Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2024 – 02:08 PM JST

PDB ID	:	4TQU
Title	:	Crystal structure of a bacterial ABC transporter involved in the import of the acidic polysaccharide alginate
Authors	:	Maruyama, Y.; Itoh, T.; Kaneko, A.; Nishitani, Y.; Mikami, B.; Hashimoto, W.; Murata, K.
Deposited on	:	2014-06-12
Resolution	:	3.20 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:

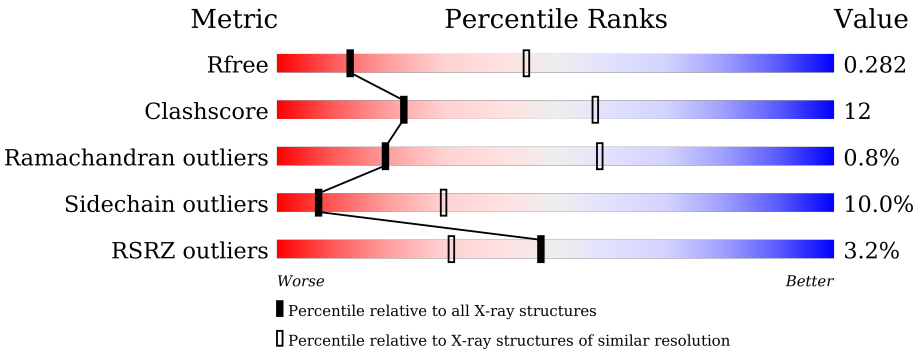
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.20 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))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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% 64% 26% 6%
2	N	305	68% 20% 5% 7%
3	S	363	4% 64% 31%
3	T	363	5% 61% 35%
4	Q	516	3% 72% 20% 5%
5	A	4	25% 50% 25%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14198 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	284	Total	C	N	O	S	0	0	0
			2296	1539	364	383	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	24	MET	-	expression tag	UNP Q9KWT8

- Molecule 2 is a protein called AlgM2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	283	Total	C	N	O	S	0	0	0
			2251	1503	358	378	12			

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			

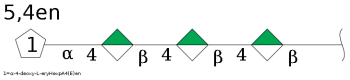
There are 2 discrepancies between the modelled and reference sequences:

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	0	0	0
			48	24	24			

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

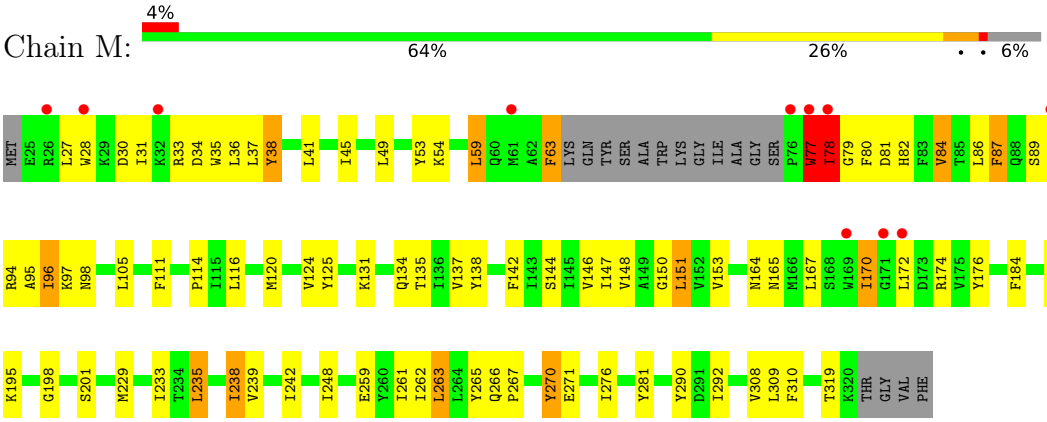
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	Q	1	Total	Ca	0	0
			1	1		

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.

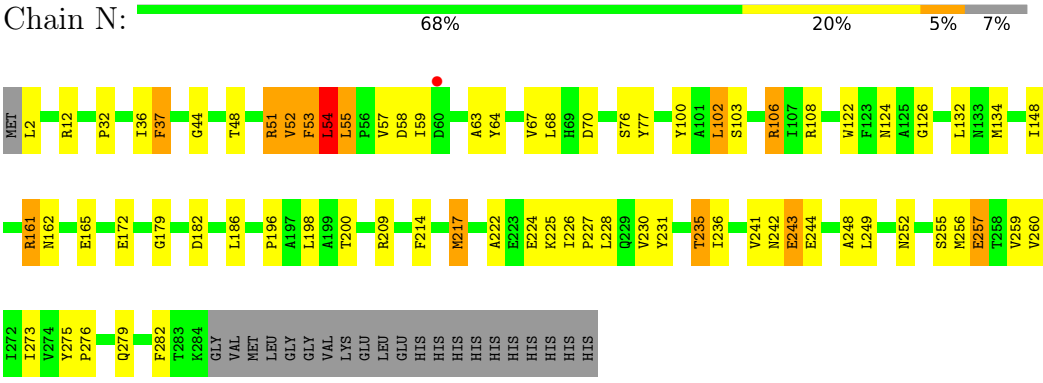
• Molecule 1: AlgM1

Chain M:



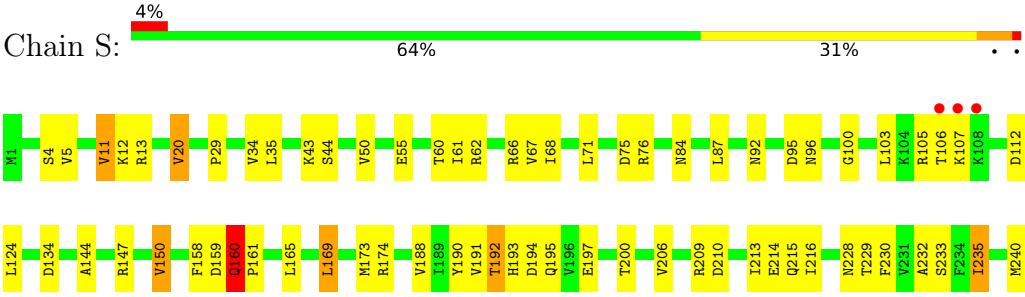
• Molecule 2: AlgM2

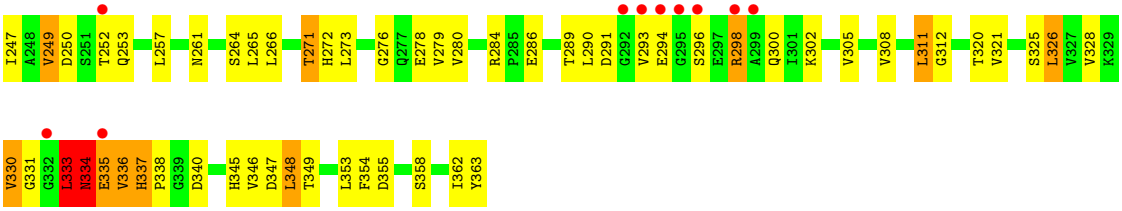
Chain N:



• Molecule 3: AlgS

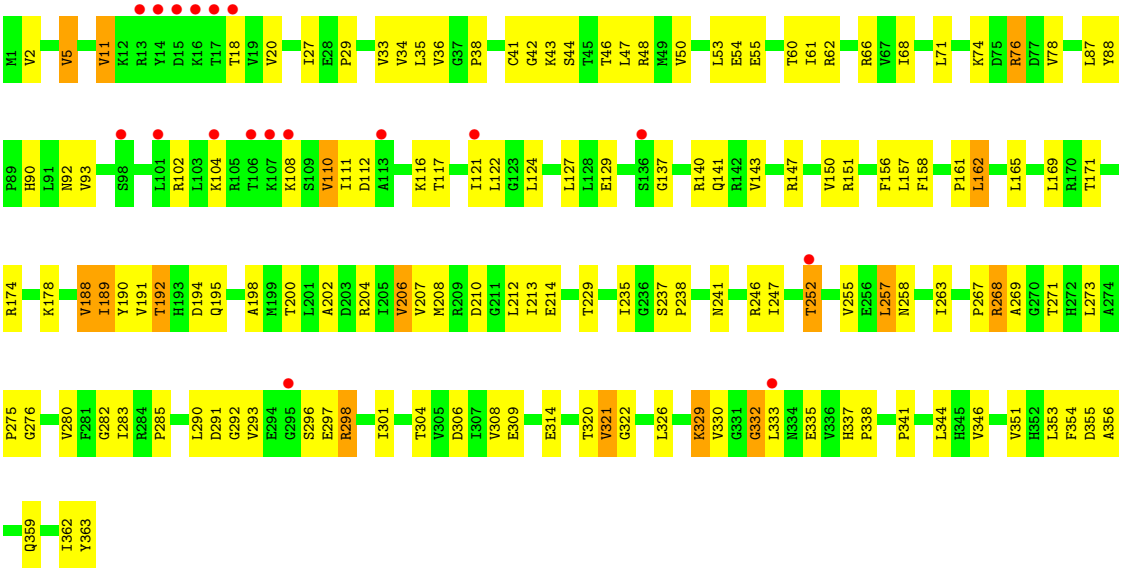
Chain S:





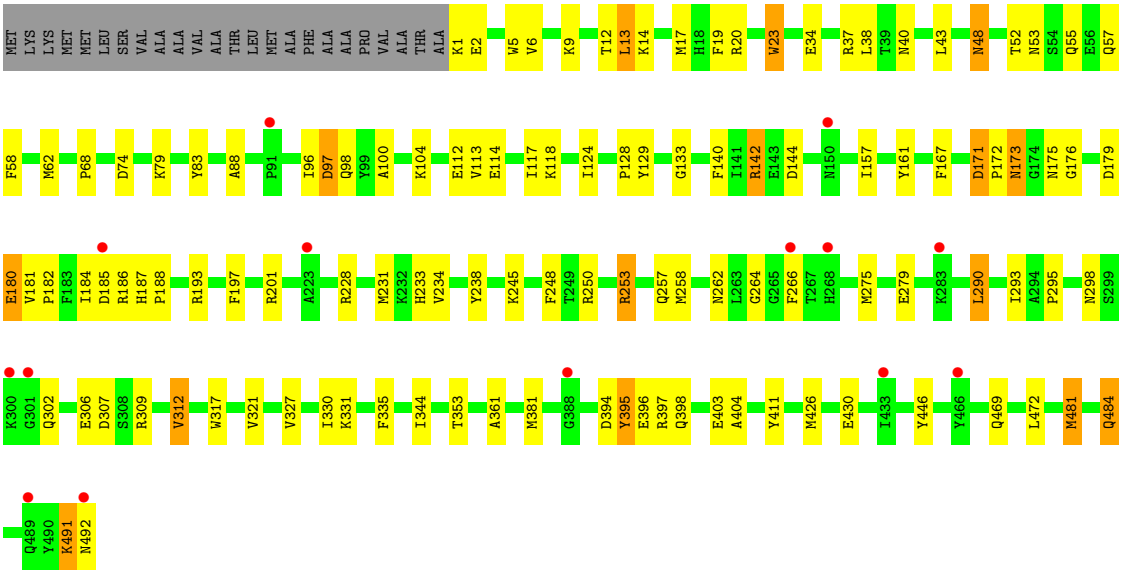
• Molecule 3: AlgS

Chain T:



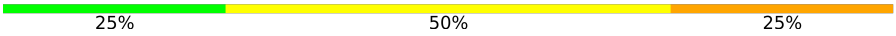
• Molecule 4: AlgQ2

Chain Q:



• 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	71.37Å 134.18Å 273.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.64 – 3.20 29.64 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.64-3.20) 97.5 (29.64-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.22 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.237 , 0.282 0.237 , 0.282	Depositor DCC
R_{free} test set	2166 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	89.5	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 86.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14198	wwPDB-VP
Average B, all atoms (Å^2)	117.0	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, CA, 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	0.30	0/2359	0.53	0/3218
2	N	0.34	0/2310	0.53	1/3142 (0.0%)
3	S	0.34	0/2822	0.58	1/3826 (0.0%)
3	T	0.27	0/2822	0.51	0/3826
4	Q	0.28	0/4168	0.46	0/5640
All	All	0.30	0/14481	0.52	2/19652 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	1
3	S	0	1
3	T	0	2
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	S	160	GLN	C-N-CD	5.85	140.69	128.40
2	N	55	LEU	C-N-CD	5.81	140.60	128.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	77	TRP	Peptide
3	S	333	LEU	Peptide
3	T	293	VAL	Peptide
3	T	332	GLY	Peptide

5.2 Too-close contacts (i)

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	2296	0	2381	66	0
2	N	2251	0	2315	53	0
3	S	2777	0	2854	80	0
3	T	2777	0	2854	74	0
4	Q	4048	0	3920	69	0
5	A	48	0	25	3	0
6	Q	1	0	0	0	0
All	All	14198	0	14349	329	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 12.

All (329) 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:M:34:ASP:O	1:M:38:TYR:HB2	1.57	1.03
1:M:30:ASP:OD1	1:M:33:ARG:NH1	1.93	1.02
1:M:35:TRP:O	1:M:38:TYR:N	1.97	0.96
3:S:334:ASN:HD21	3:S:336:VAL:HG23	1.31	0.94
2:N:76:SER:HB3	2:N:228:LEU:H	1.34	0.92
1:M:30:ASP:HA	1:M:33:ARG:NH1	1.87	0.89
1:M:30:ASP:O	1:M:34:ASP:N	2.08	0.85
1:M:27:LEU:O	1:M:31:ILE:HG13	1.76	0.85
3:S:247:ILE:HB	3:S:276:GLY:H	1.41	0.84
3:S:290:LEU:HG	3:S:330:VAL:HG21	1.62	0.82
3:S:195:GLN:HG3	3:S:235:ILE:HA	1.61	0.80
1:M:35:TRP:CG	1:M:36:LEU:N	2.47	0.80
4:Q:184:ILE:HD13	4:Q:258:MET:HB2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:34:ASP:O	1:M:38:TYR:CD2	2.36	0.78
1:M:35:TRP:O	1:M:36:LEU:C	2.25	0.75
1:M:148:VAL:HG21	1:M:195:LYS:HD2	1.70	0.73
3:T:195:GLN:HG3	3:T:235:ILE:HA	1.71	0.73
1:M:34:ASP:O	1:M:38:TYR:HD2	1.71	0.72
1:M:35:TRP:O	1:M:37:LEU:N	2.22	0.72
1:M:34:ASP:O	1:M:38:TYR:CB	2.37	0.71
2:N:102:LEU:HD12	2:N:161:ARG:HE	1.54	0.71
1:M:30:ASP:O	1:M:33:ARG:N	2.23	0.70
3:T:41:CYS:HB3	3:T:43:LYS:HZ3	1.57	0.69
3:S:334:ASN:ND2	3:S:336:VAL:HG23	2.07	0.69
2:N:256:MET:SD	4:Q:253:ARG:NH1	2.66	0.68
2:N:200:THR:HG22	2:N:282:PHE:HE2	1.57	0.68
3:S:12:LYS:NZ	3:S:55:GLU:O	2.26	0.68
2:N:54:LEU:HB3	2:N:55:LEU:HD22	1.75	0.68
3:T:353:LEU:HB2	3:T:363:TYR:HB2	1.75	0.67
3:S:214:GLU:HG3	3:S:228:ASN:HD21	1.60	0.67
2:N:52:VAL:O	2:N:54:LEU:N	2.28	0.66
3:T:141:GLN:NE2	3:T:161:PRO:O	2.27	0.66
1:M:98:ASN:ND2	1:M:271:GLU:O	2.29	0.65
3:T:48:ARG:HG3	3:T:53:LEU:HB2	1.79	0.65
4:Q:309:ARG:NH1	4:Q:396:GLU:OE1	2.29	0.65
4:Q:395:TYR:OH	5:A:4:MAW:O3	2.08	0.64
2:N:76:SER:HB3	2:N:228:LEU:N	2.10	0.64
4:Q:298:ASN:ND2	4:Q:302:GLN:O	2.31	0.64
3:S:336:VAL:HG12	3:S:337:HIS:N	2.11	0.64
1:M:135:THR:HA	2:N:279:GLN:HE22	1.63	0.64
4:Q:430:GLU:HB2	4:Q:481:MET:HG3	1.79	0.63
2:N:63:ALA:HB1	2:N:259:VAL:HA	1.81	0.63
1:M:146:VAL:HG12	1:M:263:LEU:HD21	1.80	0.62
2:N:106:ARG:NH2	2:N:172:GLU:OE2	2.31	0.62
4:Q:34:GLU:OE1	4:Q:37:ARG:NH2	2.32	0.62
3:S:253:GLN:O	3:S:265:LEU:N	2.32	0.61
2:N:51:ARG:HG2	2:N:57:VAL:HG11	1.82	0.61
3:S:34:VAL:HG22	3:S:190:TYR:HB3	1.81	0.61
3:T:11:VAL:HA	3:T:20:VAL:HG23	1.82	0.61
3:S:158:PHE:HD2	3:S:161:PRO:HG2	1.65	0.61
3:T:93:VAL:HG13	3:T:143:VAL:HG21	1.81	0.61
3:S:174:ARG:HD2	3:S:197:GLU:HA	1.81	0.61
3:T:92:ASN:ND2	3:T:129:GLU:OE2	2.34	0.61
3:S:335:GLU:O	3:S:337:HIS:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:192:THR:HG22	3:T:194:ASP:H	1.66	0.60
3:T:36:VAL:HG21	3:T:198:ALA:HB2	1.84	0.60
3:T:41:CYS:SG	3:T:42:GLY:N	2.75	0.60
4:Q:20:ARG:HA	5:A:1:BEM:O3	2.02	0.59
2:N:52:VAL:HG12	2:N:53:PHE:N	2.17	0.59
4:Q:113:VAL:HG13	4:Q:312:VAL:HB	1.84	0.59
4:Q:96:ILE:HA	4:Q:100:ALA:HB3	1.85	0.59
1:M:89:SER:HB2	1:M:92:PHE:HB3	1.85	0.59
3:T:355:ASP:HB2	3:T:362:ILE:HD11	1.84	0.58
4:Q:20:ARG:N	4:Q:74:ASP:OD1	2.35	0.58
2:N:217:MET:HB3	2:N:230:VAL:HG22	1.85	0.58
1:M:137:VAL:HG12	1:M:198:GLY:HA3	1.87	0.57
1:M:262:ILE:HD11	1:M:281:TYR:CE2	2.40	0.57
1:M:164:ASN:HB3	1:M:174:ARG:HG2	1.87	0.57
3:T:124:LEU:HB2	3:T:127:LEU:HB2	1.86	0.57
4:Q:188:PRO:HB3	4:Q:248:PHE:HA	1.86	0.56
3:S:68:ILE:HB	3:S:76:ARG:HG2	1.87	0.56
4:Q:173:ASN:HD22	4:Q:173:ASN:H	1.52	0.56
3:T:257:LEU:HD21	3:T:263:ILE:HG12	1.87	0.56
1:M:49:LEU:HA	1:M:53:TYR:HB2	1.88	0.56
3:S:264:SER:HB3	3:S:298:ARG:HG3	1.87	0.56
3:T:296:SER:O	3:T:298:ARG:NH1	2.38	0.56
1:M:235:LEU:O	1:M:239:VAL:HG23	2.06	0.56
1:M:308:VAL:HG21	2:N:122:TRP:CE3	2.41	0.56
2:N:51:ARG:HB3	2:N:57:VAL:HG21	1.86	0.56
3:S:66:ARG:NH2	3:S:75:ASP:O	2.39	0.56
4:Q:14:LYS:O	4:Q:68:PRO:HB2	2.06	0.55
3:T:38:PRO:O	3:T:43:LYS:NZ	2.36	0.55
1:M:150:GLY:HA3	2:N:236:ILE:HG22	1.89	0.55
3:S:4:SER:HB3	3:S:29:PRO:HG3	1.88	0.55
3:S:169:LEU:HD22	3:S:173:MET:HG2	1.89	0.55
3:T:208:MET:HG2	3:T:213:ILE:HA	1.88	0.55
1:M:35:TRP:HA	1:M:38:TYR:HB2	1.89	0.55
4:Q:142:ARG:NH2	4:Q:262:ASN:OD1	2.38	0.55
1:M:78:ILE:HG23	1:M:79:GLY:O	2.07	0.55
4:Q:481:MET:O	4:Q:484:GLN:HG3	2.07	0.55
3:S:158:PHE:CD2	3:S:161:PRO:HG2	2.41	0.55
3:T:247:ILE:HB	3:T:276:GLY:H	1.72	0.54
2:N:52:VAL:C	2:N:54:LEU:H	2.11	0.54
3:S:330:VAL:HG13	3:S:331:GLY:N	2.23	0.54
3:T:124:LEU:HD23	3:T:124:LEU:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:128:PRO:HB2	4:Q:312:VAL:HG23	1.90	0.54
1:M:90:GLU:O	1:M:94:ARG:HG2	2.07	0.54
4:Q:167:PHE:O	4:Q:180:GLU:HG3	2.07	0.54
3:T:290:LEU:O	3:T:292:GLY:N	2.41	0.53
3:S:96:ASN:O	3:S:147:ARG:HD3	2.08	0.53
1:M:170:ILE:HG23	1:M:172:LEU:HD13	1.91	0.53
3:T:36:VAL:HG12	3:T:207:VAL:HG12	1.90	0.53
2:N:179:GLY:HA2	3:T:74:LYS:HE2	1.91	0.53
3:T:301:ILE:HG22	3:T:344:LEU:HB2	1.91	0.53
3:T:48:ARG:HG2	3:T:54:GLU:HG3	1.91	0.53
3:T:122:LEU:HB2	3:T:124:LEU:HD22	1.91	0.53
3:S:291:ASP:HA	3:S:345:HIS:CE1	2.44	0.52
3:S:308:VAL:HG11	3:S:336:VAL:HG11	1.91	0.52
3:T:162:LEU:HD22	3:T:162:LEU:H	1.73	0.52
3:S:43:LYS:HG3	3:S:44:SER:H	1.75	0.52
3:T:156:PHE:HB2	3:T:188:VAL:HB	1.91	0.52
2:N:248:ALA:O	2:N:252:ASN:ND2	2.41	0.52
3:T:87:LEU:HA	3:T:147:ARG:HH12	1.75	0.52
2:N:243:GLU:HG2	4:Q:23:TRP:CH2	2.44	0.52
1:M:35:TRP:C	1:M:37:LEU:N	2.62	0.52
1:M:111:PHE:O	1:M:114:PRO:HD2	2.10	0.52
2:N:134:MET:HE2	2:N:134:MET:HA	1.91	0.52
4:Q:97:ASP:HA	4:Q:104:LYS:HD3	1.92	0.52
3:T:5:VAL:HG13	3:T:27:ILE:HB	1.92	0.52
4:Q:426:MET:HB3	4:Q:430:GLU:HG3	1.92	0.51
1:M:165:ASN:OD1	1:M:174:ARG:NH1	2.43	0.51
3:T:241:ASN:O	3:T:282:GLY:HA2	2.10	0.51
1:M:124:VAL:HG12	1:M:125:TYR:O	2.11	0.51
2:N:55:LEU:HD22	2:N:55:LEU:N	2.25	0.51
3:S:243:MET:HE1	3:S:326:LEU:HB3	1.91	0.51
3:S:334:ASN:HD21	3:S:336:VAL:CG2	2.15	0.51
3:T:92:ASN:OD1	3:T:93:VAL:N	2.43	0.51
2:N:44:GLY:O	2:N:48:THR:OG1	2.19	0.51
3:S:213:ILE:HD11	3:S:216:ILE:HD11	1.93	0.51
3:S:305:VAL:HG13	3:S:338:PRO:HA	1.93	0.51
4:Q:48:ASN:OD1	4:Q:48:ASN:N	2.34	0.51
1:M:96:ILE:HB	1:M:276:ILE:HD11	1.92	0.51
4:Q:157:ILE:HD13	4:Q:197:PHE:HB3	1.93	0.51
3:T:88:TYR:HB3	3:T:90:HIS:CD2	2.46	0.51
3:T:76:ARG:HB3	3:T:78:VAL:HG22	1.93	0.50
4:Q:394:ASP:OD1	4:Q:397:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:275:MET:HG3	4:Q:404:ALA:HB2	1.92	0.50
3:T:34:VAL:HG22	3:T:190:TYR:HB3	1.94	0.50
3:T:296:SER:OG	3:T:297:GLU:OE2	2.28	0.50
4:Q:133:GLY:HA3	4:Q:309:ARG:HD2	1.92	0.50
3:S:159:ASP:OD1	3:S:160:GLN:HG3	2.11	0.50
4:Q:335:PHE:HE2	4:Q:344:ILE:HD11	1.76	0.50
4:Q:171:ASP:OD2	4:Q:176:GLY:N	2.37	0.50
1:M:229:MET:O	1:M:233:ILE:HG12	2.11	0.50
3:T:171:THR:HG22	3:T:174:ARG:HH12	1.76	0.50
3:T:178:LYS:NZ	3:T:200:THR:O	2.35	0.49
3:T:238:PRO:HB2	3:T:285:PRO:HG2	1.94	0.49
1:M:49:LEU:O	1:M:54:LYS:N	2.45	0.49
3:S:92:ASN:ND2	3:S:95:ASP:OD2	2.44	0.49
3:S:353:LEU:HB2	3:S:363:TYR:HB3	1.94	0.49
4:Q:231:MET:HA	4:Q:234:VAL:HG22	1.93	0.49
3:T:35:LEU:HD11	3:T:189:ILE:HD11	1.94	0.49
4:Q:201:ARG:HH11	4:Q:306:GLU:HG3	1.78	0.49
2:N:260:VAL:O	2:N:264:ILE:HG23	2.13	0.49
3:S:320:THR:HA	3:S:325:SER:HA	1.94	0.49
1:M:138:TYR:HB2	2:N:275:TYR:OH	2.14	0.48
3:S:66:ARG:HH21	3:S:71:LEU:HD21	1.78	0.48
3:S:347:ASP:OD1	3:S:349:THR:HG22	2.12	0.48
3:T:161:PRO:HG2	3:T:162:LEU:HD13	1.94	0.48
3:T:252:THR:HG22	3:T:267:PRO:HA	1.95	0.48
1:M:239:VAL:HG12	1:M:319:THR:HG21	1.95	0.48
3:S:105:ARG:O	3:S:106:THR:OG1	2.29	0.48
4:Q:491:LYS:HD3	4:Q:492:ASN:H	1.79	0.48
3:T:237:SER:HB3	3:T:238:PRO:HD3	1.95	0.48
3:T:124:LEU:HD12	3:T:127:LEU:HB2	1.95	0.48
3:S:11:VAL:HA	3:S:20:VAL:HG22	1.95	0.48
3:S:200:THR:HB	3:T:309:GLU:HB3	1.95	0.48
4:Q:83:TYR:HB3	4:Q:88:ALA:HB3	1.96	0.48
1:M:59:LEU:O	1:M:63:PHE:HB2	2.14	0.48
2:N:158:ILE:HA	2:N:161:ARG:HG2	1.96	0.48
1:M:79:GLY:C	1:M:81:ASP:H	2.17	0.48
4:Q:197:PHE:O	4:Q:298:ASN:HB2	2.13	0.48
3:T:35:LEU:HD23	3:T:206:VAL:HG13	1.95	0.48
2:N:273:ILE:O	2:N:276:PRO:HD2	2.13	0.47
1:M:81:ASP:O	1:M:84:VAL:N	2.45	0.47
2:N:100:TYR:CD1	2:N:186:LEU:HD13	2.49	0.47
4:Q:142:ARG:NH1	4:Q:144:ASP:OD2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:35:TRP:CD2	1:M:36:LEU:N	2.82	0.47
1:M:248:ILE:HG12	2:N:122:TRP:HH2	1.80	0.47
3:S:305:VAL:HG12	3:S:340:ASP:O	2.15	0.47
1:M:142:PHE:HB3	2:N:271:VAL:HG11	1.96	0.47
3:S:232:ALA:HB1	3:S:240:MET:HE2	1.96	0.47
1:M:189:ILE:O	1:M:193:ILE:HG23	2.14	0.47
3:S:271:THR:HG22	3:S:363:TYR:HA	1.97	0.47
3:S:296:SER:HB2	3:S:300:GLN:H	1.80	0.47
4:Q:182:PRO:O	4:Q:266:PHE:N	2.48	0.47
4:Q:201:ARG:NH1	4:Q:306:GLU:HG3	2.30	0.47
2:N:161:ARG:HG3	2:N:162:ASN:N	2.28	0.47
3:S:62:ARG:HB2	3:S:66:ARG:O	2.15	0.47
3:S:300:GLN:HG2	3:S:346:VAL:H	1.79	0.47
1:M:259:GLU:O	1:M:262:ILE:HG22	2.14	0.47
3:S:165:LEU:HD13	3:S:169:LEU:HD13	1.97	0.47
3:T:110:VAL:O	3:T:112:ASP:N	2.48	0.46
3:T:321:VAL:HG23	3:T:322:GLY:H	1.80	0.46
3:T:330:VAL:C	3:T:332:GLY:H	2.17	0.46
3:T:330:VAL:HG12	3:T:332:GLY:N	2.30	0.46
3:S:240:MET:HG3	3:S:284:ARG:HG2	1.97	0.46
4:Q:140:PHE:HB3	4:Q:290:LEU:HD22	1.96	0.46
1:M:92:PHE:O	1:M:95:ALA:N	2.44	0.46
3:S:293:VAL:O	3:S:294:GLU:HG3	2.15	0.46
3:S:209:ARG:HD3	3:S:230:PHE:CE1	2.51	0.46
3:S:43:LYS:HB2	3:S:191:VAL:HG13	1.98	0.46
3:S:50:VAL:HA	3:S:61:ILE:HD11	1.97	0.46
4:Q:175:ASN:ND2	4:Q:179:ASP:OD2	2.47	0.46
1:M:30:ASP:O	1:M:33:ARG:HB3	2.15	0.46
1:M:184:PHE:HZ	1:M:261:ILE:HG12	1.81	0.46
1:M:267:PRO:O	1:M:270:TYR:HB2	2.15	0.46
2:N:51:ARG:O	2:N:52:VAL:HB	2.16	0.46
1:M:34:ASP:O	1:M:38:TYR:CG	2.68	0.46
3:S:334:ASN:ND2	3:S:336:VAL:N	2.63	0.46
2:N:36:ILE:HD12	2:N:37:PHE:N	2.31	0.46
3:S:158:PHE:HD2	3:S:161:PRO:CG	2.29	0.46
3:S:246:ARG:NH1	3:S:278:GLU:OE2	2.49	0.45
1:M:77:TRP:O	1:M:78:ILE:HB	2.15	0.45
3:S:233:SER:HB2	3:S:242:LEU:HD21	1.98	0.45
3:S:280:VAL:HG13	3:S:354:PHE:HB2	1.98	0.45
3:S:144:ALA:O	3:S:147:ARG:HB2	2.16	0.45
2:N:226:ILE:HA	2:N:227:PRO:HD3	1.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:43:LYS:NZ	3:S:193:HIS:HB3	2.31	0.45
3:S:308:VAL:CG1	3:S:336:VAL:HG11	2.47	0.45
3:T:271:THR:HB	3:T:273:LEU:HD23	1.99	0.45
3:T:283:ILE:HD13	3:T:351:VAL:HG12	1.98	0.45
1:M:235:LEU:HA	1:M:238:ILE:HG22	1.99	0.45
4:Q:266:PHE:HE1	4:Q:293:ILE:HD11	1.81	0.45
4:Q:114:GLU:HG3	4:Q:124:ILE:HD11	1.99	0.45
3:T:165:LEU:HB3	3:T:169:LEU:HD23	1.99	0.45
3:T:2:VAL:HG12	3:T:29:PRO:HB2	1.99	0.45
4:Q:193:ARG:NH1	4:Q:307:ASP:HB2	2.31	0.45
4:Q:117:ILE:CG2	4:Q:312:VAL:HG21	2.47	0.44
2:N:214:PHE:O	2:N:217:MET:HG3	2.17	0.44
4:Q:114:GLU:O	4:Q:118:LYS:HG3	2.17	0.44
1:M:150:GLY:HA2	1:M:153:VAL:HG12	1.99	0.44
3:S:106:THR:O	3:S:107:LYS:HB2	2.17	0.44
3:S:311:LEU:HB3	3:S:312:GLY:H	1.66	0.44
4:Q:172:PRO:HD2	4:Q:180:GLU:CD	2.38	0.44
3:T:62:ARG:HB2	3:T:66:ARG:O	2.18	0.44
3:T:46:THR:O	3:T:50:VAL:HG23	2.18	0.44
3:T:268:ARG:HB3	3:T:269:ALA:H	1.55	0.44
2:N:222:ALA:HB3	2:N:225:LYS:HD2	2.00	0.44
3:S:50:VAL:HG22	3:S:61:ILE:HD12	2.00	0.44
3:T:68:ILE:HA	3:T:71:LEU:HD22	1.99	0.44
1:M:30:ASP:CG	1:M:33:ARG:HH12	2.04	0.43
3:S:300:GLN:CG	3:S:346:VAL:H	2.31	0.43
2:N:32:PRO:O	2:N:36:ILE:HG13	2.18	0.43
3:T:304:THR:HA	3:T:341:PRO:HA	2.00	0.43
3:S:247:ILE:HB	3:S:276:GLY:N	2.21	0.43
4:Q:1:LYS:HG3	4:Q:5:TRP:CZ3	2.54	0.43
4:Q:5:TRP:HD1	4:Q:38:LEU:O	2.02	0.43
4:Q:13:LEU:HB2	4:Q:43:LEU:CD2	2.49	0.43
2:N:243:GLU:HG2	4:Q:23:TRP:CZ3	2.54	0.43
2:N:228:LEU:HD12	2:N:228:LEU:HA	1.74	0.43
3:T:35:LEU:HD12	3:T:191:VAL:HG22	1.99	0.43
3:T:44:SER:O	3:T:48:ARG:HB2	2.18	0.43
4:Q:6:VAL:HB	4:Q:331:LYS:HB3	2.01	0.43
1:M:131:LYS:O	1:M:135:THR:HG23	2.18	0.43
3:S:100:GLY:O	3:S:103:LEU:HB2	2.18	0.43
4:Q:186:ARG:HG3	4:Q:187:HIS:ND1	2.34	0.43
3:T:280:VAL:HG13	3:T:354:PHE:HB2	2.01	0.43
2:N:255:SER:OG	2:N:257:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:361:ALA:O	4:Q:398:GLN:NE2	2.44	0.43
3:T:314:GLU:OE1	3:T:329:LYS:HE2	2.18	0.43
2:N:52:VAL:C	2:N:54:LEU:N	2.72	0.42
4:Q:17:MET:HG2	4:Q:19:PHE:HD1	1.84	0.42
3:T:47:LEU:HD11	3:T:157:LEU:HB3	2.00	0.42
2:N:70:ASP:OD2	2:N:231:TYR:OH	2.36	0.42
4:Q:53:ASN:O	4:Q:57:GLN:HG2	2.20	0.42
3:S:35:LEU:HB2	3:S:191:VAL:HG22	2.01	0.42
4:Q:295:PRO:HD3	4:Q:411:TYR:CZ	2.55	0.42
3:T:202:ALA:HB1	3:T:204:ARG:O	2.19	0.42
1:M:144:SER:HB3	1:M:147:ILE:HG13	2.01	0.42
3:S:249:VAL:HG12	3:S:250:ASP:N	2.34	0.42
4:Q:330:ILE:HD12	4:Q:330:ILE:HA	1.93	0.42
2:N:103:SER:HB2	2:N:165:GLU:HG3	2.02	0.42
2:N:150:PHE:O	2:N:209:ARG:NH2	2.53	0.42
2:N:242:ASN:HB3	2:N:244:GLU:H	1.85	0.42
3:S:321:VAL:HG23	3:S:326:LEU:HD12	2.01	0.42
4:Q:250:ARG:NH1	4:Q:257:GLN:OE1	2.45	0.42
3:T:268:ARG:HA	3:T:268:ARG:NE	2.35	0.42
1:M:151:LEU:HD21	2:N:264:ILE:HD13	2.02	0.42
4:Q:5:TRP:CG	4:Q:40:ASN:HB2	2.55	0.42
4:Q:2:GLU:HB2	4:Q:5:TRP:CD1	2.55	0.42
3:T:356:ALA:O	3:T:359:GLN:NE2	2.53	0.42
1:M:259:GLU:HA	1:M:262:ILE:HG22	2.01	0.41
3:S:122:LEU:HB2	3:S:124:LEU:HG	2.02	0.41
1:M:134:GLN:HB3	1:M:138:TYR:CE2	2.56	0.41
1:M:290:TYR:CE2	2:N:132:LEU:HD21	2.55	0.41
3:S:107:LYS:HD2	3:S:107:LYS:HA	1.91	0.41
3:T:247:ILE:HB	3:T:275:PRO:HA	2.02	0.41
3:T:337:HIS:HA	3:T:338:PRO:HD2	1.89	0.41
3:S:333:LEU:O	3:S:334:ASN:HB3	2.21	0.41
3:S:355:ASP:HB3	3:S:358:SER:O	2.20	0.41
2:N:231:TYR:O	2:N:235:THR:HG22	2.20	0.41
3:S:209:ARG:HG2	3:S:210:ASP:OD2	2.20	0.41
3:S:160:GLN:HE21	3:S:160:GLN:HB3	1.64	0.41
4:Q:144:ASP:OD1	4:Q:144:ASP:N	2.53	0.41
2:N:148:ILE:HD12	2:N:148:ILE:HA	1.97	0.41
3:S:190:TYR:HE1	3:S:192:THR:HG1	1.68	0.41
3:S:192:THR:HG22	3:S:194:ASP:H	1.85	0.41
4:Q:469:GLN:HA	4:Q:472:LEU:HG	2.02	0.41
3:T:306:ASP:HB2	3:T:320:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:3:BEM:O3	5:A:4:MAW:O5	2.31	0.41
1:M:267:PRO:HA	1:M:270:TYR:CD1	2.56	0.41
3:S:272:HIS:O	3:S:272:HIS:ND1	2.53	0.41
3:S:147:ARG:O	3:S:150:VAL:HG12	2.21	0.41
4:Q:12:THR:C	4:Q:13:LEU:HD23	2.41	0.41
4:Q:353:THR:HG21	4:Q:381:MET:HE1	2.02	0.41
3:T:207:VAL:HG23	3:T:214:GLU:HB3	2.03	0.41
1:M:36:LEU:HD23	2:N:182:ASP:HB2	2.02	0.41
1:M:120:MET:O	1:M:124:VAL:HG23	2.20	0.41
3:S:12:LYS:HD3	3:S:13:ARG:N	2.36	0.40
4:Q:58:PHE:CD2	4:Q:79:LYS:HD3	2.56	0.40
4:Q:187:HIS:HA	4:Q:188:PRO:HD2	1.81	0.40
4:Q:238:TYR:CE2	4:Q:245:LYS:HA	2.57	0.40
3:T:117:THR:O	3:T:121:ILE:HG12	2.21	0.40
1:M:30:ASP:CA	1:M:33:ARG:NH1	2.73	0.40
3:S:215:GLN:HG2	3:S:216:ILE:N	2.37	0.40
3:S:266:LEU:HG	3:S:348:LEU:HB3	2.03	0.40
3:T:290:LEU:C	3:T:292:GLY:H	2.23	0.40
1:M:84:VAL:HA	1:M:87:PHE:HB2	2.04	0.40
2:N:64:TYR:O	2:N:68:LEU:HG	2.21	0.40
3:T:156:PHE:HB3	3:T:158:PHE:CE1	2.56	0.40
2:N:124:ASN:OD1	2:N:126:GLY:N	2.41	0.40
2:N:196:PRO:O	2:N:200:THR:HG23	2.21	0.40
3:S:261:ASN:OD1	3:S:302:LYS:N	2.54	0.40
4:Q:181:VAL:O	4:Q:264:GLY:HA2	2.20	0.40
4:Q:275:MET:HE2	4:Q:403:GLU:HB2	2.04	0.40
4:Q:62:MET:HG2	4:Q:83:TYR:CE1	2.57	0.40
4:Q:253:ARG:NH1	4:Q:257:GLN:HE22	2.19	0.40
3:T:137:GLY:HA2	3:T:140:ARG:HD3	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	280/301 (93%)	254 (91%)	25 (9%)	1 (0%)	34 69
2	N	281/305 (92%)	247 (88%)	30 (11%)	4 (1%)	11 46
3	S	361/363 (99%)	325 (90%)	31 (9%)	5 (1%)	11 46
3	T	361/363 (99%)	327 (91%)	30 (8%)	4 (1%)	14 51
4	Q	490/516 (95%)	477 (97%)	12 (2%)	1 (0%)	47 79
All	All	1773/1848 (96%)	1630 (92%)	128 (7%)	15 (1%)	19 58

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	78	ILE
3	T	111	ILE
2	N	52	VAL
2	N	53	PHE
2	N	54	LEU
3	S	336	VAL
3	T	110	VAL
3	S	334	ASN
3	T	258	ASN
2	N	59	ILE
3	S	249	VAL
3	S	362	ILE
3	T	108	LYS
3	S	337	HIS
4	Q	312	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	M	248/260 (95%)	216 (87%)	32 (13%)	4 19
2	N	239/258 (93%)	217 (91%)	22 (9%)	9 33
3	S	307/307 (100%)	273 (89%)	34 (11%)	6 25
3	T	307/307 (100%)	272 (89%)	35 (11%)	5 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	Q	424/440 (96%)	395 (93%)	29 (7%)	16 49
All	All	1525/1572 (97%)	1373 (90%)	152 (10%)	7 30

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	28	TRP
1	M	38	TYR
1	M	41	LEU
1	M	45	ILE
1	M	59	LEU
1	M	63	PHE
1	M	77	TRP
1	M	78	ILE
1	M	80	PHE
1	M	82	HIS
1	M	84	VAL
1	M	86	LEU
1	M	87	PHE
1	M	96	ILE
1	M	97	LYS
1	M	105	LEU
1	M	116	LEU
1	M	151	LEU
1	M	167	LEU
1	M	170	ILE
1	M	176	TYR
1	M	201	SER
1	M	235	LEU
1	M	238	ILE
1	M	242	ILE
1	M	263	LEU
1	M	265	TYR
1	M	266	GLN
1	M	270	TYR
1	M	292	ILE
1	M	309	LEU
1	M	310	PHE
2	N	2	LEU
2	N	12	ARG
2	N	37	PHE
2	N	51	ARG

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Mol	Chain	Res	Type
2	N	54	LEU
2	N	58	ASP
2	N	67	VAL
2	N	77	TYR
2	N	102	LEU
2	N	106	ARG
2	N	108	ARG
2	N	150	PHE
2	N	161	ARG
2	N	198	LEU
2	N	217	MET
2	N	224	GLU
2	N	235	THR
2	N	241	VAL
2	N	243	GLU
2	N	249	LEU
2	N	257	GLU
2	N	264	ILE
3	S	5	VAL
3	S	11	VAL
3	S	20	VAL
3	S	60	THR
3	S	67	VAL
3	S	84	ASN
3	S	87	LEU
3	S	112	ASP
3	S	116	LYS
3	S	134	ASP
3	S	150	VAL
3	S	160	GLN
3	S	169	LEU
3	S	188	VAL
3	S	192	THR
3	S	206	VAL
3	S	229	THR
3	S	235	ILE
3	S	252	THR
3	S	257	LEU
3	S	271	THR
3	S	273	LEU
3	S	279	VAL
3	S	286	GLU

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Mol	Chain	Res	Type
3	S	289	THR
3	S	298	ARG
3	S	311	LEU
3	S	326	LEU
3	S	328	VAL
3	S	330	VAL
3	S	333	LEU
3	S	334	ASN
3	S	335	GLU
3	S	348	LEU
4	Q	9	LYS
4	Q	13	LEU
4	Q	23	TRP
4	Q	48	ASN
4	Q	52	THR
4	Q	55	GLN
4	Q	97	ASP
4	Q	98	GLN
4	Q	112	GLU
4	Q	129	TYR
4	Q	142	ARG
4	Q	161	TYR
4	Q	171	ASP
4	Q	173	ASN
4	Q	180	GLU
4	Q	185	ASP
4	Q	228	ARG
4	Q	233	HIS
4	Q	253	ARG
4	Q	279	GLU
4	Q	290	LEU
4	Q	317	TRP
4	Q	321	VAL
4	Q	327	VAL
4	Q	395	TYR
4	Q	446	TYR
4	Q	481	MET
4	Q	484	GLN
4	Q	491	LYS
3	T	5	VAL
3	T	11	VAL
3	T	18	THR

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Mol	Chain	Res	Type
3	T	33	VAL
3	T	55	GLU
3	T	60	THR
3	T	61	ILE
3	T	76	ARG
3	T	102	ARG
3	T	104	LYS
3	T	116	LYS
3	T	150	VAL
3	T	151	ARG
3	T	162	LEU
3	T	188	VAL
3	T	189	ILE
3	T	192	THR
3	T	206	VAL
3	T	210	ASP
3	T	212	LEU
3	T	229	THR
3	T	246	ARG
3	T	252	THR
3	T	255	VAL
3	T	257	LEU
3	T	268	ARG
3	T	291	ASP
3	T	298	ARG
3	T	308	VAL
3	T	321	VAL
3	T	326	LEU
3	T	329	LYS
3	T	333	LEU
3	T	335	GLU
3	T	346	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	60	GLN
2	N	279	GLN
3	S	160	GLN
3	S	334	ASN
4	Q	55	GLN
4	Q	85	GLN

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Mol	Chain	Res	Type
4	Q	123	ASN
3	T	90	HIS
3	T	160	GLN

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	0.74	0	18,19,19	0.59	0
5	BEM	A	2	5	12,12,13	0.69	0	14,17,19	0.70	0
5	BEM	A	3	5	12,12,13	0.68	0	14,17,19	0.69	0
5	MAW	A	4	5	10,11,12	3.00	3 (30%)	13,15,17	1.67	4 (30%)

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	-	1/4/24/24	0/1/1/1
5	BEM	A	2	5	-	0/4/21/24	0/1/1/1
5	BEM	A	3	5	-	1/4/21/24	0/1/1/1
5	MAW	A	4	5	-	0/4/17/20	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4	MAW	C3-C4	-6.85	1.41	1.50
5	A	4	MAW	C4-C5	4.63	1.40	1.33
5	A	4	MAW	C5-C6	-3.83	1.39	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	4	MAW	O5-C5-C6	3.06	116.11	111.52
5	A	4	MAW	O5-C5-C4	-2.85	122.41	124.81
5	A	4	MAW	C2-C3-C4	2.65	115.94	112.32
5	A	4	MAW	O6B-C6-C5	2.32	119.98	114.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

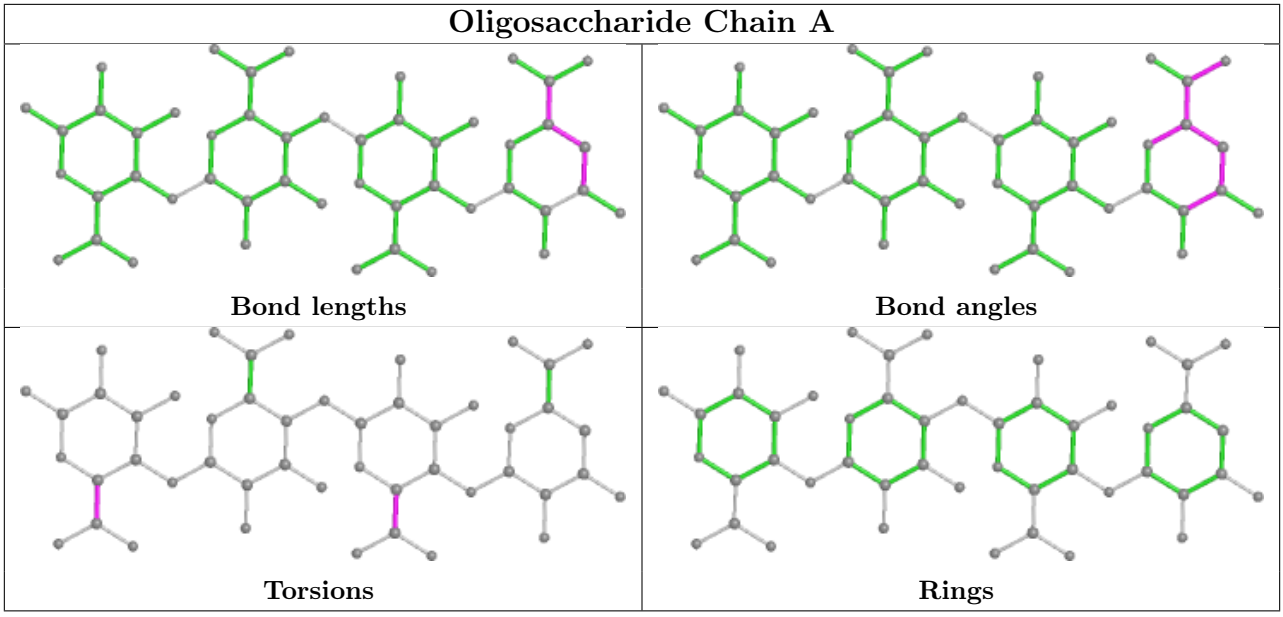
Mol	Chain	Res	Type	Atoms
5	A	1	BEM	O5-C5-C6-O6B
5	A	3	BEM	O5-C5-C6-O6B

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	BEM	1	0
5	A	4	MAW	2	0
5	A	3	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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	284/301 (94%)	-0.29	11 (3%)	39	25	63, 102, 170, 212	0
2	N	283/305 (92%)	-0.29	1 (0%)	92	89	53, 98, 143, 182	0
3	S	363/363 (100%)	-0.19	13 (3%)	42	27	42, 98, 152, 234	0
3	T	363/363 (100%)	0.08	18 (4%)	28	16	51, 122, 194, 228	0
4	Q	492/516 (95%)	-0.01	14 (2%)	53	37	88, 127, 174, 227	0
All	All	1785/1848 (96%)	-0.12	57 (3%)	47	31	42, 112, 176, 234	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	301	GLY	6.3
3	S	295	GLY	5.6
3	T	333	LEU	5.1
3	T	107	LYS	5.1
3	T	106	THR	4.5
3	T	17	THR	4.4
1	M	61	MET	4.4
3	T	136	SER	4.2
3	S	296	SER	4.1
3	T	15	ASP	3.9
3	S	298	ARG	3.8
4	Q	283	LYS	3.6
1	M	77	TRP	3.6
3	T	14	TYR	3.5
2	N	60	ASP	3.4
3	T	13	ARG	3.4
4	Q	492	ASN	3.4
4	Q	150	ASN	3.2
3	S	106	THR	3.1
3	S	332	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
3	T	295	GLY	2.9
3	T	108	LYS	2.8
3	S	292	GLY	2.8
3	T	16	LYS	2.8
3	S	294	GLU	2.7
4	Q	185	ASP	2.6
3	T	18	THR	2.6
1	M	78	ILE	2.6
3	S	293	VAL	2.6
3	S	299	ALA	2.5
3	S	108	LYS	2.5
3	S	107	LYS	2.5
3	T	98	SER	2.5
1	M	76	PRO	2.5
1	M	171	GLY	2.5
3	S	335	GLU	2.4
4	Q	268	HIS	2.4
3	T	104	LYS	2.3
3	T	113	ALA	2.3
4	Q	388	GLY	2.2
1	M	26	ARG	2.2
4	Q	91	PRO	2.2
4	Q	466	TYR	2.2
4	Q	266	PHE	2.2
1	M	90	GLU	2.2
4	Q	433	ILE	2.2
1	M	169	TRP	2.2
3	T	101	LEU	2.2
1	M	28	TRP	2.1
1	M	172	LEU	2.1
4	Q	489	GLN	2.1
3	S	252	THR	2.0
3	T	121	ILE	2.0
4	Q	300	LYS	2.0
4	Q	223	ALA	2.0
1	M	32	LYS	2.0
3	T	252	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)

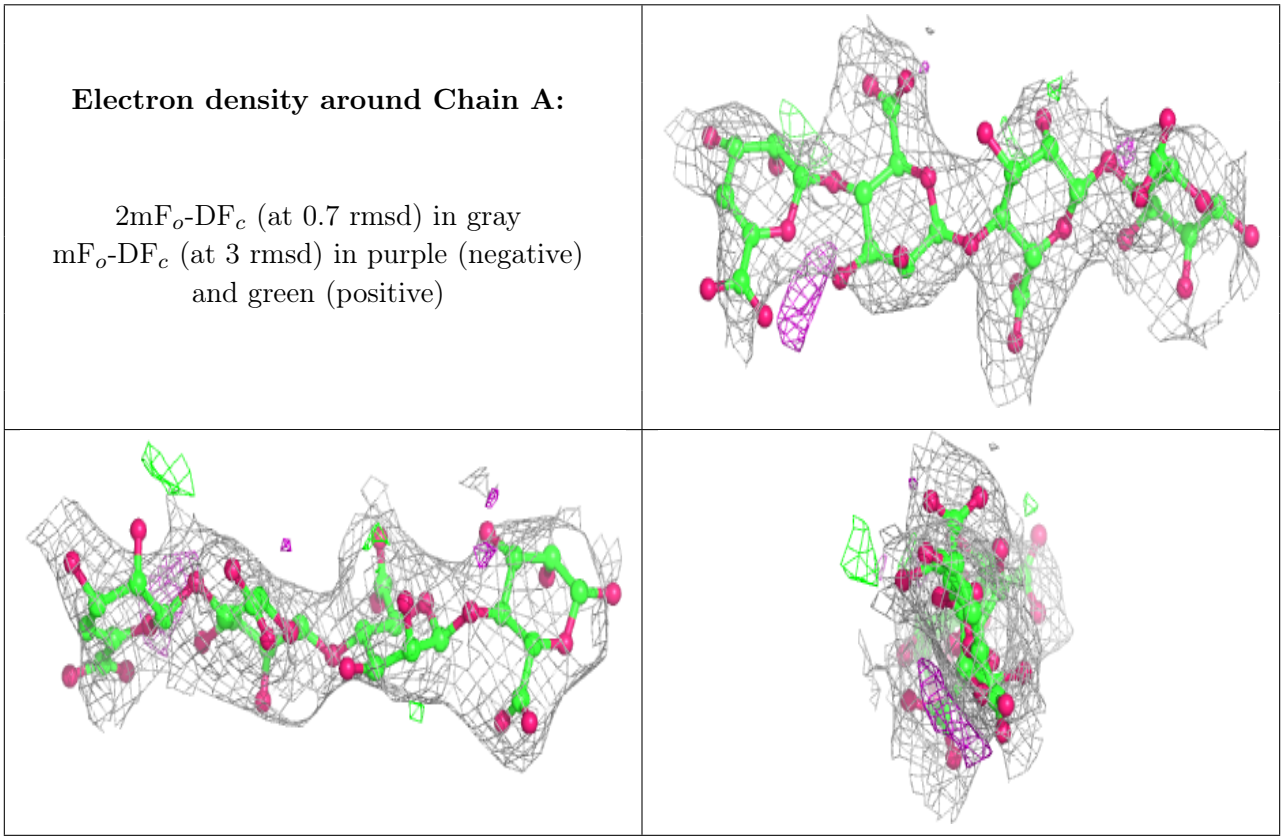
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	1	13/13	0.85	0.24	114,127,135,156	0
5	BEM	A	2	12/13	0.89	0.22	95,114,134,160	0
5	BEM	A	3	12/13	0.90	0.25	87,125,137,148	0
5	MAW	A	4	11/12	0.90	0.23	103,135,143,152	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 (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
6	CA	Q	501	1/1	0.82	0.12	246,246,246,246	0

6.5 Other polymers (i)

There are no such residues in this entry.