



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:37 PM UTC

PDB ID : 3M3R / pdb_00003m3r
Title : Crystal structure of the M113F alpha-hemolysin mutant complexed with beta-cyclodextrin
Authors : Montoya, M.; Gouaux, E.
Deposited on : 2010-03-09
Resolution : 2.20 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

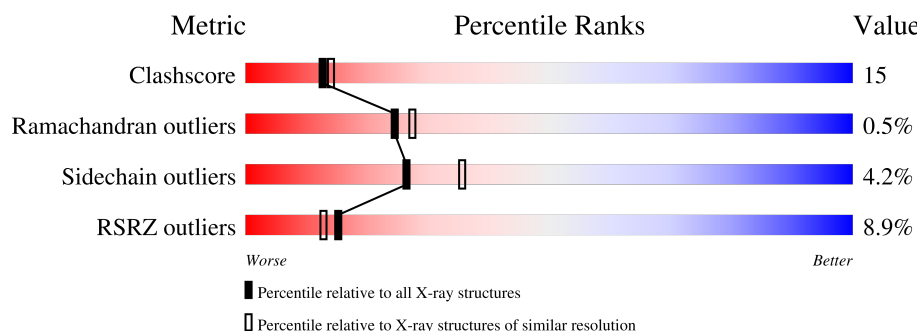
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	293	10% 70% 27% .
1	B	293	9% 66% 31% .
1	C	293	9% 69% 28% .
1	D	293	8% 76% 20% .
1	E	293	10% 73% 24% .
1	F	293	10% 67% 30% .

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Mol	Chain	Length	Quality of chain
1	G	293	6% 69% 28% .
2	H	7	29% 71%
2	I	7	29% 71%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16831 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.

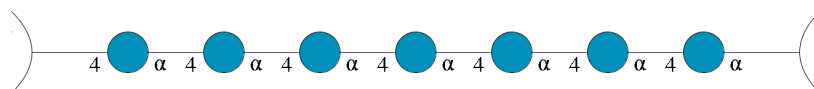
- Molecule 1 is a protein called Alpha-hemolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	41	0	0
			2348	1476	401	465	6			
1	B	293	Total	C	N	O	S	45	0	0
			2348	1476	401	465	6			
1	C	293	Total	C	N	O	S	59	0	0
			2348	1476	401	465	6			
1	D	293	Total	C	N	O	S	66	0	0
			2348	1476	401	465	6			
1	E	293	Total	C	N	O	S	49	0	0
			2348	1476	401	465	6			
1	F	293	Total	C	N	O	S	62	0	0
			2348	1476	401	465	6			
1	G	293	Total	C	N	O	S	52	0	0
			2348	1476	401	465	6			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	PHE	MET	engineered mutation	UNP P09616
B	113	PHE	MET	engineered mutation	UNP P09616
C	113	PHE	MET	engineered mutation	UNP P09616
D	113	PHE	MET	engineered mutation	UNP P09616
E	113	PHE	MET	engineered mutation	UNP P09616
F	113	PHE	MET	engineered mutation	UNP P09616
G	113	PHE	MET	engineered mutation	UNP P09616

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	H	7	Total	C	O	0	0	0
			77	42	35			
2	I	7	Total	C	O	0	0	0
			77	42	35			

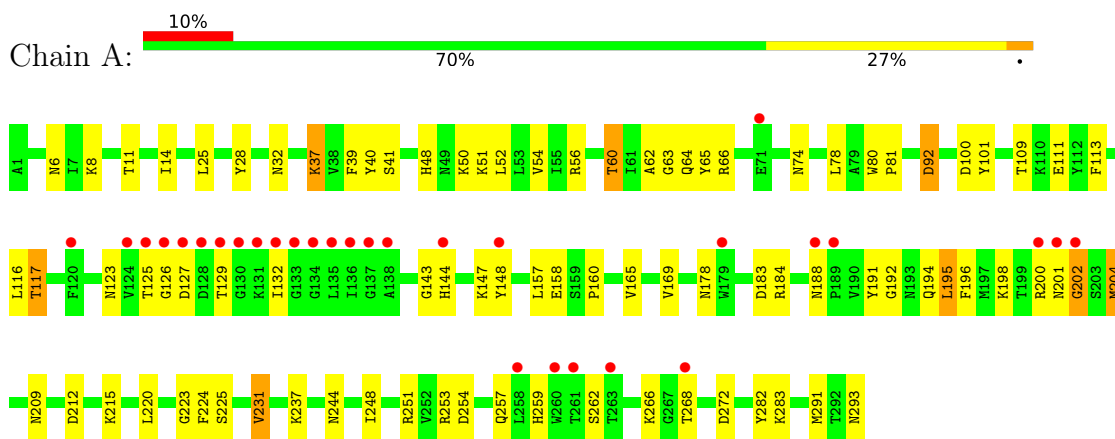
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		
3	B	33	Total	O	0	0
			33	33		
3	C	40	Total	O	0	0
			40	40		
3	D	32	Total	O	0	0
			32	32		
3	E	27	Total	O	0	0
			27	27		
3	F	43	Total	O	0	0
			43	43		
3	G	31	Total	O	0	0
			31	31		

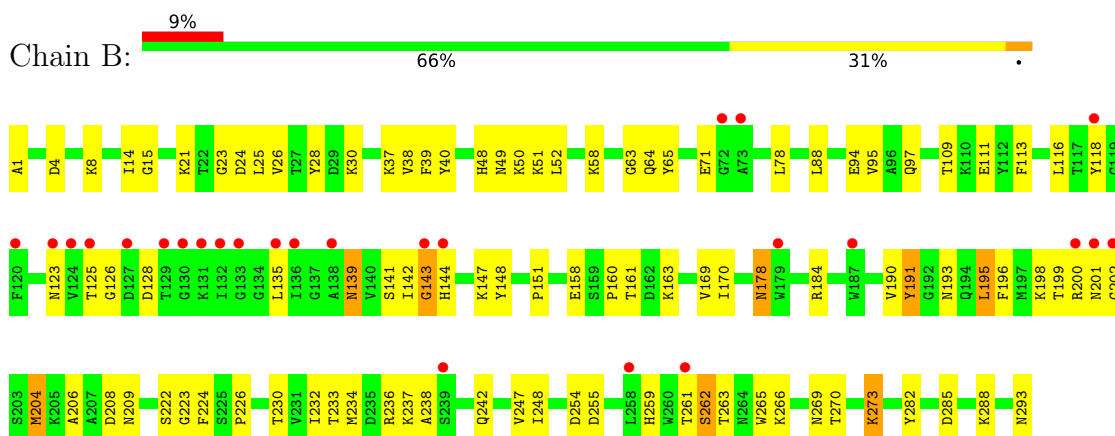
3 Residue-property plots [i](#)

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.

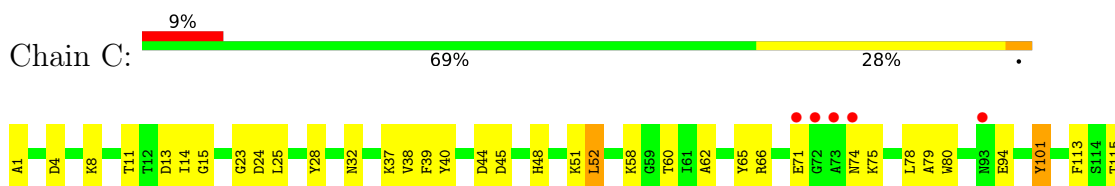
- Molecule 1: Alpha-hemolysin

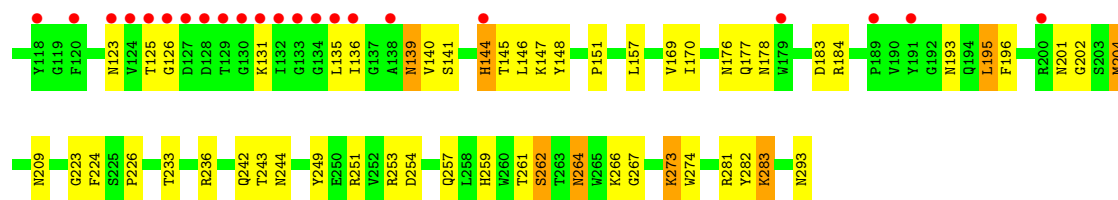


- Molecule 1: Alpha-hemolysin

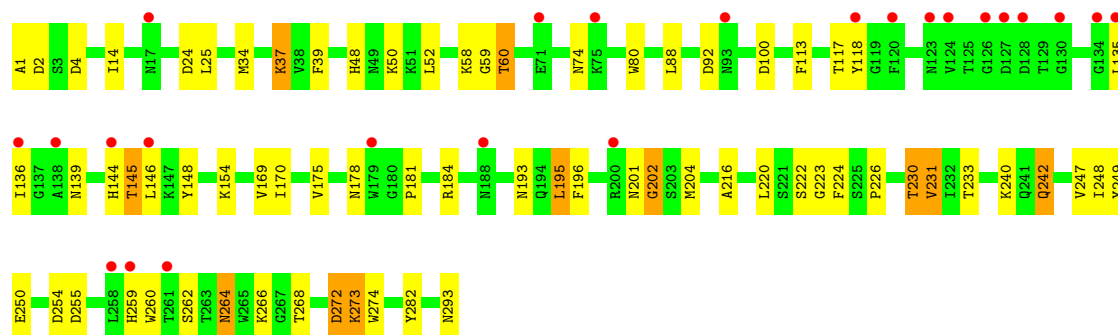
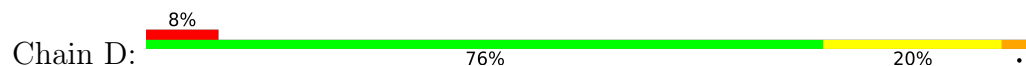


- Molecule 1: Alpha-hemolysin

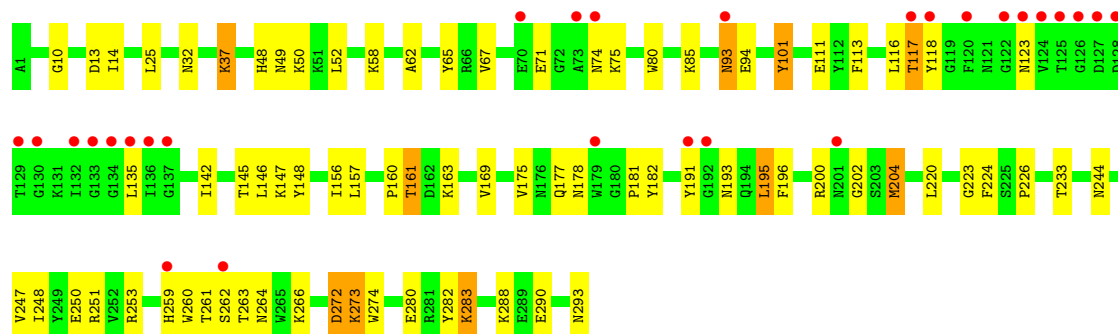
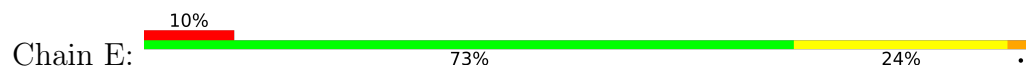




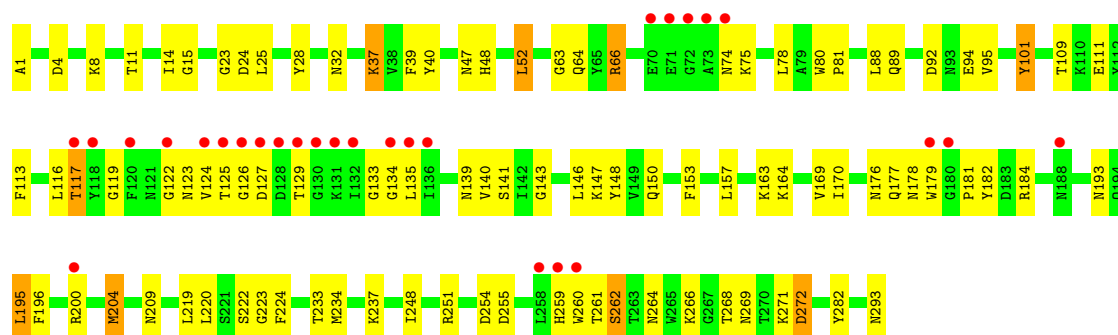
• Molecule 1: Alpha-hemolysin



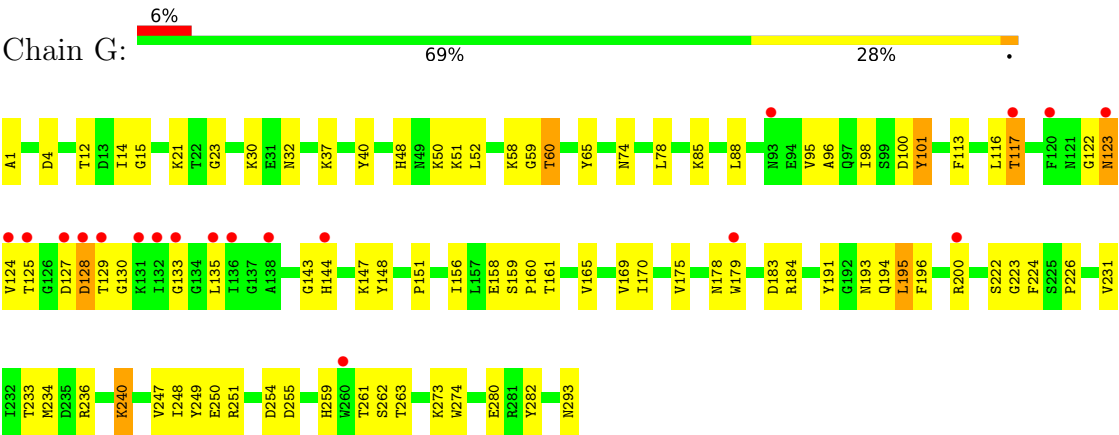
• Molecule 1: Alpha-hemolysin



• Molecule 1: Alpha-hemolysin



• Molecule 1: Alpha-hemolysin



• Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)



• Molecule 2: Cycloheptakis-(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	151.67Å 135.40Å 133.01Å 90.00° 90.77° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.0 (20.00-2.20) 90.0 (20.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.242 , 0.283 0.252 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16831	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% 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

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	0.41	0/2401	0.86	4/3249 (0.1%)
1	B	0.73	3/2401 (0.1%)	0.93	6/3249 (0.2%)
1	C	0.42	0/2401	0.89	5/3249 (0.2%)
1	D	0.42	0/2401	0.88	4/3249 (0.1%)
1	E	0.41	0/2401	0.88	3/3249 (0.1%)
1	F	0.40	0/2401	0.88	6/3249 (0.2%)
1	G	0.41	0/2401	0.89	6/3249 (0.2%)
All	All	0.47	3/16807 (0.0%)	0.89	34/22743 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	143	GLY	CA-C	21.13	1.73	1.51
1	B	143	GLY	C-O	16.42	1.43	1.23
1	B	143	GLY	C-N	5.74	1.41	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	223	GLY	N-CA-C	7.78	121.18	111.85
1	E	223	GLY	N-CA-C	7.66	121.05	111.85
1	A	92	ASP	N-CA-C	7.18	120.94	111.75
1	F	92	ASP	N-CA-C	7.12	119.04	111.28
1	G	223	GLY	N-CA-C	6.96	119.11	112.08
1	B	223	GLY	N-CA-C	6.60	118.74	112.08
1	G	15	GLY	N-CA-C	6.56	120.60	113.58
1	D	92	ASP	N-CA-C	6.50	120.08	111.75
1	D	170	ILE	N-CA-C	6.48	117.93	108.53
1	F	170	ILE	N-CA-C	6.34	117.73	108.53
1	A	223	GLY	N-CA-C	6.14	118.29	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	223	GLY	N-CA-C	6.05	118.21	112.04
1	B	170	ILE	N-CA-C	6.02	117.68	108.71
1	E	156	ILE	N-CA-C	5.80	116.23	108.11
1	D	249	TYR	N-CA-C	-5.75	100.34	109.59
1	E	161	THR	N-CA-C	-5.53	101.09	108.34
1	F	223	GLY	N-CA-C	5.50	117.63	112.08
1	B	15	GLY	N-CA-C	5.49	121.01	114.48
1	C	66	ARG	N-CA-C	5.43	117.65	109.23
1	G	156	ILE	N-CA-C	5.43	116.30	108.48
1	B	191	TYR	N-CA-C	5.39	119.92	113.23
1	C	249	TYR	N-CA-C	-5.39	100.92	109.76
1	A	6	ASN	N-CA-C	5.31	119.04	112.24
1	F	15	GLY	N-CA-C	5.24	121.92	114.85
1	F	271	LYS	N-CA-C	5.24	117.88	110.50
1	C	170	ILE	N-CA-C	5.22	116.49	108.71
1	B	143	GLY	CA-C-O	-5.18	116.81	121.47
1	F	66	ARG	N-CA-C	5.08	116.57	108.79
1	B	97	GLN	N-CA-C	5.07	117.09	109.23
1	G	98	ILE	N-CA-C	-5.07	102.20	108.89
1	G	30	LYS	N-CA-C	5.04	116.47	111.07
1	A	51	LYS	N-CA-C	-5.03	103.90	110.53
1	G	249	TYR	N-CA-C	-5.02	101.50	109.59
1	C	15	GLY	N-CA-C	5.02	120.45	114.48

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	2348	0	2270	81	0
1	B	2348	0	2270	95	0
1	C	2348	0	2270	86	0
1	D	2348	0	2270	59	0
1	E	2348	0	2270	72	0
1	F	2348	0	2270	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2348	0	2270	91	0
2	H	77	0	62	11	0
2	I	77	0	60	12	0
3	A	35	0	0	2	0
3	B	33	0	0	1	0
3	C	40	0	0	2	0
3	D	32	0	0	1	0
3	E	27	0	0	1	0
3	F	43	0	0	0	0
3	G	31	0	0	1	0
All	All	16831	0	16012	482	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (482) 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:117:THR:HG23	1:B:143:GLY:HA3	1.45	0.98
1:C:123:ASN:HB3	1:C:135:LEU:HB3	1.46	0.96
1:E:117:THR:HG23	1:F:143:GLY:CA	1.97	0.94
1:A:117:THR:CG2	1:B:143:GLY:HA3	1.99	0.93
1:C:52:LEU:HD22	1:C:233:THR:HG22	1.51	0.92
1:E:117:THR:HG23	1:F:143:GLY:HA3	1.51	0.92
1:B:125:THR:HG22	1:B:126:GLY:H	1.36	0.90
1:B:123:ASN:HB3	1:B:135:LEU:HB3	1.52	0.89
1:B:160:PRO:HD2	1:C:60:THR:HG21	1.53	0.87
1:G:51:LYS:HE3	1:G:236:ARG:HG2	1.59	0.82
1:G:240:LYS:HB2	1:G:240:LYS:NZ	1.95	0.81
1:A:143:GLY:HA3	1:G:117:THR:CG2	2.10	0.81
1:C:125:THR:HG22	1:D:135:LEU:HB2	1.62	0.81
1:B:160:PRO:CD	1:C:60:THR:HG21	2.11	0.81
1:D:52:LEU:CD2	1:D:233:THR:HG22	2.12	0.79
1:E:123:ASN:HB3	1:E:135:LEU:HB3	1.65	0.78
1:G:96:ALA:HB2	1:G:234:MET:HE2	1.64	0.78
1:D:135:LEU:HD12	1:D:136:ILE:N	1.99	0.78
1:D:240:LYS:HE3	1:D:242:GLN:HE21	1.48	0.77
1:F:184:ARG:HD2	1:F:254:ASP:OD2	1.85	0.76
1:F:204:MET:HE1	1:F:209:ASN:OD1	1.85	0.76
1:D:282:TYR:CD1	1:D:293:ASN:HB3	2.21	0.75
1:G:123:ASN:HB3	1:G:135:LEU:HB3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:ILE:HD11	1:C:48:HIS:CE1	2.22	0.75
1:B:160:PRO:CG	1:C:60:THR:HG21	2.17	0.75
1:F:14:ILE:HD11	1:F:48:HIS:CE1	2.21	0.74
1:B:52:LEU:HD23	1:B:233:THR:HG22	1.67	0.74
1:E:117:THR:HG23	1:F:143:GLY:HA2	1.69	0.74
1:B:199:THR:H	1:B:209:ASN:HD21	1.35	0.74
1:A:143:GLY:HA3	1:G:117:THR:HG23	1.69	0.74
1:E:14:ILE:HD11	1:E:48:HIS:CE1	2.23	0.73
1:C:242:GLN:HB2	1:C:283:LYS:HE3	1.68	0.73
1:F:117:THR:HG23	1:G:143:GLY:HA3	1.71	0.72
1:B:14:ILE:HD11	1:C:39:PHE:HE1	1.54	0.72
1:D:240:LYS:HG3	1:D:242:GLN:NE2	2.05	0.72
1:E:52:LEU:CD2	1:E:233:THR:HG22	2.20	0.72
1:D:240:LYS:HE3	1:D:242:GLN:NE2	2.05	0.71
1:B:8:LYS:HD2	1:C:13:ASP:HB2	1.71	0.71
1:A:204:MET:HE1	1:A:209:ASN:OD1	1.89	0.71
1:D:135:LEU:HD12	1:D:136:ILE:H	1.57	0.70
2:H:2:GLC:HO3	2:I:1:GLC:HO3	1.39	0.69
1:A:116:LEU:HD23	1:B:144:HIS:HE1	1.57	0.69
1:C:144:HIS:C	1:C:144:HIS:CD2	2.71	0.69
1:D:255:ASP:HB2	1:D:273:LYS:HG3	1.75	0.69
1:F:282:TYR:CD1	1:F:293:ASN:HB3	2.29	0.68
1:C:125:THR:HG23	1:D:135:LEU:HD13	1.75	0.68
1:A:132:ILE:HB	1:G:128:ASP:HB3	1.75	0.68
1:A:56:ARG:NH2	1:G:12:THR:HG21	2.08	0.67
1:C:37:LYS:HD2	1:C:37:LYS:C	2.19	0.67
1:E:202:GLY:HA3	1:E:204:MET:CE	2.24	0.67
1:F:259:HIS:CE1	1:F:266:LYS:HB3	2.29	0.67
1:D:52:LEU:HD23	1:D:233:THR:HG22	1.74	0.67
1:E:32:ASN:O	1:E:251:ARG:NH1	2.28	0.67
1:G:96:ALA:HB2	1:G:234:MET:CE	2.23	0.67
1:G:191:TYR:CE2	1:G:200:ARG:HB3	2.30	0.67
1:F:123:ASN:HB3	1:F:135:LEU:HB3	1.76	0.66
1:B:52:LEU:CD2	1:B:233:THR:HG22	2.25	0.66
1:E:259:HIS:CE1	1:E:266:LYS:HB3	2.30	0.66
1:G:74:ASN:O	1:G:259:HIS:HA	1.96	0.66
2:H:2:GLC:O3	2:I:1:GLC:O3	2.13	0.66
1:G:37:LYS:HD2	1:G:37:LYS:C	2.22	0.65
1:E:116:LEU:HD23	1:E:142:ILE:HG12	1.78	0.65
1:D:148:TYR:OH	1:E:178:ASN:ND2	2.29	0.65
1:A:143:GLY:HA3	1:G:117:THR:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LEU:CD2	1:C:233:THR:HG22	2.24	0.64
1:B:123:ASN:CG	1:C:135:LEU:HD11	2.22	0.64
1:C:148:TYR:OH	1:D:178:ASN:ND2	2.31	0.64
1:E:273:LYS:HD2	1:E:274:TRP:CE2	2.33	0.64
1:B:191:TYR:CE2	1:B:200:ARG:HB3	2.33	0.63
1:F:74:ASN:O	1:F:259:HIS:HA	1.98	0.63
1:G:240:LYS:HB2	1:G:240:LYS:HZ3	1.63	0.63
1:C:51:LYS:HE3	1:C:236:ARG:HG2	1.81	0.63
1:D:14:ILE:HD11	1:D:48:HIS:CE1	2.34	0.63
1:A:14:ILE:HD11	1:A:48:HIS:CE1	2.34	0.62
1:E:117:THR:CG2	1:F:143:GLY:HA3	2.28	0.62
1:F:124:VAL:O	1:G:135:LEU:HD12	1.97	0.62
1:B:178:ASN:N	1:B:178:ASN:HD22	1.97	0.62
1:A:123:ASN:OD1	1:B:135:LEU:HD11	1.99	0.62
1:A:123:ASN:ND2	1:B:135:LEU:HD11	2.14	0.62
1:A:32:ASN:O	1:A:251:ARG:NH1	2.31	0.62
1:B:116:LEU:HD21	1:B:118:TYR:HE1	1.64	0.62
1:F:123:ASN:ND2	1:G:135:LEU:HD11	2.14	0.62
1:E:146:LEU:HD13	1:F:181:PRO:HD3	1.82	0.62
1:E:148:TYR:OH	1:F:178:ASN:ND2	2.32	0.62
1:B:199:THR:N	1:B:209:ASN:HD21	1.97	0.61
1:B:184:ARG:HD2	1:B:254:ASP:OD2	2.00	0.61
1:G:100:ASP:HB3	1:G:231:VAL:CG1	2.30	0.61
1:A:117:THR:HG22	1:B:143:GLY:HA3	1.82	0.61
1:B:169:VAL:HG21	1:B:224:PHE:CZ	2.36	0.61
1:B:199:THR:H	1:B:209:ASN:ND2	1.98	0.61
1:E:74:ASN:HB3	1:E:260:TRP:HB3	1.83	0.61
1:E:117:THR:CG2	1:F:143:GLY:CA	2.76	0.61
1:G:282:TYR:CD1	1:G:293:ASN:HB3	2.36	0.61
1:A:56:ARG:HH22	1:G:12:THR:HG21	1.66	0.61
1:F:193:ASN:OD1	1:F:195:LEU:HB2	2.01	0.61
1:A:123:ASN:HD21	1:B:135:LEU:HD11	1.65	0.60
1:A:178:ASN:ND2	1:G:148:TYR:OH	2.34	0.60
1:C:204:MET:HE3	1:C:209:ASN:HB2	1.83	0.60
1:A:14:ILE:HD11	1:B:39:PHE:HE1	1.65	0.60
1:A:37:LYS:HD2	1:A:37:LYS:C	2.27	0.60
1:D:264:ASN:C	1:D:264:ASN:HD22	2.09	0.60
1:F:148:TYR:OH	1:G:178:ASN:ND2	2.35	0.60
1:G:123:ASN:CB	1:G:135:LEU:HB3	2.32	0.60
1:C:139:ASN:HD22	1:C:139:ASN:N	2.00	0.60
1:D:169:VAL:HG21	1:D:224:PHE:CZ	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:ILE:HD11	1:F:39:PHE:HE1	1.66	0.59
1:F:125:THR:HB	1:F:133:GLY:HA3	1.84	0.59
1:B:113:PHE:O	1:B:144:HIS:HA	2.02	0.59
1:B:8:LYS:HD2	1:C:13:ASP:CB	2.32	0.59
1:G:125:THR:HB	1:G:133:GLY:HA3	1.85	0.59
1:B:139:ASN:N	1:B:139:ASN:HD22	2.01	0.59
1:F:32:ASN:O	1:F:251:ARG:NH2	2.33	0.59
1:G:160:PRO:HB3	1:G:165:VAL:HG23	1.85	0.59
1:A:41:SER:OG	1:G:12:THR:HG23	2.03	0.58
1:F:119:GLY:HA3	1:F:139:ASN:OD1	2.03	0.58
1:F:177:GLN:O	1:F:179:TRP:HD1	1.86	0.58
1:C:51:LYS:HG3	1:C:236:ARG:HG3	1.84	0.58
1:C:58:LYS:HA	1:C:226:PRO:O	2.03	0.58
1:D:273:LYS:HD2	1:D:274:TRP:CE2	2.39	0.58
1:F:117:THR:CG2	1:G:143:GLY:HA3	2.32	0.58
1:D:146:LEU:HD21	1:E:175:VAL:HG22	1.86	0.58
1:D:195:LEU:HD13	1:D:196:PHE:CE2	2.39	0.58
1:A:65:TYR:CE1	1:A:78:LEU:HD21	2.39	0.58
1:B:195:LEU:HD13	1:B:196:PHE:CE2	2.39	0.58
1:C:139:ASN:HD22	1:C:139:ASN:H	1.51	0.58
1:G:184:ARG:HD2	1:G:254:ASP:OD2	2.04	0.58
1:A:39:PHE:HE1	1:G:14:ILE:HD11	1.69	0.57
1:A:178:ASN:N	1:A:178:ASN:HD22	2.02	0.57
1:C:146:LEU:HD13	1:D:181:PRO:HD3	1.86	0.57
1:E:248:ILE:N	1:E:248:ILE:HD12	2.19	0.57
1:D:37:LYS:C	1:D:37:LYS:HD2	2.29	0.57
1:G:58:LYS:HA	1:G:226:PRO:O	2.05	0.57
1:B:125:THR:HG22	1:B:126:GLY:N	2.15	0.57
1:C:144:HIS:C	1:C:144:HIS:HD2	2.13	0.57
1:E:62:ALA:O	1:E:251:ARG:NH2	2.37	0.57
1:F:123:ASN:CG	1:G:135:LEU:HD11	2.30	0.57
1:C:195:LEU:HD13	1:C:196:PHE:CE2	2.39	0.57
1:E:49:ASN:O	1:E:50:LYS:HG3	2.04	0.57
1:E:195:LEU:HD13	1:E:196:PHE:CE2	2.40	0.57
1:A:123:ASN:CG	1:B:135:LEU:HD11	2.30	0.56
1:C:125:THR:CG2	1:D:135:LEU:HD13	2.34	0.56
1:A:60:THR:HG22	1:G:101:TYR:OH	2.05	0.56
1:A:191:TYR:CE2	1:A:200:ARG:HB3	2.40	0.56
1:G:240:LYS:HB2	1:G:240:LYS:HZ2	1.68	0.56
1:A:282:TYR:CD1	1:A:293:ASN:HB3	2.41	0.56
1:C:193:ASN:OD1	1:C:195:LEU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:THR:HG22	1:G:12:THR:O	2.06	0.56
1:C:183:ASP:HB2	3:C:314:HOH:O	2.05	0.56
1:B:204:MET:HE1	1:B:265:TRP:HE1	1.71	0.56
1:E:71:GLU:O	1:E:75:LYS:HB3	2.06	0.56
1:G:32:ASN:O	1:G:251:ARG:NH1	2.35	0.56
1:A:111:GLU:OE1	1:B:147:LYS:HE3	2.06	0.55
1:D:100:ASP:HB3	1:D:231:VAL:HG13	1.87	0.55
1:F:37:LYS:HD2	1:F:37:LYS:C	2.31	0.55
1:F:176:ASN:OD1	1:F:177:GLN:HG3	2.07	0.55
1:B:49:ASN:O	1:B:50:LYS:HG3	2.06	0.55
1:E:10:GLY:HA2	1:E:13:ASP:OD2	2.06	0.55
1:D:74:ASN:O	1:D:259:HIS:HA	2.06	0.55
1:G:100:ASP:HB3	1:G:231:VAL:HG11	1.87	0.55
1:G:248:ILE:HD12	1:G:248:ILE:N	2.21	0.55
2:H:2:GLC:C3	2:I:1:GLC:HO3	2.19	0.55
1:A:144:HIS:HE1	1:G:116:LEU:HD23	1.71	0.55
1:G:170:ILE:HD12	1:G:170:ILE:C	2.32	0.55
1:B:282:TYR:CD1	1:B:293:ASN:HB3	2.42	0.55
2:H:1:GLC:HO3	2:I:2:GLC:HO2	1.53	0.55
1:A:100:ASP:N	1:A:231:VAL:HG22	2.22	0.55
1:C:184:ARG:HD2	1:C:254:ASP:OD2	2.06	0.55
1:E:85:LYS:HD2	1:E:250:GLU:OE1	2.07	0.54
1:E:113:PHE:HB2	1:E:145:THR:HB	1.88	0.54
1:F:179:TRP:HZ3	1:F:200:ARG:CZ	2.21	0.54
1:G:48:HIS:O	1:G:236:ARG:NH2	2.31	0.54
1:F:66:ARG:C	1:F:78:LEU:HD12	2.32	0.54
1:F:123:ASN:HD21	1:G:135:LEU:HD11	1.73	0.54
1:F:195:LEU:HD13	1:F:196:PHE:CE2	2.42	0.54
1:A:191:TYR:CZ	1:A:200:ARG:HD3	2.43	0.54
1:E:282:TYR:CD1	1:E:293:ASN:HB3	2.43	0.54
1:F:146:LEU:HD21	1:G:175:VAL:HG22	1.90	0.54
1:G:50:LYS:HD3	1:G:233:THR:HB	1.89	0.54
1:F:123:ASN:OD1	1:G:135:LEU:HD11	2.08	0.54
1:G:23:GLY:HA3	1:G:40:TYR:CE1	2.43	0.54
1:C:51:LYS:O	1:C:52:LEU:HD23	2.08	0.53
1:D:264:ASN:C	1:D:264:ASN:ND2	2.65	0.53
1:A:184:ARG:HD2	1:A:254:ASP:OD2	2.08	0.53
1:B:94:GLU:O	1:B:163:LYS:NZ	2.41	0.53
1:E:111:GLU:OE2	1:E:147:LYS:HD3	2.08	0.53
1:C:201:ASN:O	1:C:202:GLY:C	2.52	0.53
1:D:259:HIS:CE1	1:D:266:LYS:HB3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:GLN:O	1:E:178:ASN:HB2	2.08	0.53
1:F:122:GLY:O	1:F:123:ASN:HB2	2.07	0.53
2:H:2:GLC:HO3	2:I:1:GLC:HO2	1.55	0.53
1:F:157:LEU:O	1:G:222:SER:HB3	2.08	0.53
1:G:193:ASN:OD1	1:G:195:LEU:HB2	2.09	0.53
1:A:259:HIS:CE1	1:A:266:LYS:HB3	2.43	0.53
1:E:58:LYS:HA	1:E:226:PRO:O	2.09	0.53
1:C:48:HIS:O	1:C:236:ARG:NH2	2.39	0.52
1:B:160:PRO:HG2	1:C:60:THR:HG21	1.90	0.52
1:C:169:VAL:HG21	1:C:224:PHE:CZ	2.44	0.52
1:F:169:VAL:HG21	1:F:224:PHE:CZ	2.45	0.52
1:D:34:MET:HE1	1:D:250:GLU:HA	1.91	0.52
1:G:124:VAL:HA	1:G:133:GLY:O	2.09	0.52
1:A:212:ASP:HB3	1:A:215:LYS:HD2	1.91	0.52
1:F:261:THR:O	1:F:262:SER:CB	2.57	0.52
1:F:125:THR:HG22	1:F:126:GLY:H	1.75	0.52
1:C:113:PHE:HB2	1:C:145:THR:HB	1.91	0.52
1:C:257:GLN:O	1:C:267:GLY:HA2	2.10	0.52
1:G:170:ILE:HD12	1:G:170:ILE:O	2.10	0.52
1:B:116:LEU:HD13	1:B:142:ILE:HD11	1.92	0.51
1:B:160:PRO:HG2	1:C:60:THR:CG2	2.40	0.51
1:G:123:ASN:HD22	1:G:135:LEU:CB	2.23	0.51
1:A:160:PRO:HB3	1:A:165:VAL:HG23	1.90	0.51
1:A:248:ILE:N	1:A:248:ILE:HD12	2.25	0.51
1:B:37:LYS:HD2	1:B:37:LYS:C	2.35	0.51
1:D:184:ARG:HD2	1:D:254:ASP:OD2	2.09	0.51
1:E:191:TYR:CZ	1:E:200:ARG:HD3	2.46	0.51
1:A:109:THR:HG22	1:B:151:PRO:HA	1.93	0.51
1:B:111:GLU:OE2	1:C:147:LYS:HE3	2.11	0.51
1:B:259:HIS:CE1	1:B:266:LYS:HB3	2.46	0.51
1:E:52:LEU:HD21	1:E:233:THR:HG22	1.90	0.51
1:E:202:GLY:HA3	1:E:204:MET:HE3	1.91	0.51
1:B:37:LYS:HD2	1:B:38:VAL:N	2.26	0.51
1:A:100:ASP:H	1:A:231:VAL:HG22	1.75	0.51
1:C:115:THR:OG1	1:D:145:THR:HB	2.11	0.51
1:F:282:TYR:CE1	1:F:293:ASN:HB3	2.46	0.51
1:E:169:VAL:HG21	1:E:224:PHE:CZ	2.46	0.51
1:G:52:LEU:CD2	1:G:233:THR:HG22	2.41	0.50
1:A:195:LEU:HD13	1:A:196:PHE:CE2	2.46	0.50
1:B:160:PRO:HD2	1:C:60:THR:CG2	2.33	0.50
1:B:51:LYS:HE3	1:B:236:ARG:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:VAL:C	1:D:248:ILE:HD12	2.36	0.50
1:D:52:LEU:HD21	1:D:233:THR:HG22	1.93	0.50
1:G:1:ALA:O	1:G:4:ASP:HB2	2.11	0.50
2:H:3:GLC:HO3	2:I:7:GLC:HO2	1.60	0.50
1:A:80:TRP:O	1:A:253:ARG:HA	2.12	0.50
1:D:293:ASN:CG	1:D:293:ASN:O	2.54	0.50
1:C:74:ASN:O	1:C:259:HIS:HA	2.12	0.50
1:E:260:TRP:NE1	1:E:262:SER:HA	2.27	0.50
1:B:247:VAL:C	1:B:248:ILE:HD12	2.37	0.50
1:A:117:THR:HG23	1:B:143:GLY:CA	2.31	0.49
1:B:58:LYS:HA	1:B:226:PRO:O	2.12	0.49
1:E:244:ASN:OD1	1:E:283:LYS:HE3	2.12	0.49
1:C:101:TYR:OH	1:D:60:THR:HG23	2.12	0.49
1:B:1:ALA:HB3	1:B:4:ASP:OD1	2.12	0.49
1:C:261:THR:OG1	1:C:264:ASN:ND2	2.44	0.49
1:A:62:ALA:O	1:A:251:ARG:NH2	2.42	0.49
1:A:244:ASN:OD1	1:A:283:LYS:HE2	2.12	0.49
1:C:23:GLY:HA3	1:C:40:TYR:CZ	2.47	0.49
1:C:264:ASN:N	1:C:264:ASN:HD22	2.10	0.49
1:G:125:THR:CB	1:G:133:GLY:HA3	2.43	0.49
1:D:118:TYR:HA	1:D:139:ASN:O	2.12	0.49
1:G:273:LYS:HD3	1:G:274:TRP:CZ2	2.47	0.49
1:G:12:THR:O	1:G:12:THR:CG2	2.60	0.49
1:C:78:LEU:HD12	1:C:79:ALA:N	2.27	0.49
1:E:37:LYS:HD2	1:E:37:LYS:C	2.38	0.49
1:A:14:ILE:CD1	1:A:48:HIS:CE1	2.96	0.49
1:A:215:LYS:NZ	1:G:183:ASP:OD1	2.46	0.49
1:B:141:SER:C	1:B:142:ILE:HD12	2.38	0.49
1:F:148:TYR:OH	1:G:178:ASN:HA	2.12	0.49
1:F:272:ASP:OD2	1:F:272:ASP:N	2.46	0.49
2:I:1:GLC:H62	2:I:2:GLC:O5	2.12	0.49
1:F:248:ILE:N	1:F:248:ILE:HD12	2.28	0.49
1:G:65:TYR:CE2	1:G:78:LEU:HD21	2.48	0.49
1:C:261:THR:O	1:C:262:SER:HB3	2.13	0.48
1:A:74:ASN:O	1:A:259:HIS:HA	2.13	0.48
1:D:216:ALA:HB1	1:D:220:LEU:HD12	1.95	0.48
1:E:191:TYR:CE1	1:E:200:ARG:HB3	2.48	0.48
1:A:28:TYR:CZ	1:G:161:THR:HG22	2.49	0.48
1:A:40:TYR:HA	1:A:54:VAL:O	2.13	0.48
1:A:257:GLN:HB2	1:A:268:THR:CG2	2.43	0.48
1:F:179:TRP:CZ3	1:F:200:ARG:CZ	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:GLY:HA3	1:G:40:TYR:CZ	2.48	0.48
1:B:191:TYR:O	1:B:266:LYS:HA	2.13	0.48
1:F:261:THR:O	1:F:262:SER:HB2	2.13	0.48
1:C:32:ASN:O	1:C:251:ARG:NH1	2.41	0.48
1:C:125:THR:HG22	1:D:135:LEU:CB	2.40	0.48
1:F:23:GLY:HA3	1:F:40:TYR:CZ	2.49	0.48
1:A:14:ILE:HD11	1:B:39:PHE:CE1	2.47	0.48
1:E:74:ASN:O	1:E:259:HIS:HA	2.13	0.48
1:E:288:LYS:HE2	1:E:290:GLU:OE1	2.14	0.48
1:A:158:GLU:O	1:A:160:PRO:HD3	2.14	0.48
1:C:51:LYS:C	1:C:52:LEU:HD23	2.40	0.47
1:C:65:TYR:CE2	1:C:78:LEU:HD21	2.49	0.47
1:C:157:LEU:O	1:D:222:SER:HB3	2.15	0.47
1:F:89:GLN:HG3	1:F:164:LYS:HB3	1.97	0.47
1:C:8:LYS:O	1:C:11:THR:OG1	2.26	0.47
1:E:261:THR:C	1:E:263:THR:H	2.23	0.47
1:E:263:THR:HG23	1:E:264:ASN:OD1	2.14	0.47
1:F:75:LYS:HG2	1:F:259:HIS:CB	2.45	0.47
1:A:148:TYR:OH	1:B:178:ASN:ND2	2.48	0.47
1:B:95:VAL:CG1	1:B:234:MET:HE1	2.44	0.47
1:C:259:HIS:CE1	1:C:266:LYS:HB3	2.50	0.47
1:F:125:THR:HG22	1:F:126:GLY:N	2.29	0.47
1:F:125:THR:H	1:F:133:GLY:C	2.23	0.47
1:E:261:THR:O	1:E:262:SER:HB2	2.14	0.47
1:A:80:TRP:CE2	1:A:254:ASP:HB2	2.50	0.47
1:B:109:THR:HG22	1:C:151:PRO:HA	1.97	0.47
1:A:8:LYS:O	1:A:11:THR:OG1	2.31	0.46
1:A:50:LYS:NZ	3:A:296:HOH:O	2.48	0.46
1:B:255:ASP:HB3	1:B:270:THR:OG1	2.15	0.46
1:F:52:LEU:HD23	1:F:233:THR:HG22	1.97	0.46
1:F:153:PHE:CD2	1:F:219:LEU:HD22	2.50	0.46
1:F:47:ASN:OD1	1:G:21:LYS:HE2	2.15	0.46
1:D:201:ASN:O	1:D:202:GLY:C	2.58	0.46
1:D:260:TRP:CZ3	1:D:264:ASN:HA	2.50	0.46
1:G:195:LEU:HD13	1:G:196:PHE:CE2	2.50	0.46
1:G:247:VAL:C	1:G:248:ILE:HD12	2.41	0.46
1:B:23:GLY:HA3	1:B:40:TYR:CZ	2.50	0.46
1:B:248:ILE:HD12	1:B:248:ILE:N	2.30	0.46
1:E:161:THR:HA	1:F:28:TYR:CD2	2.51	0.46
1:F:111:GLU:OE1	1:F:147:LYS:HD3	2.16	0.46
2:H:1:GLC:HO2	2:I:2:GLC:HO3	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLY:O	1:A:64:GLN:HB2	2.15	0.46
1:B:204:MET:HE2	1:B:204:MET:N	2.31	0.46
1:D:88:LEU:HD22	1:D:230:THR:HG21	1.97	0.46
1:D:272:ASP:OD2	1:D:272:ASP:N	2.49	0.46
1:E:80:TRP:O	1:E:253:ARG:HA	2.16	0.46
1:F:80:TRP:CE2	1:F:254:ASP:HB2	2.50	0.46
1:B:193:ASN:OD1	1:B:195:LEU:HB2	2.15	0.46
1:C:101:TYR:OH	1:D:60:THR:CG2	2.64	0.46
1:D:146:LEU:HD21	1:E:175:VAL:CG2	2.46	0.46
1:E:182:TYR:HB2	1:E:195:LEU:HD23	1.97	0.46
1:E:202:GLY:C	1:E:204:MET:HE3	2.40	0.46
1:F:140:VAL:HG12	1:F:141:SER:N	2.31	0.46
1:B:199:THR:OG1	1:B:209:ASN:ND2	2.49	0.46
1:E:93:ASN:H	1:E:93:ASN:ND2	2.14	0.46
1:G:280:GLU:OE1	1:G:293:ASN:ND2	2.49	0.46
1:E:116:LEU:C	1:E:116:LEU:HD13	2.40	0.46
1:B:178:ASN:N	1:B:178:ASN:ND2	2.61	0.45
1:C:273:LYS:HB3	1:C:274:TRP:CE3	2.51	0.45
1:F:88:LEU:HD12	1:F:88:LEU:N	2.31	0.45
1:G:14:ILE:HD11	1:G:48:HIS:CE1	2.51	0.45
1:A:132:ILE:H	1:G:128:ASP:CG	2.24	0.45
1:A:282:TYR:C	1:A:283:LYS:HD2	2.41	0.45
1:D:58:LYS:HA	1:D:226:PRO:O	2.15	0.45
1:C:14:ILE:CD1	1:C:48:HIS:CE1	2.97	0.45
1:D:146:LEU:HD13	1:E:181:PRO:HD3	1.98	0.45
1:D:282:TYR:CE1	1:D:293:ASN:HB3	2.51	0.45
1:E:193:ASN:OD1	1:E:195:LEU:HB2	2.15	0.45
1:A:144:HIS:CE1	1:G:116:LEU:HB3	2.52	0.45
1:A:191:TYR:HE2	1:A:200:ARG:HB3	1.82	0.45
1:B:14:ILE:HD11	1:B:48:HIS:CE1	2.51	0.45
1:B:111:GLU:HB3	1:B:147:LYS:HB3	1.98	0.45
1:G:85:LYS:HB2	1:G:250:GLU:HB3	1.99	0.45
2:H:3:GLC:HO2	2:I:7:GLC:HO3	1.64	0.45
1:A:183:ASP:C	1:A:183:ASP:OD2	2.60	0.45
1:G:100:ASP:CB	1:G:231:VAL:CG1	2.95	0.45
1:B:190:VAL:HB	1:B:191:TYR:CD1	2.52	0.44
1:E:93:ASN:C	1:E:93:ASN:HD22	2.25	0.44
1:A:113:PHE:O	1:A:144:HIS:HA	2.17	0.44
1:D:14:ILE:CD1	1:D:48:HIS:CE1	3.00	0.44
1:B:230:THR:HG22	1:B:232:ILE:HD12	1.99	0.44
1:B:237:LYS:O	1:B:238:ALA:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:52:LEU:HD22	1:G:233:THR:HG22	1.98	0.44
2:H:7:GLC:HO3	2:I:3:GLC:HO2	1.64	0.44
1:B:255:ASP:HB2	1:B:273:LYS:HG3	2.00	0.44
1:A:237:LYS:HA	1:A:237:LYS:HE2	1.99	0.44
1:B:65:TYR:CE2	1:B:78:LEU:HD21	2.53	0.44
1:B:191:TYR:HE2	1:B:200:ARG:HB3	1.78	0.44
1:D:100:ASP:HB3	1:D:231:VAL:CG1	2.47	0.44
1:F:116:LEU:HB3	1:G:144:HIS:CE1	2.53	0.44
1:C:126:GLY:HA2	1:C:131:LYS:O	2.17	0.44
1:E:52:LEU:HD23	1:E:233:THR:HG22	1.98	0.44
1:F:63:GLY:O	1:F:64:GLN:HB2	2.18	0.44
1:G:122:GLY:O	1:G:123:ASN:HB2	2.17	0.44
1:G:194:GLN:O	1:G:195:LEU:C	2.61	0.44
1:C:135:LEU:HD12	1:C:136:ILE:H	1.82	0.44
1:A:188:ASN:O	1:A:192:GLY:N	2.47	0.44
1:B:261:THR:O	1:B:262:SER:HB3	2.18	0.44
1:B:293:ASN:CG	1:B:293:ASN:O	2.60	0.44
1:E:260:TRP:CD1	1:E:262:SER:H	2.35	0.44
1:B:26:VAL:HG22	1:B:37:LYS:HG2	2.00	0.43
1:B:206:ALA:C	1:B:208:ASP:H	2.25	0.43
1:C:80:TRP:CE2	1:C:254:ASP:HB2	2.52	0.43
1:E:14:ILE:CD1	1:E:48:HIS:CE1	2.98	0.43
1:B:25:LEU:HD21	1:B:40:TYR:HE1	1.83	0.43
1:G:169:VAL:HG21	1:G:224:PHE:CZ	2.53	0.43
2:H:4:GLC:HO2	2:I:6:GLC:HO3	1.66	0.43
1:B:28:TYR:CE1	1:B:30:LYS:HA	2.53	0.43
1:D:1:ALA:HB3	1:D:4:ASP:OD1	2.18	0.43
1:F:52:LEU:CD2	1:F:233:THR:HG22	2.48	0.43
1:G:59:GLY:C	1:G:60:THR:HG22	2.43	0.43
1:C:94:GLU:OE1	1:C:243:THR:HG23	2.19	0.43
1:F:101:TYR:OH	1:G:60:THR:CG2	2.67	0.43
1:A:14:ILE:CD1	1:B:39:PHE:HE1	2.30	0.43
1:C:244:ASN:HB3	1:C:281:ARG:HD2	2.01	0.43
1:B:198:LYS:HB3	1:B:209:ASN:ND2	2.34	0.43
1:B:201:ASN:O	1:B:202:GLY:C	2.62	0.43
1:F:95:VAL:HG23	1:F:234:MET:SD	2.59	0.43
1:A:253:ARG:NH1	3:A:316:HOH:O	2.52	0.43
1:C:71:GLU:HB2	1:C:75:LYS:HB3	2.00	0.43
1:B:24:ASP:OD1	1:B:37:LYS:HD3	2.19	0.42
1:B:50:LYS:NZ	3:B:317:HOH:O	2.52	0.42
1:E:50:LYS:NZ	3:E:299:HOH:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:N	1:B:88:LEU:HD12	2.34	0.42
1:C:62:ALA:O	1:C:251:ARG:NH2	2.47	0.42
1:C:202:GLY:HA3	1:C:204:MET:HE1	1.99	0.42
1:E:101:TYR:CZ	1:E:160:PRO:HG3	2.54	0.42
1:F:124:VAL:HA	1:F:134:GLY:HA2	2.01	0.42
1:G:255:ASP:HB2	1:G:273:LYS:HD2	2.01	0.42
1:B:204:MET:CE	1:B:265:TRP:HE1	2.32	0.42
1:D:50:LYS:NZ	3:D:301:HOH:O	2.52	0.42
1:D:113:PHE:O	1:D:144:HIS:HA	2.20	0.42
1:E:118:TYR:O	1:F:141:SER:HB2	2.19	0.42
1:F:148:TYR:HE2	1:F:150:GLN:OE1	2.03	0.42
1:G:261:THR:O	1:G:263:THR:N	2.47	0.42
1:D:80:TRP:CE2	1:D:254:ASP:HB2	2.54	0.42
1:F:113:PHE:CE2	1:G:147:LYS:HD2	2.55	0.42
1:F:127:ASP:C	1:F:129:THR:H	2.27	0.42
1:G:183:ASP:HB2	3:G:311:HOH:O	2.18	0.42
2:H:7:GLC:HO2	2:I:3:GLC:HO3	1.68	0.42
1:B:14:ILE:HD11	1:C:39:PHE:CE1	2.45	0.42
1:F:81:PRO:CG	1:F:220:LEU:HA	2.49	0.42
1:A:191:TYR:C	1:A:266:LYS:HG3	2.44	0.42
1:B:148:TYR:OH	1:C:178:ASN:ND2	2.53	0.42
1:F:1:ALA:HB3	1:F:4:ASP:OD1	2.20	0.42
1:G:100:ASP:HB3	1:G:231:VAL:HG12	2.01	0.42
1:A:117:THR:CG2	1:B:143:GLY:CA	2.85	0.42
1:C:178:ASN:N	1:C:178:ASN:HD22	2.18	0.42
1:E:195:LEU:HD13	1:E:196:PHE:CZ	2.55	0.42
1:C:44:ASP:HB3	3:C:302:HOH:O	2.20	0.42
1:C:282:TYR:CD1	1:C:293:ASN:HB3	2.55	0.42
1:E:75:LYS:HE3	1:E:75:LYS:HB2	1.87	0.42
1:C:14:ILE:CD1	1:D:39:PHE:HE1	2.33	0.41
1:E:116:LEU:HD13	1:E:117:THR:N	2.35	0.41
1:F:8:LYS:HB3	1:F:11:THR:OG1	2.20	0.41
1:F:94:GLU:O	1:F:163:LYS:NZ	2.53	0.41
1:C:113:PHE:N	1:C:113:PHE:CD1	2.88	0.41
1:C:140:VAL:HG12	1:C:141:SER:N	2.35	0.41
1:E:247:VAL:C	1:E:248:ILE:HD12	2.44	0.41
1:F:177:GLN:O	1:F:178:ASN:HB2	2.20	0.41
1:G:113:PHE:CD1	1:G:113:PHE:N	2.88	0.41
1:G:127:ASP:C	1:G:129:THR:H	2.28	0.41
1:G:273:LYS:HD3	1:G:274:TRP:CH2	2.55	0.41
1:A:157:LEU:O	1:B:222:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:THR:HG22	1:C:28:TYR:CZ	2.55	0.41
1:C:1:ALA:HB3	1:C:4:ASP:OD1	2.21	0.41
1:A:127:ASP:C	1:A:129:THR:H	2.28	0.41
1:C:23:GLY:HA3	1:C:40:TYR:CE1	2.55	0.41
1:F:75:LYS:HG2	1:F:259:HIS:HB3	2.02	0.41
1:G:88:LEU:N	1:G:88:LEU:HD12	2.35	0.41
1:B:285:ASP:OD1	1:B:288:LYS:HG3	2.20	0.41
1:C:45:ASP:OD2	1:C:45:ASP:C	2.62	0.41
1:F:182:TYR:HB2	1:F:195:LEU:HD23	2.03	0.41
1:A:147:LYS:HD2	1:G:113:PHE:CE2	2.56	0.41
1:D:59:GLY:C	1:D:60:THR:HG22	2.46	0.41
1:G:158:GLU:O	1:G:159:SER:C	2.63	0.41
1:G:282:TYR:CE1	1:G:293:ASN:HB3	2.56	0.41
1:C:139:ASN:N	1:C:139:ASN:ND2	2.68	0.41
1:C:176:ASN:OD1	1:C:177:GLN:HG3	2.21	0.41
1:C:195:LEU:HD13	1:C:196:PHE:CZ	2.55	0.41
1:E:85:LYS:HB2	1:E:250:GLU:HB3	2.03	0.41
1:G:51:LYS:HG3	1:G:236:ARG:HG3	2.02	0.41
1:A:60:THR:HB	1:A:225:SER:OG	2.20	0.41
1:C:37:LYS:HD2	1:C:38:VAL:N	2.36	0.41
1:C:80:TRP:O	1:C:253:ARG:HA	2.21	0.41
1:C:146:LEU:HD11	1:D:181:PRO:HG3	2.03	0.41
1:E:148:TYR:CD1	1:E:148:TYR:N	2.89	0.41
1:A:40:TYR:CE1	1:A:291:MET:HB2	2.56	0.40
1:A:169:VAL:HG21	1:A:224:PHE:CZ	2.55	0.40
1:B:63:GLY:O	1:B:64:GLN:HB2	2.21	0.40
1:C:146:LEU:HD21	1:D:175:VAL:HG22	2.03	0.40
1:D:1:ALA:O	1:D:2:ASP:C	2.64	0.40
1:F:109:THR:HG22	1:G:151:PRO:HA	2.02	0.40
1:A:66:ARG:C	1:A:78:LEU:HD12	2.47	0.40
1:E:272:ASP:OD2	1:E:272:ASP:N	2.53	0.40
1:F:260:TRP:CZ3	1:F:264:ASN:HA	2.56	0.40
1:A:81:PRO:HG2	1:A:220:LEU:HD23	2.04	0.40
1:A:194:GLN:O	1:A:195:LEU:C	2.65	0.40
1:A:201:ASN:O	1:A:202:GLY:C	2.63	0.40
1:B:158:GLU:O	1:B:160:PRO:HD3	2.22	0.40
1:E:94:GLU:O	1:E:163:LYS:NZ	2.54	0.40
1:E:157:LEU:O	1:F:222:SER:HB3	2.21	0.40
1:F:255:ASP:O	1:F:269:ASN:HA	2.22	0.40
1:A:125:THR:HG22	1:A:126:GLY:N	2.36	0.40
1:D:154:LYS:O	1:D:169:VAL:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:ASN:OD1	1:D:195:LEU:HB2	2.21	0.40
1:E:280:GLU:OE1	1:E:293:ASN:ND2	2.54	0.40
1:A:123:ASN:HD21	1:B:135:LEU:CD1	2.32	0.40
1:A:178:ASN:ND2	1:A:178:ASN:N	2.67	0.40
1:B:255:ASP:O	1:B:269:ASN:HA	2.22	0.40
1:E:65:TYR:HB2	1:E:220:LEU:O	2.21	0.40
1:E:293:ASN:O	1:E:293:ASN:CG	2.64	0.40
1:G:261:THR:O	1:G:262:SER:HB3	2.21	0.40

There are no symmetry-related clashes.

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	291/293 (99%)	273 (94%)	16 (6%)	2 (1%)	18	19
1	B	291/293 (99%)	265 (91%)	24 (8%)	2 (1%)	18	19
1	C	291/293 (99%)	275 (94%)	15 (5%)	1 (0%)	36	42
1	D	291/293 (99%)	273 (94%)	16 (6%)	2 (1%)	18	19
1	E	291/293 (99%)	276 (95%)	15 (5%)	0	100	100
1	F	291/293 (99%)	271 (93%)	19 (6%)	1 (0%)	36	42
1	G	291/293 (99%)	268 (92%)	20 (7%)	3 (1%)	12	11
All	All	2037/2051 (99%)	1901 (93%)	125 (6%)	11 (0%)	24	27

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	SER
1	B	262	SER
1	C	262	SER

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Mol	Chain	Res	Type
1	D	262	SER
1	D	202	GLY
1	A	202	GLY
1	F	262	SER
1	G	128	ASP
1	B	128	ASP
1	G	123	ASN
1	G	130	GLY

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	259/259 (100%)	247 (95%)	12 (5%)	24	32
1	B	259/259 (100%)	250 (96%)	9 (4%)	32	43
1	C	259/259 (100%)	248 (96%)	11 (4%)	26	36
1	D	259/259 (100%)	244 (94%)	15 (6%)	18	22
1	E	259/259 (100%)	248 (96%)	11 (4%)	26	36
1	F	259/259 (100%)	248 (96%)	11 (4%)	26	36
1	G	259/259 (100%)	252 (97%)	7 (3%)	39	53
All	All	1813/1813 (100%)	1737 (96%)	76 (4%)	26	36

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	37	LYS
1	A	52	LEU
1	A	60	THR
1	A	92	ASP
1	A	101	TYR
1	A	117	THR
1	A	195	LEU
1	A	198	LYS

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Mol	Chain	Res	Type
1	A	204	MET
1	A	231	VAL
1	A	272	ASP
1	B	21	LYS
1	B	71	GLU
1	B	139	ASN
1	B	178	ASN
1	B	195	LEU
1	B	204	MET
1	B	242	GLN
1	B	263	THR
1	B	273	LYS
1	C	24	ASP
1	C	25	LEU
1	C	52	LEU
1	C	101	TYR
1	C	139	ASN
1	C	144	HIS
1	C	195	LEU
1	C	204	MET
1	C	264	ASN
1	C	273	LYS
1	C	283	LYS
1	D	24	ASP
1	D	25	LEU
1	D	37	LYS
1	D	60	THR
1	D	117	THR
1	D	145	THR
1	D	195	LEU
1	D	204	MET
1	D	230	THR
1	D	231	VAL
1	D	242	GLN
1	D	264	ASN
1	D	268	THR
1	D	272	ASP
1	D	273	LYS
1	E	25	LEU
1	E	37	LYS
1	E	67	VAL
1	E	93	ASN

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Mol	Chain	Res	Type
1	E	101	TYR
1	E	117	THR
1	E	195	LEU
1	E	204	MET
1	E	272	ASP
1	E	273	LYS
1	E	283	LYS
1	F	24	ASP
1	F	25	LEU
1	F	37	LYS
1	F	52	LEU
1	F	101	TYR
1	F	117	THR
1	F	195	LEU
1	F	204	MET
1	F	237	LYS
1	F	268	THR
1	F	272	ASP
1	G	60	THR
1	G	95	VAL
1	G	101	TYR
1	G	117	THR
1	G	179	TRP
1	G	195	LEU
1	G	240	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	64	GLN
1	A	74	ASN
1	A	123	ASN
1	A	144	HIS
1	A	178	ASN
1	A	259	HIS
1	B	64	GLN
1	B	74	ASN
1	B	89	GLN
1	B	139	ASN
1	B	144	HIS
1	B	178	ASN

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Mol	Chain	Res	Type
1	B	209	ASN
1	B	242	GLN
1	B	259	HIS
1	C	64	GLN
1	C	74	ASN
1	C	89	GLN
1	C	139	ASN
1	C	150	GLN
1	C	178	ASN
1	C	201	ASN
1	C	257	GLN
1	C	259	HIS
1	C	264	ASN
1	D	64	GLN
1	D	74	ASN
1	D	89	GLN
1	D	144	HIS
1	D	178	ASN
1	D	242	GLN
1	D	244	ASN
1	D	257	GLN
1	D	259	HIS
1	D	264	ASN
1	E	64	GLN
1	E	74	ASN
1	E	93	ASN
1	E	144	HIS
1	E	150	GLN
1	E	178	ASN
1	E	201	ASN
1	F	74	ASN
1	F	89	GLN
1	F	144	HIS
1	F	178	ASN
1	F	259	HIS
1	G	17	ASN
1	G	74	ASN
1	G	89	GLN
1	G	123	ASN
1	G	144	HIS
1	G	178	ASN
1	G	194	GLN

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Mol	Chain	Res	Type
1	G	201	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 ⓘ

14 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	H	1	2	11,11,12	1.67	3 (27%)	15,15,17	0.74	0
2	GLC	H	2	2	11,11,12	2.98	2 (18%)	15,15,17	2.68	6 (40%)
2	GLC	H	3	2	11,11,12	0.79	0	15,15,17	0.87	1 (6%)
2	GLC	H	4	2	11,11,12	1.29	1 (9%)	15,15,17	1.13	1 (6%)
2	GLC	H	5	2	11,11,12	0.99	0	15,15,17	1.28	2 (13%)
2	GLC	H	6	2	11,11,12	1.76	4 (36%)	15,15,17	1.10	0
2	GLC	H	7	2	11,11,12	1.43	2 (18%)	15,15,17	0.85	0
2	GLC	I	1	2	11,11,12	2.08	4 (36%)	15,15,17	1.02	1 (6%)
2	GLC	I	2	2	11,11,12	3.05	2 (18%)	15,15,17	2.63	5 (33%)
2	GLC	I	3	2	11,11,12	0.88	0	15,15,17	1.08	1 (6%)
2	GLC	I	4	2	11,11,12	1.58	2 (18%)	15,15,17	2.15	3 (20%)
2	GLC	I	5	2	11,11,12	0.86	0	15,15,17	1.13	2 (13%)
2	GLC	I	6	2	11,11,12	2.02	6 (54%)	15,15,17	1.44	3 (20%)
2	GLC	I	7	2	11,11,12	1.60	2 (18%)	15,15,17	1.00	1 (6%)

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	H	1	2	-	0/2/19/22	0/1/1/1
2	GLC	H	2	2	-	2/2/19/22	0/1/1/1
2	GLC	H	3	2	-	2/2/19/22	0/1/1/1
2	GLC	H	4	2	-	0/2/19/22	0/1/1/1
2	GLC	H	5	2	-	2/2/19/22	0/1/1/1
2	GLC	H	6	2	-	2/2/19/22	0/1/1/1
2	GLC	H	7	2	-	2/2/19/22	0/1/1/1
2	GLC	I	1	2	-	0/2/19/22	0/1/1/1
2	GLC	I	2	2	-	2/2/19/22	0/1/1/1
2	GLC	I	3	2	-	0/2/19/22	0/1/1/1
2	GLC	I	4	2	-	0/2/19/22	0/1/1/1
2	GLC	I	5	2	-	0/2/19/22	0/1/1/1
2	GLC	I	6	2	-	1/2/19/22	0/1/1/1
2	GLC	I	7	2	-	2/2/19/22	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	GLC	O5-C5	-9.33	1.25	1.43
2	I	2	GLC	O5-C5	-9.12	1.25	1.43
2	H	1	GLC	O5-C5	3.95	1.51	1.43
2	H	7	GLC	O5-C5	3.83	1.50	1.43
2	I	4	GLC	C1-C2	3.59	1.60	1.52
2	I	7	GLC	C2-C3	3.58	1.58	1.52
2	I	6	GLC	C4-C3	-3.42	1.43	1.52
2	I	7	GLC	O5-C5	3.33	1.49	1.43
2	I	2	GLC	C4-C5	3.28	1.60	1.53
2	H	4	GLC	C1-C2	3.26	1.60	1.52
2	H	6	GLC	O6-C6	-3.18	1.29	1.42
2	I	1	GLC	O5-C1	3.07	1.48	1.43
2	I	1	GLC	O5-C5	2.95	1.49	1.43
2	I	1	GLC	C2-C3	2.88	1.56	1.52
2	I	6	GLC	O6-C6	-2.83	1.30	1.42
2	H	6	GLC	O5-C5	2.81	1.48	1.43
2	I	6	GLC	O4-C4	2.68	1.49	1.43
2	H	2	GLC	C4-C5	2.59	1.58	1.53
2	H	1	GLC	O5-C1	2.48	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	4	GLC	O2-C2	-2.44	1.38	1.43
2	I	6	GLC	C2-C3	2.42	1.56	1.52
2	I	1	GLC	C4-C3	-2.34	1.46	1.52
2	H	1	GLC	C1-C2	2.23	1.57	1.52
2	H	6	GLC	O5-C1	2.22	1.47	1.43
2	I	6	GLC	O5-C5	2.21	1.47	1.43
2	H	7	GLC	C2-C3	2.09	1.55	1.52
2	H	6	GLC	C4-C3	-2.08	1.46	1.52
2	I	6	GLC	C6-C5	-2.06	1.44	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	GLC	C1-O5-C5	7.41	122.12	112.19
2	H	2	GLC	C1-O5-C5	7.12	121.72	112.19
2	I	4	GLC	C1-O5-C5	6.11	120.38	112.19
2	I	4	GLC	C6-C5-C4	-3.92	103.40	113.02
2	I	2	GLC	O5-C5-C6	3.87	115.19	107.66
2	H	2	GLC	O5-C5-C6	3.80	115.06	107.66
2	H	2	GLC	O4-C4-C5	3.21	117.23	109.32
2	H	5	GLC	O4-C4-C3	-3.20	102.82	110.38
2	H	4	GLC	C1-O5-C5	3.20	116.47	112.19
2	I	2	GLC	O4-C4-C5	3.02	116.76	109.32
2	I	3	GLC	C1-O5-C5	2.97	116.17	112.19
2	H	5	GLC	C1-O5-C5	2.76	115.88	112.19
2	I	7	GLC	C1-O5-C5	2.72	115.83	112.19
2	I	5	GLC	O4-C4-C3	-2.53	104.41	110.38
2	I	6	GLC	O6-C6-C5	-2.53	102.73	111.33
2	H	2	GLC	O6-C6-C5	-2.49	102.86	111.33
2	H	2	GLC	O2-C2-C3	2.40	115.13	110.15
2	I	5	GLC	C1-O5-C5	2.35	115.34	112.19
2	I	2	GLC	O2-C2-C3	2.31	114.94	110.15
2	I	4	GLC	C3-C4-C5	2.29	114.38	110.23
2	I	2	GLC	O6-C6-C5	-2.12	104.10	111.33
2	I	6	GLC	C1-C2-C3	2.09	112.68	109.64
2	H	2	GLC	O4-C4-C3	-2.07	105.50	110.38
2	I	1	GLC	O5-C1-C2	-2.07	105.86	110.79
2	I	6	GLC	O5-C5-C4	-2.05	105.85	110.83
2	H	3	GLC	C1-O5-C5	2.01	114.89	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	6	GLC	O5-C5-C6-O6
2	H	5	GLC	O5-C5-C6-O6
2	I	7	GLC	O5-C5-C6-O6
2	H	5	GLC	C4-C5-C6-O6
2	H	6	GLC	C4-C5-C6-O6
2	I	7	GLC	C4-C5-C6-O6
2	H	2	GLC	C4-C5-C6-O6
2	I	2	GLC	O5-C5-C6-O6
2	H	7	GLC	C4-C5-C6-O6
2	H	3	GLC	C4-C5-C6-O6
2	H	7	GLC	O5-C5-C6-O6
2	I	6	GLC	C4-C5-C6-O6
2	H	3	GLC	O5-C5-C6-O6
2	I	2	GLC	C4-C5-C6-O6
2	H	2	GLC	O5-C5-C6-O6

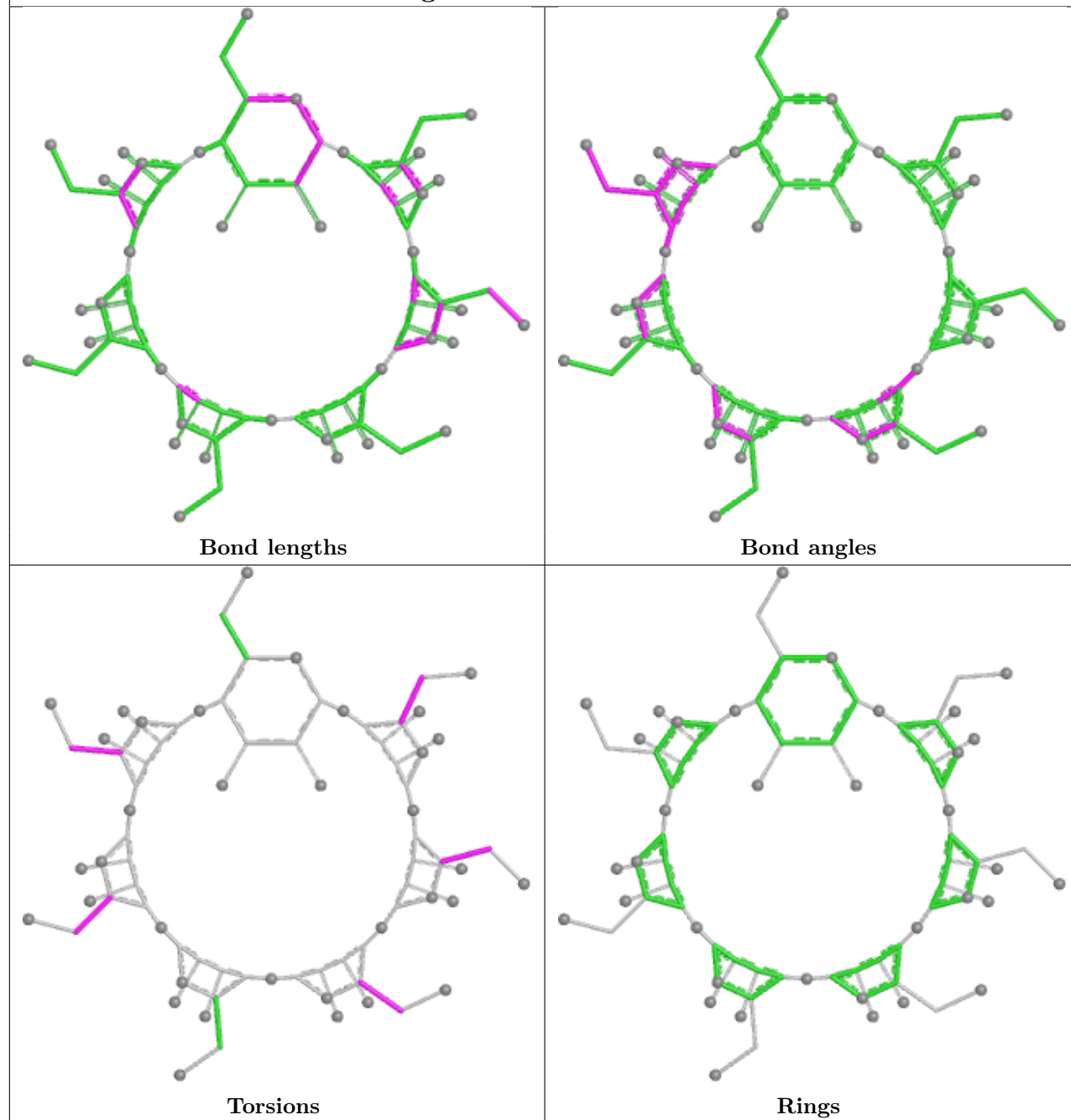
There are no ring outliers.

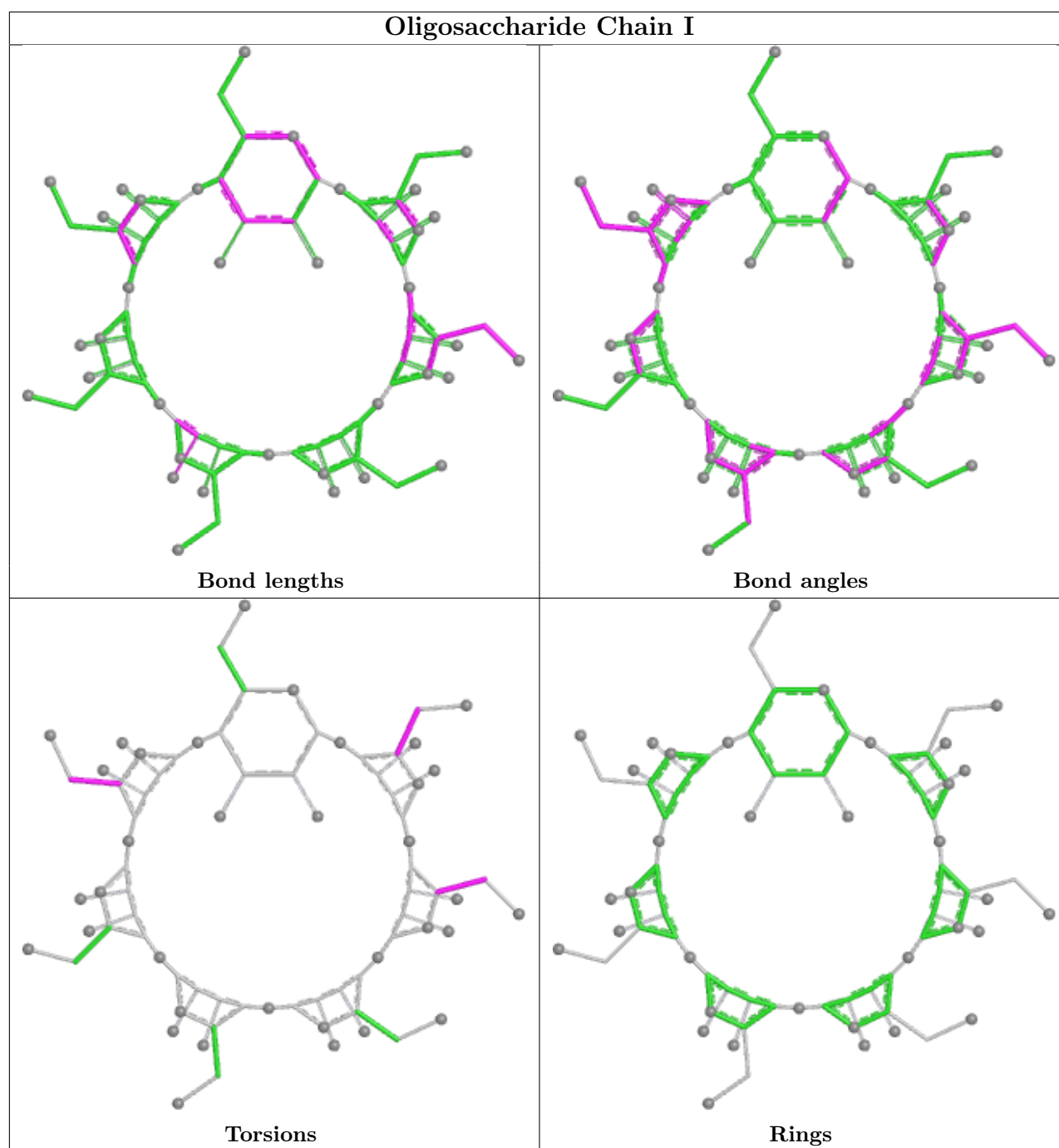
10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	GLC	4	0
2	I	2	GLC	3	0
2	H	4	GLC	1	0
2	H	3	GLC	2	0
2	I	3	GLC	2	0
2	H	1	GLC	2	0
2	I	1	GLC	5	0
2	I	6	GLC	1	0
2	H	7	GLC	2	0
2	I	7	GLC	2	0

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

Oligosaccharide Chain H





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	293/293 (100%)	0.42	30 (10%) 12 9	12, 38, 71, 96	13 (4%)
1	B	292/293 (99%)	0.35	26 (8%) 15 13	20, 36, 70, 95	12 (4%)
1	C	293/293 (100%)	0.23	27 (9%) 14 12	15, 36, 67, 92	16 (5%)
1	D	292/293 (99%)	0.28	24 (8%) 17 15	15, 37, 64, 81	19 (6%)
1	E	293/293 (100%)	0.41	28 (9%) 13 11	21, 39, 66, 88	17 (5%)
1	F	293/293 (100%)	0.39	28 (9%) 13 11	22, 38, 69, 90	19 (6%)
1	G	292/293 (99%)	0.33	19 (6%) 25 22	17, 38, 65, 91	16 (5%)
All	All	2048/2051 (99%)	0.35	182 (8%) 15 13	12, 38, 68, 96	112 (5%)

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	127	ASP	13.1
1	F	127	ASP	8.7
1	D	128	ASP	7.6
1	D	127	ASP	6.7
1	G	127	ASP	6.0
1	F	179	TRP	5.9
1	B	127	ASP	5.9
1	B	129	THR	5.8
1	D	124	VAL	5.7
1	G	125	THR	5.4
1	A	127	ASP	5.4
1	G	128	ASP	5.3
1	B	124	VAL	5.2
1	F	120	PHE	5.0
1	B	120	PHE	5.0
1	C	127	ASP	5.0
1	D	123	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	132	ILE	4.7
1	G	129	THR	4.7
1	G	120	PHE	4.6
1	G	179	TRP	4.5
1	E	126	GLY	4.5
1	A	144	HIS	4.5
1	E	118	TYR	4.4
1	E	124	VAL	4.4
1	F	136	ILE	4.3
1	A	129	THR	4.2
1	G	132	ILE	4.0
1	C	123	ASN	4.0
1	E	132	ILE	4.0
1	C	124	VAL	3.9
1	F	132	ILE	3.9
1	B	118	TYR	3.9
1	F	134	GLY	3.9
1	B	132	ILE	3.9
1	G	124	VAL	3.9
1	A	135	LEU	3.9
1	A	120	PHE	3.8
1	A	179	TRP	3.8
1	C	126	GLY	3.8
1	E	128	ASP	3.8
1	C	132	ILE	3.8
1	F	258	LEU	3.8
1	A	136	ILE	3.8
1	G	144	HIS	3.8
1	C	133	GLY	3.8
1	D	130	GLY	3.8
1	C	118	TYR	3.7
1	F	118	TYR	3.7
1	E	179	TRP	3.6
1	E	120	PHE	3.6
1	F	126	GLY	3.6
1	G	138	ALA	3.6
1	D	126	GLY	3.6
1	F	135	LEU	3.5
1	B	123	ASN	3.5
1	E	125	THR	3.5
1	F	124	VAL	3.5
1	C	144	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	134	GLY	3.4
1	E	135	LEU	3.4
1	A	133	GLY	3.4
1	E	122	GLY	3.4
1	B	144	HIS	3.3
1	D	179	TRP	3.3
1	F	200	ARG	3.2
1	A	131	LYS	3.2
1	E	130	GLY	3.2
1	D	136	ILE	3.2
1	A	261	THR	3.2
1	D	71	GLU	3.1
1	F	117	THR	3.1
1	C	72	GLY	3.1
1	E	136	ILE	3.1
1	C	179	TRP	3.1
1	A	126	GLY	3.1
1	C	120	PHE	3.1
1	C	128	ASP	3.1
1	B	136	ILE	3.0
1	G	136	ILE	3.0
1	B	130	GLY	3.0
1	C	130	GLY	3.0
1	G	133	GLY	3.0
1	B	138	ALA	3.0
1	C	138	ALA	3.0
1	A	200	ARG	3.0
1	G	200	ARG	3.0
1	C	93	ASN	3.0
1	A	258	LEU	2.9
1	F	131	LYS	2.9
1	A	128	ASP	2.9
1	B	133	GLY	2.9
1	F	72	GLY	2.9
1	A	124	VAL	2.9
1	A	71	GLU	2.9
1	F	128	ASP	2.9
1	E	117	THR	2.9
1	D	120	PHE	2.8
1	A	260	TRP	2.8
1	G	135	LEU	2.8
1	B	261	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	136	ILE	2.7
1	B	135	LEU	2.7
1	E	259	HIS	2.7
1	C	125	THR	2.7
1	E	137	GLY	2.7
1	F	180	GLY	2.7
1	F	73	ALA	2.7
1	B	125	THR	2.7
1	E	134	GLY	2.6
1	C	71	GLU	2.6
1	E	74	ASN	2.5
1	B	72	GLY	2.5
1	E	192	GLY	2.5
1	B	258	LEU	2.5
1	B	202	GLY	2.5
1	F	122	GLY	2.5
1	B	187	TRP	2.5
1	G	260	TRP	2.5
1	F	71	GLU	2.5
1	A	138	ALA	2.5
1	D	135	LEU	2.4
1	E	93	ASN	2.4
1	A	137	GLY	2.4
1	A	188	ASN	2.4
1	F	74	ASN	2.4
1	F	70	GLU	2.4
1	E	129	THR	2.4
1	G	117	THR	2.4
1	C	135	LEU	2.4
1	B	200	ARG	2.4
1	D	261	THR	2.4
1	A	148	TYR	2.3
1	E	201	ASN	2.3
1	G	93	ASN	2.3
1	A	130	GLY	2.3
1	E	73	ALA	2.3
1	D	144	HIS	2.3
1	B	179	TRP	2.3
1	D	118	TYR	2.3
1	A	202	GLY	2.3
1	D	200	ARG	2.3
1	F	259	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	189	PRO	2.3
1	A	134	GLY	2.3
1	C	200	ARG	2.3
1	F	129	THR	2.3
1	E	262	SER	2.3
1	C	74	ASN	2.2
1	B	143	GLY	2.2
1	B	73	ALA	2.2
1	F	130	GLY	2.2
1	B	131	LYS	2.2
1	A	263	THR	2.2
1	F	125	THR	2.2
1	E	123	ASN	2.2
1	C	73	ALA	2.2
1	D	134	GLY	2.2
1	C	191	TYR	2.1
1	B	201	ASN	2.1
1	D	188	ASN	2.1
1	D	75	LYS	2.1
1	G	131	LYS	2.1
1	A	268	THR	2.1
1	D	138	ALA	2.1
1	E	191	TYR	2.1
1	D	146	LEU	2.1
1	A	125	THR	2.1
1	C	131	LYS	2.1
1	E	70	GLU	2.1
1	F	188	ASN	2.1
1	C	129	THR	2.1
1	D	258	LEU	2.1
1	D	17	ASN	2.1
1	D	259	HIS	2.1
1	E	133	GLY	2.1
1	F	260	TRP	2.1
1	B	239	SER	2.0
1	A	201	ASN	2.0
1	A	189	PRO	2.0
1	D	93	ASN	2.0
1	G	123	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

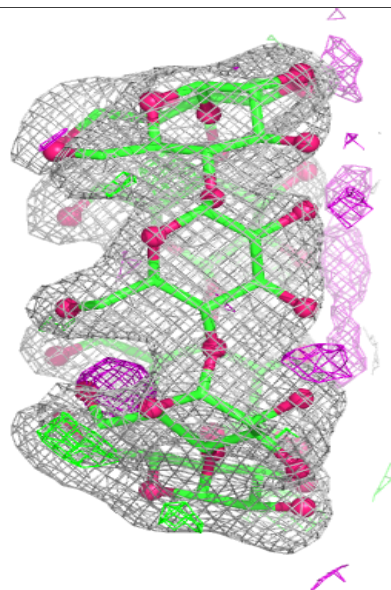
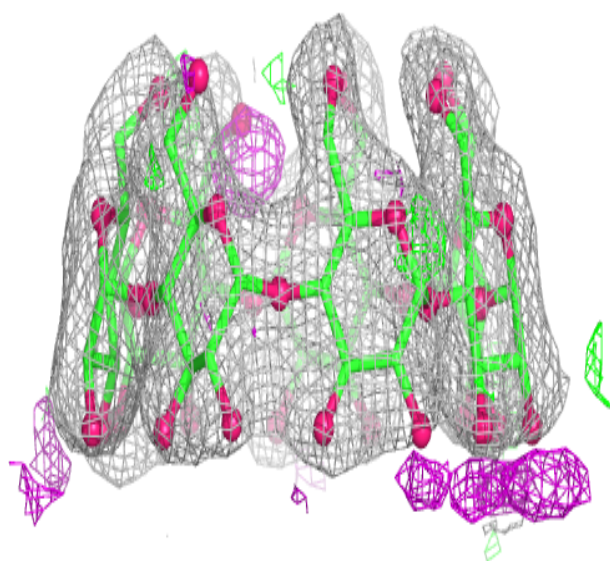
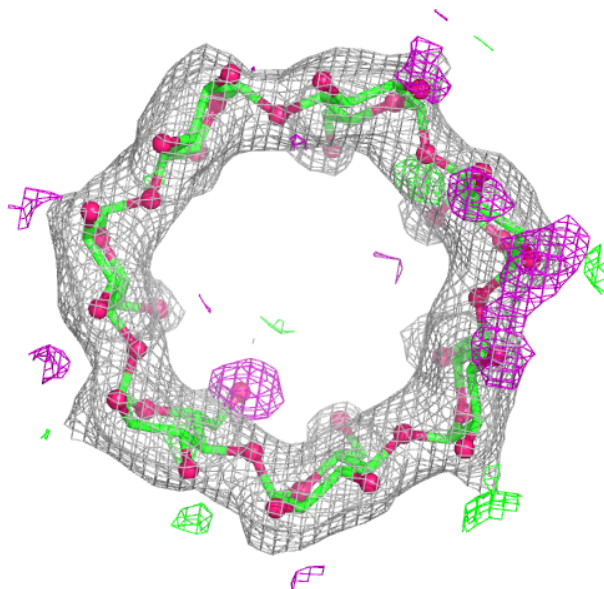
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

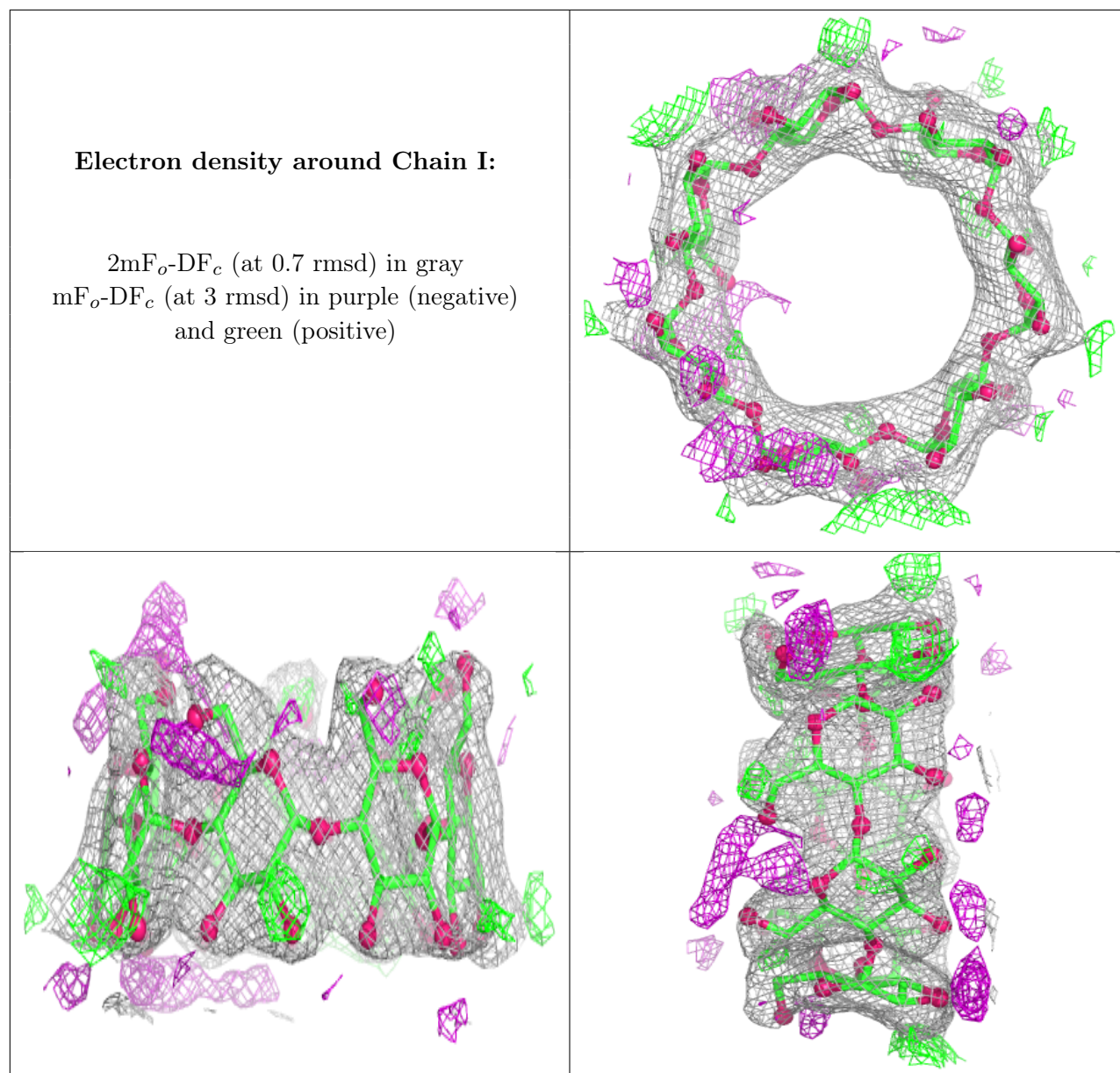
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	I	1	11/12	0.69	0.19	53,54,55,56	0
2	GLC	I	2	11/12	0.72	0.16	43,46,49,51	0
2	GLC	H	2	11/12	0.76	0.14	46,47,49,50	0
2	GLC	H	6	11/12	0.76	0.14	41,46,50,56	0
2	GLC	I	6	11/12	0.76	0.15	49,50,54,59	0
2	GLC	I	7	11/12	0.76	0.14	49,51,53,58	0
2	GLC	I	5	11/12	0.78	0.15	50,52,53,55	0
2	GLC	H	4	11/12	0.80	0.14	46,47,50,58	0
2	GLC	I	4	11/12	0.81	0.13	49,53,57,57	0
2	GLC	H	3	11/12	0.83	0.12	43,45,47,50	0
2	GLC	H	1	11/12	0.83	0.11	43,45,47,47	0
2	GLC	H	5	11/12	0.83	0.11	45,47,47,49	0
2	GLC	I	3	11/12	0.83	0.12	43,47,49,50	0
2	GLC	H	7	11/12	0.85	0.10	43,44,45,49	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 H:

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.