Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2017 – 05:20 PM EST

PDB ID	:	5J72
Title	:	Cwp6 from Clostridium difficile
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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
http://wwpdb.org/validation/2016/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:

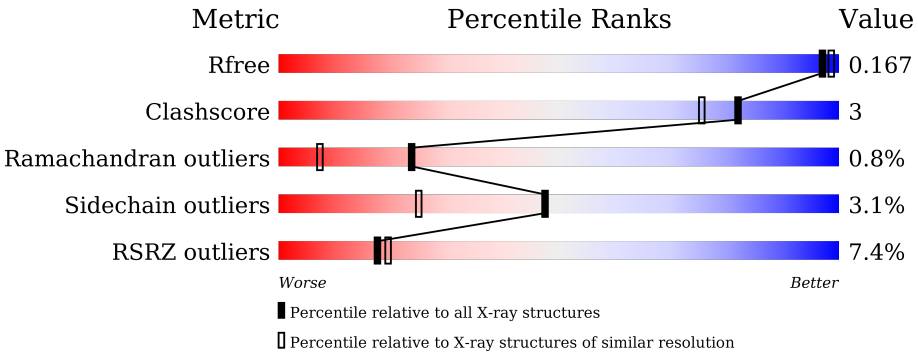
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 1.70 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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	638	7% 92% 7%
1	B	638	7% 90% 8%

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	CA	A	701[A]	-	-	-	X
6	CIT	B	708	-	-	-	X
6	CIT	B	709	-	-	-	X

2 Entry composition

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 (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

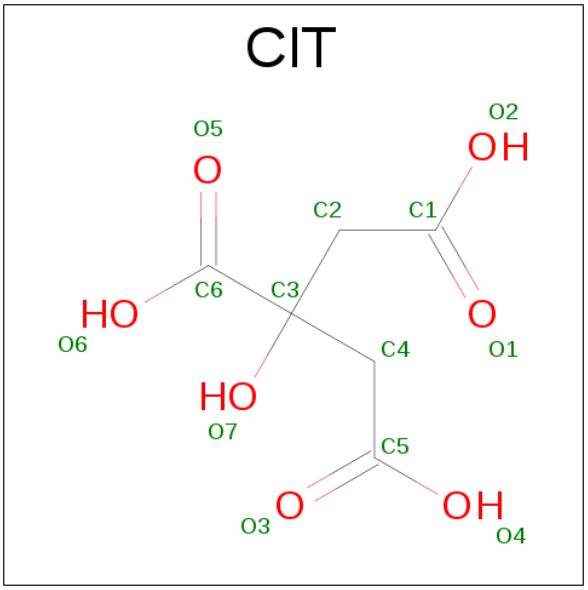
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



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

- Molecule 7 is water.

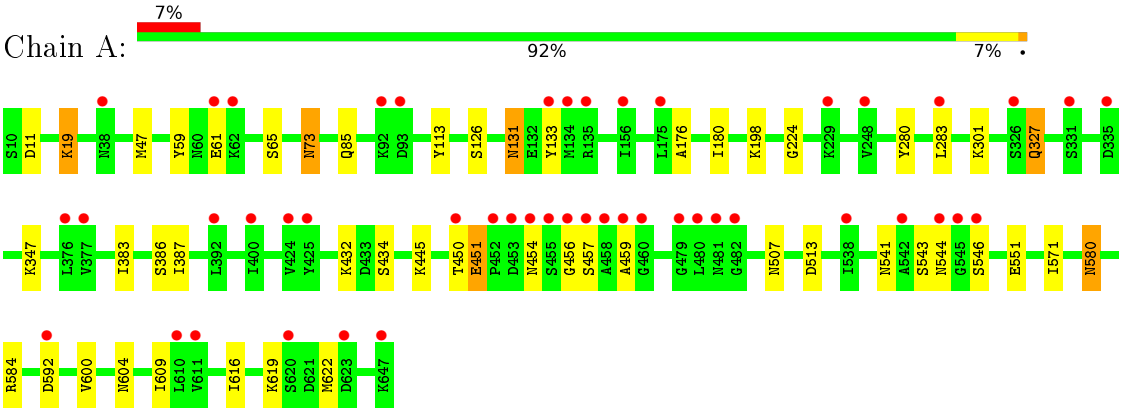
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	643	Total O 643 643	0	0
7	B	686	Total O 686 686	0	0

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 errors 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.

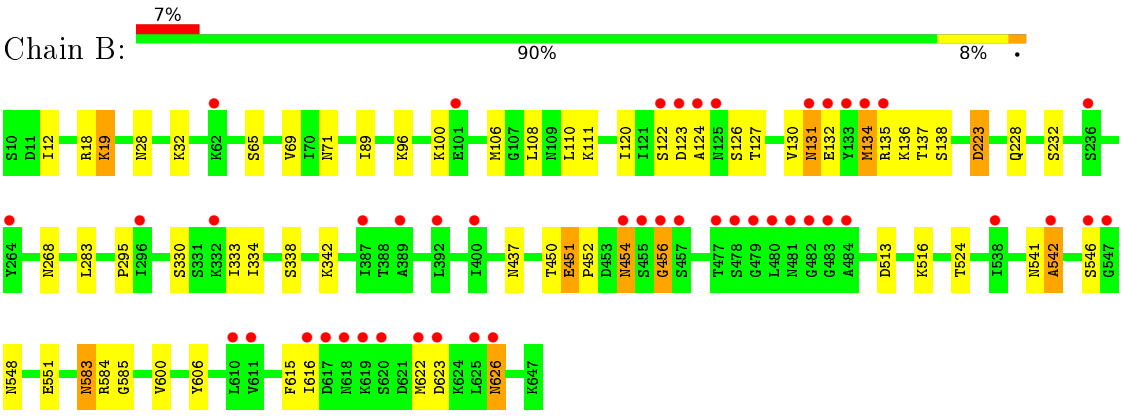
- Molecule 1: Putative N-acetylmuramoyl-L-alanine amidase,autolysin cwp6

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

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) 99.1 (29.85-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 1.70Å)	Xtriage
Refinement program	MAIN	Depositor
R, R_{free}	0.178 , 0.201 0.173 , 0.167	Depositor DCC
R_{free} test set	9036 reflections (5.26%)	DCC
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 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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: NA, ZN, CIT, CA, 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	0.85	0/5017	0.85	0/6779
1	B	0.82	0/5011	0.87	3/6771 (0.0%)
All	All	0.84	0/10028	0.86	3/13550 (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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	130	VAL	CA-CB-CG1	5.80	119.60	110.90
1	B	130	VAL	CA-CB-CG2	5.77	119.56	110.90
1	B	295	PRO	N-CA-C	5.42	126.19	112.10

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 (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	A	4918	0	4949	30	1
1	B	4921	0	4958	30	1
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	6	0
7	B	686	0	0	6	0
All	All	11210	0	9917	61	2

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 (61) 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:18[B]:ARG:HD3	7:B:1238:HOH:O	2.00	0.61
1:A:59:TYR:CE2	1:A:61:GLU:HG2	2.35	0.60
1:A:176:ALA:HB1	1:A:387:ILE:HD12	1.85	0.59
1:A:616:ILE:HA	1:A:622:MET:HE3	1.85	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LYS:NZ	7:B:802:HOH:O	2.38	0.56
1:A:327:GLN:CD	1:A:327:GLN:H	2.10	0.54
1:A:457:SER:HB3	1:A:459:ALA:O	2.07	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: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:A:600:VAL:O	1:A:604:ASN:HB2	2.15	0.47
1:B:583:ASN:HD22	1:B:583:ASN:C	2.17	0.46
1:B:12[B]:ILE:HD11	1:B:106:MET:SD	2.56	0.46
1:A:283[A]:LEU:HD13	1:A:383:ILE:HG23	1.98	0.46
1:A:434:SER:HG	1:A:456:GLY:HA2	1.77	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: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
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:A:347:LYS:NZ	7:A:813:HOH:O	2.50	0.43
1:B:616:ILE:HA	1:B:622:MET:HE3	2.01	0.42
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:283:LEU:C	1:B:283:LEU:HD23	2.40	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:28:ASN:HD22	1:B:69:VAL:HG22	1.85	0.42
1:B:122:SER:C	1:B:124:ALA:H	2.23	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:A:19:LYS:HD2	1:A:19:LYS:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (2) 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: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 (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	647/638 (101%)	625 (97%)	19 (3%)	3 (0%)	34	15
1	B	646/638 (101%)	617 (96%)	22 (3%)	7 (1%)	17	4
All	All	1293/1276 (101%)	1242 (96%)	41 (3%)	10 (1%)	24	7

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

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Mol	Chain	Res	Type
1	B	456	GLY
1	A	543	SER
1	B	134	MET

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	551/540 (102%)	533 (97%)	18 (3%)	45	22
1	B	550/540 (102%)	532 (97%)	18 (3%)	45	22
All	All	1101/1080 (102%)	1065 (97%)	36 (3%)	47	22

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	65	SER
1	A	73[A]	ASN
1	A	73[B]	ASN
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	432	LYS
1	A	445	LYS
1	A	451	GLU
1	A	541	ASN
1	A	544	ASN
1	A	580	ASN
1	A	592	ASP
1	A	619	LYS
1	B	19	LYS
1	B	71	ASN

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Mol	Chain	Res	Type
1	B	111	LYS
1	B	123	ASP
1	B	127	THR
1	B	132	GLU
1	B	135	ARG
1	B	136	LYS
1	B	138	SER
1	B	223	ASP
1	B	228	GLN
1	B	232	SER
1	B	268	ASN
1	B	342	LYS
1	B	454	ASN
1	B	516	LYS
1	B	583	ASN
1	B	626	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	241	ASN
1	A	251	HIS
1	A	306	GLN
1	A	310	ASN
1	A	447	ASN
1	A	481	ASN
1	A	507	ASN
1	A	605	ASN
1	B	28	ASN
1	B	71	ASN
1	B	268	ASN
1	B	310	ASN
1	B	481	ASN
1	B	583	ASN
1	B	626	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 carbohydrates 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	708	-	3,12,12	2.12	1 (33%)	3,17,17	2.18	2 (66%)
6	CIT	B	709	-	3,12,12	0.85	0	3,17,17	1.05	0

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	708	CIT	C2-C3	-3.32	1.49	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	708	CIT	C4-C3-C2	-2.72	103.11	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	708	CIT	C3-C4-C5	2.10	118.23	114.95

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	629/638 (98%)	0.25	47 (7%)	17	19	15, 28, 53, 166	20 (3%)
1	B	628/638 (98%)	0.26	46 (7%)	18	20	16, 27, 54, 159	16 (2%)
All	All	1257/1276 (98%)	0.25	93 (7%)	17	19	15, 27, 54, 166	36 (2%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	458	ALA	14.9
1	A	452	PRO	12.9
1	B	133	TYR	12.9
1	A	453	ASP	12.5
1	B	125	ASN	12.3
1	A	457	SER	10.5
1	B	124	ALA	10.3
1	A	459	ALA	10.0
1	B	454	ASN	9.9
1	B	134	MET	9.4
1	B	455	SER	9.1
1	A	455	SER	9.1
1	A	456	GLY	8.1
1	B	123	ASP	7.9
1	B	131	ASN	7.2
1	B	479	GLY	7.0
1	B	480	LEU	6.7
1	A	454	ASN	6.5
1	B	546	SER	5.6
1	B	482	GLY	5.3
1	B	132	GLU	5.0
1	A	545	GLY	4.9
1	B	483	GLY	4.7
1	B	620	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	134	MET	4.1
1	A	92	LYS	4.1
1	B	135	ARG	4.0
1	A	62	LYS	4.0
1	A	546	SER	3.9
1	A	480	LEU	3.9
1	B	547	GLY	3.9
1	A	620	SER	3.9
1	A	544	ASN	3.8
1	A	479	GLY	3.8
1	B	542	ALA	3.8
1	A	133	TYR	3.8
1	A	460	GLY	3.8
1	A	93	ASP	3.8
1	B	623	ASP	3.7
1	B	478	SER	3.6
1	A	482	GLY	3.6
1	A	376	LEU	3.5
1	B	538	ILE	3.5
1	A	538	ILE	3.4
1	B	481	ASN	3.3
1	B	477	THR	3.1
1	B	625	LEU	3.0
1	B	387[A]	ILE	3.0
1	B	626	ASN	2.9
1	B	456	GLY	2.9
1	A	283[A]	LEU	2.9
1	B	618	ASN	2.8
1	B	619	LYS	2.8
1	A	61	GLU	2.8
1	A	400	ILE	2.7
1	A	424	VAL	2.7
1	B	122	SER	2.7
1	A	611	VAL	2.7
1	B	484	ALA	2.6
1	A	335	ASP	2.6
1	B	617	ASP	2.6
1	B	332	LYS	2.6
1	A	592	ASP	2.6
1	A	623	ASP	2.6
1	A	156	ILE	2.6
1	A	610	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	611	VAL	2.5
1	B	622	MET	2.5
1	A	450	THR	2.5
1	B	389	ALA	2.4
1	B	392	LEU	2.4
1	A	135	ARG	2.4
1	B	616	ILE	2.3
1	B	236	SER	2.3
1	B	296	ILE	2.3
1	A	229	LYS	2.3
1	B	62	LYS	2.3
1	A	377	VAL	2.2
1	B	610	LEU	2.2
1	A	425	TYR	2.2
1	A	392	LEU	2.2
1	A	647	LYS	2.2
1	B	101	GLU	2.2
1	B	457	SER	2.1
1	A	175	LEU	2.1
1	B	400	ILE	2.1
1	A	481	ASN	2.1
1	B	264	TYR	2.1
1	A	326	SER	2.1
1	A	38	ASN	2.1
1	A	542	ALA	2.0
1	A	331	SER	2.0
1	A	248	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å^2)	Q<0.9
6	CIT	B	708	13/13	0.82	0.29	9.70	44,59,66,67	0
6	CIT	B	709	13/13	0.75	0.23	7.60	42,53,58,60	0
2	CA	A	701[A]	1/1	0.92	0.16	2.76	45,45,45,45	1
2	CA	B	701	1/1	0.98	0.15	1.37	39,39,39,39	0
2	CA	A	702	1/1	0.93	0.10	0.29	60,60,60,60	0
4	CL	B	707	1/1	0.99	0.06	-0.95	37,37,37,37	0
3	NA	B	704	1/1	0.99	0.05	-1.12	22,22,22,22	0
3	NA	A	703	1/1	0.99	0.06	-1.15	26,26,26,26	0
4	CL	B	706	1/1	0.99	0.06	-1.66	25,25,25,25	0
4	CL	A	704	1/1	0.99	0.07	-1.67	25,25,25,25	0
2	CA	B	703	1/1	0.98	0.09	-	33,33,33,33	1
4	CL	A	705	1/1	0.99	0.19	-	55,55,55,55	0
2	CA	B	702	1/1	0.79	0.26	-	61,61,61,61	0
5	ZN	A	707	1/1	0.96	0.06	-	36,36,36,36	1
4	CL	A	706	1/1	0.90	0.27	-	56,56,56,56	0
5	ZN	B	710	1/1	0.96	0.05	-	47,47,47,47	1
3	NA	B	705	1/1	0.96	0.12	-	44,44,44,44	1
2	CA	A	701[B]	1/1	0.92	0.16	-	57,57,57,57	1

6.5 Other polymers (i)

There are no such residues in this entry.