



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:54 PM UTC

PDB ID : 3FU9 / pdb_00003fu9
Title : Melanocarpus albomyces laccase crystal soaked (20 min) with 2,6-dimethoxyphenol
Authors : Kallio, J.P.; Hakulinen, N.; Rouvinen, J.
Deposited on : 2009-01-14
Resolution : 2.00 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

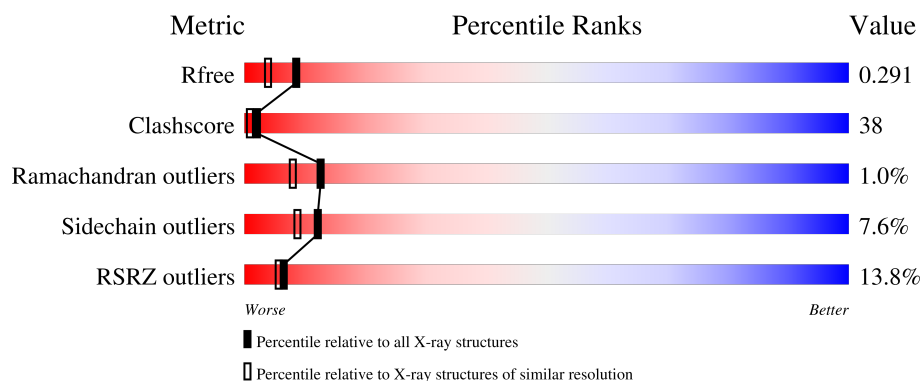
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	559	14% 44% 41% 14% .
1	B	559	13% 40% 45% 13% .
2	C	2	100%
2	D	2	50% 50%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	A	605	-	-	X	-
7	KIB	B	611	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9692 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 Laccase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4369	2764	759	831	15			
1	B	559	Total	C	N	O	S	0	0	0
			4369	2764	759	831	15			

- Molecule 2 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
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

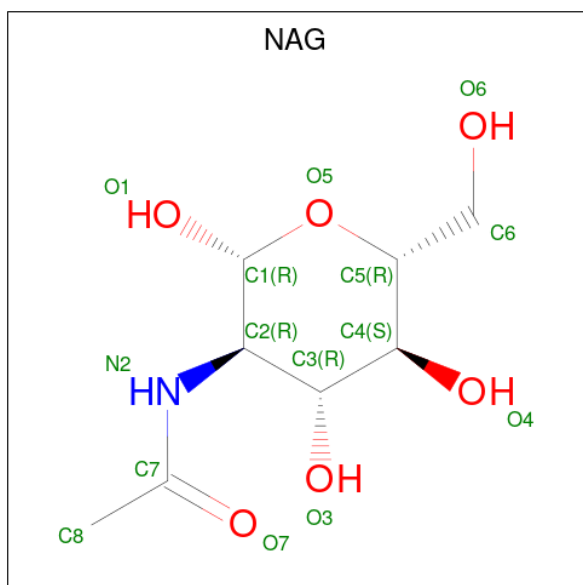
- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cu	0	0
			4	4		
3	B	4	Total	Cu	0	0
			4	4		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



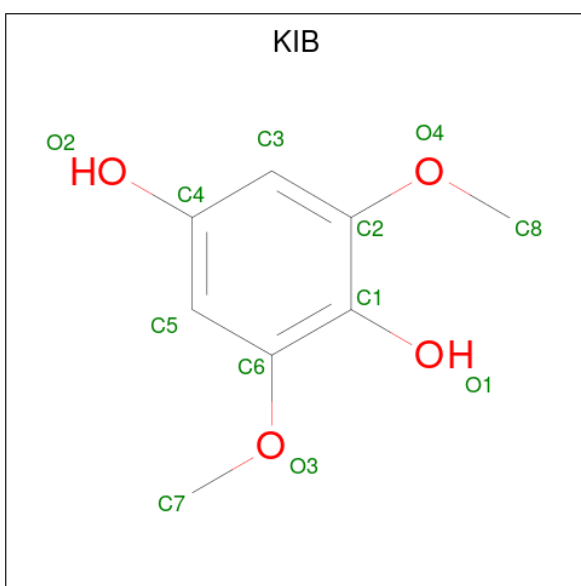
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2,6-dimethoxybenzene-1,4-diol (CCD ID: KIB) (formula: C₈H₁₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			12	8	4		
7	B	1	Total	C	O	0	0
			12	8	4		

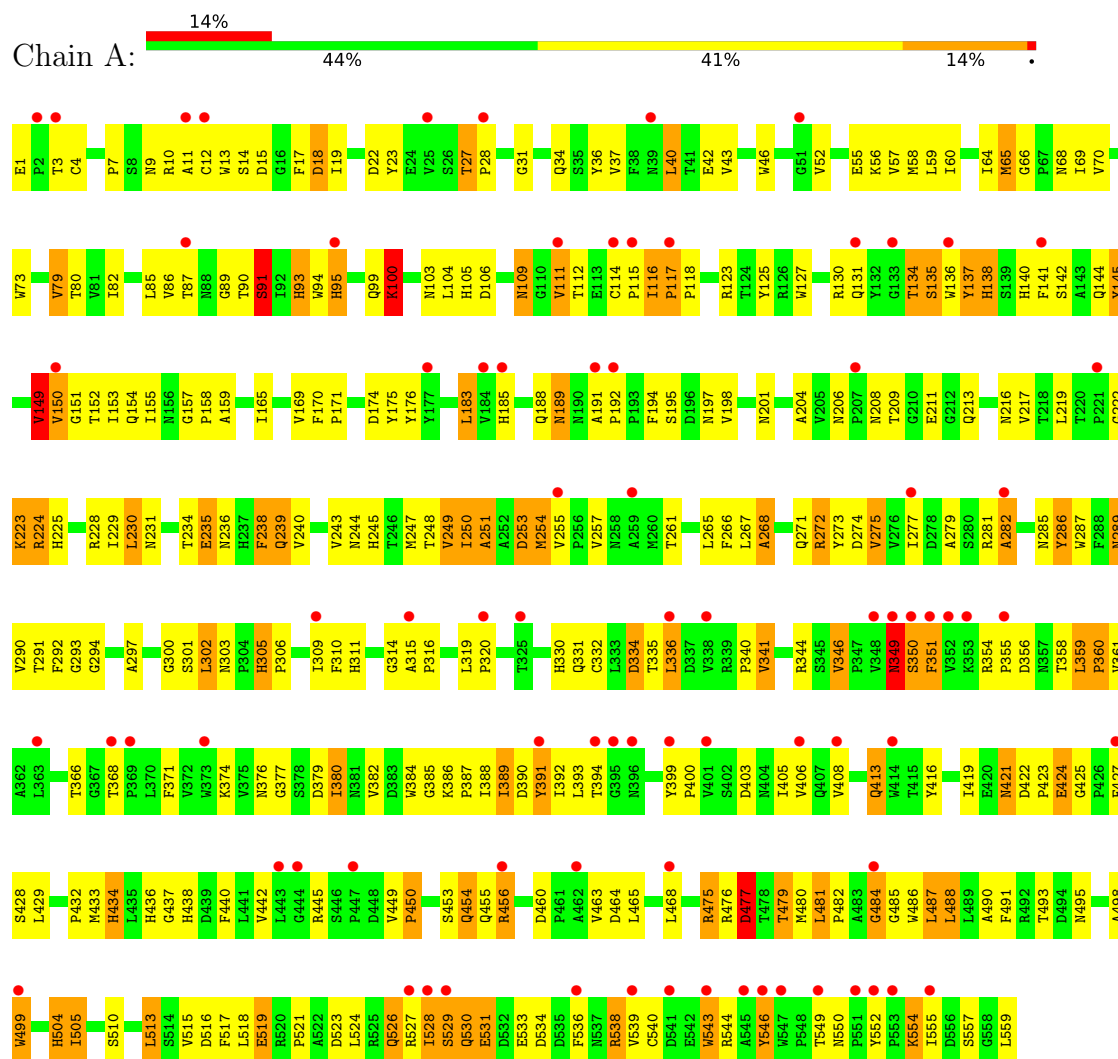
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	340	Total 340	O 340	0	0
8	B	360	Total 360	O 360	0	0

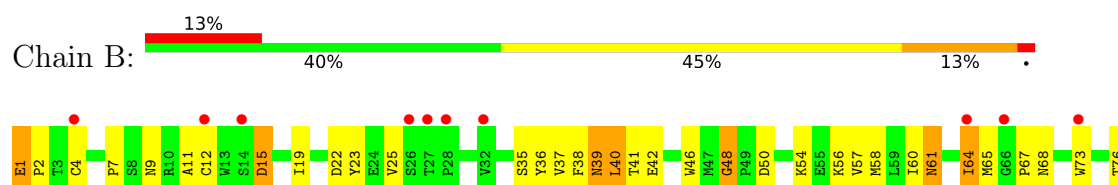
3 Residue-property plots

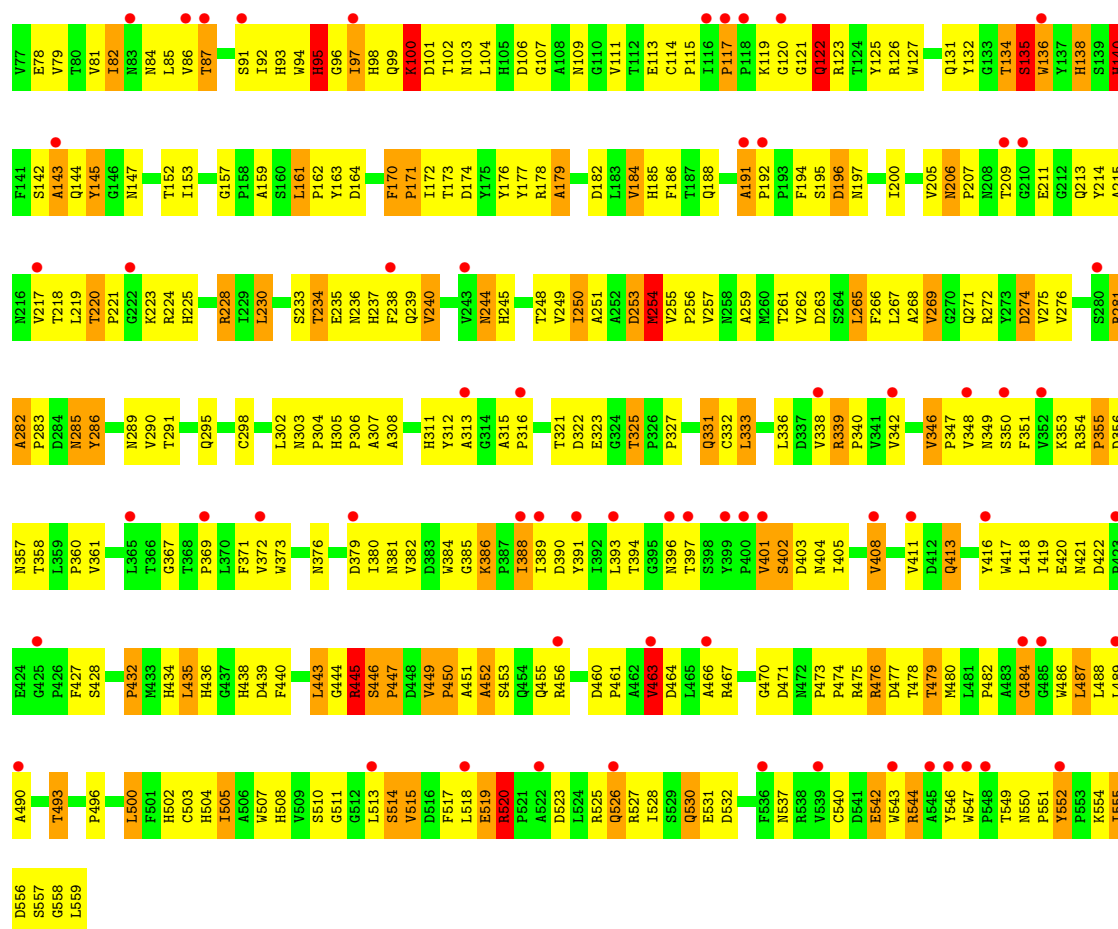
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Laccase-1



• Molecule 1: Laccase-1





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

Chain C: 100%

MAG1
MAG2

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

Chain D: 50%

MAG1
MAG2

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

Chain E: 100%

MAG1
MAG2

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

Chain F:



MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.12Å 60.23Å 117.13Å 90.00° 98.36° 90.00°	Depositor
Resolution (Å)	19.61 – 2.00 19.61 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.61-2.00) 97.3 (19.61-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.330 0.291 , 0.291	Depositor DCC
R_{free} test set	4595 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	10.1	Xtriage
Anisotropy	1.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	9692	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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: NAG, CL, KIB, CU, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.80	76/4506 (1.7%)	1.63	70/6191 (1.1%)
1	B	1.78	78/4506 (1.7%)	1.73	80/6191 (1.3%)
All	All	1.79	154/9012 (1.7%)	1.68	150/12382 (1.2%)

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

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

All (154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	GLN	C-O	-12.50	1.09	1.24
1	A	117	PRO	CA-C	11.29	1.58	1.51
1	A	361	VAL	CA-CB	10.77	1.68	1.54
1	A	346	VAL	CA-CB	-9.39	1.44	1.55
1	A	505	ILE	C-O	8.95	1.33	1.24
1	B	358	THR	CA-CB	8.59	1.66	1.53
1	A	482	PRO	C-O	8.37	1.33	1.23
1	B	388	ILE	CA-CB	8.06	1.65	1.54
1	B	73	TRP	CA-C	7.96	1.62	1.52
1	B	342	VAL	CA-C	-7.95	1.46	1.53
1	B	42	GLU	N-CA	7.73	1.55	1.46
1	B	515	VAL	CA-CB	7.71	1.65	1.54
1	A	488	LEU	C-O	7.46	1.32	1.24
1	B	230	LEU	N-CA	7.46	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	191	ALA	C-O	-7.38	1.14	1.24
1	B	251	ALA	N-CA	7.31	1.54	1.46
1	A	360	PRO	CA-C	7.24	1.59	1.52
1	A	513	LEU	C-O	7.21	1.33	1.24
1	A	238	PHE	CA-C	-7.17	1.44	1.52
1	B	266	PHE	N-CA	7.14	1.54	1.46
1	B	274	ASP	C-O	-7.10	1.15	1.23
1	A	79	VAL	CA-CB	7.02	1.63	1.54
1	B	486	TRP	C-O	6.96	1.32	1.23
1	B	339	ARG	N-CA	6.96	1.55	1.46
1	A	475	ARG	C-O	6.95	1.31	1.24
1	B	361	VAL	CA-CB	6.95	1.63	1.54
1	B	143	ALA	CA-C	6.95	1.62	1.52
1	A	191	ALA	CA-CB	6.94	1.63	1.53
1	B	452	ALA	CA-CB	6.91	1.64	1.53
1	A	243	VAL	C-O	-6.88	1.17	1.24
1	A	463	VAL	C-O	6.83	1.32	1.24
1	A	251	ALA	CA-C	-6.79	1.44	1.52
1	B	500	LEU	C-O	6.75	1.31	1.23
1	A	275	VAL	C-O	-6.73	1.16	1.23
1	A	546	TYR	N-CA	6.72	1.54	1.46
1	A	293	GLY	N-CA	6.65	1.51	1.45
1	A	366	THR	CA-CB	6.55	1.63	1.53
1	B	179	ALA	CA-CB	6.48	1.63	1.53
1	B	466	ALA	N-CA	6.47	1.54	1.46
1	A	240	VAL	N-CA	6.43	1.53	1.46
1	B	152	THR	CA-C	6.43	1.60	1.52
1	B	240	VAL	CA-CB	-6.43	1.44	1.54
1	B	488	LEU	N-CA	6.41	1.53	1.46
1	A	55	GLU	C-O	-6.35	1.16	1.24
1	A	127	TRP	N-CA	-6.30	1.38	1.45
1	B	138	HIS	N-CA	-6.29	1.38	1.46
1	B	61	ASN	C-O	6.28	1.31	1.23
1	B	220	THR	C-O	6.24	1.32	1.24
1	A	134	THR	C-O	-6.23	1.17	1.24
1	A	486	TRP	C-O	6.23	1.31	1.23
1	A	513	LEU	N-CA	6.21	1.54	1.46
1	B	339	ARG	CA-CB	6.20	1.61	1.53
1	B	39	ASN	N-CA	-6.18	1.38	1.46
1	B	152	THR	C-O	6.17	1.31	1.23
1	B	136	TRP	C-O	-6.15	1.16	1.23
1	A	499	TRP	CA-C	-6.10	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	ASP	CA-C	6.08	1.59	1.53
1	A	286	TYR	CD2-CE2	6.08	1.56	1.38
1	B	275	VAL	CA-CB	6.08	1.65	1.55
1	A	136	TRP	N-CA	-6.06	1.38	1.46
1	A	198	VAL	CA-CB	6.05	1.61	1.53
1	B	496	PRO	N-CA	6.01	1.55	1.47
1	B	518	LEU	C-O	5.98	1.31	1.23
1	B	161	LEU	CA-C	-5.96	1.44	1.52
1	B	134	THR	C-O	-5.95	1.16	1.24
1	B	419	ILE	CA-CB	-5.94	1.47	1.54
1	A	99	GLN	CA-C	5.92	1.61	1.53
1	B	257	VAL	CA-C	5.90	1.59	1.52
1	A	165	ILE	C-O	-5.88	1.18	1.24
1	B	135	SER	CA-C	-5.82	1.45	1.52
1	A	351	PHE	N-CA	5.82	1.53	1.46
1	B	357	ASN	N-CA	5.81	1.53	1.46
1	A	289	ASN	CG-ND2	5.80	1.45	1.33
1	B	173	THR	N-CA	5.79	1.53	1.46
1	B	386	LYS	C-O	5.79	1.30	1.24
1	A	230	LEU	N-CA	5.77	1.53	1.45
1	B	140	HIS	N-CA	-5.76	1.40	1.46
1	A	249	VAL	CA-CB	-5.67	1.47	1.53
1	A	197	ASN	N-CA	5.61	1.52	1.46
1	B	265	LEU	C-O	-5.61	1.17	1.23
1	B	136	TRP	N-CA	-5.60	1.39	1.46
1	B	435	LEU	C-O	5.60	1.30	1.24
1	A	194	PHE	C-O	5.59	1.30	1.23
1	A	86	VAL	C-O	-5.58	1.18	1.24
1	B	257	VAL	CA-CB	5.58	1.64	1.55
1	B	555	ILE	CA-CB	5.57	1.61	1.54
1	A	250	ILE	CB-CG2	5.56	1.71	1.52
1	A	359	LEU	C-N	5.55	1.38	1.33
1	A	484	GLY	C-O	-5.54	1.16	1.23
1	B	488	LEU	CA-C	-5.54	1.46	1.52
1	A	272	ARG	C-O	-5.54	1.17	1.23
1	B	157	GLY	C-N	5.53	1.40	1.33
1	B	519	GLU	CA-C	5.51	1.60	1.52
1	B	145	TYR	N-CA	5.49	1.53	1.46
1	B	87	THR	CA-C	5.49	1.59	1.52
1	A	136	TRP	C-O	-5.48	1.17	1.23
1	A	450	PRO	N-CA	-5.45	1.40	1.47
1	A	519	GLU	CA-CB	5.45	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	379	ASP	C-O	5.43	1.30	1.24
1	A	135	SER	CA-C	-5.42	1.45	1.52
1	A	111	VAL	CA-CB	5.41	1.61	1.54
1	A	255	VAL	CB-CG2	5.40	1.70	1.52
1	A	504	HIS	C-O	5.39	1.30	1.24
1	A	517	PHE	CA-C	5.39	1.59	1.52
1	B	445	ARG	CZ-NH2	5.39	1.40	1.33
1	B	170	PHE	C-O	-5.38	1.18	1.24
1	B	451	ALA	CA-C	-5.38	1.45	1.52
1	B	408	VAL	CA-CB	5.37	1.60	1.53
1	A	341	VAL	CA-CB	5.37	1.60	1.54
1	B	220	THR	N-CA	-5.35	1.38	1.46
1	B	479	THR	CA-CB	5.35	1.63	1.53
1	A	392	ILE	CA-CB	5.35	1.60	1.54
1	B	269	VAL	CA-CB	5.34	1.59	1.54
1	B	298	CYS	CA-C	5.33	1.60	1.52
1	B	449	VAL	CA-C	5.32	1.58	1.52
1	A	93	HIS	C-O	-5.31	1.17	1.24
1	A	235	GLU	N-CA	5.30	1.53	1.46
1	A	432	PRO	CA-C	5.30	1.59	1.52
1	A	175	TYR	CA-CB	5.29	1.61	1.53
1	B	95	HIS	C-O	5.28	1.30	1.24
1	B	486	TRP	CA-CB	5.28	1.63	1.53
1	B	269	VAL	C-O	-5.28	1.18	1.24
1	A	486	TRP	N-CA	5.26	1.52	1.46
1	A	183	LEU	N-CA	-5.23	1.40	1.46
1	B	171	PRO	C-O	5.23	1.29	1.23
1	A	477	ASP	CA-C	-5.22	1.45	1.52
1	B	511	GLY	C-O	5.22	1.29	1.24
1	A	149	VAL	C-N	5.21	1.36	1.33
1	A	104	LEU	N-CA	5.21	1.53	1.46
1	A	152	THR	CA-C	5.21	1.58	1.52
1	A	52	VAL	CA-CB	5.21	1.60	1.54
1	B	37	VAL	CA-C	5.20	1.58	1.52
1	B	254	MET	CA-C	5.18	1.60	1.52
1	A	247	MET	C-O	-5.17	1.18	1.24
1	B	551	PRO	CA-C	5.17	1.60	1.52
1	A	531	GLU	CG-CD	5.16	1.65	1.52
1	B	463	VAL	C-O	5.16	1.29	1.24
1	A	389	ILE	CG1-CD1	5.16	1.71	1.51
1	A	244	ASN	N-CA	5.15	1.52	1.46
1	A	380	ILE	CA-CB	5.13	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	VAL	CA-CB	5.12	1.61	1.54
1	A	349	ASN	CA-C	5.11	1.59	1.52
1	B	157	GLY	N-CA	5.11	1.51	1.44
1	B	286	TYR	CD1-CE1	5.10	1.53	1.38
1	A	138	HIS	C-O	-5.08	1.17	1.23
1	B	92	ILE	CA-C	-5.08	1.46	1.52
1	A	391	TYR	N-CA	5.05	1.52	1.46
1	B	87	THR	CA-CB	5.05	1.61	1.53
1	A	153	ILE	N-CA	5.05	1.52	1.46
1	B	372	VAL	N-CA	5.03	1.52	1.46
1	A	302	LEU	C-O	-5.02	1.17	1.24
1	B	544	ARG	N-CA	-5.01	1.40	1.46
1	A	481	LEU	C-O	5.01	1.30	1.24
1	B	228	ARG	N-CA	-5.01	1.39	1.46

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	446	SER	CA-C-N	-16.38	104.49	120.21
1	B	446	SER	C-N-CA	-16.38	104.49	120.21
1	A	66	GLY	CA-C-N	13.01	133.17	119.90
1	A	66	GLY	C-N-CA	13.01	133.17	119.90
1	B	386	LYS	CA-C-N	12.09	132.06	119.85
1	B	386	LYS	C-N-CA	12.09	132.06	119.85
1	B	350	SER	N-CA-C	10.52	129.93	112.99
1	B	282	ALA	CA-C-N	10.43	132.88	119.84
1	B	282	ALA	C-N-CA	10.43	132.88	119.84
1	B	97	ILE	N-CA-CB	-10.28	102.09	112.06
1	A	480	MET	N-CA-C	9.44	123.46	109.59
1	B	196	ASP	N-CA-C	-9.31	101.69	113.23
1	B	558	GLY	N-CA-C	-9.30	102.29	114.85
1	A	303	ASN	CA-C-N	-8.97	110.87	120.47
1	A	303	ASN	C-N-CA	-8.97	110.87	120.47
1	A	351	PHE	N-CA-C	8.66	122.33	109.59
1	A	70	VAL	N-CA-C	-8.64	96.43	108.27
1	B	144	GLN	N-CA-C	-8.50	101.96	111.82
1	B	255	VAL	CA-C-N	-8.38	111.15	119.78
1	B	255	VAL	C-N-CA	-8.38	111.15	119.78
1	A	425	GLY	CA-C-N	8.26	127.85	118.85
1	A	425	GLY	C-N-CA	8.26	127.85	118.85
1	A	155	ILE	N-CA-C	-8.21	95.22	107.37
1	A	421	ASN	N-CA-C	8.13	120.89	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	351	PHE	N-CA-C	8.08	122.97	110.20
1	B	161	LEU	N-CA-C	-7.85	97.99	108.11
1	B	443	LEU	N-CA-C	-7.72	103.32	112.89
1	B	73	TRP	CB-CA-C	7.62	119.17	109.80
1	B	250	ILE	N-CA-C	-7.57	105.63	112.90
1	A	249	VAL	CB-CA-C	-7.50	101.28	111.33
1	A	390	ASP	N-CA-C	-7.48	104.29	113.41
1	A	526	GLN	N-CA-C	7.45	120.27	111.71
1	A	543	TRP	N-CA-C	-7.42	103.27	111.36
1	B	120	GLY	N-CA-C	7.37	126.24	114.90
1	A	538	ARG	N-CA-C	-7.34	102.97	110.97
1	A	464	ASP	N-CA-C	7.30	121.43	112.23
1	A	350	SER	N-CA-C	7.27	126.28	110.80
1	A	149	VAL	CA-C-N	-7.14	114.83	121.97
1	A	149	VAL	C-N-CA	-7.14	114.83	121.97
1	A	27	THR	CB-CA-C	-7.10	98.12	108.84
1	B	161	LEU	CA-C-N	7.06	126.98	119.85
1	B	161	LEU	C-N-CA	7.06	126.98	119.85
1	B	444	GLY	N-CA-C	7.00	119.29	110.96
1	B	505	ILE	CA-C-N	6.97	129.50	120.44
1	B	505	ILE	C-N-CA	6.97	129.50	120.44
1	A	117	PRO	N-CA-C	6.93	117.12	110.47
1	A	379	ASP	CA-C-N	-6.75	109.46	120.13
1	A	379	ASP	C-N-CA	-6.75	109.46	120.13
1	B	544	ARG	N-CA-C	-6.62	104.15	111.36
1	B	480	MET	N-CA-C	6.61	120.28	109.76
1	A	116	ILE	CB-CA-C	-6.50	103.21	110.68
1	A	40	LEU	CA-CB-CG	6.46	138.93	116.30
1	A	528	ILE	CB-CA-C	-6.46	103.15	110.96
1	B	186	PHE	N-CA-C	6.43	118.83	111.11
1	B	525	ARG	N-CA-C	6.37	119.03	111.33
1	A	89	GLY	N-CA-C	-6.36	104.40	112.54
1	B	555	ILE	N-CA-C	6.29	118.15	112.17
1	A	554	LYS	CD-CE-NZ	-6.28	91.82	111.90
1	B	520	ARG	CA-C-N	6.25	126.44	119.32
1	B	520	ARG	C-N-CA	6.25	126.44	119.32
1	B	206	ASN	N-CA-C	-6.21	101.83	109.65
1	B	276	VAL	CB-CA-C	6.18	120.04	110.83
1	A	315	ALA	CA-C-N	-6.17	112.13	119.84
1	A	315	ALA	C-N-CA	-6.17	112.13	119.84
1	B	82	ILE	CB-CA-C	6.14	119.50	110.77
1	B	379	ASP	CA-C-N	-6.11	111.83	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	379	ASP	C-N-CA	-6.11	111.83	120.75
1	A	282	ALA	CA-C-N	6.10	127.47	119.84
1	A	282	ALA	C-N-CA	6.10	127.47	119.84
1	B	117	PRO	O-C-N	6.08	124.01	121.15
1	B	342	VAL	N-CA-C	-6.06	100.82	107.73
1	B	48	GLY	CA-C-N	6.06	125.74	119.56
1	B	48	GLY	C-N-CA	6.06	125.74	119.56
1	B	505	ILE	N-CA-C	-5.99	100.99	108.89
1	A	403	ASP	N-CA-C	5.98	119.84	112.54
1	B	346	VAL	CA-C-N	-5.96	112.20	120.25
1	B	346	VAL	C-N-CA	-5.96	112.20	120.25
1	A	192	PRO	N-CA-C	-5.92	103.48	110.70
1	A	188	GLN	N-CA-C	5.89	119.29	111.75
1	B	153	ILE	N-CA-C	5.89	116.77	108.17
1	B	68	ASN	CB-CA-C	-5.84	101.78	111.41
1	B	367	GLY	CA-C-N	5.82	130.36	122.56
1	B	367	GLY	C-N-CA	5.82	130.36	122.56
1	B	517	PHE	N-CA-C	5.82	117.94	108.63
1	B	54	LYS	N-CA-C	5.81	119.73	109.96
1	B	96	GLY	CA-C-N	5.80	128.90	122.22
1	B	96	GLY	C-N-CA	5.80	128.90	122.22
1	B	274	ASP	N-CA-C	-5.76	101.16	110.32
1	B	391	TYR	N-CA-C	5.75	117.22	111.07
1	B	234	THR	N-CA-C	-5.70	106.16	113.23
1	B	447	PRO	N-CA-C	5.69	119.19	111.22
1	A	229	ILE	CB-CA-C	-5.69	103.42	111.21
1	B	285	ASN	N-CA-C	-5.63	100.22	109.40
1	B	476	ARG	CA-CB-CG	5.62	125.34	114.10
1	B	411	VAL	CB-CA-C	-5.59	103.98	110.91
1	B	405	ILE	N-CA-C	5.57	116.25	108.89
1	B	552	TYR	N-CA-C	5.55	117.67	110.40
1	B	331	GLN	N-CA-C	5.53	119.19	111.90
1	A	145	TYR	N-CA-C	-5.51	106.06	112.89
1	A	374	LYS	N-CA-C	5.49	117.85	108.90
1	A	486	TRP	N-CA-C	5.49	118.14	108.75
1	B	530	GLN	N-CA-C	-5.49	105.45	111.82
1	B	552	TYR	CA-C-N	-5.49	114.33	120.14
1	B	552	TYR	C-N-CA	-5.49	114.33	120.14
1	B	92	ILE	N-CA-C	-5.48	99.86	107.80
1	A	460	ASP	CA-C-N	-5.47	112.89	118.85
1	A	460	ASP	C-N-CA	-5.47	112.89	118.85
1	B	239	GLN	N-CA-C	-5.36	100.17	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	GLN	O-C-N	-5.35	116.06	123.12
1	A	217	VAL	CB-CA-C	-5.35	102.86	110.83
1	A	95	HIS	N-CA-C	5.34	117.44	109.59
1	A	336	LEU	N-CA-C	-5.34	106.07	112.59
1	B	418	LEU	CA-C-N	-5.34	116.06	122.90
1	B	418	LEU	C-N-CA	-5.34	116.06	122.90
1	A	495	ASN	CA-C-N	-5.33	114.29	119.78
1	A	495	ASN	C-N-CA	-5.33	114.29	119.78
1	B	432	PRO	CA-C-N	5.31	129.47	122.30
1	B	432	PRO	C-N-CA	5.31	129.47	122.30
1	B	173	THR	N-CA-C	5.31	118.08	108.69
1	B	555	ILE	CB-CA-C	-5.31	105.11	111.85
1	A	159	ALA	CA-C-N	-5.30	113.84	122.65
1	A	159	ALA	C-N-CA	-5.30	113.84	122.65
1	A	274	ASP	CA-C-N	-5.30	115.16	122.69
1	A	274	ASP	C-N-CA	-5.30	115.16	122.69
1	A	394	THR	N-CA-C	-5.29	106.41	112.92
1	A	253	ASP	CB-CA-C	5.28	120.93	110.42
1	B	122	GLN	N-CA-C	5.28	117.10	108.55
1	A	377	GLY	N-CA-C	5.23	122.84	115.30
1	A	137	TYR	CA-C-N	5.23	132.52	121.91
1	A	137	TYR	C-N-CA	5.23	132.52	121.91
1	A	529	SER	CA-C-N	5.20	127.67	120.29
1	A	529	SER	C-N-CA	5.20	127.67	120.29
1	B	235	GLU	N-CA-C	5.18	121.84	110.80
1	A	334	ASP	N-CA-C	5.18	117.36	110.53
1	A	319	LEU	CA-C-N	5.14	125.14	119.89
1	A	319	LEU	C-N-CA	5.14	125.14	119.89
1	A	359	LEU	CB-CA-C	5.14	117.02	110.34
1	A	170	PHE	CA-C-N	-5.14	114.69	120.14
1	A	170	PHE	C-N-CA	-5.14	114.69	120.14
1	B	41	THR	N-CA-C	5.13	117.18	109.23
1	B	206	ASN	CA-C-N	-5.12	115.06	121.00
1	B	206	ASN	C-N-CA	-5.12	115.06	121.00
1	A	305	HIS	CB-CA-C	-5.10	103.77	111.27
1	A	18	ASP	N-CA-C	5.10	114.97	108.24
1	A	546	TYR	N-CA-C	5.08	116.81	111.28
1	A	255	VAL	CA-C-N	5.07	124.98	119.76
1	A	255	VAL	C-N-CA	5.07	124.98	119.76
1	B	266	PHE	CB-CA-C	-5.04	102.03	110.19
1	B	254	MET	CA-C-O	5.02	126.63	120.15
1	B	537	ASN	N-CA-C	5.01	117.47	111.71

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	437	GLY	Peptide
1	B	514	SER	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	4369	0	4114	267	0
1	B	4369	0	4114	375	1
2	C	28	0	24	5	0
2	D	28	0	24	3	0
2	E	28	0	25	8	0
2	F	28	0	25	4	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	3	0
4	B	1	0	0	0	0
5	A	42	0	39	5	1
5	B	56	0	52	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	12	0	8	1	0
7	B	12	0	8	7	0
8	A	340	0	0	110	0
8	B	360	0	0	184	0
All	All	9692	0	8433	655	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 38.

All (655) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:THR:HG22	8:B:854:HOH:O	1.28	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:GLU:HB2	8:B:717:HOH:O	1.26	1.28
1:B:143:ALA:HA	8:B:877:HOH:O	1.29	1.27
1:B:230:LEU:HB3	8:B:824:HOH:O	1.34	1.27
1:A:510:SER:HB2	8:A:702:HOH:O	1.29	1.25
1:B:505:ILE:HD13	8:B:1023:HOH:O	1.37	1.23
1:B:369:PRO:HB3	8:B:939:HOH:O	1.36	1.23
1:A:12:CYS:HB3	8:A:999:HOH:O	1.10	1.22
1:A:528:ILE:HD12	8:A:992:HOH:O	1.36	1.22
1:B:478:THR:HG22	8:B:955:HOH:O	1.36	1.21
1:B:134:THR:HG22	8:B:722:HOH:O	1.05	1.20
1:B:97:ILE:HD13	8:B:810:HOH:O	1.41	1.18
1:B:388:ILE:HG23	8:B:855:HOH:O	1.46	1.15
1:B:449:VAL:HG21	8:B:832:HOH:O	1.46	1.14
1:B:214:TYR:HA	8:B:831:HOH:O	1.44	1.13
1:B:140:HIS:CE1	8:B:701:HOH:O	1.99	1.12
1:B:217:VAL:HA	8:B:866:HOH:O	1.48	1.11
1:B:23:TYR:HB3	8:B:889:HOH:O	1.50	1.10
1:A:485:GLY:HA3	8:A:719:HOH:O	1.49	1.09
1:A:388:ILE:HD13	1:A:405:ILE:HD11	1.20	1.09
1:A:9:ASN:ND2	1:A:12:CYS:SG	2.25	1.07
1:B:447:PRO:HG2	8:B:881:HOH:O	1.55	1.06
1:B:440:PHE:HE1	8:B:781:HOH:O	1.35	1.05
1:A:64:ILE:HG13	8:A:989:HOH:O	1.55	1.04
1:B:178:ARG:HH21	1:B:182:ASP:HB3	1.23	1.03
1:B:463:VAL:HG23	8:B:952:HOH:O	1.57	1.03
1:B:85:LEU:HA	8:B:761:HOH:O	1.58	1.03
1:A:285:ASN:OD1	1:A:311:HIS:HD2	1.41	1.02
1:B:38:PHE:CE1	1:B:67:PRO:HG2	1.94	1.01
1:B:178:ARG:NH2	1:B:182:ASP:HB3	1.76	1.00
1:B:322:ASP:HA	8:B:931:HOH:O	1.62	1.00
1:A:433:MET:HB2	8:A:703:HOH:O	1.62	1.00
1:A:271:GLN:HG2	1:A:476:ARG:NH2	1.77	0.99
1:B:57:VAL:HG22	8:B:758:HOH:O	1.62	0.99
1:A:382:VAL:HG13	8:A:845:HOH:O	1.63	0.98
1:B:172:ILE:HG13	8:B:702:HOH:O	1.63	0.97
1:B:417:TRP:HD1	8:B:990:HOH:O	1.48	0.97
1:A:141:PHE:CD1	8:A:743:HOH:O	2.19	0.96
1:B:46:TRP:HB2	8:B:758:HOH:O	1.66	0.96
1:A:115:PRO:HD2	8:A:862:HOH:O	1.64	0.96
1:A:309:ILE:HD12	5:A:607:NAG:H81	1.45	0.95
1:B:50:ASP:HB2	8:B:770:HOH:O	1.62	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ILE:CD1	1:A:405:ILE:HD11	1.96	0.95
1:A:301:SER:HB3	8:A:812:HOH:O	1.66	0.94
1:B:19:ILE:HG13	8:B:720:HOH:O	1.65	0.94
1:B:308:ALA:HB2	8:B:791:HOH:O	1.67	0.94
1:B:82:ILE:HG12	1:B:122:GLN:HB2	1.48	0.93
8:A:725:HOH:O	1:B:191:ALA:HB3	1.69	0.92
1:B:140:HIS:ND1	8:B:701:HOH:O	1.96	0.92
1:B:461:PRO:HG3	8:B:992:HOH:O	1.69	0.92
1:A:510:SER:CB	8:A:702:HOH:O	1.96	0.92
1:B:46:TRP:CB	8:B:758:HOH:O	2.18	0.91
1:B:295:GLN:OE1	1:B:452:ALA:HB3	1.68	0.91
1:A:498:ALA:HB2	8:A:830:HOH:O	1.70	0.91
7:B:611:KIB:H7	8:B:821:HOH:O	1.68	0.91
1:B:107:GLY:HA2	1:B:113:GLU:OE1	1.71	0.90
1:A:388:ILE:HD13	1:A:405:ILE:CD1	2.02	0.90
1:A:358:THR:O	5:A:608:NAG:H82	1.73	0.89
1:A:491:PHE:HB2	8:A:878:HOH:O	1.71	0.89
1:B:460:ASP:HB3	1:B:463:VAL:CG1	2.02	0.89
1:B:261:THR:CG2	8:B:854:HOH:O	1.95	0.87
1:A:438:HIS:NE2	1:A:519:GLU:OE1	2.06	0.87
1:B:428:SER:HB3	1:B:484:GLY:H	1.35	0.87
1:B:540:CYS:HB3	8:B:765:HOH:O	1.74	0.87
1:B:413:GLN:HG2	8:B:841:HOH:O	1.74	0.86
1:A:429:LEU:HD23	8:A:957:HOH:O	1.74	0.86
1:A:43:VAL:HB	1:A:57:VAL:HG23	1.57	0.86
1:B:161:LEU:HG	8:B:940:HOH:O	1.75	0.86
1:B:265:LEU:HB2	8:B:814:HOH:O	1.76	0.86
1:B:38:PHE:HE1	1:B:67:PRO:HG2	1.40	0.86
1:A:314:GLY:HA3	8:A:727:HOH:O	1.76	0.85
1:B:256:PRO:HB3	8:B:867:HOH:O	1.75	0.85
1:A:523:ASP:HA	8:A:960:HOH:O	1.75	0.85
1:B:381:ASN:OD1	1:B:554:LYS:NZ	2.10	0.85
1:B:520:ARG:HH21	1:B:523:ASP:CG	1.85	0.85
1:A:273:TYR:CZ	8:A:724:HOH:O	2.28	0.84
1:B:267:LEU:HD11	8:B:814:HOH:O	1.77	0.84
1:B:347:PRO:HD3	8:B:1013:HOH:O	1.76	0.84
1:B:295:GLN:HG2	8:B:820:HOH:O	1.78	0.84
1:B:228:ARG:HG2	1:B:274:ASP:OD2	1.78	0.84
1:B:61:ASN:HB3	8:B:918:HOH:O	1.79	0.83
1:B:455:GLN:HG2	8:B:991:HOH:O	1.77	0.83
1:A:518:LEU:HG	1:A:521:PRO:HG3	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:PRO:HA	8:B:825:HOH:O	1.78	0.83
1:B:145:TYR:CE2	8:B:1006:HOH:O	2.31	0.83
1:A:271:GLN:HG2	1:A:476:ARG:HH21	1.40	0.83
1:B:479:THR:HB	8:B:781:HOH:O	1.79	0.82
1:B:244:ASN:ND2	1:B:281:ARG:HH12	1.78	0.82
1:A:285:ASN:OD1	1:A:311:HIS:CD2	2.31	0.82
1:B:206:ASN:HA	8:B:770:HOH:O	1.78	0.82
1:B:540:CYS:CB	8:B:765:HOH:O	2.28	0.82
1:A:95:HIS:O	1:A:135:SER:HB3	1.80	0.82
1:B:91:SER:HB3	8:B:825:HOH:O	1.79	0.81
7:B:611:KIB:H7	8:B:749:HOH:O	1.79	0.81
1:B:523:ASP:HA	1:B:526:GLN:HE22	1.43	0.81
1:B:549:THR:HA	8:B:885:HOH:O	1.80	0.81
1:A:9:ASN:CG	1:A:12:CYS:SG	2.63	0.81
1:A:201:ASN:ND2	8:A:706:HOH:O	2.13	0.81
1:A:306:PRO:CG	8:A:812:HOH:O	2.29	0.80
1:A:302:LEU:HD11	8:B:991:HOH:O	1.81	0.80
1:A:429:LEU:CD2	8:A:957:HOH:O	2.29	0.80
1:B:401:VAL:HG23	1:B:402:SER:H	1.47	0.80
1:A:438:HIS:HA	8:A:774:HOH:O	1.81	0.79
1:B:271:GLN:NE2	1:B:476:ARG:CZ	2.46	0.79
1:A:9:ASN:OD1	1:A:12:CYS:SG	2.41	0.79
1:A:189:ASN:ND2	8:A:705:HOH:O	2.13	0.79
1:B:114:CYS:SG	8:B:765:HOH:O	2.40	0.79
1:B:170:PHE:O	8:B:702:HOH:O	2.01	0.78
1:B:306:PRO:HG3	8:B:744:HOH:O	1.83	0.78
1:A:114:CYS:HB3	8:A:862:HOH:O	1.83	0.78
1:A:484:GLY:HA2	8:A:715:HOH:O	1.82	0.78
1:A:36:TYR:HB2	1:A:79:VAL:HG22	1.65	0.78
1:B:380:ILE:HG13	1:B:402:SER:O	1.83	0.78
1:A:456:ARG:HD2	8:A:791:HOH:O	1.83	0.78
1:B:440:PHE:CE1	8:B:781:HOH:O	2.17	0.78
1:B:95:HIS:CD2	1:B:272:ARG:HH12	2.02	0.77
1:B:267:LEU:CD1	8:B:814:HOH:O	2.32	0.77
1:B:95:HIS:O	1:B:135:SER:HB2	1.84	0.77
1:B:40:LEU:HD22	1:B:60:ILE:HG12	1.66	0.77
1:B:36:TYR:HB2	1:B:79:VAL:HG22	1.65	0.76
1:A:453:SER:HB2	8:A:1006:HOH:O	1.84	0.76
1:B:479:THR:HG22	8:B:971:HOH:O	1.83	0.76
1:B:1:GLU:HG3	1:B:2:PRO:HD2	1.68	0.76
1:B:540:CYS:SG	8:B:765:HOH:O	2.44	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:ARG:HG3	8:B:781:HOH:O	1.85	0.75
1:B:290:VAL:HG23	8:B:950:HOH:O	1.87	0.75
1:B:303:ASN:O	8:B:703:HOH:O	2.03	0.75
1:A:249:VAL:HA	1:A:275:VAL:HG12	1.69	0.75
1:B:393:LEU:HD21	1:B:528:ILE:HD13	1.69	0.75
1:A:423:PRO:HA	8:A:715:HOH:O	1.85	0.75
1:A:65:MET:HB3	1:A:150:VAL:O	1.87	0.74
1:B:138:HIS:HE1	8:B:894:HOH:O	1.69	0.74
1:B:200:ILE:HD12	8:B:791:HOH:O	1.87	0.74
1:B:4:CYS:HG	1:B:12:CYS:HG	1.35	0.74
1:B:373:TRP:HZ3	8:B:860:HOH:O	1.70	0.74
1:B:142:SER:OG	1:B:556:ASP:OD1	2.06	0.74
1:A:505:ILE:HG23	8:A:720:HOH:O	1.86	0.73
1:B:393:LEU:HD21	1:B:528:ILE:CD1	2.18	0.73
1:A:118:PRO:HG3	1:A:546:TYR:CZ	2.22	0.73
1:B:447:PRO:HD2	8:B:921:HOH:O	1.88	0.73
1:B:138:HIS:CE1	8:B:894:HOH:O	2.42	0.73
1:A:109:ASN:HB2	1:A:115:PRO:HD3	1.71	0.72
1:B:447:PRO:CD	8:B:921:HOH:O	2.35	0.72
1:A:95:HIS:CD2	1:A:272:ARG:HH12	2.08	0.72
1:B:428:SER:CB	1:B:484:GLY:H	2.01	0.72
1:B:439:ASP:HB2	8:B:718:HOH:O	1.89	0.72
1:B:515:VAL:C	8:B:793:HOH:O	2.31	0.72
1:A:106:ASP:HB3	1:A:112:THR:HG21	1.69	0.72
8:B:1019:HOH:O	2:E:1:NAG:H82	1.88	0.71
1:B:113:GLU:OE1	8:B:704:HOH:O	2.06	0.71
1:A:56:LYS:HE3	2:C:1:NAG:O6	1.90	0.71
1:A:479:THR:O	8:A:703:HOH:O	2.09	0.71
1:A:219:LEU:HD21	1:A:310:PHE:HD2	1.55	0.71
1:A:95:HIS:CD2	1:A:272:ARG:NH1	2.59	0.71
1:A:31:GLY:CA	8:A:723:HOH:O	2.40	0.70
1:A:115:PRO:CD	8:A:862:HOH:O	2.28	0.70
1:B:200:ILE:CD1	8:B:950:HOH:O	2.40	0.70
1:A:302:LEU:HD21	8:B:991:HOH:O	1.90	0.70
1:B:546:TYR:OH	1:B:550:ASN:ND2	2.25	0.70
1:A:42:GLU:OE1	8:A:701:HOH:O	2.08	0.70
1:B:446:SER:HB2	8:B:921:HOH:O	1.91	0.69
1:A:43:VAL:HB	1:A:57:VAL:CG2	2.21	0.69
1:A:176:TYR:CE2	1:A:195:SER:HA	2.26	0.69
1:B:50:ASP:CB	8:B:770:HOH:O	2.29	0.69
1:B:172:ILE:CG1	8:B:702:HOH:O	2.31	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:PRO:CG	8:B:744:HOH:O	2.39	0.69
1:B:285:ASN:OD1	1:B:311:HIS:HD2	1.76	0.68
1:B:520:ARG:NH2	1:B:523:ASP:OD2	2.17	0.68
1:B:244:ASN:O	1:B:281:ARG:NH1	2.24	0.68
1:B:455:GLN:CD	8:B:832:HOH:O	2.35	0.68
1:A:131:GLN:HG2	1:A:254:MET:SD	2.33	0.68
1:A:297:ALA:HB1	8:A:957:HOH:O	1.93	0.68
1:A:445:ARG:HD3	8:A:748:HOH:O	1.93	0.68
1:B:436:HIS:O	8:B:705:HOH:O	2.12	0.68
1:B:554:LYS:NZ	1:B:557:SER:O	2.27	0.68
1:B:254:MET:SD	8:B:810:HOH:O	2.51	0.67
1:B:460:ASP:HB3	1:B:463:VAL:HG12	1.75	0.67
1:B:97:ILE:HA	8:B:810:HOH:O	1.93	0.67
7:B:611:KIB:O1	7:B:611:KIB:C7	2.43	0.67
1:A:9:ASN:CG	1:A:12:CYS:HG	1.99	0.67
1:B:380:ILE:HD12	8:B:793:HOH:O	1.93	0.67
1:A:23:TYR:O	8:A:704:HOH:O	2.11	0.67
1:A:224:ARG:HG3	8:A:857:HOH:O	1.94	0.67
1:B:436:HIS:C	8:B:705:HOH:O	2.37	0.67
1:B:291:THR:HG21	8:B:1028:HOH:O	1.95	0.67
1:A:309:ILE:HD12	5:A:607:NAG:C8	2.22	0.67
1:A:389:ILE:CG2	1:A:389:ILE:O	2.43	0.67
1:A:368:THR:HG21	8:A:1032:HOH:O	1.94	0.67
1:A:389:ILE:O	1:A:389:ILE:HG22	1.95	0.67
1:A:306:PRO:HG3	8:A:812:HOH:O	1.89	0.66
1:A:484:GLY:C	8:A:715:HOH:O	2.39	0.66
1:B:307:ALA:HB2	2:F:1:NAG:H62	1.77	0.66
1:A:219:LEU:HD21	1:A:310:PHE:CD2	2.30	0.66
1:B:196:ASP:OD1	8:B:706:HOH:O	2.13	0.66
1:B:135:SER:N	8:B:722:HOH:O	2.28	0.66
4:A:605:CL:CL	8:A:789:HOH:O	2.51	0.65
1:A:37:VAL:CG1	1:A:82:ILE:HD12	2.26	0.65
1:A:311:HIS:CE1	5:A:607:NAG:O4	2.49	0.65
1:A:301:SER:CB	8:A:812:HOH:O	2.35	0.65
1:B:438:HIS:N	8:B:705:HOH:O	2.18	0.65
1:B:117:PRO:HG2	1:B:542:GLU:HB2	1.78	0.65
1:B:200:ILE:HD11	8:B:950:HOH:O	1.96	0.65
1:B:520:ARG:O	1:B:523:ASP:HB2	1.95	0.65
1:B:107:GLY:CA	1:B:113:GLU:OE1	2.45	0.65
1:A:236:ASN:HB3	1:A:238:PHE:CE1	2.31	0.65
1:B:240:VAL:HG22	8:B:814:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:TRP:CD1	8:A:862:HOH:O	2.49	0.64
1:A:468:LEU:HD13	1:A:488:LEU:CD2	2.27	0.64
1:B:420:GLU:OE2	8:B:707:HOH:O	2.15	0.64
1:A:13:TRP:HB2	1:A:158:PRO:HG3	1.78	0.64
1:B:371:PHE:CG	8:B:749:HOH:O	2.50	0.64
1:A:31:GLY:HA3	8:A:723:HOH:O	1.97	0.64
1:A:222:GLY:N	1:A:279:ALA:O	2.31	0.64
1:A:349:ASN:O	1:A:351:PHE:N	2.25	0.64
1:A:559:LEU:CD1	8:A:845:HOH:O	2.45	0.64
1:A:235:GLU:HB2	8:A:720:HOH:O	1.98	0.64
1:A:289:ASN:HB2	8:A:752:HOH:O	1.97	0.63
1:B:178:ARG:NH2	1:B:182:ASP:CB	2.59	0.63
1:B:179:ALA:CB	2:E:2:NAG:H81	2.28	0.63
1:B:303:ASN:HB3	8:B:744:HOH:O	1.97	0.63
1:B:332:CYS:O	1:B:333:LEU:HD23	1.98	0.63
1:A:68:ASN:OD1	8:A:707:HOH:O	2.15	0.63
1:B:455:GLN:HB2	8:B:832:HOH:O	1.97	0.63
1:A:204:ALA:HB1	8:A:800:HOH:O	1.98	0.62
1:B:523:ASP:HA	1:B:526:GLN:NE2	2.12	0.62
7:B:611:KIB:O1	7:B:611:KIB:H7B	1.99	0.62
1:B:347:PRO:HA	8:B:979:HOH:O	1.98	0.62
1:B:500:LEU:HD11	8:B:701:HOH:O	1.99	0.62
1:B:523:ASP:O	1:B:527:ARG:HD2	1.98	0.62
1:A:540:CYS:O	1:A:544:ARG:HG3	1.99	0.62
1:B:179:ALA:HB3	2:E:2:NAG:H81	1.82	0.62
1:B:382:VAL:HG13	1:B:559:LEU:HD11	1.81	0.62
1:B:449:VAL:HG11	8:B:832:HOH:O	1.98	0.61
1:A:273:TYR:CE1	8:A:724:HOH:O	2.49	0.61
1:B:131:GLN:HE21	1:B:254:MET:HB3	1.65	0.61
1:A:216:ASN:CG	5:A:607:NAG:H82	2.24	0.61
1:B:95:HIS:CD2	1:B:95:HIS:C	2.79	0.61
1:A:31:GLY:N	8:A:723:HOH:O	2.33	0.61
1:B:286:TYR:HA	8:B:828:HOH:O	1.99	0.61
1:B:455:GLN:CB	8:B:832:HOH:O	2.49	0.60
1:B:131:GLN:O	1:B:254:MET:HE2	2.00	0.60
1:B:209:THR:OG1	1:B:211:GLU:OE2	2.17	0.60
1:B:327:PRO:HA	8:B:1026:HOH:O	2.00	0.60
1:B:502:HIS:HB3	1:B:514:SER:OG	2.01	0.60
1:B:95:HIS:CD2	1:B:272:ARG:NH1	2.69	0.60
1:B:382:VAL:CG1	1:B:559:LEU:HD11	2.31	0.60
1:B:371:PHE:HB3	8:B:749:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LEU:O	1:B:221:PRO:HD3	2.02	0.60
1:B:38:PHE:CE1	1:B:67:PRO:CG	2.80	0.59
1:B:307:ALA:CB	2:F:1:NAG:H62	2.32	0.59
1:B:323:GLU:O	2:F:1:NAG:H83	2.03	0.59
1:B:302:LEU:HD11	8:B:706:HOH:O	2.03	0.59
1:A:286:TYR:OH	8:A:708:HOH:O	2.16	0.59
8:A:1022:HOH:O	2:C:2:NAG:H61	2.02	0.59
1:B:196:ASP:O	1:B:197:ASN:HB2	2.03	0.59
1:A:116:ILE:HG22	1:A:117:PRO:O	2.03	0.58
1:B:206:ASN:CA	8:B:770:HOH:O	2.44	0.58
1:B:432:PRO:O	1:B:503:CYS:HA	2.02	0.58
1:A:185:HIS:CD2	8:A:705:HOH:O	2.56	0.58
1:A:546:TYR:OH	1:A:550:ASN:ND2	2.36	0.58
1:B:176:TYR:CE2	1:B:195:SER:HA	2.39	0.58
1:A:231:ASN:HB3	1:A:268:ALA:O	2.03	0.58
1:B:417:TRP:CD1	8:B:990:HOH:O	2.34	0.58
1:B:447:PRO:CG	8:B:881:HOH:O	2.26	0.58
1:A:453:SER:OG	1:A:455:GLN:HG3	2.04	0.57
1:B:353:LYS:HD2	8:B:707:HOH:O	2.03	0.57
1:A:294:GLY:CA	1:A:331:GLN:HA	2.34	0.57
1:B:46:TRP:HH2	1:B:64:ILE:HD12	1.70	0.57
1:B:174:ASP:HB3	1:B:236:ASN:HB2	1.86	0.57
1:B:230:LEU:HD21	8:B:722:HOH:O	2.04	0.57
1:B:380:ILE:CD1	8:B:793:HOH:O	2.50	0.57
1:B:446:SER:CB	8:B:921:HOH:O	2.48	0.57
1:B:46:TRP:HB3	8:B:758:HOH:O	1.98	0.57
1:B:87:THR:HG21	1:B:552:TYR:HE2	1.70	0.57
1:A:436:HIS:HA	4:A:605:CL:CL	2.42	0.57
1:A:174:ASP:HB3	1:A:236:ASN:HB2	1.87	0.57
1:B:174:ASP:HB2	1:B:195:SER:HB3	1.87	0.57
1:B:416:TYR:CD1	1:B:416:TYR:N	2.73	0.57
1:A:141:PHE:HA	8:A:743:HOH:O	2.04	0.57
1:B:87:THR:HG21	1:B:552:TYR:CE2	2.39	0.57
8:A:1006:HOH:O	1:B:194:PHE:CD2	2.52	0.56
1:B:520:ARG:NH2	1:B:523:ASP:CG	2.59	0.56
1:A:60:ILE:HD11	1:A:149:VAL:HG13	1.88	0.56
1:A:479:THR:HG22	8:A:703:HOH:O	2.04	0.56
1:B:385:GLY:O	1:B:544:ARG:NH1	2.31	0.56
1:A:100:LYS:HG3	8:A:764:HOH:O	2.05	0.56
1:A:103:ASN:HB2	8:A:759:HOH:O	2.05	0.56
1:A:117:PRO:HG3	1:A:543:TRP:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:ASP:CG	1:B:233:SER:HB3	2.30	0.56
1:A:42:GLU:OE2	1:A:56:LYS:NZ	2.33	0.55
1:B:184:VAL:O	1:B:188:GLN:HG3	2.05	0.55
1:B:220:THR:HB	1:B:223:LYS:HG3	1.88	0.55
1:B:249:VAL:HG21	1:B:265:LEU:HD21	1.88	0.55
1:B:360:PRO:HG2	1:B:376:ASN:HA	1.88	0.55
1:B:237:HIS:HE1	1:B:505:ILE:HD11	1.71	0.55
1:B:464:ASP:OD1	1:B:467:ARG:HD3	2.06	0.55
8:B:1040:HOH:O	2:E:2:NAG:H61	2.06	0.55
1:A:555:ILE:HD11	8:A:985:HOH:O	2.06	0.55
1:B:145:TYR:CD2	8:B:1006:HOH:O	2.57	0.55
1:A:90:THR:O	1:A:91:SER:HB3	2.07	0.55
1:B:302:LEU:CD1	8:B:706:HOH:O	2.55	0.55
1:B:373:TRP:CZ3	8:B:860:HOH:O	2.53	0.55
1:A:65:MET:HE1	1:A:171:PRO:HG3	1.89	0.55
1:B:162:PRO:HG2	8:B:940:HOH:O	2.07	0.55
1:A:388:ILE:HD12	1:A:516:ASP:OD2	2.08	0.54
1:B:35:SER:HB3	8:B:980:HOH:O	2.07	0.54
1:A:34:GLN:HA	8:A:858:HOH:O	2.06	0.54
1:B:295:GLN:CD	8:B:802:HOH:O	2.49	0.54
1:B:315:ALA:HB1	1:B:316:PRO:HD2	1.90	0.54
1:B:427:PHE:HA	1:B:456:ARG:HH22	1.73	0.54
1:B:100:LYS:HE3	8:B:1000:HOH:O	2.07	0.54
1:A:27:THR:OG1	1:A:130:ARG:NH1	2.40	0.54
1:B:473:PRO:O	1:B:474:PRO:C	2.47	0.54
1:A:223:LYS:O	1:A:225:HIS:CE1	2.60	0.54
1:A:290:VAL:HB	1:A:306:PRO:HB2	1.89	0.54
1:A:306:PRO:HG2	8:A:812:HOH:O	2.00	0.54
1:B:348:VAL:HG21	1:B:470:GLY:H	1.72	0.54
1:A:422:ASP:N	1:A:423:PRO:CD	2.69	0.54
1:B:36:TYR:O	1:B:79:VAL:HA	2.08	0.54
8:B:757:HOH:O	2:E:1:NAG:H62	2.07	0.54
1:A:292:PHE:CE1	1:A:300:GLY:HA2	2.43	0.54
1:A:559:LEU:HD11	8:A:845:HOH:O	2.04	0.54
1:B:559:LEU:HD22	8:B:701:HOH:O	2.08	0.54
7:B:611:KIB:C7	8:B:749:HOH:O	2.45	0.54
1:B:104:LEU:HD22	1:B:532:ASP:HB3	1.89	0.53
1:B:117:PRO:O	1:B:121:GLY:HA3	2.08	0.53
1:B:371:PHE:CB	8:B:749:HOH:O	2.55	0.53
1:A:384:TRP:NE1	8:A:743:HOH:O	2.39	0.53
1:B:64:ILE:HG13	1:B:64:ILE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:HIS:NE2	1:A:316:PRO:O	2.40	0.53
1:A:413:GLN:NE2	8:A:740:HOH:O	2.39	0.53
1:B:354:ARG:CB	1:B:356:ASP:OD1	2.57	0.53
1:A:419:ILE:N	1:A:419:ILE:HD12	2.23	0.53
1:A:424:GLU:HB3	8:A:846:HOH:O	2.08	0.53
1:A:433:MET:HE3	8:A:760:HOH:O	2.07	0.53
1:B:163:TYR:HA	1:B:224:ARG:HB2	1.91	0.53
1:A:302:LEU:CD1	8:B:991:HOH:O	2.47	0.53
1:B:217:VAL:HG13	8:B:866:HOH:O	2.09	0.53
1:B:104:LEU:CD2	1:B:528:ILE:HG23	2.39	0.52
1:B:82:ILE:CD1	1:B:122:GLN:NE2	2.72	0.52
1:B:263:ASP:HB2	8:B:963:HOH:O	2.09	0.52
1:B:438:HIS:NE2	1:B:519:GLU:OE1	2.34	0.52
1:B:268:ALA:O	1:B:269:VAL:C	2.50	0.52
1:B:308:ALA:CA	8:B:791:HOH:O	2.58	0.52
1:A:19:ILE:HG13	1:A:341:VAL:HG11	1.92	0.52
1:B:87:THR:HG23	8:B:757:HOH:O	2.09	0.52
1:B:355:PRO:HB3	8:B:748:HOH:O	2.09	0.52
1:B:384:TRP:HH2	8:B:1019:HOH:O	1.93	0.52
1:A:406:VAL:HB	8:A:877:HOH:O	2.10	0.52
1:A:305:HIS:O	1:A:306:PRO:C	2.53	0.52
1:B:39:ASN:OD1	1:B:84:ASN:ND2	2.39	0.52
1:A:344:ARG:NH2	8:A:749:HOH:O	2.42	0.51
1:B:450:PRO:HB2	1:B:453:SER:HB3	1.91	0.51
1:A:384:TRP:CZ2	8:A:743:HOH:O	2.62	0.51
1:B:249:VAL:CG2	1:B:265:LEU:HD21	2.41	0.51
1:B:487:LEU:HD21	8:B:971:HOH:O	2.09	0.51
1:A:423:PRO:CA	8:A:715:HOH:O	2.49	0.51
1:B:200:ILE:HD13	8:B:950:HOH:O	2.04	0.51
8:A:1022:HOH:O	2:C:2:NAG:C6	2.58	0.51
1:B:321:THR:HG21	8:B:898:HOH:O	2.11	0.51
1:A:58:MET:HG2	1:A:85:LEU:HD22	1.92	0.51
1:B:104:LEU:HD22	1:B:528:ILE:HG23	1.93	0.51
1:B:493:THR:O	1:B:520:ARG:HD2	2.11	0.51
1:A:302:LEU:CD2	8:B:991:HOH:O	2.56	0.50
1:A:371:PHE:CD1	7:A:610:KIB:C8	2.95	0.50
1:A:46:TRP:CE3	1:A:57:VAL:HG11	2.46	0.50
1:B:82:ILE:HD11	1:B:122:GLN:NE2	2.26	0.50
1:B:267:LEU:HD12	1:B:267:LEU:N	2.26	0.50
1:B:332:CYS:C	1:B:333:LEU:HD23	2.35	0.50
1:A:282:ALA:O	1:A:286:TYR:OH	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:TYR:HD1	8:A:907:HOH:O	1.94	0.50
1:A:440:PHE:O	1:A:475:ARG:HA	2.12	0.50
1:B:346:VAL:O	8:B:710:HOH:O	2.19	0.50
1:B:393:LEU:HD21	1:B:528:ILE:HD12	1.93	0.50
1:B:23:TYR:CD2	1:B:23:TYR:N	2.78	0.50
1:B:552:TYR:OH	8:B:708:HOH:O	2.15	0.50
8:A:734:HOH:O	2:C:1:NAG:H61	2.11	0.50
1:B:271:GLN:HE21	1:B:476:ARG:NE	2.09	0.50
1:B:559:LEU:O	8:B:709:HOH:O	2.19	0.50
1:A:250:ILE:O	1:A:251:ALA:HB2	2.12	0.50
1:A:490:ALA:CB	8:A:1009:HOH:O	2.60	0.50
1:B:99:GLN:HB3	1:B:102:THR:O	2.12	0.50
1:A:239:GLN:HG2	1:A:330:HIS:CD2	2.47	0.50
1:B:245:HIS:CE1	1:B:281:ARG:HG3	2.47	0.50
1:B:46:TRP:CE3	1:B:57:VAL:HG11	2.47	0.50
1:B:98:HIS:NE2	1:B:131:GLN:OE1	2.45	0.50
1:A:141:PHE:CG	8:A:743:HOH:O	2.58	0.49
1:A:428:SER:CB	1:A:484:GLY:H	2.24	0.49
1:B:234:THR:O	1:B:505:ILE:HA	2.12	0.49
1:A:131:GLN:HB2	8:A:945:HOH:O	2.11	0.49
1:A:543:TRP:CG	8:A:862:HOH:O	2.65	0.49
1:A:169:VAL:HA	1:A:228:ARG:HB2	1.94	0.49
1:A:546:TYR:O	1:A:549:THR:OG1	2.26	0.49
1:B:95:HIS:O	1:B:135:SER:CB	2.58	0.49
1:B:122:GLN:CG	8:B:779:HOH:O	2.61	0.49
1:B:285:ASN:OD1	1:B:311:HIS:CD2	2.62	0.49
1:A:134:THR:HG21	1:A:228:ARG:HB3	1.94	0.49
1:A:206:ASN:C	1:A:208:ASN:H	2.20	0.49
1:B:355:PRO:CB	8:B:748:HOH:O	2.60	0.49
1:A:287:TRP:CE2	1:A:320:PRO:HB2	2.48	0.49
1:A:552:TYR:CD1	2:C:2:NAG:H62	2.48	0.49
1:A:64:ILE:CG2	8:A:1029:HOH:O	2.61	0.49
1:B:209:THR:CB	1:B:211:GLU:OE2	2.61	0.49
1:A:454:GLN:HG2	8:B:812:HOH:O	2.13	0.49
1:B:435:LEU:HG	8:B:705:HOH:O	2.13	0.49
1:B:237:HIS:NE2	1:B:432:PRO:HD3	2.28	0.48
1:B:530:GLN:N	1:B:531:GLU:OE1	2.46	0.48
1:A:427:PHE:HA	1:A:456:ARG:HH12	1.78	0.48
1:A:523:ASP:O	1:A:527:ARG:HG3	2.13	0.48
1:A:393:LEU:CD2	8:A:992:HOH:O	2.62	0.48
1:B:200:ILE:CD1	8:B:791:HOH:O	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:GLN:O	1:B:332:CYS:HB2	2.11	0.48
1:B:428:SER:HB3	1:B:484:GLY:N	2.16	0.48
1:B:467:ARG:NH2	8:B:732:HOH:O	2.34	0.48
1:B:544:ARG:NH1	8:B:765:HOH:O	2.46	0.48
1:B:103:ASN:HB2	8:B:899:HOH:O	2.12	0.48
1:A:103:ASN:N	8:A:759:HOH:O	2.46	0.48
1:B:447:PRO:CB	8:B:881:HOH:O	2.57	0.48
1:B:76:THR:CG2	1:B:126:ARG:HG3	2.43	0.48
1:A:484:GLY:CA	8:A:715:HOH:O	2.46	0.48
1:B:479:THR:CG2	8:B:971:HOH:O	2.54	0.48
1:B:543:TRP:CZ2	1:B:547:TRP:CE3	3.02	0.48
1:A:266:PHE:CE1	1:A:332:CYS:HA	2.49	0.48
1:A:331:GLN:OE1	1:A:450:PRO:HA	2.13	0.48
1:A:449:VAL:HB	1:A:455:GLN:NE2	2.29	0.48
1:A:434:HIS:CD2	1:A:504:HIS:HD2	2.32	0.47
1:A:529:SER:OG	1:A:531:GLU:HG2	2.14	0.47
1:B:97:ILE:CD1	8:B:810:HOH:O	2.23	0.47
1:B:174:ASP:OD1	1:B:233:SER:HB3	2.14	0.47
1:B:308:ALA:CB	8:B:791:HOH:O	2.40	0.47
1:A:530:GLN:HA	1:A:530:GLN:OE1	2.14	0.47
1:B:184:VAL:HG12	1:B:185:HIS:N	2.29	0.47
1:B:304:PRO:O	8:B:713:HOH:O	2.20	0.47
1:A:267:LEU:HG	1:A:273:TYR:HD2	1.79	0.47
1:A:384:TRP:CZ3	1:A:554:LYS:HD2	2.49	0.47
1:B:445:ARG:HD3	8:B:721:HOH:O	2.13	0.47
1:B:7:PRO:HB3	1:B:164:ASP:HA	1.95	0.47
1:B:336:LEU:HD22	1:B:474:PRO:HG2	1.96	0.47
1:B:476:ARG:CG	8:B:781:HOH:O	2.55	0.47
1:A:1:GLU:HG3	8:A:851:HOH:O	2.13	0.47
1:A:95:HIS:O	1:A:135:SER:CB	2.56	0.47
8:B:1040:HOH:O	2:E:2:NAG:C6	2.63	0.47
1:A:245:HIS:CE1	1:A:281:ARG:HG3	2.49	0.47
1:A:336:LEU:HD21	1:A:442:VAL:HG11	1.96	0.47
1:B:381:ASN:O	1:B:402:SER:HB3	2.14	0.47
1:A:100:LYS:HB2	1:A:100:LYS:HE3	1.82	0.47
1:A:449:VAL:HG21	8:A:986:HOH:O	2.14	0.47
1:B:79:VAL:CG2	8:B:930:HOH:O	2.63	0.47
1:B:248:THR:CG2	1:B:259:ALA:HB1	2.44	0.47
1:B:354:ARG:HB3	1:B:356:ASP:OD1	2.14	0.47
1:B:449:VAL:CG2	8:B:832:HOH:O	2.28	0.47
1:A:4:CYS:SG	8:A:999:HOH:O	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PRO:HG2	8:A:862:HOH:O	2.14	0.47
1:A:434:HIS:HD2	1:A:504:HIS:HD2	1.63	0.47
1:B:228:ARG:O	1:B:230:LEU:HD12	2.14	0.47
1:A:251:ALA:HA	1:A:257:VAL:HG22	1.95	0.47
1:B:22:ASP:HB3	1:B:25:VAL:HG22	1.96	0.47
1:B:111:VAL:HG21	1:B:500:LEU:HD21	1.97	0.47
1:B:185:HIS:CD2	1:B:185:HIS:C	2.93	0.47
1:A:64:ILE:HA	8:A:989:HOH:O	2.15	0.46
1:B:500:LEU:CD1	8:B:701:HOH:O	2.60	0.46
1:A:359:LEU:HD22	1:A:515:VAL:HG11	1.97	0.46
1:A:434:HIS:HE1	4:A:605:CL:CL	2.35	0.46
1:B:93:HIS:HA	1:B:106:ASP:O	2.15	0.46
1:B:306:PRO:O	8:B:712:HOH:O	2.20	0.46
1:B:104:LEU:CD2	1:B:532:ASP:HB3	2.45	0.46
1:B:58:MET:HG3	1:B:147:ASN:HB3	1.97	0.46
1:B:100:LYS:HA	1:B:100:LYS:HD3	1.52	0.46
1:A:434:HIS:HA	1:A:477:ASP:O	2.15	0.46
1:A:533:GLU:O	1:A:536:PHE:HB3	2.16	0.46
1:A:354:ARG:NH1	1:A:356:ASP:OD1	2.49	0.46
1:B:91:SER:O	1:B:91:SER:OG	2.33	0.46
1:B:122:GLN:HG2	8:B:779:HOH:O	2.15	0.46
1:B:131:GLN:O	1:B:254:MET:CE	2.64	0.46
1:B:386:LYS:HE3	1:B:390:ASP:OD2	2.15	0.46
1:A:253:ASP:OD2	1:A:476:ARG:HB2	2.15	0.46
1:B:19:ILE:CG1	8:B:720:HOH:O	2.44	0.46
1:B:305:HIS:O	1:B:306:PRO:C	2.59	0.46
1:B:349:ASN:HB3	8:B:1015:HOH:O	2.16	0.46
1:A:138:HIS:HB2	1:A:145:TYR:CB	2.46	0.46
1:B:65:MET:HE1	1:B:171:PRO:HG3	1.98	0.46
1:B:91:SER:CB	8:B:825:HOH:O	2.52	0.46
1:B:315:ALA:HB1	1:B:316:PRO:CD	2.46	0.46
1:B:131:GLN:HB3	8:B:808:HOH:O	2.16	0.45
1:B:215:ALA:HB3	1:B:308:ALA:HB2	1.97	0.45
1:A:145:TYR:OH	1:A:234:THR:HA	2.15	0.45
1:A:335:THR:CG2	8:A:724:HOH:O	2.65	0.45
1:A:344:ARG:CZ	8:A:749:HOH:O	2.63	0.45
1:A:454:GLN:HB3	8:A:896:HOH:O	2.16	0.45
1:B:348:VAL:HG21	1:B:470:GLY:N	2.31	0.45
1:B:1:GLU:HG3	1:B:2:PRO:CD	2.42	0.45
1:A:138:HIS:HE1	8:A:771:HOH:O	1.99	0.45
1:A:65:MET:HE2	1:A:151:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LEU:CD1	1:A:488:LEU:CD2	2.94	0.45
1:B:23:TYR:CB	8:B:889:HOH:O	2.32	0.45
1:A:13:TRP:CE3	1:A:157:GLY:HA2	2.52	0.45
1:A:111:VAL:HG13	1:A:516:ASP:OD2	2.17	0.45
1:A:248:THR:HA	1:A:261:THR:HA	1.98	0.45
1:B:223:LYS:O	1:B:225:HIS:CE1	2.70	0.45
1:B:244:ASN:HD22	1:B:244:ASN:HA	1.59	0.45
1:A:271:GLN:CG	1:A:476:ARG:NH2	2.66	0.45
1:A:384:TRP:CE2	8:A:743:HOH:O	2.55	0.45
1:B:76:THR:HG21	1:B:126:ARG:HG3	1.98	0.45
1:A:118:PRO:CG	1:A:546:TYR:CE1	2.99	0.45
1:A:384:TRP:CE3	1:A:554:LYS:HD2	2.52	0.45
1:B:432:PRO:O	1:B:504:HIS:N	2.45	0.45
1:A:22:ASP:OD1	1:A:22:ASP:C	2.61	0.44
1:A:64:ILE:HG21	8:A:1029:HOH:O	2.16	0.44
1:A:118:PRO:HG3	1:A:546:TYR:CE1	2.52	0.44
1:A:391:TYR:OH	1:A:400:PRO:HD3	2.17	0.44
1:B:122:GLN:NE2	8:B:779:HOH:O	2.50	0.44
1:B:132:TYR:CD1	1:B:132:TYR:N	2.85	0.44
1:B:215:ALA:HB3	1:B:308:ALA:CB	2.47	0.44
1:A:386:LYS:N	1:A:387:PRO:HD3	2.32	0.44
1:A:468:LEU:HD13	1:A:488:LEU:HD23	1.99	0.44
1:B:86:VAL:O	1:B:119:LYS:HE2	2.18	0.44
1:B:192:PRO:HD3	7:B:611:KIB:C1	2.47	0.44
1:B:19:ILE:CD1	8:B:720:HOH:O	2.64	0.44
1:B:325:THR:HG23	8:B:1034:HOH:O	2.17	0.44
1:A:94:TRP:O	8:A:710:HOH:O	2.21	0.44
1:B:136:TRP:CZ3	1:B:138:HIS:CD2	3.05	0.44
1:A:287:TRP:CH2	2:D:1:NAG:H62	2.52	0.44
1:A:427:PHE:HB3	8:A:725:HOH:O	2.17	0.44
1:B:111:VAL:HG21	1:B:500:LEU:CD2	2.48	0.44
1:B:440:PHE:O	1:B:475:ARG:HA	2.18	0.44
1:A:141:PHE:O	1:A:142:SER:C	2.61	0.44
1:A:518:LEU:CG	1:A:521:PRO:HG3	2.41	0.44
1:B:136:TRP:CH2	1:B:138:HIS:CD2	3.06	0.44
1:B:209:THR:HG21	1:B:211:GLU:OE2	2.18	0.44
1:B:177:TYR:CE2	1:B:196:ASP:HB3	2.53	0.44
1:B:182:ASP:OD1	8:B:714:HOH:O	2.21	0.44
1:B:394:THR:C	1:B:396:ASN:N	2.76	0.44
1:B:333:LEU:CD2	8:B:975:HOH:O	2.66	0.43
1:B:443:LEU:HD11	1:B:490:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:PRO:HA	8:B:975:HOH:O	2.16	0.43
1:B:552:TYR:CD1	2:E:2:NAG:H62	2.52	0.43
1:A:287:TRP:CZ2	2:D:1:NAG:H62	2.53	0.43
1:B:230:LEU:HG	1:B:272:ARG:HG2	2.00	0.43
1:B:449:VAL:HB	1:B:455:GLN:NE2	2.33	0.43
1:A:490:ALA:HB1	8:A:1009:HOH:O	2.18	0.43
1:A:292:PHE:CD1	1:A:300:GLY:HA2	2.53	0.43
1:A:427:PHE:CA	1:A:456:ARG:HH12	2.31	0.43
1:A:453:SER:CB	8:A:1006:HOH:O	2.55	0.43
1:B:403:ASP:O	1:B:404:ASN:C	2.59	0.43
1:A:58:MET:HG2	1:A:85:LEU:CD2	2.47	0.43
1:B:15:ASP:HA	8:B:844:HOH:O	2.19	0.43
1:B:438:HIS:HE2	1:B:519:GLU:CD	2.23	0.43
1:A:37:VAL:CG1	1:A:82:ILE:CD1	2.95	0.43
1:A:213:GLN:NE2	8:A:731:HOH:O	2.35	0.43
1:A:393:LEU:HD23	8:A:992:HOH:O	2.19	0.43
1:B:218:THR:CG2	1:B:313:ALA:HB2	2.48	0.43
1:B:253:ASP:OD2	1:B:476:ARG:HB2	2.19	0.43
1:B:389:ILE:O	1:B:393:LEU:HG	2.18	0.43
1:A:37:VAL:HG13	1:A:82:ILE:HD12	1.97	0.43
1:A:109:ASN:C	1:A:109:ASN:HD22	2.25	0.43
1:B:170:PHE:C	8:B:702:HOH:O	2.57	0.43
1:B:354:ARG:HB2	1:B:356:ASP:OD1	2.18	0.43
1:A:103:ASN:ND2	1:A:499:TRP:CZ3	2.82	0.43
1:A:479:THR:HG23	1:A:487:LEU:HD21	2.00	0.43
1:B:446:SER:OG	1:B:482:PRO:HG2	2.18	0.43
1:A:10:ARG:O	1:A:158:PRO:HA	2.19	0.43
1:B:440:PHE:CD1	1:B:489:LEU:HD22	2.53	0.43
1:B:100:LYS:O	1:B:101:ASP:C	2.61	0.42
1:B:339:ARG:HG3	8:B:1027:HOH:O	2.17	0.42
1:B:531:GLU:OE1	1:B:531:GLU:N	2.48	0.42
1:A:105:HIS:ND1	1:A:125:TYR:HA	2.34	0.42
1:B:271:GLN:NE2	1:B:476:ARG:NE	2.65	0.42
1:B:446:SER:CA	8:B:921:HOH:O	2.67	0.42
1:A:11:ALA:O	1:A:158:PRO:HB3	2.20	0.42
1:A:36:TYR:O	1:A:79:VAL:HA	2.19	0.42
1:A:149:VAL:C	1:A:150:VAL:HG12	2.45	0.42
1:B:244:ASN:ND2	1:B:281:ARG:NH1	2.58	0.42
1:A:93:HIS:O	1:A:137:TYR:HA	2.20	0.42
1:A:95:HIS:CD2	1:A:95:HIS:C	2.98	0.42
1:A:206:ASN:OD1	1:A:208:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ASP:OD1	1:A:334:ASP:N	2.51	0.42
1:B:38:PHE:HE1	1:B:67:PRO:CG	2.21	0.42
1:B:200:ILE:O	1:B:215:ALA:HB2	2.18	0.42
1:A:385:GLY:N	8:A:779:HOH:O	2.52	0.42
1:A:421:ASN:C	1:A:423:PRO:HD3	2.44	0.42
1:B:48:GLY:HA3	8:B:734:HOH:O	2.19	0.42
1:B:421:ASN:O	1:B:422:ASP:C	2.62	0.42
1:B:434:HIS:HA	1:B:477:ASP:O	2.20	0.42
1:B:526:GLN:HE21	1:B:526:GLN:HB2	1.65	0.42
1:B:197:ASN:ND2	8:B:770:HOH:O	2.48	0.42
1:B:244:ASN:OD1	8:B:715:HOH:O	2.22	0.42
1:B:65:MET:HE1	1:B:171:PRO:CG	2.49	0.42
1:B:283:PRO:HA	1:B:312:TYR:CD2	2.54	0.42
1:B:295:GLN:CG	8:B:820:HOH:O	2.48	0.42
1:B:311:HIS:NE2	1:B:316:PRO:O	2.53	0.42
1:B:353:LYS:CD	8:B:707:HOH:O	2.65	0.42
1:A:95:HIS:HD2	1:A:272:ARG:HH12	1.61	0.42
8:A:1006:HOH:O	1:B:194:PHE:HD2	1.95	0.42
1:A:100:LYS:CG	8:A:764:HOH:O	2.68	0.42
1:A:380:ILE:HG23	1:A:557:SER:HB2	2.01	0.42
1:B:11:ALA:HB2	8:B:1018:HOH:O	2.20	0.42
1:B:456:ARG:CG	8:B:922:HOH:O	2.67	0.42
1:A:530:GLN:O	1:A:534:ASP:CG	2.63	0.41
1:B:220:THR:O	1:B:221:PRO:C	2.63	0.41
1:B:461:PRO:HG2	8:B:951:HOH:O	2.20	0.41
1:A:46:TRP:CG	1:A:57:VAL:HG21	2.55	0.41
1:A:360:PRO:HG2	1:A:376:ASN:HA	2.02	0.41
1:B:233:SER:O	1:B:269:VAL:HG13	2.20	0.41
1:B:508:HIS:NE2	7:B:611:KIB:H7B	2.36	0.41
1:A:340:PRO:HG2	8:A:821:HOH:O	2.19	0.41
1:A:346:VAL:HG21	8:A:1009:HOH:O	2.21	0.41
1:A:421:ASN:C	1:A:423:PRO:CD	2.94	0.41
1:B:56:LYS:HE3	2:E:1:NAG:O6	2.20	0.41
1:B:104:LEU:HD21	1:B:528:ILE:CG2	2.50	0.41
1:B:135:SER:HB2	1:B:136:TRP:H	1.68	0.41
1:A:36:TYR:CB	1:A:79:VAL:HG22	2.43	0.41
1:A:423:PRO:HG3	8:A:848:HOH:O	2.20	0.41
1:A:538:ARG:O	1:A:539:VAL:C	2.63	0.41
1:B:471:ASP:OD2	8:B:711:HOH:O	2.20	0.41
1:B:289:ASN:OD1	2:F:1:NAG:H82	2.20	0.41
1:A:12:CYS:CB	8:A:999:HOH:O	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:VAL:HG21	1:B:125:TYR:HE1	1.85	0.41
1:A:87:THR:O	1:A:550:ASN:ND2	2.53	0.41
1:B:394:THR:C	1:B:396:ASN:H	2.29	0.41
1:A:428:SER:OG	1:A:484:GLY:N	2.44	0.41
1:B:197:ASN:ND2	1:B:205:VAL:O	2.51	0.41
1:A:36:TYR:CE1	1:A:69:ILE:HG23	2.56	0.41
1:A:454:GLN:NE2	8:A:785:HOH:O	2.53	0.41
1:A:481:LEU:HA	1:A:487:LEU:HD22	2.02	0.41
1:B:97:ILE:CA	8:B:810:HOH:O	2.60	0.41
1:B:99:GLN:OE1	1:B:127:TRP:HB3	2.21	0.41
1:B:237:HIS:CD2	1:B:268:ALA:CB	3.03	0.41
1:B:282:ALA:HA	1:B:283:PRO:HD3	1.77	0.41
1:B:401:VAL:HG23	1:B:402:SER:N	2.26	0.41
1:B:505:ILE:CD1	8:B:1023:HOH:O	2.22	0.41
1:B:546:TYR:O	1:B:549:THR:OG1	2.34	0.41
1:B:555:ILE:HD13	8:B:1049:HOH:O	2.20	0.41
1:A:14:SER:OG	1:A:17:PHE:HB2	2.21	0.41
1:A:291:THR:HG23	8:A:772:HOH:O	2.21	0.41
1:A:521:PRO:HA	1:A:524:LEU:HD23	2.03	0.41
1:B:94:TRP:CD1	1:B:94:TRP:N	2.86	0.41
1:B:336:LEU:C	8:B:815:HOH:O	2.64	0.41
1:B:401:VAL:CG2	1:B:402:SER:H	2.22	0.41
1:B:460:ASP:HA	1:B:461:PRO:HD2	1.88	0.41
1:A:28:PRO:HD3	1:A:73:TRP:CE2	2.56	0.40
1:B:78:GLU:HA	1:B:125:TYR:O	2.21	0.40
1:B:94:TRP:O	1:B:97:ILE:HB	2.21	0.40
1:B:159:ALA:HB1	1:B:250:ILE:HD12	2.03	0.40
1:A:176:TYR:CB	1:A:183:LEU:HD11	2.52	0.40
1:B:207:PRO:HG3	1:B:303:ASN:HA	2.04	0.40
1:A:521:PRO:O	1:A:524:LEU:HB3	2.21	0.40
1:B:131:GLN:NE2	1:B:254:MET:HB3	2.35	0.40
1:A:206:ASN:HB3	1:A:209:THR:OG1	2.21	0.40
1:A:265:LEU:CD2	8:A:724:HOH:O	2.70	0.40
1:B:479:THR:HG21	1:B:489:LEU:HD21	2.03	0.40
1:A:18:ASP:HB2	1:A:19:ILE:H	1.67	0.40
1:A:287:TRP:CE2	2:D:1:NAG:H5	2.57	0.40
1:A:399:TYR:CZ	1:A:518:LEU:CD2	3.04	0.40
1:A:555:ILE:HG12	8:A:898:HOH:O	2.21	0.40
1:B:236:ASN:HB3	1:B:238:PHE:CE1	2.55	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:B:78:GLU:OE2	5:A:606:NAG:O7[3_545]	2.04	0.16

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	557/559 (100%)	504 (90%)	47 (8%)	6 (1%)	11	7
1	B	557/559 (100%)	502 (90%)	50 (9%)	5 (1%)	14	9
All	All	1114/1118 (100%)	1006 (90%)	97 (9%)	11 (1%)	12	8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	SER
1	B	402	SER
1	A	91	SER
1	A	493	THR
1	B	15	ASP
1	B	100	LYS
1	B	484	GLY
1	A	268	ALA
1	B	401	VAL
1	A	100	LYS
1	A	149	VAL

5.3.2 Protein sidechains [i](#)

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	478/478 (100%)	441 (92%)	37 (8%)	12	8
1	B	478/478 (100%)	442 (92%)	36 (8%)	12	9
All	All	956/956 (100%)	883 (92%)	73 (8%)	12	9

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	7	PRO
1	A	15	ASP
1	A	40	LEU
1	A	59	LEU
1	A	65	MET
1	A	80	THR
1	A	91	SER
1	A	100	LYS
1	A	109	ASN
1	A	123	ARG
1	A	140	HIS
1	A	144	GLN
1	A	150	VAL
1	A	189	ASN
1	A	211	GLU
1	A	223	LYS
1	A	224	ARG
1	A	230	LEU
1	A	239	GLN
1	A	254	MET
1	A	277	ILE
1	A	349	ASN
1	A	355	PRO
1	A	408	VAL
1	A	413	GLN
1	A	424	GLU
1	A	434	HIS
1	A	454	GLN
1	A	456	ARG
1	A	465	LEU
1	A	477	ASP
1	A	479	THR
1	A	487	LEU
1	A	513	LEU

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Mol	Chain	Res	Type
1	A	526	GLN
1	A	530	GLN
1	B	1	GLU
1	B	9	ASN
1	B	40	LEU
1	B	64	ILE
1	B	95	HIS
1	B	100	LYS
1	B	109	ASN
1	B	122	GLN
1	B	123	ARG
1	B	135	SER
1	B	140	HIS
1	B	184	VAL
1	B	213	GLN
1	B	244	ASN
1	B	254	MET
1	B	262	VAL
1	B	281	ARG
1	B	325	THR
1	B	333	LEU
1	B	338	VAL
1	B	340	PRO
1	B	355	PRO
1	B	397	THR
1	B	408	VAL
1	B	413	GLN
1	B	445	ARG
1	B	450	PRO
1	B	463	VAL
1	B	487	LEU
1	B	493	THR
1	B	507	TRP
1	B	510	SER
1	B	513	LEU
1	B	520	ARG
1	B	526	GLN
1	B	542	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	34	GLN
1	A	72	ASN
1	A	95	HIS
1	A	122	GLN
1	A	154	GLN
1	A	156	ASN
1	A	185	HIS
1	A	190	ASN
1	A	236	ASN
1	A	311	HIS
1	A	349	ASN
1	A	396	ASN
1	A	413	GLN
1	B	20	ASN
1	B	63	ASN
1	B	72	ASN
1	B	122	GLN
1	B	131	GLN
1	B	154	GLN
1	B	185	HIS
1	B	190	ASN
1	B	244	ASN
1	B	311	HIS
1	B	413	GLN
1	B	455	GLN
1	B	526	GLN
1	B	550	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	C	1	1,2	14,14,15	1.23	1 (7%)	17,19,21	3.08	5 (29%)
2	NAG	C	2	2	14,14,15	0.98	1 (7%)	17,19,21	2.17	5 (29%)
2	NAG	D	1	1,2	14,14,15	1.41	2 (14%)	17,19,21	3.74	10 (58%)
2	NAG	D	2	2	14,14,15	1.65	5 (35%)	17,19,21	2.75	7 (41%)
2	NAG	E	1	1,2	14,14,15	1.13	1 (7%)	17,19,21	2.37	7 (41%)
2	NAG	E	2	2	14,14,15	0.88	0	17,19,21	1.35	2 (11%)
2	NAG	F	1	1,2	14,14,15	1.71	3 (21%)	17,19,21	4.75	13 (76%)
2	NAG	F	2	2	14,14,15	1.53	2 (14%)	17,19,21	3.91	12 (70%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	6/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	O5-C5	-4.05	1.35	1.43
2	D	1	NAG	C2-N2	3.92	1.52	1.46
2	F	2	NAG	O5-C5	-3.55	1.36	1.43
2	D	2	NAG	C1-C2	-3.36	1.47	1.52
2	F	1	NAG	C3-C2	-3.11	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	NAG	O5-C1	-3.07	1.38	1.43
2	D	1	NAG	O5-C1	-2.83	1.38	1.43
2	F	1	NAG	O5-C1	-2.77	1.39	1.43
2	D	2	NAG	C2-N2	-2.60	1.42	1.46
2	E	1	NAG	C1-C2	2.55	1.55	1.52
2	C	1	NAG	C1-C2	2.45	1.55	1.52
2	D	2	NAG	O5-C1	-2.44	1.39	1.43
2	D	2	NAG	O7-C7	2.24	1.28	1.23
2	D	2	NAG	O5-C5	-2.14	1.39	1.43
2	C	2	NAG	O3-C3	-2.02	1.38	1.43

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C1-O5-C5	11.20	127.20	112.19
2	D	1	NAG	C1-C2-N2	9.73	125.77	110.43
2	F	2	NAG	C1-O5-C5	-9.42	99.56	112.19
2	C	1	NAG	C1-O5-C5	9.29	124.64	112.19
2	F	1	NAG	C2-N2-C7	7.87	133.44	122.90
2	F	1	NAG	O4-C4-C3	-7.67	92.31	110.38
2	F	2	NAG	C1-C2-N2	-7.13	99.20	110.43
2	D	2	NAG	C2-N2-C7	-6.94	113.59	122.90
2	D	1	NAG	C8-C7-N2	6.45	126.81	116.12
2	D	2	NAG	O5-C1-C2	-5.50	102.79	111.29
2	D	1	NAG	C2-N2-C7	-5.10	116.07	122.90
2	F	1	NAG	O7-C7-C8	-5.06	113.05	122.05
2	F	2	NAG	O6-C6-C5	-5.02	94.24	111.33
2	D	2	NAG	O5-C5-C4	-4.68	99.44	110.83
2	F	1	NAG	O5-C5-C6	-4.58	98.75	107.66
2	E	1	NAG	O5-C5-C6	-4.57	98.77	107.66
2	C	1	NAG	C2-N2-C7	-4.51	116.86	122.90
2	F	2	NAG	C6-C5-C4	4.49	124.05	113.02
2	C	2	NAG	C1-C2-N2	4.39	117.35	110.43
2	F	1	NAG	O7-C7-N2	4.04	129.12	121.98
2	F	1	NAG	C6-C5-C4	3.94	122.69	113.02
2	C	2	NAG	C3-C4-C5	-3.91	103.14	110.23
2	D	1	NAG	O7-C7-C8	-3.84	115.21	122.05
2	E	1	NAG	C1-O5-C5	3.82	117.31	112.19
2	C	2	NAG	O4-C4-C5	3.81	118.71	109.32
2	D	1	NAG	O3-C3-C2	3.75	117.19	109.40
2	F	1	NAG	C1-C2-N2	3.69	116.25	110.43
2	E	1	NAG	C1-C2-N2	3.66	116.19	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	C4-C3-C2	3.63	116.34	111.02
2	E	1	NAG	C4-C3-C2	-3.58	105.77	111.02
2	F	2	NAG	O4-C4-C3	-3.57	101.95	110.38
2	C	1	NAG	O7-C7-C8	-3.45	115.91	122.05
2	D	1	NAG	O5-C5-C6	3.43	114.35	107.66
2	F	1	NAG	C4-C3-C2	3.43	116.05	111.02
2	F	2	NAG	O5-C5-C4	-3.41	102.52	110.83
2	C	1	NAG	C3-C4-C5	3.29	116.19	110.23
2	D	1	NAG	C1-O5-C5	-3.27	107.80	112.19
2	C	1	NAG	O5-C5-C4	3.22	118.66	110.83
2	C	2	NAG	O3-C3-C2	-3.22	102.72	109.40
2	F	1	NAG	O5-C5-C4	-3.09	103.32	110.83
2	F	2	NAG	C2-N2-C7	3.06	127.00	122.90
2	F	2	NAG	C8-C7-N2	3.01	121.12	116.12
2	F	1	NAG	O3-C3-C4	2.92	117.25	110.38
2	E	1	NAG	C8-C7-N2	-2.84	111.40	116.12
2	E	2	NAG	O5-C1-C2	-2.75	107.04	111.29
2	D	2	NAG	C3-C4-C5	-2.73	105.29	110.23
2	D	2	NAG	C6-C5-C4	2.71	119.68	113.02
2	D	1	NAG	C4-C3-C2	2.68	114.94	111.02
2	F	2	NAG	O3-C3-C2	2.64	114.88	109.40
2	E	2	NAG	C1-C2-N2	2.56	114.46	110.43
2	E	1	NAG	O5-C5-C4	2.47	116.85	110.83
2	F	2	NAG	O5-C5-C6	-2.37	103.04	107.66
2	D	1	NAG	O7-C7-N2	-2.32	117.87	121.98
2	D	2	NAG	C8-C7-N2	-2.32	112.27	116.12
2	D	1	NAG	O5-C5-C4	-2.22	105.44	110.83
2	F	1	NAG	O3-C3-C2	-2.18	104.86	109.40
2	F	1	NAG	O4-C4-C5	-2.12	104.09	109.32
2	E	1	NAG	O7-C7-N2	2.07	125.64	121.98
2	D	2	NAG	O4-C4-C5	2.02	114.31	109.32
2	C	2	NAG	O5-C1-C2	-2.01	108.19	111.29
2	F	2	NAG	O7-C7-C8	-2.00	118.48	122.05

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2

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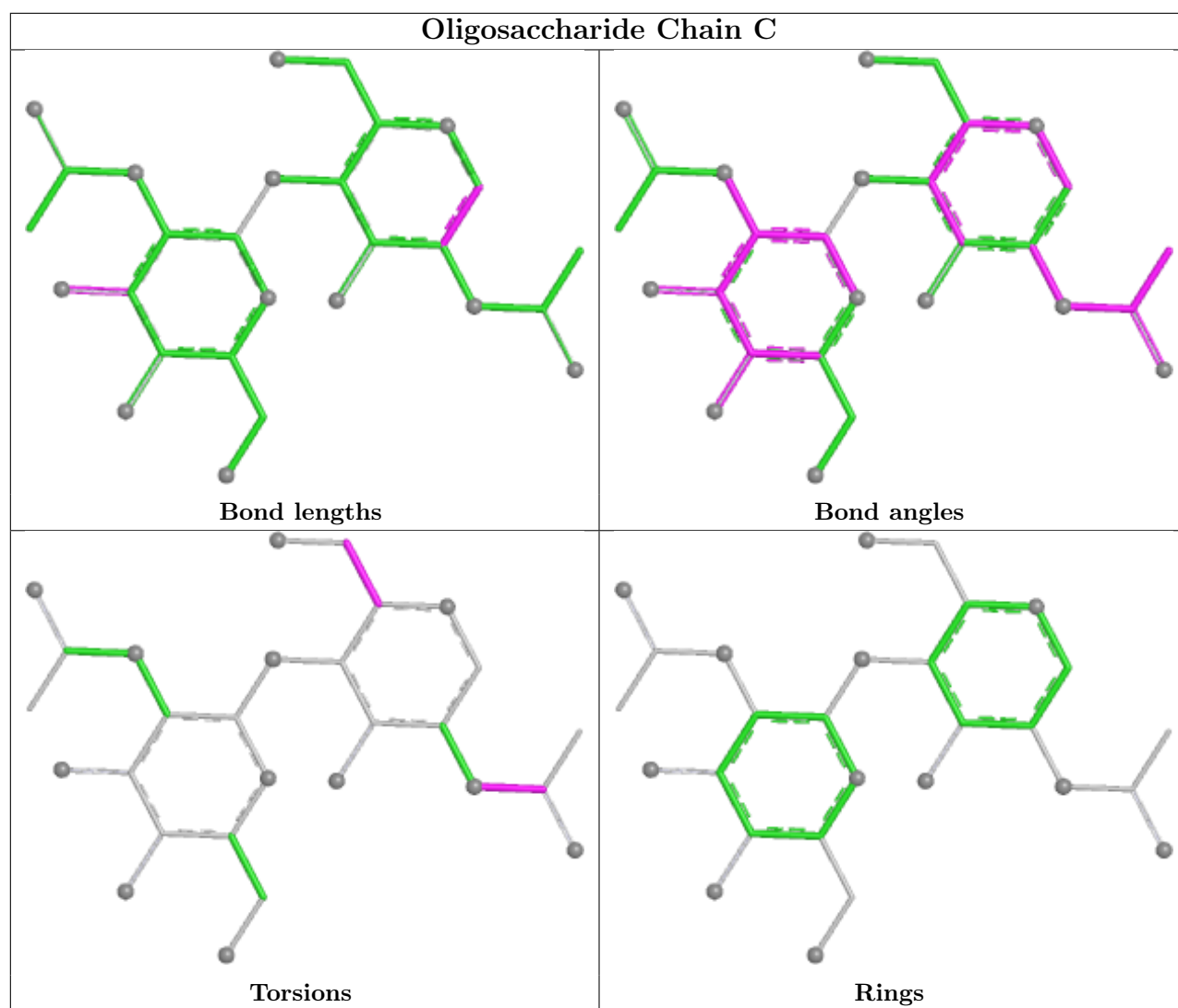
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C1-C2-N2-C7
2	F	2	NAG	C1-C2-N2-C7
2	F	2	NAG	C3-C2-N2-C7
2	D	1	NAG	C4-C5-C6-O6

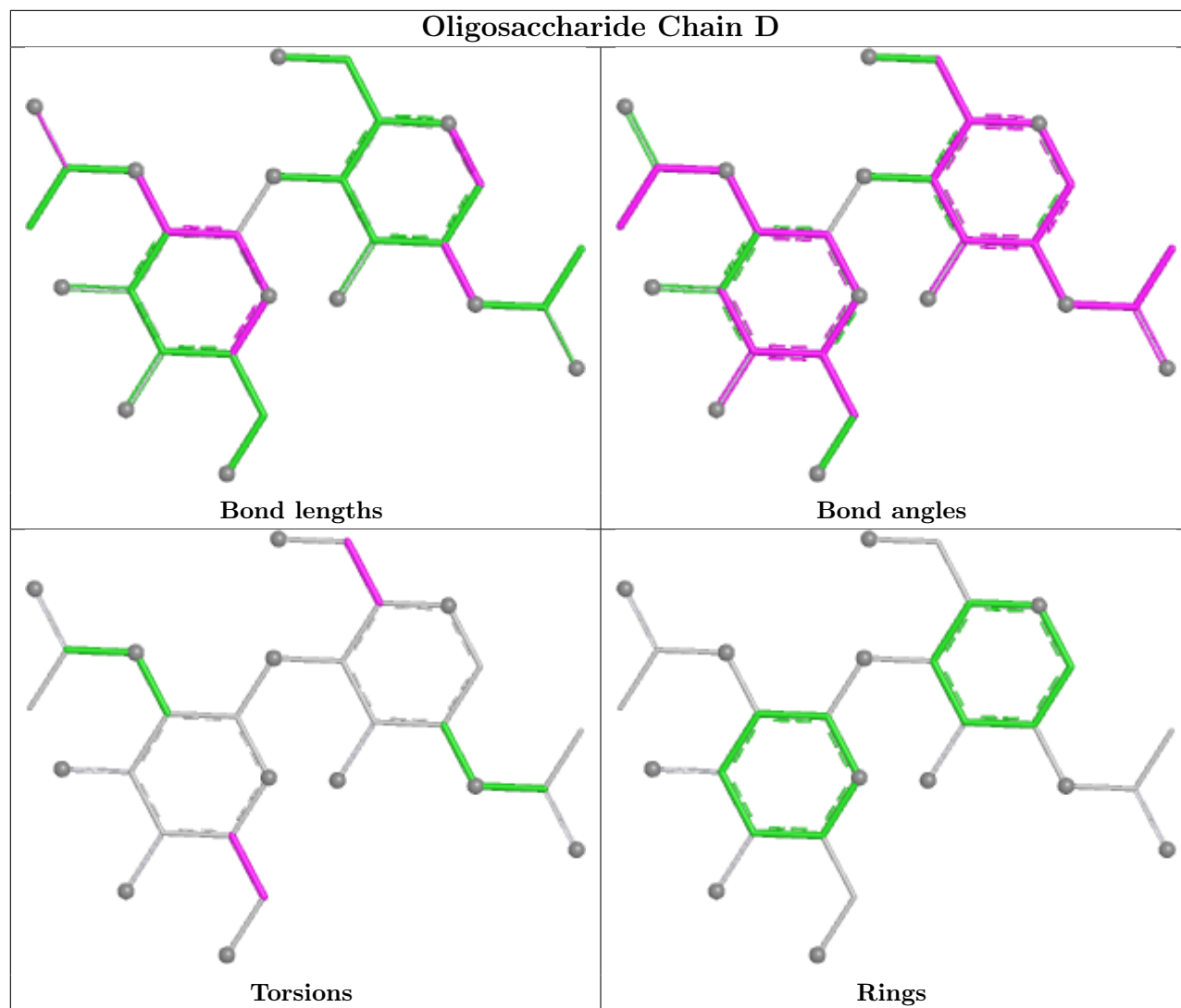
There are no ring outliers.

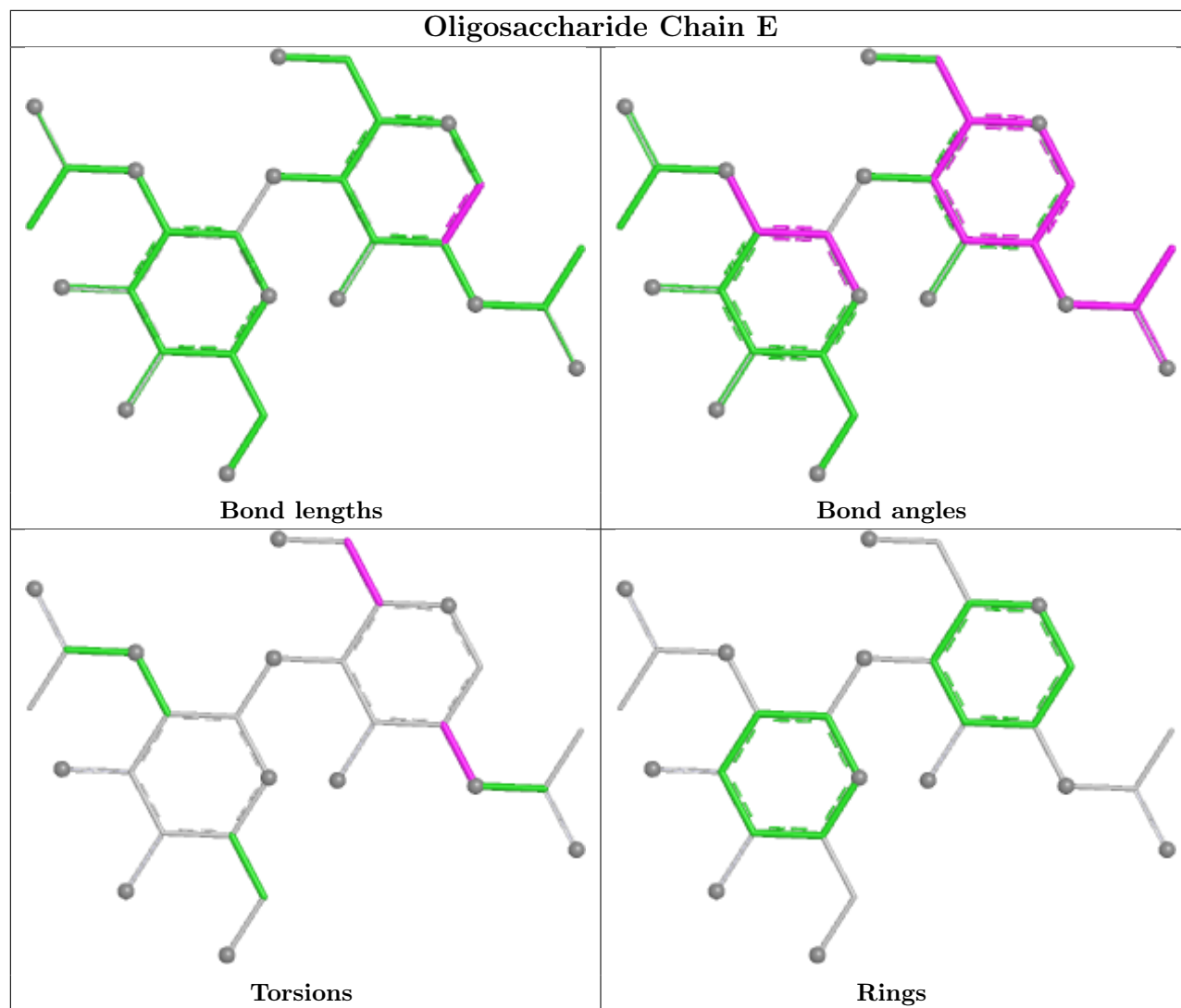
6 monomers are involved in 20 short contacts:

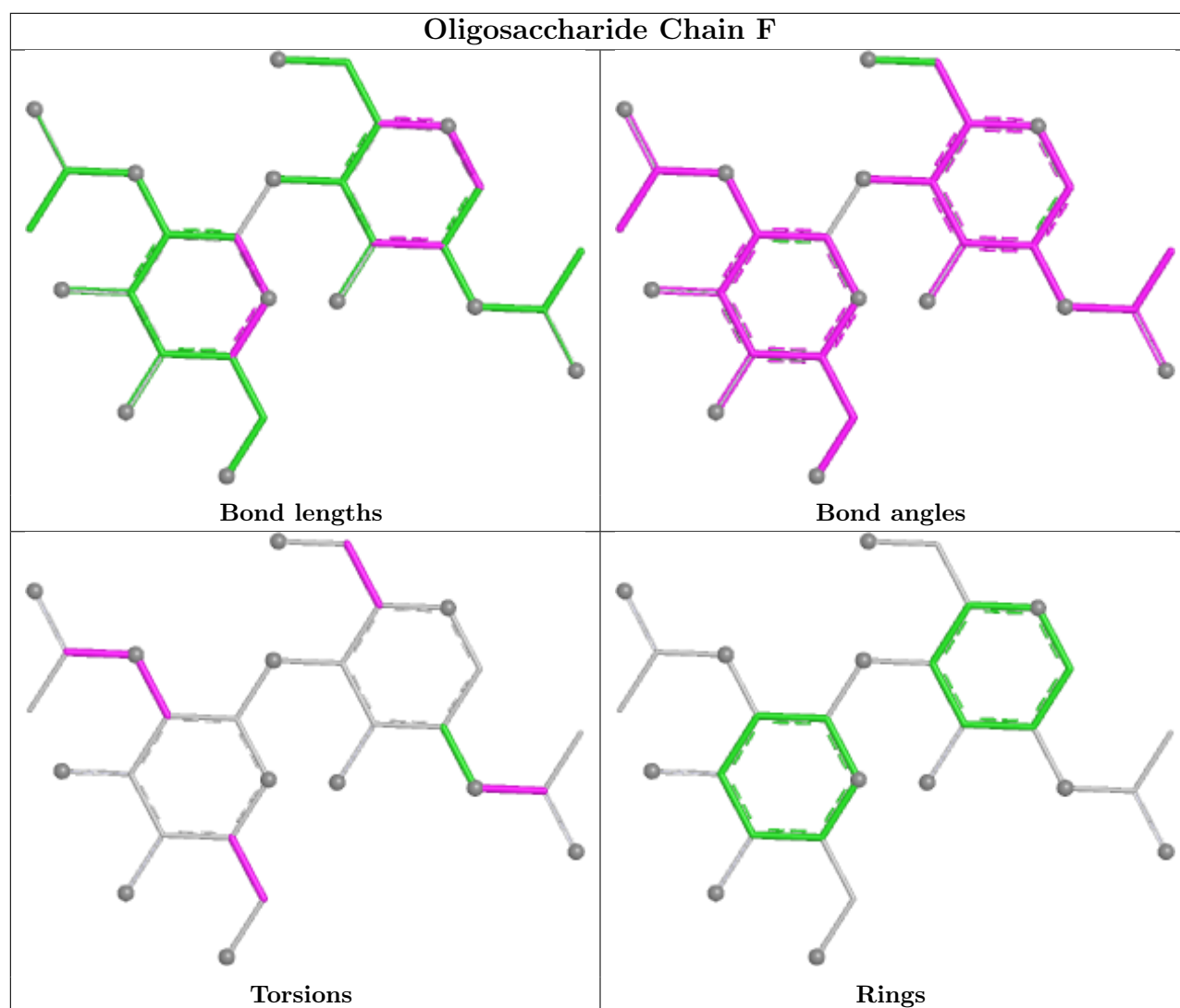
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	3	0
2	C	1	NAG	2	0
2	E	2	NAG	5	0
2	F	1	NAG	4	0
2	D	1	NAG	3	0
2	C	2	NAG	3	0

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 21 ligands modelled in this entry, 10 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SO4	A	609	-	4,4,4	0.37	0	6,6,6	0.53	0
5	NAG	B	609	1	14,14,15	0.95	1 (7%)	17,19,21	2.03	6 (35%)
6	SO4	B	610	-	4,4,4	0.36	0	6,6,6	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	606	1	14,14,15	1.07	1 (7%)	17,19,21	1.48	3 (17%)
5	NAG	A	607	1	14,14,15	1.08	0	17,19,21	2.62	8 (47%)
5	NAG	B	608	1	14,14,15	0.85	1 (7%)	17,19,21	2.26	5 (29%)
5	NAG	A	608	1	14,14,15	0.78	0	17,19,21	2.48	6 (35%)
5	NAG	B	607	1	14,14,15	0.74	0	17,19,21	1.45	2 (11%)
7	KIB	B	611	-	12,12,12	3.64	6 (50%)	16,16,16	2.07	5 (31%)
7	KIB	A	610	-	12,12,12	3.08	4 (33%)	16,16,16	2.12	7 (43%)
5	NAG	B	606	1	14,14,15	1.00	1 (7%)	17,19,21	2.54	6 (35%)

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
5	NAG	B	609	1	-	2/6/23/26	0/1/1/1
5	NAG	A	606	1	-	4/6/23/26	0/1/1/1
5	NAG	A	607	1	-	2/6/23/26	0/1/1/1
5	NAG	B	608	1	-	2/6/23/26	0/1/1/1
5	NAG	A	608	1	-	0/6/23/26	0/1/1/1
5	NAG	B	607	1	-	0/6/23/26	0/1/1/1
7	KIB	B	611	-	-	2/4/4/4	0/1/1/1
7	KIB	A	610	-	-	0/4/4/4	0/1/1/1
5	NAG	B	606	1	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	611	KIB	C6-C1	8.18	1.51	1.40
7	A	610	KIB	C2-C1	7.48	1.50	1.40
7	B	611	KIB	C2-C1	5.80	1.48	1.40
7	A	610	KIB	O1-C1	-4.41	1.26	1.36
7	B	611	KIB	C5-C4	4.17	1.45	1.39
7	A	610	KIB	O2-C4	-3.93	1.28	1.37
7	A	610	KIB	C6-C1	3.82	1.45	1.40
7	B	611	KIB	O4-C2	3.55	1.42	1.37
7	B	611	KIB	C3-C4	3.16	1.43	1.39
7	B	611	KIB	O2-C4	-3.07	1.30	1.37
5	A	606	NAG	O5-C1	-3.00	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	609	NAG	C1-C2	2.45	1.55	1.52
5	B	606	NAG	C4-C3	-2.15	1.46	1.52
5	B	608	NAG	C1-C2	2.12	1.55	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	NAG	O4-C4-C3	-6.66	94.67	110.38
5	A	608	NAG	C3-C4-C5	-5.71	99.88	110.23
5	B	608	NAG	C2-N2-C7	-5.41	115.65	122.90
5	B	609	NAG	O5-C1-C2	-4.93	103.66	111.29
7	B	611	KIB	C3-C2-C1	-4.69	116.13	120.59
5	A	607	NAG	C4-C3-C2	4.56	117.70	111.02
5	A	607	NAG	C1-C2-N2	4.48	117.49	110.43
5	A	608	NAG	O5-C1-C2	-4.45	104.41	111.29
5	A	607	NAG	O7-C7-C8	-4.33	114.34	122.05
5	B	608	NAG	C8-C7-N2	4.24	123.15	116.12
5	B	606	NAG	C1-C2-N2	-3.98	104.16	110.43
5	B	607	NAG	O5-C1-C2	-3.81	105.39	111.29
7	A	610	KIB	C5-C6-C1	-3.77	117.01	120.59
5	A	607	NAG	O7-C7-N2	3.64	128.41	121.98
5	A	608	NAG	C1-O5-C5	-3.60	107.36	112.19
7	A	610	KIB	C7-O3-C6	3.50	122.65	117.51
7	A	610	KIB	O4-C2-C1	3.47	118.16	114.53
5	B	608	NAG	C3-C4-C5	3.42	116.43	110.23
5	A	608	NAG	C2-N2-C7	3.41	127.47	122.90
7	B	611	KIB	O4-C2-C1	3.37	118.06	114.53
5	A	607	NAG	O5-C5-C6	3.30	114.08	107.66
7	B	611	KIB	C2-C3-C4	3.27	124.13	118.98
7	A	610	KIB	C8-O4-C2	3.26	122.29	117.51
5	A	606	NAG	O5-C1-C2	-3.23	106.29	111.29
5	B	606	NAG	O3-C3-C4	-3.22	102.78	110.38
5	B	606	NAG	O3-C3-C2	3.05	115.73	109.40
5	B	609	NAG	O3-C3-C2	2.99	115.61	109.40
5	A	607	NAG	C3-C4-C5	2.90	115.48	110.23
5	B	609	NAG	C2-N2-C7	-2.89	119.03	122.90
5	A	607	NAG	C2-N2-C7	2.76	126.59	122.90
5	B	609	NAG	O5-C5-C6	2.74	112.99	107.66
5	B	609	NAG	C1-O5-C5	-2.71	108.55	112.19
5	A	607	NAG	O3-C3-C2	-2.68	103.84	109.40
5	B	606	NAG	O6-C6-C5	-2.67	102.23	111.33
5	B	608	NAG	O7-C7-N2	-2.57	117.43	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	610	KIB	O1-C1-C2	2.45	124.47	119.21
5	A	606	NAG	C1-C2-N2	-2.44	106.58	110.43
7	B	611	KIB	C7-O3-C6	2.42	121.07	117.51
7	A	610	KIB	C6-C5-C4	2.38	122.73	118.98
5	A	608	NAG	C6-C5-C4	2.36	118.83	113.02
5	B	609	NAG	C1-C2-N2	-2.35	106.73	110.43
5	B	606	NAG	C3-C4-C5	-2.35	105.97	110.23
5	A	606	NAG	C8-C7-N2	2.31	119.95	116.12
5	B	607	NAG	O7-C7-C8	-2.29	117.98	122.05
5	A	608	NAG	O7-C7-N2	2.26	125.97	121.98
7	B	611	KIB	C5-C6-C1	2.21	122.69	120.59
7	A	610	KIB	O3-C6-C1	2.18	116.81	114.53
5	B	608	NAG	O5-C5-C4	2.01	115.73	110.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	607	NAG	C8-C7-N2-C2
5	A	607	NAG	O7-C7-N2-C2
7	B	611	KIB	C1-C6-O3-C7
7	B	611	KIB	C5-C6-O3-C7
5	A	606	NAG	C8-C7-N2-C2
5	A	606	NAG	C4-C5-C6-O6
5	B	609	NAG	C4-C5-C6-O6
5	B	608	NAG	C4-C5-C6-O6
5	A	606	NAG	O5-C5-C6-O6
5	A	606	NAG	O7-C7-N2-C2
5	B	608	NAG	O5-C5-C6-O6
5	B	609	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	606	NAG	0	1
5	A	607	NAG	4	0
5	A	608	NAG	1	0
7	B	611	KIB	7	0
7	A	610	KIB	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	559/559 (100%)	1.27	80 (14%) 6 5	2, 12, 24, 31	0
1	B	559/559 (100%)	1.26	74 (13%) 7 6	3, 13, 23, 32	0
All	All	1118/1118 (100%)	1.27	154 (13%) 6 6	2, 13, 24, 32	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	ALA	4.1
1	B	120	GLY	3.7
1	A	12	CYS	3.6
1	B	316	PRO	3.6
1	B	391	TYR	3.6
1	B	401	VAL	3.5
1	B	393	LEU	3.5
1	A	401	VAL	3.5
1	B	352	VAL	3.5
1	B	388	ILE	3.4
1	A	111	VAL	3.3
1	A	546	TYR	3.3
1	A	552	TYR	3.2
1	B	547	TRP	3.2
1	A	394	THR	3.2
1	A	528	ILE	3.2
1	B	28	PRO	3.1
1	B	348	VAL	3.1
1	B	369	PRO	3.0
1	A	2	PRO	3.0
1	A	255	VAL	3.0
1	A	547	TRP	3.0
1	B	136	TRP	3.0
1	B	536	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	338	VAL	2.9
1	A	363	LEU	2.9
1	B	408	VAL	2.9
1	A	543	TRP	2.9
1	A	499	TRP	2.9
1	A	51	GLY	2.8
1	A	351	PHE	2.8
1	B	238	PHE	2.8
1	B	66	GLY	2.8
1	B	87	THR	2.8
1	A	396	ASN	2.8
1	B	14	SER	2.8
1	B	379	ASP	2.8
1	B	27	THR	2.7
1	B	350	SER	2.7
1	A	414	TRP	2.7
1	B	543	TRP	2.7
1	A	133	GLY	2.7
1	B	400	PRO	2.7
1	B	64	ILE	2.6
1	A	395	GLY	2.6
1	A	368	THR	2.6
1	A	553	PRO	2.6
1	A	539	VAL	2.5
1	B	32	VAL	2.5
1	B	210	GLY	2.5
1	B	12	CYS	2.5
1	A	39	ASN	2.5
1	A	117	PRO	2.5
1	A	315	ALA	2.5
1	A	355	PRO	2.5
1	B	91	SER	2.5
1	B	389	ILE	2.5
1	A	349	ASN	2.5
1	A	527	ARG	2.5
1	B	83	ASN	2.5
1	A	325	THR	2.5
1	A	462	ALA	2.5
1	A	406	VAL	2.5
1	B	539	VAL	2.5
1	B	526	GLN	2.5
1	A	282	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	217	VAL	2.4
1	B	118	PRO	2.4
1	B	313	ALA	2.4
1	A	484	GLY	2.4
1	A	131	GLN	2.4
1	B	416	TYR	2.4
1	A	207	PRO	2.4
1	A	444	GLY	2.4
1	A	555	ILE	2.4
1	B	243	VAL	2.4
1	B	372	VAL	2.4
1	B	397	THR	2.4
1	B	552	TYR	2.4
1	B	365	LEU	2.4
1	A	141	PHE	2.4
1	B	86	VAL	2.4
1	B	97	ILE	2.4
1	A	87	THR	2.4
1	A	545	ALA	2.3
1	A	336	LEU	2.3
1	A	468	LEU	2.3
1	B	513	LEU	2.3
1	B	342	VAL	2.3
1	B	411	VAL	2.3
1	A	136	TRP	2.3
1	B	73	TRP	2.3
1	B	425	GLY	2.3
1	A	529	SER	2.3
1	A	150	VAL	2.3
1	B	522	ALA	2.3
1	B	545	ALA	2.3
1	B	26	SER	2.3
1	A	259	ALA	2.3
1	B	399	TYR	2.3
1	A	427	PHE	2.2
1	B	116	ILE	2.2
1	A	399	TYR	2.2
1	A	456	ARG	2.2
1	A	184	VAL	2.2
1	A	353	LYS	2.2
1	B	117	PRO	2.2
1	B	4	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	546	TYR	2.2
1	B	423	PRO	2.2
1	A	408	VAL	2.2
1	B	280	SER	2.2
1	A	177	TYR	2.2
1	A	391	TYR	2.2
1	A	115	PRO	2.1
1	A	320	PRO	2.1
1	A	352	VAL	2.1
1	A	185	HIS	2.1
1	B	466	ALA	2.1
1	B	489	LEU	2.1
1	A	28	PRO	2.1
1	A	549	THR	2.1
1	A	11	ALA	2.1
1	B	191	ALA	2.1
1	A	114	CYS	2.1
1	A	369	PRO	2.1
1	A	551	PRO	2.1
1	A	277	ILE	2.1
1	A	373	TRP	2.1
1	A	536	PHE	2.1
1	A	25	VAL	2.1
1	B	338	VAL	2.1
1	A	541	ASP	2.1
1	A	192	PRO	2.1
1	B	209	THR	2.1
1	B	548	PRO	2.1
1	B	484	GLY	2.1
1	A	309	ILE	2.1
1	A	348	VAL	2.1
1	B	143	ALA	2.1
1	A	95	HIS	2.0
1	A	3	THR	2.0
1	A	221	PRO	2.0
1	B	222	GLY	2.0
1	B	485	GLY	2.0
1	B	463	VAL	2.0
1	A	350	SER	2.0
1	B	490	ALA	2.0
1	B	396	ASN	2.0
1	A	443	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	518	LEU	2.0
1	B	456	ARG	2.0
1	A	447	PRO	2.0
1	B	192	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

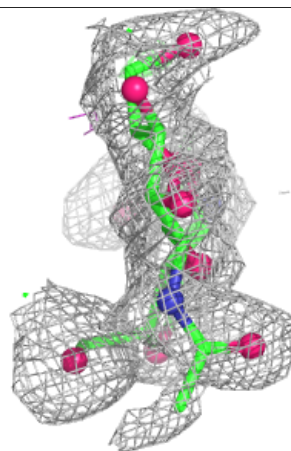
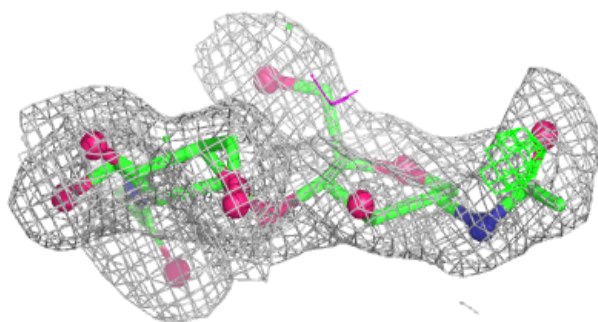
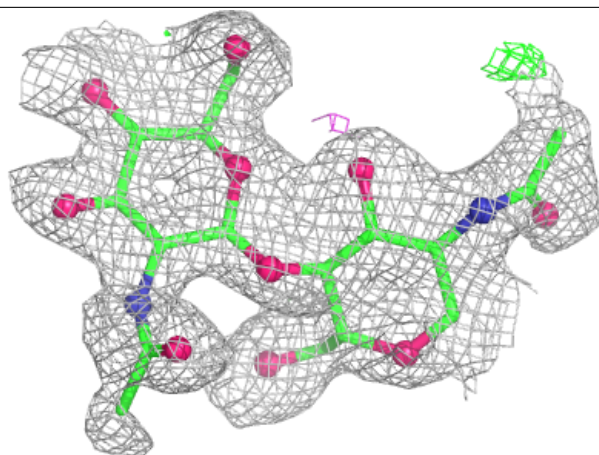
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	2	14/15	0.77	0.13	16,22,28,28	0
2	NAG	D	1	14/15	0.79	0.14	10,13,19,20	0
2	NAG	F	2	14/15	0.83	0.11	7,18,24,25	0
2	NAG	E	2	14/15	0.84	0.11	9,14,18,22	0
2	NAG	E	1	14/15	0.84	0.12	8,15,16,17	0
2	NAG	C	1	14/15	0.86	0.11	8,16,18,18	0
2	NAG	F	1	14/15	0.89	0.13	5,12,23,23	0
2	NAG	C	2	14/15	0.89	0.10	9,15,19,19	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.

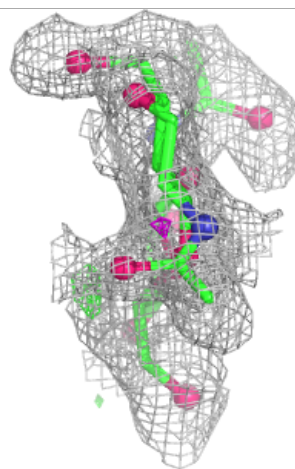
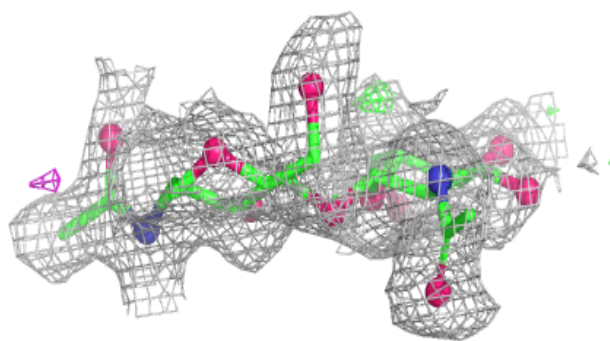
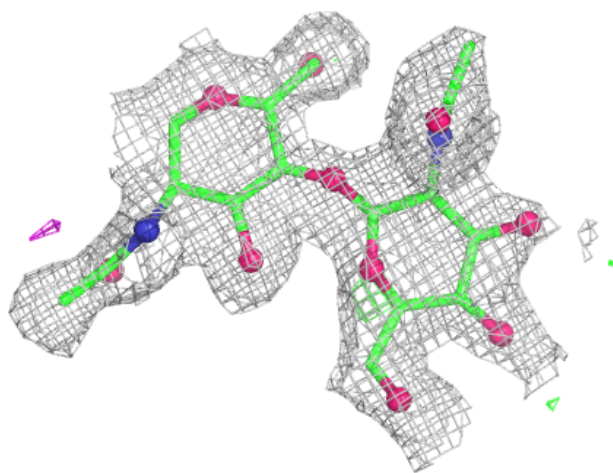
Electron density around Chain C:

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



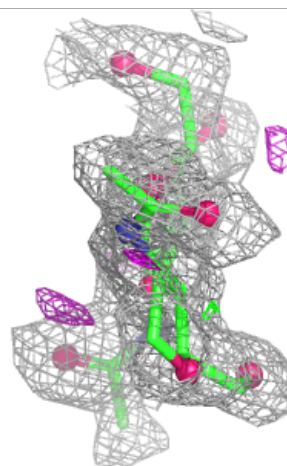
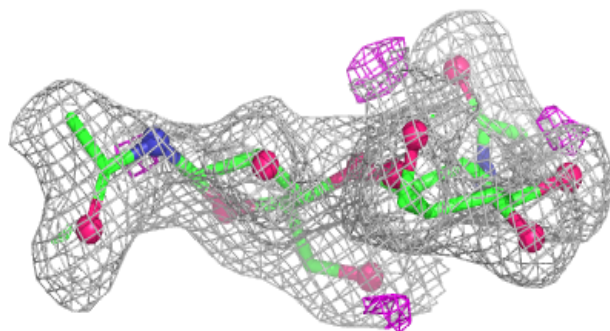
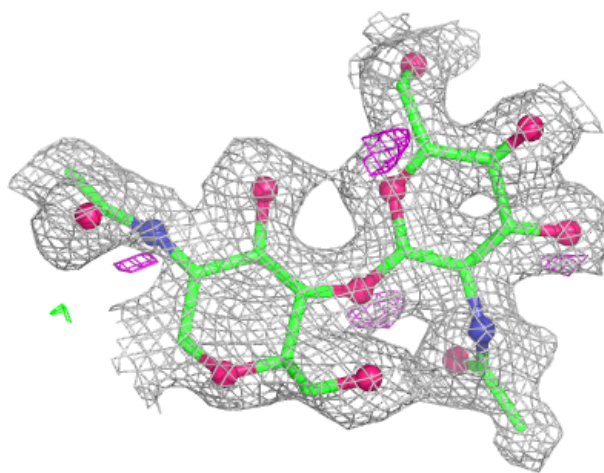
Electron density around Chain D:

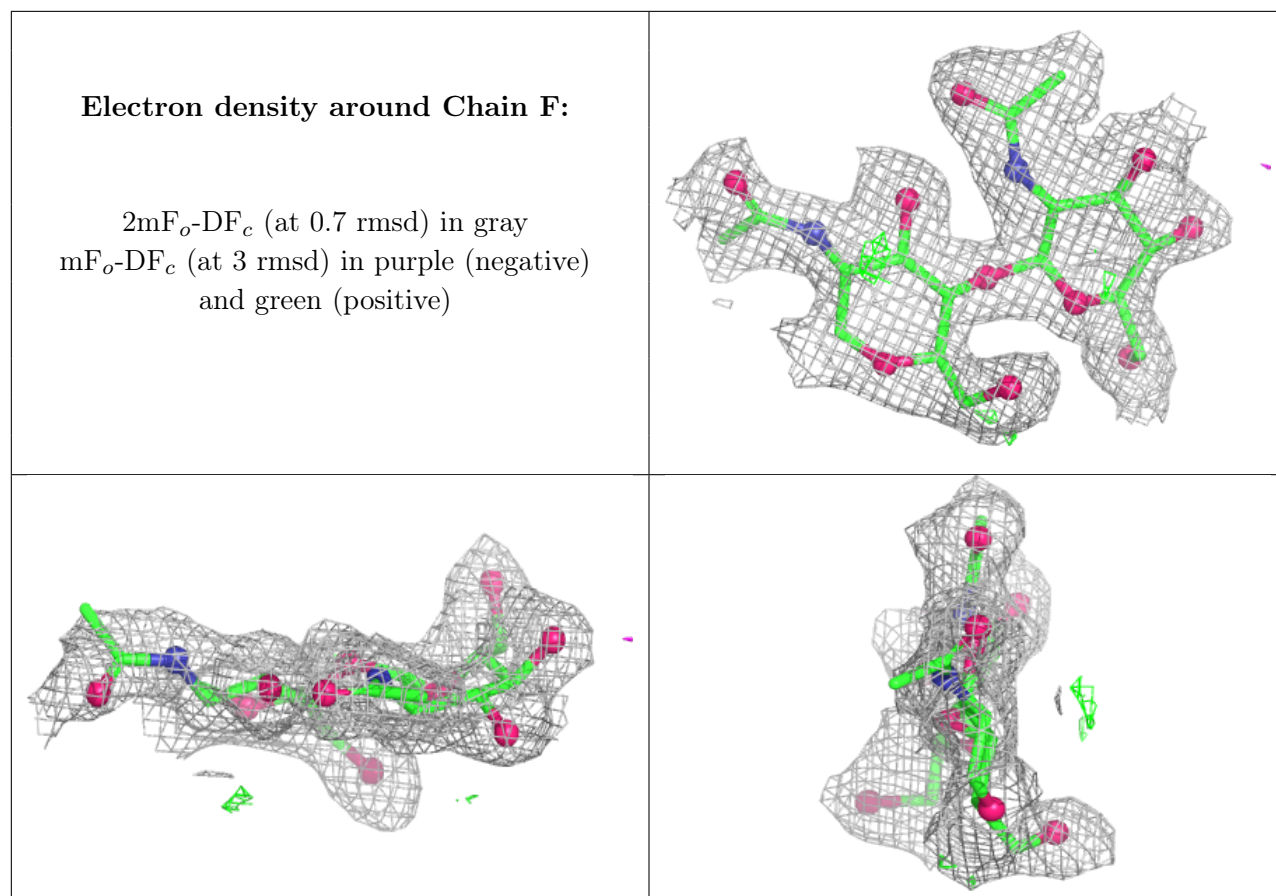
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

$2mF_o-DF_c$ (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
5	NAG	A	606	14/15	0.69	0.17	26,29,32,34	0
5	NAG	A	608	14/15	0.72	0.14	8,23,27,28	0
7	KIB	A	610	12/12	0.74	0.16	7,17,20,23	0
5	NAG	B	608	14/15	0.77	0.13	17,20,25,26	0
4	CL	A	605	1/1	0.77	0.28	41,41,41,41	0
5	NAG	A	607	14/15	0.82	0.13	16,22,33,33	0
5	NAG	B	607	14/15	0.82	0.12	13,19,24,24	0
5	NAG	B	606	14/15	0.84	0.11	9,17,19,24	0
5	NAG	B	609	14/15	0.85	0.12	8,15,27,28	0
6	SO4	B	610	5/5	0.86	0.11	17,25,25,29	0
7	KIB	B	611	12/12	0.87	0.11	2,7,15,16	0
6	SO4	A	609	5/5	0.92	0.10	22,23,26,29	0
3	CU	A	602	1/1	0.92	0.06	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CU	B	604	1/1	0.93	0.05	15,15,15,15	0
4	CL	B	605	1/1	0.94	0.09	26,26,26,26	0
3	CU	A	601	1/1	0.94	0.04	15,15,15,15	0
3	CU	B	602	1/1	0.94	0.06	18,18,18,18	0
3	CU	A	603	1/1	0.95	0.04	11,11,11,11	0
3	CU	B	601	1/1	0.97	0.04	12,12,12,12	0
3	CU	A	604	1/1	0.97	0.03	14,14,14,14	0
3	CU	B	603	1/1	0.98	0.04	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.