



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:46 AM UTC

PDB ID : 5J6Q / pdb_00005j6q
Title : Cwp8 from Clostridium difficile
Authors : Renko, M.; Usenik, A.; Turk, D.
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 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

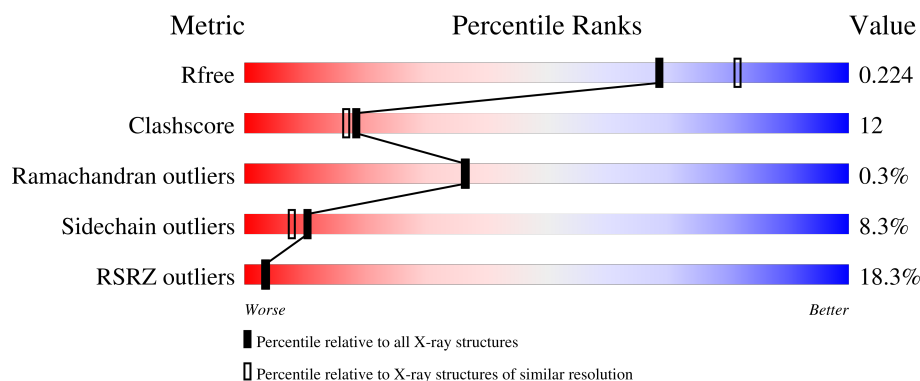
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	A	595	18% 65% 30% 5%

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 [i](#)

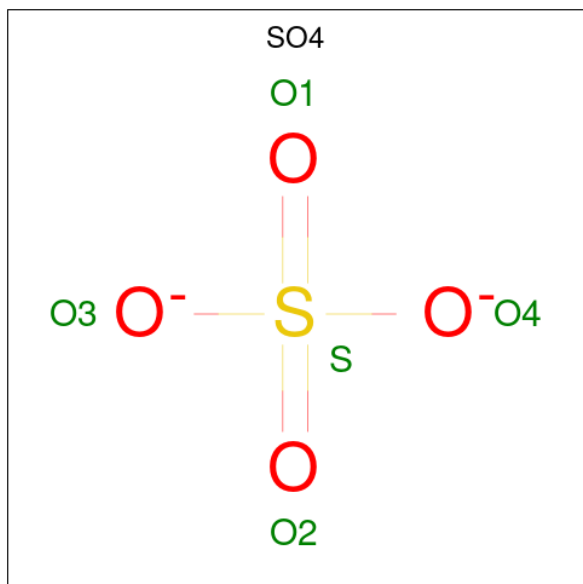
There are 4 unique types of molecules in this entry. The entry contains 10474 atoms, of which 5468 are hydrogens and 0 are deuteriums.

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 (CCD ID: SO4) (formula: O₄S).



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	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		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

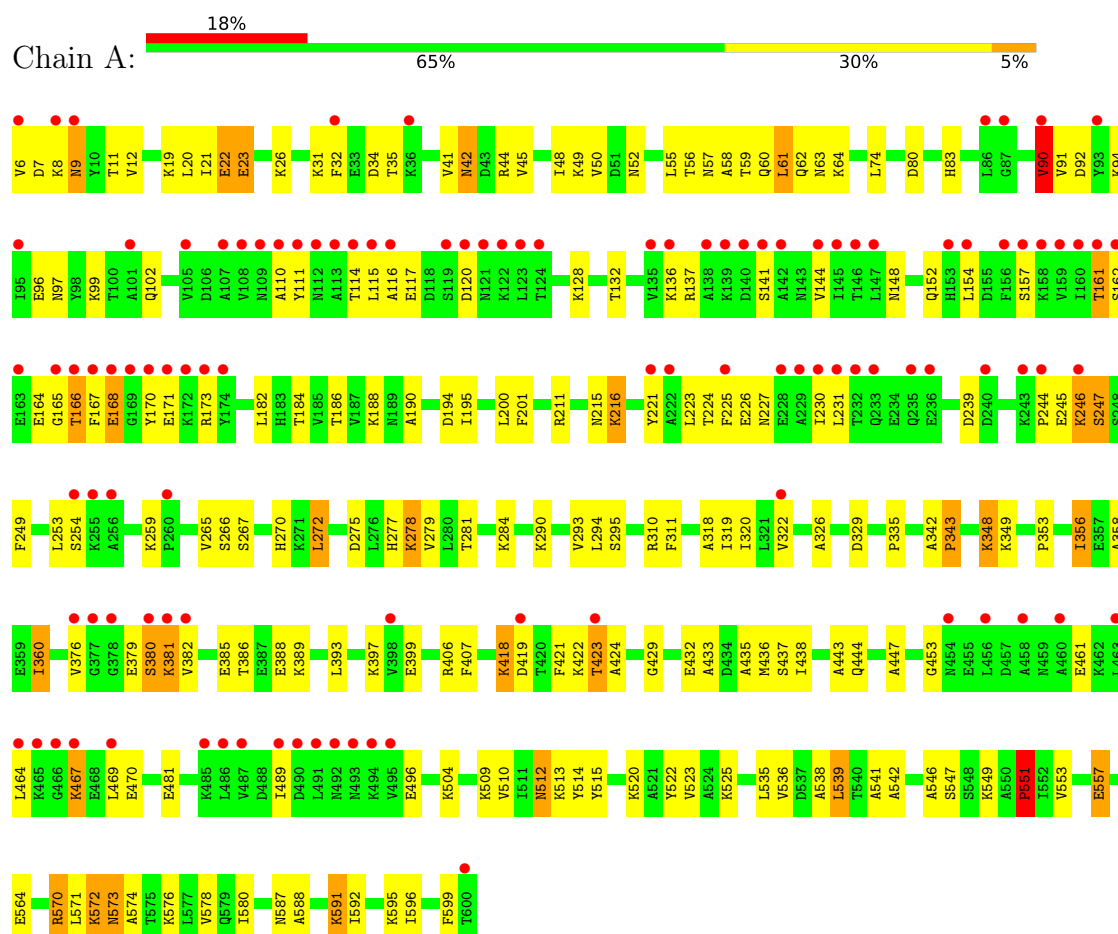
- Molecule 4 is water.

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

3 Residue-property plots

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: Cell wall binding protein cwp8



4 Data and refinement statistics

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) 95.1 (42.09-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.34 , 78.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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: 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	1.40	37/4591 (0.8%)	1.38	33/6186 (0.5%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	564	GLU	CA-C	11.30	1.67	1.52
1	A	551	PRO	CA-C	9.92	1.62	1.53
1	A	525	LYS	CA-C	-9.62	1.40	1.52
1	A	186	THR	CA-C	-8.21	1.42	1.52
1	A	542	ALA	CA-C	7.64	1.62	1.52
1	A	57	ASN	N-CA	7.63	1.55	1.46
1	A	12	VAL	CA-C	-7.29	1.44	1.52
1	A	525	LYS	N-CA	7.02	1.54	1.46
1	A	290	LYS	CA-C	6.96	1.62	1.52
1	A	59	THR	CA-C	6.81	1.61	1.52
1	A	21	ILE	CA-C	6.77	1.61	1.52
1	A	56	THR	CA-C	6.76	1.61	1.52
1	A	200	LEU	CA-C	6.50	1.61	1.52
1	A	587	ASN	CA-C	6.48	1.61	1.52
1	A	295	SER	C-N	6.31	1.42	1.33
1	A	58	ALA	CA-C	-6.27	1.44	1.52
1	A	358	ALA	C-N	6.05	1.42	1.33
1	A	294	LEU	CA-C	6.02	1.60	1.53
1	A	279	VAL	CA-C	-5.93	1.45	1.52
1	A	184	THR	CA-C	-5.86	1.45	1.52
1	A	293	VAL	CA-C	5.83	1.59	1.52
1	A	356	ILE	CA-C	5.76	1.60	1.52
1	A	433	ALA	C-N	5.75	1.42	1.33
1	A	48	ILE	CA-CB	-5.68	1.47	1.54
1	A	553	VAL	CA-C	5.61	1.59	1.52
1	A	278	LYS	C-N	5.56	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	523	VAL	N-CA	5.53	1.52	1.46
1	A	360	ILE	CA-C	5.52	1.59	1.52
1	A	278	LYS	N-CA	5.41	1.52	1.46
1	A	504	LYS	CA-C	5.30	1.59	1.52
1	A	538	ALA	N-CA	-5.24	1.40	1.46
1	A	509	LYS	N-CA	5.20	1.52	1.46
1	A	522	TYR	CA-C	5.17	1.59	1.52
1	A	571	LEU	CA-C	-5.17	1.46	1.53
1	A	102	GLN	CA-C	5.15	1.59	1.52
1	A	249	PHE	CA-C	-5.09	1.46	1.52
1	A	547	SER	N-CA	5.01	1.52	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ASN	CA-C-N	-7.33	114.11	123.19
1	A	52	ASN	C-N-CA	-7.33	114.11	123.19
1	A	599	PHE	N-CA-C	7.05	121.52	110.17
1	A	281	THR	N-CA-C	-6.76	103.84	111.14
1	A	57	ASN	OD1-CG-ND2	-6.45	116.15	122.60
1	A	23	GLU	N-CA-C	-6.34	104.37	111.28
1	A	21	ILE	N-CA-CB	-6.28	102.63	110.47
1	A	348	LYS	N-CA-C	-6.23	102.14	110.55
1	A	389	LYS	N-CA-C	-6.07	104.78	111.82
1	A	165	GLY	N-CA-C	-5.80	99.44	113.18
1	A	60	GLN	N-CA-C	-5.79	105.10	111.82
1	A	45	VAL	CA-CB-CG2	5.74	120.16	110.40
1	A	249	PHE	CA-CB-CG	5.68	119.48	113.80
1	A	573	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	A	570	ARG	CA-C-N	-5.65	113.58	122.79
1	A	570	ARG	C-N-CA	-5.65	113.58	122.79
1	A	90	VAL	CA-CB-CG2	5.59	119.91	110.40
1	A	164	GLU	N-CA-C	-5.51	100.62	109.39
1	A	45	VAL	CA-CB-CG1	5.49	119.73	110.40
1	A	599	PHE	CA-CB-CG	-5.43	108.37	113.80
1	A	512	ASN	CA-CB-CG	5.42	118.03	112.60
1	A	311	PHE	N-CA-C	5.40	117.89	108.76
1	A	90	VAL	CA-CB-CG1	5.38	119.55	110.40
1	A	386	THR	N-CA-C	-5.35	105.53	111.36
1	A	353	PRO	CA-C-O	-5.30	115.41	121.56
1	A	294	LEU	CA-C-O	-5.30	114.66	120.70
1	A	514	TYR	CA-C-N	-5.26	114.23	122.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	TYR	C-N-CA	-5.26	114.23	122.49
1	A	320	ILE	N-CA-C	-5.11	100.39	107.80
1	A	61	LEU	N-CA-C	-5.10	105.36	111.03
1	A	215	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	A	343	PRO	CA-C-N	-5.01	116.37	122.93
1	A	343	PRO	C-N-CA	-5.01	116.37	122.93

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	108	1
2	A	40	0	0	2	0
3	A	1	0	0	1	0
4	A	412	824	0	14	0
All	All	5006	5468	4638	108	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 (108) 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:436:MET:HE3	1:A:535:LEU:HB3	1.68	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:380:SER:C	1:A:381:LYS:HD2	2.32	0.55
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:74:LEU:C	1:A:74:LEU:HD12	2.35	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
1:A:227:ASN:HA	4:A:1118:HOH:O	2.10	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:9:ASN:HD22	1:A:9:ASN:N	2.11	0.49
1:A:444:GLN:O	1:A:444:GLN:HG2	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:349:LYS:HE3	1:A:379:GLU:O	2.14	0.47
1:A:74:LEU:HD12	1:A:74:LEU:O	2.15	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: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:HA	1:A:591:LYS:HD3	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:N	1:A:9:ASN:ND2	2.64	0.45
1:A:94:LYS:NZ	4:A:812:HOH:O	2.49	0.45
1:A:246:LYS:HG3	1:A:267:SER:C	2.40	0.45
1:A:55:LEU:HD21	1:A:61:LEU:HB2	1.98	0.45
1:A:116:ALA:O	1:A:117:GLU:HB2	2.17	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
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:O	1:A:245:GLU:HG2	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:32:PHE:HA	1:A:90:VAL:HG22	2.01	0.42
1:A:318:ALA:HB3	1:A:342:ALA:HB2	2.00	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:182:LEU:C	1:A:182:LEU:HD13	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:94:LYS:HE3	1:A:96:GLU:CD	2.45	0.41
1:A:536:VAL:HA	1:A:539:LEU:CD2	2.51	0.41
1:A:41:VAL:HG23	4:A:958:HOH:O	2.21	0.41
1:A:230:ILE:HA	1:A:247:SER:OG	2.20	0.41
1:A:22:GLU:OE1	1:A:26:LYS:HE3	2.20	0.41
1:A:168:GLU:H	1:A:168:GLU:HG3	1.66	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: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%)	36	36

All (2) Ramachandran outliers are listed below:

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

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	504/504 (100%)	462 (92%)	42 (8%)	10 8

All (42) 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	22	GLU
1	A	42	ASN
1	A	49	LYS
1	A	62	GLN
1	A	90	VAL
1	A	99	LYS
1	A	128	LYS
1	A	157	SER
1	A	161	THR
1	A	162	SER
1	A	166	THR
1	A	168	GLU
1	A	171	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

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Mol	Chain	Res	Type
1	A	348	LYS
1	A	380	SER
1	A	381	LYS
1	A	393	LEU
1	A	418	LYS
1	A	422	LYS
1	A	423	THR
1	A	432	GLU
1	A	467	LYS
1	A	470	GLU
1	A	481	GLU
1	A	539	LEU
1	A	551	PRO
1	A	557	GLU
1	A	570	ARG
1	A	572	LYS
1	A	591	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	66	ASN
1	A	83	HIS
1	A	143	ASN
1	A	148	ASN
1	A	219	ASN
1	A	270	HIS
1	A	444	GLN
1	A	454	ASN
1	A	476	ASN
1	A	493	ASN
1	A	512	ASN
1	A	573	ASN
1	A	587	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	706	-	4,4,4	0.97	0	6,6,6	0.43	0
2	SO4	A	701	-	4,4,4	1.44	0	6,6,6	0.47	0
2	SO4	A	707	-	4,4,4	1.27	1 (25%)	6,6,6	1.50	1 (16%)
2	SO4	A	705	-	4,4,4	0.43	0	6,6,6	0.34	0
2	SO4	A	704	-	4,4,4	0.49	0	6,6,6	0.44	0
2	SO4	A	702	-	4,4,4	0.81	0	6,6,6	0.20	0
2	SO4	A	708	-	4,4,4	0.30	0	6,6,6	0.14	0
2	SO4	A	703	-	4,4,4	0.99	0	6,6,6	0.32	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	2.47	1.59	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	707	SO4	O4-S-O1	-2.89	94.44	109.56

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, 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	A	595/595 (100%)	0.96	109 (18%) 3 3	11, 30, 87, 131	29 (4%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	LEU	7.3
1	A	159	VAL	6.7
1	A	170	TYR	6.3
1	A	156	PHE	6.2
1	A	169	GLY	5.9
1	A	108	VAL	5.9
1	A	230	ILE	5.8
1	A	111	TYR	5.2
1	A	172	LYS	5.0
1	A	116	ALA	4.9
1	A	86	LEU	4.9
1	A	6	VAL	4.8
1	A	229	ALA	4.8
1	A	232	THR	4.8
1	A	145	ILE	4.5
1	A	487	VAL	4.4
1	A	456	LEU	4.4
1	A	486	LEU	4.3
1	A	123	LEU	4.3
1	A	124	THR	4.3
1	A	160	ILE	4.3
1	A	144	VAL	4.2
1	A	489	ILE	4.2
1	A	244	PRO	4.2
1	A	495	VAL	4.2
1	A	115	LEU	4.1
1	A	491	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	423	THR	4.0
1	A	138	ALA	4.0
1	A	158	LYS	4.0
1	A	107	ALA	3.9
1	A	600	THR	3.9
1	A	154	LEU	3.9
1	A	376	VAL	3.8
1	A	157	SER	3.7
1	A	168	GLU	3.7
1	A	114	THR	3.6
1	A	466	GLY	3.6
1	A	240	ASP	3.6
1	A	8	LYS	3.5
1	A	467	LYS	3.4
1	A	464	LEU	3.4
1	A	142	ALA	3.2
1	A	162	SER	3.2
1	A	167	PHE	3.2
1	A	165	GLY	3.2
1	A	260	PRO	3.2
1	A	236	GLU	3.1
1	A	119	SER	3.1
1	A	494	LYS	3.1
1	A	161	THR	3.1
1	A	378	GLY	3.1
1	A	243	LYS	3.1
1	A	463	LEU	3.0
1	A	136	LYS	3.0
1	A	121	ASN	3.0
1	A	174	TYR	3.0
1	A	135	VAL	2.9
1	A	87	GLY	2.9
1	A	225	PHE	2.9
1	A	465	LYS	2.9
1	A	377	GLY	2.9
1	A	110	ALA	2.9
1	A	469	LEU	2.8
1	A	95	ILE	2.8
1	A	36	LYS	2.8
1	A	32	PHE	2.8
1	A	112	ASN	2.8
1	A	256	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	460	ALA	2.7
1	A	147	LEU	2.7
1	A	221	TYR	2.7
1	A	140	ASP	2.7
1	A	233	GLN	2.7
1	A	380	SER	2.7
1	A	490	ASP	2.6
1	A	105	VAL	2.6
1	A	173	ARG	2.6
1	A	235	GLN	2.6
1	A	9	ASN	2.6
1	A	141	SER	2.6
1	A	485	LYS	2.5
1	A	419	ASP	2.5
1	A	109	ASN	2.5
1	A	228	GLU	2.4
1	A	90	VAL	2.4
1	A	493	ASN	2.4
1	A	222	ALA	2.3
1	A	246	LYS	2.3
1	A	166	THR	2.3
1	A	93	TYR	2.3
1	A	254	SER	2.3
1	A	492	ASN	2.3
1	A	101	ALA	2.3
1	A	398	VAL	2.2
1	A	171	GLU	2.2
1	A	458	ALA	2.2
1	A	122	LYS	2.2
1	A	139	LYS	2.2
1	A	146	THR	2.2
1	A	382	VAL	2.1
1	A	113	ALA	2.1
1	A	255	LYS	2.1
1	A	120	ASP	2.1
1	A	381	LYS	2.1
1	A	454	ASN	2.0
1	A	153	HIS	2.0
1	A	163	GLU	2.0
1	A	322	VAL	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 oligosaccharides 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, 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($\text{\AA}^2$)	Q<0.9
2	SO4	A	708	5/5	0.66	0.09	155,156,157,157	0
2	SO4	A	705	5/5	0.85	0.10	98,102,102,105	0
2	SO4	A	707	5/5	0.86	0.15	69,71,75,77	0
2	SO4	A	701	5/5	0.90	0.09	58,60,65,67	0
2	SO4	A	703	5/5	0.90	0.12	79,79,80,82	0
2	SO4	A	704	5/5	0.90	0.10	95,96,98,98	0
2	SO4	A	706	5/5	0.93	0.10	80,82,83,87	0
2	SO4	A	702	5/5	0.96	0.07	52,52,53,59	0
3	CL	A	709	1/1	0.99	0.09	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.