Full wwPDB X-ray Structure Validation Report (i)

Mar 13, 2024 – 02:48 PM JST

PDB ID	:	4XIG
Title	:	Crystal structure of bacterial alginate ABC transporter determined through humid air and glue-coating method
Authors	:	Kaneko, A.; Maruyama, Y.; Mizuno, N.; Baba, S.; Kumasaka, T.; Mikami, B.; Murata, K.; Hashimoto, W.
Deposited on	:	2015-01-07
Resolution	:	3.40 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 (i) 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 (i)) were used in the production of this report:

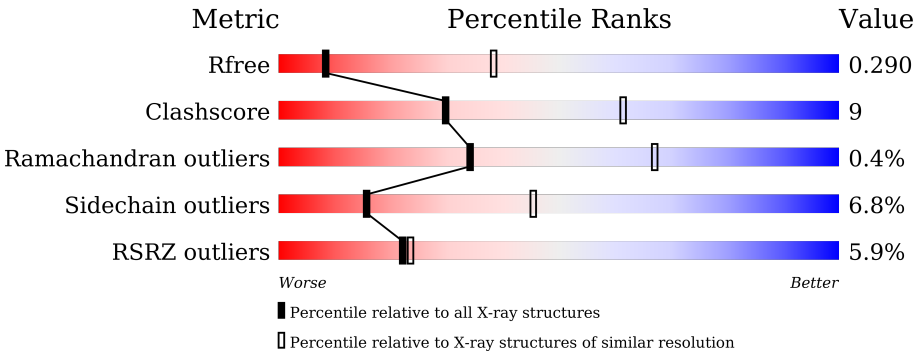
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 <=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	M	301	5% 69% 26%
2	N	305	4% 74% 18% 5%
3	S	363	6% 71% 24%
3	T	363	9% 63% 33%
4	Q	516	5% 71% 22% 5%
5	A	4	50% 50%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14266 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 AlgM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	M	288	2323	1554	369	390	10	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	?	-	THR	deletion	UNP Q9KWT8
M	?	-	SER	deletion	UNP Q9KWT8
M	?	-	ALA	deletion	UNP Q9KWT8
M	?	-	THR	deletion	UNP Q9KWT8
M	?	-	LYS	deletion	UNP Q9KWT8
M	?	-	ALA	deletion	UNP Q9KWT8
M	?	-	GLN	deletion	UNP Q9KWT8
M	?	-	SER	deletion	UNP Q9KWT8
M	?	-	ILE	deletion	UNP Q9KWT8
M	?	-	PRO	deletion	UNP Q9KWT8
M	?	-	LEU	deletion	UNP Q9KWT8
M	?	-	PRO	deletion	UNP Q9KWT8
M	?	-	ALA	deletion	UNP Q9KWT8
M	?	-	ALA	deletion	UNP Q9KWT8
M	?	-	THR	deletion	UNP Q9KWT8
M	?	-	LEU	deletion	UNP Q9KWT8
M	?	-	ASP	deletion	UNP Q9KWT8
M	?	-	VAL	deletion	UNP Q9KWT8
M	?	-	ARG	deletion	UNP Q9KWT8
M	?	-	SER	deletion	UNP Q9KWT8
M	?	-	LYS	deletion	UNP Q9KWT8
M	?	-	PRO	deletion	UNP Q9KWT8
M	?	-	LEU	deletion	UNP Q9KWT8

- Molecule 2 is a protein called AlgM2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	290	Total	C	N	O	S	0	0	0
			2293	1530	365	385	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	294	LEU	-	expression tag	UNP Q9KWT7
N	295	GLU	-	expression tag	UNP Q9KWT7
N	296	HIS	-	expression tag	UNP Q9KWT7
N	297	HIS	-	expression tag	UNP Q9KWT7
N	298	HIS	-	expression tag	UNP Q9KWT7
N	299	HIS	-	expression tag	UNP Q9KWT7
N	300	HIS	-	expression tag	UNP Q9KWT7
N	301	HIS	-	expression tag	UNP Q9KWT7
N	302	HIS	-	expression tag	UNP Q9KWT7
N	303	HIS	-	expression tag	UNP Q9KWT7
N	304	HIS	-	expression tag	UNP Q9KWT7
N	305	HIS	-	expression tag	UNP Q9KWT7

- Molecule 3 is a protein called AlgS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	363	Total	C	N	O	S	0	0	0
			2777	1745	503	518	11			
3	T	363	Total	C	N	O	S	0	0	0
			2777	1745	503	518	11			

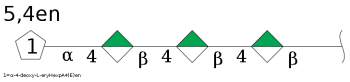
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	160	GLN	GLU	engineered mutation	UNP Q9KWT9
T	160	GLN	GLU	engineered mutation	UNP Q9KWT9

- Molecule 4 is a protein called AlgQ2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Q	492	Total	C	N	O	S	0	0	0
			4048	2604	693	735	16			

- Molecule 5 is an oligosaccharide called 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid.

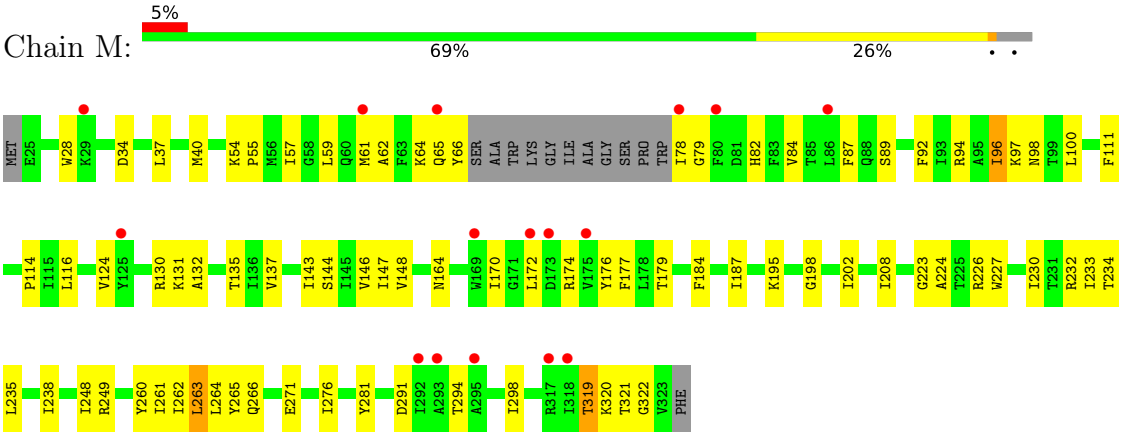


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	A	4	Total C O 48 24 24	0	0	0

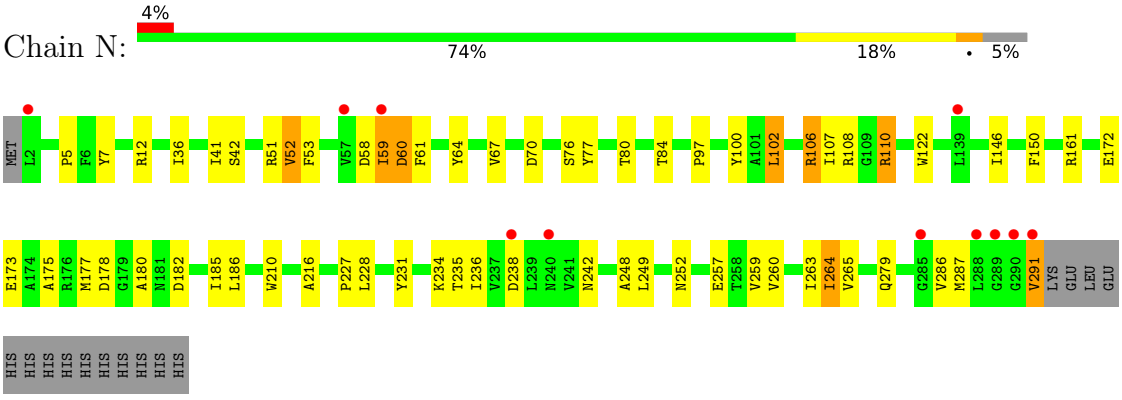
3 Residue-property plots (i)

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.

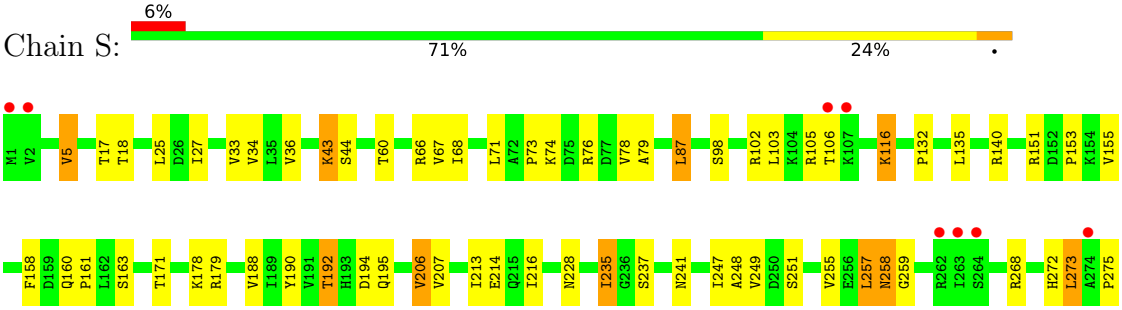
• Molecule 1: AlgM1

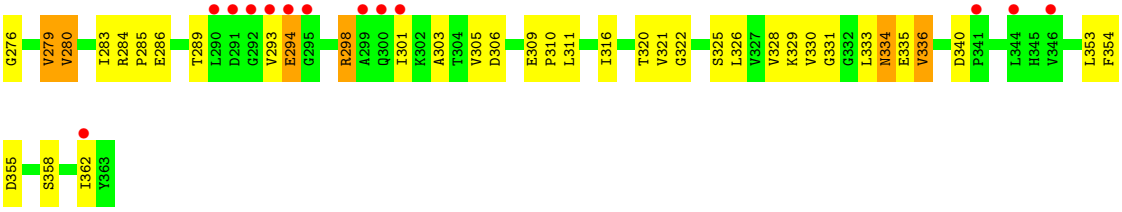


• Molecule 2: AlgM2

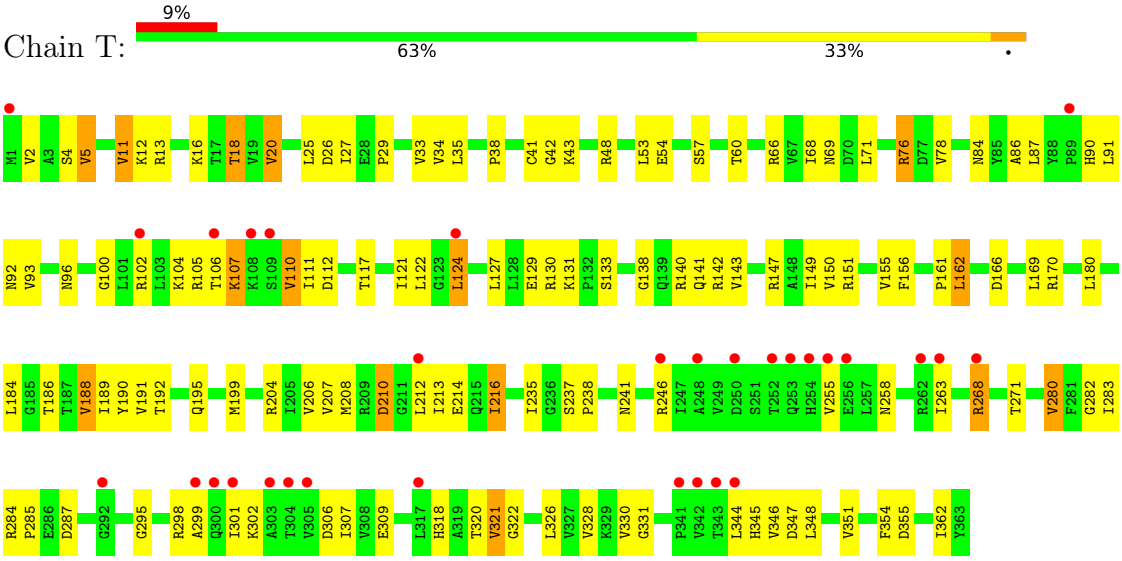


• Molecule 3: AlgS

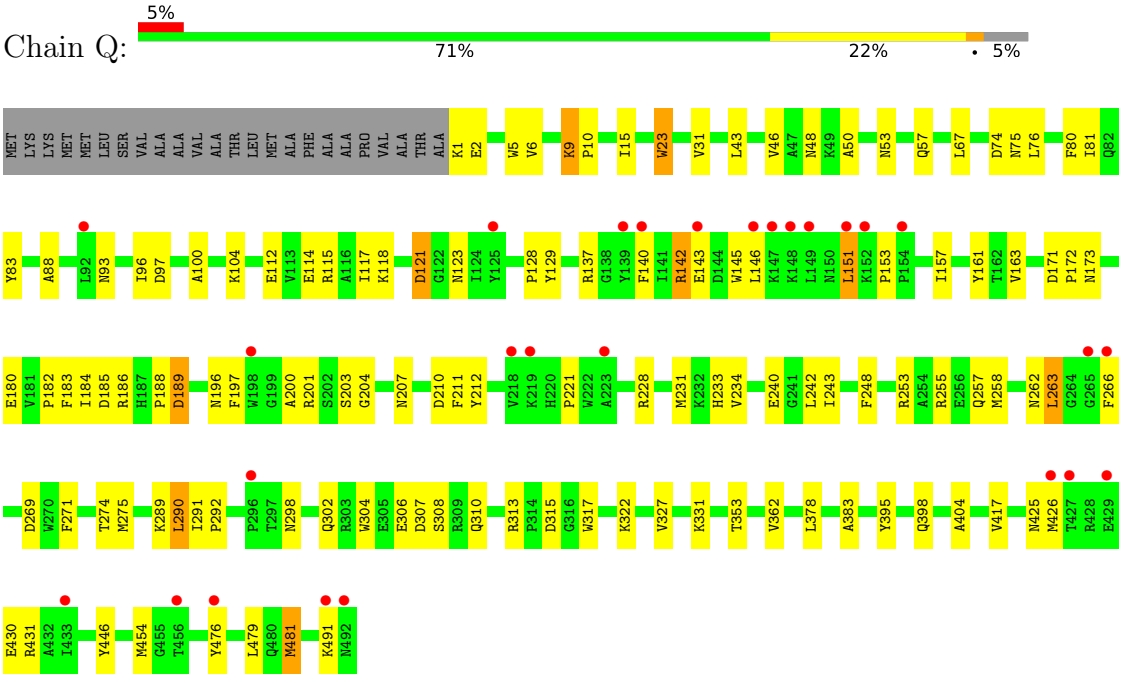




• Molecule 3: AlgS



• Molecule 4: AlgQ2



• Molecule 5: 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid

Chain A:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.17Å 133.41Å 272.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.56 – 3.40 37.56 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (37.56-3.40) 99.7 (37.56-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.29 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.236 , 0.289 0.239 , 0.290	Depositor DCC
R_{free} test set	1846 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	110.5	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 68.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14266	wwPDB-VP
Average B, all atoms (Å^2)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MAW, BEM

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	M	0.23	0/2384	0.42	0/3250
2	N	0.25	0/2352	0.44	0/3198
3	S	0.23	0/2822	0.50	0/3826
3	T	0.22	0/2822	0.48	0/3826
4	Q	0.21	0/4168	0.37	0/5640
All	All	0.23	0/14548	0.44	0/19740

There are no bond length outliers.

There are no bond angle outliers.

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	M	2323	0	2412	43	0
2	N	2293	0	2362	41	0
3	S	2777	0	2854	58	0
3	T	2777	0	2854	80	0
4	Q	4048	0	3920	67	0
5	A	48	0	25	0	0
All	All	14266	0	14427	270	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 9.

All (270) 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)
3:S:43:LYS:HD3	3:S:44:SER:H	1.43	0.84
3:T:34:VAL:HG22	3:T:190:TYR:HB3	1.68	0.75
3:T:48:ARG:HG3	3:T:53:LEU:HB2	1.69	0.75
3:S:34:VAL:HG22	3:S:190:TYR:HB3	1.69	0.74
3:T:141:GLN:NE2	3:T:161:PRO:O	2.24	0.71
1:M:98:ASN:ND2	1:M:271:GLU:O	2.23	0.71
2:N:52:VAL:HG13	2:N:53:PHE:H	1.57	0.70
3:T:207:VAL:HG23	3:T:214:GLU:HB3	1.73	0.69
4:Q:142:ARG:NH2	4:Q:262:ASN:OD1	2.26	0.69
2:N:248:ALA:O	2:N:252:ASN:ND2	2.26	0.69
3:S:248:ALA:H	3:S:276:GLY:H	1.41	0.68
2:N:287:MET:SD	2:N:287:MET:N	2.67	0.67
1:M:143:ILE:O	1:M:195:LYS:NZ	2.27	0.67
3:S:78:VAL:HG12	3:S:155:VAL:HB	1.77	0.67
3:S:241:ASN:ND2	3:S:283:ILE:O	2.27	0.67
3:T:41:CYS:SG	3:T:42:GLY:N	2.68	0.66
3:T:93:VAL:HG13	3:T:143:VAL:HG21	1.78	0.65
1:M:148:VAL:HG21	1:M:195:LYS:HD2	1.78	0.65
2:N:42:SER:HA	2:N:59:ILE:HA	1.77	0.65
3:S:258:ASN:ND2	3:S:322:GLY:HA3	2.12	0.65
3:T:280:VAL:HG13	3:T:354:PHE:HB2	1.79	0.65
4:Q:97:ASP:HA	4:Q:104:LYS:HD3	1.77	0.64
3:T:48:ARG:HG2	3:T:54:GLU:HG3	1.78	0.64
3:T:5:VAL:HG13	3:T:27:ILE:HB	1.78	0.64
3:T:78:VAL:HG12	3:T:155:VAL:HB	1.80	0.64
3:T:238:PRO:HB2	3:T:285:PRO:HG2	1.79	0.64
4:Q:255:ARG:NH1	4:Q:269:ASP:OD2	2.32	0.63
3:T:237:SER:HB3	3:T:238:PRO:HD3	1.80	0.63
3:T:20:VAL:HG13	3:T:42:GLY:HA3	1.81	0.62
3:S:235:ILE:HD11	3:S:284:ARG:HH12	1.65	0.61
4:Q:378:LEU:HB3	4:Q:383:ALA:HB3	1.82	0.61
3:T:12:LYS:H	3:T:20:VAL:HG23	1.65	0.61
4:Q:157:ILE:HD13	4:Q:197:PHE:HB3	1.83	0.61
3:T:213:ILE:HD11	3:T:216:ILE:HG12	1.83	0.61
4:Q:96:ILE:HA	4:Q:100:ALA:HB3	1.83	0.60
3:S:195:GLN:HG3	3:S:235:ILE:HA	1.82	0.60
4:Q:146:LEU:HD13	4:Q:153:PRO:HG3	1.81	0.60
3:T:355:ASP:HB2	3:T:362:ILE:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:253:ARG:HH11	4:Q:257:GLN:HE22	1.48	0.60
3:T:4:SER:HB3	3:T:29:PRO:HD3	1.83	0.60
3:T:110:VAL:O	3:T:112:ASP:N	2.34	0.60
1:M:54:LYS:HD2	1:M:57:ILE:HD12	1.82	0.60
3:S:74:LYS:O	3:S:151:ARG:NH2	2.34	0.59
3:S:273:LEU:HD23	3:S:273:LEU:H	1.67	0.59
1:M:146:VAL:HG12	1:M:263:LEU:HD21	1.83	0.59
2:N:80:THR:HG23	2:N:228:LEU:H	1.67	0.58
2:N:58:ASP:O	2:N:59:ILE:HG13	2.03	0.58
4:Q:188:PRO:HB3	4:Q:248:PHE:HA	1.86	0.58
4:Q:196:ASN:ND2	4:Q:200:ALA:O	2.37	0.58
1:M:34:ASP:OD1	2:N:106:ARG:NH1	2.36	0.57
3:T:26:ASP:O	3:T:204:ARG:NH2	2.37	0.57
2:N:234:LYS:HD2	4:Q:50:ALA:HA	1.86	0.57
3:S:247:ILE:HG12	3:S:255:VAL:HG22	1.87	0.57
3:S:207:VAL:HG13	3:S:214:GLU:HB3	1.87	0.57
3:T:110:VAL:C	3:T:112:ASP:H	2.09	0.57
4:Q:430:GLU:HB2	4:Q:481:MET:HG3	1.87	0.56
1:M:291:ASP:OD1	1:M:291:ASP:N	2.39	0.56
2:N:102:LEU:HB3	2:N:161:ARG:HD3	1.88	0.56
2:N:107:ILE:HB	2:N:110:ARG:HB2	1.87	0.56
2:N:106:ARG:NH2	2:N:172:GLU:OE2	2.39	0.56
3:S:213:ILE:HD11	3:S:216:ILE:HG12	1.89	0.55
3:T:105:ARG:O	3:T:106:THR:OG1	2.24	0.55
3:T:38:PRO:O	3:T:43:LYS:NZ	2.34	0.55
4:Q:74:ASP:OD2	4:Q:75:ASN:ND2	2.35	0.54
3:T:258:ASN:HB3	3:T:322:GLY:HA3	1.88	0.54
1:M:223:GLY:HA3	3:S:74:LYS:HD3	1.89	0.54
3:S:5:VAL:HG13	3:S:27:ILE:HB	1.89	0.54
3:S:306:ASP:HB2	3:S:320:THR:HG23	1.89	0.54
2:N:41:ILE:O	2:N:60:ASP:N	2.41	0.54
3:S:98:SER:OG	3:S:102:ARG:NH1	2.40	0.54
4:Q:67:LEU:HB2	4:Q:322:LYS:HD2	1.88	0.54
4:Q:171:ASP:OD1	4:Q:173:ASN:ND2	2.41	0.54
1:M:94:ARG:HA	1:M:97:LYS:HB3	1.90	0.54
2:N:234:LYS:O	2:N:238:ASP:HB2	2.08	0.53
3:T:106:THR:HG22	3:T:107:LYS:H	1.73	0.53
3:S:192:THR:HG22	3:S:194:ASP:H	1.74	0.53
3:S:280:VAL:HG13	3:S:354:PHE:HB2	1.89	0.53
3:S:286:GLU:HG3	3:S:329:LYS:HD3	1.91	0.53
4:Q:140:PHE:CZ	4:Q:271:PHE:HA	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:362:VAL:HA	4:Q:398:GLN:HE22	1.73	0.53
1:M:321:THR:OG1	1:M:322:GLY:N	2.40	0.52
3:T:107:LYS:O	3:T:110:VAL:N	2.33	0.52
3:S:355:ASP:HB3	3:S:358:SER:O	2.10	0.52
3:T:195:GLN:HG3	3:T:235:ILE:HA	1.90	0.52
1:M:226:ARG:HH12	2:N:5:PRO:HG2	1.74	0.52
1:M:248:ILE:HG12	2:N:122:TRP:HH2	1.75	0.52
2:N:70:ASP:OD2	2:N:231:TYR:OH	2.21	0.52
3:T:255:VAL:HG13	3:T:263:ILE:HB	1.91	0.52
4:Q:207:ASN:OD1	4:Q:310:GLN:NE2	2.35	0.51
2:N:84:THR:HG21	2:N:210:TRP:HE3	1.75	0.51
2:N:178:ASP:OD1	3:T:151:ARG:NH2	2.43	0.51
4:Q:182:PRO:HG2	4:Q:242:LEU:HA	1.92	0.51
4:Q:2:GLU:HB2	4:Q:5:TRP:CD1	2.45	0.51
3:T:184:LEU:HG	3:T:186:THR:HG23	1.93	0.51
3:S:178:LYS:HE3	3:T:307:ILE:HD11	1.92	0.51
3:T:102:ARG:NH1	3:T:106:THR:OG1	2.44	0.51
4:Q:231:MET:HA	4:Q:234:VAL:HG22	1.93	0.51
3:T:117:THR:O	3:T:121:ILE:HG12	2.10	0.51
3:S:251:SER:HB3	3:S:275:PRO:HB3	1.92	0.51
3:T:295:GLY:HA2	3:T:345:HIS:NE2	2.26	0.51
1:M:64:LYS:HG3	1:M:65:GLN:H	1.76	0.50
1:M:227:TRP:HA	1:M:230:ILE:HG12	1.94	0.50
3:S:272:HIS:O	3:S:272:HIS:ND1	2.44	0.50
4:Q:184:ILE:HD13	4:Q:258:MET:HB2	1.94	0.50
1:M:260:TYR:CZ	1:M:264:LEU:HD12	2.47	0.50
4:Q:426:MET:HB3	4:Q:430:GLU:HG3	1.93	0.50
3:T:41:CYS:HB3	3:T:43:LYS:HZ3	1.77	0.50
3:T:71:LEU:HB3	3:T:76:ARG:HH21	1.77	0.50
3:T:35:LEU:HD12	3:T:191:VAL:HG22	1.94	0.50
1:M:62:ALA:HB3	1:M:294:THR:HG21	1.92	0.50
3:T:124:LEU:HB2	3:T:127:LEU:HB2	1.93	0.50
3:T:321:VAL:HG23	3:T:322:GLY:H	1.76	0.50
2:N:59:ILE:HD13	2:N:61:PHE:HD2	1.76	0.50
3:S:214:GLU:HG3	3:S:228:ASN:HD21	1.76	0.50
4:Q:76:LEU:O	4:Q:80:PHE:N	2.38	0.50
4:Q:204:GLY:HA3	4:Q:212:TYR:HB3	1.94	0.49
4:Q:140:PHE:HB3	4:Q:290:LEU:HD22	1.94	0.49
3:S:68:ILE:HB	3:S:76:ARG:HG2	1.94	0.49
3:T:241:ASN:O	3:T:282:GLY:HA2	2.13	0.49
4:Q:114:GLU:HG2	4:Q:118:LYS:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:35:LEU:HD11	3:T:189:ILE:HD11	1.94	0.49
3:T:210:ASP:OD1	3:T:210:ASP:N	2.43	0.49
4:Q:93:ASN:HD21	4:Q:123:ASN:HA	1.78	0.49
3:T:76:ARG:HB3	3:T:78:VAL:HG22	1.94	0.49
3:T:156:PHE:HB2	3:T:188:VAL:HB	1.95	0.49
3:S:320:THR:HG22	3:S:325:SER:HB2	1.94	0.48
3:T:11:VAL:O	3:T:57:SER:OG	2.23	0.48
1:M:137:VAL:HG12	1:M:198:GLY:HA3	1.95	0.48
4:Q:15:ILE:HG21	4:Q:43:LEU:HB3	1.95	0.48
4:Q:173:ASN:ND2	4:Q:180:GLU:OE1	2.42	0.48
3:T:283:ILE:HD13	3:T:351:VAL:HG12	1.95	0.48
3:S:43:LYS:HD2	3:S:43:LYS:H	1.79	0.48
4:Q:31:VAL:HG21	4:Q:383:ALA:HB2	1.96	0.48
4:Q:143:GLU:HG2	4:Q:289:LYS:HD2	1.95	0.48
2:N:64:TYR:HA	2:N:67:VAL:HG12	1.96	0.48
1:M:184:PHE:HZ	1:M:261:ILE:HG12	1.79	0.48
1:M:224:ALA:HB2	3:S:103:LEU:HD21	1.95	0.48
1:M:208:ILE:HG23	1:M:238:ILE:HD12	1.96	0.48
4:Q:145:TRP:CD2	4:Q:172:PRO:HB2	2.49	0.48
1:M:84:VAL:HA	1:M:87:PHE:HB2	1.96	0.47
4:Q:476:TYR:HA	4:Q:479:LEU:HB2	1.97	0.47
1:M:319:THR:HG22	1:M:320:LYS:H	1.80	0.47
2:N:60:ASP:O	2:N:61:PHE:HB2	2.14	0.47
1:M:111:PHE:O	1:M:114:PRO:HD2	2.14	0.47
3:S:279:VAL:HG21	3:S:353:LEU:HD23	1.97	0.47
1:M:177:PHE:HB3	1:M:187:ILE:HD11	1.97	0.47
3:S:87:LEU:HD11	3:S:140:ARG:HB3	1.97	0.47
2:N:231:TYR:O	2:N:235:THR:HG22	2.14	0.47
3:S:43:LYS:HD3	3:S:44:SER:N	2.22	0.47
1:M:37:LEU:HD23	2:N:107:ILE:HD11	1.97	0.47
4:Q:151:LEU:HD13	4:Q:163:VAL:HG22	1.96	0.47
3:S:330:VAL:HG22	3:S:331:GLY:H	1.79	0.46
4:Q:129:TYR:HB3	4:Q:315:ASP:HB2	1.96	0.46
3:S:160:GLN:HB3	3:S:163:SER:OG	2.16	0.46
1:M:262:ILE:HD11	1:M:281:TYR:CZ	2.51	0.46
3:S:206:VAL:HB	3:S:216:ILE:HG23	1.97	0.46
3:T:2:VAL:HG12	3:T:29:PRO:HB2	1.98	0.46
4:Q:121:ASP:OD1	4:Q:123:ASN:ND2	2.36	0.46
1:M:164:ASN:HB3	1:M:174:ARG:HG2	1.97	0.46
4:Q:183:PHE:HD2	4:Q:243:ILE:HG23	1.81	0.46
4:Q:6:VAL:HB	4:Q:331:LYS:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:92:ASN:O	3:T:96:ASN:N	2.46	0.46
1:M:179:THR:OG1	4:Q:454:MET:SD	2.65	0.45
3:T:60:THR:HA	3:T:69:ASN:HD21	1.81	0.45
3:S:66:ARG:HD3	3:S:71:LEU:HD22	1.99	0.45
2:N:242:ASN:HB3	4:Q:23:TRP:CZ2	2.52	0.45
2:N:260:VAL:O	2:N:264:ILE:HG23	2.17	0.45
4:Q:203:SER:N	4:Q:306:GLU:OE1	2.49	0.45
1:M:78:ILE:HA	1:M:79:GLY:HA3	1.61	0.45
3:T:66:ARG:HH11	3:T:71:LEU:HD11	1.82	0.45
3:T:138:GLY:HA3	3:T:169:LEU:HD21	1.99	0.44
3:S:258:ASN:HB3	3:S:259:GLY:H	1.42	0.44
3:S:309:GLU:HB2	3:S:316:ILE:HB	1.98	0.44
1:M:132:ALA:O	1:M:135:THR:OG1	2.31	0.44
2:N:173:GLU:HB3	3:T:53:LEU:HD13	2.00	0.44
1:M:232:ARG:HH21	3:S:105:ARG:HH21	1.66	0.44
3:S:298:ARG:HD2	3:S:298:ARG:N	2.33	0.44
4:Q:137:ARG:NH1	4:Q:307:ASP:OD2	2.45	0.44
4:Q:258:MET:O	4:Q:263:LEU:N	2.46	0.44
3:S:116:LYS:HE3	3:S:116:LYS:HB3	1.55	0.44
3:T:301:ILE:HG22	3:T:344:LEU:HB2	2.00	0.44
3:T:87:LEU:HA	3:T:147:ARG:NH1	2.33	0.44
3:T:90:HIS:CE1	3:T:91:LEU:HG	2.53	0.44
3:S:17:THR:O	3:S:18:THR:OG1	2.34	0.43
4:Q:313:ARG:O	4:Q:315:ASP:N	2.48	0.43
3:T:330:VAL:HG12	3:T:331:GLY:H	1.83	0.43
3:T:162:LEU:HD22	3:T:162:LEU:H	1.83	0.43
4:Q:53:ASN:O	4:Q:57:GLN:HG2	2.19	0.43
3:T:129:GLU:O	3:T:130:ARG:HG2	2.18	0.43
2:N:175:ALA:HB1	2:N:180:ALA:HB3	2.01	0.43
3:T:131:LYS:HE2	3:T:133:SER:HB2	1.99	0.43
3:T:302:LYS:O	3:T:321:VAL:HG12	2.19	0.43
1:M:65:GLN:HB3	1:M:66:TYR:CD2	2.54	0.43
1:M:202:ILE:HG21	2:N:291:VAL:HG22	2.00	0.43
3:S:310:PRO:HG2	3:T:199:MET:O	2.19	0.43
3:S:334:ASN:O	3:S:334:ASN:ND2	2.52	0.43
4:Q:189:ASP:N	4:Q:189:ASP:OD1	2.51	0.43
3:T:268:ARG:O	3:T:271:THR:HG23	2.18	0.43
3:T:299:ALA:HB3	3:T:345:HIS:CD2	2.54	0.43
2:N:76:SER:HB3	2:N:228:LEU:HA	2.01	0.42
4:Q:308:SER:HB3	4:Q:417:VAL:HG13	2.01	0.42
3:T:284:ARG:HB2	3:T:287:ASP:OD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:275:MET:HG3	4:Q:404:ALA:HB2	2.01	0.42
2:N:177:MET:HG2	3:T:53:LEU:HD21	2.02	0.42
3:T:309:GLU:OE2	3:T:318:HIS:NE2	2.52	0.42
3:T:38:PRO:HD2	3:T:208:MET:O	2.19	0.42
4:Q:298:ASN:HD21	4:Q:302:GLN:HB2	1.85	0.42
3:T:25:LEU:HD21	3:T:33:VAL:HG21	2.00	0.42
3:T:149:ILE:HG22	3:T:156:PHE:CZ	2.55	0.42
2:N:286:VAL:HG12	2:N:287:MET:HG2	2.02	0.42
4:Q:129:TYR:HE2	4:Q:313:ARG:HD3	1.84	0.42
3:S:105:ARG:O	3:S:106:THR:OG1	2.33	0.42
1:M:54:LYS:HB3	1:M:55:PRO:HD3	2.01	0.42
2:N:100:TYR:CD1	2:N:186:LEU:HD13	2.54	0.42
3:T:84:ASN:C	3:T:86:ALA:H	2.23	0.42
4:Q:9:LYS:HA	4:Q:10:PRO:HD3	1.93	0.42
4:Q:302:GLN:OE1	4:Q:304:TRP:NE1	2.51	0.42
1:M:59:LEU:HD11	1:M:298:ILE:HG12	2.01	0.42
3:S:132:PRO:HA	3:S:135:LEU:HD12	2.01	0.42
3:S:303:ALA:HB2	3:S:321:VAL:HG22	2.01	0.42
4:Q:184:ILE:HG21	4:Q:258:MET:HG3	2.01	0.42
4:Q:186:ARG:NE	4:Q:269:ASP:OD1	2.52	0.42
4:Q:274:THR:HG22	4:Q:290:LEU:HD13	2.02	0.42
1:M:124:VAL:HB	1:M:130:ARG:HD3	2.02	0.41
2:N:216:ALA:HB1	2:N:227:PRO:HG3	2.01	0.41
3:S:87:LEU:H	3:S:87:LEU:HD13	1.85	0.41
4:Q:183:PHE:HD1	4:Q:266:PHE:HD2	1.68	0.41
3:T:87:LEU:HD21	3:T:140:ARG:CZ	2.50	0.41
3:T:122:LEU:HD22	3:T:142:ARG:HG3	2.02	0.41
1:M:135:THR:HG22	2:N:279:GLN:OE1	2.20	0.41
3:S:284:ARG:HA	3:S:285:PRO:HD3	1.90	0.41
4:Q:117:ILE:HD13	4:Q:128:PRO:HG3	2.02	0.41
2:N:259:VAL:O	2:N:263:ILE:HG13	2.20	0.41
3:S:79:ALA:HB3	3:S:153:PRO:HG3	2.02	0.41
3:S:334:ASN:O	3:S:336:VAL:HG23	2.20	0.41
4:Q:173:ASN:ND2	4:Q:173:ASN:H	2.19	0.41
3:T:11:VAL:HG23	3:T:20:VAL:O	2.20	0.41
1:M:40:MET:HB3	2:N:97:PRO:HB2	2.02	0.41
3:S:158:PHE:HB3	3:S:161:PRO:HG3	2.02	0.41
4:Q:201:ARG:O	4:Q:221:PRO:HB2	2.20	0.41
3:T:13:ARG:HG2	3:T:18:THR:HB	2.02	0.41
1:M:89:SER:OG	1:M:92:PHE:HB3	2.20	0.41
1:M:131:LYS:O	1:M:135:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:7:TYR:CE2	3:S:73:PRO:HD3	2.56	0.41
2:N:36:ILE:HD13	2:N:264:ILE:HD11	2.01	0.41
3:S:36:VAL:O	3:S:207:VAL:HA	2.21	0.41
3:S:257:LEU:HD21	3:S:301:ILE:HD11	2.03	0.41
3:T:100:GLY:HA3	3:T:151:ARG:HH22	1.85	0.41
1:M:144:SER:HB3	1:M:147:ILE:HG13	2.01	0.41
2:N:235:THR:HG23	2:N:236:ILE:HG12	2.03	0.41
3:S:25:LEU:HD21	3:S:33:VAL:HG21	2.02	0.41
3:T:166:ASP:O	3:T:170:ARG:N	2.51	0.41
3:S:293:VAL:C	3:S:294:GLU:HG3	2.40	0.41
4:Q:115:ARG:HG3	4:Q:425:ASN:HD21	1.84	0.41
2:N:264:ILE:HG13	2:N:265:VAL:N	2.33	0.41
3:S:305:VAL:HG12	3:S:340:ASP:O	2.21	0.41
4:Q:81:ILE:HD12	4:Q:431:ARG:NH2	2.36	0.41
4:Q:291:ILE:HA	4:Q:292:PRO:HD3	1.93	0.41
2:N:182:ASP:O	2:N:185:ILE:HB	2.21	0.40
1:M:96:ILE:HD13	1:M:276:ILE:HD11	2.03	0.40
1:M:233:ILE:HG13	1:M:234:THR:H	1.86	0.40
3:T:147:ARG:O	3:T:150:VAL:HG12	2.22	0.40
3:T:330:VAL:HG12	3:T:331:GLY:N	2.36	0.40
3:T:347:ASP:O	3:T:351:VAL:HG13	2.21	0.40
4:Q:210:ASP:OD1	4:Q:211:PHE:N	2.53	0.40
4:Q:161:TYR:OH	4:Q:240:GLU:OE2	2.40	0.40
4:Q:83:TYR:HB3	4:Q:88:ALA:HB3	2.04	0.40
4:Q:203:SER:HA	4:Q:221:PRO:HG3	2.03	0.40
3:T:68:ILE:HB	3:T:76:ARG:HD2	2.04	0.40
3:T:306:ASP:HB2	3:T:320:THR:HG23	2.04	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	M	284/301 (94%)	268 (94%)	16 (6%)	0	100	100
2	N	288/305 (94%)	258 (90%)	28 (10%)	2 (1%)	22	55
3	S	361/363 (99%)	330 (91%)	27 (8%)	4 (1%)	14	44
3	T	361/363 (99%)	334 (92%)	25 (7%)	2 (1%)	25	57
4	Q	490/516 (95%)	460 (94%)	30 (6%)	0	100	100
All	All	1784/1848 (96%)	1650 (92%)	126 (7%)	8 (0%)	34	67

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	59	ILE
3	T	111	ILE
2	N	52	VAL
3	S	249	VAL
3	S	336	VAL
3	S	334	ASN
3	T	110	VAL
3	S	362	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	251/260 (96%)	236 (94%)	15 (6%)	19	49
2	N	243/258 (94%)	229 (94%)	14 (6%)	20	50
3	S	307/307 (100%)	280 (91%)	27 (9%)	10	33
3	T	307/307 (100%)	281 (92%)	26 (8%)	10	35
4	Q	424/440 (96%)	402 (95%)	22 (5%)	23	53
All	All	1532/1572 (98%)	1428 (93%)	104 (7%)	16	45

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	28	TRP
1	M	61	MET
1	M	82	HIS
1	M	96	ILE
1	M	100	LEU
1	M	116	LEU
1	M	170	ILE
1	M	172	LEU
1	M	176	TYR
1	M	235	LEU
1	M	249	ARG
1	M	263	LEU
1	M	265	TYR
1	M	266	GLN
1	M	319	THR
2	N	12	ARG
2	N	51	ARG
2	N	60	ASP
2	N	77	TYR
2	N	102	LEU
2	N	106	ARG
2	N	108	ARG
2	N	110	ARG
2	N	146	ILE
2	N	150	PHE
2	N	249	LEU
2	N	257	GLU
2	N	264	ILE
2	N	291	VAL
3	S	5	VAL
3	S	43	LYS
3	S	60	THR
3	S	67	VAL
3	S	87	LEU
3	S	116	LYS
3	S	171	THR
3	S	179	ARG
3	S	188	VAL
3	S	192	THR
3	S	206	VAL
3	S	235	ILE
3	S	237	SER
3	S	257	LEU

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Mol	Chain	Res	Type
3	S	258	ASN
3	S	268	ARG
3	S	273	LEU
3	S	279	VAL
3	S	280	VAL
3	S	289	THR
3	S	294	GLU
3	S	298	ARG
3	S	311	LEU
3	S	326	LEU
3	S	328	VAL
3	S	333	LEU
3	S	335	GLU
4	Q	1	LYS
4	Q	9	LYS
4	Q	23	TRP
4	Q	46	VAL
4	Q	48	ASN
4	Q	112	GLU
4	Q	121	ASP
4	Q	142	ARG
4	Q	151	LEU
4	Q	185	ASP
4	Q	189	ASP
4	Q	228	ARG
4	Q	233	HIS
4	Q	263	LEU
4	Q	290	LEU
4	Q	317	TRP
4	Q	327	VAL
4	Q	353	THR
4	Q	395	TYR
4	Q	446	TYR
4	Q	481	MET
4	Q	491	LYS
3	T	5	VAL
3	T	11	VAL
3	T	16	LYS
3	T	18	THR
3	T	20	VAL
3	T	76	ARG
3	T	104	LYS

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Mol	Chain	Res	Type
3	T	107	LYS
3	T	124	LEU
3	T	162	LEU
3	T	180	LEU
3	T	188	VAL
3	T	192	THR
3	T	206	VAL
3	T	210	ASP
3	T	212	LEU
3	T	216	ILE
3	T	246	ARG
3	T	268	ARG
3	T	280	VAL
3	T	298	ARG
3	T	321	VAL
3	T	326	LEU
3	T	328	VAL
3	T	346	VAL
3	T	348	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	S	258	ASN
3	S	324	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	$\#\|Z\| > 2$
5	BEM	A	1	5	13,13,13	0.72	0	18,19,19	1.16	2 (11%)
5	BEM	A	2	5	12,12,13	0.66	0	14,17,19	0.69	0
5	BEM	A	3	5	12,12,13	0.71	0	14,17,19	0.69	0
5	MAW	A	4	5	10,11,12	2.14	1 (10%)	13,15,17	1.74	5 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BEM	A	1	5	-	0/4/24/24	0/1/1/1
5	BEM	A	2	5	-	0/4/21/24	0/1/1/1
5	BEM	A	3	5	-	0/4/21/24	0/1/1/1
5	MAW	A	4	5	-	2/4/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4	MAW	O5-C5	6.01	1.45	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	4	MAW	O5-C5-C6	4.09	117.66	111.52
5	A	1	BEM	C3-C4-C5	2.59	113.69	109.25
5	A	1	BEM	O5-C5-C4	2.36	113.79	109.57
5	A	4	MAW	C2-C3-C4	-2.31	109.16	112.32
5	A	4	MAW	O5-C5-C4	-2.15	122.99	124.81
5	A	4	MAW	C1-C2-C3	2.12	112.27	109.67
5	A	4	MAW	C4-C5-C6	-2.00	119.33	123.65

There are no chirality outliers.

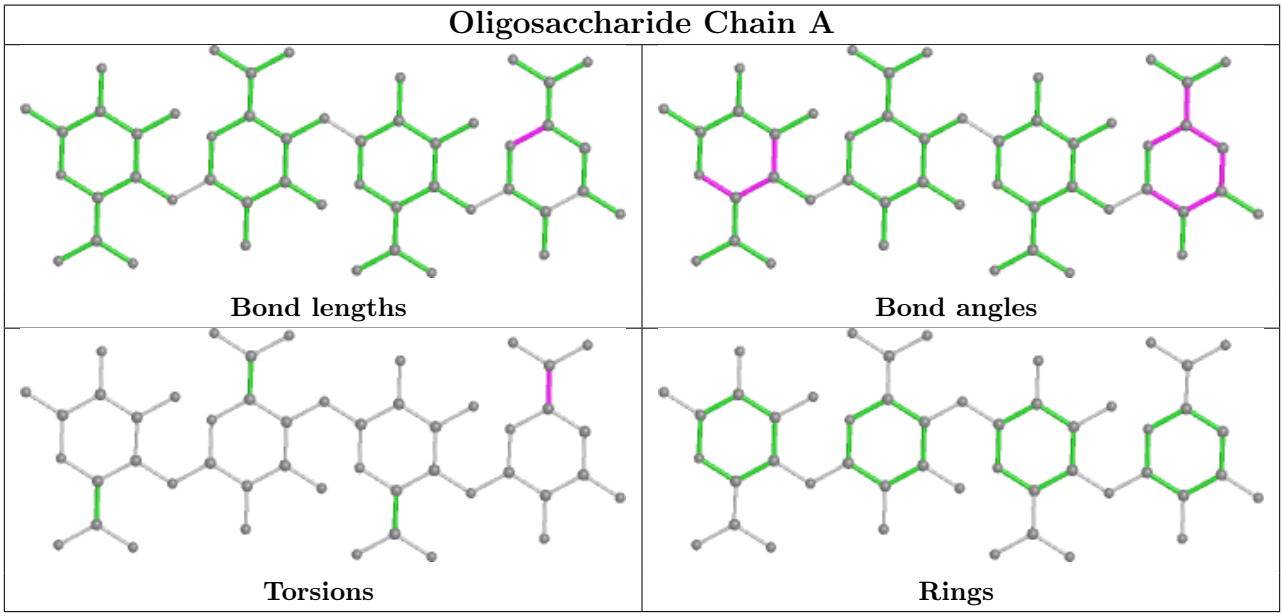
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	4	MAW	O5-C5-C6-O6A
5	A	4	MAW	O5-C5-C6-O6B

There are no ring outliers.

No monomer is involved in short contacts.

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)

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 (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, 95^{th} 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	M	288/301 (95%)	0.28	16 (5%)	24	25	63, 110, 183, 249	0
2	N	290/305 (95%)	0.12	11 (3%)	40	39	70, 108, 157, 223	0
3	S	363/363 (100%)	0.30	21 (5%)	23	24	64, 113, 172, 276	0
3	T	363/363 (100%)	0.41	31 (8%)	10	12	86, 130, 214, 269	0
4	Q	492/516 (95%)	0.30	27 (5%)	25	25	95, 140, 195, 254	0
All	All	1796/1848 (97%)	0.29	106 (5%)	22	23	63, 123, 192, 276	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	492	ASN	6.1
2	N	289	GLY	5.0
4	Q	429	GLU	4.8
3	S	290	LEU	4.7
1	M	65	GLN	4.4
3	S	295	GLY	4.4
3	T	254	HIS	4.3
4	Q	223	ALA	4.2
3	S	264	SER	4.1
3	S	291	ASP	3.9
4	Q	265	GLY	3.9
3	T	341	PRO	3.8
3	T	253	GLN	3.8
1	M	293	ALA	3.8
3	T	342	VAL	3.8
3	S	1	MET	3.8
3	T	301	ILE	3.6
3	T	268	ARG	3.6
3	T	1	MET	3.6
4	Q	154	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
3	S	300	GLN	3.6
1	M	172	LEU	3.5
4	Q	426	MET	3.5
3	T	252	THR	3.5
3	S	299	ALA	3.4
3	T	89	PRO	3.4
3	T	343	THR	3.4
3	S	263	ILE	3.3
3	T	102	ARG	3.3
3	T	344	LEU	3.3
3	T	250	ASP	3.3
2	N	290	GLY	3.3
3	T	305	VAL	3.3
4	Q	198	TRP	3.2
1	M	61	MET	3.2
3	S	106	THR	3.1
3	S	107	LYS	3.0
3	T	300	GLN	3.0
2	N	288	LEU	3.0
4	Q	427	THR	3.0
1	M	292	ILE	3.0
3	S	362	ILE	3.0
4	Q	125	TYR	3.0
4	Q	149	LEU	3.0
3	T	255	VAL	3.0
4	Q	219	LYS	2.9
1	M	78	ILE	2.9
3	S	341	PRO	2.9
3	T	212	LEU	2.8
4	Q	491	LYS	2.8
2	N	291	VAL	2.8
3	S	294	GLU	2.8
2	N	57	VAL	2.8
1	M	29	LYS	2.7
2	N	2	LEU	2.7
1	M	173	ASP	2.6
3	S	2	VAL	2.6
3	T	263	ILE	2.6
4	Q	218	VAL	2.6
3	S	301	ILE	2.6
3	T	256	GLU	2.5
2	N	238	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
4	Q	152	LYS	2.5
4	Q	143	GLU	2.5
1	M	175	VAL	2.5
1	M	125	TYR	2.4
4	Q	433	ILE	2.4
3	T	248	ALA	2.4
1	M	169	TRP	2.4
1	M	318	ILE	2.4
3	T	109	SER	2.4
1	M	317	ARG	2.4
1	M	86	LEU	2.3
4	Q	266	PHE	2.3
3	T	303	ALA	2.3
2	N	240	ASN	2.3
4	Q	139	TYR	2.3
1	M	80	PHE	2.3
3	T	304	THR	2.3
3	S	274	ALA	2.3
4	Q	92	LEU	2.2
4	Q	296	PRO	2.2
4	Q	147	LYS	2.2
4	Q	146	LEU	2.2
3	T	108	LYS	2.2
3	S	344	LEU	2.2
3	T	262	ARG	2.1
2	N	285	GLY	2.1
4	Q	476	TYR	2.1
3	T	292	GLY	2.1
3	T	246	ARG	2.1
3	S	293	VAL	2.1
3	S	262	ARG	2.1
4	Q	151	LEU	2.1
2	N	59	ILE	2.1
1	M	295	ALA	2.1
3	S	346	VAL	2.1
3	S	292	GLY	2.1
3	T	124	LEU	2.1
3	T	317	LEU	2.0
4	Q	140	PHE	2.0
3	T	299	ALA	2.0
4	Q	148	LYS	2.0
2	N	139	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	T	106	THR	2.0
4	Q	456	THR	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)

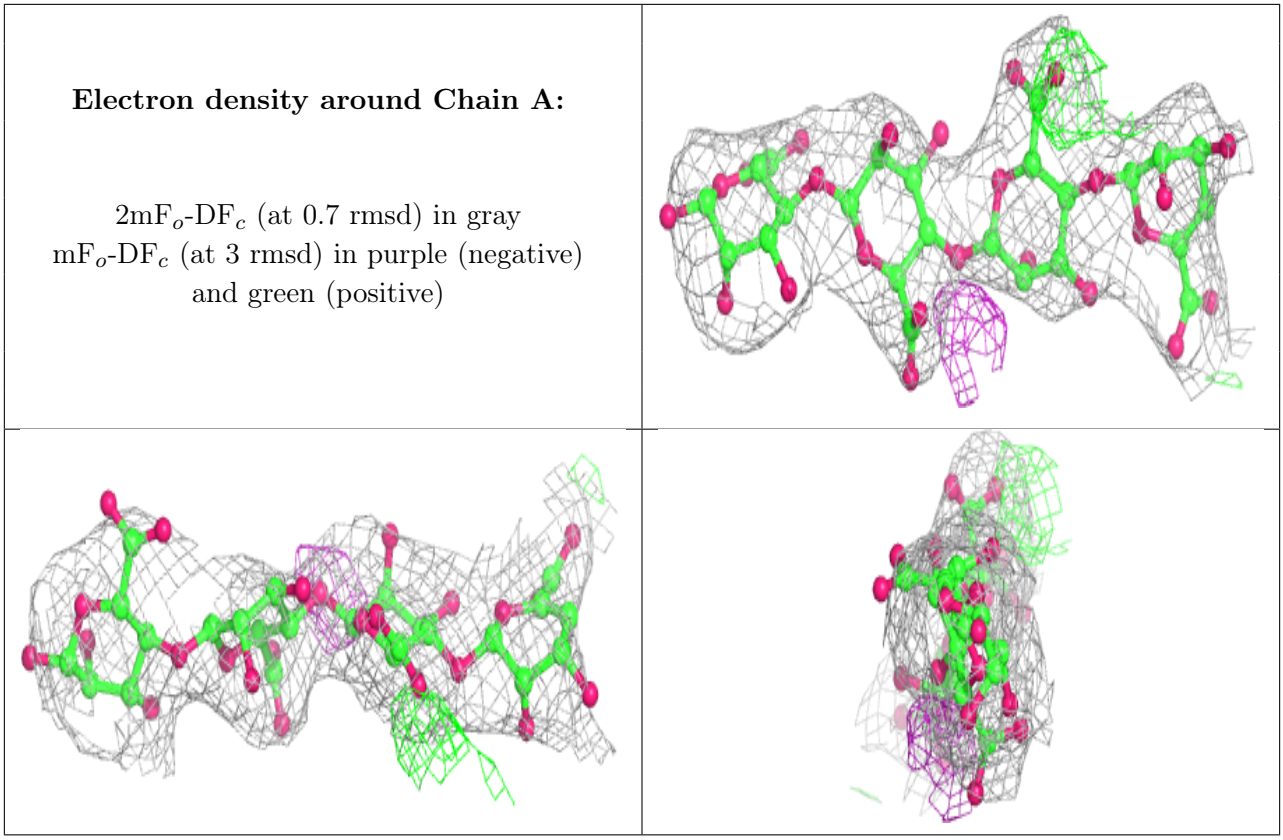
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	BEM	A	2	12/13	0.87	0.38	86,120,150,188	0
5	BEM	A	1	13/13	0.88	0.52	87,140,163,172	0
5	BEM	A	3	12/13	0.88	0.38	117,126,145,155	0
5	MAW	A	4	11/12	0.91	0.33	133,137,149,155	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 A:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.