



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:08 AM UTC

PDB ID : 1AHP / pdb_00001ahp
Title : OLIGOSACCHARIDE SUBSTRATE BINDING IN ESCHERICHIA COLI
MALTODEXTRIN PHSPHORYLASE
Authors : O'Reilly, M.; Watson, K.A.; Schinzel, R.; Palm, D.; Johnson, L.N.
Deposited on : 1997-04-10
Resolution : 3.00 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

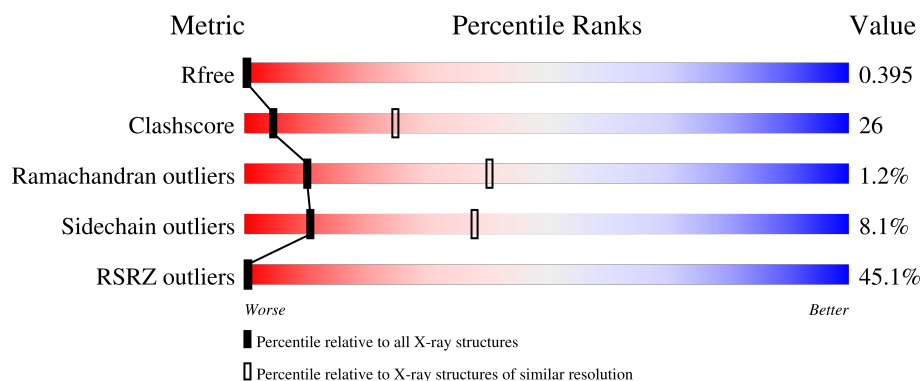
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	797	34% 53% 41% 5%
1	B	797	56% 54% 41% 5%
2	C	2	100%
2	D	2	100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12830 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 E.COLI MALTODEXTRIN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	796	Total	C	N	O	S	0	0	0
			6366	4064	1126	1156	20			
1	B	796	Total	C	N	O	S	0	0	0
			6366	4064	1126	1156	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	ALA	ASN	engineered mutation	UNP P00490
A	184	ALA	LYS	conflict	UNP P00490
A	497	ASP	GLN	conflict	UNP P00490
A	547	ARG	HIS	conflict	UNP P00490
A	681	LYS	GLU	conflict	UNP P00490
A	795	ALA	LYS	conflict	UNP P00490
B	112	ALA	ASN	engineered mutation	UNP P00490
B	184	ALA	LYS	conflict	UNP P00490
B	497	ASP	GLN	conflict	UNP P00490
B	547	ARG	HIS	conflict	UNP P00490
B	681	LYS	GLU	conflict	UNP P00490
B	795	ALA	LYS	conflict	UNP P00490

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			23	12	11			
2	D	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



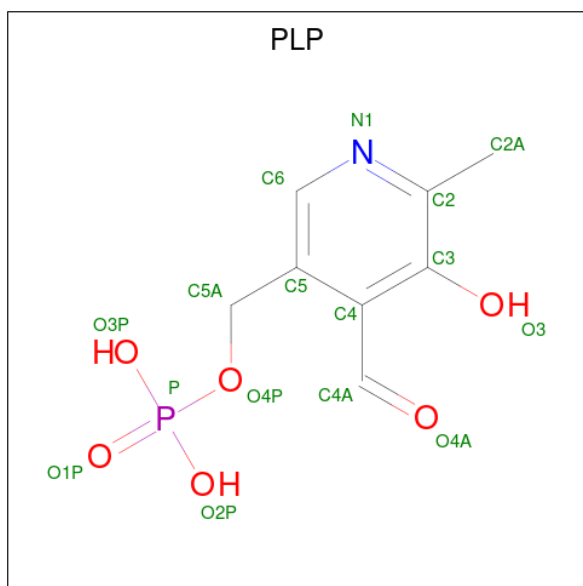
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $\text{C}_8\text{H}_{10}\text{NO}_6\text{P}$).

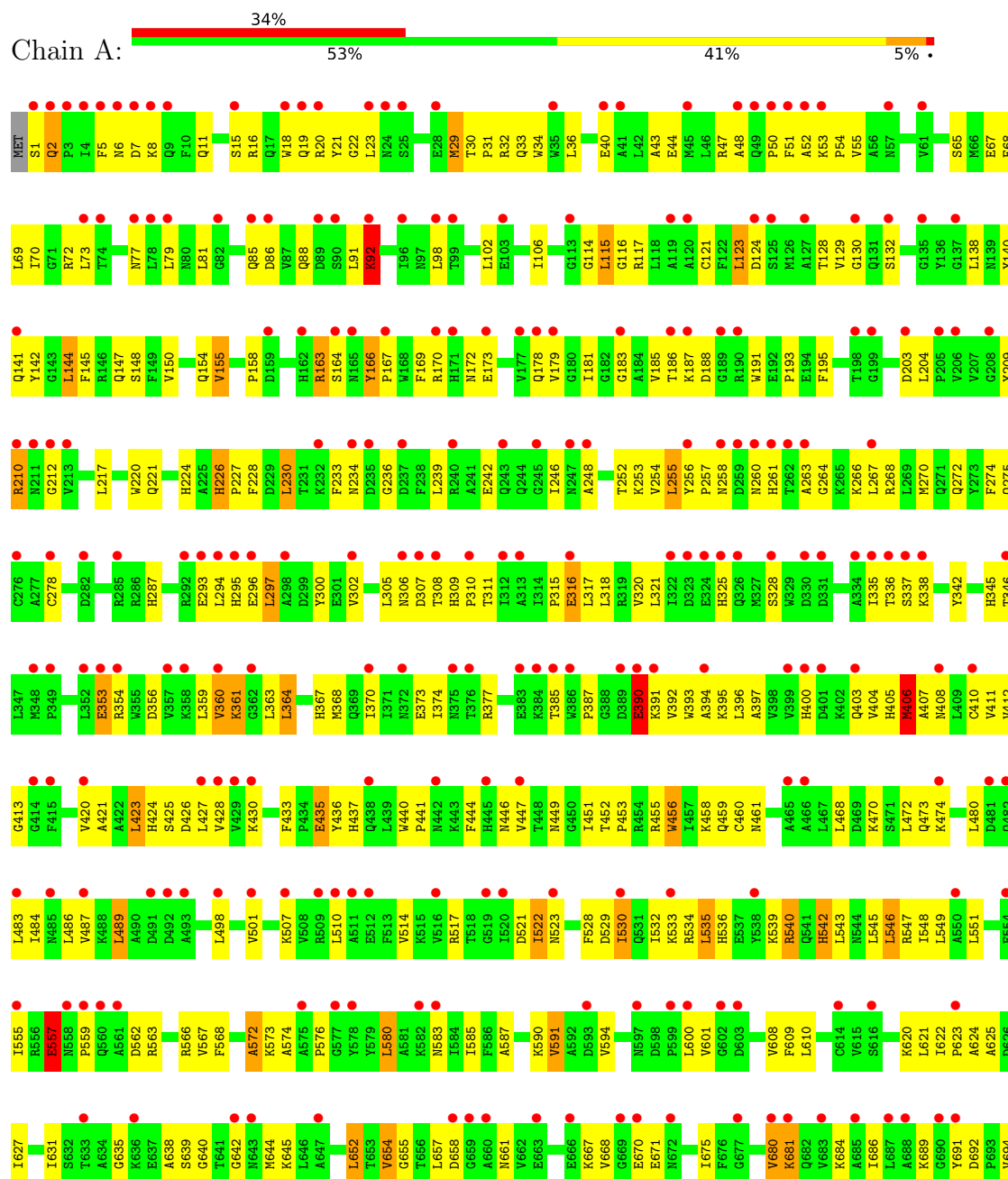


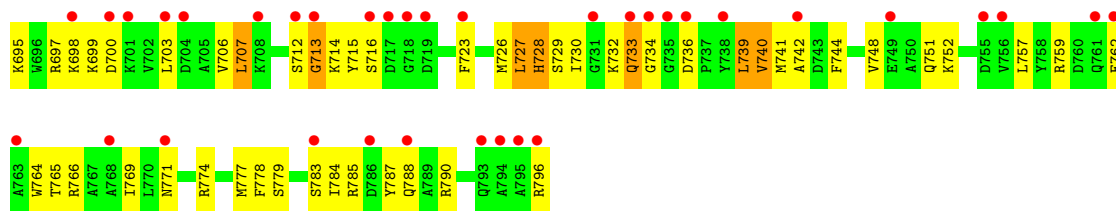
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 15	C 8	N 1	O 5	P 1	0	0
5	B	1	Total 15	C 8	N 1	O 5	P 1	0	0

3 Residue-property plots

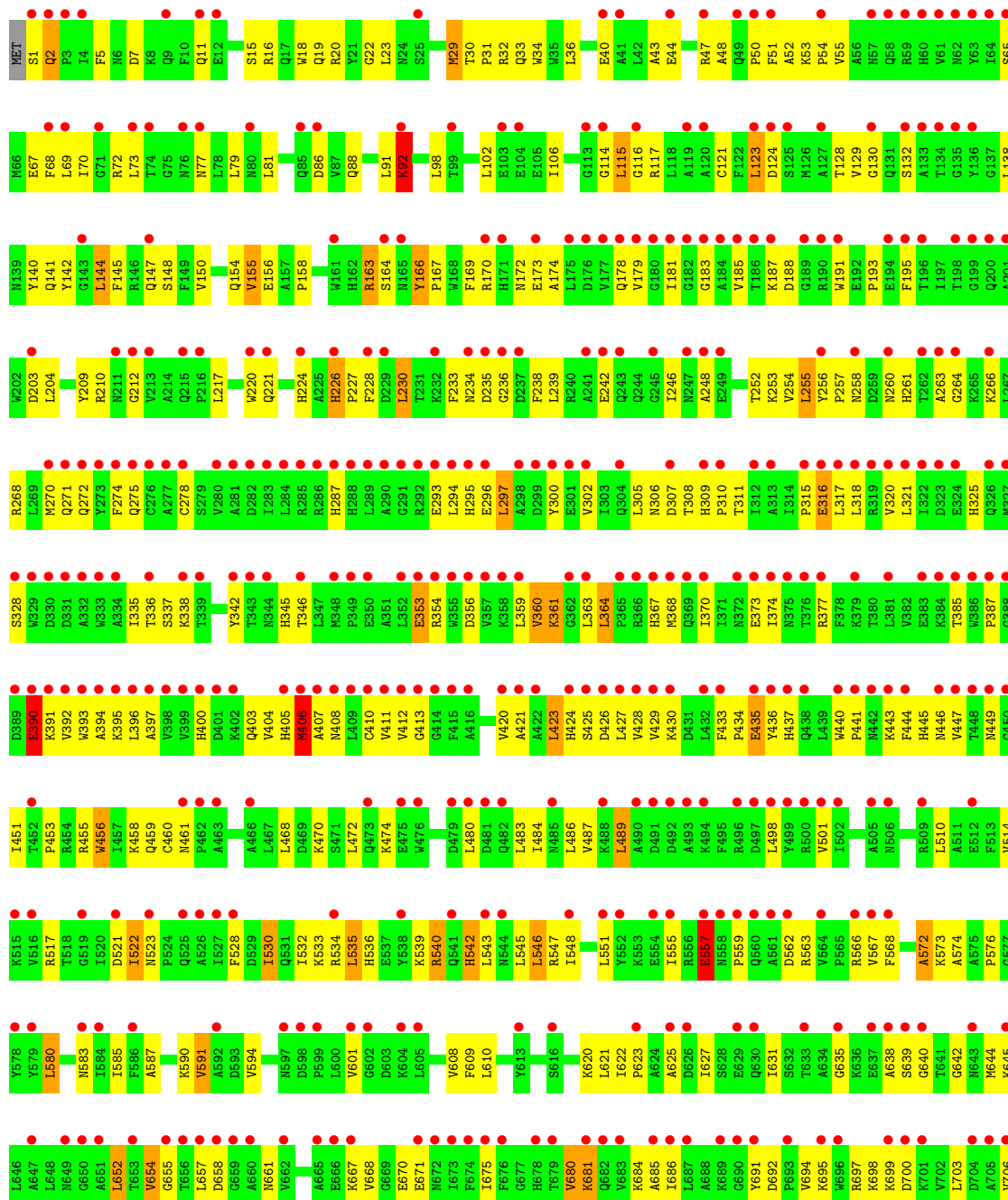
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

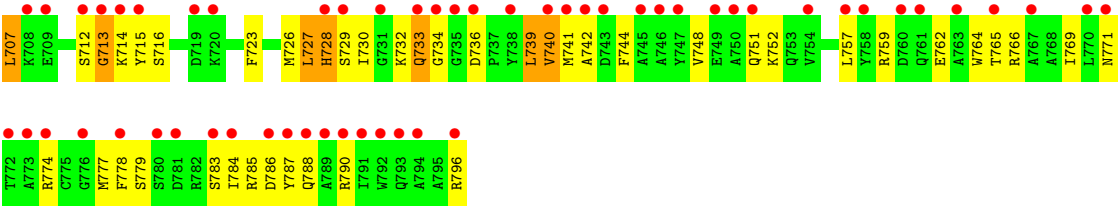
• Molecule 1: E.COLI MALTODEXTRIN PHOSPHORYLASE





● Molecule 1: E.COLI MALTODEXTRIN PHOSPHORYLASE





● Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



● Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.20Å 112.40Å 121.70Å 90.00° 119.70° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 10.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	73.0 (10.00-3.00) 71.5 (10.00-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.99Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.232 , 0.278 0.390 , 0.395	Depositor DCC
R_{free} test set	608 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.57	EDS
Total number of atoms	12830	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: GLC, PLP, SO4, GOL

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	0.49	0/6514	1.00	30/8837 (0.3%)
1	B	0.49	0/6514	1.00	30/8837 (0.3%)
All	All	0.49	0/13028	1.00	60/17674 (0.3%)

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	TYR	CA-C-N	8.70	130.71	119.84
1	A	166	TYR	C-N-CA	8.70	130.71	119.84
1	B	166	TYR	CA-C-N	8.69	130.70	119.84
1	B	166	TYR	C-N-CA	8.69	130.70	119.84
1	A	345	HIS	N-CA-C	8.53	123.78	113.12
1	B	345	HIS	N-CA-C	8.50	123.75	113.12
1	B	530	ILE	N-CA-C	8.33	120.27	108.36
1	A	530	ILE	N-CA-C	8.31	120.24	108.36
1	B	29	MET	N-CA-C	7.16	119.54	110.24
1	A	29	MET	N-CA-C	7.13	119.51	110.24
1	A	540	ARG	N-CA-C	6.97	121.02	111.54
1	B	540	ARG	N-CA-C	6.96	121.00	111.54
1	A	456	TRP	N-CA-C	6.77	121.25	113.19
1	A	461	ASN	CA-C-N	6.77	126.01	118.97
1	A	461	ASN	C-N-CA	6.77	126.01	118.97
1	B	461	ASN	CA-C-N	6.75	126.00	118.97
1	B	461	ASN	C-N-CA	6.75	126.00	118.97
1	B	456	TRP	N-CA-C	6.75	121.22	113.19
1	B	203	ASP	N-CA-C	6.72	120.41	109.59
1	A	203	ASP	N-CA-C	6.72	120.41	109.59
1	B	543	LEU	N-CA-C	-6.67	104.09	111.36
1	A	543	LEU	N-CA-C	-6.66	104.10	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	SER	N-CA-C	6.32	118.70	111.11
1	B	164	SER	N-CA-C	6.32	118.69	111.11
1	B	713	GLY	N-CA-C	-6.20	105.53	115.08
1	A	713	GLY	N-CA-C	-6.20	105.54	115.08
1	B	572	ALA	N-CA-C	6.19	118.71	108.99
1	A	572	ALA	N-CA-C	6.16	118.66	108.99
1	A	654	VAL	N-CA-C	-5.97	96.92	109.34
1	A	106	ILE	N-CA-C	-5.96	101.02	108.89
1	B	106	ILE	N-CA-C	-5.96	101.02	108.89
1	A	226	HIS	CA-C-N	5.96	125.58	119.56
1	A	226	HIS	C-N-CA	5.96	125.58	119.56
1	B	654	VAL	N-CA-C	-5.96	96.95	109.34
1	B	114	GLY	N-CA-C	5.93	120.07	112.83
1	B	226	HIS	CA-C-N	5.93	125.55	119.56
1	B	226	HIS	C-N-CA	5.93	125.55	119.56
1	A	114	GLY	N-CA-C	5.92	120.05	112.83
1	B	70	ILE	N-CA-C	5.87	119.30	111.44
1	A	70	ILE	N-CA-C	5.84	119.26	111.44
1	A	92	LYS	N-CA-C	-5.70	105.07	111.28
1	B	92	LYS	N-CA-C	-5.69	105.08	111.28
1	A	440	TRP	CA-C-N	5.60	125.21	119.56
1	A	440	TRP	C-N-CA	5.60	125.21	119.56
1	B	440	TRP	CA-C-N	5.59	125.21	119.56
1	B	440	TRP	C-N-CA	5.59	125.21	119.56
1	A	187	LYS	N-CA-C	-5.50	105.44	111.82
1	B	187	LYS	N-CA-C	-5.50	105.44	111.82
1	A	406	MET	N-CA-C	5.44	117.64	111.11
1	B	406	MET	N-CA-C	5.44	117.64	111.11
1	A	248	ALA	N-CA-C	-5.41	107.23	113.88
1	B	248	ALA	N-CA-C	-5.38	107.27	113.88
1	A	680	VAL	N-CA-C	5.36	115.98	110.36
1	B	680	VAL	N-CA-C	5.34	115.97	110.36
1	A	548	ILE	N-CA-C	-5.28	105.35	110.42
1	B	740	VAL	N-CA-C	-5.28	105.23	110.62
1	A	740	VAL	N-CA-C	-5.27	105.24	110.62
1	B	774	ARG	N-CA-C	5.27	119.72	113.28
1	A	774	ARG	N-CA-C	5.27	119.70	113.28
1	B	548	ILE	N-CA-C	-5.25	105.38	110.42

There are no chirality outliers.

There are no planarity outliers.

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	6366	0	6326	413	11
1	B	6366	0	6326	407	9
2	C	23	0	20	5	0
2	D	23	0	20	4	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	A	15	0	7	1	0
5	B	15	0	7	1	0
All	All	12830	0	12722	653	12

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 26.

All (653) 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:A:170:ARG:CG	1:B:20:ARG:O	1.67	1.40
1:A:158:PRO:HG2	1:B:228:PHE:O	1.49	1.11
1:A:253:LYS:HE3	1:B:242:GLU:OE2	1.54	1.07
1:A:20:ARG:HG3	1:B:47:ARG:CZ	1.84	1.07
1:A:19:GLN:CD	1:B:47:ARG:O	2.02	1.01
1:A:20:ARG:NH1	1:B:40:GLU:OE1	1.91	1.01
1:A:170:ARG:HG3	1:B:20:ARG:C	1.87	1.00
1:A:258:ASN:HB3	1:B:234:ASN:O	1.60	1.00
1:A:32:ARG:HB3	1:B:173:GLU:OE2	1.63	0.99
1:A:19:GLN:HB3	1:B:47:ARG:HB3	1.45	0.97
1:A:47:ARG:CZ	1:B:20:ARG:HG3	1.94	0.97
1:A:258:ASN:CB	1:B:234:ASN:O	2.16	0.94
1:A:47:ARG:HD3	1:B:20:ARG:HA	1.49	0.94
1:A:258:ASN:HB2	1:B:234:ASN:CB	1.97	0.94
1:A:20:ARG:HA	1:B:47:ARG:HD3	1.51	0.92
1:A:158:PRO:CG	1:B:228:PHE:O	2.18	0.90
1:A:261:HIS:NE2	1:B:236:GLY:CA	2.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:VAL:HG21	1:B:715:TYR:HD1	1.35	0.90
1:A:594:VAL:HG21	1:A:715:TYR:HD1	1.35	0.90
1:A:170:ARG:HG3	1:B:20:ARG:O	0.71	0.89
1:A:19:GLN:OE1	1:B:47:ARG:O	1.88	0.89
1:A:40:GLU:OE1	1:B:20:ARG:NH1	2.06	0.89
1:A:22:GLY:N	1:B:170:ARG:HD2	1.88	0.88
1:A:23:LEU:HD21	1:B:172:ASN:ND2	1.89	0.88
1:A:47:ARG:NH1	1:B:20:ARG:HG3	1.89	0.87
1:A:228:PHE:O	1:B:158:PRO:HG2	1.75	0.86
1:A:246:ILE:HD11	1:B:246:ILE:HD11	1.58	0.85
1:A:20:ARG:HG3	1:B:47:ARG:NH1	1.91	0.85
1:A:145:PHE:HB3	1:B:230:LEU:HD11	1.59	0.85
1:A:254:VAL:CG2	1:B:228:PHE:CZ	2.60	0.84
1:B:535:LEU:HB2	1:B:572:ALA:HB1	1.59	0.84
1:A:32:ARG:HD3	1:B:173:GLU:OE1	1.77	0.84
1:A:48:ALA:HA	1:B:19:GLN:OE1	1.77	0.83
1:A:535:LEU:HB2	1:A:572:ALA:HB1	1.59	0.83
1:A:142:TYR:OH	1:B:227:PRO:HG2	1.80	0.81
1:B:144:LEU:HD11	1:B:573:LYS:HE3	1.63	0.81
1:A:144:LEU:HD11	1:A:573:LYS:HE3	1.63	0.81
1:A:594:VAL:HG21	1:A:715:TYR:CD1	2.16	0.81
1:A:19:GLN:OE1	1:B:48:ALA:HA	1.81	0.80
1:A:236:GLY:CA	1:B:261:HIS:NE2	2.44	0.80
1:A:361:LYS:HD2	1:A:368:MET:HG2	1.63	0.80
1:B:361:LYS:HD2	1:B:368:MET:HG2	1.63	0.80
1:A:254:VAL:HG23	1:B:228:PHE:CZ	2.16	0.79
1:A:32:ARG:HG2	1:B:173:GLU:OE1	1.83	0.79
1:A:242:GLU:OE2	1:B:253:LYS:HE3	1.82	0.79
1:B:594:VAL:HG21	1:B:715:TYR:CD1	2.16	0.78
1:A:258:ASN:CG	1:B:234:ASN:O	2.27	0.78
1:A:258:ASN:HB3	1:B:234:ASN:C	2.07	0.78
1:A:32:ARG:CG	1:B:173:GLU:OE1	2.32	0.77
1:A:115:LEU:HD12	2:C:2:GLC:H2	1.67	0.77
1:B:423:LEU:HD22	1:B:423:LEU:H	1.50	0.77
1:A:258:ASN:CB	1:B:234:ASN:CA	2.63	0.76
1:A:16:ARG:NH1	1:B:16:ARG:NH1	2.34	0.76
1:A:423:LEU:H	1:A:423:LEU:HD22	1.50	0.76
1:A:22:GLY:CA	1:B:170:ARG:HD2	2.15	0.76
1:A:522:ILE:HG13	1:A:567:VAL:HG11	1.68	0.75
1:B:522:ILE:HG13	1:B:567:VAL:HG11	1.68	0.75
1:A:258:ASN:HB2	1:B:234:ASN:CA	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:HG23	1:A:130:GLY:HA3	1.68	0.75
1:A:253:LYS:CE	1:B:242:GLU:OE2	2.33	0.75
1:A:535:LEU:HD13	1:A:585:ILE:HG12	1.69	0.75
1:B:55:VAL:HG23	1:B:130:GLY:HA3	1.68	0.75
1:B:115:LEU:HD12	2:D:2:GLC:H2	1.66	0.75
1:A:19:GLN:OE1	1:B:47:ARG:C	2.31	0.74
1:A:309:HIS:HB2	1:A:310:PRO:HD3	1.70	0.73
1:B:535:LEU:HD13	1:B:585:ILE:HG12	1.69	0.73
1:A:261:HIS:NE2	1:B:236:GLY:HA3	2.02	0.73
1:A:258:ASN:CB	1:B:234:ASN:HA	2.19	0.73
1:B:309:HIS:HB2	1:B:310:PRO:HD3	1.70	0.72
1:A:32:ARG:CD	1:B:173:GLU:OE1	2.37	0.72
1:A:261:HIS:CE1	1:B:235:ASP:C	2.68	0.72
1:A:145:PHE:HB3	1:B:230:LEU:CD1	2.19	0.71
1:A:230:LEU:HD11	1:B:145:PHE:HB3	1.72	0.71
1:A:16:ARG:HD3	1:B:44:GLU:CG	2.20	0.71
1:B:658:ASP:O	1:B:661:ASN:HB2	1.91	0.71
1:A:258:ASN:HB2	1:B:234:ASN:HB3	1.71	0.71
1:A:47:ARG:HH12	1:B:20:ARG:NH1	1.89	0.70
1:A:547:ARG:HH22	1:A:551:LEU:HB2	1.57	0.69
1:B:530:ILE:HD12	1:B:625:ALA:HB2	1.73	0.69
1:A:658:ASP:O	1:A:661:ASN:HB2	1.91	0.69
1:B:547:ARG:HH22	1:B:551:LEU:HB2	1.57	0.69
1:A:254:VAL:CG2	1:B:228:PHE:HZ	2.04	0.68
1:A:254:VAL:HG21	1:B:228:PHE:HZ	1.58	0.68
1:A:700:ASP:HB3	1:A:703:LEU:HB3	1.76	0.68
1:A:305:LEU:HD22	1:A:310:PRO:HB2	1.75	0.68
1:A:230:LEU:CD1	1:B:156:GLU:HB3	2.23	0.68
1:A:261:HIS:CD2	1:B:236:GLY:HA3	2.28	0.68
1:A:530:ILE:HD12	1:A:625:ALA:HB2	1.74	0.68
1:B:305:LEU:HD22	1:B:310:PRO:HB2	1.75	0.68
1:B:573:LYS:NZ	2:D:1:GLC:O6	2.27	0.68
1:B:308:THR:OG1	1:B:353:GLU:HG3	1.94	0.68
1:A:573:LYS:NZ	2:C:1:GLC:O6	2.27	0.67
1:A:308:THR:OG1	1:A:353:GLU:HG3	1.94	0.67
1:A:254:VAL:HG21	1:B:228:PHE:CZ	2.28	0.67
1:A:510:LEU:HD11	1:A:621:LEU:HD23	1.77	0.67
1:B:700:ASP:HB3	1:B:703:LEU:HB3	1.75	0.67
1:A:757:LEU:HG	1:A:764:TRP:HE3	1.60	0.67
1:A:224:HIS:CD2	1:A:226:HIS:H	2.13	0.66
1:B:115:LEU:HD12	2:D:2:GLC:C2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:ILE:HA	1:A:736:ASP:HB2	1.78	0.66
1:B:224:HIS:CD2	1:B:226:HIS:H	2.13	0.66
1:B:551:LEU:O	1:B:555:ILE:HG13	1.96	0.66
1:A:551:LEU:O	1:A:555:ILE:HG13	1.96	0.66
1:A:47:ARG:O	1:B:19:GLN:OE1	2.15	0.65
1:A:258:ASN:HB3	1:B:234:ASN:CA	2.25	0.65
1:A:739:LEU:HB3	1:A:742:ALA:HB3	1.77	0.65
1:B:183:GLY:HA3	1:B:193:PRO:HA	1.79	0.65
1:A:20:ARG:CA	1:B:47:ARG:HD3	2.24	0.65
1:A:267:LEU:HD22	1:B:238:PHE:CZ	2.32	0.65
1:B:739:LEU:HB3	1:B:742:ALA:HB3	1.77	0.65
1:A:115:LEU:HD12	2:C:2:GLC:C2	2.26	0.65
1:A:183:GLY:HA3	1:A:193:PRO:HA	1.78	0.65
1:A:228:PHE:HD2	1:B:158:PRO:HG3	1.60	0.65
1:A:533:LYS:HD3	1:A:539:LYS:HD3	1.79	0.65
1:A:765:THR:O	1:A:769:ILE:HG13	1.97	0.65
1:B:533:LYS:HD3	1:B:539:LYS:HD3	1.79	0.65
1:B:510:LEU:HD11	1:B:621:LEU:HD23	1.77	0.65
1:B:757:LEU:HG	1:B:764:TRP:HE3	1.60	0.65
1:A:258:ASN:N	1:B:234:ASN:OD1	2.29	0.65
1:B:730:ILE:HA	1:B:736:ASP:HB2	1.78	0.64
1:A:47:ARG:O	1:B:19:GLN:CD	2.40	0.64
1:A:236:GLY:HA2	1:B:261:HIS:NE2	2.12	0.64
1:A:246:ILE:HG21	1:B:239:LEU:HD12	1.80	0.63
1:B:707:LEU:HD21	1:B:741:MET:HE1	1.79	0.63
1:B:765:THR:O	1:B:769:ILE:HG13	1.97	0.63
1:A:360:VAL:HG11	1:A:404:VAL:HG21	1.80	0.63
1:A:707:LEU:HD21	1:A:741:MET:HE1	1.79	0.63
1:A:532:ILE:HG21	1:A:621:LEU:HD13	1.80	0.63
1:A:236:GLY:HA3	1:B:261:HIS:NE2	2.14	0.63
1:B:423:LEU:O	1:B:427:LEU:HD12	1.99	0.63
1:B:532:ILE:HG21	1:B:621:LEU:HD13	1.80	0.63
1:B:360:VAL:HG11	1:B:404:VAL:HG21	1.80	0.63
1:A:20:ARG:NH1	1:B:47:ARG:HH12	1.97	0.62
1:A:258:ASN:HB2	1:B:234:ASN:CG	2.23	0.62
1:A:423:LEU:O	1:A:427:LEU:HD12	1.99	0.62
1:B:53:LYS:HE2	1:B:54:PRO:HD2	1.81	0.62
1:A:16:ARG:HD3	1:B:44:GLU:HG2	1.79	0.62
1:A:20:ARG:HA	1:B:47:ARG:CD	2.25	0.62
1:A:542:HIS:CD2	1:A:542:HIS:H	2.18	0.62
1:B:433:PHE:HB2	1:B:444:PHE:HE2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:HIS:CD2	1:B:441:PRO:HA	2.35	0.62
1:A:16:ARG:HD3	1:B:44:GLU:CD	2.24	0.62
1:A:437:HIS:CD2	1:A:441:PRO:HA	2.34	0.62
1:B:587:ALA:O	1:B:591:VAL:HG13	2.00	0.62
1:A:258:ASN:HB3	1:B:234:ASN:HA	1.80	0.61
1:A:53:LYS:HE2	1:A:54:PRO:HD2	1.81	0.61
1:A:385:THR:O	1:A:387:PRO:HD3	2.00	0.61
1:B:667:LYS:HE3	1:B:777:MET:SD	2.40	0.61
1:A:47:ARG:HB3	1:B:19:GLN:HB3	1.82	0.61
1:A:667:LYS:HE3	1:A:777:MET:SD	2.40	0.61
1:B:385:THR:O	1:B:387:PRO:HD3	2.00	0.61
1:B:681:LYS:HE2	1:B:681:LYS:HA	1.83	0.61
1:A:20:ARG:CZ	1:B:47:ARG:HH12	2.14	0.61
1:A:173:GLU:OE1	1:B:32:ARG:HD3	2.01	0.61
1:A:433:PHE:HB2	1:A:444:PHE:HE2	1.64	0.61
1:A:261:HIS:HD2	1:A:263:ALA:HB3	1.66	0.60
1:A:267:LEU:HD21	1:B:233:PHE:CZ	2.35	0.60
1:A:587:ALA:O	1:A:591:VAL:HG13	2.00	0.60
1:B:547:ARG:CD	1:B:751:GLN:HG3	2.31	0.60
1:B:484:ILE:O	1:B:487:VAL:HG22	2.01	0.60
1:B:98:LEU:O	1:B:102:LEU:HG	2.02	0.60
1:B:542:HIS:H	1:B:542:HIS:CD2	2.18	0.60
1:A:267:LEU:HD22	1:B:238:PHE:CE1	2.37	0.60
1:A:547:ARG:CD	1:A:751:GLN:HG3	2.31	0.59
1:A:484:ILE:O	1:A:487:VAL:HG22	2.01	0.59
1:A:315:PRO:HA	1:A:318:LEU:HD12	1.85	0.59
1:B:261:HIS:HD2	1:B:263:ALA:HB3	1.65	0.59
1:B:686:ILE:HG22	1:B:691:TYR:HB2	1.85	0.59
1:B:691:TYR:OH	1:B:741:MET:HB2	2.03	0.59
1:A:691:TYR:OH	1:A:741:MET:HB2	2.03	0.59
1:B:91:LEU:HD12	1:B:98:LEU:HD13	1.84	0.59
1:A:420:VAL:HG23	1:A:639:SER:HB2	1.85	0.59
1:B:315:PRO:HA	1:B:318:LEU:HD12	1.85	0.59
1:A:655:GLY:O	1:A:675:ILE:HA	2.03	0.59
1:A:681:LYS:HE2	1:A:681:LYS:HA	1.83	0.59
1:A:686:ILE:HG22	1:A:691:TYR:HB2	1.85	0.59
1:A:91:LEU:HD12	1:A:98:LEU:HD13	1.84	0.58
1:B:181:ILE:HB	1:B:195:PHE:HB3	1.85	0.58
1:A:19:GLN:OE1	1:B:48:ALA:CA	2.50	0.58
1:A:181:ILE:HB	1:A:195:PHE:HB3	1.85	0.58
1:A:234:ASN:HA	1:B:258:ASN:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:GLY:O	1:B:675:ILE:HA	2.03	0.58
1:B:420:VAL:HG23	1:B:639:SER:HB2	1.85	0.58
1:A:98:LEU:O	1:A:102:LEU:HG	2.02	0.58
1:B:420:VAL:H	1:B:424:HIS:HD2	1.51	0.58
1:B:311:THR:HG21	1:B:406:MET:HE2	1.86	0.57
1:A:234:ASN:HA	1:B:258:ASN:HB2	1.87	0.57
1:A:420:VAL:H	1:A:424:HIS:HD2	1.51	0.57
1:A:739:LEU:N	1:A:739:LEU:HD23	2.20	0.57
1:A:373:GLU:O	1:A:377:ARG:HB2	2.05	0.57
1:A:657:LEU:HG	1:A:675:ILE:HG21	1.87	0.57
1:B:456:TRP:HA	1:B:460:CYS:SG	2.44	0.57
1:A:321:LEU:HD21	1:A:335:ILE:HD12	1.85	0.56
1:B:268:ARG:O	1:B:272:GLN:HG3	2.05	0.56
1:B:321:LEU:HD21	1:B:335:ILE:HD12	1.85	0.56
1:B:557:GLU:O	1:B:559:PRO:HD3	2.05	0.56
1:A:258:ASN:CB	1:B:234:ASN:C	2.72	0.56
1:A:456:TRP:HA	1:A:460:CYS:SG	2.44	0.56
1:B:640:GLY:O	1:B:644:MET:HE3	2.05	0.56
1:A:268:ARG:O	1:A:272:GLN:HG3	2.05	0.56
1:A:557:GLU:O	1:A:559:PRO:HD3	2.05	0.56
1:B:254:VAL:O	1:B:257:PRO:HD3	2.06	0.56
1:A:246:ILE:HD11	1:B:246:ILE:CD1	2.35	0.56
1:A:233:PHE:HE2	1:B:257:PRO:HB3	1.69	0.56
1:A:254:VAL:O	1:A:257:PRO:HD3	2.06	0.56
1:A:311:THR:HG21	1:A:406:MET:HE2	1.86	0.56
1:A:757:LEU:HG	1:A:764:TRP:CE3	2.41	0.56
1:B:739:LEU:N	1:B:739:LEU:HD23	2.20	0.56
1:A:228:PHE:HD2	1:B:158:PRO:CG	2.19	0.56
1:A:234:ASN:ND2	1:B:576:PRO:CB	2.69	0.56
1:A:166:TYR:HB3	1:A:169:PHE:CD2	2.41	0.56
1:A:316:GLU:HG2	1:A:367:HIS:HE1	1.71	0.56
1:B:373:GLU:O	1:B:377:ARG:HB2	2.05	0.56
1:B:115:LEU:HD21	1:B:306:ASN:CG	2.31	0.56
1:A:21:TYR:C	1:B:170:ARG:HG2	2.31	0.55
1:A:640:GLY:O	1:A:644:MET:HE3	2.05	0.55
1:B:166:TYR:HB3	1:B:169:PHE:CD2	2.41	0.55
1:B:498:LEU:HA	1:B:501:VAL:HG22	1.89	0.55
1:B:610:LEU:HD12	1:B:621:LEU:HD21	1.88	0.55
1:A:142:TYR:OH	1:B:227:PRO:CG	2.53	0.55
1:A:228:PHE:O	1:B:158:PRO:CG	2.50	0.55
1:A:261:HIS:NE2	1:B:236:GLY:HA2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:LEU:HA	1:B:325:HIS:HB2	1.89	0.55
1:A:20:ARG:CG	1:B:47:ARG:NH1	2.68	0.55
1:A:47:ARG:CD	1:B:20:ARG:HA	2.30	0.55
1:A:703:LEU:HD21	1:A:741:MET:SD	2.46	0.55
1:B:316:GLU:HG2	1:B:367:HIS:HE1	1.71	0.55
1:B:703:LEU:HD21	1:B:741:MET:SD	2.46	0.55
1:A:321:LEU:HA	1:A:325:HIS:HB2	1.89	0.55
1:B:757:LEU:HG	1:B:764:TRP:CE3	2.41	0.55
1:A:16:ARG:NH1	1:B:16:ARG:HH11	2.05	0.55
1:A:115:LEU:HD21	1:A:306:ASN:CG	2.31	0.55
1:A:236:GLY:HA3	1:B:261:HIS:CD2	2.42	0.55
1:A:444:PHE:N	1:A:444:PHE:CD1	2.74	0.54
1:B:433:PHE:HB2	1:B:444:PHE:CE2	2.42	0.54
1:B:580:LEU:HD21	1:B:726:MET:HA	1.89	0.54
1:B:657:LEU:HG	1:B:675:ILE:HG21	1.87	0.54
1:A:47:ARG:NH1	1:B:20:ARG:CG	2.68	0.54
1:A:261:HIS:NE2	1:B:236:GLY:N	2.54	0.54
1:A:580:LEU:HD21	1:A:726:MET:HA	1.89	0.54
1:A:729:SER:HA	1:A:734:GLY:HA3	1.90	0.54
1:B:420:VAL:HB	1:B:449:ASN:ND2	2.22	0.54
1:A:234:ASN:O	1:B:258:ASN:CG	2.50	0.54
1:A:433:PHE:HB2	1:A:444:PHE:CE2	2.42	0.54
1:A:261:HIS:HE1	1:B:234:ASN:O	1.88	0.54
1:B:444:PHE:N	1:B:444:PHE:CD1	2.74	0.54
1:B:534:ARG:HG2	1:B:573:LYS:HD3	1.90	0.54
1:A:733:GLN:CD	1:A:733:GLN:H	2.16	0.54
1:B:433:PHE:HB3	1:B:436:TYR:HB2	1.90	0.54
1:A:33:GLN:HE22	1:B:172:ASN:CG	2.15	0.54
1:B:455:ARG:HA	1:B:459:GLN:HB3	1.90	0.54
1:A:455:ARG:HA	1:A:459:GLN:HB3	1.90	0.54
1:A:234:ASN:O	1:B:258:ASN:CB	2.56	0.54
1:A:117:ARG:HD3	1:A:456:TRP:HZ2	1.73	0.54
1:A:498:LEU:HA	1:A:501:VAL:HG22	1.89	0.54
1:A:47:ARG:HD3	1:B:20:ARG:CA	2.33	0.53
1:A:270:MET:HG2	1:A:363:LEU:HD21	1.90	0.53
1:A:420:VAL:HB	1:A:449:ASN:ND2	2.22	0.53
1:A:610:LEU:HD12	1:A:621:LEU:HD21	1.88	0.53
1:A:267:LEU:HD21	1:B:233:PHE:CE2	2.44	0.53
1:B:1:SER:O	1:B:2:GLN:HG2	2.09	0.53
1:B:729:SER:HA	1:B:734:GLY:HA3	1.90	0.53
1:A:172:ASN:ND2	1:B:23:LEU:HD21	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ARG:HG2	1:A:573:LYS:HD3	1.90	0.52
1:B:270:MET:HG2	1:B:363:LEU:HD21	1.90	0.52
1:B:733:GLN:CD	1:B:733:GLN:H	2.16	0.52
1:B:293:GLU:HG2	1:B:295:HIS:H	1.74	0.52
1:B:117:ARG:HD3	1:B:456:TRP:HZ2	1.73	0.52
1:A:23:LEU:HD21	1:B:172:ASN:HD21	1.73	0.52
1:A:293:GLU:HB3	1:A:296:GLU:HG2	1.92	0.52
1:A:424:HIS:O	1:A:428:VAL:HG23	2.10	0.52
1:A:287:HIS:CE1	1:A:297:LEU:HA	2.45	0.52
1:B:447:VAL:HG11	1:B:787:TYR:CD2	2.44	0.52
1:A:1:SER:O	1:A:2:GLN:HG2	2.09	0.52
1:B:150:VAL:HG23	1:B:155:VAL:HG21	1.92	0.52
1:A:293:GLU:HG2	1:A:295:HIS:H	1.74	0.52
1:A:433:PHE:HB3	1:A:436:TYR:HB2	1.90	0.52
1:B:424:HIS:O	1:B:428:VAL:HG23	2.10	0.52
1:A:576:PRO:CB	1:B:234:ASN:ND2	2.73	0.52
1:B:783:SER:O	1:B:787:TYR:HD2	1.93	0.52
1:A:48:ALA:CA	1:B:19:GLN:OE1	2.56	0.51
1:A:783:SER:O	1:A:787:TYR:HD2	1.93	0.51
1:A:140:TYR:CE2	1:A:255:LEU:HG	2.45	0.51
1:B:140:TYR:CE2	1:B:255:LEU:HG	2.45	0.51
1:A:20:ARG:CZ	1:B:47:ARG:NH1	2.73	0.51
1:B:453:PRO:HB3	1:B:480:LEU:HD13	1.91	0.51
1:A:2:GLN:HG3	1:A:52:ALA:HB2	1.92	0.51
1:A:16:ARG:CZ	1:B:16:ARG:NH1	2.73	0.51
1:A:230:LEU:HD12	1:B:156:GLU:HB3	1.92	0.51
1:A:453:PRO:HB3	1:A:480:LEU:HD13	1.91	0.51
1:A:44:GLU:CG	1:B:16:ARG:HD3	2.41	0.51
1:B:363:LEU:O	1:B:364:LEU:HD13	2.11	0.51
1:A:16:ARG:HH11	1:B:16:ARG:HH11	1.58	0.51
1:A:72:ARG:O	1:A:455:ARG:NH2	2.44	0.51
1:A:447:VAL:HG11	1:A:787:TYR:CD2	2.44	0.51
1:B:287:HIS:CE1	1:B:297:LEU:HA	2.45	0.51
1:B:364:LEU:HB3	1:B:367:HIS:CD2	2.46	0.51
1:B:547:ARG:HD2	1:B:751:GLN:HG3	1.93	0.51
1:A:517:ARG:NH2	1:A:610:LEU:HB3	2.26	0.51
1:A:547:ARG:HD2	1:A:751:GLN:HG3	1.93	0.51
1:A:5:PHE:CD2	1:A:86:ASP:HB3	2.46	0.50
1:A:47:ARG:HH12	1:B:20:ARG:CZ	2.23	0.50
1:A:150:VAL:HG23	1:A:155:VAL:HG21	1.92	0.50
1:A:239:LEU:HD12	1:B:246:ILE:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LEU:HB3	1:A:367:HIS:CD2	2.46	0.50
1:B:72:ARG:O	1:B:455:ARG:NH2	2.44	0.50
1:B:536:HIS:HB3	1:B:539:LYS:HG3	1.93	0.50
1:B:293:GLU:HB3	1:B:296:GLU:HG2	1.92	0.50
1:A:44:GLU:HG2	1:B:16:ARG:HD3	1.92	0.50
1:A:534:ARG:O	1:A:539:LYS:HD2	2.11	0.50
1:A:141:GLN:HG3	1:A:142:TYR:CD2	2.46	0.50
1:A:293:GLU:CD	1:A:295:HIS:HB2	2.37	0.50
1:B:5:PHE:CD2	1:B:86:ASP:HB3	2.46	0.50
1:B:141:GLN:HG3	1:B:142:TYR:CD2	2.46	0.50
1:B:566:ARG:HD2	1:B:568:PHE:CZ	2.47	0.50
1:A:67:GLU:O	1:A:116:GLY:HA2	2.12	0.50
1:A:228:PHE:CZ	1:B:254:VAL:CG2	2.95	0.50
1:A:576:PRO:HG2	1:B:234:ASN:HD21	1.77	0.50
1:B:2:GLN:HG3	1:B:52:ALA:HB2	1.92	0.50
1:B:138:LEU:HD21	1:B:275:GLN:HB2	1.93	0.50
1:B:318:LEU:HG	1:B:336:THR:HG21	1.93	0.50
1:A:472:LEU:HD21	1:A:486:LEU:HG	1.93	0.50
1:B:293:GLU:CD	1:B:295:HIS:HB2	2.37	0.50
1:B:517:ARG:NH2	1:B:610:LEU:HB3	2.26	0.50
1:A:185:VAL:HA	1:A:191:TRP:HA	1.94	0.50
1:A:228:PHE:CD2	1:B:158:PRO:HG3	2.45	0.50
1:B:423:LEU:H	1:B:423:LEU:CD2	2.23	0.50
1:A:32:ARG:HB3	1:B:173:GLU:CD	2.37	0.50
1:A:363:LEU:O	1:A:364:LEU:HD13	2.11	0.50
1:A:536:HIS:HB3	1:A:539:LYS:HG3	1.93	0.50
1:B:7:ASP:O	1:B:11:GLN:HG2	2.12	0.50
1:B:534:ARG:O	1:B:539:LYS:HD2	2.11	0.49
1:A:170:ARG:HD2	1:B:22:GLY:N	2.27	0.49
1:A:566:ARG:HD2	1:A:568:PHE:CZ	2.47	0.49
1:B:472:LEU:HD21	1:B:486:LEU:HG	1.93	0.49
1:A:138:LEU:HD21	1:A:275:GLN:HB2	1.93	0.49
1:A:234:ASN:ND2	1:B:576:PRO:HB3	2.27	0.49
1:B:337:SER:HA	1:B:413:GLY:O	2.13	0.49
1:A:234:ASN:O	1:B:258:ASN:HB3	2.13	0.49
1:A:246:ILE:CD1	1:B:246:ILE:HD11	2.38	0.49
1:B:67:GLU:O	1:B:116:GLY:HA2	2.12	0.49
1:B:354:ARG:HA	1:B:404:VAL:O	2.13	0.49
1:A:19:GLN:CD	1:B:48:ALA:HA	2.36	0.49
1:A:33:GLN:NE2	1:B:172:ASN:OD1	2.46	0.49
1:A:318:LEU:HG	1:A:336:THR:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:LEU:H	1:A:423:LEU:CD2	2.23	0.49
1:A:7:ASP:O	1:A:11:GLN:HG2	2.12	0.49
1:A:258:ASN:HB2	1:B:234:ASN:HA	1.86	0.49
1:B:185:VAL:HA	1:B:191:TRP:HA	1.94	0.49
1:B:535:LEU:HD13	1:B:585:ILE:CG1	2.41	0.49
1:A:234:ASN:CA	1:B:258:ASN:HB2	2.42	0.49
1:B:668:VAL:HG11	1:B:771:ASN:OD1	2.13	0.49
1:B:15:SER:HA	1:B:18:TRP:NE1	2.28	0.48
1:B:77:ASN:O	1:B:81:LEU:HG	2.14	0.48
1:B:407:ALA:O	1:B:411:VAL:HG23	2.13	0.48
1:B:681:LYS:HE2	1:B:681:LYS:CA	2.43	0.48
1:A:77:ASN:O	1:A:81:LEU:HG	2.13	0.48
1:A:230:LEU:HD13	1:B:156:GLU:HB3	1.93	0.48
1:A:261:HIS:CE1	1:B:236:GLY:N	2.80	0.48
1:A:681:LYS:HE2	1:A:681:LYS:CA	2.43	0.48
1:A:15:SER:HA	1:A:18:TRP:NE1	2.28	0.48
1:A:317:LEU:HD23	1:A:336:THR:HG22	1.96	0.48
1:A:342:TYR:HB2	1:A:410:CYS:HB3	1.96	0.48
1:A:668:VAL:HG11	1:A:771:ASN:OD1	2.13	0.48
1:A:242:GLU:OE2	1:B:253:LYS:CE	2.60	0.48
1:A:713:GLY:HA2	1:A:716:SER:OG	2.14	0.48
1:A:583:ASN:HD21	1:A:723:PHE:HA	1.79	0.48
1:B:583:ASN:HD21	1:B:723:PHE:HA	1.79	0.48
1:B:697:ARG:NH2	1:B:707:LEU:HB3	2.29	0.48
1:A:2:GLN:HE22	1:A:50:PRO:HB2	1.79	0.48
1:A:267:LEU:CD2	1:B:238:PHE:CE1	2.97	0.48
1:A:407:ALA:O	1:A:411:VAL:HG23	2.13	0.48
1:B:342:TYR:HB2	1:B:410:CYS:HB3	1.96	0.48
1:A:354:ARG:HA	1:A:404:VAL:O	2.13	0.48
1:A:47:ARG:NH1	1:B:20:ARG:CZ	2.76	0.47
1:A:337:SER:HA	1:A:413:GLY:O	2.13	0.47
1:A:257:PRO:HB3	1:B:233:PHE:CE2	2.49	0.47
1:A:363:LEU:C	1:A:364:LEU:HD13	2.39	0.47
1:B:317:LEU:HD23	1:B:336:THR:HG22	1.96	0.47
1:B:542:HIS:H	1:B:542:HIS:HD2	1.59	0.47
1:A:542:HIS:H	1:A:542:HIS:HD2	1.59	0.47
1:B:36:LEU:HD23	1:B:167:PRO:HG3	1.96	0.47
1:B:421:ALA:C	1:B:446:ASN:HD21	2.22	0.47
1:A:36:LEU:HD23	1:A:167:PRO:HG3	1.97	0.47
1:A:145:PHE:CB	1:B:230:LEU:CD1	2.90	0.47
1:A:421:ALA:C	1:A:446:ASN:HD21	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:713:GLY:HA2	1:B:716:SER:OG	2.14	0.47
1:A:117:ARG:HG2	5:A:999:PLP:C4A	2.45	0.47
1:A:697:ARG:NH2	1:A:707:LEU:HB3	2.29	0.47
1:B:363:LEU:C	1:B:364:LEU:HD13	2.39	0.47
1:B:423:LEU:HD22	1:B:423:LEU:N	2.26	0.47
1:B:523:ASN:O	1:B:528:PHE:HE1	1.98	0.47
1:A:23:LEU:HD21	1:B:172:ASN:HD22	1.77	0.47
1:B:43:ALA:O	1:B:47:ARG:HG3	2.15	0.47
1:B:540:ARG:HA	1:B:542:HIS:CD2	2.50	0.47
1:B:692:ASP:HB3	1:B:695:LYS:HE2	1.97	0.47
1:B:2:GLN:HE22	1:B:50:PRO:HB2	1.79	0.47
1:B:117:ARG:HG2	5:B:999:PLP:C4A	2.45	0.47
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.71	0.47
1:A:311:THR:HG23	1:A:410:CYS:SG	2.55	0.47
1:A:426:ASP:O	1:A:430:LYS:HG2	2.15	0.47
1:A:540:ARG:HA	1:A:542:HIS:CD2	2.50	0.46
1:A:148:SER:OG	1:A:155:VAL:HB	2.15	0.46
1:A:523:ASN:O	1:A:528:PHE:HE1	1.98	0.46
1:A:170:ARG:HD2	1:B:22:GLY:CA	2.45	0.46
1:A:258:ASN:HD22	1:B:234:ASN:HB3	1.81	0.46
1:B:311:THR:HG23	1:B:410:CYS:SG	2.55	0.46
1:B:346:THR:HA	1:B:638:ALA:HB2	1.98	0.46
1:A:532:ILE:O	1:A:532:ILE:HG13	2.16	0.46
1:A:642:GLY:HA2	1:A:645:LYS:HD2	1.98	0.46
1:A:227:PRO:HG2	1:B:142:TYR:OH	2.15	0.46
1:A:480:LEU:HD22	1:A:779:SER:HB2	1.98	0.46
1:B:2:GLN:HB2	1:B:212:GLY:HA3	1.98	0.46
1:B:129:VAL:HG13	1:B:785:ARG:CZ	2.46	0.46
1:A:354:ARG:HD3	1:A:403:GLN:OE1	2.15	0.46
1:B:654:VAL:HG11	1:B:751:GLN:NE2	2.31	0.46
1:A:2:GLN:HB2	1:A:212:GLY:HA3	1.98	0.46
1:A:692:ASP:HB3	1:A:695:LYS:HE2	1.97	0.46
1:B:148:SER:OG	1:B:155:VAL:HB	2.15	0.46
1:B:224:HIS:HD2	1:B:226:HIS:C	2.24	0.46
1:B:266:LYS:HG2	1:B:270:MET:HE2	1.98	0.46
1:B:354:ARG:HD3	1:B:403:GLN:OE1	2.15	0.46
1:B:426:ASP:O	1:B:430:LYS:HG2	2.15	0.46
1:B:480:LEU:CD2	1:B:779:SER:HB2	2.46	0.46
1:A:158:PRO:HG3	1:B:228:PHE:O	2.10	0.46
1:B:338:LYS:HE2	1:B:338:LYS:HB3	1.77	0.46
1:A:115:LEU:HD21	1:A:306:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:LYS:HE2	1:A:681:LYS:O	2.16	0.46
1:A:43:ALA:O	1:A:47:ARG:HG3	2.15	0.45
1:A:246:ILE:CD1	1:B:239:LEU:HD12	2.46	0.45
1:A:390:GLU:HG2	1:A:394:ALA:HB2	1.98	0.45
1:A:405:HIS:N	1:A:405:HIS:CD2	2.84	0.45
1:B:480:LEU:HD22	1:B:779:SER:HB2	1.98	0.45
1:B:681:LYS:HE2	1:B:681:LYS:O	2.16	0.45
1:A:397:ALA:O	1:A:400:HIS:ND1	2.49	0.45
1:B:209:TYR:OH	1:B:458:LYS:HE2	2.16	0.45
1:A:16:ARG:NH1	1:B:16:ARG:CZ	2.79	0.45
1:A:129:VAL:HG13	1:A:785:ARG:CZ	2.46	0.45
1:A:423:LEU:HD22	1:A:423:LEU:N	2.26	0.45
1:B:356:ASP:HA	1:B:403:GLN:HG2	1.98	0.45
1:B:532:ILE:O	1:B:532:ILE:HG13	2.16	0.45
1:A:480:LEU:CD2	1:A:779:SER:HB2	2.46	0.45
1:A:654:VAL:HG11	1:A:751:GLN:NE2	2.31	0.45
1:B:221:GLN:HA	1:B:252:THR:HG21	1.99	0.45
1:A:209:TYR:OH	1:A:458:LYS:HE2	2.16	0.45
1:A:224:HIS:HD2	1:A:226:HIS:C	2.24	0.45
1:A:221:GLN:HA	1:A:252:THR:HG21	1.99	0.45
1:B:390:GLU:HG2	1:B:394:ALA:HB2	1.98	0.45
1:A:228:PHE:HZ	1:B:254:VAL:HG21	1.81	0.45
1:A:19:GLN:CG	1:B:47:ARG:O	2.62	0.45
1:A:406:MET:HA	1:A:406:MET:CE	2.47	0.45
1:B:115:LEU:HD21	1:B:306:ASN:ND2	2.31	0.45
1:B:144:LEU:HD23	1:B:144:LEU:HA	1.71	0.45
1:B:405:HIS:CD2	1:B:405:HIS:N	2.84	0.45
1:A:234:ASN:HA	1:B:258:ASN:HB3	1.98	0.45
1:B:406:MET:CE	1:B:406:MET:HA	2.47	0.45
1:B:642:GLY:HA2	1:B:645:LYS:HD2	1.98	0.45
1:A:141:GLN:HG3	1:A:142:TYR:CE2	2.52	0.45
1:A:166:TYR:HA	1:A:167:PRO:HD3	1.75	0.45
1:A:267:LEU:CD2	1:B:238:PHE:CZ	3.00	0.45
1:A:346:THR:HA	1:A:638:ALA:HB2	1.98	0.45
1:A:356:ASP:HA	1:A:403:GLN:HG2	1.98	0.45
1:A:406:MET:HE2	1:A:406:MET:HA	1.99	0.45
1:B:141:GLN:HG3	1:B:142:TYR:CE2	2.52	0.45
1:B:542:HIS:CD2	1:B:542:HIS:N	2.85	0.45
1:B:545:LEU:HD23	1:B:726:MET:HE1	1.98	0.45
1:A:535:LEU:HD13	1:A:585:ILE:CG1	2.41	0.44
1:B:266:LYS:HE3	1:B:363:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:ALA:O	1:B:400:HIS:CE1	2.70	0.44
1:B:397:ALA:O	1:B:400:HIS:ND1	2.49	0.44
1:A:627:ILE:HG23	1:A:654:VAL:HG23	2.00	0.44
1:A:30:THR:CG2	1:B:174:ALA:HB2	2.47	0.44
1:A:338:LYS:HB3	1:A:338:LYS:HE2	1.77	0.44
1:A:1:SER:N	1:A:210:ARG:O	2.47	0.44
1:B:396:LEU:HD21	1:B:435:GLU:HG3	1.99	0.44
1:B:563:ARG:HH12	1:B:752:LYS:HA	1.82	0.44
1:A:266:LYS:HG2	1:A:270:MET:HE2	1.98	0.44
1:A:563:ARG:HH12	1:A:752:LYS:HA	1.82	0.44
1:B:408:ASN:O	1:B:412:VAL:HG23	2.18	0.44
1:B:480:LEU:O	1:B:483:LEU:HD13	2.18	0.44
1:A:257:PRO:HB3	1:B:233:PHE:HE2	1.81	0.44
1:A:338:LYS:HE3	1:A:796:ARG:HB3	2.00	0.44
1:A:396:LEU:HD21	1:A:435:GLU:HG3	1.99	0.44
1:A:51:PHE:HD1	1:A:51:PHE:H	1.66	0.44
1:A:408:ASN:O	1:A:412:VAL:HG23	2.18	0.44
1:B:29:MET:HE3	1:B:34:TRP:CD2	2.52	0.44
1:B:517:ARG:HH21	1:B:610:LEU:HB3	1.82	0.44
1:A:510:LEU:O	1:A:514:VAL:HG23	2.18	0.44
1:A:545:LEU:HD23	1:A:726:MET:HE1	1.98	0.44
1:B:166:TYR:HB3	1:B:169:PHE:HD2	1.83	0.44
1:B:287:HIS:HE1	1:B:300:TYR:CD2	2.36	0.44
1:A:179:VAL:HG21	1:A:274:PHE:HD1	1.83	0.43
1:A:397:ALA:O	1:A:400:HIS:CE1	2.70	0.43
1:A:546:LEU:HD12	1:A:546:LEU:HA	1.81	0.43
1:A:574:ALA:HB2	1:A:585:ILE:HD11	2.00	0.43
1:A:234:ASN:CB	1:B:258:ASN:HB2	2.48	0.43
1:A:266:LYS:HE3	1:A:363:LEU:HD13	1.99	0.43
1:B:65:SER:O	1:B:275:GLN:NE2	2.50	0.43
1:B:179:VAL:HG21	1:B:274:PHE:HD1	1.83	0.43
1:B:220:TRP:CE2	1:B:278:CYS:HB3	2.53	0.43
1:B:451:ILE:HD12	1:B:456:TRP:HB2	1.99	0.43
1:A:30:THR:HG21	1:B:174:ALA:HB2	2.00	0.43
1:A:65:SER:HB3	1:A:68:PHE:CE1	2.53	0.43
1:A:228:PHE:CZ	1:B:254:VAL:HG21	2.53	0.43
1:B:744:PHE:O	1:B:748:VAL:HG23	2.19	0.43
1:A:29:MET:HE3	1:A:34:TRP:CD2	2.52	0.43
1:A:173:GLU:OE2	1:B:32:ARG:HB3	2.18	0.43
1:A:220:TRP:CE2	1:A:278:CYS:HB3	2.53	0.43
1:A:233:PHE:CE2	1:B:257:PRO:HB3	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:HIS:HE1	1:A:300:TYR:CD2	2.36	0.43
1:B:406:MET:HE2	1:B:406:MET:HA	1.99	0.43
1:B:446:ASN:O	1:B:790:ARG:NH1	2.51	0.43
1:A:230:LEU:HD11	1:B:145:PHE:CB	2.46	0.43
1:A:540:ARG:HD2	1:A:740:VAL:HG22	2.01	0.43
1:A:732:LYS:HG3	1:A:733:GLN:N	2.34	0.43
1:B:123:LEU:HD21	1:B:217:LEU:HD13	2.00	0.43
1:B:338:LYS:HE3	1:B:796:ARG:HB3	2.00	0.43
1:A:21:TYR:C	1:B:170:ARG:CG	2.91	0.43
1:A:456:TRP:C	1:A:460:CYS:SG	3.01	0.43
1:B:456:TRP:C	1:B:460:CYS:SG	3.01	0.43
1:B:562:ASP:O	1:B:759:ARG:NH2	2.52	0.43
1:B:574:ALA:HB2	1:B:585:ILE:HD11	2.00	0.43
1:B:622:ILE:HB	1:B:623:PRO:HD3	2.01	0.43
1:A:234:ASN:CA	1:B:258:ASN:CB	2.96	0.43
1:A:562:ASP:O	1:A:759:ARG:NH2	2.52	0.43
1:A:635:GLY:H	1:A:658:ASP:CG	2.27	0.43
1:B:30:THR:OG1	1:B:33:GLN:HG3	2.19	0.43
1:B:421:ALA:C	1:B:446:ASN:ND2	2.77	0.43
1:B:635:GLY:H	1:B:658:ASP:CG	2.27	0.43
1:A:321:LEU:CD2	1:A:335:ILE:HD12	2.49	0.43
1:B:65:SER:HB3	1:B:68:PHE:CE1	2.53	0.43
1:B:627:ILE:HG23	1:B:654:VAL:HG23	2.00	0.43
1:A:451:ILE:HD12	1:A:456:TRP:HB2	1.99	0.43
1:B:51:PHE:HD1	1:B:51:PHE:H	1.66	0.43
1:B:179:VAL:HG21	1:B:274:PHE:CD1	2.54	0.43
1:B:510:LEU:O	1:B:514:VAL:HG23	2.18	0.43
1:B:784:ILE:O	1:B:788:GLN:HG3	2.19	0.43
1:B:390:GLU:O	1:B:392:VAL:N	2.52	0.42
1:B:728:HIS:CG	1:B:733:GLN:HG3	2.54	0.42
1:A:16:ARG:HH11	1:B:16:ARG:CD	2.32	0.42
1:A:20:ARG:NH1	1:B:40:GLU:CD	2.72	0.42
1:A:150:VAL:CG2	1:A:155:VAL:HG21	2.49	0.42
1:A:480:LEU:O	1:A:483:LEU:HD13	2.18	0.42
1:A:517:ARG:HH21	1:A:610:LEU:HB3	1.82	0.42
1:B:141:GLN:HB3	1:B:163:ARG:CZ	2.49	0.42
1:B:144:LEU:CD1	1:B:573:LYS:HE3	2.42	0.42
1:B:533:LYS:HB3	1:B:533:LYS:HE2	1.75	0.42
1:A:30:THR:OG1	1:A:33:GLN:HG3	2.19	0.42
1:A:145:PHE:CB	1:B:230:LEU:HD12	2.49	0.42
1:A:370:ILE:O	1:A:374:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:TRP:C	1:A:395:LYS:H	2.26	0.42
1:A:726:MET:HG3	1:A:727:LEU:N	2.34	0.42
1:A:728:HIS:CG	1:A:733:GLN:HG3	2.54	0.42
1:A:744:PHE:O	1:A:748:VAL:HG23	2.19	0.42
1:B:393:TRP:C	1:B:395:LYS:H	2.26	0.42
1:B:585:ILE:HG23	1:B:609:PHE:CE2	2.55	0.42
1:B:726:MET:HG3	1:B:727:LEU:N	2.34	0.42
1:A:233:PHE:HE2	1:B:257:PRO:CB	2.33	0.42
1:B:540:ARG:HD2	1:B:740:VAL:HG22	2.00	0.42
1:B:695:LYS:O	1:B:699:LYS:HG2	2.20	0.42
1:A:390:GLU:O	1:A:392:VAL:N	2.52	0.42
1:A:585:ILE:HG23	1:A:609:PHE:CE2	2.55	0.42
1:A:234:ASN:OD1	1:B:258:ASN:HB2	2.19	0.42
1:A:547:ARG:HH22	1:A:551:LEU:CB	2.28	0.42
1:A:784:ILE:O	1:A:788:GLN:HG3	2.19	0.42
1:B:622:ILE:HD13	1:B:645:LYS:CB	2.49	0.42
1:B:739:LEU:CB	1:B:742:ALA:HB3	2.45	0.42
1:A:16:ARG:CD	1:B:44:GLU:CG	2.92	0.42
1:A:123:LEU:HD21	1:A:217:LEU:HD13	2.00	0.42
1:A:316:GLU:O	1:A:320:VAL:HG23	2.20	0.42
1:A:421:ALA:C	1:A:446:ASN:ND2	2.77	0.42
1:B:255:LEU:HD22	1:B:256:TYR:CG	2.55	0.42
1:B:370:ILE:O	1:B:374:ILE:HG13	2.19	0.42
1:A:128:THR:HG23	1:A:209:TYR:HB3	2.01	0.42
1:A:166:TYR:HB3	1:A:169:PHE:HD2	1.83	0.42
1:A:739:LEU:CB	1:A:742:ALA:HB3	2.45	0.42
1:A:92:LYS:HA	1:A:92:LYS:HE3	2.02	0.42
1:A:141:GLN:HB3	1:A:163:ARG:CZ	2.49	0.42
1:A:622:ILE:HD13	1:A:645:LYS:CB	2.49	0.42
1:A:707:LEU:HD12	1:A:707:LEU:HA	1.87	0.42
1:B:128:THR:HG23	1:B:209:TYR:HB3	2.01	0.42
1:B:732:LYS:HG3	1:B:733:GLN:N	2.33	0.42
1:B:762:GLU:O	1:B:766:ARG:HG3	2.20	0.42
1:A:44:GLU:CD	1:B:16:ARG:HD3	2.45	0.42
1:A:691:TYR:HH	1:A:741:MET:HB2	1.85	0.42
1:A:694:VAL:O	1:A:698:LYS:HG2	2.20	0.42
1:B:297:LEU:C	1:B:297:LEU:HD23	2.45	0.42
1:A:446:ASN:O	1:A:790:ARG:NH1	2.51	0.41
1:A:549:LEU:HD23	1:A:549:LEU:HA	1.93	0.41
1:A:622:ILE:HB	1:A:623:PRO:HD3	2.01	0.41
1:A:712:SER:OG	1:A:714:LYS:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LYS:HE3	1:B:92:LYS:HA	2.02	0.41
1:A:179:VAL:HG21	1:A:274:PHE:CD1	2.54	0.41
1:A:255:LEU:HD22	1:A:256:TYR:CG	2.55	0.41
1:B:150:VAL:CG2	1:B:155:VAL:HG21	2.49	0.41
1:B:316:GLU:O	1:B:320:VAL:HG23	2.20	0.41
1:A:115:LEU:HD21	1:A:306:ASN:OD1	2.20	0.41
1:B:147:GLN:HG3	1:B:154:GLN:HG3	2.01	0.41
1:A:121:CYS:O	1:A:124:ASP:HB3	2.21	0.41
1:A:147:GLN:HG3	1:A:154:GLN:HG3	2.01	0.41
1:A:695:LYS:O	1:A:699:LYS:HG2	2.20	0.41
1:B:657:LEU:HD23	1:B:657:LEU:HA	1.91	0.41
1:B:777:MET:HE2	1:B:778:PHE:CE1	2.55	0.41
1:A:5:PHE:CE2	1:A:86:ASP:HB3	2.55	0.41
1:A:547:ARG:NH2	1:A:551:LEU:HB2	2.32	0.41
1:A:652:LEU:HD23	1:A:764:TRP:CZ2	2.56	0.41
1:B:115:LEU:HD21	1:B:306:ASN:OD1	2.20	0.41
1:B:486:LEU:O	1:B:489:LEU:N	2.54	0.41
1:A:425:SER:O	1:A:428:VAL:HB	2.20	0.41
1:B:5:PHE:CE2	1:B:86:ASP:HB3	2.55	0.41
1:A:680:VAL:O	1:A:684:LYS:HG3	2.20	0.41
1:B:712:SER:OG	1:B:714:LYS:HB2	2.20	0.41
1:A:22:GLY:CA	1:B:170:ARG:CD	2.93	0.41
1:A:762:GLU:O	1:A:766:ARG:HG3	2.20	0.41
1:A:777:MET:HE2	1:A:778:PHE:CE1	2.55	0.41
1:A:16:ARG:CD	1:B:44:GLU:CD	2.92	0.41
1:A:88:GLN:O	1:A:92:LYS:HD2	2.21	0.41
1:A:529:ASP:O	1:A:568:PHE:HA	2.21	0.41
1:B:261:HIS:CD2	1:B:263:ALA:HB3	2.52	0.41
1:B:610:LEU:HD23	1:B:610:LEU:HA	1.95	0.41
1:A:16:ARG:CG	1:B:44:GLU:HG3	2.51	0.41
1:A:115:LEU:CD1	2:C:2:GLC:H2	2.43	0.41
1:A:261:HIS:CD2	1:A:263:ALA:HB3	2.52	0.41
1:A:297:LEU:HD23	1:A:297:LEU:C	2.45	0.41
1:B:144:LEU:HD23	1:B:255:LEU:O	2.21	0.41
1:A:22:GLY:N	1:B:170:ARG:CD	2.72	0.40
1:A:258:ASN:O	1:A:264:GLY:HA3	2.21	0.40
1:A:739:LEU:HB3	1:A:742:ALA:CB	2.50	0.40
1:B:88:GLN:O	1:B:92:LYS:HD2	2.21	0.40
1:B:258:ASN:O	1:B:264:GLY:HA3	2.21	0.40
1:B:447:VAL:HG13	1:B:786:ASP:CB	2.51	0.40
1:B:694:VAL:O	1:B:698:LYS:HG2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:GLY:HA2	1:B:170:ARG:HD2	1.98	0.40
1:B:121:CYS:O	1:B:124:ASP:HB3	2.21	0.40
1:B:425:SER:O	1:B:428:VAL:HB	2.20	0.40
1:B:652:LEU:HD23	1:B:764:TRP:CZ2	2.56	0.40
1:B:680:VAL:O	1:B:684:LYS:HG3	2.20	0.40
1:A:6:ASN:OD1	1:A:8:LYS:HB3	2.21	0.40
1:A:452:THR:HA	1:A:453:PRO:HD2	1.89	0.40
3:A:997:SO4:O3	2:C:2:GLC:H61	2.21	0.40
1:A:129:VAL:O	1:A:129:VAL:CG1	2.69	0.40
1:A:144:LEU:HD23	1:A:255:LEU:O	2.21	0.40
1:A:144:LEU:CD1	1:A:573:LYS:HE3	2.42	0.40
1:A:224:HIS:CD2	1:A:226:HIS:N	2.85	0.40
1:A:486:LEU:O	1:A:489:LEU:N	2.54	0.40
1:A:542:HIS:CD2	1:A:542:HIS:N	2.85	0.40
1:B:268:ARG:HA	1:B:271:GLN:OE1	2.21	0.40
1:B:429:VAL:O	1:B:434:PRO:HA	2.21	0.40
1:A:507:LYS:HA	1:A:624:ALA:HB1	2.04	0.40
1:B:115:LEU:CD1	2:D:2:GLC:H2	2.43	0.40
1:B:129:VAL:O	1:B:129:VAL:CG1	2.69	0.40
1:B:443:LYS:O	1:B:445:HIS:CD2	2.75	0.40
1:B:546:LEU:HD12	1:B:546:LEU:HA	1.81	0.40

All (12) 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:600:LEU:CD2	1:A:714:LYS:CE[2_555]	0.84	1.36
1:A:600:LEU:CD2	1:A:714:LYS:NZ[2_555]	1.14	1.06
1:A:85:GLN:OE1	1:B:474:LYS:NZ[4_546]	1.22	0.98
1:A:85:GLN:CD	1:B:474:LYS:NZ[4_546]	1.50	0.70
1:A:689:LYS:NZ	1:B:685:ALA:CA[1_545]	1.61	0.59
1:A:474:LYS:NZ	1:B:2:GLN:OE1[4_546]	1.62	0.58
1:A:689:LYS:NZ	1:B:685:ALA:CB[1_545]	1.69	0.51
1:B:235:ASP:OD2	1:B:732:LYS:NZ[4_545]	1.81	0.39
1:A:85:GLN:NE2	1:B:474:LYS:NZ[4_546]	1.87	0.33
1:A:473:GLN:CD	1:B:2:GLN:O[4_546]	1.99	0.21
1:A:473:GLN:NE2	1:B:2:GLN:O[4_546]	2.08	0.12
1:A:600:LEU:CG	1:A:714:LYS:NZ[2_555]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	794/797 (100%)	716 (90%)	68 (9%)	10 (1%)	9	38
1	B	794/797 (100%)	717 (90%)	68 (9%)	9 (1%)	11	43
All	All	1588/1594 (100%)	1433 (90%)	136 (9%)	19 (1%)	10	40

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	B	2	GLN
1	A	210	ARG
1	A	390	GLU
1	A	391	LYS
1	A	670	GLU
1	B	210	ARG
1	B	390	GLU
1	B	391	LYS
1	B	670	GLU
1	A	557	GLU
1	B	557	GLU
1	A	69	LEU
1	A	132	SER
1	B	69	LEU
1	B	132	SER
1	A	631	ILE
1	B	631	ILE
1	A	186	THR

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	664/665 (100%)	610 (92%)	54 (8%)	11	38
1	B	664/665 (100%)	610 (92%)	54 (8%)	11	38
All	All	1328/1330 (100%)	1220 (92%)	108 (8%)	11	38

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	PRO
1	A	73	LEU
1	A	79	LEU
1	A	92	LYS
1	A	115	LEU
1	A	123	LEU
1	A	144	LEU
1	A	155	VAL
1	A	163	ARG
1	A	178	GLN
1	A	188	ASP
1	A	204	LEU
1	A	230	LEU
1	A	255	LEU
1	A	260	ASN
1	A	294	LEU
1	A	297	LEU
1	A	302	VAL
1	A	307	ASP
1	A	316	GLU
1	A	328	SER
1	A	353	GLU
1	A	359	LEU
1	A	360	VAL
1	A	361	LYS
1	A	364	LEU
1	A	390	GLU
1	A	406	MET
1	A	423	LEU
1	A	435	GLU
1	A	468	LEU
1	A	470	LYS
1	A	489	LEU

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Mol	Chain	Res	Type
1	A	521	ASP
1	A	522	ILE
1	A	535	LEU
1	A	542	HIS
1	A	546	LEU
1	A	557	GLU
1	A	580	LEU
1	A	590	LYS
1	A	591	VAL
1	A	601	VAL
1	A	608	VAL
1	A	620	LYS
1	A	652	LEU
1	A	671	GLU
1	A	681	LYS
1	A	706	VAL
1	A	707	LEU
1	A	727	LEU
1	A	728	HIS
1	A	733	GLN
1	A	739	LEU
1	B	31	PRO
1	B	73	LEU
1	B	79	LEU
1	B	92	LYS
1	B	115	LEU
1	B	123	LEU
1	B	144	LEU
1	B	155	VAL
1	B	163	ARG
1	B	178	GLN
1	B	188	ASP
1	B	204	LEU
1	B	230	LEU
1	B	255	LEU
1	B	260	ASN
1	B	294	LEU
1	B	297	LEU
1	B	302	VAL
1	B	307	ASP
1	B	316	GLU
1	B	328	SER

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Mol	Chain	Res	Type
1	B	353	GLU
1	B	359	LEU
1	B	360	VAL
1	B	361	LYS
1	B	364	LEU
1	B	390	GLU
1	B	406	MET
1	B	423	LEU
1	B	435	GLU
1	B	468	LEU
1	B	470	LYS
1	B	489	LEU
1	B	521	ASP
1	B	522	ILE
1	B	535	LEU
1	B	542	HIS
1	B	546	LEU
1	B	557	GLU
1	B	580	LEU
1	B	590	LYS
1	B	591	VAL
1	B	601	VAL
1	B	608	VAL
1	B	620	LYS
1	B	652	LEU
1	B	671	GLU
1	B	681	LYS
1	B	706	VAL
1	B	707	LEU
1	B	727	LEU
1	B	728	HIS
1	B	733	GLN
1	B	739	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	9	GLN
1	A	11	GLN
1	A	33	GLN
1	A	85	GLN

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Mol	Chain	Res	Type
1	A	139	ASN
1	A	141	GLN
1	A	171	HIS
1	A	215	GLN
1	A	221	GLN
1	A	224	HIS
1	A	295	HIS
1	A	367	HIS
1	A	424	HIS
1	A	437	HIS
1	A	445	HIS
1	A	446	ASN
1	A	531	GLN
1	A	542	HIS
1	A	589	ASN
1	A	728	HIS
1	B	2	GLN
1	B	9	GLN
1	B	11	GLN
1	B	85	GLN
1	B	139	ASN
1	B	141	GLN
1	B	215	GLN
1	B	221	GLN
1	B	224	HIS
1	B	367	HIS
1	B	424	HIS
1	B	437	HIS
1	B	445	HIS
1	B	446	ASN
1	B	531	GLN
1	B	542	HIS
1	B	589	ASN
1	B	728	HIS

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 ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	GLC	C	1	2	12,12,12	1.75	4 (33%)	17,17,17	2.40	7 (41%)
2	GLC	C	2	2	11,11,12	2.00	4 (36%)	15,15,17	3.13	9 (60%)
2	GLC	D	1	2	12,12,12	1.75	4 (33%)	17,17,17	2.40	7 (41%)
2	GLC	D	2	2	11,11,12	2.02	4 (36%)	15,15,17	3.13	9 (60%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	GLC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	GLC	C4-C5	3.61	1.60	1.53
2	C	2	GLC	C4-C5	3.58	1.60	1.53
2	D	1	GLC	O2-C2	-3.49	1.34	1.43
2	C	1	GLC	O2-C2	-3.48	1.34	1.43
2	C	1	GLC	C6-C5	3.08	1.62	1.51
2	D	1	GLC	C6-C5	3.06	1.62	1.51
2	C	2	GLC	C1-C2	2.94	1.59	1.52
2	D	2	GLC	C1-C2	2.94	1.59	1.52
2	C	1	GLC	C1-C2	2.73	1.58	1.52
2	D	1	GLC	C1-C2	2.72	1.58	1.52
2	D	2	GLC	O5-C5	2.59	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GLC	O5-C5	2.58	1.48	1.43
2	D	2	GLC	C4-C3	-2.54	1.45	1.52
2	C	2	GLC	C4-C3	-2.52	1.45	1.52
2	D	1	GLC	O5-C1	2.07	1.47	1.42
2	C	1	GLC	O5-C1	2.05	1.47	1.42

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLC	C6-C5-C4	-6.15	97.91	113.02
2	C	2	GLC	C6-C5-C4	-6.14	97.94	113.02
2	C	2	GLC	C1-C2-C3	5.89	118.22	109.64
2	D	2	GLC	C1-C2-C3	5.85	118.17	109.64
2	C	1	GLC	O5-C1-C2	-5.33	100.92	110.30
2	D	1	GLC	O5-C1-C2	-5.31	100.96	110.30
2	D	2	GLC	O2-C2-C3	-4.92	99.96	110.15
2	C	2	GLC	O2-C2-C3	-4.91	99.98	110.15
2	D	1	GLC	O2-C2-C1	4.81	120.34	109.25
2	C	1	GLC	O2-C2-C1	4.81	120.34	109.25
2	D	2	GLC	O4-C4-C3	-3.81	101.39	110.38
2	C	2	GLC	O4-C4-C3	-3.80	101.43	110.38
2	C	1	GLC	C1-O5-C5	3.35	120.14	113.65
2	D	1	GLC	C1-O5-C5	3.35	120.13	113.65
2	D	1	GLC	O2-C2-C3	-3.23	102.77	110.38
2	C	1	GLC	O2-C2-C3	-3.22	102.78	110.38
2	D	2	GLC	C1-O5-C5	-2.95	108.23	112.19
2	C	2	GLC	C1-O5-C5	-2.92	108.27	112.19
2	C	2	GLC	O5-C1-C2	-2.85	103.99	110.79
2	D	2	GLC	O5-C1-C2	-2.85	104.00	110.79
2	D	1	GLC	O1-C1-O5	-2.69	102.42	110.41
2	C	1	GLC	O1-C1-O5	-2.68	102.44	110.41
2	C	1	GLC	O3-C3-C2	-2.24	105.10	110.38
2	D	1	GLC	O3-C3-C2	-2.23	105.12	110.38
2	C	2	GLC	O3-C3-C2	2.21	114.56	110.05
2	D	1	GLC	O6-C6-C5	-2.19	103.89	111.33
2	C	1	GLC	O6-C6-C5	-2.18	103.90	111.33
2	D	2	GLC	O3-C3-C2	2.18	114.51	110.05
2	C	2	GLC	C2-C3-C4	-2.15	107.07	110.86
2	D	2	GLC	C2-C3-C4	-2.15	107.08	110.86
2	D	2	GLC	O5-C5-C4	2.15	116.06	110.83
2	C	2	GLC	O5-C5-C4	2.15	116.06	110.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

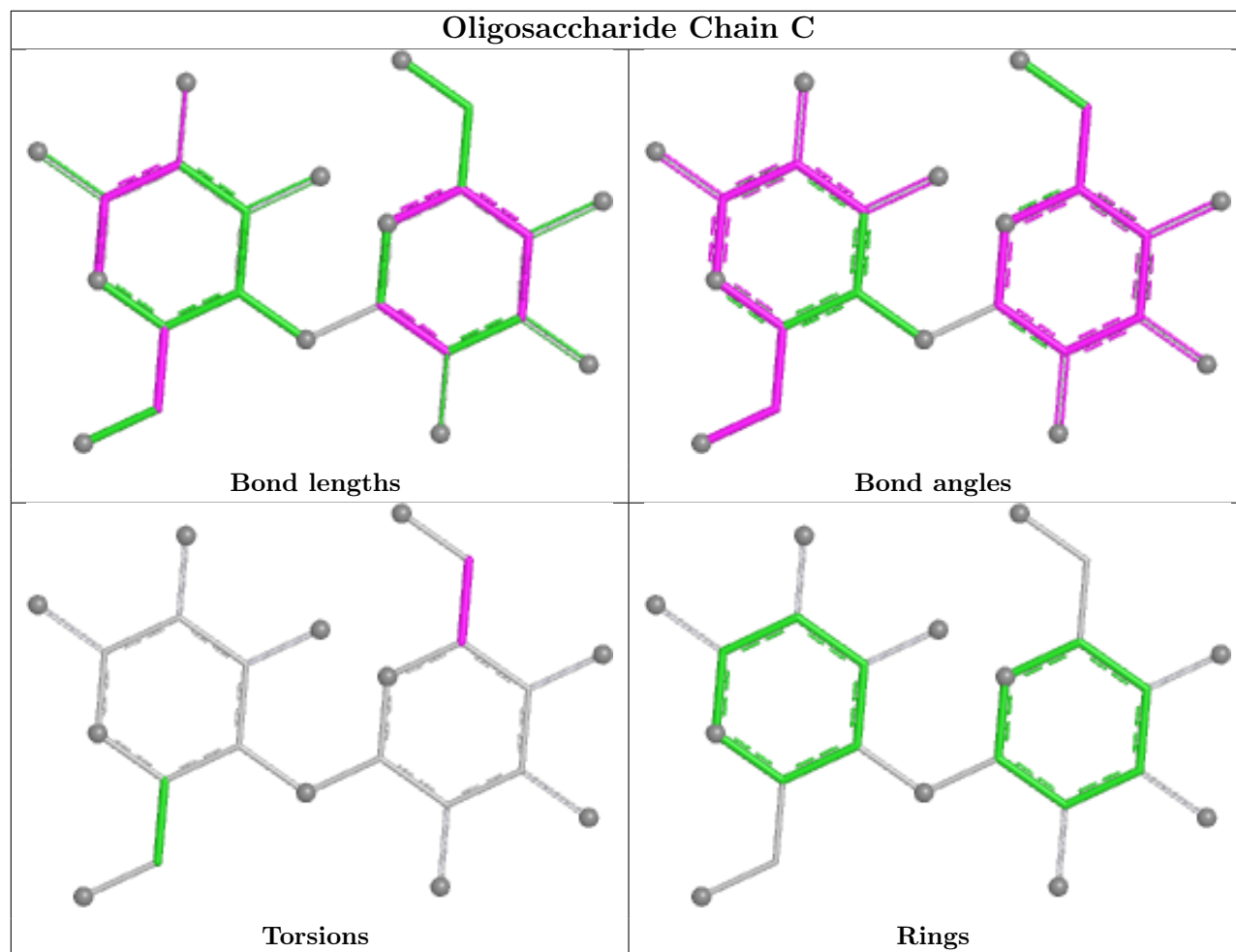
Mol	Chain	Res	Type	Atoms
2	C	2	GLC	O5-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6

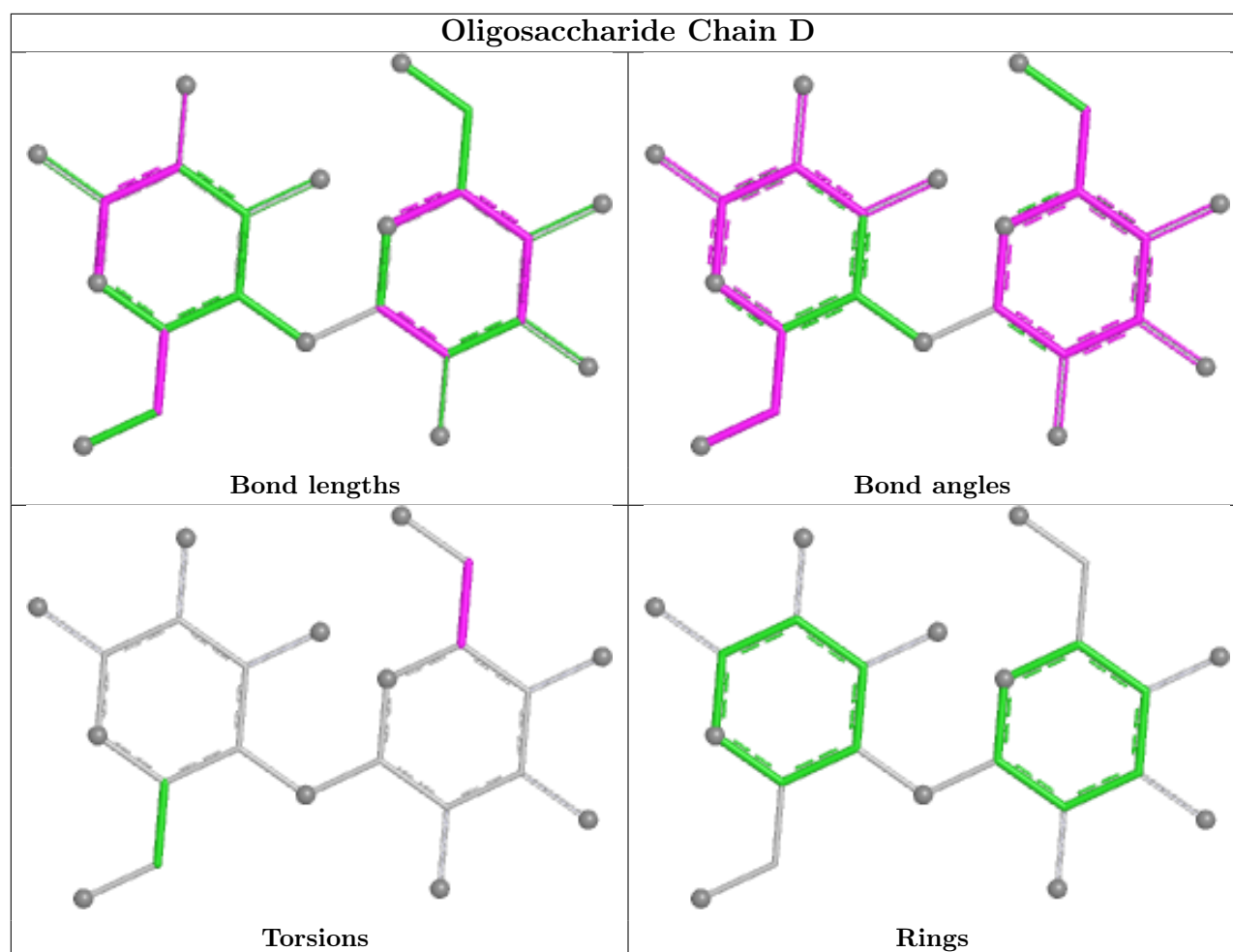
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	GLC	1	0
2	D	2	GLC	3	0
2	C	2	GLC	4	0
2	D	1	GLC	1	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](#)

6 ligands 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$
5	PLP	B	999	1	15,15,16	2.01	3 (20%)	21,22,23	1.55	5 (23%)
4	GOL	A	998	-	5,5,5	0.33	0	5,5,5	0.77	0
4	GOL	B	998	-	5,5,5	0.32	0	5,5,5	0.78	0
3	SO4	B	997	-	4,4,4	0.56	0	6,6,6	0.89	0
5	PLP	A	999	1	15,15,16	2.00	3 (20%)	21,22,23	1.55	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	997	-	4,4,4	0.56	0	6,6,6	0.89	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
4	GOL	A	998	-	-	0/4/4/4	-
5	PLP	A	999	1	-	3/6/6/8	0/1/1/1
5	PLP	B	999	1	-	3/6/6/8	0/1/1/1
4	GOL	B	998	-	-	0/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	999	PLP	C3-C2	-6.38	1.34	1.41
5	A	999	PLP	C3-C2	-6.36	1.34	1.41
5	A	999	PLP	C5-C4	-2.16	1.38	1.40
5	B	999	PLP	C5-C4	-2.13	1.38	1.40
5	A	999	PLP	P-O2P	2.12	1.62	1.54
5	B	999	PLP	P-O2P	2.12	1.62	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	999	PLP	C4A-C4-C5	-3.30	117.54	120.94
5	A	999	PLP	C4A-C4-C5	-3.27	117.57	120.94
5	B	999	PLP	O3P-P-O1P	2.90	122.14	110.83
5	A	999	PLP	O3P-P-O1P	2.90	122.14	110.83
5	A	999	PLP	C5-C6-N1	-2.64	119.53	123.83
5	B	999	PLP	C5-C6-N1	-2.63	119.55	123.83
5	B	999	PLP	O4P-C5A-C5	2.39	113.83	109.36
5	A	999	PLP	O4P-C5A-C5	2.37	113.80	109.36
5	B	999	PLP	O3P-P-O2P	-2.23	99.43	107.80
5	A	999	PLP	O3P-P-O2P	-2.23	99.43	107.80

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	999	PLP	C5A-O4P-P-O1P
5	A	999	PLP	C5A-O4P-P-O2P
5	A	999	PLP	C5A-O4P-P-O3P
5	B	999	PLP	C5A-O4P-P-O1P
5	B	999	PLP	C5A-O4P-P-O2P
5	B	999	PLP	C5A-O4P-P-O3P

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	999	PLP	1	0
5	A	999	PLP	1	0
3	A	997	SO4	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	796/797 (99%)	1.75	271 (34%) 1 1	2, 20, 61, 115	0
1	B	796/797 (99%)	2.43	447 (56%) 0 0	2, 20, 61, 115	0
All	All	1592/1594 (99%)	2.09	718 (45%) 0 0	2, 20, 61, 115	0

All (718) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	ALA	11.6
1	B	780	SER	8.6
1	A	561	ALA	8.2
1	B	760	ASP	7.9
1	B	410	CYS	7.8
1	B	372	ASN	7.7
1	B	704	ASP	7.6
1	A	713	GLY	7.4
1	B	561	ALA	7.3
1	B	281	ALA	7.2
1	B	558	ASN	7.1
1	A	717	ASP	6.9
1	B	320	VAL	6.8
1	B	331	ASP	6.8
1	B	438	GLN	6.5
1	B	783	SER	6.4
1	B	332	ALA	6.2
1	B	390	GLU	6.2
1	B	387	PRO	6.2
1	A	243	GLN	6.1
1	A	119	ALA	6.0
1	B	196	THR	6.0
1	B	400	HIS	5.9
1	A	390	GLU	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	300	TYR	5.8
1	A	353	GLU	5.8
1	B	442	ASN	5.8
1	A	362	GLY	5.7
1	B	761	GLN	5.7
1	A	99	THR	5.6
1	B	771	ASN	5.5
1	B	186	THR	5.5
1	A	2	GLN	5.5
1	B	116	GLY	5.5
1	B	262	THR	5.4
1	B	61	VAL	5.4
1	B	370	ILE	5.4
1	B	60	HIS	5.4
1	A	25	SER	5.4
1	B	394	ALA	5.4
1	B	655	GLY	5.4
1	A	324	GLU	5.3
1	B	178	GLN	5.3
1	B	512	GLU	5.3
1	B	389	ASP	5.2
1	B	391	LYS	5.2
1	B	420	VAL	5.2
1	B	745	ALA	5.2
1	B	436	TYR	5.2
1	B	735	GLY	5.2
1	A	593	ASP	5.1
1	B	525	GLN	5.1
1	B	353	GLU	5.1
1	B	287	HIS	5.1
1	B	313	ALA	5.0
1	A	7	ASP	5.0
1	B	700	ASP	5.0
1	A	8	LYS	5.0
1	A	482	GLN	5.0
1	B	383	GLU	5.0
1	B	298	ALA	4.9
1	B	132	SER	4.9
1	B	713	GLY	4.9
1	B	425	SER	4.9
1	B	195	PHE	4.9
1	B	184	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	321	LEU	4.9
1	B	296	GLU	4.8
1	B	237	ASP	4.8
1	A	19	GLN	4.8
1	B	329	TRP	4.8
1	B	426	ASP	4.8
1	B	789	ALA	4.8
1	B	784	ILE	4.7
1	B	47	ARG	4.7
1	A	712	SER	4.7
1	B	185	VAL	4.7
1	A	400	HIS	4.7
1	B	294	LEU	4.7
1	B	374	ILE	4.6
1	B	65	SER	4.6
1	B	120	ALA	4.6
1	B	77	ASN	4.6
1	B	326	GLN	4.6
1	B	696	TRP	4.6
1	A	50	PRO	4.6
1	B	742	ALA	4.6
1	B	386	TRP	4.5
1	A	92	LYS	4.5
1	A	578	TYR	4.5
1	B	293	GLU	4.5
1	B	180	GLY	4.5
1	B	323	ASP	4.5
1	B	224	HIS	4.5
1	A	171	HIS	4.5
1	B	301	GLU	4.5
1	A	6	ASN	4.4
1	B	447	VAL	4.4
1	A	9	GLN	4.4
1	B	59	ARG	4.4
1	B	203	ASP	4.4
1	B	660	ALA	4.4
1	B	189	GLY	4.4
1	B	343	THR	4.4
1	B	135	GLY	4.4
1	B	424	HIS	4.3
1	A	385	THR	4.3
1	B	562	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	211	ASN	4.3
1	B	336	THR	4.3
1	B	430	LYS	4.3
1	B	2	GLN	4.3
1	A	20	ARG	4.3
1	B	776	GLY	4.3
1	A	178	GLN	4.3
1	B	348	MET	4.2
1	B	274	PHE	4.2
1	B	368	MET	4.2
1	A	3	PRO	4.2
1	B	190	ARG	4.2
1	B	678	HIS	4.2
1	B	498	LEU	4.2
1	B	328	SER	4.2
1	B	330	ASP	4.2
1	A	346	THR	4.2
1	B	466	ALA	4.1
1	B	187	LYS	4.1
1	B	416	ALA	4.1
1	B	422	ALA	4.1
1	B	338	LYS	4.1
1	B	781	ASP	4.1
1	B	69	LEU	4.1
1	B	302	VAL	4.1
1	A	383	GLU	4.1
1	B	201	ALA	4.1
1	A	658	ASP	4.1
1	A	132	SER	4.0
1	B	492	ASP	4.0
1	B	369	GLN	4.0
1	B	41	ALA	4.0
1	B	693	PRO	4.0
1	A	189	GLY	4.0
1	A	442	ASN	4.0
1	A	415	PHE	4.0
1	B	444	PHE	4.0
1	B	384	LYS	4.0
1	A	512	GLU	4.0
1	B	462	PRO	4.0
1	B	623	PRO	4.0
1	A	391	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	479	ASP	3.9
1	A	127	ALA	3.9
1	A	308	THR	3.9
1	A	328	SER	3.9
1	B	182	GLY	3.9
1	B	682	GLN	3.9
1	B	437	HIS	3.9
1	A	408	ASN	3.9
1	B	695	LYS	3.9
1	A	394	ALA	3.9
1	A	177	VAL	3.8
1	B	62	ASN	3.8
1	B	80	ASN	3.8
1	B	604	LYS	3.8
1	A	670	GLU	3.8
1	B	249	GLU	3.8
1	A	295	HIS	3.8
1	B	687	LEU	3.8
1	A	704	ASP	3.8
1	B	177	VAL	3.8
1	A	734	GLY	3.8
1	B	278	CYS	3.8
1	B	381	LEU	3.8
1	A	203	ASP	3.8
1	A	52	ALA	3.7
1	A	85	GLN	3.7
1	A	57	ASN	3.7
1	B	659	GLY	3.7
1	A	575	ALA	3.7
1	B	446	ASN	3.7
1	B	440	TRP	3.7
1	B	124	ASP	3.7
1	B	245	GLY	3.7
1	B	749	GLU	3.7
1	B	307	ASP	3.7
1	B	3	PRO	3.7
1	B	448	THR	3.7
1	B	665	ALA	3.7
1	B	191	TRP	3.7
1	B	672	ASN	3.7
1	A	15	SER	3.7
1	B	235	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	493	ALA	3.7
1	B	638	ALA	3.7
1	B	280	VAL	3.7
1	B	494	LYS	3.7
1	B	554	GLU	3.6
1	B	647	ALA	3.6
1	B	161	TRP	3.6
1	B	164	SER	3.6
1	B	179	VAL	3.6
1	B	241	ALA	3.6
1	A	348	MET	3.6
1	A	438	GLN	3.6
1	B	228	PHE	3.6
1	A	795	ALA	3.6
1	B	421	ALA	3.6
1	B	312	ILE	3.6
1	A	51	PHE	3.6
1	B	433	PHE	3.6
1	B	50	PRO	3.6
1	A	258	ASN	3.6
1	B	363	LEU	3.6
1	B	559	PRO	3.6
1	A	165	ASN	3.6
1	B	85	GLN	3.5
1	A	498	LEU	3.5
1	B	375	ASN	3.5
1	B	788	GLN	3.5
1	B	264	GLY	3.5
1	B	260	ASN	3.5
1	B	496	ARG	3.5
1	B	560	GLN	3.5
1	B	395	LYS	3.5
1	B	310	PRO	3.5
1	A	370	ILE	3.5
1	A	519	GLY	3.5
1	B	793	GLN	3.5
1	B	773	ALA	3.5
1	B	327	MET	3.5
1	B	136	TYR	3.5
1	A	53	LYS	3.5
1	A	260	ASN	3.5
1	B	706	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	323	ASP	3.5
1	B	415	PHE	3.4
1	B	49	GLN	3.4
1	B	651	ALA	3.4
1	B	181	ILE	3.4
1	B	675	ILE	3.4
1	B	475	GLU	3.4
1	A	735	GLY	3.4
1	B	248	ALA	3.4
1	A	262	THR	3.4
1	A	771	ASN	3.4
1	B	315	PRO	3.4
1	B	401	ASP	3.4
1	B	557	GLU	3.4
1	A	516	VAL	3.4
1	B	99	THR	3.4
1	A	247	ASN	3.4
1	B	349	PRO	3.4
1	A	738	TYR	3.4
1	B	289	LEU	3.3
1	A	293	GLU	3.3
1	B	658	ASP	3.3
1	B	758	TYR	3.3
1	B	316	GLU	3.3
1	B	54	PRO	3.3
1	B	408	ASN	3.3
1	A	636	LYS	3.3
1	A	511	ALA	3.3
1	B	578	TYR	3.3
1	A	232	LYS	3.3
1	A	558	ASN	3.3
1	A	73	LEU	3.3
1	B	9	GLN	3.3
1	B	772	THR	3.3
1	A	360	VAL	3.3
1	B	379	LYS	3.3
1	B	592	ALA	3.3
1	A	603	ASP	3.2
1	B	276	CYS	3.2
1	B	452	THR	3.2
1	B	393	TRP	3.2
1	A	749	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	602	GLY	3.2
1	B	774	ARG	3.2
1	B	229	ASP	3.2
1	B	411	VAL	3.2
1	B	270	MET	3.2
1	A	685	ALA	3.2
1	A	285	ARG	3.2
1	B	57	ASN	3.2
1	B	449	ASN	3.2
1	B	243	GLN	3.2
1	B	482	GLN	3.2
1	B	373	GLU	3.2
1	A	485	ASN	3.2
1	B	708	LYS	3.2
1	B	405	HIS	3.2
1	A	330	ASP	3.2
1	A	560	GLN	3.2
1	B	428	VAL	3.1
1	A	761	GLN	3.1
1	B	147	GLN	3.1
1	B	443	LYS	3.1
1	A	235	ASP	3.1
1	B	216	PRO	3.1
1	B	322	ILE	3.1
1	A	742	ALA	3.1
1	B	272	GLN	3.1
1	B	275	GLN	3.1
1	B	733	GLN	3.1
1	B	376	THR	3.1
1	A	137	GLY	3.1
1	A	690	GLY	3.1
1	B	731	GLY	3.1
1	B	743	ASP	3.1
1	A	756	VAL	3.1
1	A	23	LEU	3.1
1	A	74	THR	3.1
1	B	765	THR	3.1
1	A	237	ASP	3.1
1	B	796	ARG	3.1
1	A	647	ALA	3.1
1	A	79	LEU	3.1
1	A	483	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	288	HIS	3.1
1	B	199	GLY	3.1
1	B	212	GLY	3.1
1	B	362	GLY	3.1
1	A	357	VAL	3.1
1	B	194	GLU	3.1
1	B	637	GLU	3.1
1	B	258	ASN	3.0
1	A	354	ARG	3.0
1	B	690	GLY	3.0
1	B	357	VAL	3.0
1	B	429	VAL	3.0
1	A	430	LYS	3.0
1	B	173	GLU	3.0
1	B	441	PRO	3.0
1	B	481	ASP	3.0
1	A	687	LEU	3.0
1	B	183	GLY	3.0
1	B	397	ALA	3.0
1	B	295	HIS	3.0
1	A	326	GLN	3.0
1	A	583	ASN	3.0
1	B	392	VAL	3.0
1	B	92	LYS	3.0
1	B	123	LEU	3.0
1	B	729	SER	3.0
1	B	767	ALA	3.0
1	A	719	ASP	3.0
1	B	367	HIS	3.0
1	B	653	THR	3.0
1	A	796	ARG	2.9
1	B	342	TYR	2.9
1	A	501	VAL	2.9
1	A	680	VAL	2.9
1	B	601	VAL	2.9
1	A	389	ASP	2.9
1	B	751	GLN	2.9
1	B	509	ARG	2.9
1	B	103	GLU	2.9
1	A	493	ALA	2.9
1	B	794	ALA	2.9
1	B	715	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	199	GLY	2.9
1	B	778	PHE	2.9
1	B	292	ARG	2.9
1	A	336	THR	2.9
1	A	205	PRO	2.9
1	A	763	ALA	2.9
1	B	435	GLU	2.9
1	B	691	TYR	2.9
1	B	291	GLY	2.9
1	A	597	ASN	2.9
1	A	113	GLY	2.9
1	B	579	TYR	2.9
1	A	352	LEU	2.9
1	A	248	ALA	2.9
1	A	554	GLU	2.9
1	B	40	GLU	2.9
1	A	179	VAL	2.9
1	B	567	VAL	2.9
1	A	190	ARG	2.9
1	A	322	ILE	2.9
1	B	352	LEU	2.9
1	A	159	ASP	2.8
1	A	465	ALA	2.8
1	B	242	GLU	2.8
1	B	412	VAL	2.8
1	B	506	ASN	2.8
1	B	413	GLY	2.8
1	A	312	ILE	2.8
1	A	186	THR	2.8
1	A	683	VAL	2.8
1	B	501	VAL	2.8
1	B	629	GLU	2.8
1	A	642	GLY	2.8
1	B	113	GLY	2.8
1	B	480	LEU	2.8
1	B	519	GLY	2.8
1	A	278	CYS	2.8
1	B	613	TYR	2.8
1	A	41	ALA	2.8
1	A	263	ALA	2.8
1	A	429	VAL	2.8
1	B	402	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	720	LYS	2.8
1	B	736	ASP	2.8
1	A	731	GLY	2.8
1	A	120	ALA	2.8
1	A	688	ALA	2.8
1	B	58	GLN	2.8
1	B	119	ALA	2.8
1	A	164	SER	2.8
1	B	175	LEU	2.8
1	A	386	TRP	2.8
1	B	555	ILE	2.8
1	B	544	ASN	2.8
1	A	538	TYR	2.8
1	B	133	ALA	2.8
1	B	790	ARG	2.8
1	A	358	LYS	2.8
1	A	474	LYS	2.8
1	B	232	LYS	2.8
1	B	125	SER	2.8
1	B	74	THR	2.8
1	A	183	GLY	2.7
1	A	577	GLY	2.7
1	A	187	LYS	2.7
1	A	681	LYS	2.7
1	B	114	GLY	2.7
1	B	299	ASP	2.7
1	B	398	VAL	2.7
1	A	4	ILE	2.7
1	A	555	ILE	2.7
1	B	143	GLY	2.7
1	A	298	ALA	2.7
1	B	523	ASN	2.7
1	B	635	GLY	2.7
1	B	671	GLU	2.7
1	A	86	ASP	2.7
1	B	548	ILE	2.7
1	A	296	GLU	2.7
1	A	614	CYS	2.7
1	B	712	SER	2.7
1	B	399	VAL	2.7
1	B	409	LEU	2.7
1	A	523	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	672	ASN	2.7
1	B	51	PHE	2.6
1	B	271	GLN	2.6
1	A	384	LYS	2.6
1	A	533	LYS	2.6
1	B	236	GLY	2.6
1	B	728	HIS	2.6
1	A	481	ASP	2.6
1	B	521	ASP	2.6
1	A	211	ASN	2.6
1	B	11	GLN	2.6
1	B	165	ASN	2.6
1	B	266	LYS	2.6
1	B	12	GLU	2.6
1	A	410	CYS	2.6
1	B	277	ALA	2.6
1	B	639	SER	2.6
1	B	63	TYR	2.6
1	B	226	HIS	2.6
1	A	212	GLY	2.6
1	B	130	GLY	2.6
1	B	734	GLY	2.6
1	A	666	GLU	2.6
1	B	666	GLU	2.6
1	B	366	ARG	2.6
1	B	667	LYS	2.6
1	A	162	HIS	2.6
1	B	568	PHE	2.6
1	A	89	ASP	2.6
1	A	491	ASP	2.6
1	A	77	ASN	2.6
1	A	414	GLY	2.6
1	B	234	ASN	2.6
1	B	396	LEU	2.6
1	A	206	VAL	2.6
1	B	526	ALA	2.6
1	A	335	ILE	2.6
1	B	791	ILE	2.6
1	B	317	LEU	2.6
1	B	359	LEU	2.6
1	A	701	LYS	2.6
1	B	354	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	18	TRP	2.5
1	B	656	THR	2.6
1	A	372	ASN	2.5
1	B	285	ARG	2.5
1	B	497	ASP	2.5
1	B	786	ASP	2.5
1	B	346	THR	2.5
1	B	502	ILE	2.5
1	B	633	THR	2.5
1	A	125	SER	2.5
1	B	616	SER	2.5
1	B	701	LYS	2.5
1	B	714	LYS	2.5
1	B	491	ASP	2.5
1	A	520	ILE	2.5
1	B	792	TRP	2.5
1	A	141	GLN	2.5
1	A	337	SER	2.5
1	A	403	GLN	2.5
1	A	492	ASP	2.5
1	A	349	PRO	2.5
1	B	488	LYS	2.5
1	A	447	VAL	2.5
1	B	679	THR	2.5
1	A	210	ARG	2.5
1	A	240	ARG	2.5
1	A	509	ARG	2.5
1	A	698	LYS	2.5
1	B	551	LEU	2.5
1	A	82	GLY	2.5
1	B	683	VAL	2.5
1	A	96	ILE	2.4
1	B	68	PHE	2.4
1	B	676	PHE	2.4
1	A	170	ARG	2.4
1	A	623	PRO	2.4
1	B	740	VAL	2.4
1	A	466	ALA	2.4
1	B	215	GLN	2.4
1	B	673	ILE	2.4
1	A	28	GLU	2.4
1	B	709	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	24	ASN	2.4
1	A	198	THR	2.4
1	A	331	ASP	2.4
1	B	339	THR	2.4
1	B	538	TYR	2.4
1	B	685	ALA	2.4
1	A	716	SER	2.4
1	B	657	LEU	2.4
1	A	643	ASN	2.4
1	B	599	PRO	2.4
1	B	626	ASP	2.4
1	B	719	ASP	2.4
1	A	602	GLY	2.4
1	B	450	GLY	2.4
1	B	64	ILE	2.4
1	B	527	ILE	2.4
1	A	45	MET	2.4
1	B	473	GLN	2.4
1	A	267	LEU	2.4
1	B	318	LEU	2.4
1	A	1	SER	2.4
1	A	616	SER	2.4
1	A	783	SER	2.4
1	B	643	ASN	2.4
1	A	700	ASP	2.4
1	A	794	ALA	2.4
1	B	584	ILE	2.4
1	B	750	ALA	2.4
1	B	787	TYR	2.4
1	A	292	ARG	2.4
1	B	200	GLN	2.4
1	B	256	TYR	2.3
1	B	334	ALA	2.3
1	B	583	ASN	2.3
1	B	597	ASN	2.3
1	B	649	ASN	2.3
1	B	566	ARG	2.3
1	B	738	TYR	2.3
1	B	427	LEU	2.3
1	A	40	GLU	2.3
1	A	399	VAL	2.3
1	A	167	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	633	THR	2.3
1	B	358	LYS	2.3
1	A	48	ALA	2.3
1	B	757	LEU	2.3
1	B	645	LYS	2.3
1	B	1	SER	2.3
1	B	499	TYR	2.3
1	A	427	LEU	2.3
1	B	485	ASN	2.3
1	B	282	ASP	2.3
1	B	104	GLU	2.3
1	A	302	VAL	2.3
1	B	286	ARG	2.3
1	B	534	ARG	2.3
1	B	686	ILE	2.3
1	B	763	ALA	2.3
1	A	325	HIS	2.3
1	B	309	HIS	2.3
1	A	691	TYR	2.3
1	A	316	GLU	2.3
1	A	487	VAL	2.3
1	B	754	VAL	2.3
1	B	650	GLY	2.3
1	A	510	LEU	2.3
1	A	5	PHE	2.3
1	A	582	LYS	2.3
1	B	681	LYS	2.3
1	A	401	ASP	2.3
1	A	103	GLU	2.2
1	B	4	ILE	2.2
1	A	245	GLY	2.2
1	B	365	PRO	2.2
1	B	388	GLY	2.2
1	B	490	ALA	2.2
1	A	78	LEU	2.2
1	B	605	LEU	2.2
1	B	476	TRP	2.2
1	B	171	HIS	2.2
1	A	256	TYR	2.2
1	B	747	TYR	2.2
1	B	662	VAL	2.2
1	A	310	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	660	ALA	2.2
1	B	414	GLY	2.2
1	B	463	ALA	2.2
1	B	705	ALA	2.2
1	B	741	MET	2.2
1	B	221	GLN	2.2
1	B	304	GLN	2.2
1	A	306	ASN	2.2
1	B	76	ASN	2.2
1	A	755	ASP	2.2
1	A	786	ASP	2.2
1	A	130	GLY	2.2
1	B	220	TRP	2.2
1	B	355	TRP	2.2
1	B	528	PHE	2.2
1	A	445	HIS	2.2
1	A	762	GLU	2.2
1	B	344	ASN	2.2
1	B	432	LEU	2.2
1	A	313	ALA	2.2
1	A	334	ALA	2.2
1	A	677	GLY	2.2
1	B	586	PHE	2.2
1	A	261	HIS	2.2
1	A	663	GLU	2.2
1	B	350	GLU	2.2
1	A	669	GLY	2.2
1	A	708	LYS	2.2
1	B	505	ALA	2.2
1	B	625	ALA	2.2
1	B	377	ARG	2.2
1	A	124	ASP	2.2
1	A	736	ASP	2.2
1	B	598	ASP	2.2
1	A	428	VAL	2.1
1	A	550	ALA	2.1
1	B	407	ALA	2.1
1	B	746	ALA	2.1
1	A	559	PRO	2.1
1	A	659	GLY	2.1
1	B	247	ASN	2.1
1	B	674	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	282	ASP	2.1
1	A	35	TRP	2.1
1	A	61	VAL	2.1
1	B	213	VAL	2.1
1	B	516	VAL	2.1
1	A	376	THR	2.1
1	A	600	LEU	2.1
1	B	284	LEU	2.1
1	B	689	LYS	2.1
1	A	768	ALA	2.1
1	B	170	ARG	2.1
1	A	135	GLY	2.1
1	A	208	GLY	2.1
1	B	44	GLU	2.1
1	B	324	GLU	2.1
1	A	307	ASP	2.1
1	B	176	ASP	2.1
1	A	530	ILE	2.1
1	B	515	LYS	2.1
1	B	406	MET	2.1
1	A	49	GLN	2.1
1	B	263	ALA	2.1
1	B	640	GLY	2.1
1	A	723	PHE	2.1
1	B	25	SER	2.1
1	A	375	ASN	2.1
1	B	461	ASN	2.1
1	A	276	CYS	2.1
1	B	86	ASP	2.1
1	B	319	ARG	2.1
1	A	733	GLN	2.1
1	A	788	GLN	2.1
1	B	541	GLN	2.1
1	B	630	GLN	2.1
1	A	90	SER	2.1
1	A	420	VAL	2.1
1	B	564	VAL	2.1
1	A	234	ASN	2.1
1	A	294	LEU	2.1
1	B	500	ARG	2.1
1	B	273	TYR	2.1
1	A	173	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	699	LYS	2.0
1	A	98	LEU	2.0
1	B	73	LEU	2.0
1	B	283	ILE	2.0
1	B	333	TRP	2.0
1	A	259	ASP	2.0
1	B	134	THR	2.0
1	B	290	ALA	2.0
1	B	356	ASP	2.0
1	B	385	THR	2.0
1	B	552	TYR	2.0
1	A	793	GLN	2.0
1	B	71	GLY	2.0
1	A	599	PRO	2.0
1	A	338	LYS	2.0
1	B	543	LEU	2.0
1	B	770	LEU	2.0
1	B	198	THR	2.0
1	A	718	GLY	2.0
1	A	507	LYS	2.0
1	A	213	VAL	2.0
1	A	703	LEU	2.0

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

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

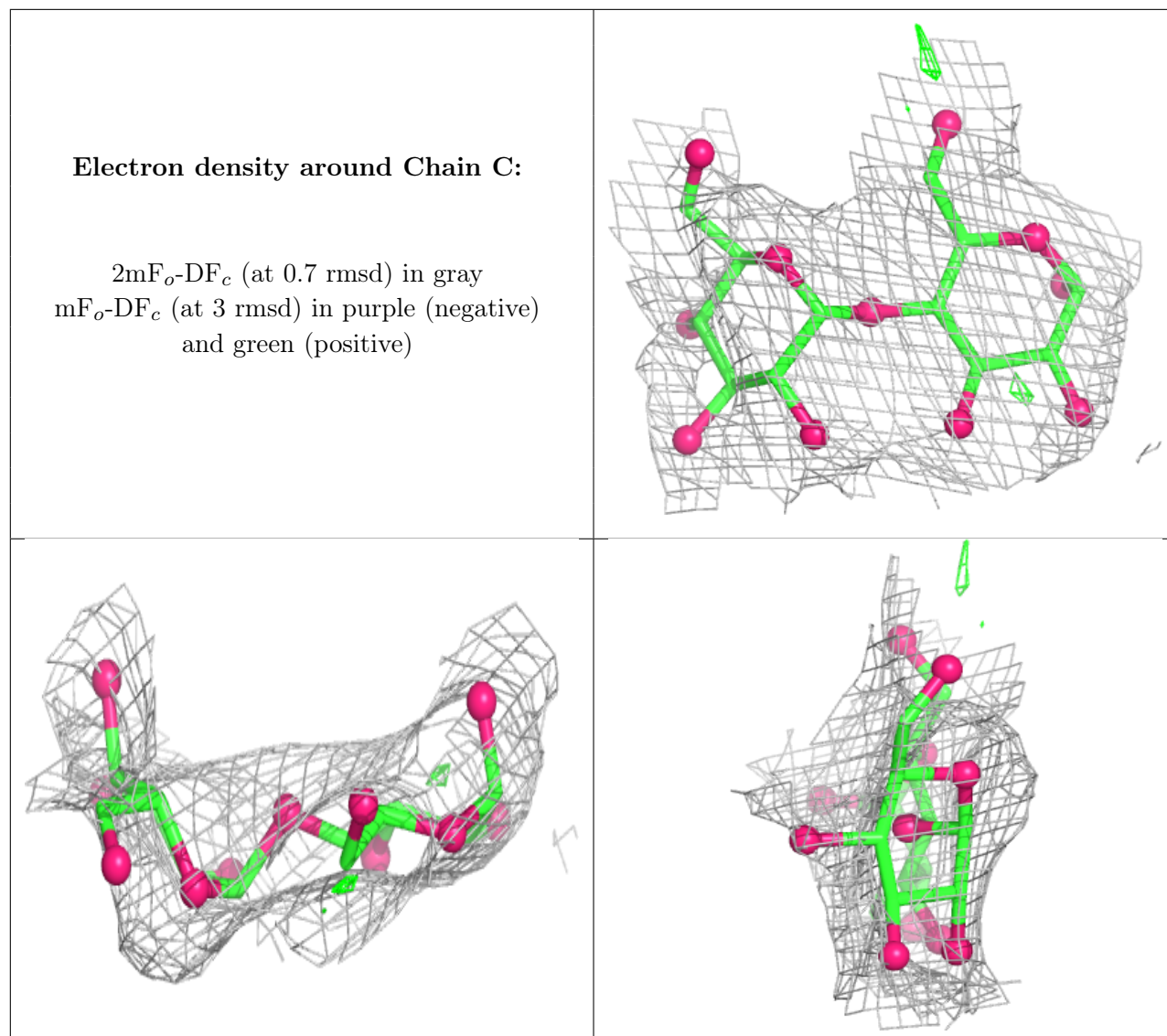
6.3 Carbohydrates [i](#)

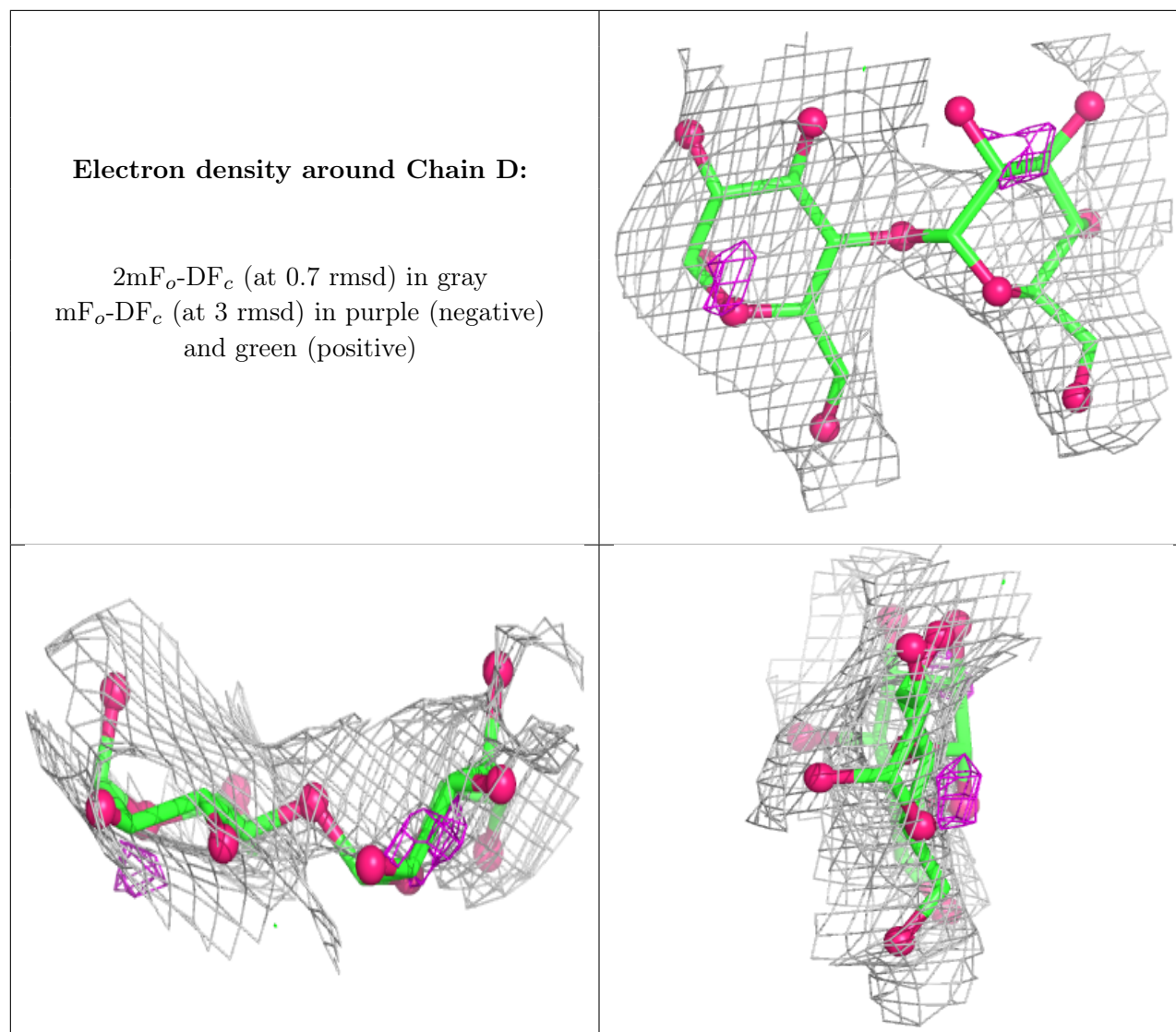
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	D	2	11/12	0.37	0.32	35,35,35,35	0
2	GLC	D	1	12/12	0.59	0.22	35,35,35,35	0
2	GLC	C	2	11/12	0.66	0.22	35,35,35,35	0
2	GLC	C	1	12/12	0.70	0.20	35,35,35,35	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	998	6/6	0.47	0.31	91,91,91,91	0
4	GOL	A	998	6/6	0.53	0.27	91,91,91,91	0
3	SO4	B	997	5/5	0.63	0.23	77,77,77,77	0
5	PLP	B	999	15/16	0.68	0.30	25,25,25,25	0
5	PLP	A	999	15/16	0.81	0.21	25,25,25,25	0
3	SO4	A	997	5/5	0.83	0.22	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.