Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 07:06 am BST

PDB ID	:	5J6Q
Title	:	Cwp8 from Clostridium difficile
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Deposited on	:	2016-04-05
Resolution	:	2.10 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 following versions of software and data (see references ⓘ) were used in the production of this report:

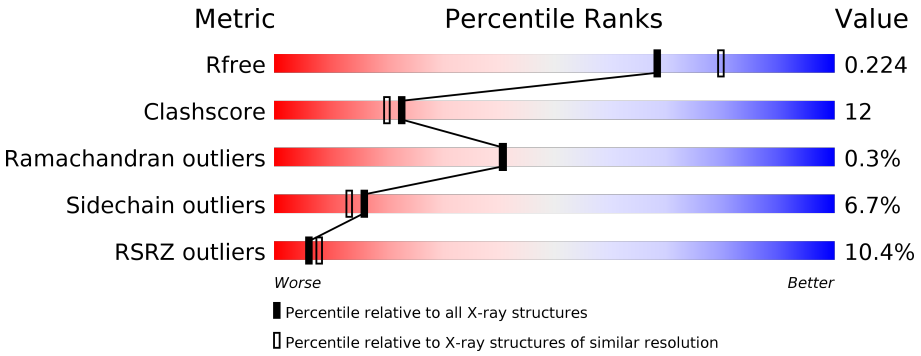
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	595	10% 73% 24% .

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
2	SO4	A	707	-	-	X	-

2 Entry composition

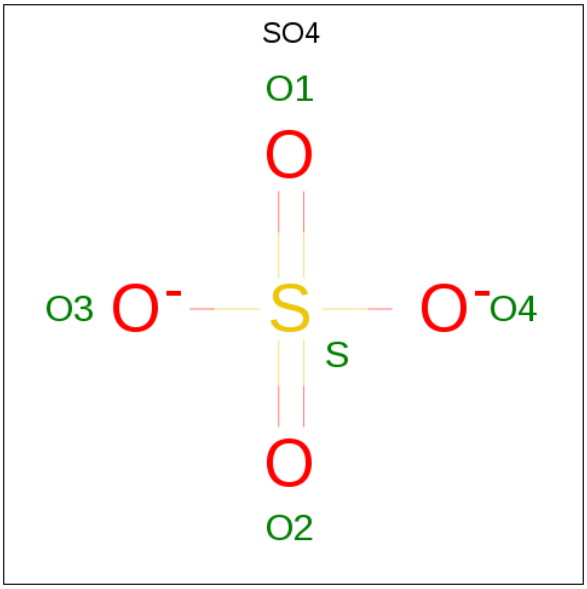
There are 4 unique types of molecules in this entry. The entry contains 10474 atoms, of which 5468 are hydrogens and 0 are deuteriums.

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 Cell wall binding protein cwp8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	H	N	O	S	4725	0	0
			9197	2835	4644	772	945	1			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is water.

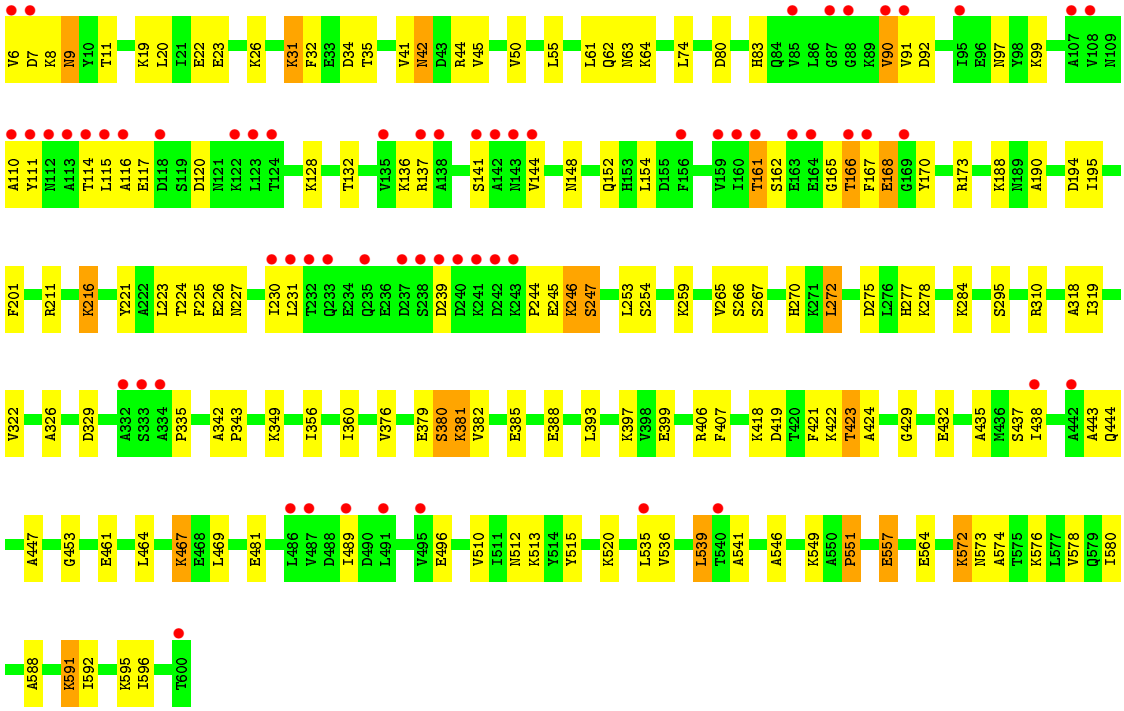
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	412	Total H O 1236 824 412	824	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Cell wall binding protein cwp8

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	45.45Å 63.43Å 86.41Å 97.25° 100.53° 91.96°	Depositor
Resolution (Å)	42.09 – 2.10 42.09 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.0 (42.09-2.10) 95.0 (42.09-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.10Å)	Xtriage
Refinement program	MAIN	Depositor
R, R_{free}	0.229 , 0.255 0.222 , 0.224	Depositor DCC
R_{free} test set	2610 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 74.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10474	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% 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: SO4, CL

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	0.92	2/4591 (0.0%)	0.88	7/6186 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	564	GLU	CA-C	5.47	1.67	1.52
1	A	295	SER	C-N	5.37	1.42	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	45	VAL	CA-CB-CG2	6.18	120.16	110.90
1	A	90	VAL	CA-CB-CG2	6.00	119.91	110.90
1	A	45	VAL	CA-CB-CG1	5.89	119.73	110.90
1	A	90	VAL	CA-CB-CG1	5.76	119.55	110.90
1	A	165	GLY	N-CA-C	-5.46	99.44	113.10
1	A	90	VAL	CG1-CB-CG2	5.34	119.44	110.90
1	A	535	LEU	CB-CG-CD1	-5.24	102.09	111.00

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	4553	4644	4638	104	1
2	A	40	0	0	2	0
3	A	1	0	0	1	0
4	A	412	824	0	13	0
All	All	5006	5468	4638	104	1

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 (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:THR:HA	1:A:167:PHE:O	1.92	0.69
1:A:464:LEU:HB3	1:A:469:LEU:HD21	1.74	0.68
1:A:319:ILE:HD12	1:A:360:ILE:HD13	1.77	0.66
1:A:385:GLU:O	1:A:388:GLU:HG2	1.96	0.66
1:A:97:ASN:OD1	1:A:152:GLN:HA	1.97	0.65
1:A:11:THR:HG21	1:A:188:LYS:HE3	1.79	0.65
1:A:154:LEU:HD23	1:A:170:TYR:HB3	1.79	0.64
1:A:549:LYS:HE3	4:A:995:HOH:O	1.98	0.63
1:A:44:ARG:HB3	4:A:851:HOH:O	2.00	0.61
1:A:435:ALA:O	1:A:438:ILE:HG22	2.01	0.60
1:A:329:ASP:HB3	1:A:376:VAL:HG12	1.81	0.60
1:A:195:ILE:HG13	1:A:265:VAL:HG12	1.83	0.59
1:A:423:THR:HG22	4:A:1137:HOH:O	2.02	0.59
1:A:461:GLU:HG3	1:A:489:ILE:HG21	1.85	0.58
1:A:424:ALA:HB3	1:A:469:LEU:HD23	1.85	0.58
1:A:277:HIS:HD2	4:A:1081:HOH:O	1.86	0.58
1:A:356:ILE:O	1:A:360:ILE:HG12	2.05	0.57
1:A:223:LEU:O	1:A:284:LYS:HD2	2.05	0.57
1:A:595:LYS:HE2	4:A:1014:HOH:O	2.05	0.56
1:A:335:PRO:HA	1:A:443:ALA:HA	1.88	0.56
1:A:461:GLU:HG3	1:A:489:ILE:HD13	1.89	0.54
1:A:572:LYS:HB2	4:A:825:HOH:O	2.08	0.53
1:A:132:THR:HG22	1:A:148:ASN:ND2	2.22	0.53
1:A:201:PHE:HD2	1:A:272:LEU:HD13	1.74	0.53
1:A:225:PHE:O	1:A:226:GLU:HG3	2.09	0.52
1:A:31:LYS:HG2	1:A:42:ASN:O	2.10	0.52
1:A:154:LEU:HD23	1:A:170:TYR:CB	2.40	0.51
1:A:322:VAL:HG22	1:A:326:ALA:HB3	1.92	0.51
1:A:418:LYS:O	1:A:421:PHE:HD2	1.93	0.51
1:A:19:LYS:O	1:A:23:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ASN:HA	4:A:1118:HOH:O	2.10	0.50
1:A:380:SER:C	1:A:381:LYS:HD2	2.32	0.50
1:A:111:TYR:O	1:A:115:LEU:HB3	2.12	0.50
1:A:247:SER:O	1:A:266:SER:HA	2.12	0.50
1:A:34:ASP:HB3	1:A:91:VAL:HG12	1.94	0.49
1:A:515:TYR:CD1	1:A:551:PRO:HB3	2.48	0.49
1:A:211:ARG:HD3	3:A:709:CL:CL	2.49	0.49
1:A:381:LYS:HD2	1:A:381:LYS:N	2.27	0.49
1:A:444:GLN:O	1:A:444:GLN:HG2	2.13	0.49
1:A:9:ASN:HD22	1:A:9:ASN:N	2.11	0.49
1:A:310:ARG:NH2	1:A:343:PRO:HA	2.27	0.49
1:A:195:ILE:CG1	1:A:265:VAL:HG12	2.42	0.49
1:A:437:SER:O	1:A:510:VAL:HG11	2.13	0.49
1:A:379:GLU:HA	1:A:382:VAL:O	2.12	0.49
1:A:253:LEU:HD22	1:A:253:LEU:N	2.28	0.48
1:A:578:VAL:HG11	2:A:707:SO4:O1	2.14	0.48
1:A:190:ALA:CA	1:A:259:LYS:HE2	2.43	0.48
1:A:406:ARG:NH2	1:A:429:GLY:O	2.47	0.48
1:A:20:LEU:O	1:A:23:GLU:HB2	2.14	0.48
1:A:247:SER:HB2	1:A:270:HIS:CD2	2.49	0.48
1:A:223:LEU:HD23	1:A:224:THR:N	2.29	0.48
1:A:74:LEU:HD12	1:A:74:LEU:C	2.35	0.47
1:A:349:LYS:HE3	1:A:379:GLU:O	2.14	0.47
1:A:190:ALA:HA	1:A:259:LYS:HE2	1.95	0.47
1:A:453:GLY:HA3	4:A:1048:HOH:O	2.14	0.47
1:A:74:LEU:HD12	1:A:74:LEU:O	2.15	0.47
1:A:137:ARG:O	1:A:141:SER:HA	2.15	0.47
1:A:319:ILE:HG21	1:A:360:ILE:CD1	2.45	0.47
1:A:557:GLU:HG3	4:A:1145:HOH:O	2.14	0.47
1:A:591:LYS:HD3	1:A:591:LYS:HA	1.71	0.46
1:A:80:ASP:OD1	1:A:83:HIS:HD2	1.99	0.46
1:A:50:VAL:HG11	1:A:64:LYS:HD2	1.97	0.46
1:A:578:VAL:HG21	2:A:707:SO4:O1	2.16	0.46
1:A:541:ALA:CB	1:A:580:ILE:HG13	2.46	0.45
1:A:9:ASN:ND2	1:A:9:ASN:N	2.64	0.45
1:A:116:ALA:O	1:A:117:GLU:HB2	2.17	0.45
1:A:55:LEU:HD21	1:A:61:LEU:HB2	1.98	0.45
1:A:419:ASP:HA	1:A:421:PHE:CE2	2.53	0.44
1:A:201:PHE:HD2	1:A:272:LEU:CD1	2.29	0.44
1:A:421:PHE:CE1	1:A:467:LYS:HD2	2.52	0.44
1:A:349:LYS:HA	1:A:381:LYS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLN:O	1:A:154:LEU:HD12	2.17	0.44
1:A:520:LYS:HE2	1:A:576:LYS:HD3	2.00	0.44
1:A:231:LEU:HD11	1:A:244:PRO:HG2	1.99	0.44
1:A:536:VAL:HA	1:A:539:LEU:HD23	2.00	0.43
1:A:110:ALA:O	1:A:114:THR:HB	2.18	0.43
1:A:216:LYS:O	1:A:221:TYR:HD1	2.00	0.43
1:A:35:THR:HA	1:A:92:ASP:OD1	2.19	0.43
1:A:423:THR:HG23	1:A:447:ALA:HB2	2.00	0.43
1:A:245:GLU:HG2	1:A:245:GLU:O	2.17	0.43
1:A:406:ARG:CG	1:A:407:PHE:N	2.82	0.43
1:A:319:ILE:HD12	1:A:360:ILE:CD1	2.47	0.43
1:A:318:ALA:HB3	1:A:342:ALA:HB2	2.00	0.42
1:A:32:PHE:HA	1:A:90:VAL:HG22	2.01	0.42
1:A:397:LYS:HE2	1:A:399:GLU:HB2	2.02	0.42
1:A:329:ASP:HB3	1:A:376:VAL:CG1	2.48	0.42
1:A:19:LYS:HB3	4:A:849:HOH:O	2.18	0.42
1:A:443:ALA:HB3	1:A:546:ALA:HB2	2.02	0.42
1:A:275:ASP:O	1:A:278:LYS:HB2	2.20	0.42
1:A:278:LYS:HG3	4:A:871:HOH:O	2.18	0.42
1:A:201:PHE:CD2	1:A:272:LEU:HD13	2.54	0.42
1:A:136:LYS:HB3	1:A:144:VAL:HG22	2.02	0.41
1:A:588:ALA:O	1:A:592:ILE:HG13	2.20	0.41
1:A:536:VAL:HA	1:A:539:LEU:CD2	2.51	0.41
1:A:230:ILE:HA	1:A:247:SER:OG	2.20	0.41
1:A:41:VAL:HG23	4:A:958:HOH:O	2.21	0.41
1:A:168:GLU:HG3	1:A:168:GLU:H	1.66	0.41
1:A:22:GLU:OE1	1:A:26:LYS:HE3	2.20	0.41
1:A:195:ILE:O	1:A:265:VAL:HA	2.21	0.41
1:A:573:ASN:HB2	4:A:918:HOH:O	2.21	0.40
1:A:246:LYS:HG3	1:A:267:SER:C	2.40	0.40
1:A:496:GLU:OE2	1:A:513:LYS:NZ	2.54	0.40
1:A:574:ALA:HB3	1:A:596:ILE:HD12	2.03	0.40
1:A:246:LYS:HG3	1:A:267:SER:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASN:ND2	1:A:512:ASN:HD21[1_445]	1.59	0.01

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	A	593/595 (100%)	561 (95%)	30 (5%)	2 (0%)	41 41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	ASP
1	A	166	THR

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	504/504 (100%)	470 (93%)	34 (7%)	16 13

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	7	ASP
1	A	8	LYS
1	A	9	ASN
1	A	31	LYS
1	A	42	ASN
1	A	62	GLN
1	A	99	LYS
1	A	128	LYS

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Mol	Chain	Res	Type
1	A	161	THR
1	A	162	SER
1	A	166	THR
1	A	168	GLU
1	A	173	ARG
1	A	194	ASP
1	A	216	LYS
1	A	239	ASP
1	A	246	LYS
1	A	247	SER
1	A	254	SER
1	A	272	LEU
1	A	380	SER
1	A	381	LYS
1	A	393	LEU
1	A	422	LYS
1	A	423	THR
1	A	432	GLU
1	A	467	LYS
1	A	481	GLU
1	A	539	LEU
1	A	551	PRO
1	A	557	GLU
1	A	572	LYS
1	A	591	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	83	HIS
1	A	143	ASN
1	A	148	ASN
1	A	215	ASN
1	A	219	ASN
1	A	270	HIS
1	A	444	GLN
1	A	476	ASN
1	A	493	ASN
1	A	573	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\#\|Z\| > 2$
2	SO4	A	703	-	4,4,4	1.09	0	6,6,6	0.31	0
2	SO4	A	704	-	4,4,4	0.41	0	6,6,6	0.43	0
2	SO4	A	706	-	4,4,4	1.00	0	6,6,6	0.41	0
2	SO4	A	702	-	4,4,4	1.00	0	6,6,6	0.20	0
2	SO4	A	705	-	4,4,4	0.35	0	6,6,6	0.32	0
2	SO4	A	701	-	4,4,4	1.42	0	6,6,6	0.52	0
2	SO4	A	707	-	4,4,4	1.27	1 (25%)	6,6,6	1.51	1 (16%)
2	SO4	A	708	-	4,4,4	0.19	0	6,6,6	0.16	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	707	SO4	O2-S	2.49	1.59	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	707	SO4	O4-S-O1	-2.85	94.44	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	707	SO4	2	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	595/595 (100%)	0.65	62 (10%) 6 8	25, 62, 178, 199	29 (4%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	PHE	6.7
1	A	600	THR	6.2
1	A	169	GLY	5.8
1	A	113	ALA	5.7
1	A	231	LEU	5.7
1	A	114	THR	5.5
1	A	142	ALA	5.4
1	A	7	ASP	5.4
1	A	118	ASP	5.2
1	A	156	PHE	5.1
1	A	240	ASP	4.7
1	A	166	THR	4.6
1	A	123	LEU	4.1
1	A	6	VAL	3.9
1	A	238	SER	3.6
1	A	243	LYS	3.6
1	A	239	ASP	3.5
1	A	85	VAL	3.4
1	A	143	ASN	3.4
1	A	163	GLU	3.3
1	A	489	ILE	3.3
1	A	122	LYS	3.2
1	A	230	ILE	3.1
1	A	232	THR	3.1
1	A	138	ALA	3.1
1	A	242	ASP	2.9
1	A	233	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	491	LEU	2.9
1	A	141	SER	2.9
1	A	164	GLU	2.9
1	A	90	VAL	2.8
1	A	438	ILE	2.8
1	A	112	ASN	2.8
1	A	161	THR	2.7
1	A	160	ILE	2.7
1	A	111	TYR	2.7
1	A	95	ILE	2.6
1	A	137	ARG	2.6
1	A	91	VAL	2.6
1	A	108	VAL	2.6
1	A	116	ALA	2.5
1	A	144	VAL	2.5
1	A	110	ALA	2.5
1	A	241	LYS	2.5
1	A	487	VAL	2.4
1	A	235	GLN	2.4
1	A	495	VAL	2.4
1	A	107	ALA	2.3
1	A	124	THR	2.3
1	A	486	LEU	2.3
1	A	237	ASP	2.2
1	A	159	VAL	2.1
1	A	442	ALA	2.1
1	A	333	SER	2.1
1	A	535	LEU	2.1
1	A	88	GLY	2.1
1	A	332	ALA	2.1
1	A	135	VAL	2.0
1	A	540	THR	2.0
1	A	115	LEU	2.0
1	A	334	ALA	2.0
1	A	87	GLY	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 carbohydrates 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
2	SO4	A	707	5/5	0.91	0.15	69,71,75,77	0
2	SO4	A	708	5/5	0.91	0.21	155,156,157,157	0
2	SO4	A	705	5/5	0.92	0.17	98,102,102,105	0
2	SO4	A	703	5/5	0.94	0.19	79,79,80,82	0
2	SO4	A	701	5/5	0.94	0.13	58,60,65,67	0
2	SO4	A	704	5/5	0.95	0.17	95,96,98,98	0
2	SO4	A	706	5/5	0.96	0.12	80,82,83,87	0
2	SO4	A	702	5/5	0.99	0.18	52,52,53,59	0
3	CL	A	709	1/1	0.99	0.08	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.