Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2021 – 02:09 PM JST

PDB ID	:	6JQ9
Title	:	Crystal structure of a lyase from Alteromonas sp.
Authors	:	Qin, H.M.; Guo, Q.Q.
Deposited on	:	2019-03-29
Resolution	:	1.81 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 following versions of software and data (see references (1)) were used in the production of this report:

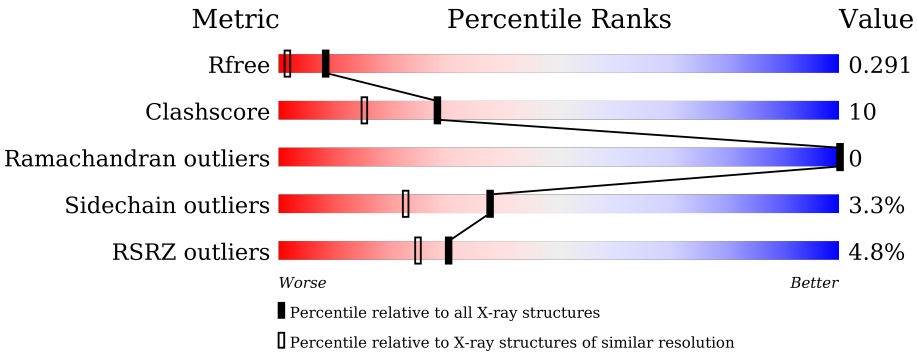
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.81 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	A	483	4% 84% 15%
1	B	483	6% 82% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	603	-	-	X	-
3	SO4	A	604	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9042 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.

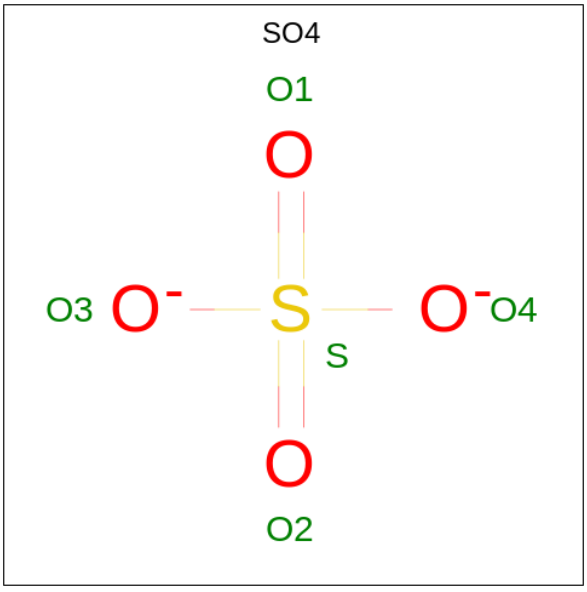
- Molecule 1 is a protein called Short ulvan lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	1	0
			3851	2452	657	733	9			
1	B	483	Total	C	N	O	S	0	0	0
			3816	2430	648	729	9			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

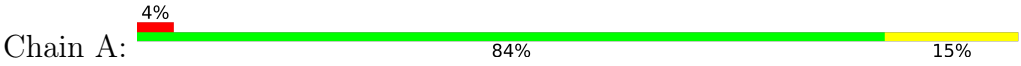
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	676	Total O 676 676	0	0
4	B	680	Total O 680 680	0	0

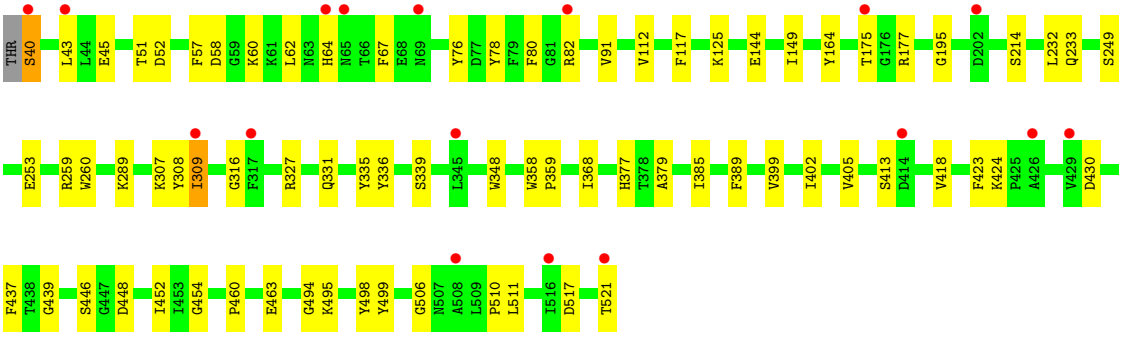
3 Residue-property plots (i)

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: Short ulvan lyase

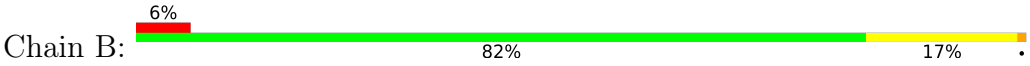
Chain A:

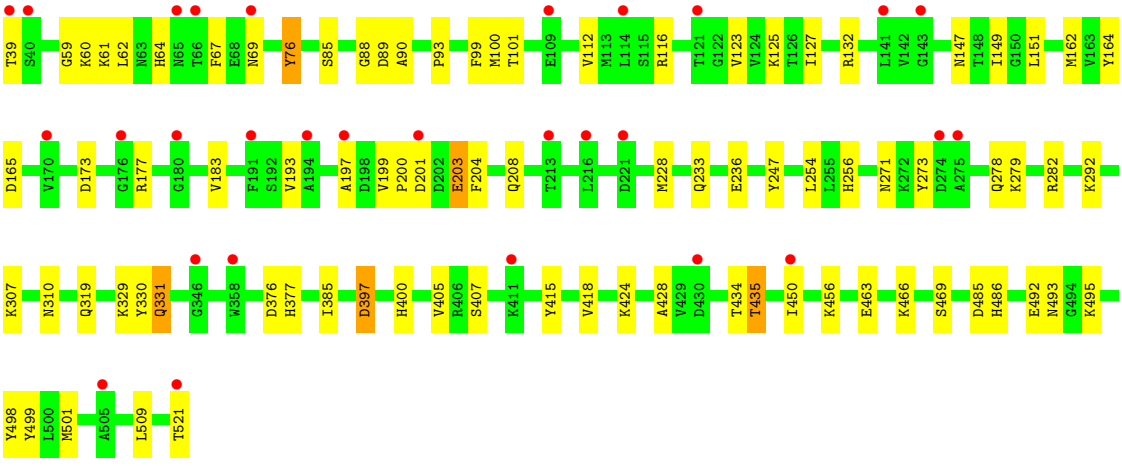




• Molecule 1: Short ulvan lyase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.05Å 121.77Å 124.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.89 – 1.81 24.88 – 1.81	Depositor EDS
% Data completeness (in resolution range)	99.0 (24.89-1.81) 99.1 (24.88-1.81)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.84 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.235 , 0.288 0.243 , 0.291	Depositor DCC
R_{free} test set	5736 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9042	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9476e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: SO4, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.77	0/3966	0.92	0/5377
1	B	0.79	0/3927	0.94	0/5331
All	All	0.78	0/7893	0.93	0/10708

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	A	3851	0	3576	56	0
1	B	3816	0	3501	88	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	10	0	0	3	0
3	B	5	0	0	1	0
4	A	676	0	0	17	0
4	B	680	0	0	51	0
All	All	9042	0	7077	144	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 (144) 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:B:116:ARG:HG2	4:B:914:HOH:O	1.49	1.12
1:B:236:GLU:HB2	4:B:1148:HOH:O	1.49	1.11
1:B:125:LYS:HB2	4:B:873:HOH:O	1.52	1.07
1:B:200:PRO:HD3	4:B:1125:HOH:O	1.59	1.02
1:A:499:TYR:CZ	4:A:763:HOH:O	2.20	0.94
1:B:85:SER:O	1:B:486:HIS:HE1	1.58	0.87
1:B:200:PRO:HD2	1:B:203:GLU:HG3	1.56	0.87
1:A:144:GLU:HA	4:A:819:HOH:O	1.77	0.84
1:A:45:GLU:OE1	1:A:495:LYS:HE3	1.79	0.83
1:B:99:PHE:CZ	4:B:910:HOH:O	2.32	0.82
1:B:149:ILE:HG12	4:B:772:HOH:O	1.80	0.81
1:A:82[B]:ARG:H	1:A:82[B]:ARG:HH21	1.29	0.81
1:B:521:THR:HG22	4:B:811:HOH:O	1.82	0.80
1:A:45:GLU:OE1	1:A:495:LYS:CE	2.32	0.78
1:B:197:ALA:HB1	4:B:910:HOH:O	1.85	0.76
1:A:80:PHE:HD2	4:A:819:HOH:O	1.69	0.73
1:B:112:VAL:HG22	4:B:772:HOH:O	1.88	0.72
1:B:162:MET:SD	4:B:1098:HOH:O	2.47	0.72
1:A:117:PHE:CD2	4:A:1138:HOH:O	2.41	0.72
1:A:379:ALA:N	3:A:603:SO4:O1	2.21	0.71
1:A:511:LEU:HD13	4:A:763:HOH:O	1.91	0.71
1:B:228:MET:O	1:B:279:LYS:HD2	1.92	0.70
1:B:123:VAL:HG12	4:B:873:HOH:O	1.91	0.70
1:B:99:PHE:HZ	4:B:910:HOH:O	1.73	0.69
1:B:424:LYS:NZ	1:B:428:ALA:O	2.25	0.69
1:B:418:VAL:HG21	1:B:435:THR:OG1	1.93	0.69
1:A:43:LEU:C	1:A:43:LEU:HD12	2.13	0.69
1:A:80:PHE:CD2	4:A:819:HOH:O	2.45	0.68
1:A:309:ILE:HD11	4:A:1307:HOH:O	1.93	0.67
1:B:64:HIS:CB	4:B:1208:HOH:O	2.45	0.65
1:B:292:LYS:CB	4:B:1271:HOH:O	2.45	0.65
1:B:125:LYS:NZ	1:B:201:ASP:O	2.25	0.64
1:B:204:PHE:CE2	4:B:764:HOH:O	2.50	0.64
1:A:259:ARG:CG	4:A:741:HOH:O	2.46	0.64
1:A:82[B]:ARG:HD3	1:A:82[B]:ARG:H	1.63	0.63
1:B:495:LYS:HE3	4:B:741:HOH:O	1.97	0.63
1:B:183:VAL:HB	4:B:805:HOH:O	1.98	0.63
1:B:278:GLN:O	1:B:279:LYS:HG2	1.99	0.62
1:B:279:LYS:HG3	4:B:1183:HOH:O	1.98	0.62
1:B:162:MET:CG	4:B:1098:HOH:O	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:LYS:CG	4:B:1183:HOH:O	2.47	0.62
1:A:78:TYR:CZ	1:A:82[B]:ARG:HD2	2.34	0.62
1:A:377:HIS:HB3	3:A:603:SO4:O2	2.00	0.62
1:A:214:SER:HB2	1:A:232:LEU:HD11	1.82	0.61
1:A:40:SER:HB3	4:A:1120:HOH:O	1.99	0.61
1:A:195:GLY:HA2	4:A:744:HOH:O	2.01	0.61
1:B:228:MET:O	1:B:279:LYS:CD	2.49	0.60
1:B:456:LYS:HE3	4:B:1243:HOH:O	2.01	0.60
1:B:162:MET:HG3	4:B:1098:HOH:O	2.00	0.60
1:B:199:VAL:HA	4:B:1125:HOH:O	2.01	0.60
1:B:88:GLY:C	4:B:706:HOH:O	2.38	0.60
1:B:183:VAL:HG22	4:B:905:HOH:O	2.02	0.59
1:B:279:LYS:HB2	4:B:1057:HOH:O	2.03	0.58
1:B:60:LYS:CB	4:B:1326:HOH:O	2.51	0.58
1:B:89:ASP:N	4:B:706:HOH:O	2.37	0.57
1:B:310:ASN:ND2	1:B:397:ASP:OD1	2.36	0.57
1:B:495:LYS:CE	4:B:741:HOH:O	2.50	0.57
1:A:446:SER:OG	1:A:494:GLY:HA2	2.05	0.55
1:B:127:ILE:HG13	4:B:764:HOH:O	2.06	0.55
1:B:99:PHE:CE1	4:B:910:HOH:O	2.57	0.55
1:B:101:THR:HG23	1:B:151:LEU:HD22	1.89	0.55
1:B:90:ALA:HB2	4:B:706:HOH:O	2.06	0.55
1:B:282:ARG:HD2	4:B:997:HOH:O	2.08	0.54
1:B:233:GLN:CB	4:B:925:HOH:O	2.55	0.54
1:A:253:GLU:HG3	4:A:1072:HOH:O	2.08	0.54
1:B:85:SER:O	1:B:486:HIS:CE1	2.50	0.53
1:B:93:PRO:CG	1:B:492:GLU:HG2	2.39	0.53
1:B:147:ASN:HB3	1:B:165:ASP:HA	1.90	0.52
1:A:389:PHE:HA	1:A:402:ILE:O	2.10	0.52
1:A:385:ILE:HG12	1:A:405:VAL:HG22	1.92	0.52
1:B:521:THR:O	1:B:521:THR:HG23	2.10	0.52
1:A:316:GLY:HA2	1:A:335:TYR:O	2.10	0.51
1:B:485:ASP:OD2	1:B:486:HIS:HD2	1.94	0.51
1:A:452:ILE:HB	1:A:463:GLU:HB2	1.92	0.51
1:A:377:HIS:CB	3:A:603:SO4:O2	2.59	0.51
1:B:199:VAL:HB	1:B:203:GLU:HB2	1.94	0.50
1:B:486:HIS:NE2	1:B:501:MET:HE1	2.26	0.50
1:B:377:HIS:HB3	3:B:603:SO4:O3	2.12	0.50
1:B:93:PRO:HG2	1:B:492:GLU:HG2	1.94	0.49
1:A:499:TYR:CE1	4:A:763:HOH:O	2.59	0.49
1:A:57:PHE:O	1:A:82[B]:ARG:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:VAL:O	1:A:91:VAL:HG13	2.13	0.49
1:B:418:VAL:CG2	1:B:435:THR:OG1	2.59	0.49
1:B:385:ILE:HG12	1:B:405:VAL:HG22	1.94	0.49
1:B:193:VAL:HG22	1:B:208:GLN:O	2.13	0.48
1:B:466:LYS:O	1:B:469:SER:OG	2.25	0.48
1:A:82[B]:ARG:H	1:A:82[B]:ARG:CD	2.27	0.48
1:B:69:ASN:CB	4:B:1046:HOH:O	2.60	0.48
1:B:112:VAL:CG2	4:B:772:HOH:O	2.54	0.48
1:B:486:HIS:CD2	1:B:501:MET:HE1	2.49	0.48
1:B:329:LYS:HG2	1:B:330:TYR:CE2	2.49	0.47
1:B:247:TYR:CZ	1:B:307:LYS:HA	2.49	0.47
1:B:282:ARG:CD	4:B:997:HOH:O	2.62	0.47
1:A:175:THR:HB	4:A:1050:HOH:O	2.15	0.47
1:A:149:ILE:HG23	1:A:164:TYR:HB3	1.97	0.47
1:B:319:GLN:O	1:B:331:GLN:HA	2.15	0.47
1:B:173:ASP:OD1	1:B:173:ASP:C	2.54	0.46
1:B:279:LYS:HE3	4:B:1183:HOH:O	2.16	0.46
1:B:271:ASN:HA	4:B:729:HOH:O	2.16	0.46
1:A:259:ARG:HG3	4:A:741:HOH:O	2.14	0.46
1:A:308:TYR:C	1:A:309:ILE:HG12	2.36	0.45
1:B:495:LYS:NZ	4:B:741:HOH:O	2.50	0.45
1:A:43:LEU:C	1:A:43:LEU:CD1	2.84	0.45
1:A:43:LEU:HD12	1:A:43:LEU:O	2.16	0.45
1:B:39:THR:N	4:B:740:HOH:O	2.50	0.45
1:B:256:HIS:HB3	1:B:271:ASN:OD1	2.16	0.45
1:B:400:HIS:CE1	1:B:450:ILE:HD13	2.52	0.45
1:B:100:MET:HG2	1:B:499:TYR:CE1	2.52	0.44
1:A:358:TRP:HA	1:A:359:PRO:C	2.37	0.44
1:B:39:THR:CB	4:B:1056:HOH:O	2.66	0.44
1:A:424:LYS:HG3	1:A:430:ASP:O	2.18	0.44
1:A:260:TRP:CH2	1:A:289:LYS:HD3	2.53	0.44
1:A:233:GLN:CB	4:A:1176:HOH:O	2.66	0.43
1:A:307:LYS:CB	1:A:309:ILE:HG13	2.47	0.43
1:A:58:ASP:OD2	1:A:506:GLY:HA2	2.17	0.43
1:A:117:PHE:CE2	4:A:1138:HOH:O	2.69	0.43
1:B:39:THR:HA	4:B:1056:HOH:O	2.17	0.43
1:A:112:VAL:HG21	1:A:164:TYR:CD1	2.54	0.43
1:A:494:GLY:HA3	1:A:521:THR:HG22	2.01	0.43
1:A:437:PHE:CE2	1:A:439:GLY:HA2	2.54	0.43
1:B:463:GLU:OE2	4:B:701:HOH:O	2.21	0.43
1:B:132:ARG:NE	4:B:752:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ARG:NE	4:A:741:HOH:O	2.52	0.42
1:A:399:VAL:O	1:A:423:PHE:HA	2.19	0.42
1:B:127:ILE:CG1	4:B:764:HOH:O	2.64	0.42
1:A:339:SER:HB2	1:A:348:TRP:CE2	2.55	0.41
1:B:254:LEU:HB2	1:B:273:TYR:HB3	2.01	0.41
1:B:59:GLY:N	1:B:76:TYR:O	2.47	0.41
1:B:100:MET:HG2	1:B:499:TYR:CZ	2.55	0.41
1:B:127:ILE:HD12	4:B:764:HOH:O	2.20	0.41
1:B:39:THR:CB	4:B:740:HOH:O	2.69	0.41
1:A:51:THR:O	1:A:510:PRO:HA	2.21	0.41
1:B:62:LEU:HD13	1:B:67:PHE:HA	2.02	0.41
1:A:249:SER:HA	1:A:308:TYR:CE2	2.56	0.41
1:B:39:THR:CA	4:B:1056:HOH:O	2.69	0.41
1:B:164:TYR:HB2	4:B:772:HOH:O	2.20	0.40
1:B:407:SER:HB2	1:B:415:TYR:CD1	2.57	0.40
1:B:521:THR:O	1:B:521:THR:CG2	2.69	0.40
1:A:62:LEU:HD13	1:A:67:PHE:HA	2.03	0.40
1:A:336:TYR:HB3	1:A:368:ILE:HD11	2.02	0.40
1:A:454:GLY:O	1:A:460:PRO:HA	2.22	0.40
1:B:61:LYS:HE3	4:B:705:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	481/483 (100%)	462 (96%)	19 (4%)	0	100	100
1	B	481/483 (100%)	459 (95%)	22 (5%)	0	100	100
All	All	962/966 (100%)	921 (96%)	41 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	A	402/412 (98%)	387 (96%)	15 (4%)	34 19
1	B	392/412 (95%)	381 (97%)	11 (3%)	43 29
All	All	794/824 (96%)	768 (97%)	26 (3%)	38 23

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	52	ASP
1	A	60	LYS
1	A	64	HIS
1	A	76	TYR
1	A	125	LYS
1	A	177	ARG
1	A	309	ILE
1	A	327	ARG
1	A	331	GLN
1	A	413	SER
1	A	418	VAL
1	A	448	ASP
1	A	498	TYR
1	A	517	ASP
1	B	76	TYR
1	B	177	ARG
1	B	203	GLU
1	B	331	GLN
1	B	376	ASP
1	B	397	ASP
1	B	434	THR
1	B	435	THR
1	B	493	ASN
1	B	498	TYR
1	B	509	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	69	ASN
1	A	111	ASN
1	B	318	GLN
1	B	347	ASN
1	B	486	HIS
1	B	493	ASN

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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	$\#\|Z\| > 2$
3	SO4	A	604	-	4,4,4	0.39	0	6,6,6	0.05	0
3	SO4	A	603	-	4,4,4	0.38	0	6,6,6	0.18	0
3	SO4	B	603	-	4,4,4	0.37	0	6,6,6	0.12	0

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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	SO4	3	0
3	B	603	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	482/483 (99%)	0.55	17 (3%)	44	38	12, 21, 35, 49	0
1	B	483/483 (100%)	0.71	29 (6%)	21	17	11, 21, 36, 49	0
All	All	965/966 (99%)	0.63	46 (4%)	30	25	11, 21, 36, 49	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	THR	6.3
1	A	64	HIS	5.2
1	B	197	ALA	4.6
1	B	275	ALA	4.4
1	B	65	ASN	4.4
1	B	221	ASP	3.8
1	A	202	ASP	3.8
1	B	176	GLY	3.6
1	A	429	VAL	3.3
1	B	40	SER	3.3
1	B	170	VAL	3.2
1	B	194	ALA	3.0
1	B	411	LYS	3.0
1	B	66	THR	3.0
1	A	65	ASN	2.8
1	A	521	THR	2.8
1	B	505	ALA	2.7
1	B	201	ASP	2.7
1	A	508	ALA	2.6
1	A	345	LEU	2.6
1	B	521	THR	2.6
1	A	317	PHE	2.6
1	A	175	THR	2.6
1	B	216	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	141	LEU	2.5
1	B	69	ASN	2.5
1	B	274	ASP	2.4
1	B	358	TRP	2.4
1	A	69	ASN	2.4
1	B	121	THR	2.4
1	A	309	ILE	2.3
1	B	180	GLY	2.3
1	A	426	ALA	2.3
1	B	109	GLU	2.3
1	A	82[A]	ARG	2.2
1	B	114	LEU	2.2
1	A	516	ILE	2.1
1	A	414	ASP	2.1
1	B	213	THR	2.1
1	B	430	ASP	2.1
1	B	191	PHE	2.1
1	B	450	ILE	2.1
1	B	143	GLY	2.1
1	A	43	LEU	2.0
1	B	346	GLY	2.0
1	A	40	SER	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)

There are no monosaccharides in this entry.

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
3	SO4	A	604	5/5	0.69	0.52	152,154,161,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	603	5/5	0.93	0.39	34,45,48,48	0
3	SO4	B	603	5/5	0.96	0.36	39,48,54,55	0
2	CA	A	601	1/1	0.99	0.07	15,15,15,15	0
2	CA	A	602	1/1	0.99	0.04	14,14,14,14	0
2	CA	B	602	1/1	0.99	0.03	17,17,17,17	0
2	CA	B	601	1/1	1.00	0.03	11,11,11,11	0

6.5 Other polymers

There are no such residues in this entry.