



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:35 AM UTC

PDB ID : 4XTC / pdb_00004xtc
Title : Crystal structure of bacterial alginate ABC transporter in complex with alginate pentasaccharide-bound periplasmic protein
Authors : Kaneko, A.; Maruyama, Y.; Mizuno, N.; Baba, S.; Kumasaka, T.; Mikami, B.; Murata, K.; Hashimoto, W.
Deposited on : 2015-01-23
Resolution : 3.60 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

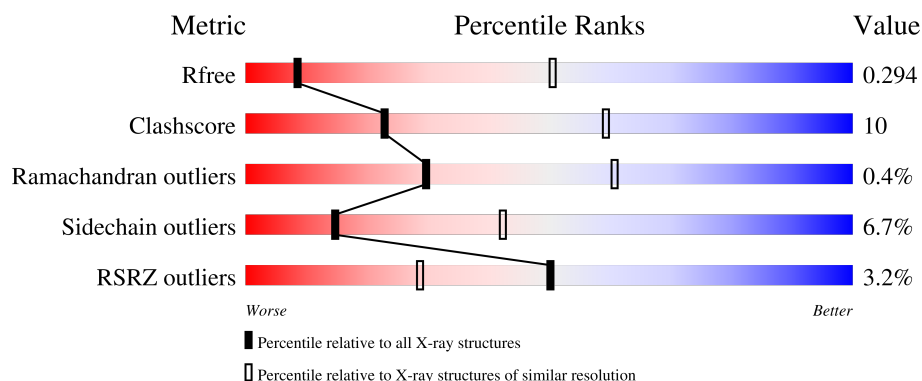
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	M	301	4% 69% 26% • •
2	N	305	4% 69% 23% • 6%
3	S	363	2% 64% 30% 6%
3	T	363	0% 67% 28% 5%
4	Q	516	4% 70% 24% • 5%

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Mol	Chain	Length	Quality of chain
5	A	5	 60% 40%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14264 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
1	M	288	Total	C	N	O	S	0	0	0
			2323	1554	369	390	10			

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	287	Total	C	N	O	S	0	0	0
			2278	1521	362	382	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			

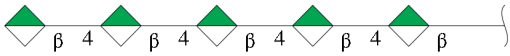
There are 2 discrepancies between the modelled and reference sequences:

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

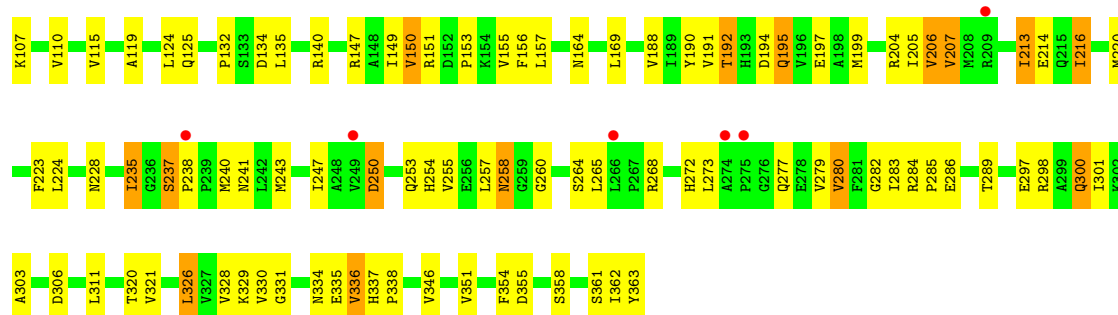
- Molecule 4 is a protein called AlgQ2.

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

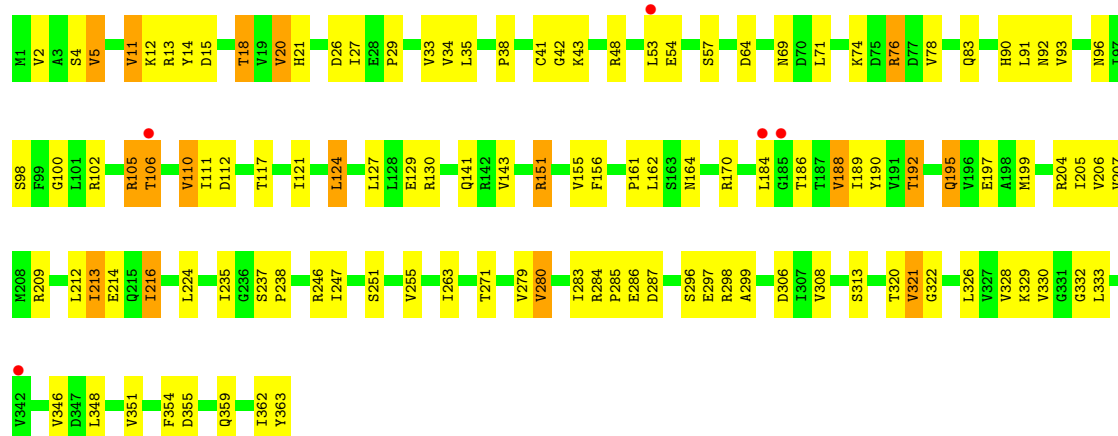
- Molecule 5 is an oligosaccharide called beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid.



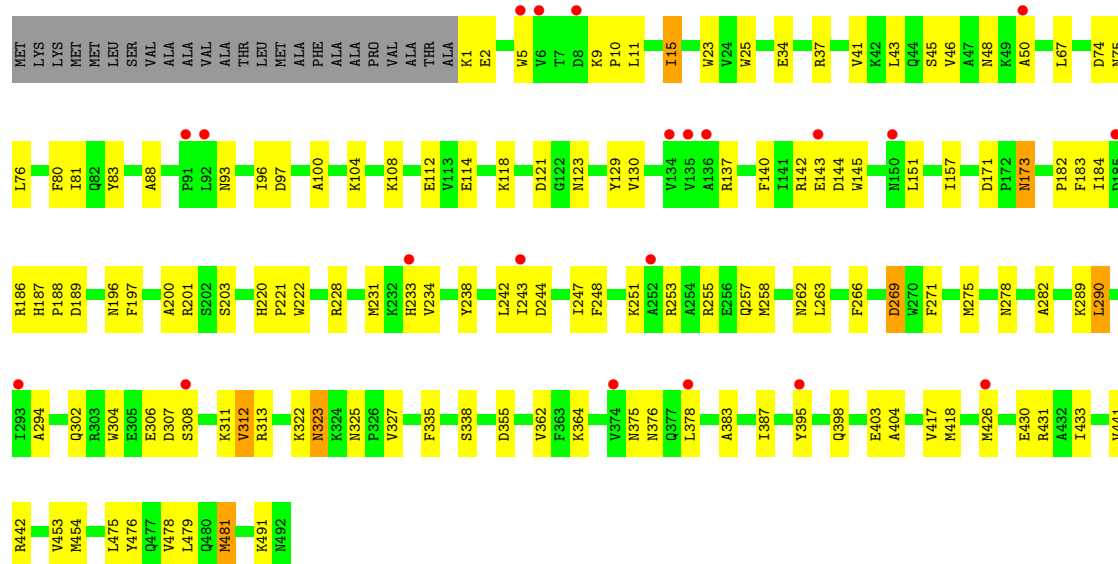
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	A	5	Total	C	O	0	0	0
			61	30	31			



• Molecule 3: AlgS



• Molecule 4: AlgQ2



- Molecule 5: beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid

Chain A:  60% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.61Å 132.96Å 272.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.42 – 3.60 37.42 – 3.60	Depositor EDS
% Data completeness (in resolution range)	95.2 (37.42-3.60) 95.5 (37.42-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.238 , 0.288 0.247 , 0.294	Depositor DCC
R_{free} test set	1516 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	108.1	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 107.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	14264	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: 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	0.32	0/2384	0.76	1/3250 (0.0%)
2	N	0.34	0/2337	0.78	1/3178 (0.0%)
3	S	0.31	0/2822	0.84	9/3826 (0.2%)
3	T	0.30	0/2822	0.82	3/3826 (0.1%)
4	Q	0.26	0/4168	0.72	3/5640 (0.1%)
All	All	0.30	0/14533	0.78	17/19720 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	237	SER	CA-C-N	-6.27	113.92	120.38
3	S	237	SER	C-N-CA	-6.27	113.92	120.38
3	S	106	THR	CB-CA-C	-5.88	108.80	115.79
3	S	301	ILE	N-CA-C	5.81	117.82	109.51
4	Q	251	LYS	CB-CA-C	-5.79	109.92	116.63
3	T	15	ASP	CB-CA-C	-5.64	110.06	116.54
4	Q	294	ALA	CA-C-N	5.39	125.94	120.38
4	Q	294	ALA	C-N-CA	5.39	125.94	120.38
3	S	258	ASN	N-CA-C	5.37	117.83	111.33
3	T	64	ASP	CB-CA-C	-5.30	110.44	116.54
3	S	125	GLN	CA-C-N	-5.28	114.22	119.56
3	S	125	GLN	C-N-CA	-5.28	114.22	119.56
2	N	96	VAL	CB-CA-C	-5.23	108.73	113.70
3	T	105	ARG	CB-CA-C	-5.14	109.14	116.34
3	S	64	ASP	CB-CA-C	-5.07	110.75	116.63
1	M	239	VAL	CB-CA-C	-5.04	108.92	113.70
3	S	300	GLN	N-CA-C	5.02	116.41	110.19

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	50	0
2	N	2278	0	2347	57	0
3	S	2777	0	2854	66	0
3	T	2777	0	2854	69	0
4	Q	4048	0	3920	81	0
5	A	61	0	33	2	0
All	All	14264	0	14420	297	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 10.

All (297) 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:34:VAL:HG22	3:S:190:TYR:HB3	1.63	0.79
3:T:34:VAL:HG22	3:T:190:TYR:HB3	1.63	0.79
3:S:235:ILE:HD11	3:S:284:ARG:HH12	1.50	0.76
3:S:192:THR:HG22	3:S:194:ASP:H	1.55	0.72
4:Q:201:ARG:NH1	4:Q:418:MET:SD	2.64	0.71
2:N:52:VAL:HG13	2:N:53:PHE:H	1.55	0.71
3:T:141:GLN:NE2	3:T:161:PRO:O	2.25	0.69
1:M:34:ASP:OD1	2:N:106:ARG:NH1	2.25	0.69
1:M:98:ASN:ND2	1:M:271:GLU:O	2.26	0.69
3:T:48:ARG:HG3	3:T:53:LEU:HB2	1.74	0.68
3:S:102:ARG:O	3:S:105:ARG:NH1	2.27	0.68
2:N:43:SER:HA	2:N:60:ASP:HB2	1.75	0.67
2:N:234:LYS:HD2	4:Q:50:ALA:HA	1.77	0.67
1:M:179:THR:OG1	4:Q:454:MET:SD	2.54	0.66
1:M:143:ILE:O	1:M:195:LYS:NZ	2.29	0.66
2:N:248:ALA:O	2:N:252:ASN:ND2	2.29	0.66
3:T:195:GLN:HG3	3:T:235:ILE:HA	1.78	0.65
4:Q:81:ILE:HD12	4:Q:431:ARG:HH21	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:97:ASP:HA	4:Q:104:LYS:HD3	1.80	0.64
4:Q:255:ARG:NH1	4:Q:269:ASP:OD2	2.31	0.63
2:N:178:ASP:OD1	3:T:151:ARG:NH2	2.32	0.63
3:S:84:ASN:OD1	3:S:164:ASN:ND2	2.29	0.63
3:T:41:CYS:SG	3:T:42:GLY:N	2.72	0.63
1:M:148:VAL:HG21	1:M:195:LYS:HD2	1.80	0.63
3:S:195:GLN:HG3	3:S:235:ILE:HA	1.81	0.63
3:S:5:VAL:HG13	3:S:27:ILE:HB	1.81	0.63
3:T:4:SER:HB3	3:T:29:PRO:HD3	1.80	0.63
3:S:286:GLU:HG3	3:S:329:LYS:HD3	1.80	0.62
3:S:26:ASP:O	3:S:204:ARG:NH2	2.32	0.62
3:S:241:ASN:ND2	3:S:283:ILE:O	2.32	0.62
3:T:237:SER:HB3	3:T:238:PRO:HD3	1.80	0.62
2:N:80:THR:HG23	2:N:228:LEU:H	1.64	0.62
4:Q:157:ILE:HD13	4:Q:197:PHE:HB3	1.81	0.62
3:T:13:ARG:HG2	3:T:18:THR:HB	1.80	0.62
2:N:107:ILE:HB	2:N:110:ARG:HB2	1.82	0.61
4:Q:313:ARG:NH2	5:A:3:BEM:O3	2.34	0.61
4:Q:142:ARG:NH2	4:Q:262:ASN:OD1	2.33	0.61
3:T:5:VAL:HG13	3:T:27:ILE:HB	1.83	0.60
3:S:78:VAL:HG12	3:S:155:VAL:HB	1.82	0.60
3:S:223:PHE:O	3:S:284:ARG:NH1	2.30	0.60
3:T:207:VAL:HG23	3:T:214:GLU:HB3	1.82	0.60
3:S:206:VAL:HB	3:S:216:ILE:HG23	1.83	0.60
4:Q:323:ASN:HD22	4:Q:325:ASN:H	1.48	0.60
3:S:97:ILE:HA	3:S:147:ARG:HB3	1.84	0.60
4:Q:130:VAL:HA	4:Q:312:VAL:HA	1.83	0.60
4:Q:143:GLU:HG2	4:Q:289:LYS:HD2	1.83	0.60
3:S:213:ILE:HD11	3:S:216:ILE:HG12	1.83	0.59
3:T:286:GLU:HG3	3:T:329:LYS:HD2	1.83	0.59
3:T:110:VAL:C	3:T:112:ASP:H	2.10	0.59
4:Q:238:TYR:HD2	4:Q:453:VAL:HG12	1.68	0.59
4:Q:96:ILE:HA	4:Q:100:ALA:HB3	1.84	0.59
2:N:84:THR:HG21	2:N:210:TRP:HE3	1.68	0.58
3:T:110:VAL:O	3:T:112:ASP:N	2.37	0.58
3:S:107:LYS:HB3	3:S:110:VAL:HG23	1.86	0.58
4:Q:171:ASP:OD1	4:Q:173:ASN:ND2	2.37	0.58
2:N:102:LEU:HB3	2:N:161:ARG:HD3	1.86	0.58
3:T:12:LYS:H	3:T:20:VAL:HG23	1.69	0.58
3:S:247:ILE:HG12	3:S:255:VAL:HG22	1.86	0.57
3:S:250:ASP:OD2	3:S:254:HIS:N	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:130:ARG:HG2	2:N:287:MET:HE2	1.86	0.57
3:T:298:ARG:HB3	3:T:348:LEU:HB2	1.87	0.57
2:N:42:SER:HG	2:N:57:VAL:H	1.51	0.57
3:S:253:GLN:O	3:S:265:LEU:N	2.33	0.57
1:M:209:MET:HE1	2:N:287:MET:HB2	1.87	0.57
3:T:298:ARG:HB3	3:T:348:LEU:H	1.70	0.56
3:T:238:PRO:HB2	3:T:285:PRO:HG2	1.86	0.56
3:S:18:THR:O	3:S:21:HIS:NE2	2.38	0.56
4:Q:362:VAL:HA	4:Q:398:GLN:HE22	1.70	0.56
3:S:87:LEU:HD11	3:S:140:ARG:HB3	1.88	0.56
3:T:2:VAL:HG12	3:T:29:PRO:HB2	1.88	0.56
3:T:20:VAL:HG13	3:T:42:GLY:HA3	1.88	0.56
3:S:273:LEU:HD23	3:S:273:LEU:H	1.71	0.56
3:T:162:LEU:HB3	3:T:170:ARG:HG3	1.88	0.56
2:N:36:ILE:HD13	2:N:264:ILE:HD11	1.89	0.55
3:T:78:VAL:HG12	3:T:155:VAL:HB	1.86	0.55
3:S:94:ARG:HG3	3:S:115:VAL:HG11	1.88	0.55
4:Q:441:VAL:HG11	4:Q:475:LEU:HD13	1.89	0.55
2:N:33:ILE:HA	2:N:36:ILE:HD12	1.88	0.55
3:T:11:VAL:O	3:T:57:SER:OG	2.17	0.54
2:N:177:MET:HE1	3:T:78:VAL:HG23	1.88	0.54
4:Q:378:LEU:HB3	4:Q:383:ALA:HB3	1.89	0.54
3:T:124:LEU:HD23	3:T:124:LEU:H	1.72	0.54
3:T:156:PHE:HB2	3:T:188:VAL:HB	1.90	0.54
1:M:159:SER:H	1:M:174:ARG:HE	1.54	0.54
3:S:102:ARG:HA	3:S:105:ARG:HA	1.89	0.54
3:S:220:MET:HG3	3:S:224:LEU:HD13	1.91	0.53
3:S:223:PHE:HD2	3:S:224:LEU:HD12	1.73	0.53
2:N:75:THR:O	2:N:79:ASN:ND2	2.41	0.53
3:S:74:LYS:O	3:S:151:ARG:NH2	2.33	0.53
3:T:41:CYS:HB3	3:T:43:LYS:HZ3	1.73	0.53
4:Q:188:PRO:HB3	4:Q:248:PHE:HA	1.91	0.53
3:T:48:ARG:HG2	3:T:54:GLU:HG3	1.90	0.53
2:N:287:MET:SD	2:N:287:MET:N	2.82	0.53
3:T:355:ASP:HB2	3:T:362:ILE:HD11	1.91	0.53
1:M:61:MET:C	1:M:63:PHE:H	2.17	0.52
4:Q:142:ARG:NH1	4:Q:144:ASP:OD1	2.42	0.52
3:T:263:ILE:HD12	3:T:299:ALA:HB1	1.91	0.52
2:N:242:ASN:HB3	4:Q:23:TRP:CZ2	2.45	0.52
4:Q:143:GLU:HB3	4:Q:289:LYS:HB3	1.91	0.52
3:S:238:PRO:HB2	3:S:285:PRO:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:203:SER:N	4:Q:306:GLU:OE1	2.43	0.52
4:Q:196:ASN:ND2	4:Q:200:ALA:O	2.43	0.52
4:Q:275:MET:HE2	4:Q:403:GLU:HB2	1.90	0.52
4:Q:140:PHE:HB3	4:Q:290:LEU:HD22	1.92	0.51
4:Q:140:PHE:CZ	4:Q:271:PHE:HA	2.45	0.51
3:T:124:LEU:HD12	3:T:127:LEU:HB2	1.93	0.51
4:Q:130:VAL:HG22	4:Q:312:VAL:HG23	1.90	0.51
1:M:41:LEU:HD11	2:N:102:LEU:HD23	1.92	0.51
2:N:64:TYR:HA	2:N:67:VAL:HG12	1.93	0.51
4:Q:74:ASP:OD2	4:Q:75:ASN:ND2	2.35	0.51
1:M:37:LEU:HD23	2:N:107:ILE:HD11	1.91	0.51
1:M:47:TRP:HZ2	2:N:150:PHE:HA	1.74	0.51
3:T:199:MET:HA	3:T:205:ILE:HD11	1.92	0.51
4:Q:244:ASP:HB3	4:Q:247:ILE:HB	1.92	0.51
4:Q:312:VAL:HG22	4:Q:313:ARG:H	1.75	0.51
4:Q:83:TYR:HB3	4:Q:88:ALA:HB3	1.93	0.51
4:Q:183:PHE:HD2	4:Q:243:ILE:HG23	1.76	0.51
4:Q:430:GLU:HB2	4:Q:481:MET:HG3	1.93	0.51
4:Q:203:SER:HA	4:Q:221:PRO:HG3	1.94	0.50
1:M:146:VAL:HG12	1:M:263:LEU:HD21	1.93	0.50
3:S:132:PRO:HA	3:S:135:LEU:HD12	1.92	0.50
4:Q:173:ASN:HD22	4:Q:173:ASN:H	1.60	0.50
2:N:38:SER:HA	2:N:56:PRO:HG3	1.92	0.50
1:M:162:VAL:HG23	2:N:53:PHE:HD2	1.75	0.50
3:T:92:ASN:O	3:T:96:ASN:ND2	2.42	0.50
1:M:96:ILE:HG13	1:M:276:ILE:HD11	1.93	0.49
4:Q:355:ASP:OD1	4:Q:364:LYS:NZ	2.45	0.49
3:T:38:PRO:HG3	3:T:209:ARG:HG3	1.93	0.49
1:M:252:HIS:C	1:M:254:LEU:H	2.20	0.49
1:M:140:PRO:HB2	1:M:195:LYS:HA	1.95	0.49
3:S:277:GLN:NE2	3:S:355:ASP:OD1	2.42	0.49
3:S:280:VAL:HG13	3:S:354:PHE:HB2	1.95	0.49
2:N:7:TYR:CE2	3:S:73:PRO:HD3	2.47	0.49
3:S:330:VAL:HG22	3:S:331:GLY:H	1.77	0.49
1:M:35:TRP:CG	1:M:36:LEU:N	2.81	0.49
3:S:199:MET:HA	3:S:205:ILE:HD11	1.95	0.49
3:T:280:VAL:HG13	3:T:354:PHE:HB2	1.95	0.49
3:T:306:ASP:HB2	3:T:320:THR:HG23	1.95	0.49
3:T:26:ASP:O	3:T:204:ARG:NH2	2.45	0.48
3:T:71:LEU:HB3	3:T:76:ARG:HH21	1.78	0.48
4:Q:426:MET:HB3	4:Q:430:GLU:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:90:HIS:CE1	3:T:91:LEU:HG	2.48	0.48
3:T:98:SER:O	3:T:102:ARG:HG2	2.14	0.48
3:T:255:VAL:HG13	3:T:263:ILE:HB	1.96	0.48
3:S:207:VAL:HG13	3:S:214:GLU:HB3	1.96	0.48
3:S:334:ASN:O	3:S:334:ASN:ND2	2.47	0.48
4:Q:114:GLU:HG2	4:Q:118:LYS:HE3	1.96	0.47
3:T:93:VAL:HG13	3:T:143:VAL:HG21	1.95	0.47
3:T:117:THR:O	3:T:121:ILE:HG12	2.13	0.47
3:S:68:ILE:HB	3:S:76:ARG:HG2	1.96	0.47
3:S:272:HIS:O	3:S:272:HIS:ND1	2.47	0.47
1:M:64:LYS:HG3	1:M:65:GLN:H	1.79	0.47
4:Q:308:SER:HB3	4:Q:417:VAL:HG13	1.96	0.47
3:S:300:GLN:HG3	3:S:346:VAL:H	1.79	0.47
1:M:250:LEU:HD23	1:M:253:ILE:HD12	1.95	0.47
3:S:149:ILE:HG22	3:S:156:PHE:CZ	2.50	0.47
4:Q:228:ARG:HA	4:Q:231:MET:HB2	1.95	0.47
2:N:213:TYR:CG	2:N:214:PHE:N	2.82	0.47
3:S:192:THR:HG21	3:S:197:GLU:HB2	1.95	0.47
3:T:12:LYS:HD3	3:T:14:TYR:HE1	1.79	0.47
3:T:184:LEU:HG	3:T:186:THR:HG23	1.96	0.47
2:N:178:ASP:HB3	3:T:100:GLY:HA2	1.97	0.47
3:S:214:GLU:HG3	3:S:228:ASN:HD21	1.80	0.47
1:M:227:TRP:HA	1:M:230:ILE:HG12	1.97	0.47
4:Q:275:MET:HG3	4:Q:404:ALA:HB2	1.96	0.47
3:T:83:GLN:O	3:T:164:ASN:ND2	2.49	0.46
3:T:283:ILE:HD13	3:T:351:VAL:HG12	1.98	0.46
1:M:120:MET:HE2	2:N:22:LEU:HB2	1.97	0.46
1:M:284:GLY:HA3	2:N:128:ILE:HD11	1.97	0.46
4:Q:11:LEU:HB3	4:Q:41:VAL:HG22	1.96	0.46
4:Q:433:ILE:HG22	4:Q:478:VAL:HG22	1.97	0.46
3:T:129:GLU:O	3:T:130:ARG:HG2	2.15	0.46
4:Q:302:GLN:OE1	4:Q:304:TRP:NE1	2.38	0.46
3:S:25:LEU:HD21	3:S:33:VAL:HG21	1.98	0.46
3:S:223:PHE:HA	3:S:235:ILE:HG13	1.96	0.46
3:T:12:LYS:NZ	3:T:54:GLU:HB3	2.31	0.46
1:M:111:PHE:O	1:M:114:PRO:HD2	2.16	0.46
4:Q:184:ILE:HG21	4:Q:258:MET:HG3	1.96	0.46
3:T:35:LEU:HD11	3:T:189:ILE:HD11	1.98	0.46
2:N:36:ILE:HG21	2:N:264:ILE:HD11	1.98	0.45
2:N:286:VAL:HG12	2:N:287:MET:HG2	1.99	0.45
4:Q:137:ARG:NH1	4:Q:307:ASP:OD2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:335:PHE:O	4:Q:338:SER:OG	2.25	0.45
4:Q:93:ASN:HD21	4:Q:123:ASN:HA	1.81	0.45
1:M:55:PRO:HD3	2:N:133:ASN:ND2	2.32	0.45
4:Q:476:TYR:HA	4:Q:479:LEU:HB2	1.98	0.45
4:Q:2:GLU:HB2	4:Q:5:TRP:CD1	2.52	0.45
4:Q:278:ASN:CG	4:Q:290:LEU:H	2.25	0.45
1:M:150:GLY:HA3	2:N:236:ILE:HG22	1.99	0.45
4:Q:442:ARG:NE	5:A:1:BEM:O2	2.50	0.45
1:M:54:LYS:HD2	1:M:57:ILE:HD12	1.99	0.45
2:N:42:SER:OG	2:N:57:VAL:N	2.37	0.45
2:N:70:ASP:OD2	2:N:231:TYR:OH	2.21	0.44
2:N:243:GLU:HG2	4:Q:23:TRP:CZ3	2.52	0.44
3:T:192:THR:HG21	3:T:197:GLU:HB2	1.98	0.44
3:S:361:SER:C	3:S:363:TYR:H	2.25	0.44
4:Q:15:ILE:HG21	4:Q:43:LEU:HB3	1.99	0.44
3:S:119:ALA:HA	3:S:124:LEU:HB2	1.99	0.44
4:Q:25:TRP:HD1	4:Q:45:SER:HB2	1.82	0.44
4:Q:278:ASN:ND2	4:Q:290:LEU:O	2.45	0.44
1:M:208:ILE:HG23	1:M:238:ILE:HD12	1.99	0.44
2:N:100:TYR:CD1	2:N:186:LEU:HD13	2.52	0.44
3:T:284:ARG:HB2	3:T:287:ASP:OD2	2.17	0.44
2:N:137:LEU:HB3	2:N:139:LEU:HG	1.99	0.44
1:M:260:TYR:CZ	1:M:264:LEU:HD12	2.52	0.44
1:M:321:THR:OG1	1:M:322:GLY:N	2.50	0.44
4:Q:186:ARG:HG3	4:Q:187:HIS:ND1	2.32	0.44
3:S:240:MET:HE3	3:S:282:GLY:HA3	1.99	0.44
4:Q:253:ARG:HH11	4:Q:257:GLN:HE22	1.65	0.44
1:M:132:ALA:O	1:M:135:THR:OG1	2.34	0.44
1:M:259:GLU:HB3	2:N:213:TYR:HE2	1.83	0.44
4:Q:129:TYR:CE2	4:Q:313:ARG:HD3	2.53	0.44
1:M:162:VAL:HG23	2:N:53:PHE:CD2	2.53	0.43
2:N:231:TYR:O	2:N:235:THR:HG22	2.18	0.43
3:S:104:LYS:C	3:S:106:THR:H	2.26	0.43
3:S:355:ASP:HB3	3:S:358:SER:O	2.17	0.43
3:S:147:ARG:O	3:S:150:VAL:HG12	2.18	0.43
4:Q:182:PRO:HG2	4:Q:242:LEU:HA	1.99	0.43
4:Q:231:MET:HA	4:Q:234:VAL:HG22	2.00	0.43
4:Q:278:ASN:OD1	4:Q:290:LEU:N	2.42	0.43
3:S:79:ALA:HB3	3:S:153:PRO:HG3	1.99	0.43
3:S:98:SER:O	3:S:102:ARG:HG3	2.19	0.43
2:N:73:PHE:HD2	2:N:74:TRP:HD1	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:236:ILE:HD12	2:N:260:VAL:HG13	2.00	0.43
4:Q:258:MET:O	4:Q:263:LEU:N	2.51	0.43
2:N:76:SER:HB3	2:N:227:PRO:C	2.44	0.43
3:S:47:LEU:HD11	3:S:157:LEU:HB3	2.01	0.43
3:S:334:ASN:C	3:S:336:VAL:HG23	2.44	0.43
4:Q:76:LEU:O	4:Q:80:PHE:N	2.43	0.43
4:Q:220:HIS:CD2	4:Q:222:TRP:HB2	2.53	0.43
2:N:179:GLY:HA2	3:T:74:LYS:HB2	2.01	0.43
3:S:43:LYS:HD3	3:S:191:VAL:HG13	2.00	0.43
4:Q:34:GLU:CD	4:Q:37:ARG:HH22	2.27	0.43
3:T:156:PHE:HE2	3:T:184:LEU:HD23	1.83	0.43
1:M:90:GLU:O	1:M:94:ARG:HG2	2.19	0.42
3:S:264:SER:HB2	3:S:298:ARG:HG2	2.00	0.42
4:Q:312:VAL:HG13	4:Q:313:ARG:N	2.34	0.42
2:N:76:SER:HB3	2:N:228:LEU:HA	2.01	0.42
1:M:185:ARG:HB2	1:M:186:PRO:HD3	2.02	0.42
2:N:6:PHE:HB3	2:N:7:TYR:H	1.59	0.42
3:S:306:ASP:HB2	3:S:320:THR:HG23	2.01	0.42
3:S:337:HIS:HA	3:S:338:PRO:HD3	1.88	0.42
4:Q:221:PRO:HG2	4:Q:222:TRP:HD1	1.84	0.42
1:M:226:ARG:HH12	2:N:5:PRO:HG2	1.85	0.42
1:M:274:ASP:OD2	1:M:282:ARG:NH2	2.46	0.42
3:S:42:GLY:O	3:S:46:THR:N	2.46	0.42
4:Q:67:LEU:HB2	4:Q:322:LYS:HD2	2.00	0.42
2:N:265:VAL:O	2:N:269:ILE:HG13	2.20	0.42
3:S:264:SER:CB	3:S:298:ARG:HG2	2.50	0.42
2:N:235:THR:HG23	2:N:236:ILE:HG12	2.00	0.42
1:M:65:GLN:HB3	1:M:66:TYR:CD2	2.53	0.42
2:N:260:VAL:O	2:N:264:ILE:HG23	2.20	0.42
1:M:227:TRP:CD1	1:M:230:ILE:HD11	2.55	0.42
1:M:184:PHE:HZ	1:M:261:ILE:HG12	1.85	0.42
2:N:134:MET:HE2	2:N:134:MET:HA	2.02	0.42
4:Q:375:ASN:ND2	4:Q:376:ASN:OD1	2.53	0.42
3:T:321:VAL:HG23	3:T:322:GLY:H	1.83	0.42
3:S:258:ASN:C	3:S:260:GLY:H	2.27	0.41
3:T:235:ILE:O	3:T:284:ARG:NH2	2.33	0.41
3:S:283:ILE:HD13	3:S:351:VAL:HA	2.01	0.41
4:Q:114:GLU:O	4:Q:118:LYS:HG3	2.19	0.41
1:M:37:LEU:HD21	2:N:104:LYS:HB2	2.02	0.41
3:S:13:ARG:NH1	3:S:57:SER:HB3	2.35	0.41
3:T:313:SER:O	3:T:332:GLY:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:90:HIS:CD2	3:S:91:LEU:HG	2.54	0.41
3:T:247:ILE:HG21	3:T:251:SER:HA	2.02	0.41
3:T:105:ARG:HB3	3:T:106:THR:H	1.65	0.41
3:T:271:THR:HG22	3:T:363:TYR:HA	2.03	0.41
2:N:259:VAL:O	2:N:263:ILE:HG13	2.20	0.41
1:M:238:ILE:O	1:M:242:ILE:HG23	2.20	0.41
4:Q:142:ARG:HB2	4:Q:145:TRP:HB2	2.02	0.41
1:M:56:MET:HA	1:M:59:LEU:HB3	2.02	0.41
1:M:212:ASN:OD1	1:M:212:ASN:N	2.54	0.41
1:M:267:PRO:HA	1:M:270:TYR:CD2	2.56	0.41
2:N:178:ASP:HA	3:T:151:ARG:HH21	1.86	0.41
3:T:21:HIS:HB2	3:T:212:LEU:HD23	2.01	0.41
3:T:284:ARG:HA	3:T:285:PRO:HD3	1.95	0.41
4:Q:9:LYS:HA	4:Q:10:PRO:HD3	1.99	0.41
4:Q:278:ASN:O	4:Q:282:ALA:HB2	2.20	0.41
3:T:12:LYS:HZ2	3:T:54:GLU:HB3	1.86	0.41
1:M:131:LYS:HE2	1:M:131:LYS:HB3	1.90	0.40
1:M:137:VAL:HG12	1:M:198:GLY:HA3	2.02	0.40
1:M:262:ILE:HD11	1:M:281:TYR:CZ	2.57	0.40
4:Q:183:PHE:HD1	4:Q:266:PHE:HD2	1.70	0.40
3:T:102:ARG:HA	3:T:102:ARG:HD2	1.89	0.40
1:M:308:VAL:HG21	2:N:122:TRP:CE3	2.57	0.40
4:Q:129:TYR:CD2	4:Q:313:ARG:HD3	2.56	0.40
4:Q:311:LYS:O	4:Q:312:VAL:HG12	2.21	0.40
3:T:90:HIS:ND1	3:T:91:LEU:HG	2.36	0.40
4:Q:129:TYR:HB2	4:Q:387:ILE:O	2.21	0.40
3:T:296:SER:N	3:T:297:GLU:HA	2.36	0.40
1:M:204:TYR:CE1	1:M:242:ILE:HG22	2.56	0.40
3:S:243:MET:HE3	3:S:326:LEU:HB3	2.03	0.40
3:S:303:ALA:HB2	3:S:321:VAL:HG22	2.02	0.40
4:Q:25:TRP:CD1	4:Q:45:SER:HB2	2.56	0.40
4:Q:189:ASP:OD1	4:Q:189:ASP:N	2.54	0.40
3:T:213:ILE:HD11	3:T:216:ILE:HG12	2.03	0.40

There are no symmetry-related clashes.

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	M	284/301 (94%)	264 (93%)	19 (7%)	1 (0%)	30	61
2	N	285/305 (93%)	263 (92%)	20 (7%)	2 (1%)	18	51
3	S	361/363 (99%)	336 (93%)	23 (6%)	2 (1%)	21	54
3	T	361/363 (99%)	335 (93%)	24 (7%)	2 (1%)	21	54
4	Q	490/516 (95%)	464 (95%)	25 (5%)	1 (0%)	43	72
All	All	1781/1848 (96%)	1662 (93%)	111 (6%)	8 (0%)	30	61

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	253	ILE
3	S	362	ILE
3	T	111	ILE
4	Q	312	VAL
3	T	110	VAL
2	N	52	VAL
3	S	336	VAL
2	N	59	ILE

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	M	251/260 (96%)	241 (96%)	10 (4%)	28	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	242/258 (94%)	225 (93%)	17 (7%)	14	41
3	S	307/307 (100%)	277 (90%)	30 (10%)	7	31
3	T	307/307 (100%)	279 (91%)	28 (9%)	9	33
4	Q	424/440 (96%)	407 (96%)	17 (4%)	28	54
All	All	1531/1572 (97%)	1429 (93%)	102 (7%)	15	42

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	59	LEU
1	M	82	HIS
1	M	127	LYS
1	M	170	ILE
1	M	235	LEU
1	M	253	ILE
1	M	262	ILE
1	M	265	TYR
1	M	266	GLN
1	M	309	LEU
2	N	6	PHE
2	N	42	SER
2	N	55	LEU
2	N	71	LYS
2	N	77	TYR
2	N	80	THR
2	N	102	LEU
2	N	108	ARG
2	N	140	LEU
2	N	146	ILE
2	N	150	PHE
2	N	189	VAL
2	N	217	MET
2	N	226	ILE
2	N	237	VAL
2	N	241	VAL
2	N	264	ILE
3	S	5	VAL
3	S	11	VAL
3	S	20	VAL
3	S	33	VAL
3	S	43	LYS

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Mol	Chain	Res	Type
3	S	87	LEU
3	S	103	LEU
3	S	134	ASP
3	S	150	VAL
3	S	169	LEU
3	S	188	VAL
3	S	192	THR
3	S	195	GLN
3	S	206	VAL
3	S	207	VAL
3	S	213	ILE
3	S	216	ILE
3	S	235	ILE
3	S	237	SER
3	S	250	ASP
3	S	257	LEU
3	S	268	ARG
3	S	279	VAL
3	S	280	VAL
3	S	289	THR
3	S	297	GLU
3	S	311	LEU
3	S	326	LEU
3	S	328	VAL
3	S	335	GLU
4	Q	1	LYS
4	Q	15	ILE
4	Q	46	VAL
4	Q	48	ASN
4	Q	108	LYS
4	Q	112	GLU
4	Q	121	ASP
4	Q	151	LEU
4	Q	173	ASN
4	Q	233	HIS
4	Q	269	ASP
4	Q	290	LEU
4	Q	323	ASN
4	Q	327	VAL
4	Q	395	TYR
4	Q	481	MET
4	Q	491	LYS

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Mol	Chain	Res	Type
3	T	5	VAL
3	T	11	VAL
3	T	18	THR
3	T	20	VAL
3	T	33	VAL
3	T	69	ASN
3	T	76	ARG
3	T	106	THR
3	T	124	LEU
3	T	151	ARG
3	T	188	VAL
3	T	192	THR
3	T	195	GLN
3	T	206	VAL
3	T	213	ILE
3	T	216	ILE
3	T	224	LEU
3	T	246	ARG
3	T	279	VAL
3	T	280	VAL
3	T	308	VAL
3	T	321	VAL
3	T	326	LEU
3	T	328	VAL
3	T	330	VAL
3	T	333	LEU
3	T	346	VAL
3	T	359	GLN

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

Mol	Chain	Res	Type
2	N	133	ASN
2	N	181	ASN
2	N	252	ASN
3	S	160	GLN
3	S	193	HIS
3	S	253	GLN
3	S	334	ASN
3	S	359	GLN
4	Q	55	GLN
4	Q	85	GLN

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Mol	Chain	Res	Type
4	Q	372	GLN
4	Q	375	ASN
3	T	141	GLN
3	T	225	HIS
3	T	359	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

5 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	0.74	0	18,19,19	0.68	0
5	BEM	A	2	5	12,12,13	0.70	0	14,17,19	0.68	0
5	BEM	A	3	5	12,12,13	0.69	0	14,17,19	0.74	0
5	BEM	A	4	5	12,12,13	0.69	0	14,17,19	0.60	0
5	BEM	A	5	5	12,12,13	0.72	0	14,17,19	0.65	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
5	BEM	A	1	5	-	0/4/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	BEM	A	4	5	-	0/4/21/24	0/1/1/1
5	BEM	A	5	5	-	1/4/21/24	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

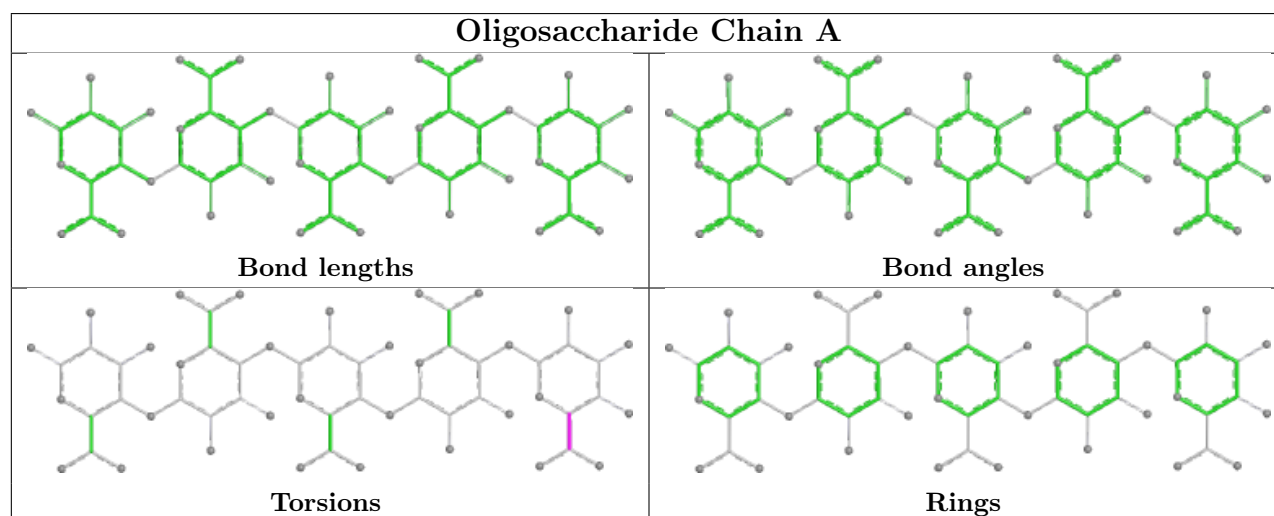
Mol	Chain	Res	Type	Atoms
5	A	5	BEM	C4-C5-C6-O6B

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3	BEM	1	0
5	A	1	BEM	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](#)

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, 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	M	288/301 (95%)	0.17	12 (4%)	40 22	58, 103, 179, 224	0
2	N	287/305 (94%)	0.29	11 (3%)	44 25	60, 99, 148, 213	0
3	S	363/363 (100%)	0.23	9 (2%)	58 34	59, 103, 178, 259	0
3	T	363/363 (100%)	0.23	5 (1%)	73 46	75, 126, 201, 281	0
4	Q	492/516 (95%)	0.29	21 (4%)	40 22	89, 137, 196, 252	0
All	All	1793/1848 (97%)	0.25	58 (3%)	50 29	58, 118, 186, 281	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	48	THR	5.0
4	Q	135	VAL	3.9
4	Q	378	LEU	3.8
4	Q	5	TRP	3.8
2	N	47	VAL	3.7
3	S	209	ARG	3.7
2	N	152	CYS	3.4
3	S	69	ASN	3.4
4	Q	91	PRO	3.3
4	Q	252	ALA	3.3
2	N	226	ILE	3.2
3	S	249	VAL	3.2
4	Q	50	ALA	3.1
1	M	290	TYR	2.9
3	S	274	ALA	2.9
4	Q	233	HIS	2.9
1	M	295	ALA	2.9
3	T	53	LEU	2.9
1	M	323	VAL	2.8
4	Q	6	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
4	Q	136	ALA	2.7
4	Q	395	TYR	2.6
3	S	55	GLU	2.6
3	T	185	GLY	2.6
4	Q	185	ASP	2.6
4	Q	134	VAL	2.6
1	M	138	TYR	2.5
3	T	184	LEU	2.5
3	T	106	THR	2.5
2	N	78	ALA	2.4
1	M	48	PHE	2.4
1	M	197	ALA	2.4
4	Q	8	ASP	2.4
1	M	159	SER	2.4
4	Q	374	VAL	2.4
1	M	318	ILE	2.4
2	N	210	TRP	2.4
3	S	266	LEU	2.3
2	N	267	SER	2.3
4	Q	243	ILE	2.3
4	Q	150	ASN	2.3
1	M	292	ILE	2.3
1	M	274	ASP	2.3
3	S	275	PRO	2.3
1	M	105	LEU	2.2
2	N	3	ALA	2.1
2	N	288	LEU	2.2
3	T	342	VAL	2.1
4	Q	92	LEU	2.1
4	Q	308	SER	2.1
2	N	173	GLU	2.1
4	Q	293	ILE	2.1
4	Q	426	MET	2.1
1	M	212	ASN	2.1
2	N	286	VAL	2.1
3	S	238	PRO	2.1
4	Q	143	GLU	2.1
3	S	57	SER	2.0

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

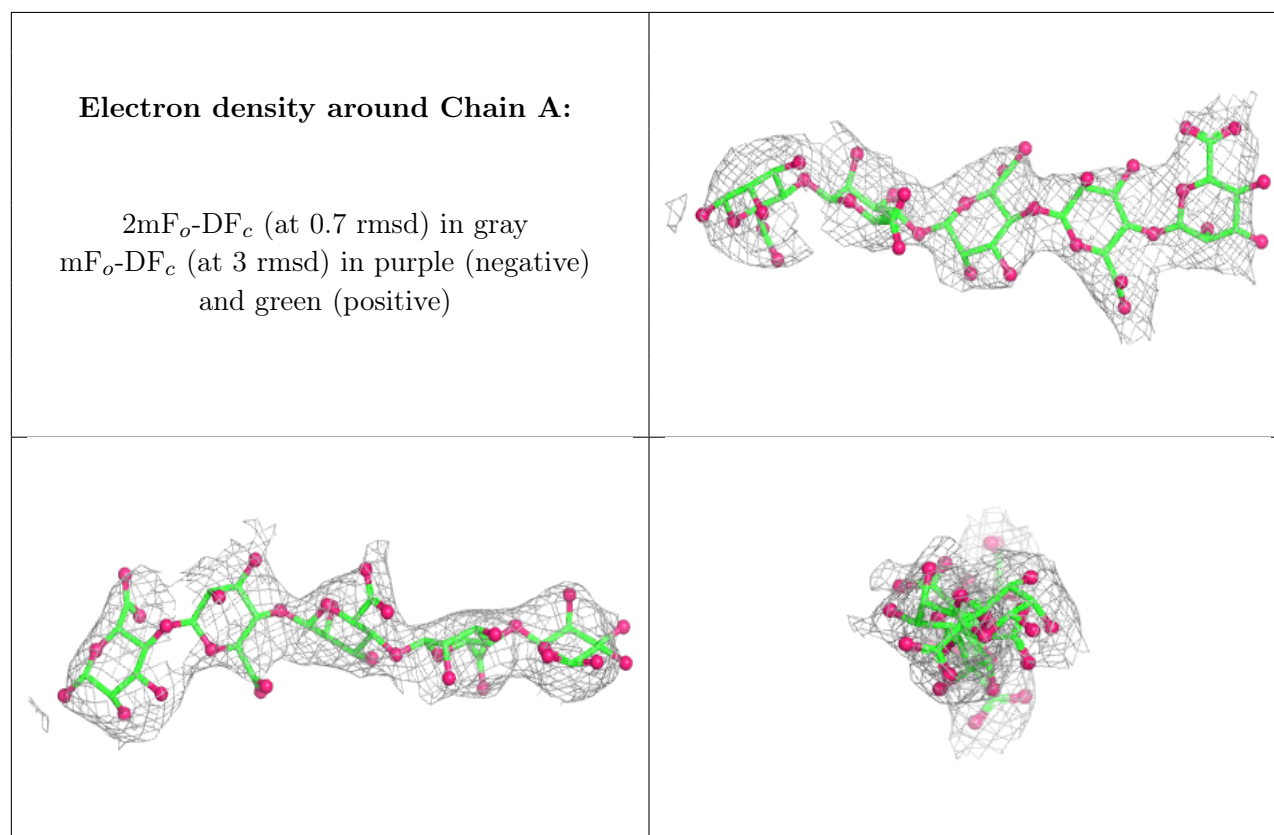
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [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(Å ²)	Q<0.9
5	BEM	A	1	13/13	-	-	119,137,147,156	0
5	BEM	A	2	12/13	-	-	87,122,132,136	0
5	BEM	A	3	12/13	-	-	93,114,122,125	0
5	BEM	A	4	12/13	-	-	100,116,124,125	0
5	BEM	A	5	12/13	-	-	95,121,135,144	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.



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.