



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:08 AM UTC

PDB ID : 5K8D / pdb_00005k8d
Title : Crystal structure of rFVIIIFc
Authors : Leksa, N.; Quan, C.
Deposited on : 2016-05-29
Resolution : 4.19 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

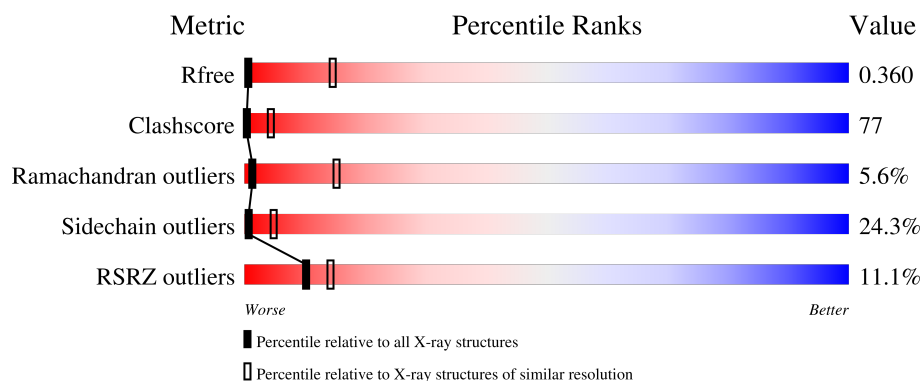
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.19 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	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	740	9% 19% 45% 16% • 17%
2	B	865	8% 18% 37% 15% • 28%
3	C	4	75% 25%
4	D	2	100%
5	E	7	14% 43% 43%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10138 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 Coagulation factor VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4937	3190	824	898	25			

- Molecule 2 is a protein called Coagulation factor VIII,Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	619	Total	C	N	O	S	0	0	0
			5035	3234	862	908	31			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2332	TYR	-	linker	UNP P00451

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



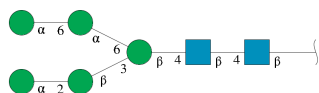
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O		0	0	0
			50	28	2	20				

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-beta-D-mannopyranos e-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Ca	0	0
			3	3		

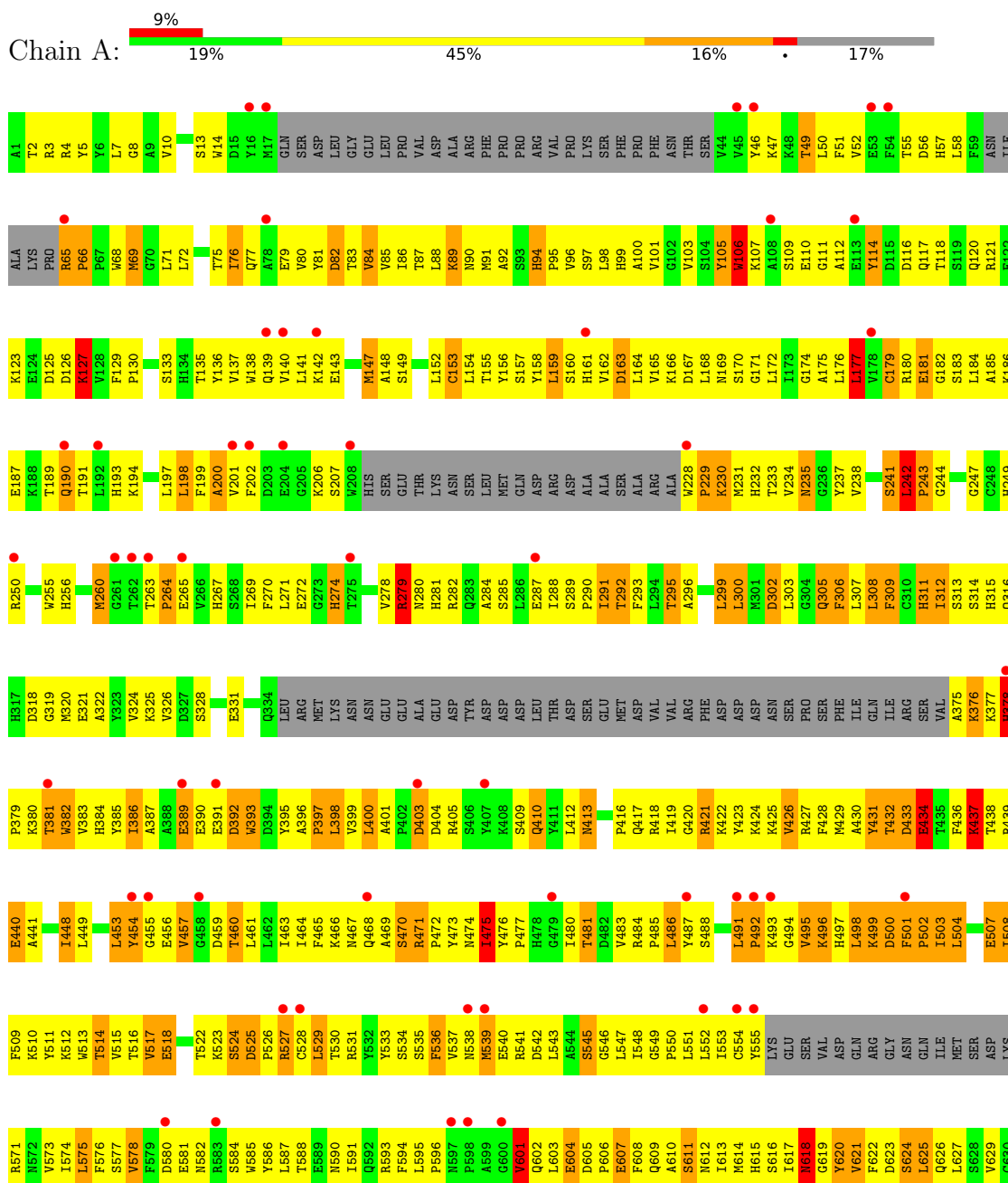
- Molecule 7 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

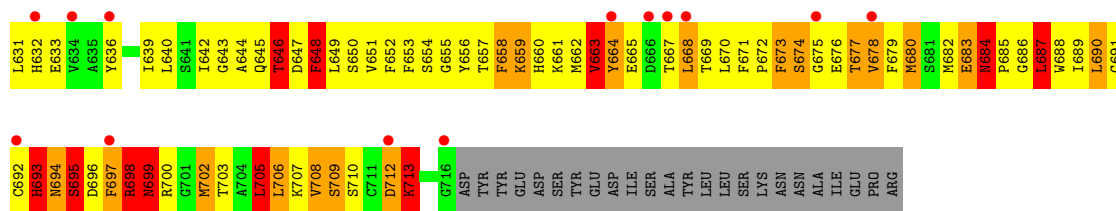
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cu	0	0
			1	1		
7	B	1	Total	Cu	0	0
			1	1		

3 Residue-property plots

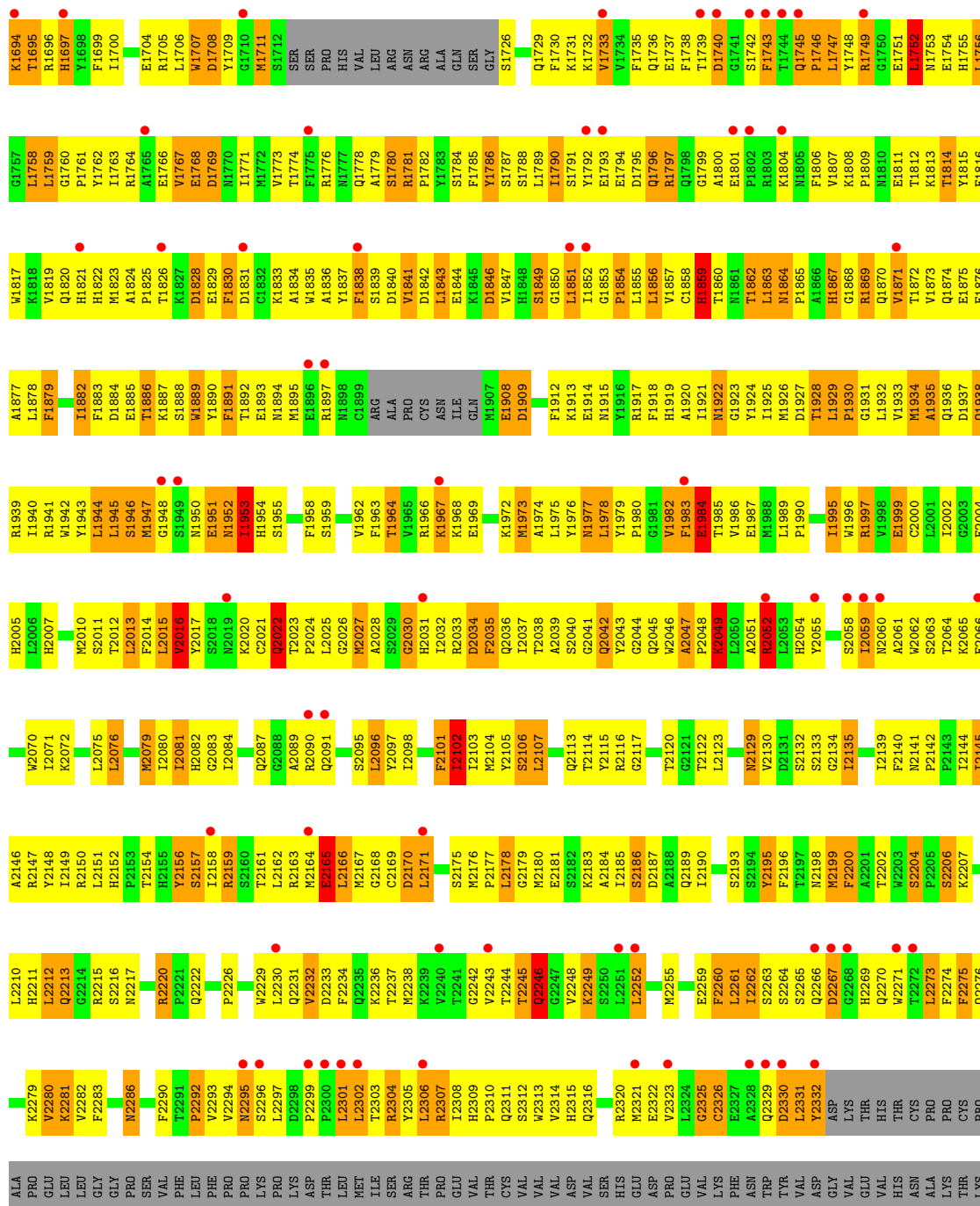
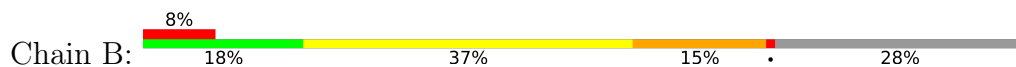
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Coagulation factor VIII





● Molecule 2: Coagulation factor VIII,Ig gamma-1 chain C region



PRO ARG
LEU PRO
GLU SER
GLN ARG
TYR ASP
ASN SER
THR THR
TYR TYR
ARG ASN
VAL VAL
SER SER
VAL VAL
THR THR
CYS VAL
LEU VAL
HIS HIS
GLN GLN
PHE ASP
TYR TYR
PRO LEU
SER ASN
GLY ASP
LYS ILE
GLU ALA
TYR VAL
CYS GLU
TRP TRP
CYS CYS
LYS VAL
SER VAL
ASN ASN
GLN GLN
LYS LYS
ALA ALA
LEU LEU
PRO PRO
ASN ASN
ALA ALA
TYR TYR
LYS LYS
THR THR
GLU GLU
LYS THR
THR THR
PRO PRO
ILE ILE
SER VAL
LEU LEU
LYS LYS
ASP ASP
SER SER
GLY GLY
GLN GLN
PRO PRO
ARG ARG
GLU GLU
PRO PRO
GLN GLN
VAL VAL
TYR TYR
LYS LYS
THR THR

LEU PRO
PRO PRO
SER SER
ARG ARG
ASP ASP
GLU GLU
LEU LEU
THR THR
LYS LYS
ASN ASN
GLN GLN
VAL VAL
PHE PHE
SER SER
LEU LEU
THR THR
CYS CYS
VAL VAL
MET MET
HIS HIS
GLU GLU
ALA ALA
HIS HIS
LEU LEU
ASN ASN
HIS HIS
TYR TYR
THR THR
GLN GLN
LYS LYS
SER SER
LEU LEU
SER SER
LEU LEU
PRO PRO
PRO PRO
GLY GLY
ASN ASN
GLU GLU
PRO PRO
GLU GLU
ASN ASN
TYR TYR
LYS LYS
THR THR
THR THR
PRO PRO
ILE ILE
SER VAL
LEU LEU
LYS LYS
ASP ASP
SER SER
ASP ASP
GLY GLY
GLN GLN
PRO PRO
PHE PHE
PHE PHE
LEU LEU
TYR TYR
SER SER
LYS LYS
VAL VAL
TYR TYR
LEU LEU

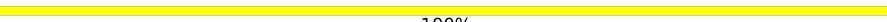
THR VAL
ASP ASP
LYS LYS
SER SER
ARG ARG
TRP TRP
GLN GLN
GLY GLY
VAL VAL
PHE PHE
SER SER
CYS CYS
SER SER
VAL VAL
MET MET
HIS HIS
GLU GLU
ALA ALA
HIS HIS
LEU LEU
ASN ASN
HIS HIS
TYR TYR
THR THR
GLN GLN
LYS LYS
SER SER
LEU LEU
SER SER
LEU LEU
PRO PRO
PRO PRO
GLY GLY

- Molecule 3: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  75% 25%

MAG1
MAG2
BMA3
MAN4

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

MAG1
MAG2

- Molecule 5: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  14% 43% 43%

MAG1
MAG2
BMA3
BMA4
MAN5
MAN6
MAN7

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	136.29Å 136.29Å 365.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.60 – 4.19 37.60 – 4.19	Depositor EDS
% Data completeness (in resolution range)	98.8 (37.60-4.19) 98.8 (37.60-4.19)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 4.13Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.298 , 0.362 0.298 , 0.360	Depositor DCC
R_{free} test set	1309 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	126.3	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 293.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10138	wwPDB-VP
Average B, all atoms (Å ²)	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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: MAN, NAG, CA, CU, BMA

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	0.94	14/5077 (0.3%)	1.23	34/6890 (0.5%)
2	B	0.89	14/5178 (0.3%)	1.19	29/7011 (0.4%)
All	All	0.91	28/10255 (0.3%)	1.21	63/13901 (0.5%)

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	2
2	B	0	2
All	All	0	4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	PHE	CG-CD2	9.64	1.59	1.38
2	B	1897	ARG	NE-CZ	9.64	1.43	1.33
1	A	712	ASP	CG-OD2	9.18	1.42	1.25
1	A	712	ASP	CG-OD1	8.84	1.42	1.25
1	A	434	GLU	CD-OE1	8.79	1.42	1.25
1	A	618	ASN	C-O	8.77	1.35	1.24
1	A	697	PHE	CG-CD1	8.40	1.56	1.38
1	A	389	GLU	CD-OE2	8.32	1.41	1.25
2	B	2165	GLU	CA-C	-7.51	1.46	1.53
2	B	1838	PHE	CG-CD1	6.71	1.52	1.38
2	B	1983	PHE	CG-CD1	6.53	1.52	1.38
2	B	1801	GLU	C-N	6.46	1.38	1.33
2	B	2330	ASP	CG-OD1	6.38	1.37	1.25
2	B	1745	GLN	CG-CD	6.27	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1983	PHE	CG-CD2	6.23	1.51	1.38
1	A	697	PHE	CE1-CZ	6.21	1.57	1.38
2	B	2267	ASP	CG-OD2	6.16	1.37	1.25
1	A	434	GLU	CD-OE2	5.59	1.35	1.25
1	A	190	GLN	CG-CD	5.45	1.65	1.52
1	A	190	GLN	CD-OE1	5.44	1.33	1.23
1	A	434	GLU	CG-CD	5.40	1.65	1.52
2	B	1742	SER	CB-OG	5.31	1.52	1.42
2	B	2266	GLN	CD-OE1	5.24	1.33	1.23
2	B	1838	PHE	CG-CD2	5.21	1.49	1.38
2	B	1897	ARG	CZ-NH2	5.21	1.40	1.33
2	B	1743	PHE	CG-CD1	5.20	1.49	1.38
1	A	697	PHE	CE2-CZ	5.16	1.54	1.38
1	A	694	ASN	CA-C	5.04	1.59	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2325	GLY	N-CA-C	9.91	123.96	110.58
1	A	149	SER	N-CA-C	-9.33	101.91	113.38
1	A	228	TRP	CA-C-N	8.37	130.30	119.84
1	A	228	TRP	C-N-CA	8.37	130.30	119.84
1	A	694	ASN	N-CA-C	-8.36	102.52	112.89
2	B	2162	LEU	N-CA-C	7.90	121.24	108.76
2	B	2047	ALA	CA-C-N	-7.65	112.87	120.21
2	B	2047	ALA	C-N-CA	-7.65	112.87	120.21
2	B	1982	VAL	N-CA-C	7.61	118.40	110.72
1	A	495	VAL	N-CA-C	7.33	119.28	108.65
1	A	677	THR	N-CA-C	7.16	119.28	108.46
2	B	2260	PHE	N-CA-C	6.74	119.31	109.07
1	A	475	ILE	N-CA-C	6.58	116.36	106.42
2	B	1859	HIS	N-CA-C	6.47	118.71	108.67
1	A	687	LEU	N-CA-C	6.40	116.90	107.88
1	A	507	GLU	N-CA-C	6.35	118.33	109.31
1	A	693	HIS	N-CA-C	6.33	118.90	109.59
1	A	648	PHE	N-CA-C	6.32	119.83	109.72
2	B	2059	ILE	N-CA-C	6.31	117.20	107.99
2	B	1953	ILE	N-CA-C	-6.28	105.23	111.77
1	A	200	ALA	N-CA-C	6.10	119.49	108.69
1	A	440	GLU	N-CA-C	6.10	118.62	108.13
1	A	675	GLY	N-CA-C	-6.07	104.93	114.10
2	B	2030	GLY	N-CA-C	6.07	120.54	112.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	664	TYR	N-CA-C	-6.02	99.90	109.59
2	B	2246	GLN	N-CA-C	6.01	116.03	108.45
2	B	1760	GLY	CA-C-N	-5.99	114.59	120.52
2	B	1760	GLY	C-N-CA	-5.99	114.59	120.52
2	B	2052	ARG	N-CA-C	5.98	123.54	110.80
2	B	2296	SER	N-CA-C	5.98	117.80	111.28
1	A	698	ARG	N-CA-C	-5.87	105.01	111.82
1	A	491	LEU	CA-C-N	5.87	127.17	119.84
1	A	491	LEU	C-N-CA	5.87	127.17	119.84
2	B	1920	ALA	N-CA-C	5.86	118.67	108.76
2	B	1801	GLU	CA-C-N	-5.86	114.20	121.00
2	B	1801	GLU	C-N-CA	-5.86	114.20	121.00
2	B	2016	VAL	N-CA-C	5.76	117.14	109.37
2	B	2022	GLN	N-CA-C	5.73	118.66	110.24
1	A	181	GLU	N-CA-C	5.72	117.97	111.11
2	B	1864	ASN	N-CA-C	5.72	116.90	109.64
1	A	279	ARG	N-CA-C	-5.70	106.18	113.02
2	B	2044	GLY	N-CA-C	-5.70	105.24	112.65
2	B	2106	SER	N-CA-C	5.67	116.88	108.60
2	B	1748	TYR	N-CA-C	5.54	118.48	109.24
1	A	230	LYS	N-CA-C	5.53	118.06	109.60
1	A	308	LEU	N-CA-C	-5.51	102.37	110.52
1	A	300	LEU	N-CA-C	5.43	119.12	111.52
2	B	2066	GLU	CA-C-N	-5.42	114.37	119.85
2	B	2066	GLU	C-N-CA	-5.42	114.37	119.85
1	A	229	PRO	N-CA-C	5.42	123.62	112.47
1	A	177	LEU	N-CA-C	5.39	117.87	108.76
1	A	179	CYS	N-CA-C	5.38	117.57	109.23
2	B	2102	ILE	CB-CA-C	-5.37	102.31	110.95
1	A	441	ALA	N-CA-C	-5.21	100.53	108.76
1	A	695	SER	N-CA-C	5.20	121.87	110.80
2	B	2122	THR	N-CA-C	5.14	118.33	111.75
1	A	488	SER	N-CA-C	5.12	116.19	108.46
2	B	1780	SER	N-CA-C	5.09	116.82	111.28
1	A	678	VAL	CB-CA-C	5.06	118.86	110.30
1	A	65	ARG	CA-C-N	5.05	125.58	120.38
1	A	65	ARG	C-N-CA	5.05	125.58	120.38
1	A	274	HIS	N-CA-C	5.05	117.64	109.06
1	A	432	THR	N-CA-C	5.03	116.84	111.36

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	430	ALA	Peptide
1	A	693	HIS	Peptide
2	B	1790	ILE	Peptide
2	B	1828	ASP	Peptide

5.2 Too-close contacts

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	4937	0	4820	828	1
2	B	5035	0	4902	803	0
3	C	50	0	43	1	0
4	D	28	0	25	0	0
5	E	83	0	70	4	0
6	A	3	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
All	All	10138	0	9860	1540	1

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 77.

All (1540) 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)
2:B:2046:TRP:CZ3	2:B:2059:ILE:HA	1.37	1.59
1:A:287:GLU:HB3	1:A:673:PHE:CE2	1.51	1.42
2:B:1934:MET:CE	2:B:1940:ILE:HD13	1.46	1.41
2:B:1934:MET:HE3	2:B:1940:ILE:CD1	1.55	1.37
2:B:1738:PHE:CD2	2:B:1747:LEU:HD12	1.57	1.36
1:A:65:ARG:CG	1:A:66:PRO:HD3	1.57	1.35
2:B:1738:PHE:CB	2:B:1746:PRO:O	1.75	1.34
2:B:1738:PHE:HB2	2:B:1746:PRO:O	1.19	1.33
2:B:1830:PHE:CD1	2:B:1966:ARG:NH1	2.03	1.26
1:A:114:TYR:CE2	2:B:1997:ARG:HB2	1.69	1.26
2:B:1758:LEU:HD11	2:B:1923:GLY:CA	1.63	1.25
2:B:1786:TYR:HA	2:B:1790:ILE:CD1	1.65	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1944:LEU:O	2:B:1978:LEU:HD11	1.29	1.25
1:A:395:TYR:HB3	1:A:621:VAL:CG2	1.65	1.25
2:B:2180:MET:HB2	2:B:2322:GLU:OE2	1.32	1.25
2:B:1828:ASP:OD2	2:B:1968:LYS:HA	1.31	1.23
1:A:625:LEU:CD1	1:A:706:LEU:HD11	1.68	1.23
1:A:5:TYR:CE2	1:A:76:ILE:HB	1.72	1.22
2:B:2264:SER:OG	2:B:2301:LEU:HD21	1.35	1.21
2:B:1945:LEU:HG	2:B:1983:PHE:CB	1.68	1.21
1:A:453:LEU:HD21	1:A:533:TYR:CE2	1.75	1.20
2:B:2046:TRP:CZ3	2:B:2059:ILE:CA	2.24	1.18
1:A:417:GLN:OE1	1:A:601:VAL:HG22	1.39	1.18
1:A:657:THR:HG21	2:B:1788:SER:HA	1.25	1.17
2:B:1830:PHE:HD1	2:B:1966:ARG:NH1	1.40	1.17
2:B:1813:LYS:HD2	2:B:1814:THR:H	1.04	1.17
2:B:1945:LEU:CG	2:B:1983:PHE:HB2	1.75	1.16
2:B:2046:TRP:CH2	2:B:2059:ILE:HA	1.81	1.15
2:B:2032:ILE:HG23	2:B:2036:GLN:OE1	1.43	1.15
2:B:2046:TRP:HH2	2:B:2058:SER:O	1.27	1.15
1:A:114:TYR:CD2	2:B:1997:ARG:HD3	1.82	1.14
1:A:395:TYR:CB	1:A:621:VAL:CG2	2.26	1.14
2:B:2329:GLN:HG3	2:B:2332:TYR:O	1.44	1.13
2:B:2052:ARG:HD3	2:B:2165:GLU:HB2	1.25	1.12
2:B:2087:GLN:HB3	2:B:2163:ARG:HB2	1.13	1.12
1:A:651:VAL:H	1:A:693:HIS:HB2	1.09	1.12
2:B:1946:SER:CB	2:B:1978:LEU:HD12	1.80	1.12
1:A:621:VAL:HG12	1:A:622:PHE:H	1.07	1.11
1:A:625:LEU:HD13	1:A:706:LEU:CG	1.79	1.11
1:A:105:TYR:HB3	1:A:109:SER:HB3	1.29	1.11
1:A:663:VAL:HG22	2:B:1968:LYS:HD2	1.21	1.10
2:B:1886:THR:CG2	2:B:1913:LYS:NZ	2.16	1.09
2:B:1947:MET:CE	2:B:1948:GLY:H	1.65	1.09
2:B:2083:GLY:HA2	2:B:2140:PHE:CD2	1.87	1.09
2:B:1758:LEU:HD11	2:B:1923:GLY:HA3	1.09	1.09
2:B:1886:THR:HG21	2:B:1913:LYS:NZ	1.67	1.09
2:B:1947:MET:HE2	2:B:1948:GLY:H	0.93	1.08
2:B:1786:TYR:HA	2:B:1790:ILE:HD11	1.18	1.08
2:B:2027:MET:HE3	2:B:2032:ILE:HD13	1.29	1.08
2:B:2330:ASP:HB3	2:B:2331:LEU:HD23	1.32	1.08
1:A:700:ARG:HH22	2:B:1844:GLU:CB	1.67	1.07
2:B:1891:PHE:HD1	2:B:1892:THR:N	1.51	1.07
2:B:1945:LEU:HA	2:B:1983:PHE:HA	1.27	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2087:GLN:CB	2:B:2163:ARG:HB2	1.84	1.07
2:B:1743:PHE:CE1	2:B:1778:GLN:NE2	2.21	1.07
1:A:75:THR:HG22	1:A:175:ALA:HB3	1.37	1.07
1:A:287:GLU:CB	1:A:673:PHE:CE2	2.37	1.07
2:B:1813:LYS:HD2	2:B:1814:THR:N	1.68	1.06
2:B:1886:THR:HG21	2:B:1913:LYS:HZ3	0.96	1.06
2:B:2169:CYS:O	2:B:2170:ASP:HB3	1.34	1.06
2:B:2187:ASP:HB2	2:B:2206:SER:HB3	1.37	1.06
1:A:65:ARG:CG	1:A:66:PRO:CD	2.33	1.06
1:A:5:TYR:HE2	1:A:76:ILE:HB	1.07	1.06
1:A:148:ALA:HA	1:A:180:ARG:NH2	1.69	1.06
1:A:100:ALA:HB2	1:A:138:TRP:CZ3	1.90	1.05
1:A:395:TYR:HB3	1:A:621:VAL:HG23	1.07	1.05
2:B:1828:ASP:OD2	2:B:1968:LYS:CA	2.03	1.05
1:A:471:ARG:HG2	1:A:585:TRP:CE3	1.91	1.05
2:B:2052:ARG:CD	2:B:2165:GLU:HB2	1.87	1.05
1:A:65:ARG:HG2	1:A:66:PRO:HD3	1.12	1.05
2:B:1707:TRP:HE1	2:B:1758:LEU:HD21	1.18	1.05
2:B:1838:PHE:HZ	2:B:1947:MET:HG3	1.15	1.04
1:A:141:LEU:HD23	1:A:143:GLU:H	1.22	1.03
2:B:1963:PHE:CD1	2:B:1986:VAL:HG11	1.94	1.03
2:B:2096:LEU:HB3	2:B:2161:THR:HG21	1.08	1.03
2:B:2273:LEU:HD21	2:B:2280:VAL:CG2	1.88	1.03
1:A:491:LEU:O	1:A:493:LYS:N	1.92	1.02
1:A:625:LEU:CD1	1:A:706:LEU:CD1	2.36	1.02
2:B:1790:ILE:HA	2:B:1817:TRP:CE3	1.95	1.02
2:B:1886:THR:CG2	2:B:1913:LYS:HZ3	1.70	1.02
2:B:1909:ASP:O	2:B:1913:LYS:HB2	1.58	1.02
2:B:2273:LEU:HD21	2:B:2280:VAL:HG21	1.36	1.02
1:A:531:ARG:HB2	1:A:551:LEU:O	1.58	1.01
1:A:700:ARG:HH22	2:B:1844:GLU:HB2	1.20	1.01
1:A:615:HIS:HB2	1:A:703:THR:HB	1.40	1.01
2:B:1946:SER:HB3	2:B:1978:LEU:HD12	1.36	1.01
2:B:1983:PHE:CD1	2:B:1984:GLU:N	2.29	1.01
2:B:2038:THR:HG21	2:B:2072:LYS:HE2	1.42	1.01
1:A:432:THR:OG1	1:A:440:GLU:HB3	1.61	1.01
2:B:1758:LEU:HD11	2:B:1923:GLY:N	1.75	1.01
1:A:622:PHE:O	1:A:705:LEU:HB2	1.60	1.00
2:B:1707:TRP:NE1	2:B:1758:LEU:CD2	2.24	0.99
1:A:395:TYR:HB2	1:A:621:VAL:HG21	1.45	0.99
2:B:1829:GLU:H	2:B:1966:ARG:HD2	1.26	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2083:GLY:HA2	2:B:2140:PHE:HD2	1.22	0.98
1:A:287:GLU:HB3	1:A:673:PHE:CD2	1.97	0.98
1:A:625:LEU:HD13	1:A:706:LEU:CD1	1.91	0.98
2:B:1758:LEU:CD1	2:B:1923:GLY:HA3	1.92	0.98
1:A:663:VAL:CG2	2:B:1968:LYS:HD2	1.93	0.98
2:B:2046:TRP:CH2	2:B:2058:SER:O	2.17	0.98
2:B:2306:LEU:HD23	2:B:2307:ARG:H	1.25	0.98
1:A:389:GLU:OE1	1:A:431:TYR:CE2	2.16	0.98
2:B:2052:ARG:H	2:B:2163:ARG:HB3	1.25	0.98
2:B:2169:CYS:O	2:B:2170:ASP:CB	2.09	0.97
2:B:2329:GLN:O	2:B:2332:TYR:O	1.81	0.97
2:B:1743:PHE:HE1	2:B:1778:GLN:CD	1.72	0.97
1:A:622:PHE:CE1	1:A:702:MET:O	2.16	0.97
1:A:617:ILE:O	1:A:618:ASN:HB2	1.60	0.97
2:B:1946:SER:HB3	2:B:1978:LEU:CD1	1.94	0.97
2:B:1964:THR:O	2:B:1986:VAL:HG13	1.64	0.97
2:B:1947:MET:HE2	2:B:1948:GLY:N	1.78	0.97
1:A:180:ARG:O	1:A:183:SER:HB3	1.65	0.96
1:A:625:LEU:HD13	1:A:706:LEU:HG	1.43	0.96
2:B:1944:LEU:O	2:B:1978:LEU:CD1	2.12	0.96
2:B:1738:PHE:HD2	2:B:1747:LEU:HD12	0.91	0.96
2:B:1934:MET:HB3	2:B:2016:VAL:HB	1.45	0.96
1:A:287:GLU:HB3	1:A:673:PHE:HE2	1.15	0.96
2:B:1829:GLU:H	2:B:1966:ARG:CD	1.79	0.96
1:A:433:ASP:O	1:A:434:GLU:HG3	1.65	0.95
2:B:2051:ALA:HB1	2:B:2164:MET:H	1.31	0.95
1:A:398:LEU:HD23	1:A:399:VAL:HG12	1.43	0.95
1:A:656:TYR:CZ	2:B:1791:SER:HB2	2.01	0.95
1:A:642:ILE:HG22	1:A:643:GLY:H	1.29	0.95
1:A:114:TYR:HE2	2:B:1997:ARG:HB2	1.01	0.95
1:A:501:PHE:O	1:A:503:ILE:HG12	1.64	0.95
1:A:663:VAL:HG22	2:B:1968:LYS:CD	1.95	0.95
2:B:2273:LEU:CD2	2:B:2280:VAL:CG2	2.45	0.94
1:A:312:ILE:HD12	1:A:315:HIS:CE1	2.03	0.94
2:B:1829:GLU:N	2:B:1966:ARG:HD2	1.82	0.94
2:B:2034:ASP:HB3	2:B:2049:LYS:HD2	1.49	0.94
2:B:2087:GLN:HB3	2:B:2163:ARG:CB	1.97	0.94
2:B:2264:SER:CB	2:B:2301:LEU:CD2	2.46	0.94
1:A:395:TYR:CB	1:A:621:VAL:HG21	1.94	0.94
1:A:187:GLU:HA	1:A:190:GLN:HB3	1.47	0.94
2:B:2046:TRP:HZ3	2:B:2060:ASN:N	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1738:PHE:HB3	2:B:1746:PRO:O	1.67	0.94
1:A:10:VAL:HG23	1:A:52:VAL:HG21	1.50	0.93
2:B:1838:PHE:CZ	2:B:1947:MET:HG3	2.02	0.93
1:A:109:SER:HB2	1:A:137:VAL:O	1.68	0.93
1:A:617:ILE:HD13	1:A:706:LEU:HD13	1.50	0.93
1:A:306:PHE:HD1	1:A:306:PHE:N	1.65	0.93
2:B:2096:LEU:HB3	2:B:2161:THR:CG2	1.99	0.93
1:A:700:ARG:NH2	2:B:1844:GLU:HB2	1.83	0.93
2:B:2046:TRP:HZ3	2:B:2059:ILE:CA	1.70	0.93
2:B:1829:GLU:HB2	2:B:1966:ARG:HD2	1.51	0.93
2:B:2052:ARG:HD3	2:B:2165:GLU:CB	1.98	0.92
1:A:114:TYR:HD2	2:B:1997:ARG:HD3	1.24	0.92
1:A:147:MET:HE1	2:B:1972:LYS:NZ	1.84	0.92
1:A:114:TYR:HE2	2:B:1997:ARG:CB	1.80	0.92
1:A:157:SER:HB2	1:A:174:GLY:O	1.67	0.92
1:A:498:LEU:HD12	1:A:498:LEU:H	1.32	0.92
1:A:656:TYR:CB	1:A:686:GLY:HA2	1.99	0.92
1:A:615:HIS:HB2	1:A:703:THR:CB	2.00	0.91
2:B:1707:TRP:NE1	2:B:1758:LEU:HD21	1.83	0.91
2:B:1738:PHE:CD2	2:B:1747:LEU:CD1	2.51	0.91
2:B:2039:ALA:HB2	2:B:2048:PRO:HG2	1.49	0.91
1:A:688:TRP:HE1	2:B:1800:ALA:N	1.68	0.91
2:B:1789:LEU:HD23	2:B:1823:MET:HB3	1.53	0.91
2:B:1946:SER:HB3	2:B:1978:LEU:HB3	1.50	0.91
2:B:2245:THR:C	2:B:2286:ASN:HD21	1.78	0.91
1:A:287:GLU:CB	1:A:673:PHE:HE2	1.79	0.91
1:A:480:ILE:HG22	1:A:481:THR:H	1.35	0.91
1:A:57:HIS:HB2	1:A:89:LYS:NZ	1.85	0.91
1:A:186:LYS:O	1:A:190:GLN:N	2.05	0.90
1:A:471:ARG:CG	1:A:585:TRP:CZ3	2.55	0.90
2:B:1790:ILE:HG12	2:B:1817:TRP:CZ3	2.07	0.90
2:B:1934:MET:CB	2:B:2016:VAL:HB	2.02	0.89
2:B:1983:PHE:O	2:B:1984:GLU:HB2	1.71	0.89
2:B:2264:SER:CB	2:B:2301:LEU:HD21	2.01	0.89
1:A:621:VAL:HG12	1:A:622:PHE:N	1.88	0.89
1:A:660:HIS:ND1	1:A:680:MET:HE3	1.87	0.89
2:B:2213:GLN:HA	2:B:2217:ASN:HD22	1.38	0.89
1:A:656:TYR:CE1	2:B:1791:SER:HB2	2.08	0.89
1:A:670:LEU:HD12	1:A:671:PHE:H	1.36	0.89
1:A:105:TYR:CB	1:A:109:SER:HB3	2.02	0.88
1:A:105:TYR:CD2	1:A:110:GLU:HB3	2.08	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1791:SER:O	2:B:1793:GLU:HG3	1.74	0.88
2:B:1934:MET:HE3	2:B:1940:ILE:HD13	0.90	0.88
1:A:165:VAL:HG12	1:A:206:LYS:HG2	1.54	0.88
2:B:1829:GLU:CB	2:B:1966:ARG:HD2	2.02	0.87
1:A:65:ARG:CB	1:A:66:PRO:CD	2.52	0.87
1:A:651:VAL:N	1:A:693:HIS:HB2	1.89	0.87
2:B:1819:VAL:HA	2:B:1823:MET:HE2	1.55	0.87
1:A:7:LEU:HD11	1:A:51:PHE:HB3	1.56	0.87
1:A:396:ALA:HB1	1:A:397:PRO:HA	1.57	0.86
2:B:2048:PRO:HG3	2:B:2062:TRP:CD1	2.10	0.86
2:B:2096:LEU:CB	2:B:2161:THR:HG21	2.01	0.86
1:A:147:MET:HE1	2:B:1972:LYS:HZ2	1.38	0.86
2:B:2055:TYR:HD1	2:B:2060:ASN:ND2	1.73	0.86
1:A:617:ILE:CD1	1:A:706:LEU:HD13	2.05	0.86
2:B:2262:ILE:H	2:B:2262:ILE:HD12	1.41	0.86
1:A:625:LEU:HD11	1:A:706:LEU:HD11	1.57	0.85
1:A:656:TYR:HB2	1:A:686:GLY:HA2	1.57	0.85
2:B:1707:TRP:HE1	2:B:1758:LEU:CD2	1.88	0.85
1:A:395:TYR:HE2	1:A:614:MET:HG3	1.39	0.85
1:A:656:TYR:HB2	1:A:686:GLY:CA	2.05	0.85
2:B:1829:GLU:HB2	2:B:1966:ARG:NH1	1.92	0.85
2:B:1758:LEU:CD1	2:B:1922:ASN:C	2.50	0.84
1:A:65:ARG:CB	1:A:66:PRO:HD3	2.06	0.84
2:B:1738:PHE:CE2	2:B:1747:LEU:HD12	2.12	0.84
1:A:453:LEU:CD2	1:A:533:TYR:CE2	2.61	0.84
1:A:182:GLY:O	1:A:186:LYS:HE3	1.77	0.84
1:A:705:LEU:O	1:A:706:LEU:HB2	1.77	0.84
2:B:1786:TYR:CA	2:B:1790:ILE:HD11	2.06	0.84
2:B:1830:PHE:CE1	2:B:1966:ARG:NH1	2.45	0.84
1:A:389:GLU:OE1	1:A:429:MET:CE	2.25	0.84
1:A:448:ILE:HD13	1:A:448:ILE:H	1.42	0.83
2:B:1829:GLU:HB2	2:B:1966:ARG:CD	2.07	0.83
1:A:237:TYR:CG	1:A:242:LEU:HB3	2.13	0.83
1:A:656:TYR:OH	2:B:1792:TYR:CE1	2.29	0.83
2:B:1790:ILE:HG12	2:B:1817:TRP:HZ3	1.42	0.83
1:A:141:LEU:CD2	1:A:143:GLU:HB3	2.08	0.83
1:A:696:ASP:O	1:A:699:ASN:HB2	1.77	0.83
2:B:1786:TYR:HA	2:B:1790:ILE:HD12	1.60	0.83
2:B:2180:MET:CB	2:B:2322:GLU:OE2	2.21	0.83
1:A:485:PRO:HD3	1:A:498:LEU:HD21	1.59	0.83
2:B:1707:TRP:NE1	2:B:1758:LEU:HD23	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:HIS:HB3	1:A:379:PRO:HD2	1.59	0.83
2:B:2055:TYR:HD1	2:B:2060:ASN:HD22	1.24	0.83
1:A:541:ARG:HG2	1:A:585:TRP:HE1	1.44	0.83
2:B:1732:LYS:HG2	2:B:1849:SER:O	1.78	0.83
2:B:1738:PHE:HB3	2:B:1747:LEU:HA	1.61	0.83
1:A:281:HIS:ND1	1:A:524:SER:HB3	1.94	0.83
1:A:686:GLY:O	1:A:687:LEU:HD23	1.79	0.83
1:A:649:LEU:O	1:A:695:SER:HB3	1.77	0.82
2:B:2055:TYR:HA	2:B:2060:ASN:HB3	1.60	0.82
1:A:271:LEU:HD22	1:A:274:HIS:HB2	1.61	0.82
1:A:471:ARG:HG2	1:A:585:TRP:HE3	1.41	0.82
2:B:2083:GLY:CA	2:B:2140:PHE:HD2	1.91	0.82
2:B:2264:SER:OG	2:B:2301:LEU:CD2	2.24	0.82
2:B:2330:ASP:HB3	2:B:2331:LEU:CD2	2.09	0.82
1:A:169:ASN:O	1:A:170:SER:OG	1.98	0.82
1:A:285:SER:HB2	1:A:676:GLU:OE2	1.78	0.82
1:A:287:GLU:CB	1:A:673:PHE:CD2	2.61	0.82
2:B:2262:ILE:HD12	2:B:2262:ILE:N	1.94	0.82
1:A:428:PHE:HE1	1:A:547:LEU:HB3	1.42	0.82
2:B:1934:MET:CE	2:B:1940:ILE:CD1	2.34	0.82
1:A:615:HIS:CB	1:A:703:THR:HB	2.09	0.82
2:B:1983:PHE:HD1	2:B:1984:GLU:H	1.23	0.81
2:B:2046:TRP:HZ3	2:B:2059:ILE:C	1.88	0.81
2:B:1829:GLU:CA	2:B:1966:ARG:HD2	2.10	0.81
1:A:65:ARG:HG3	1:A:66:PRO:N	1.96	0.81
2:B:1883:PHE:O	2:B:1917:ARG:HA	1.80	0.81
1:A:471:ARG:HG2	1:A:585:TRP:CZ3	2.16	0.81
2:B:1946:SER:CB	2:B:1978:LEU:HB3	2.08	0.81
1:A:471:ARG:CG	1:A:585:TRP:HZ3	1.93	0.81
2:B:1934:MET:HE1	2:B:1940:ILE:HG21	1.62	0.81
2:B:1940:ILE:HD12	2:B:1990:PRO:HD3	1.63	0.81
1:A:534:SER:HB3	1:A:536:PHE:HE1	1.45	0.81
2:B:1885:GLU:O	2:B:1887:LYS:N	2.13	0.81
1:A:575:LEU:N	1:A:618:ASN:OD1	2.14	0.81
2:B:1973:MET:HE3	2:B:1976:TYR:HB2	1.62	0.81
1:A:495:VAL:HG21	1:A:501:PHE:HB2	1.63	0.80
2:B:1934:MET:HB3	2:B:2016:VAL:CB	2.10	0.80
2:B:2306:LEU:HD23	2:B:2307:ARG:N	1.95	0.80
1:A:100:ALA:HB2	1:A:138:TRP:CE3	2.15	0.80
1:A:664:TYR:CE1	2:B:1826:THR:HG23	2.14	0.80
1:A:191:THR:OG1	1:A:193:HIS:ND1	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1736:GLN:OE1	2:B:1747:LEU:HD21	1.81	0.80
2:B:2052:ARG:N	2:B:2163:ARG:HB3	1.96	0.80
2:B:1849:SER:OG	2:B:1888:SER:HB2	1.81	0.80
2:B:2036:GLN:NE2	2:B:2076:LEU:HD11	1.96	0.80
1:A:83:THR:HG22	1:A:140:VAL:H	1.46	0.80
2:B:1909:ASP:O	2:B:1913:LYS:CB	2.30	0.80
1:A:7:LEU:HD21	1:A:51:PHE:CD2	2.17	0.80
1:A:249:HIS:NE2	1:A:303:LEU:HD11	1.97	0.79
1:A:285:SER:CB	1:A:676:GLU:OE2	2.30	0.79
2:B:2273:LEU:CD2	2:B:2280:VAL:HG23	2.12	0.79
1:A:461:LEU:HB2	1:A:513:TRP:HB2	1.63	0.79
2:B:1739:THR:H	2:B:1746:PRO:HG2	1.48	0.79
1:A:656:TYR:CG	1:A:686:GLY:HA2	2.17	0.79
2:B:1945:LEU:HD12	2:B:1945:LEU:H	1.47	0.79
1:A:293:PHE:CD1	2:B:1975:LEU:HD21	2.18	0.79
1:A:656:TYR:O	1:A:658:PHE:N	2.16	0.79
1:A:428:PHE:CE1	1:A:547:LEU:HB3	2.18	0.79
2:B:1982:VAL:O	2:B:1983:PHE:CD2	2.36	0.79
2:B:1829:GLU:HB2	2:B:1966:ARG:CZ	2.12	0.79
2:B:1790:ILE:HA	2:B:1817:TRP:CZ3	2.18	0.78
2:B:1952:ASN:HB3	2:B:1954:HIS:NE2	1.98	0.78
1:A:464:ILE:HG23	1:A:510:LYS:HG2	1.65	0.78
2:B:1865:PRO:O	2:B:1867:HIS:N	2.15	0.78
1:A:530:THR:OG1	1:A:679:PHE:HB3	1.82	0.78
1:A:647:ASP:OD1	2:B:1950:ASN:ND2	2.16	0.78
2:B:2081:ILE:HD12	2:B:2149:ILE:HD11	1.64	0.78
2:B:2329:GLN:HG3	2:B:2332:TYR:C	2.09	0.78
1:A:157:SER:HA	1:A:176:LEU:H	1.45	0.78
1:A:631:LEU:HD21	1:A:632:HIS:ND1	1.98	0.78
2:B:1813:LYS:CD	2:B:1814:THR:H	1.94	0.78
2:B:1886:THR:CG2	2:B:1913:LYS:HZ1	1.96	0.78
1:A:656:TYR:HH	2:B:1792:TYR:HE1	1.28	0.78
1:A:448:ILE:HD12	1:A:619:GLY:HA3	1.63	0.78
2:B:1886:THR:HG22	2:B:1913:LYS:NZ	1.99	0.78
2:B:1945:LEU:HG	2:B:1983:PHE:HB2	0.82	0.78
1:A:289:SER:HB3	1:A:290:PRO:CD	2.13	0.77
1:A:432:THR:HA	1:A:438:THR:OG1	1.82	0.77
2:B:1838:PHE:HZ	2:B:1947:MET:CG	1.96	0.77
1:A:526:PRO:O	1:A:679:PHE:HZ	1.67	0.77
1:A:491:LEU:C	1:A:493:LYS:H	1.91	0.77
2:B:1830:PHE:HD1	2:B:1966:ARG:HH12	0.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ALA:HB2	1:A:138:TRP:HZ3	1.49	0.77
1:A:700:ARG:HH22	2:B:1844:GLU:HB3	1.49	0.77
1:A:278:VAL:HG23	1:A:279:ARG:H	1.49	0.77
1:A:662:MET:HG3	1:A:680:MET:HE1	1.64	0.77
2:B:1699:PHE:CG	2:B:1740:ASP:OD1	2.38	0.77
1:A:529:LEU:CD1	1:A:553:ILE:HB	2.15	0.77
2:B:1863:LEU:HB2	2:B:1870:GLN:H	1.48	0.77
2:B:1891:PHE:CD1	2:B:1892:THR:N	2.40	0.77
1:A:278:VAL:HG12	1:A:296:ALA:HB2	1.67	0.77
2:B:2081:ILE:HG13	2:B:2144:ILE:HB	1.66	0.77
1:A:456:GLU:O	1:A:459:ASP:HB2	1.83	0.77
2:B:2042:GLN:HE21	2:B:2047:ALA:HA	1.47	0.77
2:B:2089:ALA:O	2:B:2096:LEU:HB2	1.85	0.77
2:B:1773:VAL:HG11	2:B:1785:PHE:CE1	2.20	0.76
2:B:2187:ASP:HB2	2:B:2206:SER:CB	2.16	0.76
2:B:2042:GLN:OE1	2:B:2042:GLN:N	2.17	0.76
1:A:529:LEU:HA	1:A:679:PHE:CE1	2.20	0.76
2:B:2234:PHE:HB2	2:B:2304:ARG:O	1.85	0.76
1:A:375:ALA:C	1:A:376:LYS:HG2	2.10	0.76
1:A:474:ASN:O	1:A:535:SER:HA	1.85	0.76
2:B:1882:ILE:HD11	2:B:1919:HIS:ND1	1.99	0.76
1:A:100:ALA:CB	1:A:138:TRP:CZ3	2.68	0.76
1:A:148:ALA:CA	1:A:180:ARG:NH2	2.49	0.76
2:B:1758:LEU:HD11	2:B:1922:ASN:C	2.10	0.76
2:B:2000:CYS:SG	2:B:2002:ILE:HD12	2.25	0.76
1:A:77:GLN:HB3	1:A:177:LEU:HD12	1.68	0.76
1:A:491:LEU:HB3	1:A:492:PRO:HD2	1.68	0.76
2:B:1751:GLU:HG3	2:B:2117:GLY:H	1.51	0.76
2:B:1789:LEU:CD2	2:B:1823:MET:HB3	2.16	0.76
2:B:1735:PHE:HE1	2:B:1851:LEU:HG	1.50	0.76
2:B:2013:LEU:HD22	2:B:2013:LEU:N	2.01	0.75
1:A:281:HIS:CE1	1:A:524:SER:HB3	2.22	0.75
1:A:613:ILE:O	1:A:613:ILE:HG13	1.85	0.75
2:B:1795:ASP:OD2	2:B:1800:ALA:HB2	1.87	0.75
1:A:382:TRP:HE1	1:A:454:TYR:HB3	1.51	0.75
1:A:622:PHE:CZ	1:A:702:MET:O	2.39	0.75
2:B:1707:TRP:CE2	2:B:1758:LEU:HD23	2.22	0.75
1:A:624:SER:C	1:A:625:LEU:HD12	2.10	0.75
1:A:287:GLU:CA	1:A:673:PHE:HE2	2.00	0.74
1:A:688:TRP:CZ2	2:B:1799:GLY:HA2	2.22	0.74
2:B:1731:LYS:H	2:B:1893:GLU:CD	1.96	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2027:MET:HB3	2:B:2165:GLU:HG2	1.67	0.74
1:A:668:LEU:HG	2:B:1788:SER:OG	1.86	0.74
2:B:1758:LEU:HD12	2:B:1922:ASN:C	2.12	0.74
1:A:311:HIS:O	1:A:312:ILE:HG12	1.87	0.74
1:A:454:TYR:HE1	1:A:456:GLU:HG2	1.50	0.74
1:A:651:VAL:HG13	1:A:668:LEU:HA	1.67	0.74
2:B:1743:PHE:CE1	2:B:1778:GLN:CD	2.57	0.74
2:B:2034:ASP:CB	2:B:2049:LYS:HD2	2.17	0.74
1:A:662:MET:HG3	1:A:680:MET:CE	2.17	0.74
1:A:385:TYR:CD2	1:A:436:PHE:O	2.40	0.74
1:A:503:ILE:O	1:A:504:LEU:HD12	1.86	0.74
1:A:393:TRP:CD1	1:A:395:TYR:HE1	2.05	0.74
1:A:105:TYR:O	1:A:106:TRP:HB2	1.86	0.74
2:B:1738:PHE:HD2	2:B:1747:LEU:CD1	1.87	0.74
1:A:306:PHE:N	1:A:306:PHE:CD1	2.40	0.73
1:A:453:LEU:HD21	1:A:533:TYR:HE2	1.49	0.73
1:A:90:ASN:OD1	1:A:92:ALA:HB3	1.87	0.73
1:A:105:TYR:CE2	1:A:110:GLU:HB3	2.23	0.73
2:B:1997:ARG:HD2	2:B:2011:SER:OG	1.88	0.73
1:A:471:ARG:CG	1:A:585:TRP:CE3	2.67	0.73
1:A:480:ILE:HG22	1:A:481:THR:N	2.03	0.73
1:A:471:ARG:HG3	1:A:585:TRP:HZ3	1.53	0.73
1:A:617:ILE:HD11	1:A:705:LEU:O	1.88	0.73
2:B:1964:THR:O	2:B:1986:VAL:CG1	2.36	0.73
1:A:148:ALA:HA	1:A:180:ARG:HH22	1.53	0.73
2:B:1889:TRP:HA	2:B:1889:TRP:CE3	2.22	0.73
1:A:123:LYS:HA	1:A:126:ASP:HB2	1.69	0.73
1:A:389:GLU:OE1	1:A:431:TYR:CZ	2.42	0.72
1:A:495:VAL:HG22	1:A:496:LYS:N	2.04	0.72
2:B:1759:LEU:HD22	2:B:1854:PRO:HG3	1.71	0.72
2:B:1891:PHE:HD1	2:B:1892:THR:H	0.80	0.72
2:B:2081:ILE:HA	2:B:2168:GLY:HA3	1.71	0.72
1:A:412:LEU:HA	1:A:420:GLY:HA3	1.72	0.72
1:A:65:ARG:HG3	1:A:66:PRO:CD	2.17	0.72
1:A:114:TYR:O	1:A:116:ASP:N	2.22	0.72
1:A:653:PHE:HB2	1:A:693:HIS:HE1	1.55	0.72
1:A:664:TYR:CD1	2:B:1826:THR:HG23	2.25	0.72
1:A:416:PRO:HA	1:A:596:PRO:HG3	1.71	0.72
2:B:1997:ARG:HG2	2:B:1999:GLU:HG3	1.72	0.72
2:B:2032:ILE:CG2	2:B:2036:GLN:OE1	2.30	0.72
2:B:2036:GLN:HG2	2:B:2076:LEU:HD21	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:ARG:NH1	2:B:1843:LEU:HB3	2.05	0.72
2:B:1830:PHE:HD2	2:B:1985:THR:HG1	1.34	0.72
1:A:50:LEU:HB3	1:A:171:GLY:HA3	1.72	0.71
1:A:663:VAL:HG13	2:B:1968:LYS:HB2	1.72	0.71
1:A:473:TYR:CD2	1:A:547:LEU:HD11	2.25	0.71
1:A:651:VAL:CG1	1:A:668:LEU:HA	2.19	0.71
2:B:1963:PHE:CG	2:B:1986:VAL:HG11	2.24	0.71
1:A:375:ALA:O	1:A:376:LYS:HG2	1.90	0.71
1:A:616:SER:O	1:A:620:TYR:N	2.21	0.71
2:B:1707:TRP:HA	2:B:1707:TRP:CE3	2.26	0.71
2:B:1943:TYR:C	2:B:1944:LEU:HD23	2.15	0.71
1:A:98:LEU:HB3	1:A:136:TYR:CZ	2.25	0.71
1:A:605:ASP:O	1:A:609:GLN:HG3	1.91	0.71
2:B:2055:TYR:CD1	2:B:2060:ASN:ND2	2.55	0.71
2:B:2273:LEU:CD2	2:B:2280:VAL:HG21	2.12	0.71
1:A:4:ARG:HG3	1:A:85:VAL:HG23	1.71	0.71
1:A:420:GLY:O	1:A:421:ARG:HG2	1.91	0.71
2:B:1789:LEU:N	2:B:1789:LEU:HD12	2.06	0.71
2:B:1878:LEU:HA	2:B:1922:ASN:HD21	1.55	0.71
2:B:2087:GLN:HG2	2:B:2163:ARG:CD	2.20	0.71
2:B:2149:ILE:HD12	2:B:2166:LEU:HD22	1.72	0.71
1:A:667:THR:O	1:A:669:THR:N	2.24	0.71
1:A:667:THR:OG1	1:A:668:LEU:N	2.24	0.71
2:B:2097:TYR:CZ	2:B:2157:SER:OG	2.41	0.70
2:B:2264:SER:HB3	2:B:2301:LEU:CD2	2.21	0.70
1:A:428:PHE:HE2	1:A:475:ILE:HG12	1.55	0.70
1:A:663:VAL:CG1	2:B:1968:LYS:HB2	2.21	0.70
2:B:1786:TYR:CA	2:B:1790:ILE:CD1	2.58	0.70
1:A:147:MET:CE	2:B:1972:LYS:HE3	2.21	0.70
2:B:1819:VAL:HA	2:B:1823:MET:CE	2.21	0.70
2:B:1945:LEU:HA	2:B:1983:PHE:CA	2.15	0.70
5:E:3:BMA:O3	5:E:5:MAN:C1	2.39	0.70
1:A:646:THR:OG1	2:B:1950:ASN:OD1	2.09	0.70
1:A:522:THR:N	1:A:525:ASP:OD1	2.24	0.70
2:B:1735:PHE:HE1	2:B:1851:LEU:CG	2.04	0.70
1:A:412:LEU:HA	1:A:420:GLY:CA	2.21	0.70
2:B:1973:MET:HE1	2:B:1976:TYR:CD1	2.25	0.70
1:A:287:GLU:HG2	1:A:673:PHE:HD2	1.57	0.70
2:B:1948:GLY:HA3	2:B:1952:ASN:HD21	1.57	0.70
2:B:2051:ALA:HA	2:B:2163:ARG:HA	1.73	0.70
1:A:147:MET:O	1:A:148:ALA:HB3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:VAL:HB	1:A:693:HIS:CE1	2.26	0.70
1:A:287:GLU:CG	1:A:673:PHE:CD2	2.75	0.69
1:A:534:SER:HB3	1:A:536:PHE:CE1	2.27	0.69
2:B:2306:LEU:CD2	2:B:2307:ARG:N	2.55	0.69
2:B:1997:ARG:CD	2:B:2011:SER:OG	2.41	0.69
2:B:1763:ILE:HG23	2:B:1855:LEU:HG	1.73	0.69
1:A:616:SER:O	1:A:617:ILE:HG22	1.93	0.69
2:B:1834:ALA:O	2:B:1945:LEU:HD21	1.91	0.69
2:B:2034:ASP:HB3	2:B:2049:LYS:CD	2.22	0.69
2:B:1945:LEU:H	2:B:1945:LEU:CD1	2.05	0.69
2:B:1838:PHE:CZ	2:B:1947:MET:CG	2.75	0.69
1:A:287:GLU:CG	1:A:673:PHE:HD2	2.05	0.69
1:A:395:TYR:CE2	1:A:614:MET:HG3	2.26	0.69
1:A:486:LEU:O	1:A:487:TYR:HB2	1.92	0.69
1:A:7:LEU:HD12	1:A:52:VAL:O	1.91	0.68
1:A:249:HIS:CD2	1:A:303:LEU:HD11	2.27	0.68
1:A:289:SER:HB3	1:A:290:PRO:HD2	1.73	0.68
1:A:454:TYR:CE1	1:A:456:GLU:HG2	2.28	0.68
1:A:687:LEU:HD12	2:B:1795:ASP:OD2	1.93	0.68
1:A:688:TRP:HE1	2:B:1799:GLY:C	2.01	0.68
2:B:1849:SER:CB	2:B:1888:SER:HB2	2.23	0.68
1:A:495:VAL:HG22	1:A:496:LYS:H	1.58	0.68
2:B:1963:PHE:HB2	2:B:1986:VAL:CG1	2.23	0.68
1:A:127:LYS:HG3	1:A:162:VAL:HG11	1.74	0.68
1:A:272:GLU:HB3	1:A:306:PHE:HB3	1.73	0.68
1:A:281:HIS:HB3	1:A:525:ASP:HB3	1.73	0.68
1:A:396:ALA:HB1	1:A:397:PRO:CA	2.23	0.68
2:B:2273:LEU:O	2:B:2275:PHE:CD1	2.47	0.68
2:B:1889:TRP:HA	2:B:1889:TRP:HE3	1.57	0.68
1:A:432:THR:OG1	1:A:440:GLU:CB	2.40	0.68
1:A:587:LEU:O	1:A:591:ILE:HG22	1.94	0.68
1:A:684:ASN:O	1:A:686:GLY:N	2.23	0.68
2:B:1776:ARG:HG2	2:B:1812:THR:HG22	1.76	0.68
1:A:65:ARG:HB3	1:A:66:PRO:CD	2.23	0.68
2:B:1831:ASP:O	2:B:1858:CYS:HB3	1.94	0.68
2:B:1838:PHE:CZ	2:B:1947:MET:SD	2.87	0.68
2:B:1942:TRP:HB3	2:B:1944:LEU:HD21	1.75	0.68
1:A:428:PHE:HE2	1:A:475:ILE:CG1	2.06	0.68
1:A:457:VAL:CG1	1:A:517:VAL:HA	2.24	0.68
1:A:57:HIS:HB2	1:A:89:LYS:HZ1	1.59	0.67
1:A:57:HIS:O	1:A:58:LEU:HG	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:HD22	1:A:143:GLU:HB3	1.75	0.67
1:A:480:ILE:CG2	1:A:481:THR:H	2.06	0.67
1:A:642:ILE:HG22	1:A:643:GLY:N	2.06	0.67
2:B:2262:ILE:HD11	2:B:2283:PHE:CE1	2.28	0.67
1:A:97:SER:O	1:A:160:SER:HB3	1.94	0.67
1:A:605:ASP:OD2	1:A:607:GLU:HB3	1.93	0.67
2:B:2042:GLN:HB3	2:B:2062:TRP:HE1	1.59	0.67
1:A:696:ASP:O	1:A:699:ASN:CB	2.42	0.67
2:B:2273:LEU:O	2:B:2275:PHE:CE1	2.48	0.67
1:A:581:GLU:HB2	1:A:612:ASN:O	1.95	0.67
1:A:617:ILE:HG12	1:A:706:LEU:CD2	2.25	0.67
1:A:700:ARG:CZ	2:B:1844:GLU:HB2	2.24	0.67
1:A:477:PRO:HG3	1:A:513:TRP:CE2	2.29	0.67
2:B:1784:SER:O	2:B:1839:SER:HA	1.94	0.67
2:B:2096:LEU:HD12	2:B:2159:ARG:HB3	1.77	0.67
1:A:72:LEU:HG	1:A:198:LEU:HD12	1.76	0.67
1:A:538:ASN:HD21	1:A:541:ARG:HB3	1.60	0.67
1:A:428:PHE:CE2	1:A:475:ILE:HG12	2.30	0.67
2:B:2249:LYS:HE3	2:B:2249:LYS:H	1.59	0.67
1:A:700:ARG:NH1	2:B:1844:GLU:HB2	2.10	0.67
1:A:270:PHE:HB2	1:A:309:PHE:HE1	1.59	0.66
1:A:448:ILE:HD13	1:A:448:ILE:N	2.10	0.66
1:A:640:LEU:CB	1:A:677:THR:HB	2.25	0.66
2:B:1837:TYR:CZ	2:B:1853:GLY:HA3	2.30	0.66
2:B:2087:GLN:HG2	2:B:2163:ARG:HD3	1.75	0.66
1:A:94:HIS:HB3	1:A:96:VAL:HG13	1.77	0.66
2:B:1735:PHE:CE1	2:B:1851:LEU:HB2	2.30	0.66
2:B:1849:SER:OG	2:B:1888:SER:CB	2.42	0.66
2:B:1945:LEU:CA	2:B:1983:PHE:HA	2.15	0.66
1:A:457:VAL:HG11	1:A:517:VAL:HA	1.76	0.66
1:A:687:LEU:CD1	2:B:1795:ASP:OD2	2.43	0.66
1:A:700:ARG:HH12	2:B:1844:GLU:HB2	1.59	0.66
2:B:1946:SER:HB2	2:B:1978:LEU:HD12	1.74	0.66
2:B:2036:GLN:HE21	2:B:2076:LEU:HD11	1.59	0.66
1:A:448:ILE:CD1	1:A:618:ASN:O	2.44	0.66
1:A:577:SER:O	1:A:616:SER:HB3	1.96	0.66
2:B:2022:GLN:HG3	2:B:2082:HIS:ND1	2.10	0.66
2:B:2031:HIS:HB2	2:B:2294:VAL:HG11	1.78	0.66
1:A:272:GLU:HB2	1:A:307:LEU:H	1.60	0.66
1:A:473:TYR:HA	1:A:537:VAL:CG2	2.25	0.66
1:A:697:PHE:CE1	1:A:698:ARG:HB2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:VAL:HA	1:A:140:VAL:CG1	2.25	0.66
2:B:1774:THR:HG22	2:B:1814:THR:CG2	2.25	0.66
2:B:2331:LEU:O	2:B:2332:TYR:HB2	1.95	0.66
1:A:651:VAL:HB	1:A:693:HIS:ND1	2.11	0.65
2:B:2023:THR:HB	2:B:2176:MET:HE3	1.78	0.65
1:A:657:THR:O	1:A:658:PHE:HB2	1.94	0.65
1:A:114:TYR:CE2	2:B:1997:ARG:HD3	2.31	0.65
1:A:293:PHE:HD1	2:B:1975:LEU:HD21	1.58	0.65
1:A:664:TYR:OH	2:B:1825:PRO:HA	1.95	0.65
1:A:670:LEU:HG	1:A:672:PRO:HD3	1.79	0.65
2:B:1997:ARG:HG2	2:B:1999:GLU:CG	2.26	0.65
2:B:2129:ASN:HB3	2:B:2134:GLY:HA3	1.78	0.65
1:A:398:LEU:CD2	1:A:399:VAL:HG12	2.23	0.65
1:A:417:GLN:O	1:A:418:ARG:HG2	1.97	0.65
1:A:542:ASP:O	1:A:545:SER:N	2.29	0.65
1:A:623:ASP:OD1	1:A:705:LEU:CB	2.45	0.65
2:B:1749:ARG:HG2	2:B:1749:ARG:HH11	1.62	0.65
2:B:2220:ARG:HH11	2:B:2220:ARG:HB2	1.62	0.65
1:A:87:THR:HG22	1:A:135:THR:CB	2.27	0.65
1:A:473:TYR:HA	1:A:537:VAL:HG22	1.79	0.65
1:A:234:VAL:HG23	1:A:320:MET:HA	1.79	0.65
1:A:417:GLN:HE22	1:A:602:GLN:HB2	1.62	0.65
1:A:656:TYR:CB	1:A:686:GLY:CA	2.67	0.65
2:B:1738:PHE:CE2	2:B:1747:LEU:CD1	2.79	0.65
1:A:278:VAL:HG23	1:A:279:ARG:N	2.10	0.64
2:B:1735:PHE:CD1	2:B:1851:LEU:HB2	2.31	0.64
1:A:390:GLU:OE2	1:A:470:SER:HB2	1.96	0.64
1:A:378:HIS:HB3	1:A:379:PRO:CD	2.25	0.64
1:A:530:THR:O	1:A:531:ARG:NE	2.31	0.64
1:A:486:LEU:HD22	1:A:487:TYR:CG	2.32	0.64
1:A:617:ILE:HG12	1:A:706:LEU:HD22	1.80	0.64
2:B:2046:TRP:CD1	2:B:2159:ARG:HH22	2.15	0.64
1:A:292:THR:HG23	2:B:1977:ASN:HD21	1.61	0.64
1:A:620:TYR:C	1:A:621:VAL:HG23	2.22	0.64
2:B:2276:GLN:N	2:B:2279:LYS:O	2.28	0.64
1:A:116:ASP:OD1	1:A:118:THR:HG22	1.98	0.64
2:B:2051:ALA:HB1	2:B:2164:MET:N	2.10	0.64
1:A:166:LYS:O	1:A:207:SER:HB2	1.98	0.64
1:A:686:GLY:O	1:A:687:LEU:CD2	2.45	0.64
1:A:654:SER:HB2	1:A:690:LEU:HB2	1.80	0.64
2:B:2054:HIS:O	2:B:2060:ASN:CB	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2263:SER:HB2	2:B:2307:ARG:HB3	1.79	0.64
1:A:121:ARG:HG3	1:A:121:ARG:HH11	1.63	0.64
1:A:271:LEU:HD22	1:A:274:HIS:CB	2.27	0.64
2:B:1829:GLU:HB2	2:B:1966:ARG:NE	2.13	0.64
2:B:1934:MET:HE3	2:B:1940:ILE:HD11	1.68	0.64
2:B:2105:TYR:CD2	2:B:2144:ILE:HG23	2.33	0.64
1:A:260:MET:HE2	1:A:260:MET:HA	1.80	0.63
1:A:475:ILE:HG23	1:A:475:ILE:O	1.97	0.63
2:B:1787:SER:OG	2:B:1788:SER:N	2.30	0.63
2:B:1837:TYR:CE2	2:B:1853:GLY:HA3	2.34	0.63
2:B:1976:TYR:CE2	2:B:1984:GLU:OE2	2.50	0.63
1:A:271:LEU:HD11	1:A:324:VAL:HG11	1.80	0.63
2:B:1743:PHE:CZ	2:B:1778:GLN:NE2	2.65	0.63
2:B:2046:TRP:CZ3	2:B:2060:ASN:N	2.51	0.63
1:A:448:ILE:H	1:A:448:ILE:CD1	2.10	0.63
2:B:2080:ILE:HG12	2:B:2170:ASP:O	1.98	0.63
1:A:697:PHE:CG	1:A:698:ARG:N	2.58	0.63
2:B:1758:LEU:CD1	2:B:1923:GLY:N	2.54	0.63
2:B:1953:ILE:HD12	2:B:1953:ILE:H	1.63	0.63
1:A:389:GLU:OE1	1:A:429:MET:HE3	1.99	0.63
1:A:509:PHE:HD1	1:A:510:LYS:H	1.47	0.63
1:A:147:MET:HE1	2:B:1972:LYS:CE	2.27	0.63
2:B:2052:ARG:H	2:B:2163:ARG:CB	2.07	0.63
1:A:305:GLN:C	1:A:306:PHE:HD1	2.07	0.63
1:A:623:ASP:OD1	1:A:705:LEU:HB2	1.98	0.63
2:B:1939:ARG:NH2	2:B:1987:GLU:OE1	2.21	0.63
2:B:1997:ARG:HD2	2:B:2011:SER:HG	1.64	0.62
2:B:1889:TRP:CZ3	2:B:1890:TYR:HB2	2.34	0.62
2:B:2178:LEU:HD12	2:B:2323:VAL:HB	1.80	0.62
1:A:271:LEU:CD2	1:A:274:HIS:HB2	2.28	0.62
1:A:153:CYS:N	1:A:179:CYS:SG	2.58	0.62
1:A:658:PHE:C	1:A:659:LYS:HD3	2.24	0.62
2:B:1934:MET:HE1	2:B:1940:ILE:HD13	1.70	0.62
2:B:2115:TYR:CE2	2:B:2140:PHE:HD1	2.17	0.62
2:B:2207:LYS:HD2	2:B:2216:SER:O	1.99	0.62
1:A:453:LEU:HD22	1:A:453:LEU:H	1.63	0.62
1:A:651:VAL:HG12	1:A:652:PHE:N	2.15	0.62
2:B:2042:GLN:HE21	2:B:2047:ALA:CA	2.12	0.62
2:B:2283:PHE:HD2	2:B:2295:ASN:HD22	1.47	0.62
1:A:656:TYR:CE2	2:B:1791:SER:HB2	2.35	0.62
2:B:2330:ASP:CB	2:B:2331:LEU:HD23	2.21	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LEU:HD22	1:A:453:LEU:N	2.15	0.62
2:B:1963:PHE:HB2	2:B:1986:VAL:HG12	1.81	0.62
1:A:457:VAL:HG11	1:A:517:VAL:HG23	1.81	0.62
2:B:2193:SER:HA	2:B:2229:TRP:CZ2	2.34	0.62
1:A:512:LYS:HE3	1:A:514:THR:OG1	2.00	0.61
2:B:1929:LEU:HB3	2:B:2012:THR:OG1	2.00	0.61
2:B:2087:GLN:HG2	2:B:2163:ARG:NE	2.15	0.61
1:A:651:VAL:HB	1:A:693:HIS:CG	2.35	0.61
2:B:1705:ARG:HG2	2:B:1706:LEU:H	1.64	0.61
2:B:1758:LEU:CD1	2:B:1922:ASN:O	2.48	0.61
2:B:1840:ASP:O	2:B:1841:VAL:HG23	1.99	0.61
1:A:56:ASP:O	1:A:57:HIS:HB3	2.00	0.61
1:A:473:TYR:O	1:A:504:LEU:CD1	2.49	0.61
1:A:529:LEU:HA	1:A:679:PHE:CD1	2.34	0.61
1:A:625:LEU:HD13	1:A:706:LEU:CD2	2.30	0.61
1:A:693:HIS:HB3	1:A:695:SER:HB2	1.81	0.61
2:B:1829:GLU:HB2	2:B:1966:ARG:HH11	1.63	0.61
1:A:282:ARG:HH12	1:A:299:LEU:HD22	1.65	0.61
2:B:1952:ASN:OD1	2:B:1952:ASN:N	2.32	0.61
2:B:2087:GLN:CG	2:B:2163:ARG:HD3	2.30	0.61
1:A:2:THR:OG1	1:A:83:THR:O	2.18	0.61
1:A:507:GLU:HG3	1:A:508:ILE:H	1.65	0.61
1:A:664:TYR:HE1	2:B:1826:THR:HG23	1.64	0.61
2:B:1732:LYS:HE3	2:B:1885:GLU:OE2	2.00	0.61
1:A:87:THR:HG22	1:A:135:THR:HB	1.83	0.61
1:A:615:HIS:HB2	1:A:703:THR:OG1	2.01	0.61
2:B:2193:SER:HB3	2:B:2229:TRP:CD1	2.35	0.61
1:A:291:ILE:HG23	2:B:1955:SER:CB	2.31	0.61
2:B:2083:GLY:CA	2:B:2140:PHE:CD2	2.72	0.61
1:A:85:VAL:HG12	1:A:137:VAL:HA	1.82	0.61
1:A:631:LEU:HD23	1:A:632:HIS:HB2	1.83	0.61
2:B:2052:ARG:HD2	2:B:2165:GLU:HB2	1.78	0.61
1:A:308:LEU:O	1:A:309:PHE:HB3	2.00	0.61
1:A:624:SER:HB2	1:A:625:LEU:HD12	1.83	0.61
1:A:645:GLN:CD	1:A:645:GLN:H	2.09	0.61
2:B:1951:GLU:O	2:B:1953:ILE:HD12	2.00	0.61
1:A:417:GLN:C	1:A:418:ARG:HG2	2.26	0.60
1:A:287:GLU:CA	1:A:673:PHE:CE2	2.80	0.60
1:A:395:TYR:HB2	1:A:621:VAL:CG2	2.11	0.60
2:B:1934:MET:O	2:B:1935:ALA:HB3	2.00	0.60
2:B:1979:TYR:O	2:B:1980:PRO:C	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2087:GLN:CG	2:B:2163:ARG:HB2	2.31	0.60
1:A:302:ASP:C	1:A:303:LEU:HD12	2.26	0.60
2:B:2245:THR:C	2:B:2286:ASN:ND2	2.56	0.60
1:A:664:TYR:HE1	2:B:1826:THR:H	1.46	0.60
2:B:2024:PRO:HA	2:B:2167:MET:HG2	1.84	0.60
2:B:1711:MET:HE3	2:B:1711:MET:HA	1.83	0.60
2:B:1829:GLU:CB	2:B:1966:ARG:NH1	2.64	0.60
2:B:1856:LEU:HD13	2:B:1943:TYR:CE2	2.37	0.60
1:A:697:PHE:CD1	1:A:698:ARG:N	2.57	0.60
2:B:2180:MET:H	2:B:2185:ILE:HB	1.67	0.60
1:A:622:PHE:CE1	1:A:702:MET:C	2.78	0.60
1:A:694:ASN:ND2	1:A:703:THR:O	2.34	0.60
2:B:1865:PRO:C	2:B:1867:HIS:H	2.07	0.60
1:A:237:TYR:CD2	1:A:242:LEU:HB3	2.36	0.60
1:A:688:TRP:NE1	2:B:1800:ALA:N	2.46	0.60
2:B:1912:PHE:O	2:B:1915:ASN:HB2	2.02	0.60
2:B:1962:VAL:HG12	2:B:1974:ALA:HB2	1.83	0.60
2:B:2302:LEU:O	2:B:2302:LEU:HD23	2.01	0.60
1:A:112:ALA:O	1:A:126:ASP:HB3	2.01	0.60
1:A:625:LEU:HD12	1:A:706:LEU:CD1	2.31	0.60
2:B:1767:VAL:O	2:B:1768:GLU:HB2	2.01	0.60
2:B:1774:THR:HG22	2:B:1814:THR:HG22	1.83	0.60
2:B:1875:GLU:OE1	2:B:1943:TYR:OH	2.18	0.60
1:A:312:ILE:HD12	1:A:315:HIS:ND1	2.17	0.60
1:A:393:TRP:CD1	1:A:395:TYR:CE1	2.90	0.60
2:B:1870:GLN:OE1	2:B:1872:THR:N	2.31	0.60
2:B:1945:LEU:HD12	2:B:1945:LEU:N	2.17	0.60
1:A:10:VAL:CG2	1:A:52:VAL:HG21	2.30	0.59
1:A:237:TYR:CE1	1:A:242:LEU:HB2	2.36	0.59
1:A:398:LEU:O	1:A:400:LEU:HD23	2.02	0.59
2:B:1735:PHE:CE1	2:B:1851:LEU:HD23	2.36	0.59
1:A:147:MET:HE3	2:B:1972:LYS:HE3	1.83	0.59
1:A:657:THR:HB	2:B:1788:SER:O	2.01	0.59
2:B:1842:ASP:O	2:B:1846:ASP:OD1	2.20	0.59
1:A:658:PHE:CZ	1:A:684:ASN:ND2	2.70	0.59
2:B:1733:VAL:O	2:B:1850:GLY:C	2.45	0.59
2:B:1842:ASP:HB2	2:B:1846:ASP:OD2	2.01	0.59
1:A:8:GLY:HA3	1:A:52:VAL:CG2	2.32	0.59
1:A:72:LEU:HD11	1:A:198:LEU:HB2	1.85	0.59
1:A:147:MET:O	1:A:148:ALA:CB	2.49	0.59
2:B:1787:SER:H	2:B:1790:ILE:CD1	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2075:LEU:HD22	2:B:2079:MET:HE3	1.83	0.59
1:A:529:LEU:HD11	1:A:553:ILE:HB	1.84	0.59
1:A:155:THR:HG22	1:A:256:HIS:ND1	2.17	0.59
1:A:483:VAL:HG13	1:A:513:TRP:HD1	1.67	0.59
1:A:495:VAL:CG2	1:A:496:LYS:H	2.16	0.59
1:A:623:ASP:OD1	1:A:705:LEU:HG	2.03	0.59
2:B:2213:GLN:HA	2:B:2217:ASN:ND2	2.12	0.59
1:A:386:ILE:HD11	1:A:428:PHE:HD2	1.68	0.59
1:A:685:PRO:HG2	2:B:1822:HIS:HE1	1.68	0.59
1:A:688:TRP:CE2	2:B:1799:GLY:HA2	2.38	0.59
1:A:393:TRP:O	1:A:422:LYS:HA	2.02	0.59
2:B:1849:SER:CA	2:B:1888:SER:HB2	2.33	0.59
1:A:395:TYR:CB	1:A:621:VAL:HG23	1.97	0.59
1:A:624:SER:HB2	1:A:625:LEU:CD1	2.33	0.59
2:B:1989:LEU:HG	2:B:1989:LEU:O	2.03	0.59
1:A:3:ARG:HH22	1:A:79:GLU:CD	2.11	0.58
1:A:498:LEU:O	1:A:502:PRO:HD2	2.02	0.58
2:B:1735:PHE:CE1	2:B:1851:LEU:CG	2.85	0.58
2:B:1976:TYR:CE2	2:B:1984:GLU:CD	2.80	0.58
2:B:1976:TYR:HE2	2:B:1984:GLU:OE1	1.86	0.58
2:B:2220:ARG:HH11	2:B:2220:ARG:CB	2.16	0.58
2:B:1836:ALA:HB2	2:B:1945:LEU:HD23	1.84	0.58
2:B:1934:MET:O	2:B:1935:ALA:CB	2.51	0.58
1:A:423:TYR:CE2	1:A:581:GLU:HG3	2.39	0.58
1:A:382:TRP:CD1	1:A:454:TYR:O	2.57	0.58
2:B:2198:ASN:OD1	2:B:2199:MET:N	2.36	0.58
1:A:141:LEU:HD23	1:A:143:GLU:N	2.06	0.58
1:A:263:THR:OG1	1:A:264:PRO:HD2	2.03	0.58
1:A:5:TYR:HE2	1:A:76:ILE:CB	1.99	0.58
1:A:147:MET:CE	2:B:1972:LYS:CE	2.81	0.58
2:B:1789:LEU:HD12	2:B:1789:LEU:H	1.66	0.58
1:A:389:GLU:OE1	1:A:429:MET:HE1	2.01	0.58
1:A:509:PHE:HB3	1:A:511:TYR:HE1	1.69	0.58
2:B:1813:LYS:CD	2:B:1814:THR:N	2.54	0.58
1:A:242:LEU:HD12	1:A:243:PRO:O	2.04	0.58
1:A:652:PHE:O	1:A:657:THR:O	2.22	0.58
2:B:2248:VAL:O	2:B:2255:MET:HG2	2.03	0.58
2:B:2273:LEU:HD22	2:B:2280:VAL:HB	1.85	0.58
2:B:1925:ILE:O	2:B:1928:THR:OG1	2.22	0.58
2:B:2084:ILE:HD11	2:B:2164:MET:SD	2.44	0.58
2:B:2265:SER:HB3	2:B:2267:ASP:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLU:HG3	1:A:82:ASP:HB2	1.85	0.57
2:B:1952:ASN:HB3	2:B:1954:HIS:HE2	1.69	0.57
2:B:2102:ILE:HG21	2:B:2123:LEU:HD22	1.85	0.57
1:A:688:TRP:HE1	2:B:1800:ALA:H	1.50	0.57
5:E:2:NAG:H61	5:E:3:BMA:H2	1.84	0.57
1:A:292:THR:HG23	2:B:1977:ASN:ND2	2.19	0.57
1:A:313:SER:O	1:A:316:GLN:NE2	2.37	0.57
2:B:1863:LEU:CB	2:B:1870:GLN:H	2.14	0.57
2:B:1755:HIS:CD2	2:B:1876:PHE:HD1	2.21	0.57
2:B:1983:PHE:CG	2:B:1984:GLU:N	2.72	0.57
1:A:693:HIS:CD2	1:A:695:SER:HB2	2.40	0.57
2:B:1947:MET:CE	2:B:1948:GLY:N	2.47	0.57
2:B:1977:ASN:N	2:B:1977:ASN:OD1	2.36	0.57
1:A:191:THR:OG1	1:A:193:HIS:CG	2.58	0.57
2:B:1755:HIS:HB3	2:B:1931:GLY:O	2.04	0.57
1:A:10:VAL:HG23	1:A:52:VAL:CG2	2.31	0.57
1:A:157:SER:HA	1:A:176:LEU:N	2.18	0.57
1:A:409:SER:OG	1:A:413:ASN:OD1	2.12	0.57
1:A:432:THR:HB	1:A:433:ASP:OD1	2.04	0.57
1:A:471:ARG:HB3	1:A:585:TRP:CZ3	2.40	0.57
2:B:1840:ASP:O	2:B:1841:VAL:CB	2.52	0.57
1:A:308:LEU:HD12	1:A:308:LEU:C	2.30	0.57
1:A:492:PRO:HG2	1:A:495:VAL:HG12	1.87	0.57
2:B:1756:LEU:N	2:B:1756:LEU:HD23	2.19	0.57
2:B:2061:ALA:HB2	2:B:2163:ARG:HG3	1.86	0.57
1:A:401:ALA:HB1	1:A:405:ARG:HG3	1.86	0.57
1:A:580:ASP:C	1:A:582:ASN:H	2.13	0.57
2:B:2030:GLY:HA3	2:B:2293:VAL:HG23	1.87	0.57
2:B:2105:TYR:HA	2:B:2148:TYR:O	2.05	0.57
1:A:57:HIS:CB	1:A:89:LYS:NZ	2.64	0.56
1:A:197:LEU:HD12	1:A:255:TRP:HB3	1.87	0.56
1:A:642:ILE:CG2	1:A:643:GLY:H	2.12	0.56
2:B:1763:ILE:HG23	2:B:1763:ILE:O	2.05	0.56
1:A:97:SER:O	1:A:160:SER:CB	2.54	0.56
1:A:577:SER:O	1:A:616:SER:CB	2.53	0.56
1:A:617:ILE:O	1:A:618:ASN:CB	2.41	0.56
2:B:2072:LYS:HA	2:B:2150:ARG:HA	1.86	0.56
1:A:49:THR:H	1:A:170:SER:HB2	1.71	0.56
1:A:89:LYS:CD	1:A:91:MET:HE3	2.36	0.56
1:A:184:LEU:HD23	1:A:187:GLU:HB3	1.86	0.56
1:A:453:LEU:HD21	1:A:533:TYR:CD2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:VAL:HG13	1:A:513:TRP:CD1	2.40	0.56
1:A:625:LEU:CD1	1:A:706:LEU:HG	2.29	0.56
2:B:1781:ARG:O	2:B:1781:ARG:HG3	2.04	0.56
2:B:1948:GLY:HA3	2:B:1952:ASN:ND2	2.21	0.56
2:B:2021:CYS:O	2:B:2169:CYS:SG	2.63	0.56
1:A:667:THR:HG23	1:A:668:LEU:HD12	1.88	0.56
2:B:1786:TYR:CA	2:B:1790:ILE:HD12	2.32	0.56
2:B:1940:ILE:CD1	2:B:1990:PRO:HD3	2.35	0.56
2:B:2043:TYR:HB3	2:B:2065:LYS:HG2	1.86	0.56
2:B:2170:ASP:OD1	2:B:2171:LEU:HD12	2.05	0.56
2:B:1749:ARG:HG2	2:B:1749:ARG:NH1	2.21	0.56
2:B:1766:GLU:CD	2:B:1860:THR:O	2.49	0.56
2:B:2200:PHE:CE1	2:B:2215:ARG:HD3	2.40	0.56
1:A:453:LEU:O	1:A:551:LEU:HD12	2.06	0.56
1:A:640:LEU:HB3	1:A:677:THR:HB	1.86	0.56
2:B:1709:TYR:CE2	2:B:1924:TYR:HA	2.41	0.56
2:B:1732:LYS:CG	2:B:1849:SER:O	2.51	0.56
2:B:1918:PHE:HA	2:B:1925:ILE:HD12	1.86	0.56
2:B:2027:MET:HE3	2:B:2032:ILE:CD1	2.20	0.56
2:B:2097:TYR:CE1	2:B:2157:SER:OG	2.58	0.56
1:A:648:PHE:O	1:A:671:PHE:HA	2.05	0.56
1:A:684:ASN:C	1:A:686:GLY:H	2.13	0.56
2:B:1764:ARG:NH1	2:B:1875:GLU:OE2	2.38	0.56
2:B:1946:SER:HB3	2:B:1978:LEU:CB	2.31	0.56
2:B:2233:ASP:HA	2:B:2305:TYR:CD1	2.41	0.56
1:A:448:ILE:HD13	1:A:618:ASN:O	2.06	0.55
1:A:72:LEU:HD13	1:A:235:ASN:OD1	2.06	0.55
1:A:279:ARG:O	1:A:280:ASN:HB3	2.06	0.55
1:A:526:PRO:C	1:A:679:PHE:HZ	2.14	0.55
1:A:633:GLU:O	1:A:684:ASN:HB2	2.06	0.55
2:B:1946:SER:CB	2:B:1978:LEU:CD1	2.63	0.55
2:B:2013:LEU:HD22	2:B:2013:LEU:H	1.70	0.55
2:B:2042:GLN:HG3	2:B:2047:ALA:HA	1.88	0.55
1:A:89:LYS:HD2	1:A:91:MET:HE3	1.87	0.55
1:A:278:VAL:CG1	1:A:296:ALA:HB2	2.35	0.55
1:A:384:HIS:HB3	1:A:386:ILE:CG2	2.36	0.55
2:B:1694:LYS:HG3	2:B:1769:ASP:HB3	1.89	0.55
2:B:1829:GLU:CB	2:B:1966:ARG:CD	2.75	0.55
1:A:457:VAL:HA	1:A:515:VAL:CG1	2.37	0.55
2:B:1826:THR:OG1	2:B:1828:ASP:HB2	2.07	0.55
2:B:1934:MET:CG	2:B:2016:VAL:HB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:MET:CE	2:B:1972:LYS:HB2	2.36	0.55
1:A:501:PHE:O	1:A:502:PRO:C	2.47	0.55
1:A:625:LEU:HD13	1:A:706:LEU:HD11	1.53	0.55
1:A:656:TYR:CZ	2:B:1791:SER:CB	2.84	0.55
2:B:1739:THR:HB	2:B:1746:PRO:CG	2.36	0.55
2:B:1795:ASP:CG	2:B:1800:ALA:HB2	2.32	0.55
2:B:2259:GLU:HB2	2:B:2312:SER:H	1.70	0.55
1:A:307:LEU:HD12	1:A:322:ALA:O	2.06	0.55
1:A:418:ARG:HH21	1:A:607:GLU:HG2	1.72	0.55
1:A:471:ARG:CB	1:A:585:TRP:CZ3	2.90	0.55
1:A:538:ASN:ND2	1:A:541:ARG:HB3	2.21	0.55
2:B:2023:THR:OG1	2:B:2024:PRO:HD2	2.06	0.55
2:B:2302:LEU:HD22	2:B:2302:LEU:H	1.71	0.55
2:B:1709:TYR:HE2	2:B:1924:TYR:HA	1.71	0.55
2:B:2042:GLN:HE21	2:B:2047:ALA:CB	2.20	0.55
1:A:316:GLN:CD	1:A:316:GLN:H	2.15	0.55
1:A:631:LEU:HD23	1:A:631:LEU:C	2.31	0.55
2:B:1864:ASN:HB3	2:B:1867:HIS:O	2.06	0.55
2:B:2246:GLN:OE1	2:B:2320:ARG:HB2	2.06	0.55
1:A:164:LEU:O	1:A:167:ASP:O	2.25	0.55
1:A:673:PHE:O	1:A:674:SER:HB2	2.06	0.55
2:B:1796:GLN:O	2:B:1797:ARG:HB3	2.07	0.55
1:A:647:ASP:CG	2:B:1950:ASN:HD21	2.15	0.55
1:A:660:HIS:HB2	1:A:680:MET:HG3	1.89	0.55
1:A:237:TYR:CZ	1:A:242:LEU:HB2	2.42	0.54
1:A:457:VAL:HA	1:A:515:VAL:HG12	1.88	0.54
2:B:2046:TRP:CZ3	2:B:2059:ILE:CB	2.89	0.54
1:A:536:PHE:CD1	1:A:536:PHE:N	2.75	0.54
1:A:664:TYR:HE1	2:B:1826:THR:N	2.05	0.54
2:B:1732:LYS:NZ	2:B:1918:PHE:HE2	2.04	0.54
1:A:172:LEU:N	1:A:172:LEU:HD12	2.22	0.54
1:A:475:ILE:O	1:A:475:ILE:CG2	2.56	0.54
1:A:495:VAL:CG2	1:A:496:LYS:N	2.70	0.54
2:B:1735:PHE:CE1	2:B:1851:LEU:CB	2.90	0.54
2:B:1975:LEU:N	2:B:1975:LEU:HD23	2.22	0.54
1:A:393:TRP:HA	1:A:393:TRP:CE3	2.43	0.54
1:A:626:GLN:C	1:A:627:LEU:HD12	2.32	0.54
1:A:656:TYR:HB2	1:A:686:GLY:C	2.32	0.54
2:B:1705:ARG:NH2	2:B:1707:TRP:HZ3	2.05	0.54
2:B:2026:GLY:O	2:B:2032:ILE:HB	2.07	0.54
1:A:168:LEU:H	1:A:172:LEU:HB2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ALA:CB	1:A:138:TRP:CE3	2.90	0.54
1:A:269:ILE:HD12	1:A:288:ILE:HG21	1.89	0.54
1:A:503:ILE:HG21	1:A:537:VAL:HG13	1.88	0.54
1:A:640:LEU:HB3	1:A:677:THR:CB	2.38	0.54
2:B:2273:LEU:HD22	2:B:2280:VAL:CG2	2.36	0.54
1:A:640:LEU:HB2	1:A:677:THR:HB	1.89	0.54
2:B:1828:ASP:OD2	2:B:1968:LYS:C	2.51	0.54
2:B:1833:LYS:HG3	2:B:1834:ALA:H	1.73	0.54
2:B:1840:ASP:O	2:B:1841:VAL:HB	2.07	0.54
1:A:111:GLY:O	1:A:161:HIS:HB3	2.07	0.54
1:A:688:TRP:HZ2	2:B:1799:GLY:HA2	1.73	0.54
2:B:1953:ILE:HD12	2:B:1953:ILE:N	2.23	0.54
2:B:2180:MET:CE	2:B:2232:VAL:HG11	2.38	0.54
1:A:398:LEU:HD23	1:A:399:VAL:H	1.73	0.54
1:A:662:MET:O	1:A:663:VAL:HG23	2.07	0.54
2:B:1890:TYR:O	2:B:1894:ASN:N	2.22	0.54
2:B:2070:TRP:CE3	2:B:2150:ARG:HD2	2.43	0.54
2:B:2156:TYR:HB2	2:B:2159:ARG:O	2.08	0.54
1:A:425:LYS:NZ	1:A:581:GLU:OE1	2.41	0.53
1:A:492:PRO:O	1:A:494:GLY:N	2.33	0.53
2:B:1830:PHE:CZ	2:B:1987:GLU:HG3	2.44	0.53
2:B:1963:PHE:HB2	2:B:1986:VAL:HG11	1.89	0.53
1:A:426:VAL:HG22	1:A:586:TYR:HE1	1.73	0.53
2:B:2023:THR:HB	2:B:2176:MET:CE	2.38	0.53
2:B:2200:PHE:O	2:B:2202:THR:HG23	2.08	0.53
1:A:114:TYR:CE2	2:B:1997:ARG:CB	2.62	0.53
1:A:536:PHE:N	1:A:536:PHE:HD1	2.06	0.53
2:B:1830:PHE:HE2	2:B:1986:VAL:HA	1.74	0.53
2:B:2039:ALA:HB2	2:B:2048:PRO:CG	2.31	0.53
2:B:2064:THR:OG1	2:B:2065:LYS:N	2.39	0.53
2:B:2274:PHE:CD1	2:B:2275:PHE:N	2.76	0.53
1:A:148:ALA:CA	1:A:180:ARG:HH21	2.19	0.53
1:A:267:HIS:HA	1:A:312:ILE:HD11	1.90	0.53
1:A:426:VAL:HG22	1:A:586:TYR:CE1	2.43	0.53
1:A:428:PHE:CE2	1:A:475:ILE:CG1	2.90	0.53
2:B:2325:GLY:C	2:B:2326:CYS:SG	2.91	0.53
1:A:65:ARG:HB3	1:A:66:PRO:HD3	1.87	0.53
1:A:242:LEU:HD12	1:A:243:PRO:N	2.24	0.53
1:A:465:PHE:CD1	1:A:466:LYS:N	2.77	0.53
2:B:1699:PHE:CD1	2:B:1740:ASP:OD1	2.61	0.53
2:B:1884:ASP:HA	2:B:1917:ARG:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2013:LEU:N	2:B:2013:LEU:CD2	2.72	0.53
2:B:2330:ASP:C	2:B:2331:LEU:HD23	2.33	0.53
1:A:99:HIS:HD2	1:A:161:HIS:ND1	2.06	0.53
2:B:2190:ILE:HG12	2:B:2232:VAL:HG12	1.90	0.53
1:A:385:TYR:CE1	1:A:436:PHE:HB3	2.44	0.53
1:A:527:ARG:HD2	1:A:527:ARG:N	2.23	0.53
2:B:1830:PHE:HD2	2:B:1985:THR:OG1	1.90	0.53
2:B:1870:GLN:HG3	2:B:1871:VAL:H	1.74	0.53
2:B:1976:TYR:CE2	2:B:1984:GLU:OE1	2.62	0.53
1:A:688:TRP:NE1	2:B:1799:GLY:HA2	2.24	0.53
1:A:498:LEU:H	1:A:498:LEU:CD1	2.10	0.53
1:A:542:ASP:O	1:A:543:LEU:C	2.52	0.53
1:A:578:VAL:HG23	1:A:644:ALA:H	1.73	0.53
2:B:2196:PHE:HD1	2:B:2222:GLN:O	1.92	0.53
2:B:2275:PHE:HA	2:B:2280:VAL:HA	1.91	0.53
2:B:2027:MET:CA	2:B:2032:ILE:HD12	2.39	0.53
1:A:80:VAL:O	1:A:81:TYR:HB2	2.09	0.52
1:A:670:LEU:HD12	1:A:671:PHE:N	2.16	0.52
2:B:1755:HIS:CE1	2:B:1756:LEU:CD2	2.92	0.52
2:B:2210:LEU:HG	2:B:2211:HIS:ND1	2.24	0.52
2:B:2244:THR:OG1	2:B:2322:GLU:HB3	2.09	0.52
1:A:99:HIS:ND1	1:A:100:ALA:N	2.56	0.52
1:A:308:LEU:HG	1:A:322:ALA:O	2.09	0.52
1:A:673:PHE:O	1:A:674:SER:CB	2.56	0.52
2:B:1946:SER:CA	2:B:1978:LEU:HD12	2.40	0.52
2:B:1995:ILE:N	2:B:1995:ILE:HD13	2.24	0.52
2:B:2081:ILE:HA	2:B:2168:GLY:CA	2.39	0.52
2:B:2304:ARG:HD2	2:B:2305:TYR:CZ	2.44	0.52
1:A:168:LEU:HA	1:A:172:LEU:HB2	1.91	0.52
1:A:249:HIS:O	1:A:300:LEU:O	2.26	0.52
1:A:393:TRP:HA	1:A:393:TRP:HE3	1.75	0.52
1:A:484:ARG:HH11	1:A:486:LEU:HA	1.74	0.52
1:A:518:GLU:H	1:A:518:GLU:CD	2.18	0.52
2:B:2087:GLN:N	2:B:2163:ARG:O	2.42	0.52
2:B:1855:LEU:HD23	2:B:1856:LEU:N	2.25	0.52
2:B:2226:PRO:O	2:B:2310:PRO:O	2.26	0.52
2:B:2261:LEU:HD21	2:B:2281:LYS:O	2.09	0.52
2:B:2281:LYS:HD3	2:B:2282:VAL:N	2.25	0.52
1:A:14:TRP:N	1:A:46:TYR:O	2.43	0.52
1:A:527:ARG:O	1:A:528:CYS:HB2	2.09	0.52
1:A:576:PHE:HE2	1:A:650:SER:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1732:LYS:HB3	2:B:1849:SER:O	2.10	0.52
2:B:1932:LEU:CB	2:B:2014:PHE:HA	2.40	0.52
2:B:2273:LEU:HD21	2:B:2280:VAL:HG23	1.73	0.52
1:A:278:VAL:HG12	1:A:296:ALA:CB	2.38	0.52
1:A:398:LEU:CG	1:A:399:VAL:H	2.22	0.52
2:B:1932:LEU:HB3	2:B:2014:PHE:HA	1.91	0.52
2:B:2261:LEU:CD2	2:B:2281:LYS:O	2.58	0.52
2:B:2262:ILE:HD11	2:B:2283:PHE:CD1	2.45	0.52
1:A:155:THR:HG21	1:A:256:HIS:HA	1.90	0.52
1:A:501:PHE:O	1:A:503:ILE:N	2.42	0.52
1:A:622:PHE:O	1:A:623:ASP:OD1	2.28	0.52
1:A:65:ARG:HB3	1:A:66:PRO:HD2	1.92	0.52
1:A:156:TYR:HA	1:A:293:PHE:CD2	2.45	0.52
1:A:396:ALA:CB	1:A:397:PRO:HA	2.24	0.52
2:B:1769:ASP:OD1	2:B:1769:ASP:N	2.32	0.52
2:B:2048:PRO:HG3	2:B:2062:TRP:CG	2.45	0.52
2:B:2156:TYR:HD2	2:B:2159:ARG:C	2.18	0.52
2:B:2264:SER:HB3	2:B:2301:LEU:HD22	1.91	0.52
1:A:438:THR:OG1	1:A:439:ARG:N	2.43	0.51
1:A:111:GLY:HA2	1:A:126:ASP:HA	1.91	0.51
1:A:654:SER:H	1:A:657:THR:HA	1.75	0.51
2:B:1829:GLU:CB	2:B:1966:ARG:HH11	2.22	0.51
2:B:1834:ALA:HB1	2:B:1945:LEU:HD11	1.91	0.51
1:A:51:PHE:CD2	1:A:158:TYR:HE1	2.28	0.51
1:A:65:ARG:O	1:A:66:PRO:C	2.53	0.51
2:B:2260:PHE:O	2:B:2283:PHE:HB2	2.11	0.51
1:A:14:TRP:CE2	1:A:71:LEU:CD1	2.93	0.51
1:A:237:TYR:CG	1:A:242:LEU:CB	2.90	0.51
1:A:656:TYR:CE1	2:B:1791:SER:CB	2.90	0.51
1:A:656:TYR:CD1	2:B:1791:SER:HB2	2.45	0.51
2:B:1704:GLU:HG2	2:B:1731:LYS:HE2	1.91	0.51
2:B:1975:LEU:HD23	2:B:1975:LEU:H	1.75	0.51
2:B:1733:VAL:H	2:B:1850:GLY:HA2	1.75	0.51
2:B:1840:ASP:O	2:B:1841:VAL:CG2	2.58	0.51
2:B:1983:PHE:CD1	2:B:1984:GLU:CA	2.93	0.51
2:B:2052:ARG:HH11	2:B:2165:GLU:HG3	1.76	0.51
2:B:2104:MET:HA	2:B:2113:GLN:O	2.11	0.51
1:A:80:VAL:HA	1:A:140:VAL:HG11	1.92	0.51
1:A:97:SER:O	1:A:160:SER:HA	2.11	0.51
1:A:274:HIS:HE2	1:A:306:PHE:HE2	1.59	0.51
1:A:496:LYS:O	1:A:500:ASP:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:CYS:HA	1:A:553:ILE:O	2.11	0.51
1:A:658:PHE:HZ	1:A:684:ASN:ND2	2.07	0.51
2:B:2129:ASN:CB	2:B:2134:GLY:HA3	2.41	0.51
1:A:162:VAL:HG23	1:A:167:ASP:OD2	2.11	0.51
1:A:272:GLU:CB	1:A:307:LEU:H	2.24	0.51
2:B:2171:LEU:HD12	2:B:2171:LEU:H	1.75	0.51
2:B:2322:GLU:HG3	2:B:2323:VAL:N	2.26	0.51
2:B:1889:TRP:CE3	2:B:1890:TYR:N	2.79	0.51
1:A:631:LEU:CD2	1:A:632:HIS:ND1	2.71	0.51
2:B:1952:ASN:HB3	2:B:1954:HIS:CD2	2.45	0.51
2:B:2157:SER:C	2:B:2159:ARG:H	2.19	0.51
1:A:199:PHE:CD1	1:A:269:ILE:HD13	2.46	0.51
1:A:625:LEU:O	1:A:627:LEU:N	2.39	0.51
1:A:461:LEU:HD22	1:A:513:TRP:CE3	2.46	0.50
1:A:581:GLU:O	1:A:584:SER:HB3	2.11	0.50
1:A:667:THR:C	1:A:669:THR:N	2.68	0.50
1:A:687:LEU:HA	1:A:710:SER:OG	2.10	0.50
2:B:1787:SER:H	2:B:1790:ILE:HG13	1.75	0.50
2:B:2063:SER:OG	2:B:2161:THR:HB	2.11	0.50
1:A:271:LEU:HA	1:A:308:LEU:HA	1.92	0.50
1:A:679:PHE:CD1	1:A:679:PHE:N	2.78	0.50
2:B:1707:TRP:HA	2:B:1707:TRP:HE3	1.72	0.50
2:B:2186:SER:HB2	2:B:2189:GLN:HG3	1.93	0.50
2:B:2195:TYR:HA	2:B:2220:ARG:O	2.11	0.50
1:A:688:TRP:HZ2	2:B:1799:GLY:CA	2.23	0.50
2:B:2062:TRP:CZ3	2:B:2071:ILE:HB	2.47	0.50
1:A:87:THR:HG22	1:A:135:THR:OG1	2.11	0.50
1:A:94:HIS:HD2	1:A:95:PRO:HD2	1.77	0.50
1:A:137:VAL:HG11	2:B:2329:GLN:HE22	1.76	0.50
1:A:417:GLN:NE2	1:A:602:GLN:HB2	2.26	0.50
1:A:509:PHE:HD1	1:A:510:LYS:N	2.08	0.50
2:B:2331:LEU:HD23	2:B:2331:LEU:N	2.26	0.50
1:A:2:THR:HB	1:A:82:ASP:OD2	2.11	0.50
1:A:105:TYR:HD2	1:A:110:GLU:HB3	1.71	0.50
1:A:106:TRP:CZ3	2:B:2329:GLN:HB3	2.46	0.50
1:A:206:LYS:O	1:A:207:SER:HB3	2.12	0.50
2:B:1808:LYS:O	2:B:1811:GLU:HB2	2.12	0.50
2:B:1983:PHE:O	2:B:1984:GLU:CB	2.52	0.50
1:A:270:PHE:O	1:A:308:LEU:HA	2.11	0.50
1:A:617:ILE:CG1	1:A:706:LEU:HD22	2.40	0.50
1:A:654:SER:HB2	1:A:690:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:TRP:CZ2	2:B:1799:GLY:CA	2.94	0.50
2:B:2052:ARG:HD3	2:B:2165:GLU:CG	2.42	0.50
2:B:2265:SER:OG	2:B:2271:TRP:CE3	2.61	0.50
2:B:1752:LEU:HD12	2:B:1752:LEU:N	2.27	0.50
1:A:121:ARG:HG3	1:A:121:ARG:NH1	2.24	0.50
2:B:1830:PHE:CE1	2:B:1966:ARG:CZ	2.95	0.50
2:B:1877:ALA:HA	2:B:1943:TYR:HB2	1.93	0.50
2:B:2042:GLN:HB3	2:B:2062:TRP:NE1	2.26	0.50
2:B:2046:TRP:CD1	2:B:2159:ARG:NH2	2.79	0.50
1:A:578:VAL:CG2	1:A:644:ALA:H	2.25	0.50
2:B:1708:ASP:C	2:B:1709:TYR:CD1	2.90	0.50
2:B:1908:GLU:O	2:B:1909:ASP:OD1	2.30	0.50
2:B:1941:ARG:HD2	2:B:1943:TYR:OH	2.12	0.50
1:A:5:TYR:CD2	1:A:76:ILE:HB	2.36	0.49
1:A:158:TYR:CZ	1:A:174:GLY:HA3	2.47	0.49
1:A:527:ARG:O	1:A:679:PHE:CE2	2.65	0.49
1:A:616:SER:OG	1:A:617:ILE:N	2.45	0.49
1:A:232:HIS:CD2	1:A:318:ASP:CB	2.95	0.49
1:A:299:LEU:H	1:A:299:LEU:HD23	1.77	0.49
1:A:480:ILE:CG2	1:A:481:THR:N	2.70	0.49
1:A:624:SER:O	1:A:625:LEU:HD12	2.12	0.49
1:A:653:PHE:HB2	1:A:693:HIS:CE1	2.42	0.49
1:A:687:LEU:CD1	1:A:688:TRP:H	2.25	0.49
2:B:2046:TRP:CH2	2:B:2058:SER:C	2.88	0.49
2:B:2220:ARG:HH11	2:B:2220:ARG:CG	2.25	0.49
1:A:626:GLN:HA	1:A:707:LYS:HB2	1.93	0.49
1:A:107:LYS:O	1:A:126:ASP:OD1	2.30	0.49
1:A:392:ASP:HA	1:A:424:LYS:HA	1.94	0.49
2:B:2083:GLY:HA2	2:B:2140:PHE:CE2	2.44	0.49
2:B:2195:TYR:HD2	2:B:2204:SER:HA	1.76	0.49
1:A:57:HIS:O	1:A:58:LEU:CG	2.61	0.49
1:A:125:ASP:C	1:A:127:LYS:H	2.21	0.49
1:A:267:HIS:HB2	1:A:288:ILE:HG23	1.95	0.49
1:A:386:ILE:O	1:A:465:PHE:HA	2.13	0.49
1:A:389:GLU:CD	1:A:431:TYR:CE2	2.90	0.49
2:B:1807:VAL:HG13	2:B:1811:GLU:HB3	1.94	0.49
1:A:100:ALA:HB3	1:A:105:TYR:CE1	2.48	0.49
1:A:503:ILE:C	1:A:504:LEU:HG	2.37	0.49
2:B:2210:LEU:HD13	2:B:2321:MET:HA	1.94	0.49
1:A:10:VAL:HB	1:A:52:VAL:HG11	1.95	0.49
1:A:184:LEU:O	1:A:185:ALA:C	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1735:PHE:CE1	2:B:1851:LEU:HG	2.40	0.49
2:B:1859:HIS:O	2:B:1862:THR:OG1	2.28	0.49
2:B:1895:MET:HA	2:B:1895:MET:HE2	1.93	0.49
2:B:2230:LEU:O	2:B:2308:ILE:HG22	2.11	0.49
1:A:137:VAL:HG11	2:B:2329:GLN:NE2	2.27	0.49
1:A:249:HIS:CE1	1:A:303:LEU:CD1	2.96	0.49
1:A:423:TYR:CD2	1:A:581:GLU:HG3	2.47	0.49
1:A:700:ARG:HH11	2:B:1843:LEU:HB3	1.77	0.49
2:B:2105:TYR:HB2	2:B:2146:ALA:CB	2.43	0.49
2:B:2144:ILE:HG22	2:B:2145:ILE:N	2.27	0.49
2:B:2275:PHE:CD1	2:B:2275:PHE:N	2.81	0.49
1:A:101:VAL:O	1:A:101:VAL:HG13	2.13	0.49
1:A:663:VAL:HG13	2:B:1968:LYS:HD2	1.95	0.49
1:A:688:TRP:HE1	2:B:1799:GLY:CA	2.25	0.49
2:B:1851:LEU:C	2:B:1851:LEU:HD22	2.38	0.49
1:A:95:PRO:HB3	1:A:130:PRO:HD3	1.94	0.49
1:A:660:HIS:HB3	1:A:682:MET:HG3	1.95	0.49
1:A:688:TRP:CD1	2:B:1800:ALA:HB3	2.48	0.49
2:B:1838:PHE:CE1	2:B:1852:ILE:HG13	2.48	0.49
2:B:2199:MET:HA	2:B:2199:MET:HE2	1.95	0.49
2:B:1946:SER:CB	2:B:1978:LEU:CB	2.86	0.48
2:B:1968:LYS:O	2:B:1969:GLU:HG2	2.13	0.48
1:A:417:GLN:CD	1:A:601:VAL:HG22	2.29	0.48
1:A:472:PRO:HB2	1:A:503:ILE:HB	1.96	0.48
1:A:655:GLY:HA3	1:A:687:LEU:HB3	1.95	0.48
1:A:683:GLU:H	1:A:683:GLU:CD	2.20	0.48
2:B:1738:PHE:HB2	2:B:1746:PRO:C	2.21	0.48
2:B:1755:HIS:ND1	2:B:1756:LEU:HD23	2.28	0.48
2:B:1779:ALA:O	2:B:1809:PRO:HG3	2.13	0.48
2:B:1924:TYR:HD1	2:B:1928:THR:HB	1.78	0.48
2:B:1996:TRP:HB2	2:B:2014:PHE:CE1	2.48	0.48
1:A:186:LYS:O	1:A:189:THR:N	2.46	0.48
1:A:200:ALA:CB	1:A:202:PHE:CE1	2.96	0.48
1:A:433:ASP:OD1	1:A:433:ASP:N	2.46	0.48
1:A:249:HIS:NE2	1:A:303:LEU:CD1	2.71	0.48
1:A:282:ARG:HH12	1:A:299:LEU:CD2	2.26	0.48
1:A:473:TYR:HA	1:A:537:VAL:HG21	1.95	0.48
2:B:1873:VAL:HG21	2:B:1941:ARG:NH2	2.29	0.48
2:B:1944:LEU:HD23	2:B:1944:LEU:N	2.28	0.48
1:A:653:PHE:HB3	1:A:691:GLY:O	2.13	0.48
1:A:683:GLU:C	1:A:685:PRO:HD2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2106:SER:O	2:B:2146:ALA:HB1	2.13	0.48
1:A:13:SER:HB3	1:A:47:LYS:HG2	1.95	0.48
1:A:249:HIS:CE1	1:A:303:LEU:HD12	2.48	0.48
1:A:319:GLY:O	1:A:320:MET:HB2	2.12	0.48
1:A:621:VAL:CG1	1:A:622:PHE:H	1.90	0.48
1:A:657:THR:CG2	2:B:1788:SER:HA	2.18	0.48
2:B:1732:LYS:NZ	2:B:1918:PHE:CE2	2.80	0.48
2:B:2087:GLN:HG2	2:B:2163:ARG:HB2	1.94	0.48
2:B:2246:GLN:OE1	2:B:2320:ARG:NE	2.46	0.48
2:B:2331:LEU:O	2:B:2332:TYR:CB	2.62	0.48
1:A:237:TYR:HD2	1:A:241:SER:HB2	1.79	0.48
1:A:473:TYR:O	1:A:504:LEU:HD12	2.12	0.48
1:A:664:TYR:CD1	2:B:1826:THR:CG2	2.95	0.48
1:A:412:LEU:C	1:A:420:GLY:HA3	2.39	0.48
1:A:471:ARG:CB	1:A:585:TRP:CE3	2.97	0.48
1:A:586:TYR:O	1:A:590:ASN:ND2	2.47	0.48
2:B:1735:PHE:HE1	2:B:1851:LEU:CB	2.27	0.48
2:B:1958:PHE:O	2:B:1959:SER:C	2.56	0.48
2:B:2075:LEU:C	2:B:2076:LEU:HG	2.38	0.48
2:B:2101:PHE:HD2	2:B:2151:LEU:HG	1.78	0.48
2:B:2025:LEU:HD12	2:B:2166:LEU:HD12	1.96	0.48
1:A:51:PHE:CE1	1:A:172:LEU:HA	2.49	0.47
1:A:237:TYR:CD2	1:A:242:LEU:CB	2.96	0.47
1:A:659:LYS:HE2	2:B:1822:HIS:CD2	2.49	0.47
1:A:670:LEU:CD1	1:A:671:PHE:H	2.19	0.47
2:B:2039:ALA:C	2:B:2041:GLY:H	2.22	0.47
1:A:84:VAL:HG23	1:A:138:TRP:CD1	2.49	0.47
1:A:652:PHE:C	1:A:657:THR:O	2.56	0.47
1:A:653:PHE:O	1:A:690:LEU:HA	2.14	0.47
2:B:1766:GLU:HB3	2:B:1769:ASP:OD1	2.14	0.47
2:B:2076:LEU:C	2:B:2147:ARG:HE	2.22	0.47
2:B:2238:MET:CE	2:B:2326:CYS:O	2.62	0.47
1:A:311:HIS:O	1:A:312:ILE:CG1	2.59	0.47
1:A:398:LEU:HG	1:A:399:VAL:H	1.79	0.47
1:A:542:ASP:O	1:A:545:SER:HB2	2.15	0.47
1:A:676:GLU:OE1	1:A:676:GLU:HA	2.14	0.47
2:B:1709:TYR:CD1	2:B:1709:TYR:N	2.81	0.47
2:B:1732:LYS:CB	2:B:1849:SER:O	2.62	0.47
2:B:1936:GLN:HG2	2:B:1937:ASP:OD1	2.15	0.47
2:B:2087:GLN:HB3	2:B:2163:ARG:CA	2.44	0.47
1:A:163:ASP:HA	2:B:2007:HIS:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LEU:HD12	1:A:322:ALA:C	2.40	0.47
2:B:2329:GLN:CG	2:B:2332:TYR:O	2.37	0.47
1:A:664:TYR:OH	2:B:1825:PRO:CA	2.62	0.47
1:A:712:ASP:O	1:A:713:LYS:HG2	2.14	0.47
2:B:1830:PHE:HE1	2:B:1966:ARG:NH2	2.12	0.47
2:B:1888:SER:OG	2:B:1889:TRP:N	2.46	0.47
2:B:2178:LEU:O	2:B:2185:ILE:HD12	2.14	0.47
1:A:380:LYS:CG	1:A:382:TRP:HZ3	2.27	0.47
1:A:471:ARG:N	1:A:471:ARG:HD3	2.30	0.47
1:A:654:SER:CB	1:A:690:LEU:HB2	2.45	0.47
1:A:661:LYS:HA	1:A:665:GLU:HA	1.97	0.47
2:B:1963:PHE:CB	2:B:1986:VAL:HG11	2.45	0.47
2:B:2027:MET:CB	2:B:2165:GLU:HG2	2.42	0.47
2:B:2052:ARG:HA	2:B:2163:ARG:HB3	1.95	0.47
2:B:2265:SER:O	2:B:2303:THR:HB	2.14	0.47
1:A:69:MET:HE3	1:A:69:MET:HB2	1.86	0.47
1:A:116:ASP:O	2:B:1995:ILE:HG13	2.15	0.47
1:A:199:PHE:HB3	1:A:320:MET:HE1	1.96	0.47
1:A:432:THR:OG1	1:A:440:GLU:CG	2.62	0.47
1:A:660:HIS:ND1	1:A:680:MET:CE	2.71	0.47
1:A:663:VAL:CG1	2:B:1968:LYS:HD2	2.45	0.47
1:A:663:VAL:HG11	2:B:1968:LYS:HB2	1.95	0.47
1:A:693:HIS:HD2	1:A:695:SER:HB2	1.77	0.47
2:B:1739:THR:H	2:B:1746:PRO:CG	2.24	0.47
2:B:1969:GLU:HA	2:B:1969:GLU:OE1	2.15	0.47
2:B:1996:TRP:O	2:B:2013:LEU:HA	2.14	0.47
2:B:2046:TRP:O	2:B:2062:TRP:HA	2.15	0.47
2:B:2054:HIS:O	2:B:2060:ASN:HB2	2.13	0.47
2:B:2105:TYR:HB2	2:B:2146:ALA:HB3	1.97	0.47
2:B:2231:GLN:HA	2:B:2306:LEU:O	2.14	0.47
1:A:127:LYS:CG	1:A:162:VAL:HG11	2.42	0.47
1:A:645:GLN:O	1:A:646:THR:HB	2.15	0.47
2:B:1785:PHE:HB3	2:B:1815:TYR:HE2	1.79	0.47
1:A:455:GLY:O	1:A:554:CYS:N	2.47	0.47
1:A:617:ILE:CG1	1:A:706:LEU:HD13	2.44	0.47
1:A:645:GLN:CD	1:A:645:GLN:N	2.73	0.47
2:B:1889:TRP:CE3	2:B:1890:TYR:HB2	2.48	0.47
2:B:2083:GLY:N	2:B:2140:PHE:HD2	2.13	0.47
1:A:89:LYS:HA	1:A:133:SER:HA	1.97	0.46
1:A:278:VAL:CG2	1:A:279:ARG:H	2.24	0.46
1:A:663:VAL:HG13	2:B:1968:LYS:CB	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1789:LEU:HD23	2:B:1823:MET:SD	2.54	0.46
2:B:2329:GLN:C	2:B:2332:TYR:O	2.55	0.46
1:A:398:LEU:CD2	1:A:399:VAL:H	2.28	0.46
1:A:576:PHE:HE2	1:A:650:SER:CB	2.28	0.46
1:A:607:GLU:O	1:A:611:SER:OG	2.32	0.46
2:B:2265:SER:OG	2:B:2270:GLN:O	2.33	0.46
1:A:147:MET:HE2	2:B:1972:LYS:HB2	1.97	0.46
2:B:1975:LEU:HD23	2:B:1975:LEU:O	2.15	0.46
1:A:182:GLY:O	1:A:186:LYS:CE	2.59	0.46
1:A:311:HIS:ND1	1:A:311:HIS:C	2.74	0.46
1:A:396:ALA:CB	1:A:397:PRO:CA	2.90	0.46
1:A:578:VAL:H	1:A:643:GLY:HA3	1.81	0.46
2:B:2265:SER:OG	2:B:2271:TRP:HA	2.16	0.46
2:B:2273:LEU:O	2:B:2275:PHE:HD1	1.93	0.46
3:C:1:NAG:O3	3:C:2:NAG:H62	2.15	0.46
1:A:486:LEU:CD2	1:A:487:TYR:CD2	2.98	0.46
1:A:534:SER:OG	1:A:535:SER:N	2.49	0.46
1:A:652:PHE:HD1	1:A:690:LEU:HD11	1.80	0.46
1:A:697:PHE:CD1	1:A:698:ARG:HB2	2.51	0.46
2:B:1771:ILE:HB	2:B:1817:TRP:NE1	2.31	0.46
2:B:2080:ILE:O	2:B:2080:ILE:HG13	2.15	0.46
2:B:2181:GLU:C	2:B:2183:LYS:H	2.23	0.46
1:A:181:GLU:HG3	1:A:182:GLY:N	2.30	0.46
2:B:1711:MET:SD	2:B:1711:MET:N	2.89	0.46
2:B:1882:ILE:HD11	2:B:1919:HIS:CE1	2.50	0.46
2:B:1947:MET:O	2:B:1952:ASN:ND2	2.48	0.46
2:B:2101:PHE:CE2	2:B:2103:ILE:HD11	2.50	0.46
2:B:2132:SER:O	2:B:2133:SER:HB3	2.15	0.46
2:B:2179:GLY:HA2	2:B:2184:ALA:HB3	1.98	0.46
1:A:647:ASP:CG	2:B:1950:ASN:ND2	2.72	0.46
2:B:1758:LEU:HD12	2:B:1922:ASN:O	2.14	0.46
1:A:13:SER:HA	1:A:47:LYS:HA	1.97	0.46
1:A:303:LEU:HA	1:A:326:VAL:HG13	1.97	0.46
1:A:305:GLN:HG2	1:A:325:LYS:HG2	1.98	0.46
1:A:486:LEU:HD22	1:A:487:TYR:CD2	2.51	0.46
2:B:1705:ARG:HG2	2:B:1706:LEU:N	2.29	0.46
2:B:1797:ARG:O	2:B:1797:ARG:HD3	2.16	0.46
2:B:1821:HIS:O	2:B:1824:ALA:HB3	2.16	0.46
2:B:1886:THR:HG23	2:B:1887:LYS:HD2	1.98	0.46
1:A:80:VAL:HA	1:A:140:VAL:HG12	1.98	0.46
1:A:389:GLU:HB3	1:A:429:MET:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:LEU:HD23	1:A:399:VAL:N	2.31	0.46
2:B:2097:TYR:CE1	2:B:2130:VAL:HA	2.51	0.46
2:B:2105:TYR:HD2	2:B:2146:ALA:HB2	1.80	0.46
2:B:2212:LEU:O	2:B:2217:ASN:HB2	2.16	0.46
1:A:278:VAL:CG2	1:A:279:ARG:N	2.79	0.45
1:A:421:ARG:HG2	1:A:422:LYS:N	2.31	0.45
1:A:684:ASN:N	1:A:685:PRO:CD	2.79	0.45
2:B:1891:PHE:O	2:B:1892:THR:C	2.58	0.45
2:B:2156:TYR:CD1	2:B:2156:TYR:N	2.83	0.45
2:B:2262:ILE:HG22	2:B:2306:LEU:HD21	1.97	0.45
1:A:198:LEU:H	1:A:235:ASN:HD22	1.63	0.45
1:A:200:ALA:HB3	1:A:202:PHE:CE1	2.51	0.45
1:A:426:VAL:HG11	1:A:473:TYR:HE2	1.80	0.45
1:A:433:ASP:C	1:A:434:GLU:HG3	2.40	0.45
1:A:473:TYR:O	1:A:504:LEU:HD11	2.16	0.45
1:A:688:TRP:HE1	2:B:1799:GLY:HA2	1.81	0.45
1:A:698:ARG:O	1:A:699:ASN:C	2.59	0.45
2:B:1771:ILE:O	2:B:1816:PHE:HA	2.16	0.45
2:B:2033:ARG:H	2:B:2036:GLN:NE2	2.14	0.45
1:A:137:VAL:O	1:A:137:VAL:HG13	2.16	0.45
1:A:184:LEU:HD23	1:A:184:LEU:O	2.16	0.45
1:A:187:GLU:HA	1:A:190:GLN:CB	2.33	0.45
1:A:288:ILE:HG23	1:A:288:ILE:O	2.16	0.45
1:A:503:ILE:C	1:A:504:LEU:HD12	2.41	0.45
1:A:595:LEU:HD11	1:A:601:VAL:HG21	1.98	0.45
2:B:1755:HIS:CE1	2:B:1756:LEU:HD23	2.51	0.45
2:B:1935:ALA:HB2	2:B:2017:TYR:CZ	2.52	0.45
2:B:2263:SER:HB2	2:B:2307:ARG:CB	2.46	0.45
1:A:576:PHE:N	1:A:640:LEU:O	2.49	0.45
1:A:668:LEU:HG	2:B:1788:SER:HG	1.81	0.45
2:B:1737:GLU:HG2	2:B:1761:PRO:HG2	1.98	0.45
2:B:2286:ASN:H	2:B:2293:VAL:HG11	1.82	0.45
1:A:463:ILE:N	1:A:463:ILE:HD12	2.31	0.45
1:A:501:PHE:O	1:A:503:ILE:CG1	2.52	0.45
1:A:684:ASN:C	1:A:686:GLY:N	2.73	0.45
2:B:1849:SER:OG	2:B:1888:SER:C	2.59	0.45
2:B:1889:TRP:HB3	2:B:1893:GLU:HG3	1.98	0.45
2:B:1963:PHE:CD1	2:B:1986:VAL:CG1	2.84	0.45
2:B:2274:PHE:CD1	2:B:2274:PHE:C	2.95	0.45
1:A:237:TYR:CD1	1:A:242:LEU:CB	3.00	0.45
1:A:376:LYS:C	1:A:377:LYS:HG2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:SER:O	1:A:616:SER:OG	2.35	0.45
2:B:1755:HIS:CE1	2:B:1756:LEU:HD21	2.52	0.45
2:B:1834:ALA:HB3	2:B:1983:PHE:CD1	2.51	0.45
2:B:2080:ILE:HD12	2:B:2082:HIS:NE2	2.31	0.45
1:A:419:ILE:HG22	1:A:594:PHE:HB2	1.98	0.45
2:B:1975:LEU:N	2:B:1975:LEU:CD2	2.79	0.45
2:B:2028:ALA:HB2	2:B:2052:ARG:HH11	1.82	0.45
2:B:2238:MET:HE1	2:B:2326:CYS:C	2.42	0.45
2:B:2238:MET:HE1	2:B:2326:CYS:O	2.17	0.45
1:A:163:ASP:HA	2:B:2007:HIS:CE1	2.52	0.45
1:A:184:LEU:O	1:A:187:GLU:N	2.48	0.45
1:A:453:LEU:CD2	1:A:533:TYR:HE2	2.15	0.45
1:A:548:ILE:HG13	1:A:549:GLY:N	2.32	0.45
1:A:604:GLU:HA	1:A:608:PHE:CZ	2.52	0.45
1:A:651:VAL:CG1	1:A:652:PHE:N	2.80	0.45
1:A:688:TRP:HZ2	2:B:1799:GLY:H	1.63	0.45
2:B:1735:PHE:CE1	2:B:1851:LEU:CD2	3.00	0.45
2:B:2048:PRO:O	2:B:2049:LYS:CB	2.65	0.45
2:B:2181:GLU:C	2:B:2183:LYS:N	2.75	0.45
2:B:2244:THR:HG22	2:B:2294:VAL:HB	1.99	0.45
2:B:2273:LEU:HD22	2:B:2280:VAL:CB	2.47	0.45
1:A:267:HIS:CE1	1:A:320:MET:HG3	2.52	0.45
1:A:454:TYR:CD1	1:A:454:TYR:C	2.95	0.45
1:A:499:LYS:O	1:A:536:PHE:O	2.35	0.45
1:A:610:ALA:HA	1:A:613:ILE:HG12	1.99	0.45
2:B:1789:LEU:HD23	2:B:1823:MET:HE3	1.98	0.45
2:B:1789:LEU:O	2:B:1791:SER:N	2.50	0.45
2:B:1868:GLY:O	2:B:1869:ARG:HG3	2.16	0.45
2:B:2234:PHE:HD2	2:B:2238:MET:HG3	1.82	0.45
2:B:2302:LEU:H	2:B:2302:LEU:CD2	2.30	0.45
1:A:116:ASP:O	1:A:117:GLN:C	2.59	0.45
1:A:381:THR:HB	1:A:460:THR:HB	1.99	0.45
1:A:530:THR:HB	1:A:677:THR:OG1	2.17	0.45
1:A:617:ILE:HG12	1:A:706:LEU:CD1	2.47	0.44
1:A:663:VAL:HG12	1:A:664:TYR:N	2.32	0.44
2:B:1789:LEU:HD21	2:B:1835:TRP:NE1	2.32	0.44
2:B:1919:HIS:N	2:B:1919:HIS:CD2	2.85	0.44
2:B:2102:ILE:HD12	2:B:2152:HIS:HB2	1.98	0.44
1:A:651:VAL:HG11	1:A:668:LEU:HA	1.97	0.44
2:B:1755:HIS:CD2	2:B:1876:PHE:CD1	3.04	0.44
2:B:1821:HIS:C	2:B:1823:MET:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1860:THR:O	2:B:1862:THR:OG1	2.36	0.44
2:B:1932:LEU:HB2	2:B:2015:LEU:HD12	1.97	0.44
2:B:2038:THR:HG23	2:B:2072:LYS:HB3	1.99	0.44
2:B:2200:PHE:CZ	2:B:2215:ARG:HD3	2.52	0.44
2:B:2260:PHE:CZ	2:B:2295:ASN:ND2	2.86	0.44
2:B:2081:ILE:CG1	2:B:2144:ILE:HB	2.42	0.44
2:B:2096:LEU:CD1	2:B:2159:ARG:HB3	2.44	0.44
1:A:100:ALA:O	1:A:101:VAL:C	2.59	0.44
1:A:263:THR:C	1:A:265:GLU:H	2.24	0.44
1:A:491:LEU:CB	1:A:492:PRO:HD2	2.39	0.44
1:A:625:LEU:HD13	1:A:706:LEU:HD21	1.99	0.44
1:A:705:LEU:HD22	1:A:705:LEU:H	1.80	0.44
2:B:1934:MET:HB3	2:B:2016:VAL:CA	2.47	0.44
1:A:243:PRO:HB2	1:A:244:GLY:H	1.61	0.44
2:B:1753:ASN:O	2:B:1754:GLU:C	2.58	0.44
2:B:1944:LEU:C	2:B:1978:LEU:HD11	2.24	0.44
2:B:2275:PHE:N	2:B:2275:PHE:HD1	2.16	0.44
1:A:159:LEU:CD1	1:A:168:LEU:HD21	2.48	0.44
1:A:621:VAL:HG12	1:A:622:PHE:CD2	2.53	0.44
2:B:1929:LEU:HD22	2:B:2012:THR:HG21	2.00	0.44
2:B:2264:SER:CB	2:B:2301:LEU:HD23	2.45	0.44
2:B:2264:SER:C	2:B:2271:TRP:CE3	2.96	0.44
1:A:263:THR:O	1:A:265:GLU:N	2.49	0.44
1:A:385:TYR:CG	1:A:436:PHE:O	2.70	0.44
1:A:390:GLU:CD	1:A:469:ALA:HB1	2.42	0.44
2:B:1878:LEU:HD11	2:B:1942:TRP:CZ3	2.52	0.44
2:B:1924:TYR:CD1	2:B:1928:THR:HB	2.53	0.44
2:B:1995:ILE:HD13	2:B:1995:ILE:H	1.83	0.44
2:B:2031:HIS:HB2	2:B:2294:VAL:CG1	2.47	0.44
2:B:1849:SER:HA	2:B:1888:SER:HB2	2.00	0.44
5:E:6:MAN:O5	5:E:7:MAN:H2	2.17	0.44
1:A:663:VAL:CB	2:B:1968:LYS:HD2	2.46	0.44
2:B:1820:GLN:H	2:B:1823:MET:HE2	1.83	0.44
2:B:1889:TRP:CD2	2:B:1890:TYR:N	2.82	0.44
2:B:2022:GLN:OE1	2:B:2082:HIS:HB2	2.17	0.44
1:A:477:PRO:HG3	1:A:513:TRP:CD2	2.52	0.43
1:A:648:PHE:HD1	1:A:648:PHE:HA	1.53	0.43
1:A:4:ARG:HG2	1:A:5:TYR:N	2.32	0.43
1:A:94:HIS:CE1	1:A:207:SER:OG	2.71	0.43
1:A:580:ASP:C	1:A:582:ASN:N	2.76	0.43
1:A:476:TYR:CG	1:A:477:PRO:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:TYR:HD2	1:A:659:LYS:NZ	2.16	0.43
2:B:2273:LEU:O	2:B:2275:PHE:HE1	1.96	0.43
1:A:4:ARG:HG3	1:A:85:VAL:O	2.18	0.43
1:A:234:VAL:O	1:A:235:ASN:HB2	2.18	0.43
1:A:412:LEU:CA	1:A:420:GLY:HA3	2.42	0.43
1:A:421:ARG:HG2	1:A:422:LYS:H	1.83	0.43
1:A:461:LEU:HB3	1:A:463:ILE:CD1	2.49	0.43
1:A:496:LYS:HD3	1:A:496:LYS:HA	1.69	0.43
1:A:533:TYR:CZ	1:A:549:GLY:HA3	2.54	0.43
2:B:1763:ILE:O	2:B:1763:ILE:CG2	2.66	0.43
2:B:2052:ARG:CD	2:B:2165:GLU:CB	2.72	0.43
2:B:2229:TRP:HA	2:B:2308:ILE:O	2.18	0.43
1:A:291:ILE:HG23	2:B:1955:SER:OG	2.18	0.43
1:A:509:PHE:CD1	1:A:510:LYS:N	2.86	0.43
1:A:627:LEU:HD13	1:A:707:LYS:O	2.18	0.43
1:A:137:VAL:HG11	2:B:2329:GLN:OE1	2.19	0.43
1:A:432:THR:CB	1:A:433:ASP:OD1	2.65	0.43
1:A:526:PRO:O	1:A:679:PHE:CZ	2.59	0.43
2:B:1751:GLU:CD	2:B:2115:TYR:HD1	2.26	0.43
2:B:1756:LEU:N	2:B:1756:LEU:CD2	2.81	0.43
2:B:1846:ASP:O	2:B:1847:VAL:C	2.61	0.43
2:B:1922:ASN:HD22	2:B:1929:LEU:HD11	1.82	0.43
1:A:436:PHE:O	1:A:437:LYS:C	2.62	0.43
2:B:1787:SER:H	2:B:1790:ILE:CG1	2.31	0.43
2:B:1922:ASN:HB2	2:B:1929:LEU:HD11	2.01	0.43
2:B:1934:MET:CB	2:B:2016:VAL:HA	2.48	0.43
2:B:2252:LEU:HD13	2:B:2252:LEU:O	2.18	0.43
1:A:86:ILE:HD12	1:A:98:LEU:HD21	2.01	0.43
1:A:309:PHE:HA	1:A:321:GLU:HA	2.01	0.43
1:A:580:ASP:O	1:A:582:ASN:N	2.44	0.43
1:A:198:LEU:H	1:A:235:ASN:ND2	2.17	0.43
1:A:385:TYR:CD1	1:A:436:PHE:HB3	2.53	0.43
1:A:385:TYR:CE2	1:A:436:PHE:O	2.71	0.43
1:A:393:TRP:HD1	1:A:395:TYR:HE1	1.63	0.43
2:B:2106:SER:OG	2:B:2107:LEU:N	2.51	0.43
1:A:83:THR:HG22	1:A:140:VAL:N	2.24	0.43
1:A:267:HIS:HE1	1:A:320:MET:HG3	1.84	0.43
1:A:467:ASN:HB3	1:A:504:LEU:O	2.19	0.43
1:A:651:VAL:O	1:A:693:HIS:ND1	2.49	0.43
2:B:1782:PRO:HG3	2:B:1808:LYS:HA	2.00	0.43
2:B:2180:MET:HE1	2:B:2232:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2314:VAL:O	2:B:2315:HIS:HB2	2.19	0.43
1:A:427:ARG:CD	1:A:448:ILE:HA	2.49	0.42
2:B:2052:ARG:HD3	2:B:2165:GLU:HG3	2.01	0.42
1:A:396:ALA:CB	1:A:421:ARG:HH12	2.32	0.42
1:A:688:TRP:HZ2	2:B:1799:GLY:N	2.16	0.42
2:B:2033:ARG:H	2:B:2036:GLN:CD	2.26	0.42
2:B:2286:ASN:H	2:B:2293:VAL:CG1	2.32	0.42
1:A:90:ASN:HD21	1:A:95:PRO:HA	1.84	0.42
2:B:1966:ARG:HA	2:B:1969:GLU:O	2.19	0.42
1:A:86:ILE:HG22	1:A:87:THR:N	2.35	0.42
1:A:169:ASN:O	1:A:170:SER:CB	2.65	0.42
1:A:202:PHE:O	1:A:231:MET:HB2	2.19	0.42
1:A:503:ILE:C	1:A:504:LEU:CG	2.92	0.42
1:A:602:GLN:OE1	1:A:602:GLN:HA	2.20	0.42
1:A:620:TYR:O	1:A:621:VAL:CB	2.67	0.42
1:A:656:TYR:C	1:A:658:PHE:N	2.72	0.42
2:B:1785:PHE:HB3	2:B:1815:TYR:CE2	2.55	0.42
2:B:1806:PHE:CD1	2:B:1806:PHE:C	2.97	0.42
2:B:1929:LEU:HA	2:B:1930:PRO:HD3	1.73	0.42
1:A:168:LEU:N	1:A:172:LEU:HD13	2.34	0.42
1:A:537:VAL:HB	1:A:542:ASP:OD1	2.20	0.42
1:A:542:ASP:O	1:A:545:SER:CB	2.68	0.42
2:B:1889:TRP:NE1	2:B:1892:THR:CG2	2.83	0.42
2:B:2045:GLN:O	2:B:2047:ALA:N	2.47	0.42
2:B:2193:SER:HA	2:B:2229:TRP:CE2	2.54	0.42
1:A:87:THR:HA	1:A:135:THR:HA	2.00	0.42
1:A:94:HIS:CD2	1:A:95:PRO:HD2	2.55	0.42
1:A:98:LEU:HB3	1:A:136:TYR:CE1	2.55	0.42
1:A:504:LEU:HD23	1:A:509:PHE:HB2	2.01	0.42
2:B:2000:CYS:HB3	2:B:2010:MET:HG2	2.01	0.42
2:B:2042:GLN:HB2	2:B:2063:SER:O	2.20	0.42
1:A:270:PHE:HB2	1:A:309:PHE:CE1	2.47	0.42
1:A:393:TRP:NE1	1:A:448:ILE:HG23	2.35	0.42
1:A:432:THR:HG22	1:A:433:ASP:OD1	2.19	0.42
1:A:504:LEU:CD2	1:A:509:PHE:HB2	2.50	0.42
1:A:509:PHE:HB3	1:A:511:TYR:CE1	2.53	0.42
2:B:2141:ASN:HA	2:B:2142:PRO:C	2.45	0.42
2:B:2156:TYR:N	2:B:2156:TYR:HD1	2.17	0.42
2:B:2211:HIS:CE1	2:B:2292:PRO:HG3	2.55	0.42
1:A:14:TRP:CE2	1:A:71:LEU:HD13	2.54	0.42
1:A:232:HIS:CD2	1:A:318:ASP:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:GLU:HG2	1:A:392:ASP:N	2.35	0.42
1:A:640:LEU:HB3	1:A:677:THR:OG1	2.20	0.42
2:B:1924:TYR:HB3	2:B:1928:THR:HB	2.02	0.42
2:B:1933:VAL:O	2:B:1933:VAL:HG23	2.19	0.42
2:B:1951:GLU:O	2:B:1953:ILE:CD1	2.68	0.42
1:A:89:LYS:HD3	1:A:91:MET:HE3	2.02	0.42
1:A:428:PHE:HE2	1:A:475:ILE:HG13	1.82	0.42
1:A:687:LEU:HA	1:A:687:LEU:HD22	1.89	0.42
2:B:1863:LEU:HB2	2:B:1870:GLN:N	2.27	0.42
2:B:2311:GLN:O	2:B:2313:TRP:CD1	2.73	0.42
1:A:453:LEU:CD2	1:A:533:TYR:CD2	3.00	0.42
1:A:685:PRO:HG2	2:B:1822:HIS:CE1	2.52	0.42
1:A:687:LEU:HD13	1:A:688:TRP:H	1.85	0.42
1:A:68:TRP:CE3	1:A:68:TRP:C	2.98	0.41
1:A:155:THR:HG23	1:A:295:THR:OG1	2.20	0.41
1:A:454:TYR:C	1:A:454:TYR:HD1	2.28	0.41
1:A:605:ASP:OD1	1:A:606:PRO:HD2	2.20	0.41
2:B:1697:HIS:ND1	2:B:1697:HIS:N	2.67	0.41
2:B:1699:PHE:CZ	2:B:1740:ASP:OD2	2.73	0.41
2:B:1762:TYR:HB3	2:B:1764:ARG:HE	1.84	0.41
2:B:1972:LYS:HE3	2:B:1972:LYS:HB2	1.86	0.41
1:A:305:GLN:C	1:A:306:PHE:CD1	2.89	0.41
1:A:424:LYS:H	1:A:590:ASN:CG	2.25	0.41
1:A:432:THR:C	1:A:433:ASP:OD1	2.62	0.41
1:A:616:SER:C	1:A:619:GLY:H	2.27	0.41
1:A:663:VAL:HG22	2:B:1968:LYS:HZ2	1.85	0.41
2:B:1774:THR:CG2	2:B:1814:THR:HG22	2.50	0.41
2:B:1791:SER:OG	2:B:1792:TYR:N	2.53	0.41
2:B:2295:ASN:OD1	2:B:2295:ASN:N	2.52	0.41
1:A:311:HIS:C	1:A:312:ILE:CG1	2.93	0.41
1:A:313:SER:OG	1:A:314:SER:N	2.53	0.41
1:A:492:PRO:C	1:A:494:GLY:H	2.24	0.41
1:A:543:LEU:HD11	1:A:642:ILE:HG21	2.02	0.41
2:B:1733:VAL:O	2:B:1850:GLY:CA	2.68	0.41
2:B:1739:THR:O	2:B:1740:ASP:CG	2.63	0.41
2:B:1758:LEU:HD21	2:B:1923:GLY:HA3	2.01	0.41
2:B:1790:ILE:O	2:B:1790:ILE:HG22	2.20	0.41
2:B:2002:ILE:HB	2:B:2005:HIS:HB2	2.00	0.41
2:B:2176:MET:SD	2:B:2177:PRO:HD2	2.59	0.41
2:B:2281:LYS:HE2	2:B:2282:VAL:O	2.20	0.41
1:A:83:THR:HB	1:A:139:GLN:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ALA:HB3	1:A:202:PHE:HE1	1.85	0.41
2:B:1867:HIS:ND1	2:B:1867:HIS:C	2.77	0.41
2:B:2070:TRP:HE3	2:B:2150:ARG:HD2	1.85	0.41
2:B:2246:GLN:N	2:B:2286:ASN:ND2	2.68	0.41
1:A:77:GLN:CB	1:A:177:LEU:HD12	2.44	0.41
1:A:163:ASP:HB3	1:A:166:LYS:HB3	2.01	0.41
1:A:232:HIS:CD2	1:A:318:ASP:HB2	2.56	0.41
1:A:432:THR:CB	1:A:440:GLU:HB3	2.46	0.41
1:A:8:GLY:N	1:A:52:VAL:O	2.46	0.41
1:A:68:TRP:CH2	1:A:69:MET:HE2	2.55	0.41
1:A:197:LEU:HD11	1:A:255:TRP:CE3	2.55	0.41
1:A:200:ALA:HB1	1:A:202:PHE:CE1	2.56	0.41
1:A:422:LYS:HB2	1:A:422:LYS:HE3	1.81	0.41
2:B:1839:SER:N	2:B:1851:LEU:HD21	2.35	0.41
2:B:2302:LEU:HD22	2:B:2302:LEU:N	2.35	0.41
2:B:2304:ARG:HD2	2:B:2305:TYR:CE2	2.56	0.41
5:E:3:BMA:H61	5:E:6:MAN:H2	1.36	0.41
1:A:75:THR:CG2	1:A:175:ALA:HB3	2.27	0.41
1:A:159:LEU:HD23	1:A:159:LEU:N	2.36	0.41
1:A:574:ILE:HB	1:A:639:ILE:HG22	2.03	0.41
1:A:608:PHE:HA	1:A:611:SER:OG	2.21	0.41
1:A:309:PHE:HB2	1:A:321:GLU:HG2	2.02	0.41
1:A:387:ALA:HB2	1:A:466:LYS:HG3	2.02	0.41
2:B:1946:SER:N	2:B:1978:LEU:HD12	2.36	0.41
1:A:471:ARG:HG3	1:A:585:TRP:CZ3	2.36	0.41
1:A:527:ARG:HD2	1:A:527:ARG:H	1.86	0.41
1:A:625:LEU:C	1:A:627:LEU:N	2.79	0.41
1:A:690:LEU:HB3	1:A:708:VAL:N	2.36	0.41
1:A:690:LEU:CD2	1:A:692:CYS:HB2	2.51	0.41
1:A:708:VAL:CG1	1:A:709:SER:N	2.84	0.41
2:B:1739:THR:CB	2:B:1746:PRO:HG2	2.51	0.41
2:B:1885:GLU:HB3	2:B:1886:THR:H	1.57	0.41
2:B:1929:LEU:HG	2:B:1930:PRO:CD	2.51	0.41
2:B:1997:ARG:HG2	2:B:1999:GLU:HG2	2.02	0.41
2:B:2081:ILE:HD12	2:B:2149:ILE:CD1	2.43	0.41
2:B:2105:TYR:CD2	2:B:2144:ILE:CG2	3.04	0.41
2:B:2176:MET:HE2	2:B:2177:PRO:CD	2.51	0.41
2:B:2261:LEU:O	2:B:2309:HIS:N	2.37	0.41
1:A:232:HIS:HD2	1:A:318:ASP:HB3	1.86	0.41
1:A:234:VAL:O	1:A:235:ASN:CB	2.69	0.41
1:A:461:LEU:HD22	1:A:513:TRP:HE3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:VAL:HG22	2:B:1968:LYS:NZ	2.36	0.41
2:B:1745:GLN:HA	2:B:1746:PRO:HA	1.65	0.41
2:B:1749:ARG:HH11	2:B:1749:ARG:CG	2.30	0.41
2:B:1771:ILE:HD12	2:B:1817:TRP:HE1	1.86	0.41
2:B:1921:ILE:C	2:B:1923:GLY:N	2.77	0.41
1:A:7:LEU:HG	1:A:8:GLY:O	2.21	0.40
1:A:163:ASP:O	1:A:167:ASP:HB2	2.21	0.40
1:A:271:LEU:O	1:A:272:GLU:C	2.64	0.40
1:A:663:VAL:HG22	2:B:1968:LYS:CE	2.49	0.40
2:B:1730:PHE:HA	2:B:1893:GLU:OE1	2.20	0.40
2:B:1870:GLN:O	2:B:1871:VAL:HB	2.21	0.40
2:B:2180:MET:HE1	2:B:2232:VAL:CG1	2.51	0.40
1:A:65:ARG:O	1:A:66:PRO:O	2.39	0.40
1:A:247:GLY:O	1:A:326:VAL:HG23	2.21	0.40
1:A:290:PRO:HG2	1:A:291:ILE:H	1.86	0.40
1:A:470:SER:HB3	1:A:471:ARG:H	1.64	0.40
1:A:476:TYR:HA	1:A:477:PRO:HD3	1.97	0.40
1:A:530:THR:HG1	1:A:679:PHE:HB3	1.86	0.40
1:A:683:GLU:HB2	1:A:685:PRO:HD2	2.03	0.40
2:B:2048:PRO:CG	2:B:2062:TRP:CD1	2.94	0.40
2:B:2242:GLY:HA2	2:B:2297:LEU:HD12	2.03	0.40
2:B:2322:GLU:HG3	2:B:2323:VAL:O	2.20	0.40
1:A:3:ARG:HH12	1:A:79:GLU:HG2	1.86	0.40
1:A:8:GLY:HA3	1:A:52:VAL:HG22	2.02	0.40
1:A:105:TYR:HB3	1:A:109:SER:CB	2.22	0.40
1:A:238:VAL:N	1:A:241:SER:OG	2.54	0.40
1:A:400:LEU:HD23	1:A:400:LEU:N	2.36	0.40
1:A:432:THR:CG2	1:A:433:ASP:OD1	2.70	0.40
1:A:492:PRO:C	1:A:494:GLY:N	2.80	0.40
1:A:526:PRO:HB2	1:A:679:PHE:CZ	2.56	0.40
2:B:1699:PHE:HD1	2:B:1774:THR:OG1	2.05	0.40
2:B:1739:THR:CB	2:B:1746:PRO:CG	2.99	0.40
2:B:1786:TYR:CD1	2:B:1786:TYR:C	2.99	0.40
2:B:1831:ASP:O	2:B:1858:CYS:CB	2.66	0.40
2:B:1831:ASP:OD1	2:B:1831:ASP:N	2.53	0.40
2:B:1927:ASP:OD1	2:B:2011:SER:O	2.39	0.40
2:B:2236:LYS:HB3	2:B:2330:ASP:OD1	2.21	0.40
1:A:114:TYR:N	1:A:114:TYR:CD1	2.90	0.40
1:A:448:ILE:O	1:A:449:LEU:C	2.64	0.40
1:A:694:ASN:O	1:A:696:ASP:N	2.54	0.40
2:B:1759:LEU:HD11	2:B:1879:PHE:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1884:ASP:OD1	2:B:1913:LYS:NZ	2.54	0.40
2:B:1938:GLN:O	2:B:1939:ARG:C	2.65	0.40
2:B:2032:ILE:HA	2:B:2036:GLN:HE22	1.85	0.40
2:B:2035:PHE:CE1	2:B:2036:GLN:HG3	2.57	0.40
2:B:2059:ILE:HG13	2:B:2059:ILE:O	2.21	0.40
2:B:2166:LEU:H	2:B:2166:LEU:HG	1.66	0.40
1:A:56:ASP:O	1:A:57:HIS:CB	2.66	0.40
1:A:237:TYR:CD1	1:A:242:LEU:HD22	2.57	0.40
1:A:386:ILE:CD1	1:A:428:PHE:HD2	2.31	0.40
1:A:663:VAL:HG13	2:B:1968:LYS:CG	2.52	0.40
2:B:1784:SER:HB3	2:B:1840:ASP:OD1	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ARG:NH1	1:A:496:LYS:NZ[7_555]	1.94	0.26

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	599/740 (81%)	448 (75%)	111 (18%)	40 (7%)	1	12
2	B	613/865 (71%)	498 (81%)	87 (14%)	28 (5%)	2	17
All	All	1212/1605 (76%)	946 (78%)	198 (16%)	68 (6%)	1	15

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	TRP
1	A	127	LYS

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Mol	Chain	Res	Type
1	A	229	PRO
1	A	243	PRO
1	A	312	ILE
1	A	437	LYS
1	A	492	PRO
1	A	497	HIS
1	A	621	VAL
1	A	646	THR
1	A	663	VAL
1	A	705	LEU
1	A	713	LYS
2	B	1740	ASP
2	B	1768	GLU
2	B	1841	VAL
2	B	1871	VAL
2	B	1886	THR
2	B	1930	PRO
2	B	1984	GLU
2	B	2158	ILE
1	A	403	ASP
1	A	695	SER
1	A	706	LEU
2	B	1935	ALA
2	B	2049	LYS
2	B	2170	ASP
1	A	66	PRO
1	A	159	LEU
1	A	434	GLU
1	A	501	PHE
1	A	539	MET
1	A	618	ASN
1	A	658	PHE
2	B	1695	THR
2	B	1909	ASP
2	B	2052	ARG
1	A	153	CYS
1	A	163	ASP
1	A	264	PRO
1	A	284	ALA
1	A	397	PRO
2	B	1746	PRO
2	B	1830	PHE

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Mol	Chain	Res	Type
2	B	1908	GLU
2	B	1922	ASN
2	B	1967	LYS
1	A	410	GLN
1	A	601	VAL
1	A	674	SER
1	A	689	ILE
2	B	1854	PRO
2	B	2200	PHE
2	B	2273	LEU
2	B	2286	ASN
1	A	684	ASN
1	A	699	ASN
2	B	1752	LEU
2	B	1926	MET
2	B	2299	PRO
1	A	502	PRO
1	A	103	VAL
1	A	550	PRO
1	A	378	HIS
1	A	546	GLY
2	B	2135	ILE
2	B	2292	PRO
1	A	242	LEU

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	542/660 (82%)	413 (76%)	129 (24%)	1	5
2	B	550/776 (71%)	414 (75%)	136 (25%)	1	4
All	All	1092/1436 (76%)	827 (76%)	265 (24%)	1	5

All (265) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	55	THR
1	A	69	MET
1	A	76	ILE
1	A	82	ASP
1	A	84	VAL
1	A	88	LEU
1	A	89	LYS
1	A	94	HIS
1	A	105	TYR
1	A	106	TRP
1	A	114	TYR
1	A	120	GLN
1	A	127	LYS
1	A	129	PHE
1	A	142	LYS
1	A	147	MET
1	A	152	LEU
1	A	154	LEU
1	A	177	LEU
1	A	194	LYS
1	A	198	LEU
1	A	201	VAL
1	A	230	LYS
1	A	233	THR
1	A	235	ASN
1	A	241	SER
1	A	242	LEU
1	A	260	MET
1	A	279	ARG
1	A	291	ILE
1	A	292	THR
1	A	295	THR
1	A	299	LEU
1	A	302	ASP
1	A	305	GLN
1	A	306	PHE
1	A	309	PHE
1	A	311	HIS
1	A	328	SER
1	A	331	GLU
1	A	376	LYS
1	A	378	HIS

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Mol	Chain	Res	Type
1	A	381	THR
1	A	382	TRP
1	A	383	VAL
1	A	386	ILE
1	A	392	ASP
1	A	393	TRP
1	A	398	LEU
1	A	400	LEU
1	A	403	ASP
1	A	404	ASP
1	A	410	GLN
1	A	413	ASN
1	A	421	ARG
1	A	426	VAL
1	A	431	TYR
1	A	433	ASP
1	A	437	LYS
1	A	448	ILE
1	A	453	LEU
1	A	454	TYR
1	A	457	VAL
1	A	460	THR
1	A	468	GLN
1	A	470	SER
1	A	471	ARG
1	A	475	ILE
1	A	481	THR
1	A	486	LEU
1	A	496	LYS
1	A	498	LEU
1	A	499	LYS
1	A	500	ASP
1	A	503	ILE
1	A	504	LEU
1	A	508	ILE
1	A	514	THR
1	A	516	THR
1	A	517	VAL
1	A	518	GLU
1	A	523	LYS
1	A	524	SER
1	A	525	ASP

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Mol	Chain	Res	Type
1	A	527	ARG
1	A	529	LEU
1	A	536	PHE
1	A	539	MET
1	A	540	GLU
1	A	545	SER
1	A	552	LEU
1	A	555	TYR
1	A	571	ARG
1	A	573	VAL
1	A	575	LEU
1	A	578	VAL
1	A	588	THR
1	A	593	ARG
1	A	601	VAL
1	A	603	LEU
1	A	604	GLU
1	A	607	GLU
1	A	611	SER
1	A	618	ASN
1	A	620	TYR
1	A	624	SER
1	A	625	LEU
1	A	629	VAL
1	A	636	TYR
1	A	646	THR
1	A	648	PHE
1	A	659	LYS
1	A	663	VAL
1	A	668	LEU
1	A	673	PHE
1	A	678	VAL
1	A	680	MET
1	A	683	GLU
1	A	684	ASN
1	A	687	LEU
1	A	690	LEU
1	A	698	ARG
1	A	699	ASN
1	A	702	MET
1	A	705	LEU
1	A	708	VAL

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Mol	Chain	Res	Type
1	A	709	SER
1	A	713	LYS
2	B	1694	LYS
2	B	1695	THR
2	B	1696	ARG
2	B	1697	HIS
2	B	1700	ILE
2	B	1707	TRP
2	B	1708	ASP
2	B	1711	MET
2	B	1726	SER
2	B	1729	GLN
2	B	1733	VAL
2	B	1747	LEU
2	B	1749	ARG
2	B	1752	LEU
2	B	1756	LEU
2	B	1758	LEU
2	B	1759	LEU
2	B	1767	VAL
2	B	1769	ASP
2	B	1780	SER
2	B	1781	ARG
2	B	1786	TYR
2	B	1794	GLU
2	B	1796	GLN
2	B	1797	ARG
2	B	1804	LYS
2	B	1814	THR
2	B	1843	LEU
2	B	1846	ASP
2	B	1849	SER
2	B	1851	LEU
2	B	1856	LEU
2	B	1857	VAL
2	B	1859	HIS
2	B	1862	THR
2	B	1863	LEU
2	B	1867	HIS
2	B	1869	ARG
2	B	1874	GLN
2	B	1879	PHE

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Mol	Chain	Res	Type
2	B	1882	ILE
2	B	1889	TRP
2	B	1891	PHE
2	B	1914	GLU
2	B	1928	THR
2	B	1929	LEU
2	B	1934	MET
2	B	1938	GLN
2	B	1944	LEU
2	B	1945	LEU
2	B	1946	SER
2	B	1947	MET
2	B	1951	GLU
2	B	1952	ASN
2	B	1953	ILE
2	B	1964	THR
2	B	1967	LYS
2	B	1973	MET
2	B	1977	ASN
2	B	1978	LEU
2	B	1984	GLU
2	B	1995	ILE
2	B	1997	ARG
2	B	1999	GLU
2	B	2004	GLU
2	B	2013	LEU
2	B	2015	LEU
2	B	2016	VAL
2	B	2020	LYS
2	B	2022	GLN
2	B	2027	MET
2	B	2034	ASP
2	B	2035	PHE
2	B	2037	ILE
2	B	2040	SER
2	B	2042	GLN
2	B	2049	LYS
2	B	2076	LEU
2	B	2079	MET
2	B	2081	ILE
2	B	2090	ARG
2	B	2091	GLN

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Mol	Chain	Res	Type
2	B	2095	SER
2	B	2096	LEU
2	B	2098	ILE
2	B	2101	PHE
2	B	2102	ILE
2	B	2107	LEU
2	B	2114	THR
2	B	2116	ARG
2	B	2120	THR
2	B	2129	ASN
2	B	2135	ILE
2	B	2139	ILE
2	B	2145	ILE
2	B	2154	THR
2	B	2156	TYR
2	B	2157	SER
2	B	2159	ARG
2	B	2165	GLU
2	B	2166	LEU
2	B	2171	LEU
2	B	2175	SER
2	B	2178	LEU
2	B	2186	SER
2	B	2195	TYR
2	B	2199	MET
2	B	2204	SER
2	B	2206	SER
2	B	2212	LEU
2	B	2213	GLN
2	B	2220	ARG
2	B	2232	VAL
2	B	2237	THR
2	B	2243	VAL
2	B	2245	THR
2	B	2246	GLN
2	B	2249	LYS
2	B	2252	LEU
2	B	2261	LEU
2	B	2262	ILE
2	B	2269	HIS
2	B	2275	PHE
2	B	2280	VAL

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Mol	Chain	Res	Type
2	B	2281	LYS
2	B	2290	PHE
2	B	2295	ASN
2	B	2301	LEU
2	B	2302	LEU
2	B	2304	ARG
2	B	2306	LEU
2	B	2307	ARG
2	B	2316	GLN
2	B	2326	CYS
2	B	2331	LEU
2	B	2332	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	94	HIS
1	A	232	HIS
1	A	297	GLN
1	A	612	ASN
1	A	615	HIS
1	A	684	ASN
2	B	1770	ASN
2	B	1820	GLN
2	B	1919	HIS
2	B	1938	GLN
2	B	2005	HIS
2	B	2007	HIS
2	B	2222	GLN
2	B	2287	GLN

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 ⓘ

13 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$
3	NAG	C	1	1,3	14,14,15	0.45	0	17,19,21	0.72	0
3	NAG	C	2	3	14,14,15	0.39	0	17,19,21	1.11	1 (5%)
3	BMA	C	3	3	11,11,12	0.33	0	15,15,17	1.53	3 (20%)
3	MAN	C	4	3	11,11,12	0.29	0	15,15,17	0.82	1 (6%)
4	NAG	D	1	2,4	14,14,15	0.67	0	17,19,21	1.44	2 (11%)
4	NAG	D	2	4	14,14,15	0.43	0	17,19,21	1.71	5 (29%)
5	NAG	E	1	2,5	14,14,15	0.53	0	17,19,21	2.39	5 (29%)
5	NAG	E	2	5	14,14,15	0.55	0	17,19,21	1.43	3 (17%)
5	BMA	E	3	5	11,11,12	0.57	0	15,15,17	0.98	1 (6%)
5	BMA	E	4	5	11,11,12	0.28	0	15,15,17	0.69	0
5	MAN	E	5	5	11,11,12	0.26	0	15,15,17	0.51	0
5	MAN	E	6	5	11,11,12	0.61	0	15,15,17	1.29	2 (13%)
5	MAN	E	7	5	11,11,12	0.48	0	15,15,17	0.66	0

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
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
4	NAG	D	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
5	NAG	E	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	BMA	E	4	5	-	0/2/19/22	0/1/1/1
5	MAN	E	5	5	-	0/2/19/22	0/1/1/1
5	MAN	E	6	5	-	0/2/19/22	0/1/1/1
5	MAN	E	7	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	NAG	C2-N2-C7	5.84	130.73	122.90
3	C	3	BMA	C1-C2-C3	4.40	116.05	109.64
5	E	1	NAG	O5-C5-C6	4.34	116.11	107.66
4	D	2	NAG	C4-C3-C2	3.78	116.56	111.02
4	D	2	NAG	C3-C4-C5	3.48	116.54	110.23
5	E	1	NAG	C1-C2-N2	3.47	115.90	110.43
5	E	1	NAG	C3-C4-C5	3.35	116.30	110.23
4	D	1	NAG	C2-N2-C7	3.26	127.27	122.90
5	E	6	MAN	C1-O5-C5	3.07	116.31	112.19
5	E	2	NAG	C2-N2-C7	3.00	126.92	122.90
3	C	2	NAG	O5-C5-C6	2.89	113.28	107.66
5	E	6	MAN	C1-C2-C3	2.86	113.81	109.64
5	E	2	NAG	O5-C5-C4	-2.83	103.94	110.83
5	E	3	BMA	C1-O5-C5	2.66	115.76	112.19
4	D	2	NAG	O5-C1-C2	-2.35	107.65	111.29
4	D	2	NAG	C2-N2-C7	2.33	126.02	122.90
5	E	1	NAG	O5-C1-C2	2.28	114.82	111.29
5	E	2	NAG	C6-C5-C4	2.28	118.61	113.02
3	C	3	BMA	C1-O5-C5	2.23	115.17	112.19
3	C	3	BMA	O5-C1-C2	2.18	115.98	110.79
4	D	2	NAG	C8-C7-N2	2.16	119.70	116.12
3	C	4	MAN	C1-C2-C3	2.16	112.78	109.64
4	D	1	NAG	O5-C5-C6	2.02	111.59	107.66

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	3	BMA	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

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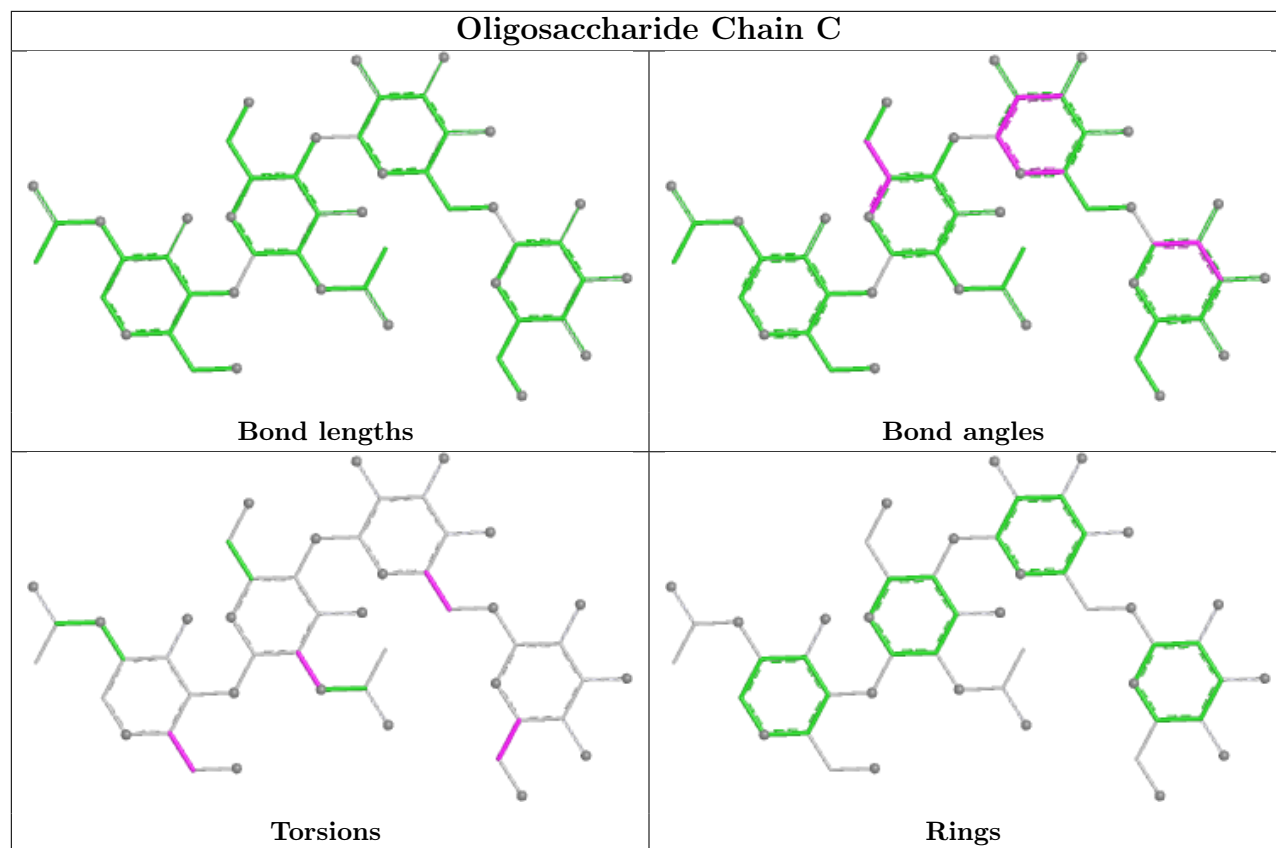
Mol	Chain	Res	Type	Atoms
5	E	3	BMA	C4-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	2	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7
3	C	3	BMA	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6

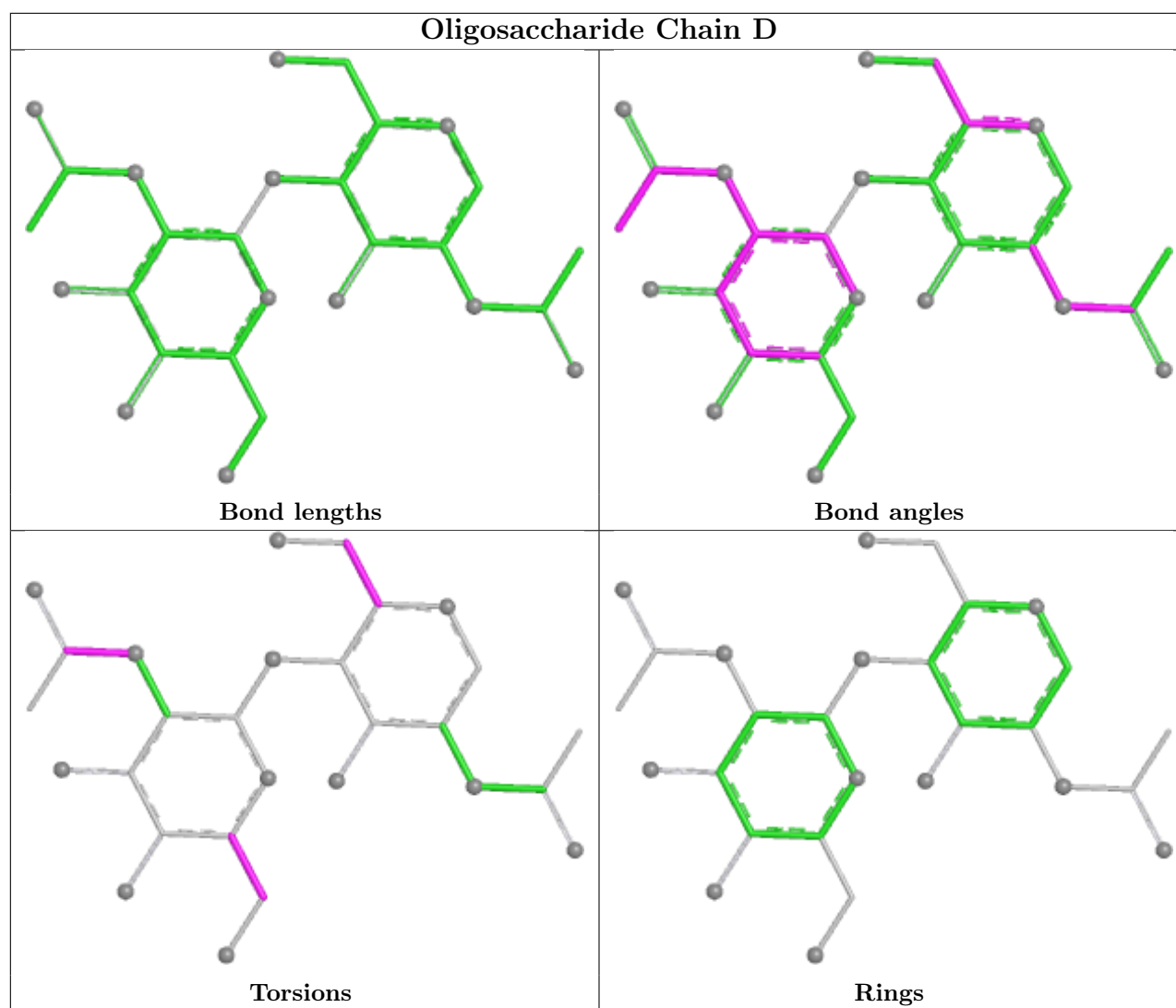
There are no ring outliers.

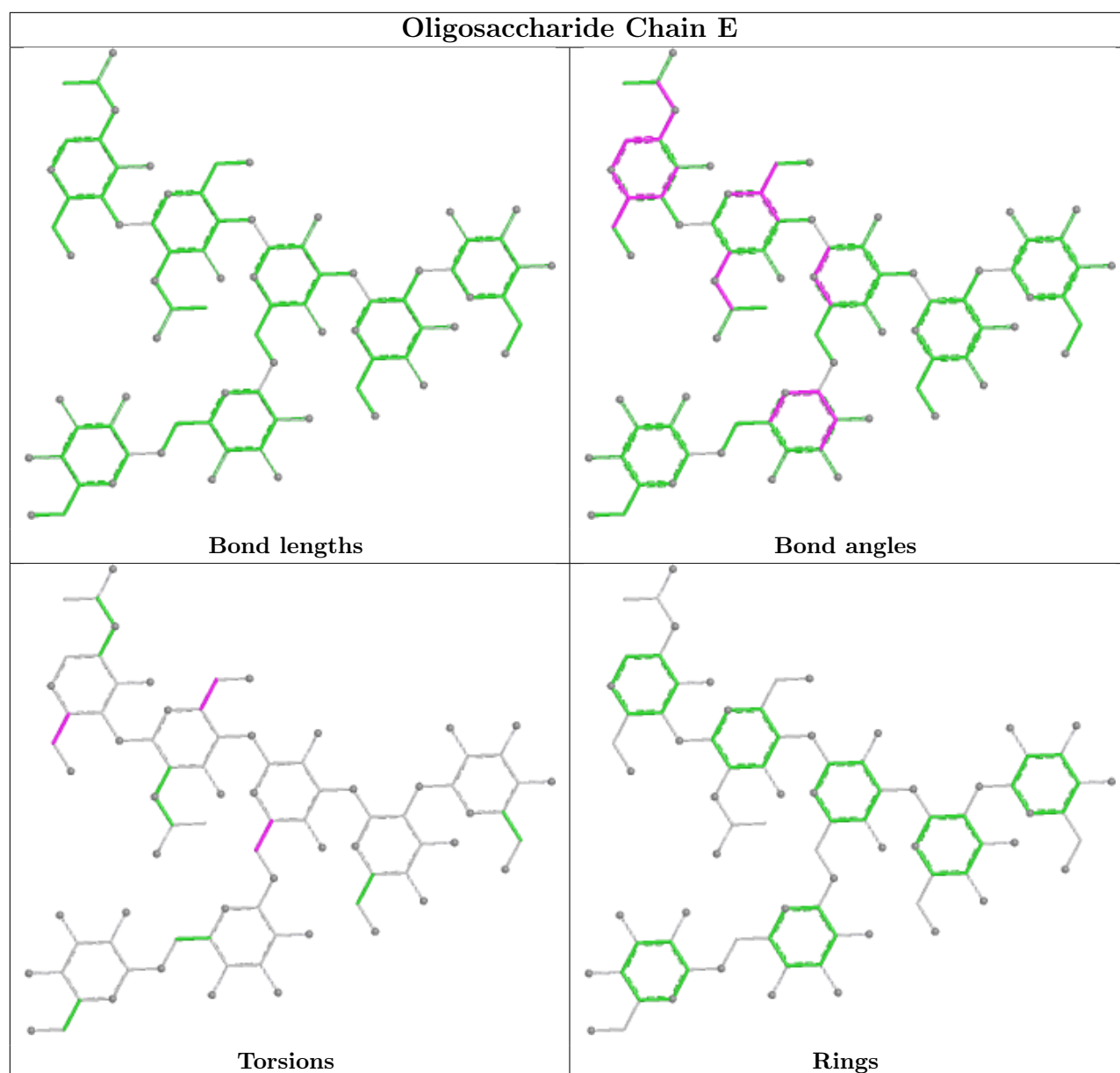
7 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
3	C	2	NAG	1	0
5	E	2	NAG	1	0
5	E	3	BMA	3	0
5	E	5	MAN	1	0
5	E	7	MAN	1	0
5	E	6	MAN	2	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 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	611/740 (82%)	0.75	70 (11%)	9 13	99, 186, 319, 397	0
2	B	619/865 (71%)	0.77	67 (10%)	11 14	106, 195, 319, 424	0
All	All	1230/1605 (76%)	0.76	137 (11%)	10 14	99, 191, 319, 424	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1838	PHE	7.1
2	B	2058	SER	6.1
1	A	190	GLN	5.7
1	A	528	CYS	4.7
1	A	491	LEU	4.4
1	A	201	VAL	4.3
2	B	1802	PRO	4.3
2	B	2158	ILE	4.2
1	A	261	GLY	4.2
2	B	1743	PHE	4.2
2	B	2059	ILE	4.1
1	A	78	ALA	4.1
2	B	2252	LEU	4.0
2	B	2171	LEU	3.9
1	A	378	HIS	3.7
2	B	1804	LYS	3.5
1	A	539	MET	3.4
2	B	1793	GLU	3.4
2	B	2306	LEU	3.4
2	B	2031	HIS	3.4
1	A	675	GLY	3.2
2	B	2332	TYR	3.2
2	B	1948	GLY	3.2
2	B	2329	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	403	ASP	3.1
2	B	1852	ILE	3.1
1	A	389	GLU	3.1
2	B	1745	GLN	3.1
1	A	202	PHE	3.1
1	A	262	THR	3.1
1	A	712	ASP	3.1
1	A	192	LEU	3.0
1	A	580	ASP	3.0
1	A	204	GLU	3.0
1	A	108	ALA	3.0
1	A	527	ARG	3.0
1	A	632	HIS	3.0
1	A	391	GLU	3.0
1	A	46	TYR	2.9
2	B	2240	VAL	2.9
2	B	1694	LYS	2.9
2	B	1896	GLU	2.9
1	A	597	ASN	2.9
2	B	1775	PHE	2.9
1	A	716	GLY	2.8
1	A	381	THR	2.8
1	A	634	VAL	2.8
2	B	2301	LEU	2.8
2	B	2271	TRP	2.8
1	A	454	TYR	2.8
1	A	65	ARG	2.7
1	A	455	GLY	2.7
2	B	1740	ASP	2.7
2	B	2268	GLY	2.7
2	B	2052	ARG	2.7
1	A	250	ARG	2.7
1	A	487	TYR	2.6
2	B	1897	ARG	2.6
2	B	2090	ARG	2.6
2	B	1749	ARG	2.6
2	B	2321	MET	2.6
2	B	2266	GLN	2.6
2	B	1710	GLY	2.6
1	A	600	GLY	2.6
2	B	1697	HIS	2.6
1	A	113	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	2328	ALA	2.6
1	A	287	GLU	2.5
2	B	2066	GLU	2.5
1	A	45	VAL	2.5
2	B	1871	VAL	2.5
1	A	554	CYS	2.5
2	B	2300	PRO	2.5
1	A	501	PHE	2.5
1	A	668	LEU	2.5
1	A	667	THR	2.5
2	B	1801	GLU	2.5
2	B	2019	ASN	2.5
1	A	555	TYR	2.4
1	A	636	TYR	2.4
1	A	493	LYS	2.4
1	A	458	GLY	2.4
1	A	492	PRO	2.4
2	B	1967	LYS	2.4
2	B	1742	SER	2.4
1	A	263	THR	2.3
1	A	678	VAL	2.3
2	B	2243	VAL	2.3
1	A	142	LYS	2.3
1	A	692	CYS	2.3
2	B	1765	ALA	2.3
1	A	407	TYR	2.3
1	A	598	PRO	2.3
2	B	1983	PHE	2.3
1	A	265	GLU	2.3
2	B	2164	MET	2.3
2	B	2055	TYR	2.3
2	B	2296	SER	2.3
1	A	666	ASP	2.3
2	B	2299	PRO	2.3
2	B	2267	ASP	2.3
2	B	2295	ASN	2.2
2	B	1851	LEU	2.2
1	A	17	MET	2.2
1	A	139	GLN	2.2
1	A	468	GLN	2.2
1	A	479	GLY	2.2
2	B	2230	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	161	HIS	2.2
2	B	1831	ASP	2.2
2	B	2330	ASP	2.2
2	B	2060	ASN	2.2
2	B	1826	THR	2.2
1	A	552	LEU	2.2
2	B	2091	GLN	2.2
1	A	664	TYR	2.1
2	B	1739	THR	2.1
1	A	54	PHE	2.1
2	B	2323	VAL	2.1
1	A	16	TYR	2.1
1	A	275	THR	2.1
2	B	1949	SER	2.1
2	B	2251	LEU	2.1
1	A	53	GLU	2.1
1	A	208	TRP	2.1
2	B	1733	VAL	2.1
1	A	583	ARG	2.1
1	A	228	TRP	2.1
1	A	178	VAL	2.1
2	B	1792	TYR	2.0
1	A	697	PHE	2.0
2	B	2302	LEU	2.0
1	A	140	VAL	2.0
1	A	538	ASN	2.0
2	B	1744	THR	2.0
2	B	2272	THR	2.0
2	B	1821	HIS	2.0

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

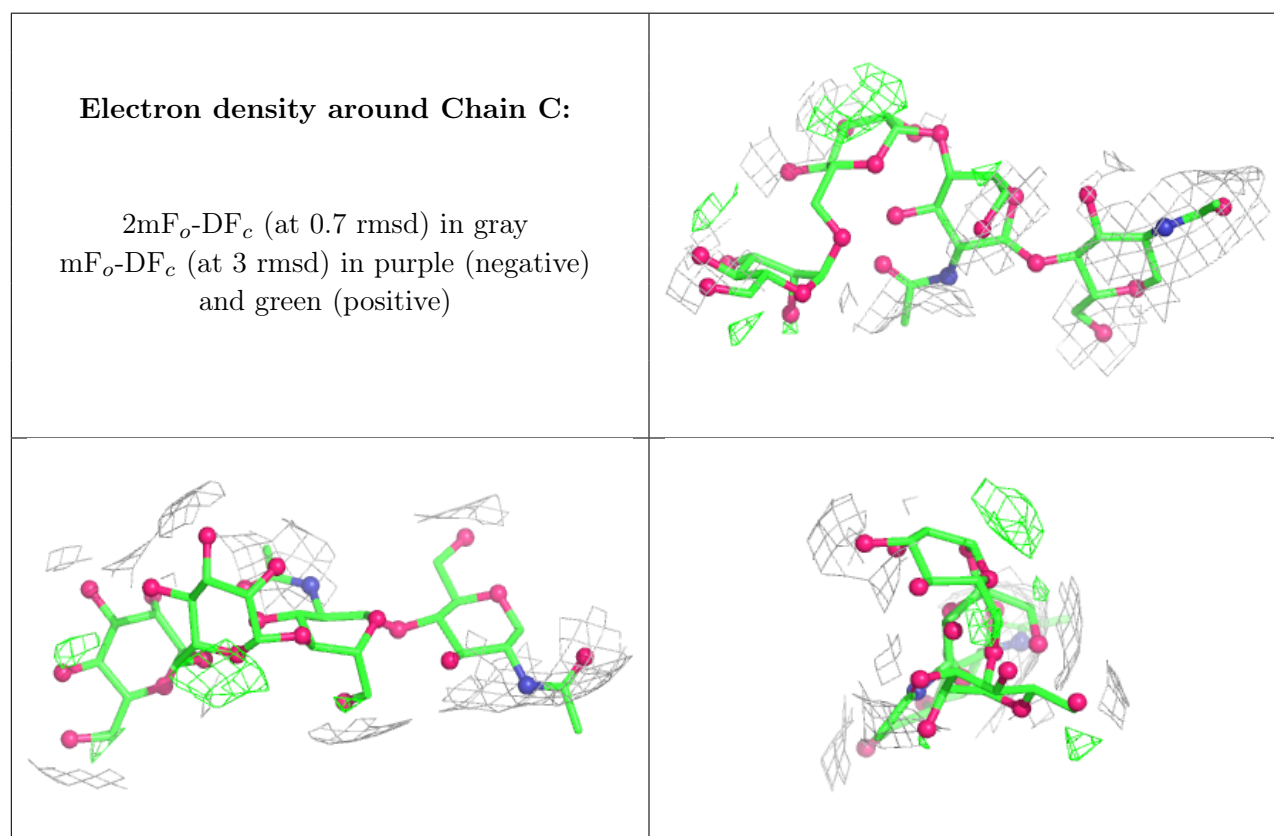
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.

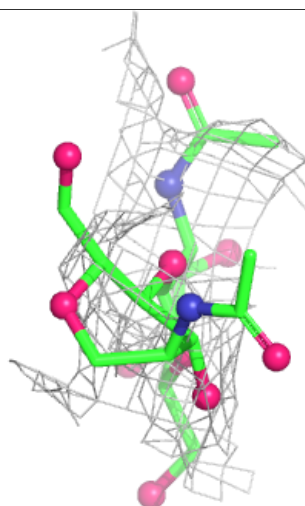
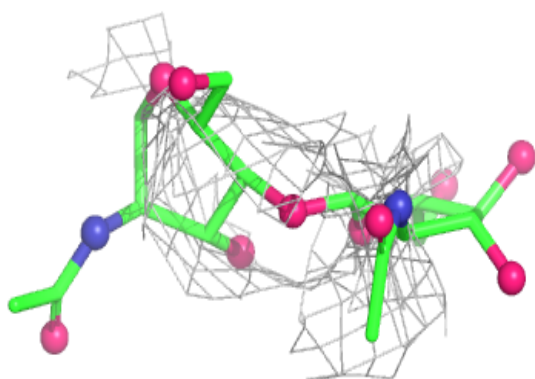
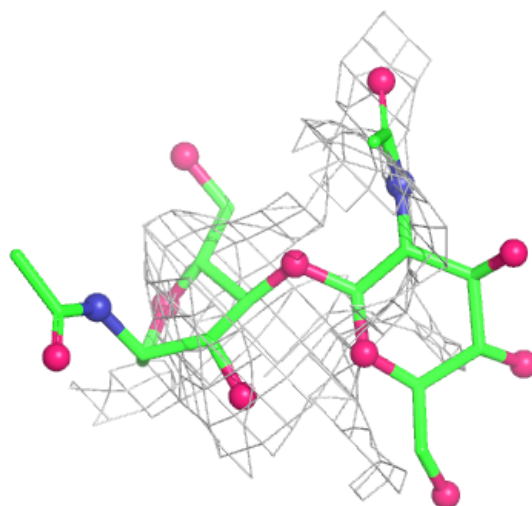
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MAN	E	5	11/12	0.25	0.18	192,215,228,233	11
4	NAG	D	2	14/15	0.27	0.14	307,363,404,410	0
3	BMA	C	3	11/12	0.39	0.12	181,207,223,224	11
3	MAN	C	4	11/12	0.41	0.15	193,218,224,226	11
5	BMA	E	4	11/12	0.61	0.24	222,241,252,258	11
5	MAN	E	6	11/12	0.65	0.14	348,364,380,392	0
4	NAG	D	1	14/15	0.66	0.16	275,361,420,429	0
5	BMA	E	3	11/12	0.67	0.13	278,295,314,335	0
5	MAN	E	7	11/12	0.79	0.16	303,330,373,383	0
3	NAG	C	1	14/15	0.87	0.22	199,244,264,269	0
3	NAG	C	2	14/15	0.88	0.11	169,231,241,258	14
5	NAG	E	2	14/15	0.91	0.18	228,247,271,273	0
5	NAG	E	1	14/15	0.95	0.16	151,202,230,232	0

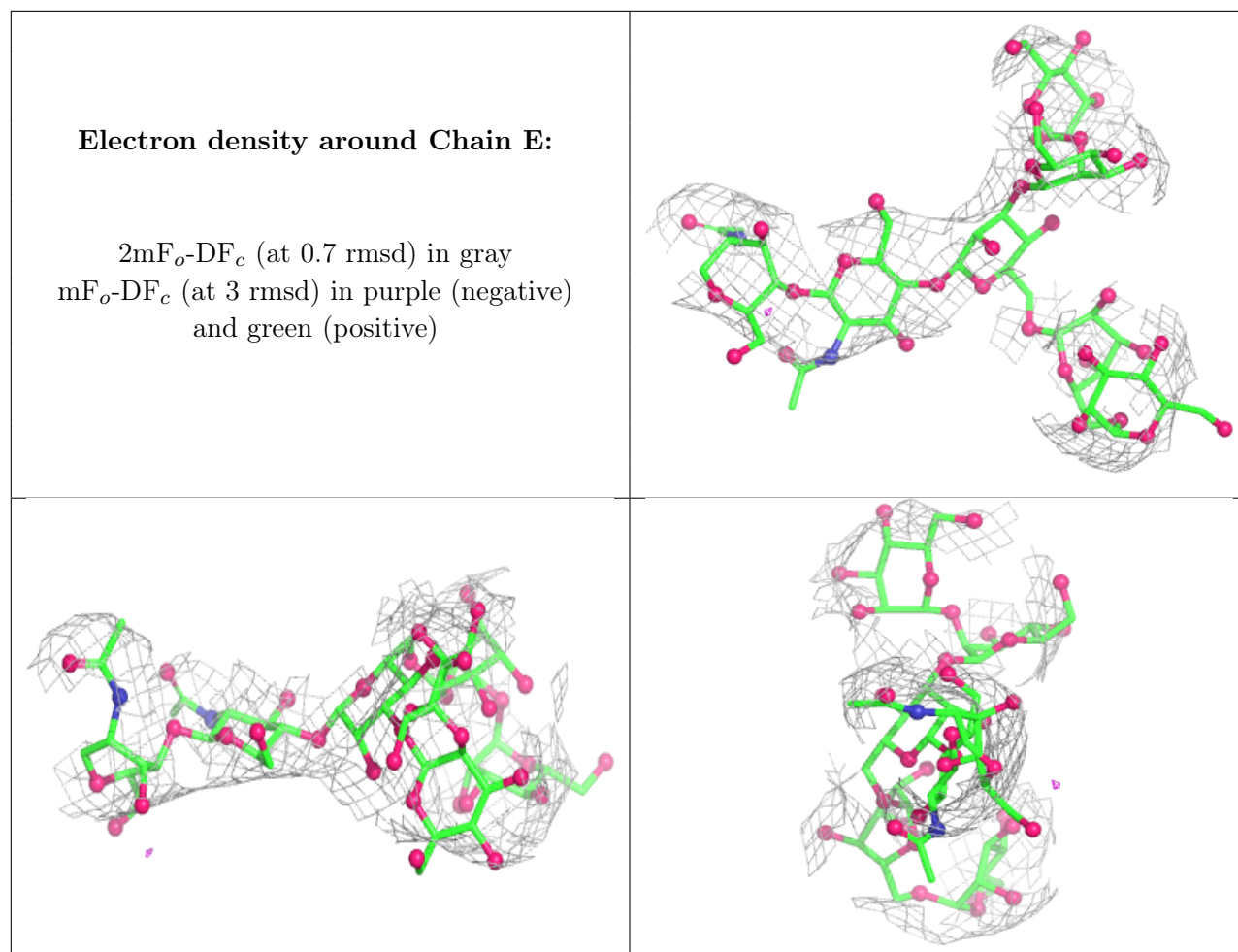
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain D:

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





6.4 Ligands [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
6	CA	A	806	1/1	0.91	0.10	236,236,236,236	0
6	CA	A	807	1/1	0.97	0.12	165,165,165,165	0
6	CA	A	805	1/1	0.99	0.09	215,215,215,215	0
7	CU	A	808	1/1	0.99	0.06	167,167,167,167	0
7	CU	B	2610	1/1	0.99	0.09	150,150,150,150	0

6.5 Other polymers [i](#)

There are no such residues in this entry.