



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:00 PM UTC

PDB ID : 5J72 / pdb_00005j72
Title : Cwp6 from Clostridium difficile
Authors : Renko, M.; Usenik, A.; Turk, D.
Deposited on : 2016-04-05
Resolution : 1.70 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

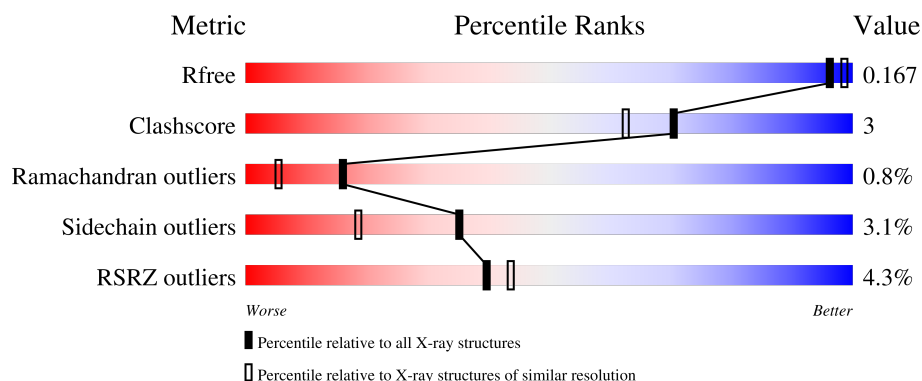
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	638	4% 89% 10%
1	B	638	5% 85% 13%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11210 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 Putative N-acetylmuramoyl-L-alanine amidase,autolysin cwp6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	117	11	0
			4918	3065	834	1004	15			
1	B	638	Total	C	N	O	S	111	10	0
			4921	3067	838	1001	15			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	1
			3	3		
2	B	3	Total	Ca	0	0
			3	3		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	2	Total	Na	0	0
			2	2		

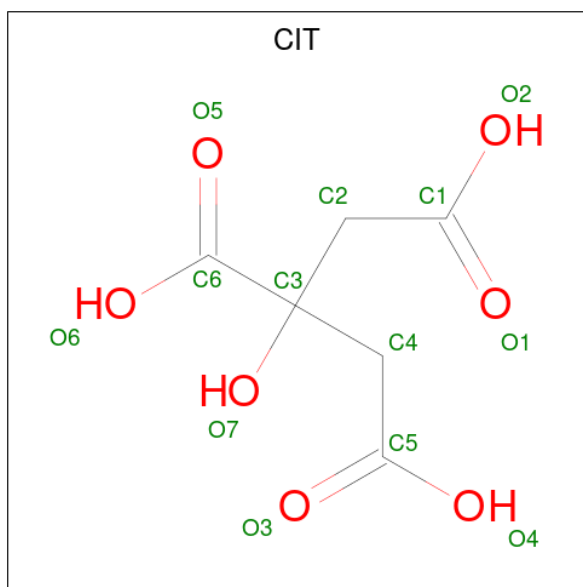
- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Cl	0	0
			3	3		
4	B	2	Total	Cl	0	0
			2	2		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		

- Molecule 6 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	6	7		
6	B	1	Total	C	O	0	0
			13	6	7		

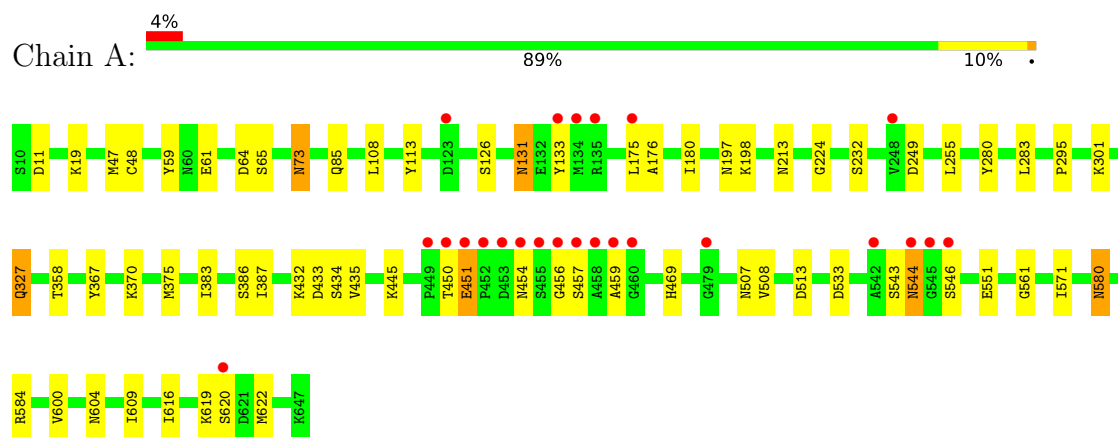
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	643	Total	O	0	0
			643	643		
7	B	686	Total	O	0	0
			686	686		

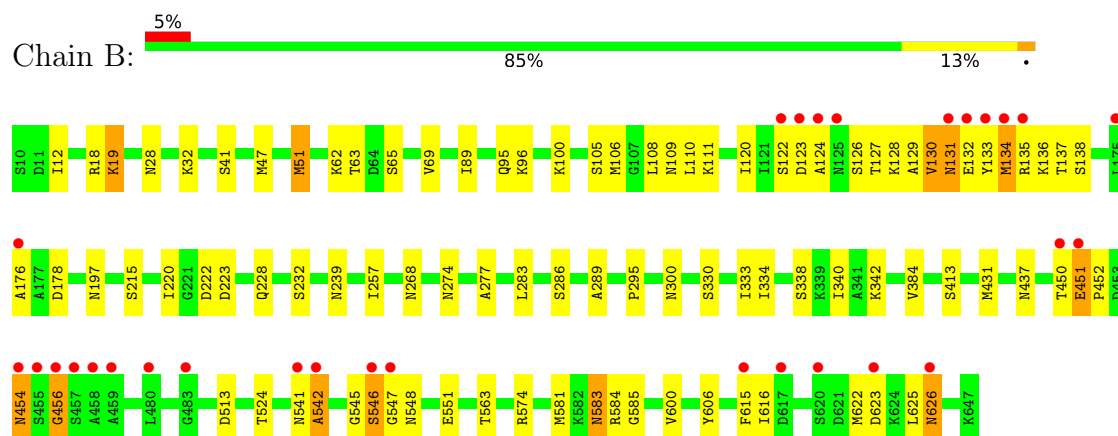
3 Residue-property plots [i](#)

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: Putative N-acetylmuramoyl-L-alanine amidase, autolysin cwp6



- Molecule 1: Putative N-acetylmuramoyl-L-alanine amidase, autolysin cwp6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.36Å 212.92Å 84.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.85 – 1.70 29.85 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.85-1.70) 99.2 (29.85-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5, MAIN	Depositor
R, R_{free}	0.178 , 0.201 0.173 , 0.167	Depositor DCC
R_{free} test set	9038 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11210	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: CA, CIT, ZN, NA, 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	1.27	13/5017 (0.3%)	1.26	10/6779 (0.1%)
1	B	1.19	11/5011 (0.2%)	1.28	21/6771 (0.3%)
All	All	1.23	24/10028 (0.2%)	1.27	31/13550 (0.2%)

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	A	0	1
1	B	0	1
All	All	0	2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375[A]	MET	CA-C	-7.11	1.44	1.52
1	A	375[B]	MET	CA-C	-7.11	1.44	1.52
1	A	255	LEU	CA-CB	6.50	1.63	1.53
1	B	105	SER	CA-C	-6.13	1.44	1.52
1	A	48	CYS	CA-C	5.78	1.59	1.52
1	A	358	THR	CA-C	5.64	1.60	1.52
1	A	433	ASP	CA-C	-5.62	1.45	1.52
1	A	367	TYR	CA-C	5.61	1.59	1.52
1	B	47	MET	SD-CE	-5.52	1.65	1.79
1	B	47	MET	CA-C	-5.41	1.45	1.52
1	B	51[A]	MET	CA-C	5.40	1.58	1.52
1	B	51[B]	MET	CA-C	5.40	1.58	1.52
1	A	232	SER	CA-C	-5.37	1.45	1.52
1	A	108	LEU	CA-C	-5.30	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	508	VAL	CA-C	-5.26	1.46	1.52
1	B	41	SER	CA-C	-5.18	1.46	1.52
1	B	431	MET	CA-C	5.16	1.59	1.52
1	A	64	ASP	CA-C	5.16	1.59	1.53
1	A	620	SER	CA-C	5.15	1.59	1.52
1	A	561	GLY	C-N	5.11	1.38	1.32
1	B	220	ILE	CA-CB	5.11	1.60	1.54
1	B	581	MET	SD-CE	5.10	1.92	1.79
1	B	257	ILE	CA-CB	5.03	1.60	1.54
1	B	574	ARG	CA-C	-5.01	1.46	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	PRO	N-CA-C	9.32	126.19	111.38
1	B	625	LEU	CA-C-N	8.74	132.86	120.28
1	B	625	LEU	C-N-CA	8.74	132.86	120.28
1	A	295	PRO	N-CA-C	8.38	123.97	111.41
1	B	384	VAL	N-CA-C	7.15	117.92	110.62
1	B	133	TYR	N-CA-C	-6.31	105.56	113.20
1	B	289	ALA	N-CA-C	-6.10	104.63	111.28
1	A	544	ASN	N-CA-C	-5.82	100.69	108.19
1	B	286	SER	N-CA-C	5.75	117.22	111.07
1	A	469	HIS	CE1-NE2-CD2	-5.65	103.35	109.00
1	B	413	SER	N-CA-C	5.57	117.03	111.07
1	B	109	ASN	CA-CB-CG	-5.49	107.11	112.60
1	A	197	ASN	N-CA-C	-5.47	102.36	110.46
1	B	130	VAL	CA-CB-CG1	5.41	119.60	110.40
1	B	197	ASN	N-CA-C	-5.39	102.19	109.95
1	A	249	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	130	VAL	CA-CB-CG2	5.39	119.56	110.40
1	B	95	GLN	N-CA-C	-5.34	101.00	109.76
1	B	563	THR	N-CA-C	5.25	117.41	111.11
1	B	215	SER	N-CA-C	-5.17	107.52	113.88
1	B	222	ASP	CA-C-N	5.14	127.69	120.28
1	B	222	ASP	C-N-CA	5.14	127.69	120.28
1	B	239	ASN	CA-CB-CG	-5.14	107.46	112.60
1	B	300	ASN	N-CA-C	-5.12	103.17	110.59
1	A	213	ASN	CA-CB-CG	-5.11	107.49	112.60
1	A	175	LEU	N-CA-CB	5.08	118.94	111.43
1	A	469	HIS	ND1-CE1-NE2	5.07	113.47	108.40
1	B	340	ILE	N-CA-C	5.07	117.04	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	ALA	N-CA-C	5.06	117.40	108.24
1	A	533	ASP	N-CA-C	-5.05	105.96	111.82
1	A	435	VAL	N-CA-CB	-5.03	104.14	110.57

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain
1	B	606	TYR	Sidechain

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	4918	0	4949	28	1
1	B	4921	0	4958	37	2
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	3	0	0	1	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	26	0	10	0	0
7	A	643	0	0	5	0
7	B	686	0	0	6	0
All	All	11210	0	9917	66	3

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 3.

All (66) 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:223:ASP:HB2	7:B:1354:HOH:O	1.68	0.93
4:A:705:CL:CL	7:A:1060:HOH:O	2.23	0.92
1:A:11:ASP:OD2	7:A:802:HOH:O	2.03	0.76
1:A:11:ASP:OD1	7:A:801:HOH:O	2.03	0.75
1:A:434:SER:OG	1:A:456:GLY:HA2	1.91	0.70
1:A:47[B]:MET:HG3	1:A:85:GLN:HG3	1.77	0.67
1:B:12[A]:ILE:HG23	1:B:108:LEU:HD21	1.76	0.67
1:B:616:ILE:HA	1:B:622:MET:HE3	1.78	0.65
1:B:18[B]:ARG:HD3	7:B:1238:HOH:O	2.00	0.61
1:B:12[B]:ILE:CG1	1:B:106:MET:HE2	2.32	0.60
1:A:59:TYR:CE2	1:A:61:GLU:HG2	2.35	0.60
1:A:327:GLN:H	1:A:327:GLN:CD	2.10	0.59
1:A:176:ALA:HB1	1:A:387:ILE:HD12	1.85	0.59
1:B:89:ILE:HD12	1:B:96:LYS:HD3	1.86	0.57
1:B:451:GLU:O	1:B:454:ASN:N	2.38	0.57
1:A:59:TYR:HE2	1:A:61:GLU:HG2	1.70	0.56
1:B:19:LYS:NZ	7:B:802:HOH:O	2.38	0.56
1:A:457:SER:HB3	1:A:459:ALA:O	2.07	0.54
1:A:616:ILE:HA	1:A:622:MET:HE3	1.90	0.54
1:B:450:THR:HG21	1:B:513:ASP:OD2	2.08	0.53
1:A:450:THR:HG22	7:A:978:HOH:O	2.07	0.53
1:B:583:ASN:C	1:B:583:ASN:HD22	2.17	0.51
1:A:280:TYR:CE1	1:A:383:ILE:HD11	2.47	0.50
1:B:18[B]:ARG:NH1	7:B:804:HOH:O	2.43	0.50
1:B:334:ILE:O	1:B:338:SER:HB2	2.12	0.49
1:B:541:ASN:O	1:B:542:ALA:HB2	2.13	0.48
1:A:457:SER:CB	1:A:507:ASN:HD21	2.28	0.47
1:B:283:LEU:C	1:B:283:LEU:HD23	2.40	0.47
1:A:600:VAL:O	1:A:604:ASN:HB2	2.15	0.47
1:B:12[B]:ILE:HD11	1:B:106:MET:SD	2.56	0.46
1:B:122:SER:C	1:B:124:ALA:H	2.23	0.46
1:A:283[A]:LEU:HD13	1:A:383:ILE:HG23	1.98	0.46
1:B:32[A]:LYS:HG2	1:B:65:SER:HB3	1.97	0.46
1:A:450:THR:HG21	1:A:513:ASP:OD2	2.17	0.45
1:B:437[B]:ASN:ND2	7:B:805:HOH:O	2.48	0.45
1:B:623:ASP:HA	1:B:626:ASN:ND2	2.32	0.45
1:B:131:ASN:HA	1:B:134:MET:HB2	1.99	0.45
1:A:571:ILE:CD1	1:A:609:ILE:HD11	2.47	0.44
1:B:32[B]:LYS:NZ	1:B:63:THR:O	2.49	0.44
1:B:456:GLY:HA3	7:B:1009:HOH:O	2.17	0.44
1:A:571:ILE:HD12	1:A:609:ILE:CD1	2.47	0.44
1:B:548:ASN:HA	1:B:615:PHE:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LYS:HG2	1:B:110:LEU:CD1	2.47	0.44
1:A:283[A]:LEU:HD21	1:A:386:SER:HB2	1.99	0.44
1:A:454:ASN:HB2	1:A:507:ASN:HB3	2.00	0.44
1:B:12[B]:ILE:HD11	1:B:106:MET:CE	2.47	0.44
1:A:73[A]:ASN:H	1:A:73[A]:ASN:ND2	2.16	0.44
1:B:546:SER:C	1:B:547:GLY:O	2.60	0.44
1:B:551:GLU:HB3	1:B:584:ARG:HB2	2.01	0.42
1:B:524:THR:HG22	1:B:600:VAL:HA	2.01	0.42
1:B:583:ASN:HD22	1:B:585:GLY:H	1.67	0.42
1:B:120:ILE:CG2	1:B:137:THR:HB	2.49	0.42
1:B:274:ASN:CG	1:B:277:ALA:HB3	2.45	0.42
1:B:28:ASN:HD22	1:B:69:VAL:HG22	1.85	0.42
1:B:330:SER:O	1:B:333:ILE:HG22	2.20	0.42
1:A:454:ASN:HA	7:A:967:HOH:O	2.20	0.42
1:B:51[B]:MET:HE3	1:B:51[B]:MET:HB2	1.94	0.41
1:A:19:LYS:HD2	1:A:19:LYS:HA	1.82	0.41
1:B:12[B]:ILE:HG12	1:B:106:MET:HE2	2.01	0.41
1:B:176:ALA:C	1:B:178:ASP:N	2.78	0.41
1:A:551:GLU:HB3	1:A:584:ARG:HB2	2.03	0.41
1:A:198:LYS:HE3	1:A:224:GLY:O	2.21	0.41
1:A:47[A]:MET:HG2	1:A:85:GLN:HG3	2.03	0.40
1:A:301:LYS:HD2	1:A:327:GLN:O	2.21	0.40
1:B:541:ASN:O	1:B:542:ALA:CB	2.69	0.40

All (3) 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:B:545:GLY:CA	1:B:547:GLY:CA[2_565]	1.58	0.62
1:B:546:SER:N	1:B:546:SER:C[2_565]	1.98	0.22
1:A:131:ASN:O	1:A:580:ASN:CG[4_455]	2.15	0.05

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	647/638 (101%)	625 (97%)	19 (3%)	3 (0%)	24	12
1	B	646/638 (101%)	617 (96%)	22 (3%)	7 (1%)	11	3
All	All	1293/1276 (101%)	1242 (96%)	41 (3%)	10 (1%)	16	5

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	542	ALA
1	A	451	GLU
1	B	451	GLU
1	B	452	PRO
1	A	546	SER
1	B	126	SER
1	B	131	ASN
1	B	456	GLY
1	A	543	SER
1	B	134	MET

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	551/540 (102%)	535 (97%)	16 (3%)	37	20
1	B	550/540 (102%)	531 (96%)	19 (4%)	32	15
All	All	1101/1080 (102%)	1066 (97%)	35 (3%)	35	17

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	SER
1	A	73[A]	ASN
1	A	73[B]	ASN

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Mol	Chain	Res	Type
1	A	126	SER
1	A	131	ASN
1	A	133	TYR
1	A	180[A]	ILE
1	A	180[B]	ILE
1	A	327	GLN
1	A	370	LYS
1	A	432	LYS
1	A	445	LYS
1	A	451	GLU
1	A	544	ASN
1	A	580	ASN
1	A	619	LYS
1	B	19	LYS
1	B	62	LYS
1	B	111	LYS
1	B	123	ASP
1	B	127	THR
1	B	128	LYS
1	B	130	VAL
1	B	132	GLU
1	B	135	ARG
1	B	136	LYS
1	B	138	SER
1	B	228	GLN
1	B	232	SER
1	B	268	ASN
1	B	342	LYS
1	B	454	ASN
1	B	546	SER
1	B	583	ASN
1	B	626	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	90	ASN
1	A	95	GLN
1	A	109	ASN
1	A	241	ASN
1	A	251	HIS

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Mol	Chain	Res	Type
1	A	306	GLN
1	A	310	ASN
1	A	437	ASN
1	A	447	ASN
1	A	481	ASN
1	A	507	ASN
1	A	605	ASN
1	B	28	ASN
1	B	481	ASN
1	B	560	ASN
1	B	583	ASN
1	B	626	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 16 are monoatomic - leaving 2 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
6	CIT	B	709	-	12,12,12	1.78	2 (16%)	17,17,17	0.98	0
6	CIT	B	708	-	12,12,12	2.35	3 (25%)	17,17,17	1.52	4 (23%)

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
6	CIT	B	709	-	-	0/16/16/16	-
6	CIT	B	708	-	-	0/16/16/16	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	708	CIT	C3-C6	5.45	1.59	1.53
6	B	709	CIT	C3-C6	4.35	1.58	1.53
6	B	708	CIT	C2-C3	-3.46	1.49	1.54
6	B	708	CIT	O2-C1	-3.36	1.19	1.30
6	B	709	CIT	O2-C1	-2.41	1.22	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	708	CIT	O6-C6-C3	2.69	118.30	113.14
6	B	708	CIT	C4-C3-C2	-2.42	103.11	109.31
6	B	708	CIT	O1-C1-C2	-2.37	116.25	122.95
6	B	708	CIT	O5-C6-C3	-2.21	117.82	122.09

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, 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	629/638 (98%)	-0.08	24 (3%)	44 48	10, 28, 51, 160	31 (4%)
1	B	628/638 (98%)	-0.14	30 (4%)	35 39	13, 26, 53, 140	26 (4%)
All	All	1257/1276 (98%)	-0.11	54 (4%)	40 44	10, 27, 52, 160	57 (4%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	452	PRO	7.9
1	B	454	ASN	7.9
1	B	546	SER	7.7
1	A	453	ASP	7.1
1	B	133	TYR	6.0
1	A	450	THR	5.9
1	B	547	GLY	5.7
1	A	133	TYR	5.5
1	B	458	ALA	5.0
1	A	459	ALA	5.0
1	B	134	MET	4.9
1	A	454	ASN	4.8
1	B	542	ALA	4.4
1	B	456	GLY	4.4
1	B	455	SER	4.3
1	B	457	SER	4.2
1	A	456	GLY	4.2
1	A	457	SER	4.0
1	B	123	ASP	3.7
1	B	124	ALA	3.6
1	B	450	THR	3.6
1	B	626	ASN	3.6
1	B	131	ASN	3.4
1	B	125	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	132	GLU	3.4
1	B	176	ALA	3.3
1	A	545	GLY	3.3
1	A	451	GLU	3.3
1	B	122	SER	3.2
1	B	459	ALA	3.2
1	A	458	ALA	3.1
1	B	541	ASN	3.1
1	A	123	ASP	3.0
1	A	135	ARG	3.0
1	B	135	ARG	2.9
1	B	451	GLU	2.8
1	B	620	SER	2.8
1	A	455	SER	2.7
1	A	134	MET	2.6
1	A	460	GLY	2.5
1	B	480	LEU	2.5
1	A	542	ALA	2.5
1	A	175	LEU	2.4
1	B	623	ASP	2.4
1	B	483	GLY	2.3
1	A	546	SER	2.2
1	A	449	PRO	2.2
1	B	175	LEU	2.2
1	A	479	GLY	2.2
1	A	544	ASN	2.2
1	A	248	VAL	2.1
1	B	615	PHE	2.1
1	A	620	SER	2.1
1	B	617	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	CIT	B	709	13/13	0.84	0.12	42,53,58,60	0
6	CIT	B	708	13/13	0.86	0.12	44,59,66,67	0
4	CL	A	706	1/1	0.90	0.32	56,56,56,56	0
2	CA	B	702	1/1	0.91	0.26	61,61,61,61	0
2	CA	A	702	1/1	0.93	0.17	60,60,60,60	0
4	CL	A	705	1/1	0.96	0.13	55,55,55,55	0
2	CA	B	701	1/1	0.97	0.20	39,39,39,39	0
5	ZN	B	710	1/1	0.97	0.12	47,47,47,47	1
2	CA	A	701[B]	1/1	0.97	0.18	57,57,57,57	1
2	CA	A	701[A]	1/1	0.97	0.18	45,45,45,45	1
5	ZN	A	707	1/1	0.98	0.10	36,36,36,36	1
3	NA	A	703	1/1	0.98	0.04	26,26,26,26	0
3	NA	B	705	1/1	0.98	0.07	44,44,44,44	1
4	CL	B	707	1/1	0.98	0.13	37,37,37,37	0
3	NA	B	704	1/1	0.99	0.05	22,22,22,22	0
2	CA	B	703	1/1	0.99	0.13	33,33,33,33	1
4	CL	B	706	1/1	0.99	0.07	25,25,25,25	0
4	CL	A	704	1/1	0.99	0.05	25,25,25,25	0

6.5 Other polymers

There are no such residues in this entry.