.68	0.42
1:D:792:ASN:HD21	1:D:796:GLU:HB2	1.84	0.42
1:G:449:GLN:HA	1:G:449:GLN:OE1	2.20	0.42
1:G:461:ASN:OD1	1:G:467:PRO:HA	2.19	0.42
1:G:951:LYS:HA	1:G:951:LYS:HD3	1.83	0.42
1:G:975:VAL:HG12	1:G:980:THR:C	2.44	0.42
1:H:298:THR:O	1:H:300:TRP:CZ3	2.66	0.42
1:H:360:ILE:O	1:H:361:SER:C	2.63	0.42
1:H:461:ASN:OD1	1:H:467:PRO:HA	2.20	0.42
1:H:860:PHE:HB2	1:H:864:GLN:HE22	1.84	0.42
1:A:273:ARG:HB2	1:A:292:PHE:CE2	2.55	0.42
1:B:267:THR:HA	1:B:1060:TYR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:551:LEU:HD22	1:C:741:PRO:CG	2.49	0.42
1:D:630:ALA:O	1:D:633:LYS:NZ	2.53	0.42
1:D:727:ILE:HD12	1:D:727:ILE:HA	1.78	0.42
1:E:367:GLN:HE21	1:E:367:GLN:HB3	1.60	0.42
1:F:432:PHE:HB2	1:F:977:LYS:HA	2.01	0.42
1:F:557:MET:O	1:F:558:ASN:C	2.61	0.42
1:F:683:LEU:O	1:F:684:LEU:C	2.63	0.42
1:G:476:VAL:HG22	1:G:956:TRP:CE3	2.51	0.42
1:G:656:ARG:HG3	1:G:856:MET:HB3	2.01	0.42
1:H:248:TYR:O	1:H:275:LYS:HB2	2.20	0.42
1:H:928:LYS:HB2	1:H:929:PRO:HD2	2.02	0.42
1:A:454:HIS:CE1	1:A:458:ASN:HD21	2.38	0.42
1:B:882:VAL:HG21	1:B:944:ALA:C	2.45	0.42
1:C:427:ILE:HG12	4:C:5001:MES:O2S	2.19	0.42
1:C:734:VAL:O	1:C:734:VAL:HG13	2.19	0.42
1:C:959:ASP:OD2	1:C:960:GLN:OE1	2.37	0.42
1:D:809:ASN:CB	1:D:810:PRO:CD	2.93	0.42
1:E:1080:LEU:HB2	1:E:1085:VAL:CG1	2.50	0.42
1:F:586:ALA:O	1:F:587:HIS:C	2.61	0.42
1:F:740:ASN:ND2	1:F:741:PRO:CD	2.73	0.42
1:F:841:ASP:CG	1:F:846:HIS:HE1	2.28	0.42
1:F:1021:GLU:HB3	1:F:1022:LEU:H	1.73	0.42
1:G:355:TRP:CZ3	1:G:359:THR:HG21	2.54	0.42
1:G:604:ASN:HD21	1:G:607:VAL:N	2.17	0.42
1:G:917:ALA:HB1	1:G:962:TYR:CG	2.55	0.42
1:H:387:LEU:HA	1:H:973:THR:O	2.19	0.42
1:H:797:LEU:HB3	1:H:799:PHE:CE2	2.54	0.42
1:A:304:GLU:OE1	1:A:304:GLU:CA	2.68	0.42
1:A:314:ASN:O	1:A:315:ALA:C	2.63	0.42
1:B:666:ASP:O	1:B:666:ASP:CG	2.60	0.42
1:C:276:TYR:HD1	1:C:285:THR:C	2.28	0.42
1:C:1004:GLN:O	1:C:1004:GLN:HG3	2.19	0.42
1:D:299:TRP:CH2	1:D:301:PRO:CA	3.00	0.42
1:D:331:GLN:O	1:D:332:LEU:C	2.63	0.42
1:E:303:GLN:H	1:E:303:GLN:HG2	1.64	0.42
1:E:306:GLN:C	1:E:309:TYR:HB3	2.41	0.42
1:E:360:ILE:HG22	1:E:361:SER:N	2.34	0.42
1:E:928:LYS:HB2	1:E:929:PRO:CD	2.50	0.42
1:F:323:TYR:HB3	1:F:327:THR:OG1	2.20	0.42
1:G:323:TYR:HB3	1:G:327:THR:OG1	2.20	0.42
1:G:604:ASN:O	1:G:604:ASN:CG	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:669:TYR:O	1:G:670:MET:CB	2.66	0.42
1:H:782:GLN:NE2	1:H:782:GLN:CA	2.83	0.42
1:A:460:GLY:CA	1:A:470:ASN:ND2	2.83	0.41
1:A:698:ARG:O	1:A:708:ILE:HA	2.20	0.41
1:A:980:THR:O	1:A:981:PRO:C	2.63	0.41
1:B:884:LYS:HA	1:B:884:LYS:HD3	1.77	0.41
1:B:912:ILE:HG23	1:B:912:ILE:HD13	1.58	0.41
1:B:987:ILE:CG1	1:B:1058:ALA:HB2	2.49	0.41
1:C:429:GLY:HA3	1:C:480:ASP:HB3	2.02	0.41
1:C:533:ILE:O	1:C:533:ILE:HG13	2.19	0.41
1:C:603:ILE:CD1	1:C:619:LYS:HG3	2.50	0.41
1:C:775:ILE:HD13	1:C:775:ILE:HG21	1.83	0.41
1:D:352:ASN:CG	1:D:354:ASN:H	2.28	0.41
1:D:424:ASP:HB3	1:D:520:ASN:ND2	2.35	0.41
1:D:681:GLU:O	1:D:682:THR:C	2.63	0.41
1:G:615:GLU:H	1:G:615:GLU:HG2	1.51	0.41
1:G:993:VAL:O	1:G:1056:ARG:NH1	2.48	0.41
1:H:300:TRP:HB3	1:H:301:PRO:HD2	2.02	0.41
1:H:355:TRP:CE3	1:H:356:LEU:N	2.88	0.41
1:H:749:ASP:C	1:H:750:ARG:CG	2.92	0.41
1:A:261:HIS:HD2	1:A:264:HIS:CA	2.33	0.41
1:A:297:MET:HG2	1:A:298:THR:CG2	2.50	0.41
1:A:339:ILE:HG22	1:A:343:ILE:HD11	2.02	0.41
1:A:868:THR:OG1	1:A:872:GLU:OE1	2.34	0.41
1:B:259:PHE:N	1:B:259:PHE:HD2	2.16	0.41
1:B:628:LEU:HD23	1:B:628:LEU:HA	1.83	0.41
1:B:702:VAL:O	1:B:703:GLY:C	2.63	0.41
1:C:460:GLY:HA3	1:C:470:ASN:ND2	2.35	0.41
1:C:974:ARG:O	1:C:981:PRO:HA	2.20	0.41
1:D:258:ASN:O	1:D:292:PHE:HE1	2.02	0.41
1:D:278:LEU:HB2	1:D:284:TRP:CZ2	2.54	0.41
1:D:375:GLU:OE1	1:D:1053:ILE:HB	2.20	0.41
1:D:457:MET:CE	1:D:493:TYR:CE2	3.02	0.41
1:E:1083:SER:C	1:E:1084:LEU:HD23	2.45	0.41
1:F:293:ARG:HB3	1:F:294:PRO:CD	2.49	0.41
1:F:327:THR:HG22	1:F:331:GLN:HB2	2.01	0.41
1:F:513:ILE:CG2	1:F:856:MET:HE1	2.50	0.41
1:H:965:PRO:HD2	1:H:997:LYS:O	2.19	0.41
1:A:305:THR:C	1:A:307:ARG:N	2.74	0.41
1:A:416:LYS:HD3	5:A:217:HOH:O	2.19	0.41
1:A:445:VAL:O	1:A:449:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:ASN:O	1:A:741:PRO:C	2.62	0.41
1:B:368:SER:HA	1:B:371:ASN:HB2	2.02	0.41
1:B:457:MET:HE2	1:B:493:TYR:CE2	2.56	0.41
1:B:557:MET:HE2	1:B:708:ILE:HG12	2.02	0.41
1:B:829:ASP:C	1:B:829:ASP:OD1	2.62	0.41
1:C:255:ASP:O	1:C:258:ASN:HB2	2.20	0.41
1:D:999:SER:C	1:D:1001:LYS:N	2.78	0.41
1:E:253:SER:H	1:E:258:ASN:ND2	2.17	0.41
1:E:279:LYS:O	1:E:279:LYS:CG	2.54	0.41
1:E:339:ILE:HG22	1:E:343:ILE:CD1	2.49	0.41
1:F:376:LYS:HA	1:F:377:PRO:C	2.44	0.41
1:F:434:LEU:HD13	1:F:962:TYR:OH	2.19	0.41
1:F:619:LYS:HA	1:F:619:LYS:HD2	1.90	0.41
1:G:513:ILE:HD13	1:G:953:MET:HE1	2.02	0.41
1:A:276:TYR:CA	1:A:285:THR:O	2.68	0.41
1:A:854:ARG:HH11	1:A:854:ARG:HD3	1.74	0.41
1:B:695:GLN:HA	1:B:711:VAL:O	2.21	0.41
1:C:503:ASN:HA	1:C:839:SER:OG	2.20	0.41
1:E:280:ASP:O	1:E:282:LYS:N	2.53	0.41
1:E:492:ASP:CG	1:E:1025:ARG:HH11	2.28	0.41
1:F:912:ILE:HG21	1:F:912:ILE:HD12	1.56	0.41
1:G:832:VAL:HG12	1:G:850:ALA:HA	2.02	0.41
1:H:251:VAL:O	1:H:252:TYR:C	2.63	0.41
1:H:278:LEU:C	1:H:283:THR:O	2.63	0.41
1:A:341:THR:O	1:A:342:LYS:C	2.64	0.41
1:A:484:ALA:O	1:A:485:ASP:C	2.62	0.41
1:A:1072:SER:OG	1:A:1074:VAL:CG1	2.68	0.41
1:B:666:ASP:HA	1:B:863:PHE:O	2.20	0.41
1:B:723:THR:O	1:B:724:GLY:C	2.64	0.41
1:B:1014:GLU:HG3	1:B:1018:LYS:HE3	2.02	0.41
1:C:321:GLN:OE1	1:C:321:GLN:HA	2.07	0.41
1:C:352:ASN:OD1	1:C:354:ASN:HB2	2.20	0.41
1:C:737:GLU:HA	1:C:815:TYR:O	2.20	0.41
1:D:464:ALA:O	1:D:465:ASN:CB	2.67	0.41
1:D:677:TYR:CD2	1:D:677:TYR:C	2.98	0.41
1:E:413:GLN:HG2	1:E:1028:ILE:CG2	2.51	0.41
1:E:504:ASP:OD1	1:E:846:HIS:CD2	2.68	0.41
1:E:625:ASN:O	1:E:628:LEU:HB2	2.21	0.41
1:F:297:MET:HE2	1:F:297:MET:HB3	1.86	0.41
1:F:358:GLN:O	1:F:358:GLN:HG2	2.18	0.41
1:F:977:LYS:H	1:F:977:LYS:HG3	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:596:ARG:HB2	1:G:612:PHE:HZ	1.84	0.41
1:A:260:GLU:OE2	1:A:357:ARG:NH2	2.37	0.41
1:A:300:TRP:HB3	1:A:301:PRO:HD2	2.01	0.41
1:B:252:TYR:CB	1:B:273:ARG:HG2	2.51	0.41
1:B:452:TRP:HB2	1:B:921:ARG:NH2	2.36	0.41
1:B:546:SER:HB2	1:B:560:LEU:HD21	2.01	0.41
1:B:682:THR:HG22	1:B:767:LEU:HD11	2.02	0.41
1:D:293:ARG:CB	1:D:297:MET:HE2	2.33	0.41
1:D:319:ILE:O	1:D:320:HIS:C	2.63	0.41
1:D:337:GLN:O	1:D:340:GLN:N	2.46	0.41
1:D:522:THR:N	1:D:523:PRO:HD2	2.36	0.41
1:D:999:SER:O	1:D:1001:LYS:N	2.53	0.41
1:E:299:TRP:C	1:E:300:TRP:CE3	2.99	0.41
1:E:300:TRP:C	1:E:302:ASP:H	2.28	0.41
1:E:492:ASP:HB3	1:E:1022:LEU:HD22	2.01	0.41
1:E:752:VAL:HG22	1:E:798:ILE:CD1	2.45	0.41
1:E:1080:LEU:HB3	1:E:1081:PRO:CD	2.51	0.41
1:F:296:LEU:HD23	1:F:296:LEU:HA	1.97	0.41
1:F:439:ASP:C	1:F:439:ASP:OD1	2.62	0.41
1:G:367:GLN:O	1:G:370:TRP:N	2.39	0.41
1:G:687:ARG:HA	1:G:691:VAL:CG2	2.50	0.41
1:H:516:ALA:HB1	1:H:521:ASP:CB	2.50	0.41
1:A:718:LEU:HD23	1:A:718:LEU:HA	1.85	0.41
1:B:461:ASN:OD1	1:B:467:PRO:HB3	2.21	0.41
1:B:614:MET:HG3	1:B:618:LYS:HE3	2.01	0.41
1:D:959:ASP:OD2	1:D:960:GLN:OE1	2.39	0.41
1:D:975:VAL:HB	1:D:979:GLY:HA2	2.02	0.41
1:F:604:ASN:HD21	1:F:607:VAL:HA	1.85	0.41
1:F:688:ILE:HG12	1:F:831:ARG:CZ	2.50	0.41
1:G:267:THR:C	1:G:269:GLU:H	2.29	0.41
1:G:280:ASP:OD1	1:G:348:THR:HB	2.20	0.41
1:G:466:ASP:HA	1:G:467:PRO:HD2	1.86	0.41
1:G:900:VAL:HG23	1:G:925:GLY:H	1.84	0.41
1:G:973:THR:HG22	1:G:974:ARG:N	2.35	0.41
2:N:2:GLC:H61	2:N:3:AC1:C5	2.39	0.41
1:B:919:THR:O	1:B:961:MET:HE2	2.21	0.41
1:B:939:VAL:HG11	1:B:943:LYS:HZ3	1.70	0.41
1:C:358:GLN:O	1:C:359:THR:C	2.63	0.41
1:C:561:ILE:HG22	1:C:562:THR:HG23	2.02	0.41
1:D:271:TRP:CH2	1:D:357:ARG:HD3	2.56	0.41
1:D:370:TRP:HA	1:D:1056:ARG:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:492:ASP:CG	1:D:1025:ARG:HH11	2.27	0.41
1:F:267:THR:HB	1:F:1060:TYR:CE2	2.55	0.41
1:F:293:ARG:HG2	1:F:293:ARG:NH1	2.27	0.41
1:F:361:SER:O	1:F:362:ALA:C	2.64	0.41
1:F:389:TYR:CE1	1:F:1050:GLY:HA2	2.56	0.41
1:F:513:ILE:CG1	1:F:953:MET:HE1	2.49	0.41
1:F:1064:ASP:O	1:F:1068:ASN:N	2.54	0.41
1:G:581:TYR:HA	1:G:654:VAL:O	2.21	0.41
1:H:619:LYS:HD2	1:H:619:LYS:HA	1.74	0.41
1:H:862:ASN:C	1:H:912:ILE:HD13	2.33	0.41
1:H:912:ILE:H	1:H:912:ILE:HG13	1.75	0.41
1:H:928:LYS:HB2	1:H:928:LYS:HE3	1.79	0.41
1:A:365:LYS:HD3	1:A:365:LYS:HA	1.62	0.41
1:A:435:ALA:HA	1:A:1052:ASN:ND2	2.36	0.41
1:B:737:GLU:HA	1:B:815:TYR:O	2.21	0.41
1:C:267:THR:HB	1:C:1060:TYR:CE2	2.56	0.41
1:C:355:TRP:CD2	1:C:356:LEU:N	2.89	0.41
1:C:558:ASN:N	1:C:559:PRO:CD	2.84	0.41
1:D:589:SER:O	1:D:590:GLU:HB2	2.21	0.41
1:D:768:LEU:HD23	1:D:777:ALA:HA	2.01	0.41
1:D:970:VAL:O	1:D:991:LEU:HA	2.21	0.41
1:D:1021:GLU:C	1:D:1023:PHE:N	2.76	0.41
1:E:249:ASN:O	1:E:250:GLN:C	2.63	0.41
1:E:412:ASN:CG	1:E:412:ASN:O	2.63	0.41
1:F:407:ASN:HD21	1:F:431:GLU:H	1.69	0.41
1:F:430:TYR:O	1:F:481:ASN:HA	2.21	0.41
1:F:585:ARG:NH1	1:F:661:ASP:OD1	2.40	0.41
1:F:765:ARG:HD2	1:F:765:ARG:C	2.46	0.41
1:F:969:VAL:HG22	1:F:993:VAL:HG22	2.03	0.41
1:G:245:PHE:O	1:G:247:GLN:N	2.53	0.41
1:G:558:ASN:N	1:G:559:PRO:CD	2.84	0.41
1:G:586:ALA:O	1:G:587:HIS:C	2.60	0.41
1:G:737:GLU:HA	1:G:815:TYR:O	2.21	0.41
1:G:1076:ASP:OD2	1:G:1077:ASN:N	2.54	0.41
1:H:278:LEU:CD2	1:H:284:TRP:CZ3	3.04	0.41
1:H:387:LEU:O	1:H:1050:GLY:HA3	2.21	0.41
1:H:584:ILE:O	1:H:584:ILE:HG13	2.19	0.41
1:H:745:LEU:N	1:H:745:LEU:HD12	2.36	0.41
1:H:877:VAL:O	1:H:878:ILE:C	2.64	0.41
1:H:964:LEU:HA	1:H:965:PRO:HD3	1.92	0.41
1:H:996:GLY:O	1:H:1044:SER:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLU:HA	1:A:344:GLU:OE1	2.21	0.41
1:B:408:ARG:HA	1:B:408:ARG:HD3	1.85	0.41
1:B:464:ALA:HA	5:B:27:HOH:O	2.22	0.41
1:C:245:PHE:CZ	1:C:337:GLN:HB3	2.56	0.41
1:C:376:LYS:CB	1:C:377:PRO:CA	2.99	0.41
1:C:439:ASP:OD1	1:C:439:ASP:C	2.64	0.41
1:D:276:TYR:CA	1:D:285:THR:O	2.69	0.41
1:D:558:ASN:N	1:D:559:PRO:CD	2.84	0.41
1:E:276:TYR:HB3	1:E:284:TRP:HE3	1.84	0.41
1:E:567:ASN:C	1:E:567:ASN:OD1	2.64	0.41
1:E:704:ASN:OD1	1:E:704:ASN:N	2.54	0.41
1:F:388:LEU:HD12	1:F:1049:ASN:O	2.21	0.41
1:F:457:MET:CE	1:F:493:TYR:CE2	3.04	0.41
1:F:726:ARG:O	1:F:729:ARG:HB3	2.20	0.41
1:F:792:ASN:ND2	1:F:796:GLU:HB2	2.36	0.41
1:G:360:ILE:O	1:G:364:VAL:HG23	2.20	0.41
1:H:267:THR:C	1:H:269:GLU:N	2.72	0.41
1:H:364:VAL:HG13	1:H:370:TRP:CE3	2.56	0.41
1:H:396:THR:HG21	1:H:970:VAL:HA	2.03	0.41
1:H:460:GLY:N	1:H:470:ASN:HD22	2.18	0.41
1:H:498:LYS:HA	1:H:498:LYS:HD3	1.89	0.41
2:M:2:GLC:H61	2:M:3:AC1:C5	2.39	0.41
1:A:279:LYS:O	1:A:280:ASP:HB2	2.22	0.40
1:A:639:ASN:O	1:A:640:THR:C	2.62	0.40
1:B:1025:ARG:O	1:B:1033:PRO:HA	2.21	0.40
1:C:651:LYS:O	1:C:652:SER:HB2	2.21	0.40
1:D:369:ALA:C	1:D:370:TRP:CD1	2.99	0.40
1:E:907:PHE:O	1:E:908:LEU:C	2.65	0.40
1:F:314:ASN:HB3	1:F:319:ILE:O	2.20	0.40
1:F:469:ALA:CB	1:F:939:VAL:HG13	2.51	0.40
1:F:698:ARG:O	1:F:708:ILE:HA	2.20	0.40
1:F:751:VAL:HG21	1:F:804:ILE:CD1	2.51	0.40
1:F:1078:THR:HG22	1:F:1079:PHE:N	2.36	0.40
1:G:267:THR:HB	1:G:1060:TYR:CE2	2.56	0.40
1:G:603:ILE:CD1	1:G:619:LYS:HG3	2.51	0.40
1:G:912:ILE:HG23	1:G:912:ILE:HD13	1.42	0.40
1:H:549:LYS:HA	1:H:549:LYS:HD3	1.92	0.40
1:H:658:TYR:O	1:H:659:TYR:C	2.63	0.40
1:H:1086:ASN:HA	1:H:1087:PRO:HD3	1.92	0.40
1:A:310:VAL:O	1:A:314:ASN:N	2.47	0.40
1:A:337:GLN:O	1:A:340:GLN:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:GLU:OE1	1:A:615:GLU:CA	2.54	0.40
1:B:965:PRO:HD2	1:B:997:LYS:O	2.21	0.40
1:B:1080:LEU:O	1:B:1081:PRO:C	2.63	0.40
1:D:342:LYS:O	1:D:346:LYS:CB	2.69	0.40
1:D:504:ASP:O	1:D:508:ASN:HB2	2.21	0.40
1:D:525:LEU:HD12	1:D:525:LEU:HA	1.93	0.40
1:D:759:HIS:CD2	1:D:764:TYR:OH	2.74	0.40
1:D:809:ASN:HB2	1:D:810:PRO:HD3	2.03	0.40
1:D:924:LEU:N	1:D:924:LEU:HD12	2.36	0.40
1:E:396:THR:HG21	1:E:969:VAL:O	2.20	0.40
1:E:430:TYR:CD1	1:E:430:TYR:C	2.98	0.40
1:E:800:THR:HG23	1:E:801:ALA:N	2.36	0.40
1:F:321:GLN:HG3	1:F:323:TYR:CZ	2.56	0.40
1:F:466:ASP:OD2	1:F:943:LYS:HD2	2.20	0.40
1:F:574:GLU:HG3	1:F:575:THR:N	2.35	0.40
1:F:606:ASN:O	1:F:607:VAL:O	2.39	0.40
1:F:987:ILE:CG1	1:F:1058:ALA:HB2	2.50	0.40
1:G:273:ARG:HB2	1:G:292:PHE:CE2	2.56	0.40
1:H:300:TRP:CD1	1:H:306:GLN:CB	3.05	0.40
1:H:606:ASN:O	1:H:607:VAL:C	2.64	0.40
1:H:988:LYS:C	1:H:990:THR:HG23	2.47	0.40
1:H:997:LYS:HA	1:H:1043:TRP:O	2.20	0.40
1:A:279:LYS:O	1:A:280:ASP:CB	2.69	0.40
1:A:334:LEU:C	1:A:336:ALA:N	2.77	0.40
1:B:744:ARG:HE	1:B:744:ARG:HB3	1.24	0.40
1:B:874:THR:HG22	1:B:875:ASN:N	2.36	0.40
1:C:481:ASN:ND2	2:K:3:AC1:O2	2.50	0.40
1:C:782:GLN:NE2	1:C:782:GLN:HA	2.35	0.40
1:C:974:ARG:HG2	1:C:987:ILE:HB	2.03	0.40
1:D:669:TYR:HE2	1:D:670:MET:HE3	1.86	0.40
1:E:298:THR:C	1:E:300:TRP:CZ3	2.99	0.40
1:G:407:ASN:ND2	1:G:430:TYR:HA	2.37	0.40
1:G:920:ASP:CG	1:G:923:ASP:HB2	2.47	0.40
1:G:965:PRO:HD2	1:G:998:SER:HA	2.02	0.40
1:H:468:ASP:O	1:H:946:HIS:ND1	2.48	0.40
1:H:604:ASN:HA	1:H:605:PRO:HD2	1.67	0.40
1:H:877:VAL:CG1	1:H:881:ASN:ND2	2.85	0.40
1:A:272:TYR:O	1:A:293:ARG:N	2.50	0.40
1:A:285:THR:HG22	1:A:286:GLN:N	2.35	0.40
1:A:316:GLN:C	1:A:318:GLY:H	2.28	0.40
1:A:341:THR:O	1:A:344:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:LEU:HA	1:A:565:LEU:HD23	1.80	0.40
1:A:670:MET:CE	1:A:885:PHE:CZ	3.02	0.40
1:A:1064:ASP:HB2	1:A:1071:PHE:CE1	2.56	0.40
1:C:367:GLN:O	1:C:368:SER:C	2.64	0.40
1:C:788:VAL:HG12	1:C:789:ARG:N	2.36	0.40
1:D:339:ILE:O	1:D:343:ILE:CG1	2.40	0.40
1:D:453:LEU:CD1	1:D:474:ILE:HG21	2.52	0.40
1:E:450:LEU:O	1:E:451:ASN:C	2.63	0.40
1:F:658:TYR:O	1:F:659:TYR:C	2.65	0.40
1:F:659:TYR:C	1:F:659:TYR:CD2	2.99	0.40
1:F:759:HIS:HA	1:F:762:GLN:OE1	2.21	0.40
1:F:809:ASN:O	1:F:810:PRO:C	2.63	0.40
1:G:444:VAL:HG23	5:G:208:HOH:O	2.21	0.40
1:G:565:LEU:HA	1:G:565:LEU:HD23	1.87	0.40
1:G:996:GLY:O	1:G:1044:SER:HA	2.21	0.40
1:A:293:ARG:HD3	1:A:293:ARG:HH11	1.74	0.40
1:A:341:THR:C	1:A:343:ILE:N	2.80	0.40
1:A:904:ASP:OD2	1:A:906:SER:OG	2.30	0.40
1:B:430:TYR:O	1:B:481:ASN:HA	2.20	0.40
1:B:613:THR:C	1:B:615:GLU:H	2.29	0.40
1:C:315:ALA:O	1:C:316:GLN:C	2.63	0.40
1:C:530:ASP:HB2	1:C:843:LYS:HB3	2.03	0.40
1:C:606:ASN:O	1:C:607:VAL:C	2.64	0.40
1:C:938:LEU:C	1:C:938:LEU:HD12	2.47	0.40
1:D:250:GLN:NE2	1:D:275:LYS:HD2	2.37	0.40
1:D:324:ASN:O	1:D:326:ALA:N	2.54	0.40
1:E:245:PHE:N	1:E:245:PHE:CG	2.90	0.40
1:F:250:GLN:CG	1:F:275:LYS:HE2	2.51	0.40
1:F:504:ASP:OD1	1:F:846:HIS:HD2	2.04	0.40
1:H:776:LYS:HG2	1:H:778:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	840/844 (100%)	772 (92%)	57 (7%)	11 (1%)	9	33
1	B	743/844 (88%)	678 (91%)	53 (7%)	12 (2%)	7	29
1	C	842/844 (100%)	777 (92%)	57 (7%)	8 (1%)	12	39
1	D	842/844 (100%)	763 (91%)	66 (8%)	13 (2%)	8	30
1	E	841/844 (100%)	758 (90%)	70 (8%)	13 (2%)	8	30
1	F	842/844 (100%)	771 (92%)	65 (8%)	6 (1%)	18	47
1	G	842/844 (100%)	776 (92%)	56 (7%)	10 (1%)	10	34
1	H	803/844 (95%)	717 (89%)	62 (8%)	24 (3%)	3	17
All	All	6595/6752 (98%)	6012 (91%)	486 (7%)	97 (2%)	8	30

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	250	GLN
1	C	321	GLN
1	C	327	THR
1	C	351	LYS
1	D	278	LEU
1	D	281	GLY
1	D	351	LYS
1	E	320	HIS
1	E	321	GLN
1	E	1066	ALA
1	F	246	ALA
1	F	1021	GLU
1	G	246	ALA
1	H	247	GLN
1	H	250	GLN
1	H	277	ILE
1	H	286	GLN
1	H	302	ASP
1	H	311	ASN
1	H	313	MET
1	H	360	ILE
1	A	247	GLN
1	A	281	GLY
1	A	315	ALA

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Mol	Chain	Res	Type
1	B	257	ALA
1	B	724	GLY
1	B	761	ASN
1	B	1066	ALA
1	C	316	GLN
1	D	246	ALA
1	D	349	ALA
1	D	1021	GLU
1	D	1066	ALA
1	E	268	ALA
1	E	312	TYR
1	E	337	GLN
1	E	360	ILE
1	F	724	GLY
1	G	281	GLY
1	G	1021	GLU
1	H	246	ALA
1	H	248	TYR
1	H	279	LYS
1	H	280	ASP
1	A	327	THR
1	A	351	LYS
1	B	384	LYS
1	B	1000	GLY
1	B	1045	ALA
1	C	268	ALA
1	C	315	ALA
1	D	304	GLU
1	D	325	THR
1	E	338	THR
1	E	351	LYS
1	F	279	LYS
1	G	253	SER
1	G	348	THR
1	G	351	LYS
1	G	362	ALA
1	G	1066	ALA
1	H	268	ALA
1	H	278	LEU
1	H	1045	ALA
1	H	1066	ALA
1	A	353	THR

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Mol	Chain	Res	Type
1	A	1066	ALA
1	D	254	THR
1	E	302	ASP
1	E	307	ARG
1	G	609	GLY
1	H	257	ALA
1	H	316	GLN
1	A	342	LYS
1	B	870	LYS
1	D	250	GLN
1	D	357	ARG
1	D	1000	GLY
1	E	362	ALA
1	H	312	TYR
1	H	357	ARG
1	H	358	GLN
1	H	364	VAL
1	A	268	ALA
1	A	384	LYS
1	B	614	MET
1	C	381	HIS
1	C	870	LYS
1	F	607	VAL
1	G	384	LYS
1	H	440	ASN
1	B	556	GLY
1	E	1008	GLY
1	A	609	GLY
1	H	310	VAL
1	B	882	VAL
1	F	603	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	713/715 (100%)	661 (93%)	52 (7%)	13	38
1	B	627/715 (88%)	588 (94%)	39 (6%)	16	44
1	C	715/715 (100%)	662 (93%)	53 (7%)	13	38
1	D	715/715 (100%)	658 (92%)	57 (8%)	11	35
1	E	714/715 (100%)	651 (91%)	63 (9%)	9	31
1	F	715/715 (100%)	653 (91%)	62 (9%)	9	32
1	G	715/715 (100%)	660 (92%)	55 (8%)	12	36
1	H	682/715 (95%)	631 (92%)	51 (8%)	12	38
All	All	5596/5720 (98%)	5164 (92%)	432 (8%)	12	36

All (432) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	253	SER
1	A	258	ASN
1	A	276	TYR
1	A	279	LYS
1	A	286	GLN
1	A	298	THR
1	A	307	ARG
1	A	309	TYR
1	A	321	GLN
1	A	342	LYS
1	A	352	ASN
1	A	353	THR
1	A	359	THR
1	A	365	LYS
1	A	368	SER
1	A	371	ASN
1	A	374	SER
1	A	394	LYS
1	A	422	THR
1	A	457	MET
1	A	465	ASN
1	A	502	LYS
1	A	532	MET

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Mol	Chain	Res	Type
1	A	574	GLU
1	A	600	LYS
1	A	604	ASN
1	A	605	PRO
1	A	615	GLU
1	A	619	LYS
1	A	622	GLU
1	A	631	THR
1	A	632	GLU
1	A	702	VAL
1	A	726	ARG
1	A	727	ILE
1	A	740	ASN
1	A	832	VAL
1	A	835	SER
1	A	870	LYS
1	A	880	LYS
1	A	882	VAL
1	A	912	ILE
1	A	928	LYS
1	A	977	LYS
1	A	985	SER
1	A	1001	LYS
1	A	1037	SER
1	A	1038	VAL
1	A	1044	SER
1	A	1052	ASN
1	A	1074	VAL
1	B	254	THR
1	B	259	PHE
1	B	374	SER
1	B	392	ASN
1	B	394	LYS
1	B	422	THR
1	B	425	ARG
1	B	465	ASN
1	B	502	LYS
1	B	532	MET
1	B	540	ARG
1	B	574	GLU
1	B	600	LYS
1	B	604	ASN

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Mol	Chain	Res	Type
1	B	612	PHE
1	B	632	GLU
1	B	708	ILE
1	B	726	ARG
1	B	727	ILE
1	B	740	ASN
1	B	744	ARG
1	B	761	ASN
1	B	793	ASP
1	B	798	ILE
1	B	800	THR
1	B	832	VAL
1	B	835	SER
1	B	882	VAL
1	B	900	VAL
1	B	912	ILE
1	B	977	LYS
1	B	985	SER
1	B	986	GLN
1	B	988	LYS
1	B	1001	LYS
1	B	1038	VAL
1	B	1052	ASN
1	B	1074	VAL
1	B	1084	LEU
1	C	245	PHE
1	C	247	GLN
1	C	253	SER
1	C	258	ASN
1	C	275	LYS
1	C	283	THR
1	C	285	THR
1	C	286	GLN
1	C	290	LYS
1	C	321	GLN
1	C	342	LYS
1	C	346	LYS
1	C	347	ILE
1	C	348	THR
1	C	350	GLU
1	C	352	ASN
1	C	353	THR

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Mol	Chain	Res	Type
1	C	368	SER
1	C	374	SER
1	C	390	SER
1	C	394	LYS
1	C	422	THR
1	C	425	ARG
1	C	457	MET
1	C	465	ASN
1	C	532	MET
1	C	574	GLU
1	C	604	ASN
1	C	607	VAL
1	C	612	PHE
1	C	619	LYS
1	C	629	LEU
1	C	631	THR
1	C	632	GLU
1	C	702	VAL
1	C	726	ARG
1	C	740	ASN
1	C	744	ARG
1	C	800	THR
1	C	832	VAL
1	C	835	SER
1	C	882	VAL
1	C	912	ILE
1	C	928	LYS
1	C	977	LYS
1	C	985	SER
1	C	988	LYS
1	C	990	THR
1	C	1001	LYS
1	C	1038	VAL
1	C	1052	ASN
1	C	1064	ASP
1	C	1074	VAL
1	D	247	GLN
1	D	277	ILE
1	D	282	LYS
1	D	287	SER
1	D	288	THR
1	D	290	LYS

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Mol	Chain	Res	Type
1	D	308	GLN
1	D	312	TYR
1	D	322	THR
1	D	325	THR
1	D	341	THR
1	D	347	ILE
1	D	351	LYS
1	D	352	ASN
1	D	359	THR
1	D	364	VAL
1	D	366	THR
1	D	368	SER
1	D	374	SER
1	D	394	LYS
1	D	396	THR
1	D	422	THR
1	D	457	MET
1	D	465	ASN
1	D	477	ASP
1	D	502	LYS
1	D	532	MET
1	D	540	ARG
1	D	551	LEU
1	D	574	GLU
1	D	600	LYS
1	D	605	PRO
1	D	619	LYS
1	D	632	GLU
1	D	726	ARG
1	D	727	ILE
1	D	734	VAL
1	D	740	ASN
1	D	748	SER
1	D	800	THR
1	D	832	VAL
1	D	880	LYS
1	D	882	VAL
1	D	900	VAL
1	D	912	ILE
1	D	928	LYS
1	D	977	LYS
1	D	986	GLN

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Mol	Chain	Res	Type
1	D	988	LYS
1	D	1001	LYS
1	D	1013	GLU
1	D	1021	GLU
1	D	1038	VAL
1	D	1052	ASN
1	D	1074	VAL
1	D	1078	THR
1	D	1084	LEU
1	E	245	PHE
1	E	247	GLN
1	E	253	SER
1	E	258	ASN
1	E	259	PHE
1	E	279	LYS
1	E	286	GLN
1	E	287	SER
1	E	289	GLU
1	E	290	LYS
1	E	291	ASP
1	E	292	PHE
1	E	295	LEU
1	E	298	THR
1	E	304	GLU
1	E	305	THR
1	E	308	GLN
1	E	310	VAL
1	E	311	ASN
1	E	316	GLN
1	E	317	LEU
1	E	322	THR
1	E	325	THR
1	E	327	THR
1	E	330	LEU
1	E	341	THR
1	E	347	ILE
1	E	359	THR
1	E	361	SER
1	E	365	LYS
1	E	368	SER
1	E	374	SER
1	E	390	SER

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Mol	Chain	Res	Type
1	E	422	THR
1	E	457	MET
1	E	477	ASP
1	E	532	MET
1	E	574	GLU
1	E	619	LYS
1	E	632	GLU
1	E	702	VAL
1	E	727	ILE
1	E	740	ASN
1	E	744	ARG
1	E	800	THR
1	E	832	VAL
1	E	835	SER
1	E	856	MET
1	E	870	LYS
1	E	882	VAL
1	E	912	ILE
1	E	928	LYS
1	E	977	LYS
1	E	985	SER
1	E	986	GLN
1	E	988	LYS
1	E	1001	LYS
1	E	1016	GLN
1	E	1038	VAL
1	E	1052	ASN
1	E	1064	ASP
1	E	1074	VAL
1	E	1075	SER
1	F	244	SER
1	F	253	SER
1	F	258	ASN
1	F	277	ILE
1	F	279	LYS
1	F	290	LYS
1	F	305	THR
1	F	308	GLN
1	F	322	THR
1	F	339	ILE
1	F	350	GLU
1	F	352	ASN

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Mol	Chain	Res	Type
1	F	356	LEU
1	F	357	ARG
1	F	361	SER
1	F	368	SER
1	F	374	SER
1	F	394	LYS
1	F	396	THR
1	F	422	THR
1	F	425	ARG
1	F	457	MET
1	F	465	ASN
1	F	532	MET
1	F	540	ARG
1	F	574	GLU
1	F	604	ASN
1	F	612	PHE
1	F	619	LYS
1	F	626	LYS
1	F	632	GLU
1	F	710	SER
1	F	719	LYS
1	F	726	ARG
1	F	727	ILE
1	F	736	ILE
1	F	750	ARG
1	F	782	GLN
1	F	787	LEU
1	F	794	ARG
1	F	800	THR
1	F	803	ASP
1	F	832	VAL
1	F	835	SER
1	F	856	MET
1	F	861	SER
1	F	868	THR
1	F	880	LYS
1	F	882	VAL
1	F	912	ILE
1	F	951	LYS
1	F	977	LYS
1	F	980	THR
1	F	988	LYS

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Mol	Chain	Res	Type
1	F	990	THR
1	F	1001	LYS
1	F	1021	GLU
1	F	1025	ARG
1	F	1038	VAL
1	F	1044	SER
1	F	1052	ASN
1	F	1074	VAL
1	G	253	SER
1	G	258	ASN
1	G	259	PHE
1	G	275	LYS
1	G	283	THR
1	G	286	GLN
1	G	288	THR
1	G	295	LEU
1	G	303	GLN
1	G	304	GLU
1	G	305	THR
1	G	308	GLN
1	G	316	GLN
1	G	319	ILE
1	G	320	HIS
1	G	322	THR
1	G	347	ILE
1	G	355	TRP
1	G	356	LEU
1	G	359	THR
1	G	366	THR
1	G	368	SER
1	G	374	SER
1	G	396	THR
1	G	422	THR
1	G	465	ASN
1	G	477	ASP
1	G	532	MET
1	G	574	GLU
1	G	600	LYS
1	G	604	ASN
1	G	670	MET
1	G	707	ILE
1	G	727	ILE

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Mol	Chain	Res	Type
1	G	736	ILE
1	G	740	ASN
1	G	794	ARG
1	G	798	ILE
1	G	800	THR
1	G	803	ASP
1	G	832	VAL
1	G	835	SER
1	G	856	MET
1	G	882	VAL
1	G	912	ILE
1	G	928	LYS
1	G	977	LYS
1	G	985	SER
1	G	990	THR
1	G	1001	LYS
1	G	1021	GLU
1	G	1038	VAL
1	G	1052	ASN
1	G	1074	VAL
1	G	1084	LEU
1	H	247	GLN
1	H	253	SER
1	H	258	ASN
1	H	267	THR
1	H	278	LEU
1	H	279	LYS
1	H	282	LYS
1	H	290	LYS
1	H	296	LEU
1	H	300	TRP
1	H	304	GLU
1	H	308	GLN
1	H	310	VAL
1	H	314	ASN
1	H	356	LEU
1	H	359	THR
1	H	360	ILE
1	H	361	SER
1	H	365	LYS
1	H	368	SER
1	H	374	SER

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Mol	Chain	Res	Type
1	H	396	THR
1	H	422	THR
1	H	465	ASN
1	H	477	ASP
1	H	505	LYS
1	H	532	MET
1	H	574	GLU
1	H	604	ASN
1	H	619	LYS
1	H	631	THR
1	H	632	GLU
1	H	728	THR
1	H	740	ASN
1	H	750	ARG
1	H	832	VAL
1	H	856	MET
1	H	882	VAL
1	H	912	ILE
1	H	928	LYS
1	H	961	MET
1	H	977	LYS
1	H	985	SER
1	H	986	GLN
1	H	988	LYS
1	H	1001	LYS
1	H	1016	GLN
1	H	1038	VAL
1	H	1052	ASN
1	H	1074	VAL
1	H	1078	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (218) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	HIS
1	A	303	GLN
1	A	311	ASN
1	A	316	GLN
1	A	407	ASN
1	A	412	ASN
1	A	440	ASN
1	A	458	ASN

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Mol	Chain	Res	Type
1	A	461	ASN
1	A	470	ASN
1	A	481	ASN
1	A	531	ASN
1	A	558	ASN
1	A	572	ASN
1	A	604	ASN
1	A	639	ASN
1	A	699	ASN
1	A	740	ASN
1	A	759	HIS
1	A	761	ASN
1	A	773	ASN
1	A	782	GLN
1	A	846	HIS
1	A	864	GLN
1	A	913	GLN
1	A	1003	GLN
1	A	1016	GLN
1	A	1052	ASN
1	A	1068	ASN
1	B	250	GLN
1	B	258	ASN
1	B	261	HIS
1	B	371	ASN
1	B	392	ASN
1	B	407	ASN
1	B	412	ASN
1	B	413	GLN
1	B	440	ASN
1	B	458	ASN
1	B	470	ASN
1	B	481	ASN
1	B	531	ASN
1	B	639	ASN
1	B	699	ASN
1	B	740	ASN
1	B	759	HIS
1	B	761	ASN
1	B	782	GLN
1	B	846	HIS
1	B	864	GLN

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Mol	Chain	Res	Type
1	B	1016	GLN
1	B	1052	ASN
1	C	247	GLN
1	C	261	HIS
1	C	306	GLN
1	C	308	GLN
1	C	311	ASN
1	C	333	ASN
1	C	367	GLN
1	C	407	ASN
1	C	412	ASN
1	C	436	ASN
1	C	440	ASN
1	C	458	ASN
1	C	470	ASN
1	C	481	ASN
1	C	558	ASN
1	C	572	ASN
1	C	639	ASN
1	C	676	ASN
1	C	699	ASN
1	C	701	GLN
1	C	740	ASN
1	C	759	HIS
1	C	782	GLN
1	C	811	GLN
1	C	846	HIS
1	C	864	GLN
1	C	1016	GLN
1	C	1052	ASN
1	C	1068	ASN
1	D	250	GLN
1	D	258	ASN
1	D	261	HIS
1	D	303	GLN
1	D	308	GLN
1	D	311	ASN
1	D	367	GLN
1	D	407	ASN
1	D	412	ASN
1	D	440	ASN
1	D	458	ASN

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Mol	Chain	Res	Type
1	D	470	ASN
1	D	531	ASN
1	D	558	ASN
1	D	639	ASN
1	D	699	ASN
1	D	700	GLN
1	D	740	ASN
1	D	759	HIS
1	D	761	ASN
1	D	782	GLN
1	D	846	HIS
1	D	864	GLN
1	D	1003	GLN
1	D	1016	GLN
1	D	1052	ASN
1	D	1068	ASN
1	E	247	GLN
1	E	258	ASN
1	E	261	HIS
1	E	306	GLN
1	E	308	GLN
1	E	311	ASN
1	E	333	ASN
1	E	354	ASN
1	E	367	GLN
1	E	392	ASN
1	E	407	ASN
1	E	440	ASN
1	E	458	ASN
1	E	465	ASN
1	E	470	ASN
1	E	481	ASN
1	E	531	ASN
1	E	558	ASN
1	E	639	ASN
1	E	699	ASN
1	E	740	ASN
1	E	759	HIS
1	E	782	GLN
1	E	811	GLN
1	E	846	HIS
1	E	864	GLN

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Mol	Chain	Res	Type
1	E	1052	ASN
1	F	258	ASN
1	F	261	HIS
1	F	308	GLN
1	F	311	ASN
1	F	316	GLN
1	F	333	ASN
1	F	354	ASN
1	F	367	GLN
1	F	407	ASN
1	F	412	ASN
1	F	440	ASN
1	F	470	ASN
1	F	481	ASN
1	F	531	ASN
1	F	558	ASN
1	F	572	ASN
1	F	639	ASN
1	F	699	ASN
1	F	740	ASN
1	F	759	HIS
1	F	782	GLN
1	F	846	HIS
1	F	864	GLN
1	F	881	ASN
1	F	913	GLN
1	F	1003	GLN
1	F	1016	GLN
1	F	1052	ASN
1	F	1068	ASN
1	G	249	ASN
1	G	250	GLN
1	G	258	ASN
1	G	261	HIS
1	G	308	GLN
1	G	311	ASN
1	G	316	GLN
1	G	340	GLN
1	G	367	GLN
1	G	407	ASN
1	G	412	ASN
1	G	440	ASN

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Mol	Chain	Res	Type
1	G	470	ASN
1	G	481	ASN
1	G	510	HIS
1	G	531	ASN
1	G	558	ASN
1	G	572	ASN
1	G	604	ASN
1	G	639	ASN
1	G	699	ASN
1	G	740	ASN
1	G	759	HIS
1	G	782	GLN
1	G	846	HIS
1	G	864	GLN
1	G	881	ASN
1	G	1052	ASN
1	G	1068	ASN
1	H	258	ASN
1	H	261	HIS
1	H	303	GLN
1	H	308	GLN
1	H	311	ASN
1	H	367	GLN
1	H	407	ASN
1	H	412	ASN
1	H	440	ASN
1	H	458	ASN
1	H	470	ASN
1	H	481	ASN
1	H	531	ASN
1	H	558	ASN
1	H	639	ASN
1	H	699	ASN
1	H	740	ASN
1	H	759	HIS
1	H	782	GLN
1	H	846	HIS
1	H	864	GLN
1	H	875	ASN
1	H	881	ASN
1	H	898	GLN
1	H	1052	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

24 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	GLC	I	1	2	12,12,12	0.68	0	17,17,17	2.03	6 (35%)
2	GLC	I	2	2	11,11,12	1.15	0	15,15,17	2.59	5 (33%)
2	AC1	I	3	2	21,22,23	1.46	4 (19%)	22,32,34	2.15	4 (18%)
2	GLC	J	1	2	12,12,12	0.77	0	17,17,17	1.91	5 (29%)
2	GLC	J	2	2	11,11,12	1.11	1 (9%)	15,15,17	2.16	4 (26%)
2	AC1	J	3	2	21,22,23	1.33	2 (9%)	22,32,34	1.52	3 (13%)
2	GLC	K	1	2	12,12,12	0.77	0	17,17,17	1.91	5 (29%)
2	GLC	K	2	2	11,11,12	1.10	1 (9%)	15,15,17	2.16	4 (26%)
2	AC1	K	3	2	21,22,23	1.32	2 (9%)	22,32,34	1.52	3 (13%)
2	GLC	L	1	2	12,12,12	0.78	0	17,17,17	1.92	5 (29%)
2	GLC	L	2	2	11,11,12	1.11	1 (9%)	15,15,17	2.16	4 (26%)
2	AC1	L	3	2	21,22,23	1.33	2 (9%)	22,32,34	1.51	3 (13%)
2	GLC	M	1	2	12,12,12	0.78	0	17,17,17	1.91	5 (29%)
2	GLC	M	2	2	11,11,12	1.12	1 (9%)	15,15,17	2.16	4 (26%)
2	AC1	M	3	2	21,22,23	1.34	2 (9%)	22,32,34	1.52	3 (13%)
2	GLC	N	1	2	12,12,12	0.77	0	17,17,17	1.92	5 (29%)
2	GLC	N	2	2	11,11,12	1.11	1 (9%)	15,15,17	2.16	4 (26%)
2	AC1	N	3	2	21,22,23	1.32	2 (9%)	22,32,34	1.52	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	O	1	2	12,12,12	0.77	0	17,17,17	1.91	5 (29%)
2	GLC	O	2	2	11,11,12	1.10	1 (9%)	15,15,17	2.17	4 (26%)
2	AC1	O	3	2	21,22,23	1.33	2 (9%)	22,32,34	1.52	3 (13%)
2	GLC	P	1	2	12,12,12	0.78	0	17,17,17	1.91	5 (29%)
2	GLC	P	2	2	11,11,12	1.11	1 (9%)	15,15,17	2.16	4 (26%)
2	AC1	P	3	2	21,22,23	1.33	2 (9%)	22,32,34	1.52	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	I	1	2	-	2/2/22/22	0/1/1/1
2	GLC	I	2	2	-	2/2/19/22	0/1/1/1
2	AC1	I	3	2	-	3/6/43/46	0/2/2/2
2	GLC	J	1	2	-	2/2/22/22	0/1/1/1
2	GLC	J	2	2	-	2/2/19/22	0/1/1/1
2	AC1	J	3	2	-	3/6/43/46	0/2/2/2
2	GLC	K	1	2	-	2/2/22/22	0/1/1/1
2	GLC	K	2	2	-	2/2/19/22	0/1/1/1
2	AC1	K	3	2	-	3/6/43/46	0/2/2/2
2	GLC	L	1	2	-	2/2/22/22	0/1/1/1
2	GLC	L	2	2	-	2/2/19/22	0/1/1/1
2	AC1	L	3	2	-	3/6/43/46	0/2/2/2
2	GLC	M	1	2	-	2/2/22/22	0/1/1/1
2	GLC	M	2	2	-	2/2/19/22	0/1/1/1
2	AC1	M	3	2	-	3/6/43/46	0/2/2/2
2	GLC	N	1	2	-	2/2/22/22	0/1/1/1
2	GLC	N	2	2	-	2/2/19/22	0/1/1/1
2	AC1	N	3	2	-	3/6/43/46	0/2/2/2
2	GLC	O	1	2	-	2/2/22/22	0/1/1/1
2	GLC	O	2	2	-	2/2/19/22	0/1/1/1
2	AC1	O	3	2	-	3/6/43/46	0/2/2/2
2	GLC	P	1	2	-	2/2/22/22	0/1/1/1
2	GLC	P	2	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AC1	P	3	2	-	3/6/43/46	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	3	AC1	C4A-C5B	-3.27	1.48	1.51
2	L	3	AC1	C4A-C5B	-2.83	1.49	1.51
2	J	3	AC1	C4A-C5B	-2.81	1.49	1.51
2	M	3	AC1	C4A-C5B	-2.80	1.49	1.51
2	P	3	AC1	C4A-C5B	-2.80	1.49	1.51
2	O	3	AC1	C4A-C5B	-2.72	1.49	1.51
2	I	3	AC1	C2B-C1B	-2.71	1.49	1.53
2	N	3	AC1	C4A-C5B	-2.71	1.49	1.51
2	K	3	AC1	C4A-C5B	-2.67	1.49	1.51
2	N	3	AC1	C3-C4	-2.60	1.48	1.53
2	M	3	AC1	C3-C4	-2.59	1.48	1.53
2	O	3	AC1	C3-C4	-2.59	1.48	1.53
2	P	3	AC1	C3-C4	-2.59	1.48	1.53
2	L	3	AC1	C3-C4	-2.59	1.48	1.53
2	J	3	AC1	C3-C4	-2.59	1.48	1.53
2	K	3	AC1	C3-C4	-2.58	1.48	1.53
2	N	2	GLC	O5-C1	-2.31	1.39	1.43
2	J	2	GLC	O5-C1	-2.30	1.39	1.43
2	M	2	GLC	O5-C1	-2.29	1.39	1.43
2	I	3	AC1	O5-C1	-2.27	1.39	1.43
2	P	2	GLC	O5-C1	-2.26	1.39	1.43
2	L	2	GLC	O5-C1	-2.26	1.39	1.43
2	K	2	GLC	O5-C1	-2.25	1.39	1.43
2	O	2	GLC	O5-C1	-2.24	1.39	1.43
2	I	3	AC1	C3-C4	-2.11	1.49	1.53

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	3	AC1	C1-C2-C3	6.91	119.71	109.64
2	I	2	GLC	C1-O5-C5	6.08	120.34	112.19
2	I	2	GLC	O2-C2-C1	-5.12	97.49	109.22
2	I	1	GLC	C3-C4-C5	-4.62	101.85	110.23
2	J	2	GLC	C6-C5-C4	-4.32	102.42	113.02
2	K	2	GLC	C6-C5-C4	-4.31	102.43	113.02
2	O	2	GLC	C6-C5-C4	-4.31	102.44	113.02
2	L	2	GLC	C6-C5-C4	-4.31	102.44	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	2	GLC	C6-C5-C4	-4.30	102.46	113.02
2	M	2	GLC	C6-C5-C4	-4.30	102.47	113.02
2	P	2	GLC	C6-C5-C4	-4.30	102.47	113.02
2	N	1	GLC	C3-C4-C5	-4.27	102.49	110.23
2	L	1	GLC	C3-C4-C5	-4.26	102.50	110.23
2	O	1	GLC	C3-C4-C5	-4.26	102.51	110.23
2	J	1	GLC	C3-C4-C5	-4.24	102.54	110.23
2	P	1	GLC	C3-C4-C5	-4.24	102.54	110.23
2	M	1	GLC	C3-C4-C5	-4.24	102.55	110.23
2	K	1	GLC	C3-C4-C5	-4.23	102.56	110.23
2	K	2	GLC	O2-C2-C1	-3.99	100.10	109.22
2	N	2	GLC	O2-C2-C1	-3.98	100.12	109.22
2	O	2	GLC	O2-C2-C1	-3.97	100.12	109.22
2	J	2	GLC	O2-C2-C1	-3.97	100.13	109.22
2	P	2	GLC	O2-C2-C1	-3.97	100.14	109.22
2	L	2	GLC	O2-C2-C1	-3.96	100.16	109.22
2	M	2	GLC	O2-C2-C1	-3.95	100.18	109.22
2	O	3	AC1	O3-C3-C2	3.81	117.84	110.05
2	M	3	AC1	O3-C3-C2	3.81	117.82	110.05
2	J	3	AC1	O3-C3-C2	3.80	117.82	110.05
2	N	3	AC1	O3-C3-C2	3.80	117.82	110.05
2	L	3	AC1	O3-C3-C2	3.80	117.81	110.05
2	K	3	AC1	O3-C3-C2	3.79	117.79	110.05
2	P	3	AC1	O3-C3-C2	3.78	117.77	110.05
2	I	2	GLC	O3-C3-C4	-3.69	101.67	110.38
2	I	2	GLC	C6-C5-C4	-3.57	104.24	113.02
2	M	1	GLC	C4-C3-C2	-3.43	104.81	110.83
2	L	1	GLC	C4-C3-C2	-3.42	104.83	110.83
2	K	1	GLC	C4-C3-C2	-3.41	104.84	110.83
2	J	1	GLC	C4-C3-C2	-3.40	104.85	110.83
2	N	1	GLC	C4-C3-C2	-3.40	104.86	110.83
2	P	1	GLC	C4-C3-C2	-3.39	104.87	110.83
2	O	1	GLC	C4-C3-C2	-3.39	104.88	110.83
2	I	3	AC1	O3-C3-C4	-3.38	102.86	109.58
2	O	2	GLC	C1-C2-C3	3.35	114.53	109.64
2	P	2	GLC	C1-C2-C3	3.34	114.51	109.64
2	M	2	GLC	C1-C2-C3	3.34	114.51	109.64
2	K	2	GLC	C1-C2-C3	3.33	114.50	109.64
2	J	2	GLC	C1-C2-C3	3.33	114.50	109.64
2	O	2	GLC	O3-C3-C4	-3.33	102.53	110.38
2	N	2	GLC	C1-C2-C3	3.32	114.48	109.64
2	P	2	GLC	O3-C3-C4	-3.32	102.55	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	2	GLC	O3-C3-C4	-3.32	102.55	110.38
2	J	2	GLC	O3-C3-C4	-3.32	102.56	110.38
2	K	2	GLC	O3-C3-C4	-3.31	102.56	110.38
2	L	2	GLC	O3-C3-C4	-3.31	102.58	110.38
2	M	2	GLC	O3-C3-C4	-3.31	102.58	110.38
2	L	2	GLC	C1-C2-C3	3.30	114.46	109.64
2	I	1	GLC	C1-C2-C3	3.18	116.84	110.36
2	I	1	GLC	O5-C5-C4	-3.11	104.09	109.70
2	M	1	GLC	O2-C2-C1	-2.89	102.56	109.25
2	N	1	GLC	O2-C2-C1	-2.89	102.57	109.25
2	P	1	GLC	O2-C2-C1	-2.88	102.59	109.25
2	O	1	GLC	O2-C2-C1	-2.88	102.60	109.25
2	J	1	GLC	O2-C2-C1	-2.88	102.60	109.25
2	K	1	GLC	O2-C2-C1	-2.88	102.60	109.25
2	L	1	GLC	O2-C2-C1	-2.88	102.61	109.25
2	I	2	GLC	O5-C5-C6	-2.83	102.16	107.66
2	I	1	GLC	O5-C1-C2	2.82	115.25	110.30
2	M	3	AC1	C3B-C4A-C5B	-2.72	107.39	111.67
2	K	3	AC1	C3B-C4A-C5B	-2.72	107.39	111.67
2	P	3	AC1	C3B-C4A-C5B	-2.72	107.40	111.67
2	J	3	AC1	C3B-C4A-C5B	-2.71	107.40	111.67
2	N	3	AC1	C3B-C4A-C5B	-2.71	107.41	111.67
2	I	3	AC1	C6-C5-C4	-2.70	108.61	113.57
2	O	3	AC1	C3B-C4A-C5B	-2.69	107.44	111.67
2	L	3	AC1	C3B-C4A-C5B	-2.68	107.45	111.67
2	I	3	AC1	C3B-C4A-C5B	-2.60	107.59	111.67
2	K	3	AC1	O4-C4A-C3B	-2.43	105.48	110.53
2	J	3	AC1	O4-C4A-C3B	-2.42	105.50	110.53
2	N	3	AC1	O4-C4A-C3B	-2.42	105.50	110.53
2	P	3	AC1	O4-C4A-C3B	-2.42	105.51	110.53
2	L	3	AC1	O4-C4A-C3B	-2.41	105.51	110.53
2	O	3	AC1	O4-C4A-C3B	-2.41	105.52	110.53
2	M	3	AC1	O4-C4A-C3B	-2.40	105.53	110.53
2	P	1	GLC	O1-C1-O5	-2.34	103.47	110.41
2	K	1	GLC	O1-C1-O5	-2.33	103.48	110.41
2	J	1	GLC	O1-C1-O5	-2.33	103.48	110.41
2	L	1	GLC	O1-C1-O5	-2.33	103.48	110.41
2	O	1	GLC	O1-C1-O5	-2.33	103.50	110.41
2	M	1	GLC	O1-C1-O5	-2.32	103.51	110.41
2	N	1	GLC	O1-C1-O5	-2.31	103.55	110.41
2	I	1	GLC	O2-C2-C1	-2.20	104.17	109.25
2	J	1	GLC	O4-C4-C5	-2.14	104.06	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	GLC	O4-C4-C5	-2.13	104.08	109.32
2	N	1	GLC	O4-C4-C5	-2.13	104.08	109.32
2	M	1	GLC	O4-C4-C5	-2.13	104.08	109.32
2	O	1	GLC	O4-C4-C5	-2.13	104.09	109.32
2	I	1	GLC	C4-C3-C2	-2.12	107.11	110.83
2	L	1	GLC	O4-C4-C5	-2.12	104.11	109.32
2	P	1	GLC	O4-C4-C5	-2.11	104.12	109.32

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	3	AC1	C7B-C1B-N4A-C4
2	I	3	AC1	C4A-C5B-C6B-O6B
2	I	3	AC1	C7B-C5B-C6B-O6B
2	J	3	AC1	C7B-C1B-N4A-C4
2	J	3	AC1	C4A-C5B-C6B-O6B
2	J	3	AC1	C7B-C5B-C6B-O6B
2	K	3	AC1	C7B-C1B-N4A-C4
2	K	3	AC1	C4A-C5B-C6B-O6B
2	K	3	AC1	C7B-C5B-C6B-O6B
2	L	3	AC1	C7B-C1B-N4A-C4
2	L	3	AC1	C4A-C5B-C6B-O6B
2	L	3	AC1	C7B-C5B-C6B-O6B
2	M	3	AC1	C7B-C1B-N4A-C4
2	M	3	AC1	C4A-C5B-C6B-O6B
2	M	3	AC1	C7B-C5B-C6B-O6B
2	N	3	AC1	C7B-C1B-N4A-C4
2	N	3	AC1	C4A-C5B-C6B-O6B
2	N	3	AC1	C7B-C5B-C6B-O6B
2	O	3	AC1	C7B-C1B-N4A-C4
2	O	3	AC1	C4A-C5B-C6B-O6B
2	O	3	AC1	C7B-C5B-C6B-O6B
2	P	3	AC1	C7B-C1B-N4A-C4
2	P	3	AC1	C4A-C5B-C6B-O6B
2	P	3	AC1	C7B-C5B-C6B-O6B
2	J	1	GLC	O5-C5-C6-O6
2	K	1	GLC	O5-C5-C6-O6
2	L	1	GLC	O5-C5-C6-O6
2	M	1	GLC	O5-C5-C6-O6
2	N	1	GLC	O5-C5-C6-O6
2	O	1	GLC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	P	1	GLC	O5-C5-C6-O6
2	I	2	GLC	O5-C5-C6-O6
2	J	2	GLC	O5-C5-C6-O6
2	K	2	GLC	O5-C5-C6-O6
2	L	2	GLC	O5-C5-C6-O6
2	M	2	GLC	O5-C5-C6-O6
2	N	2	GLC	O5-C5-C6-O6
2	O	2	GLC	O5-C5-C6-O6
2	P	2	GLC	O5-C5-C6-O6
2	I	1	GLC	O5-C5-C6-O6
2	J	1	GLC	C4-C5-C6-O6
2	K	1	GLC	C4-C5-C6-O6
2	L	1	GLC	C4-C5-C6-O6
2	M	1	GLC	C4-C5-C6-O6
2	N	1	GLC	C4-C5-C6-O6
2	O	1	GLC	C4-C5-C6-O6
2	P	1	GLC	C4-C5-C6-O6
2	I	1	GLC	C4-C5-C6-O6
2	I	2	GLC	C4-C5-C6-O6
2	J	2	GLC	C4-C5-C6-O6
2	K	2	GLC	C4-C5-C6-O6
2	L	2	GLC	C4-C5-C6-O6
2	M	2	GLC	C4-C5-C6-O6
2	N	2	GLC	C4-C5-C6-O6
2	O	2	GLC	C4-C5-C6-O6
2	P	2	GLC	C4-C5-C6-O6

There are no ring outliers.

16 monomers are involved in 62 short contacts:

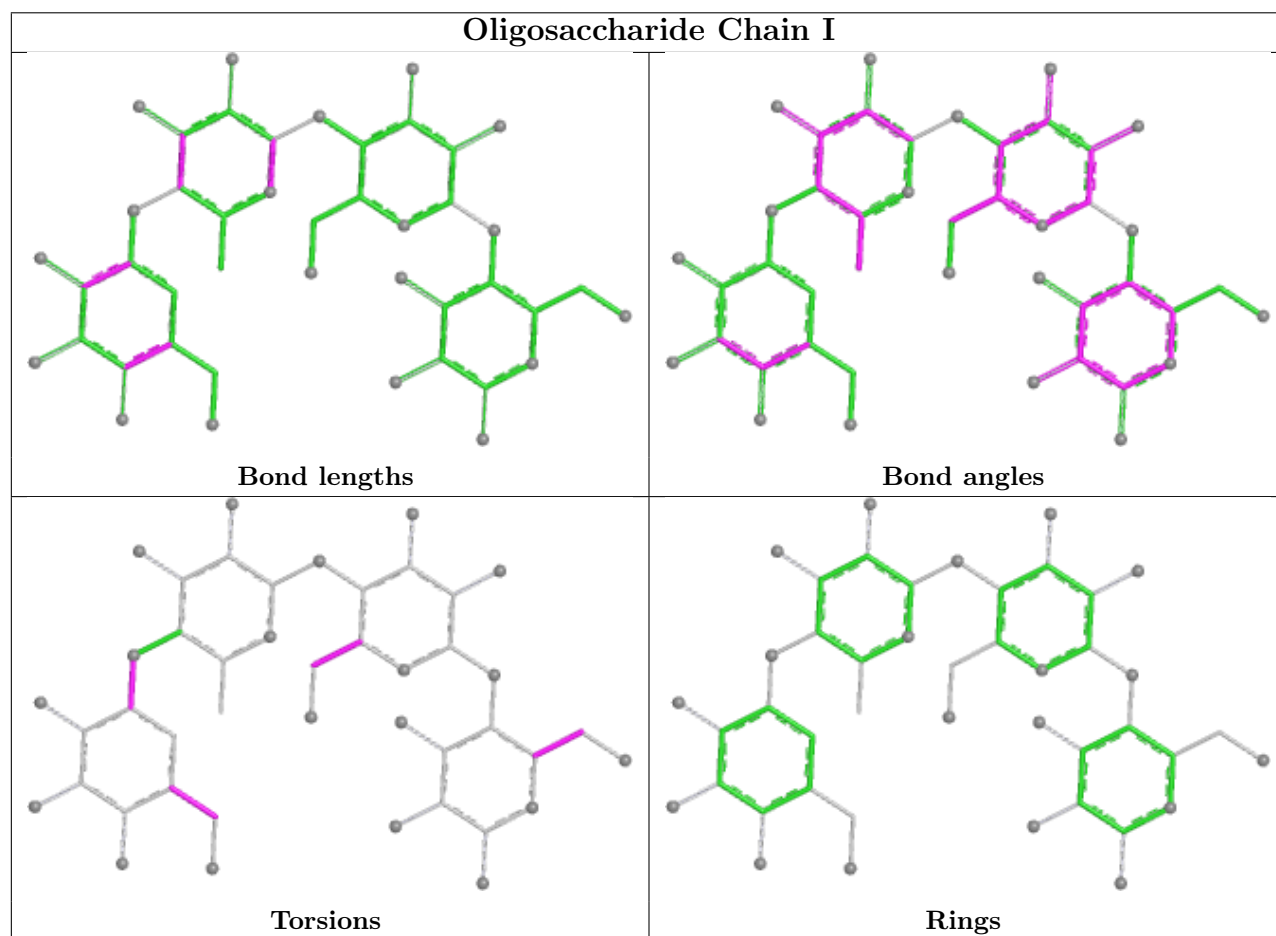
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	3	AC1	10	0
2	K	3	AC1	9	0
2	I	3	AC1	10	0
2	K	2	GLC	4	0
2	P	2	GLC	3	0
2	O	3	AC1	7	0
2	J	3	AC1	8	0
2	L	2	GLC	4	0
2	N	3	AC1	6	0
2	I	2	GLC	4	0
2	J	2	GLC	4	0

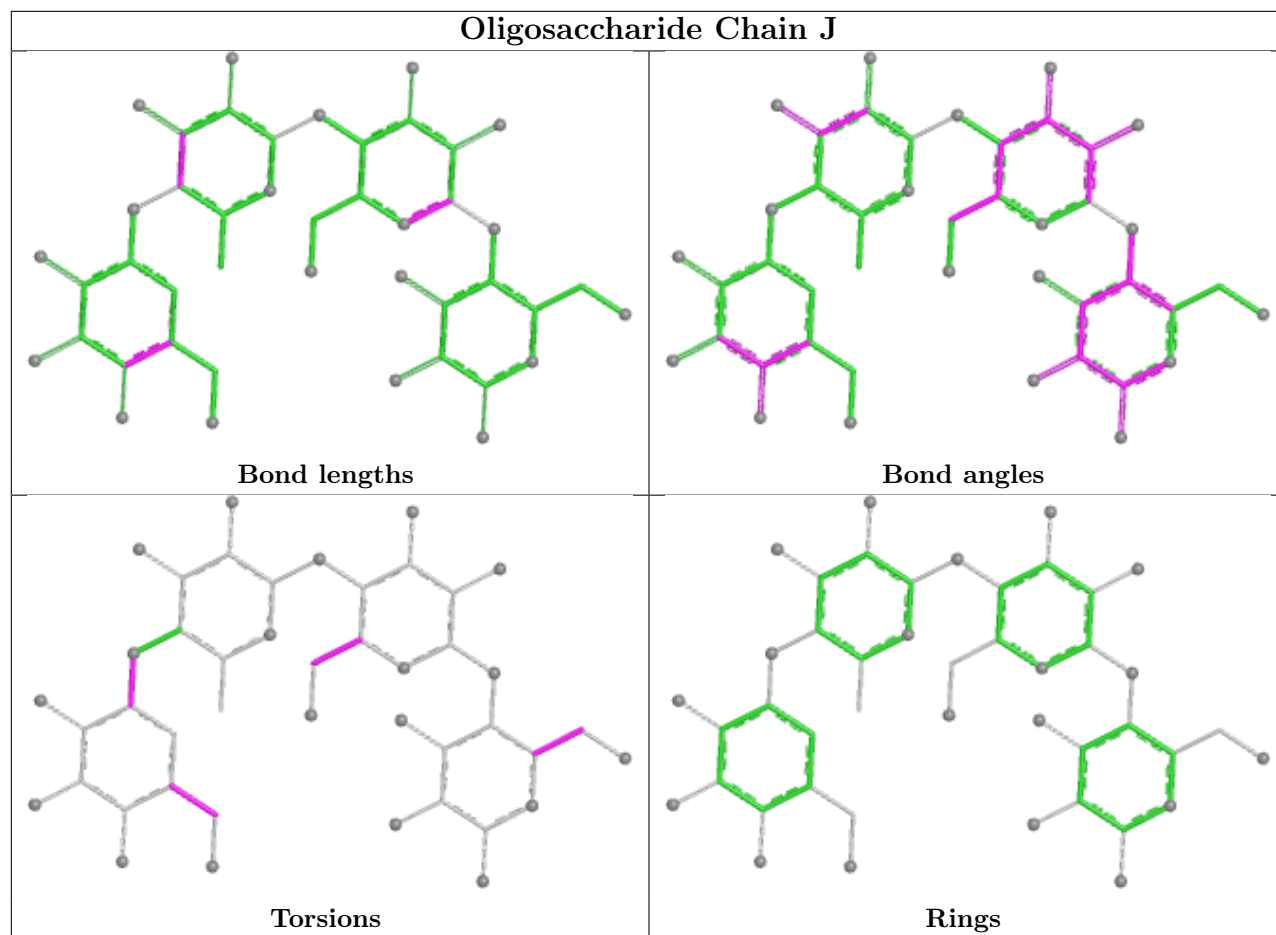
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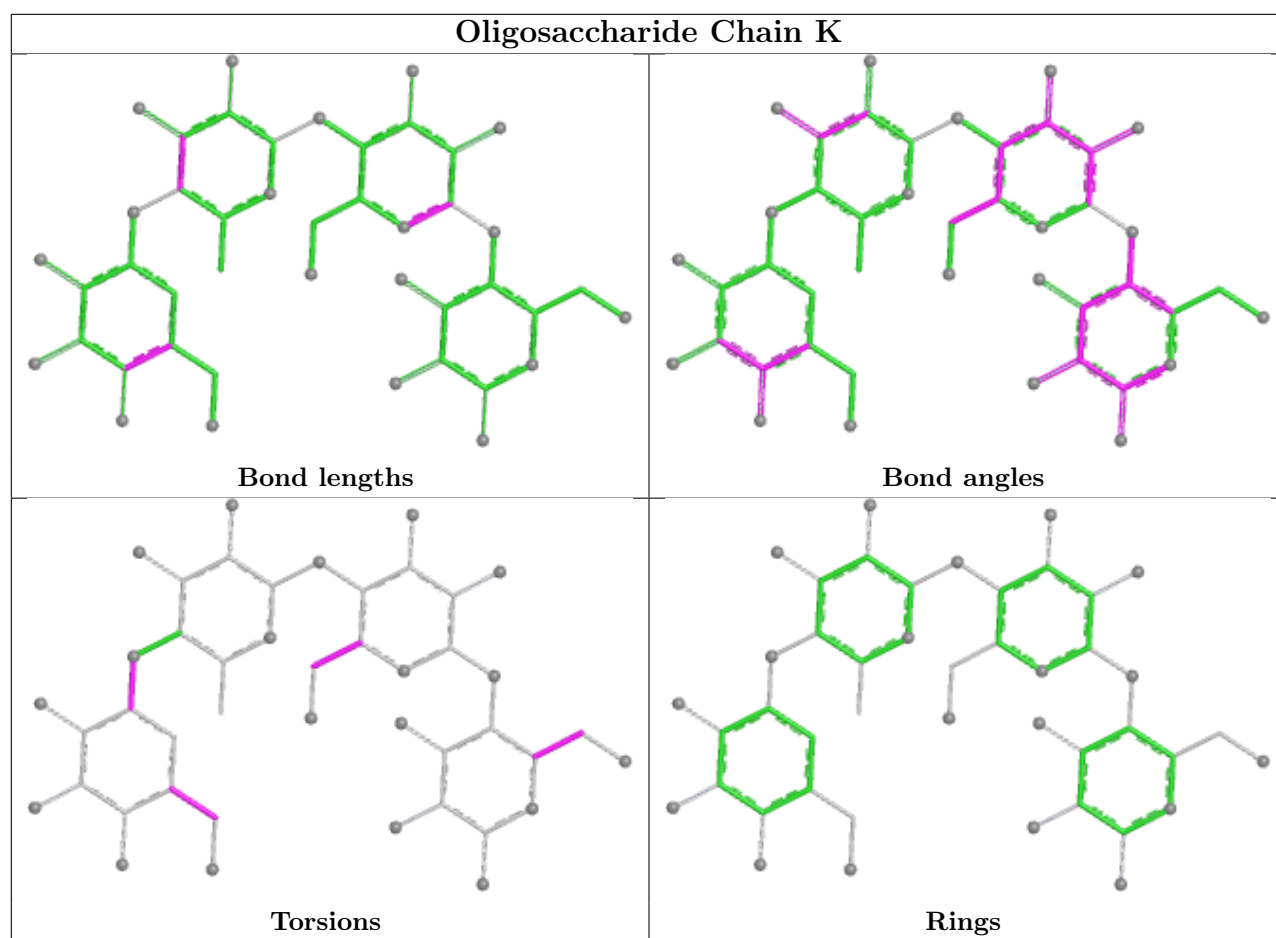
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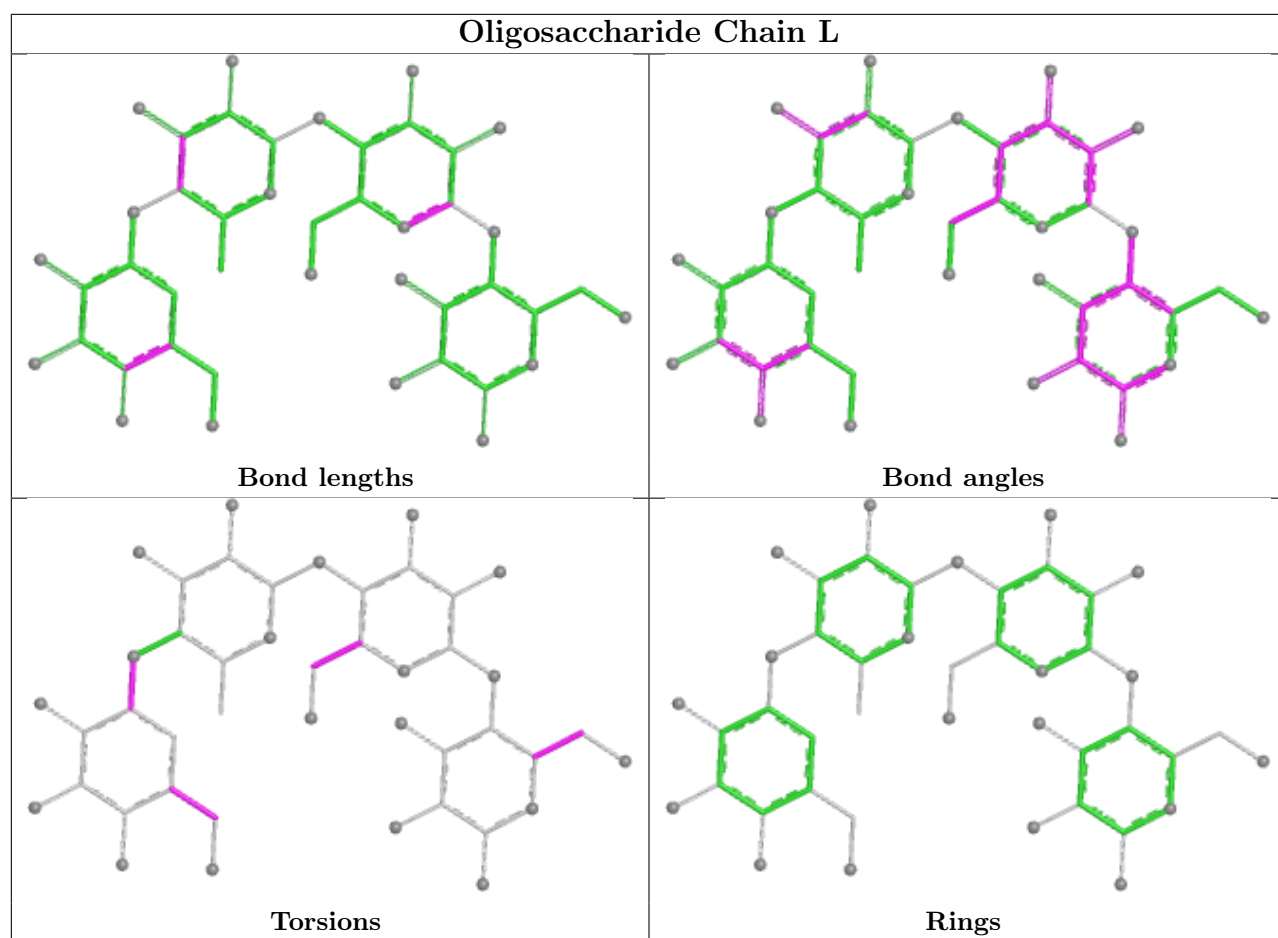
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	3	AC1	6	0
2	N	2	GLC	4	0
2	P	3	AC1	6	0
2	O	2	GLC	4	0
2	M	2	GLC	4	0

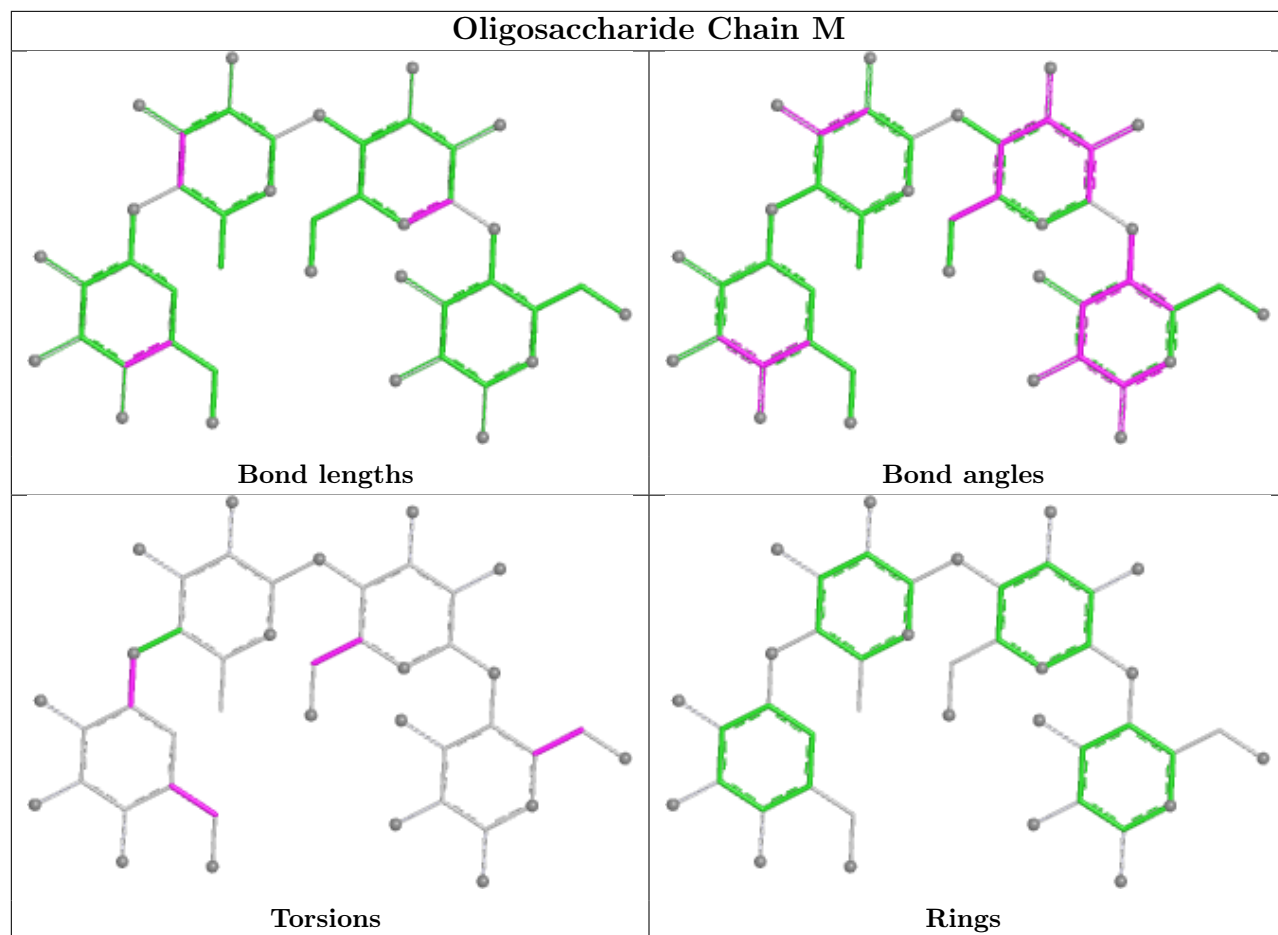
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

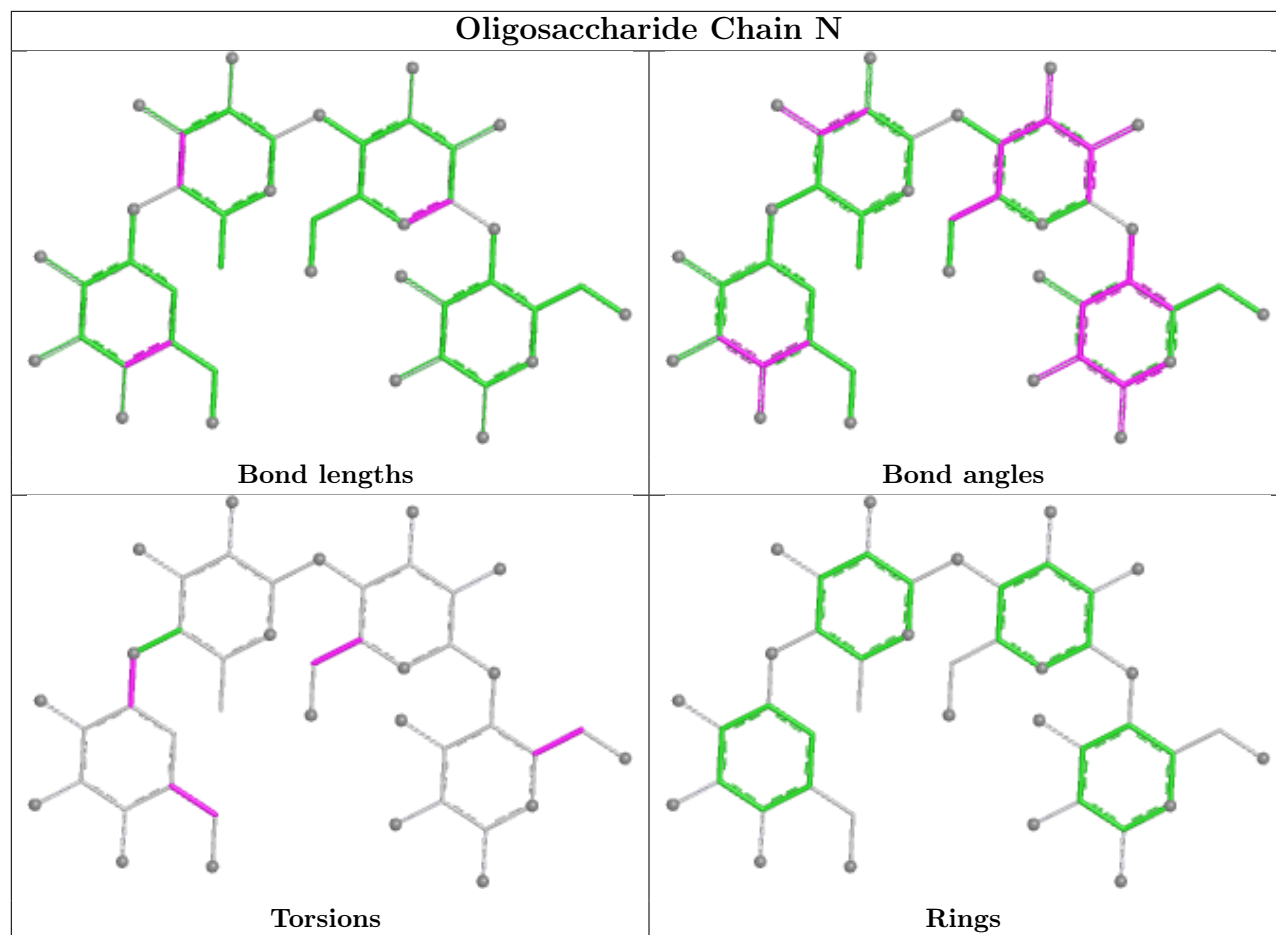


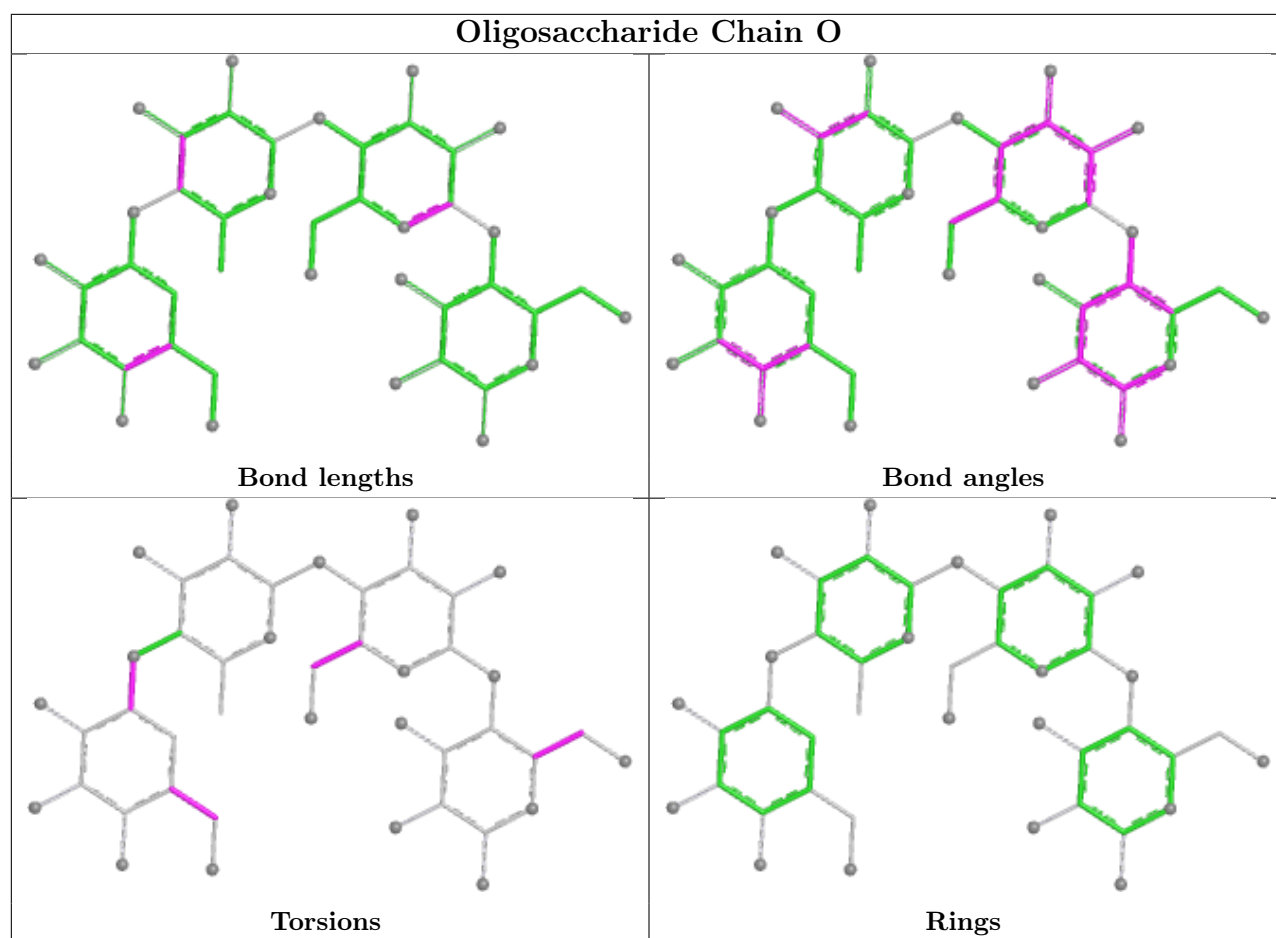


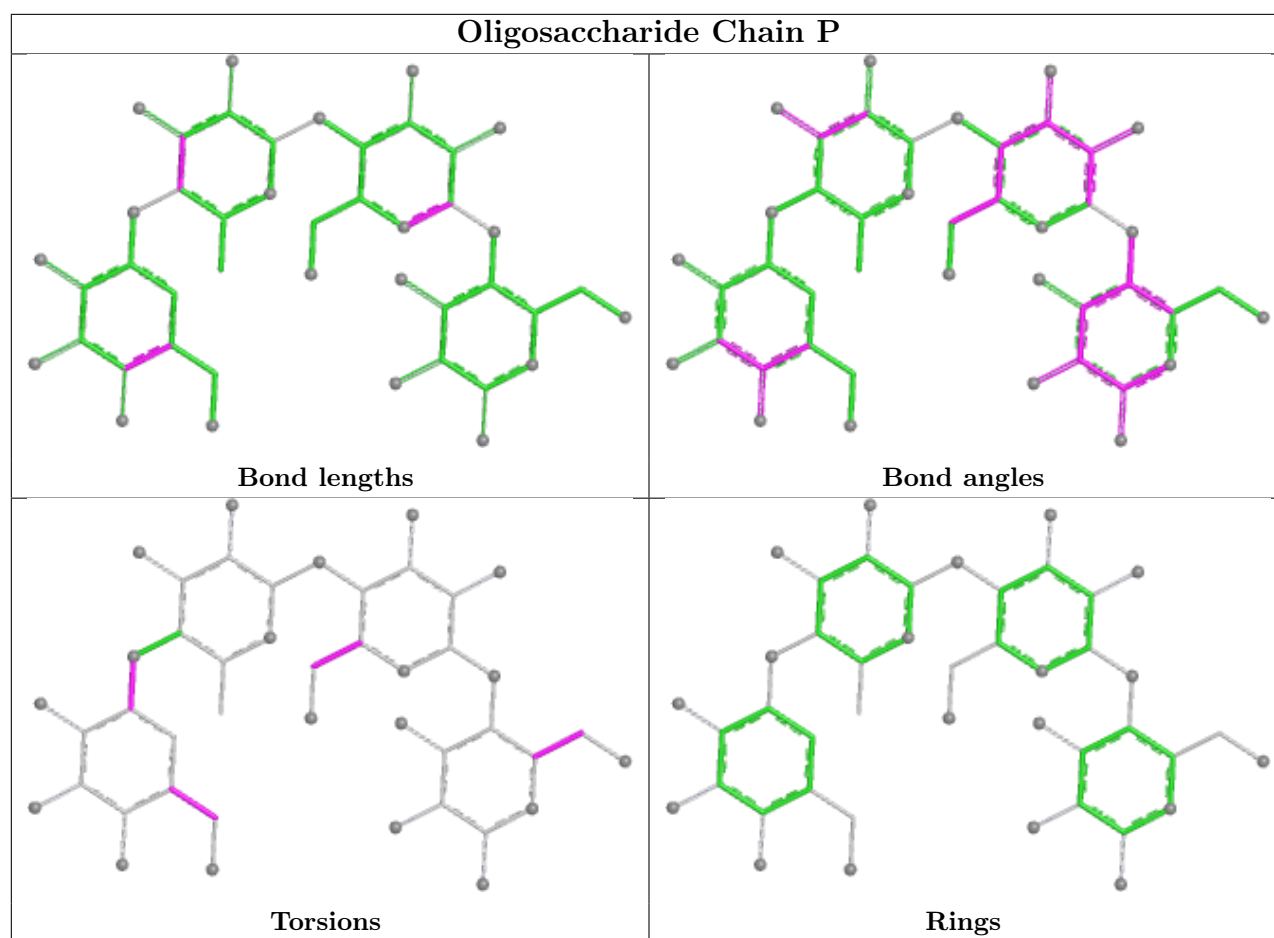












5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MES	G	5001	-	12,12,12	1.49	2 (16%)	15,16,16	5.94	11 (73%)
4	MES	C	5001	-	12,12,12	1.52	3 (25%)	15,16,16	5.54	9 (60%)
4	MES	D	5001	-	12,12,12	1.45	2 (16%)	15,16,16	5.29	9 (60%)
4	MES	F	5001	-	12,12,12	1.90	3 (25%)	15,16,16	6.27	12 (80%)
4	MES	A	5001	-	12,12,12	1.55	3 (25%)	15,16,16	6.65	10 (66%)
4	MES	E	5001	-	12,12,12	1.42	4 (33%)	15,16,16	6.07	11 (73%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MES	H	5001	-	12,12,12	1.09	1 (8%)	15,16,16	5.93	11 (73%)
4	MES	B	5001	-	12,12,12	1.73	4 (33%)	15,16,16	6.46	12 (80%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	G	5001	-	-	5/6/14/14	0/1/1/1
4	MES	C	5001	-	-	4/6/14/14	0/1/1/1
4	MES	D	5001	-	-	5/6/14/14	0/1/1/1
4	MES	F	5001	-	-	4/6/14/14	0/1/1/1
4	MES	A	5001	-	-	2/6/14/14	0/1/1/1
4	MES	E	5001	-	-	1/6/14/14	0/1/1/1
4	MES	H	5001	-	-	1/6/14/14	0/1/1/1
4	MES	B	5001	-	-	2/6/14/14	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	5001	MES	C8-S	-4.11	1.71	1.77
4	A	5001	MES	O2S-S	3.81	1.55	1.45
4	B	5001	MES	C8-S	-3.37	1.72	1.77
4	B	5001	MES	O2S-S	3.15	1.54	1.45
4	F	5001	MES	O1S-S	2.90	1.53	1.45
4	C	5001	MES	O2S-S	2.82	1.53	1.45
4	E	5001	MES	C8-S	-2.77	1.73	1.77
4	F	5001	MES	O2S-S	2.74	1.52	1.45
4	G	5001	MES	O1S-S	2.73	1.52	1.45
4	C	5001	MES	O3S-S	2.68	1.57	1.47
4	D	5001	MES	C7-C8	2.49	1.58	1.52
4	G	5001	MES	C8-S	-2.45	1.74	1.77
4	B	5001	MES	O1S-S	2.32	1.51	1.45
4	D	5001	MES	O1S-S	2.27	1.51	1.45
4	C	5001	MES	O1S-S	2.26	1.51	1.45
4	A	5001	MES	O1S-S	2.17	1.51	1.45
4	E	5001	MES	O3S-S	2.16	1.55	1.47
4	A	5001	MES	C7-C8	2.10	1.57	1.52
4	E	5001	MES	O2S-S	2.10	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5001	MES	O1S-S	2.07	1.50	1.45
4	H	5001	MES	C8-S	-2.06	1.74	1.77
4	B	5001	MES	O3S-S	2.02	1.54	1.47

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5001	MES	O2S-S-C8	-20.68	75.47	106.73
4	B	5001	MES	O1S-S-C8	-17.23	80.69	106.73
4	F	5001	MES	O2S-S-C8	-14.63	84.62	106.73
4	C	5001	MES	O1S-S-C8	-14.59	84.69	106.73
4	E	5001	MES	O2S-S-C8	-14.43	84.93	106.73
4	H	5001	MES	O1S-S-C8	-14.22	85.24	106.73
4	E	5001	MES	O1S-S-C8	-13.40	86.48	106.73
4	D	5001	MES	O3S-S-C8	-13.15	80.28	106.00
4	B	5001	MES	O2S-S-C8	-13.08	86.97	106.73
4	G	5001	MES	O1S-S-C8	-12.71	87.52	106.73
4	G	5001	MES	O3S-S-C8	-11.88	82.76	106.00
4	C	5001	MES	O2S-S-C8	-11.60	89.20	106.73
4	H	5001	MES	O2S-S-C8	-11.48	89.39	106.73
4	A	5001	MES	O1S-S-C8	-11.10	89.96	106.73
4	D	5001	MES	O1S-S-C8	-10.94	90.20	106.73
4	F	5001	MES	O1S-S-C8	-10.88	90.29	106.73
4	F	5001	MES	O3S-S-C8	-10.24	85.98	106.00
4	G	5001	MES	O2S-S-C8	-10.04	91.56	106.73
4	H	5001	MES	O3S-S-C8	-8.24	89.88	106.00
4	E	5001	MES	C5-N4-C3	6.79	123.47	108.84
4	E	5001	MES	O3S-S-C8	-6.79	92.73	106.00
4	B	5001	MES	O3S-S-C8	-6.69	92.91	106.00
4	C	5001	MES	C5-N4-C3	6.60	123.07	108.84
4	H	5001	MES	C6-C5-N4	-6.04	100.94	110.12
4	G	5001	MES	O3S-S-O1S	5.80	125.92	111.40
4	A	5001	MES	C5-N4-C3	5.76	121.24	108.84
4	F	5001	MES	C2-C3-N4	-5.72	101.43	110.12
4	D	5001	MES	O2S-S-C8	-5.67	98.15	106.73
4	G	5001	MES	C7-N4-C5	5.05	124.70	111.24
4	B	5001	MES	C5-N4-C3	5.05	119.72	108.84
4	F	5001	MES	C7-N4-C3	4.93	124.38	111.24
4	C	5001	MES	O3S-S-C8	-4.91	96.40	106.00
4	D	5001	MES	O3S-S-O1S	4.84	123.50	111.40
4	F	5001	MES	C6-C5-N4	-4.73	102.93	110.12
4	H	5001	MES	C5-N4-C3	4.61	118.77	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	5001	MES	C5-N4-C3	4.48	118.49	108.84
4	F	5001	MES	C8-C7-N4	-4.37	95.82	112.36
4	B	5001	MES	C2-C3-N4	-4.29	103.59	110.12
4	A	5001	MES	C6-C5-N4	-4.26	103.65	110.12
4	A	5001	MES	O3S-S-C8	-4.18	97.83	106.00
4	D	5001	MES	C5-N4-C3	4.07	117.61	108.84
4	E	5001	MES	O3S-S-O2S	4.02	121.46	111.40
4	F	5001	MES	O3S-S-O2S	3.97	121.33	111.40
4	G	5001	MES	C6-C5-N4	-3.86	104.26	110.12
4	H	5001	MES	C2-C3-N4	-3.85	104.26	110.12
4	B	5001	MES	C6-C5-N4	-3.81	104.33	110.12
4	E	5001	MES	C2-C3-N4	-3.80	104.34	110.12
4	D	5001	MES	C7-N4-C5	3.78	121.32	111.24
4	G	5001	MES	C7-N4-C3	3.76	121.27	111.24
4	D	5001	MES	C7-N4-C3	3.69	121.06	111.24
4	B	5001	MES	C7-N4-C5	3.60	120.83	111.24
4	H	5001	MES	C7-N4-C3	3.58	120.78	111.24
4	A	5001	MES	C7-N4-C5	3.47	120.49	111.24
4	C	5001	MES	O3S-S-O2S	3.46	120.05	111.40
4	H	5001	MES	C7-N4-C5	3.45	120.44	111.24
4	G	5001	MES	O3S-S-O2S	3.25	119.53	111.40
4	A	5001	MES	O2S-S-O1S	3.24	124.36	113.82
4	H	5001	MES	O3S-S-O2S	3.10	119.14	111.40
4	D	5001	MES	O3S-S-O2S	3.09	119.13	111.40
4	G	5001	MES	C2-C3-N4	-3.07	105.45	110.12
4	B	5001	MES	C7-N4-C3	3.07	119.41	111.24
4	B	5001	MES	O3S-S-O2S	3.06	119.06	111.40
4	G	5001	MES	C8-C7-N4	-3.06	100.79	112.36
4	E	5001	MES	C7-N4-C3	3.03	119.32	111.24
4	E	5001	MES	O2S-S-O1S	2.96	123.44	113.82
4	A	5001	MES	O3S-S-O1S	2.89	118.62	111.40
4	B	5001	MES	O3S-S-O1S	2.88	118.61	111.40
4	E	5001	MES	O1-C2-C3	-2.85	105.64	111.77
4	C	5001	MES	C7-N4-C5	2.83	118.77	111.24
4	D	5001	MES	C6-C5-N4	-2.77	105.90	110.12
4	C	5001	MES	O2S-S-O1S	2.77	122.84	113.82
4	H	5001	MES	O3S-S-O1S	2.77	118.32	111.40
4	F	5001	MES	O2S-S-O1S	2.67	122.51	113.82
4	E	5001	MES	C6-C5-N4	2.64	114.13	110.12
4	A	5001	MES	C7-N4-C3	2.62	118.23	111.24
4	C	5001	MES	C7-N4-C3	2.60	118.16	111.24
4	H	5001	MES	O2S-S-O1S	2.58	122.23	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5001	MES	C5-N4-C3	2.40	114.02	108.84
4	B	5001	MES	O2S-S-O1S	2.33	121.40	113.82
4	C	5001	MES	O3S-S-O1S	2.28	117.11	111.40
4	E	5001	MES	C7-N4-C5	2.23	117.19	111.24
4	F	5001	MES	C7-N4-C5	2.21	117.13	111.24
4	F	5001	MES	O1-C6-C5	-2.12	107.20	111.77
4	B	5001	MES	C8-C7-N4	-2.04	104.66	112.36
4	A	5001	MES	O3S-S-O2S	2.03	116.47	111.40

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5001	MES	C8-C7-N4-C5
4	A	5001	MES	N4-C7-C8-S
4	B	5001	MES	C8-C7-N4-C5
4	C	5001	MES	C8-C7-N4-C5
4	C	5001	MES	C7-C8-S-O2S
4	C	5001	MES	C7-C8-S-O3S
4	D	5001	MES	C8-C7-N4-C5
4	E	5001	MES	C8-C7-N4-C5
4	F	5001	MES	C8-C7-N4-C5
4	G	5001	MES	N4-C7-C8-S
4	G	5001	MES	C7-C8-S-O1S
4	G	5001	MES	C7-C8-S-O2S
4	H	5001	MES	C8-C7-N4-C5
4	F	5001	MES	C7-C8-S-O3S
4	G	5001	MES	C7-C8-S-O3S
4	G	5001	MES	C8-C7-N4-C3
4	C	5001	MES	C7-C8-S-O1S
4	D	5001	MES	C7-C8-S-O1S
4	F	5001	MES	C7-C8-S-O1S
4	F	5001	MES	C7-C8-S-O2S
4	B	5001	MES	N4-C7-C8-S
4	D	5001	MES	N4-C7-C8-S
4	D	5001	MES	C7-C8-S-O3S
4	D	5001	MES	C7-C8-S-O2S

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	5001	MES	1	0
4	C	5001	MES	2	0
4	D	5001	MES	2	0
4	A	5001	MES	2	0
4	E	5001	MES	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	842/844 (99%)	-0.33	17 (2%) 65 44	23, 38, 90, 113	0
1	B	747/844 (88%)	-0.21	8 (1%) 78 59	31, 50, 88, 136	0
1	C	844/844 (100%)	-0.51	5 (0%) 85 70	24, 35, 60, 70	0
1	D	844/844 (100%)	-0.33	13 (1%) 72 52	26, 39, 83, 101	0
1	E	843/844 (99%)	-0.29	25 (2%) 52 32	22, 36, 101, 126	0
1	F	844/844 (100%)	-0.22	5 (0%) 85 70	37, 53, 73, 89	0
1	G	844/844 (100%)	-0.43	5 (0%) 85 70	24, 35, 68, 79	0
1	H	807/844 (95%)	-0.30	28 (3%) 47 27	24, 42, 95, 139	0
All	All	6615/6752 (97%)	-0.33	106 (1%) 70 49	22, 40, 83, 139	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	277	ILE	7.3
1	B	248	TYR	6.4
1	B	249	ASN	5.8
1	H	282	LYS	5.7
1	H	288	THR	5.4
1	B	1087	PRO	4.8
1	H	355	TRP	4.7
1	G	1087	PRO	4.3
1	E	330	LEU	3.8
1	H	245	PHE	3.7
1	A	1087	PRO	3.6
1	E	278	LEU	3.6
1	E	277	ILE	3.6
1	A	283	THR	3.5
1	E	320	HIS	3.5
1	D	283	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	274	PRO	3.4
1	H	280	ASP	3.4
1	H	318	GLY	3.3
1	A	246	ALA	3.3
1	B	1083	SER	3.3
1	E	317	LEU	3.2
1	H	271	TRP	3.2
1	A	606	ASN	3.2
1	H	281	GLY	3.2
1	E	290	LYS	3.1
1	E	349	ALA	3.1
1	E	245	PHE	3.0
1	D	327	THR	3.0
1	E	329	PRO	2.9
1	H	303	GLN	2.9
1	H	297	MET	2.9
1	E	1085	VAL	2.9
1	A	1076	ASP	2.8
1	A	327	THR	2.8
1	C	318	GLY	2.8
1	A	320	HIS	2.8
1	D	320	HIS	2.8
1	H	293	ARG	2.8
1	A	248	TYR	2.7
1	H	357	ARG	2.7
1	G	320	HIS	2.7
1	B	272	TYR	2.7
1	F	1076	ASP	2.7
1	D	248	TYR	2.6
1	E	280	ASP	2.6
1	E	297	MET	2.6
1	H	279	LYS	2.6
1	E	279	LYS	2.6
1	E	351	LYS	2.6
1	H	356	LEU	2.6
1	C	1087	PRO	2.5
1	D	317	LEU	2.5
1	H	249	ASN	2.5
1	E	248	TYR	2.5
1	E	285	THR	2.5
1	C	320	HIS	2.5
1	E	342	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	316	GLN	2.5
1	E	289	GLU	2.5
1	C	1076	ASP	2.5
1	D	1021	GLU	2.4
1	H	306	GLN	2.4
1	H	1087	PRO	2.4
1	B	368	SER	2.4
1	C	1086	ASN	2.4
1	H	276	TYR	2.4
1	H	291	ASP	2.4
1	A	290	LYS	2.3
1	D	352	ASN	2.3
1	F	244	SER	2.3
1	D	249	ASN	2.3
1	E	249	ASN	2.3
1	E	1076	ASP	2.3
1	B	1084	LEU	2.3
1	G	606	ASN	2.3
1	A	286	GLN	2.3
1	F	574	GLU	2.2
1	H	296	LEU	2.2
1	A	615	GLU	2.2
1	E	1087	PRO	2.2
1	H	278	LEU	2.2
1	H	248	TYR	2.2
1	H	290	LYS	2.2
1	E	283	THR	2.2
1	A	314	ASN	2.2
1	A	1077	ASN	2.2
1	E	326	ALA	2.2
1	A	317	LEU	2.1
1	A	319	ILE	2.1
1	H	246	ALA	2.1
1	E	353	THR	2.1
1	H	247	GLN	2.1
1	F	1077	ASN	2.1
1	D	282	LYS	2.1
1	D	316	GLN	2.1
1	G	1086	ASN	2.1
1	G	632	GLU	2.1
1	H	275	LYS	2.0
1	A	1075	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	726	ARG	2.0
1	A	358	GLN	2.0
1	E	786	GLY	2.0
1	F	1087	PRO	2.0
1	D	279	LYS	2.0
1	D	321	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

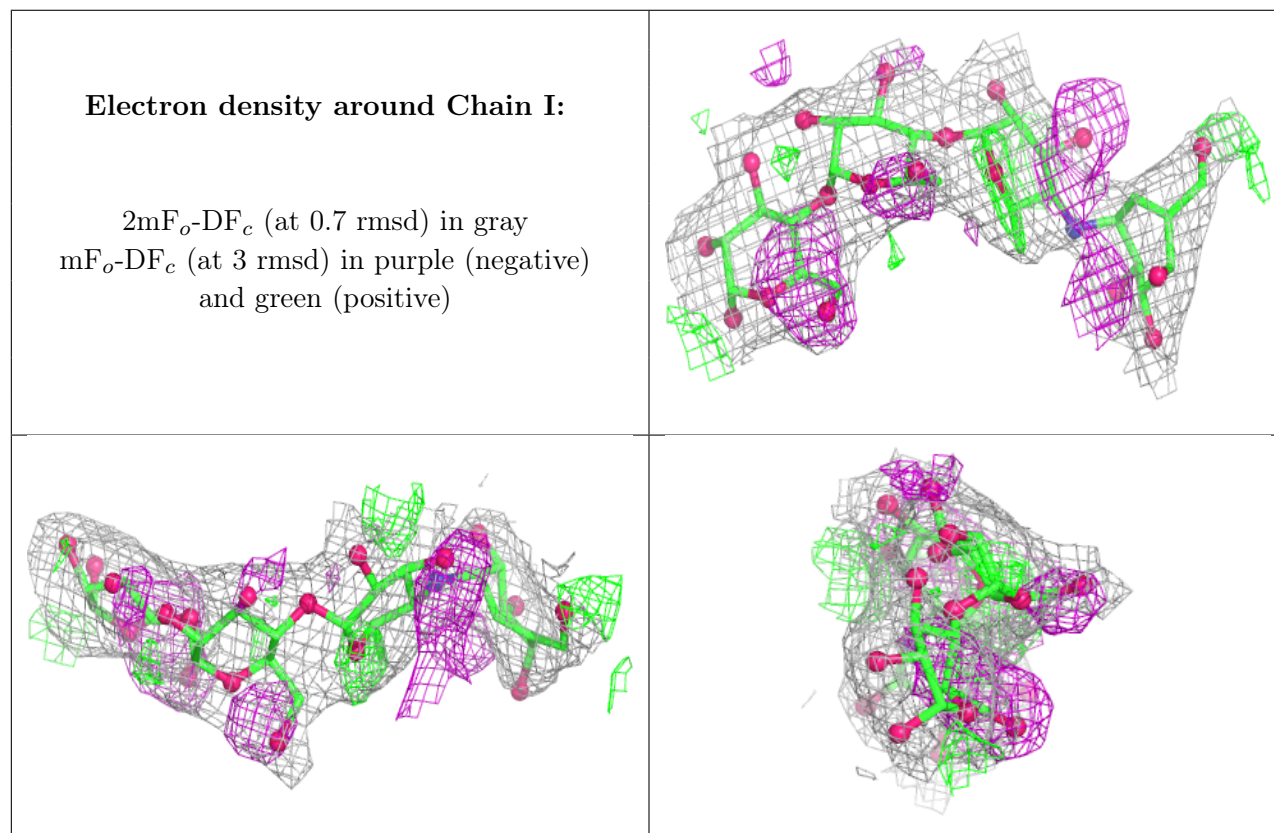
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	M	1	12/12	0.73	0.19	48,49,49,50	0
2	GLC	N	1	12/12	0.73	0.19	48,49,49,50	0
2	GLC	N	2	11/12	0.74	0.17	46,47,47,47	0
2	GLC	L	1	12/12	0.77	0.20	48,49,49,50	0
2	GLC	O	1	12/12	0.77	0.20	48,49,49,50	0
2	GLC	J	2	11/12	0.79	0.16	46,47,47,47	0
2	GLC	O	2	11/12	0.79	0.16	46,47,47,47	0
2	GLC	L	2	11/12	0.80	0.16	46,47,47,47	0
2	GLC	I	2	11/12	0.81	0.13	46,47,47,47	0
2	AC1	M	3	21/22	0.81	0.20	35,50,53,53	0
2	AC1	N	3	21/22	0.82	0.18	35,50,53,53	0
2	GLC	M	2	11/12	0.82	0.15	46,47,47,47	0
2	GLC	K	1	12/12	0.82	0.18	48,49,49,50	0
2	GLC	I	1	12/12	0.83	0.16	48,49,49,50	0
2	GLC	J	1	12/12	0.84	0.13	48,49,49,50	0
2	AC1	I	3	21/22	0.85	0.18	35,50,53,53	0
2	GLC	P	1	12/12	0.85	0.16	48,49,49,50	0
2	GLC	P	2	11/12	0.85	0.13	46,47,47,47	0
2	GLC	K	2	11/12	0.86	0.13	46,47,47,47	0
2	AC1	P	3	21/22	0.86	0.16	35,50,53,53	0
2	AC1	L	3	21/22	0.89	0.15	35,50,53,53	0
2	AC1	K	3	21/22	0.89	0.18	35,50,53,53	0

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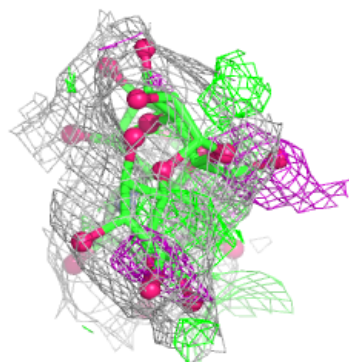
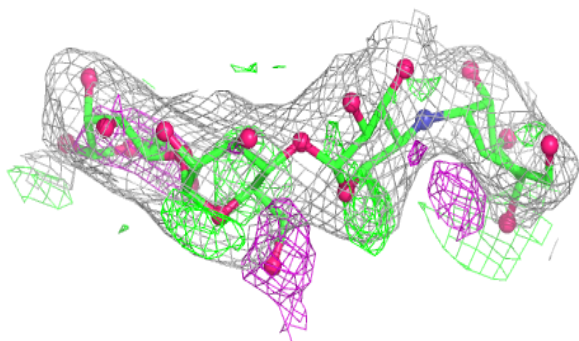
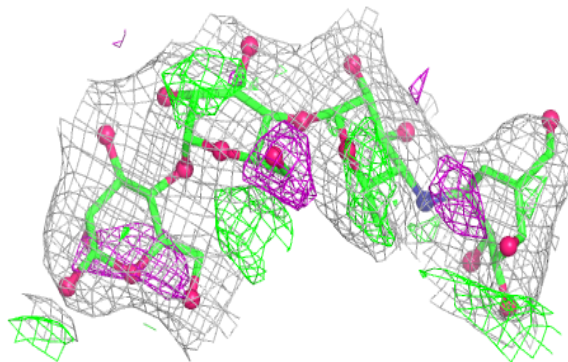
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AC1	O	3	21/22	0.91	0.16	35,50,53,53	0
2	AC1	J	3	21/22	0.91	0.16	35,50,53,53	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

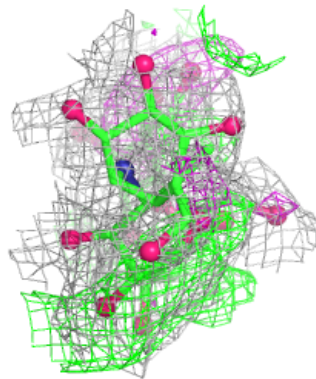
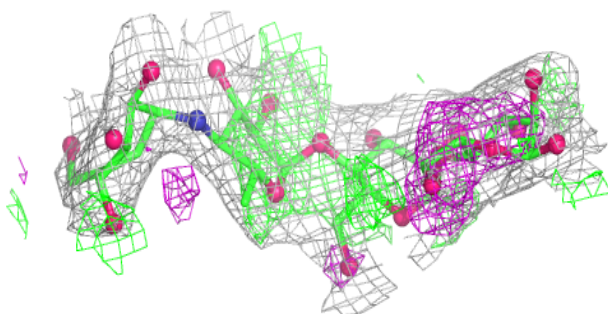
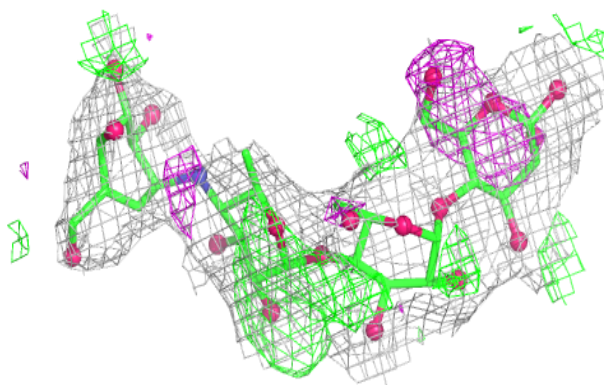


Electron density around Chain J:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

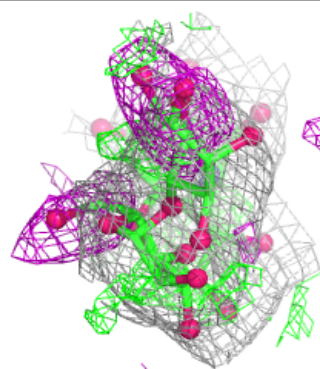
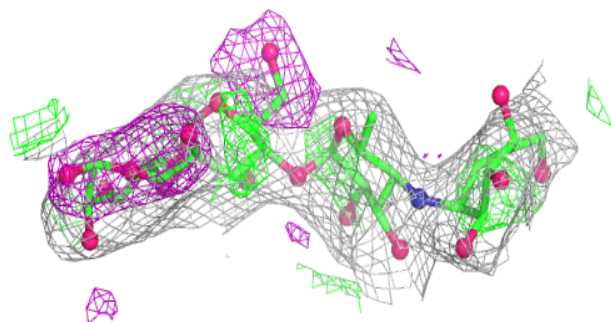
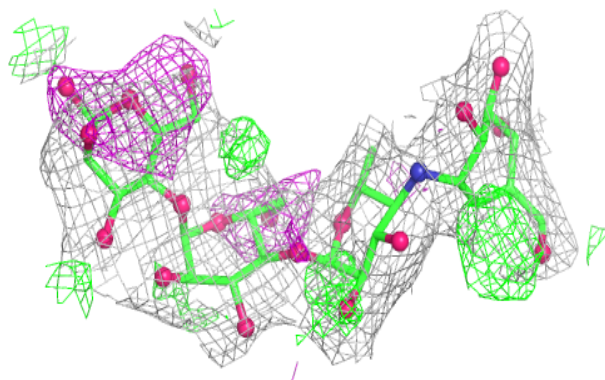
**Electron density around Chain K:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

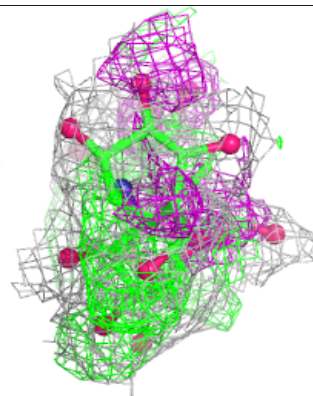
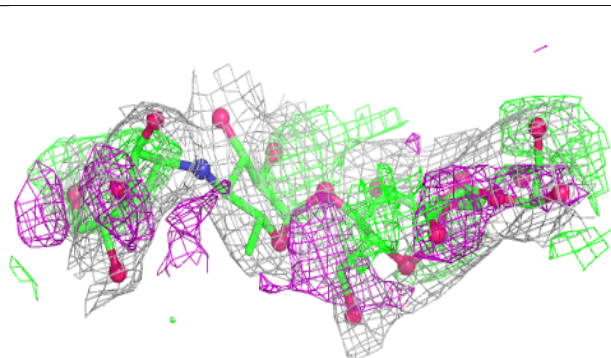
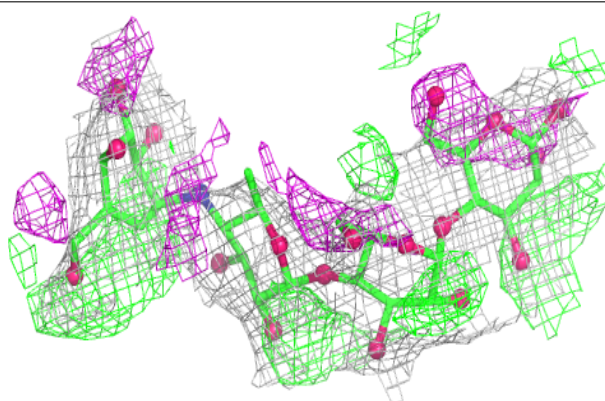


Electron density around Chain L:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

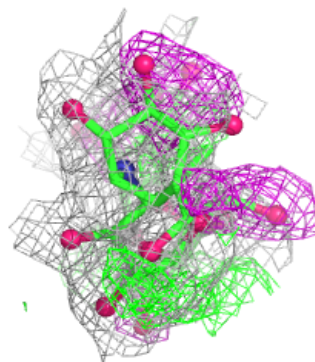
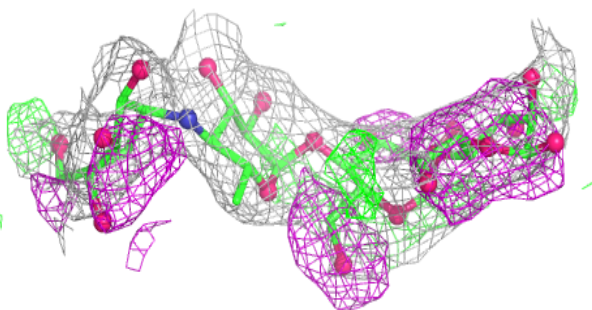
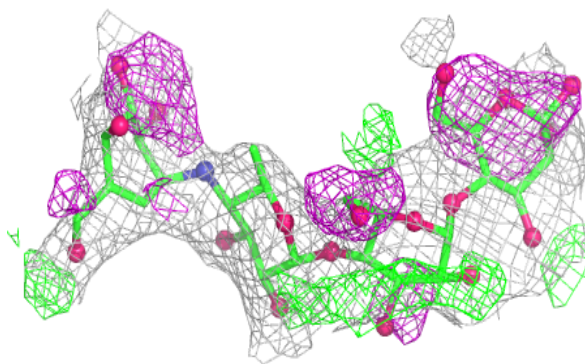
**Electron density around Chain M:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

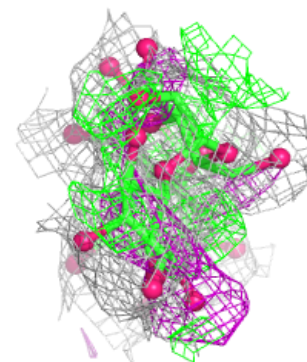
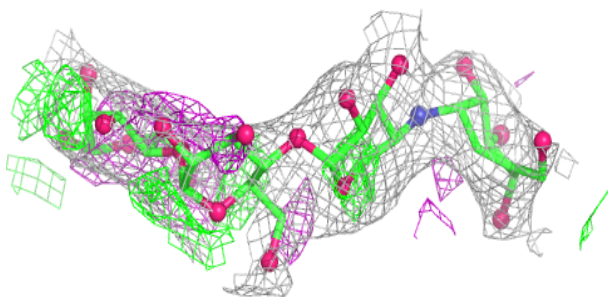
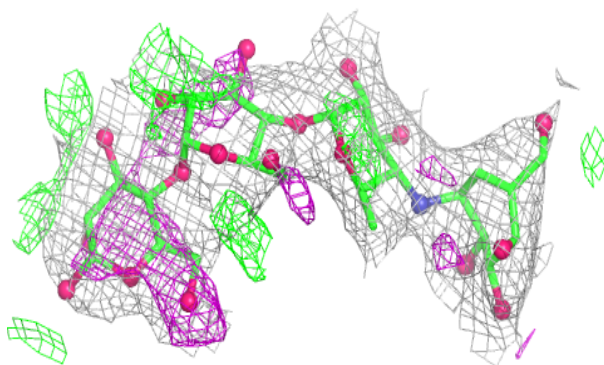


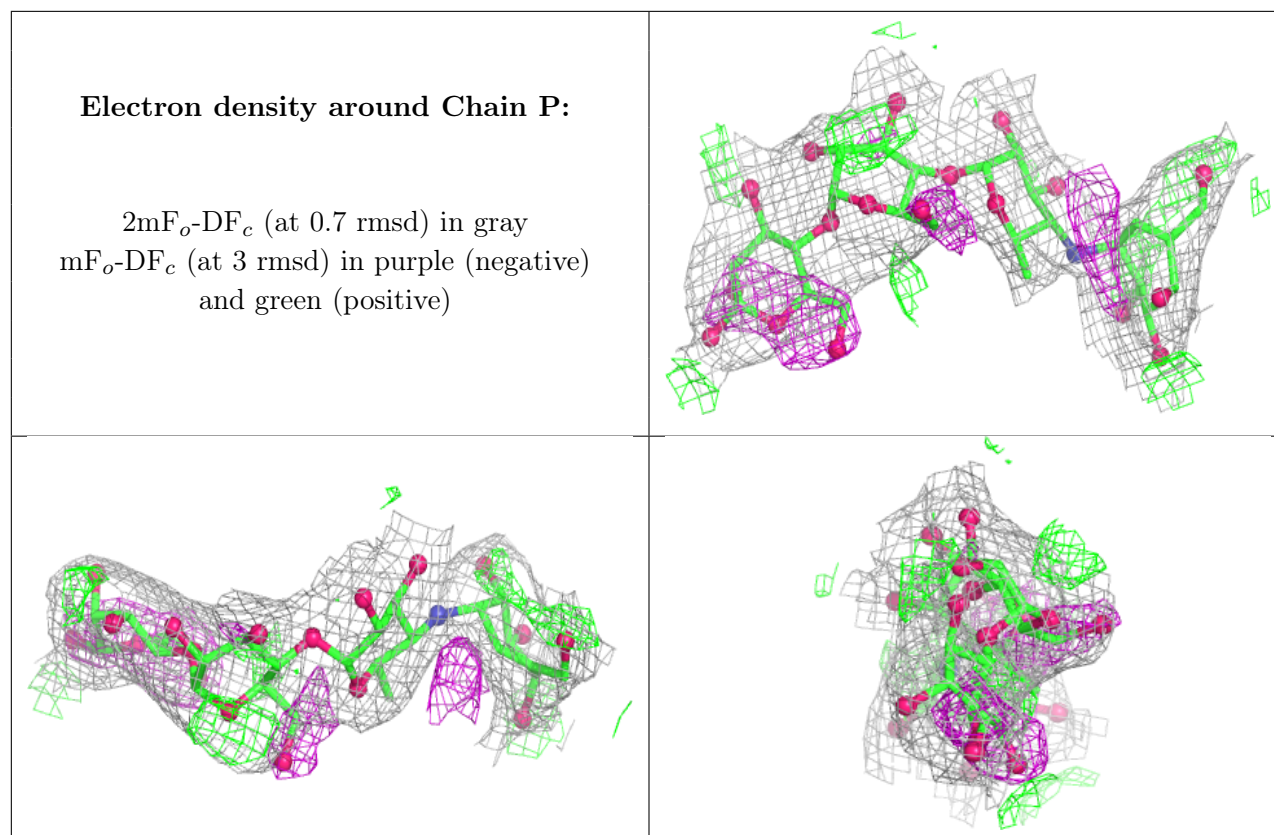
Electron density around Chain N:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain O:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MES	C	5001	12/12	0.92	0.14	29,31,32,32	0
4	MES	A	5001	12/12	0.93	0.14	29,31,33,33	0
4	MES	B	5001	12/12	0.94	0.18	39,41,43,44	0
3	CA	A	4001	1/1	0.94	0.07	28,28,28,28	0
4	MES	E	5001	12/12	0.94	0.13	30,33,35,36	0
4	MES	G	5001	12/12	0.94	0.12	30,31,33,33	0
4	MES	H	5001	12/12	0.94	0.13	28,30,32,32	0
4	MES	F	5001	12/12	0.96	0.13	36,37,37,37	0
3	CA	B	4001	1/1	0.96	0.04	33,33,33,33	0
3	CA	G	4001	1/1	0.96	0.05	28,28,28,28	0
3	CA	F	4001	1/1	0.97	0.05	38,38,38,38	0
4	MES	D	5001	12/12	0.97	0.12	31,33,35,35	0
3	CA	D	4001	1/1	0.97	0.05	32,32,32,32	0
3	CA	C	4001	1/1	0.98	0.03	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	E	4001	1/1	0.98	0.08	32,32,32,32	0
3	CA	H	4001	1/1	0.99	0.05	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.