Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:41 am BST

PDB ID	:	5W6F
Title	:	Crystal structure of Bacteriophage CBA120 tailspike protein 3 (TSP3, orf212)
Authors	:	Plattner, M.; Shneider, M.M.; Leiman, P.G.
Deposited on	:	2017-06-16
Resolution	:	2.18 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 ①) were used in the production of this report:

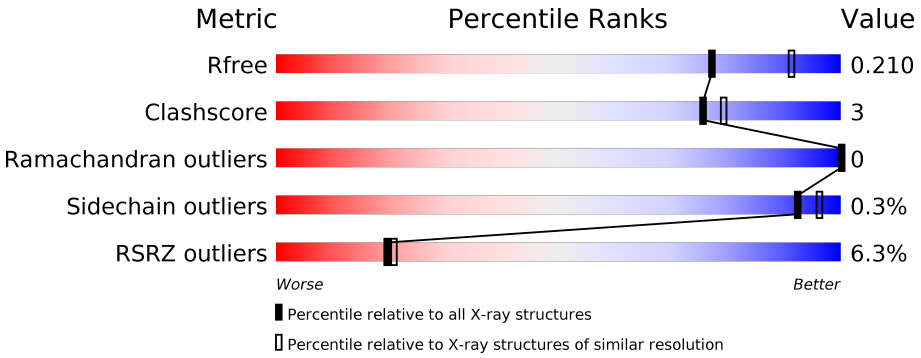
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	635	3% 92% 5% ·
1	B	635	11% 87% 9% ·
1	C	635	4% 91% 6% ·

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15366 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 tailspike protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	616	Total	C	N	O	S	0	2	0
			4719	2988	798	920	13			
1	B	616	Total	C	N	O	S	0	2	0
			4717	2982	801	921	13			
1	C	616	Total	C	N	O	S	0	0	0
			4700	2973	796	918	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	628	LEU	-	expression tag	UNP G3M191
A	629	GLU	-	expression tag	UNP G3M191
A	630	HIS	-	expression tag	UNP G3M191
A	631	HIS	-	expression tag	UNP G3M191
A	632	HIS	-	expression tag	UNP G3M191
A	633	HIS	-	expression tag	UNP G3M191
A	634	HIS	-	expression tag	UNP G3M191
A	635	HIS	-	expression tag	UNP G3M191
B	628	LEU	-	expression tag	UNP G3M191
B	629	GLU	-	expression tag	UNP G3M191
B	630	HIS	-	expression tag	UNP G3M191
B	631	HIS	-	expression tag	UNP G3M191
B	632	HIS	-	expression tag	UNP G3M191
B	633	HIS	-	expression tag	UNP G3M191
B	634	HIS	-	expression tag	UNP G3M191
B	635	HIS	-	expression tag	UNP G3M191
C	628	LEU	-	expression tag	UNP G3M191
C	629	GLU	-	expression tag	UNP G3M191
C	630	HIS	-	expression tag	UNP G3M191
C	631	HIS	-	expression tag	UNP G3M191
C	632	HIS	-	expression tag	UNP G3M191
C	633	HIS	-	expression tag	UNP G3M191
C	634	HIS	-	expression tag	UNP G3M191

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Chain	Residue	Modelled	Actual	Comment	Reference
C	635	HIS	-	expression tag	UNP G3M191

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Cl 1 1	0	0

- Molecule 3 is water.

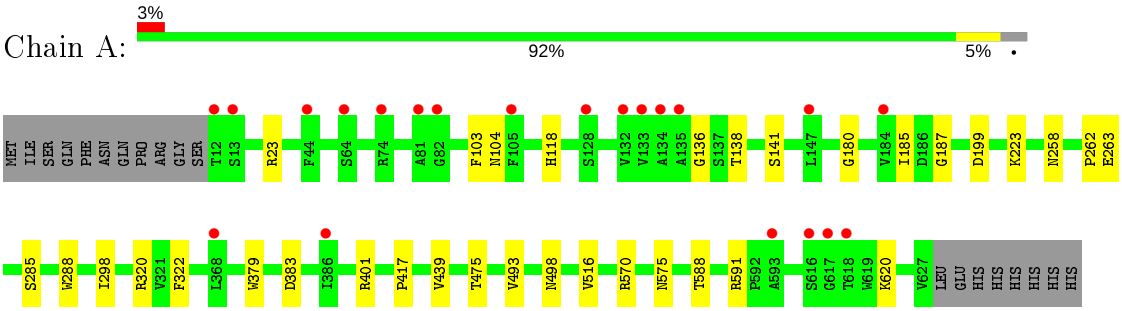
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	429	Total O 429 429	0	0
3	B	375	Total O 375 375	0	0
3	C	425	Total O 425 425	0	0

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 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.

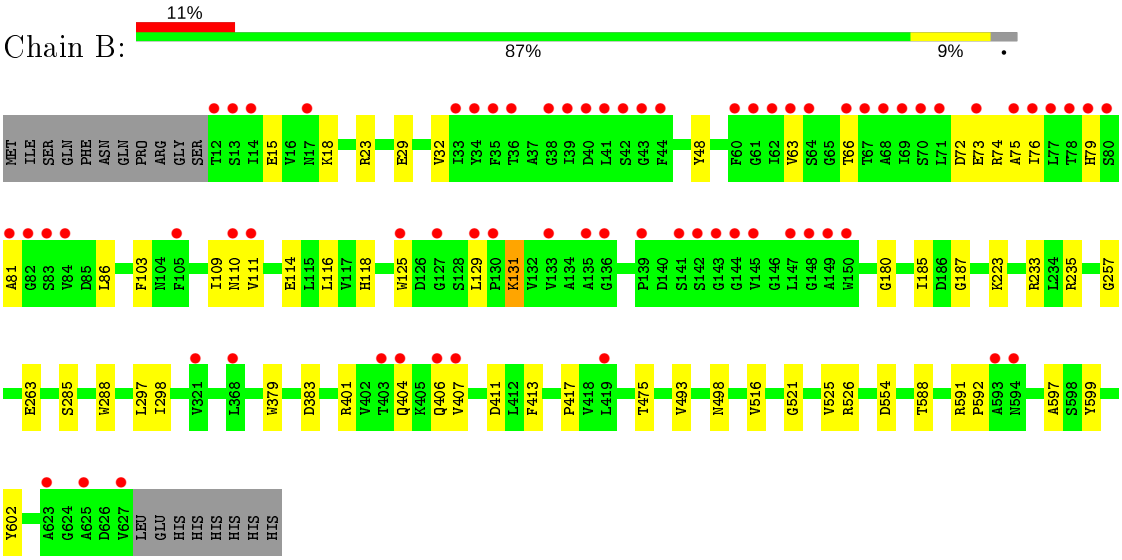
- Molecule 1: tailspike protein 3

Chain A:



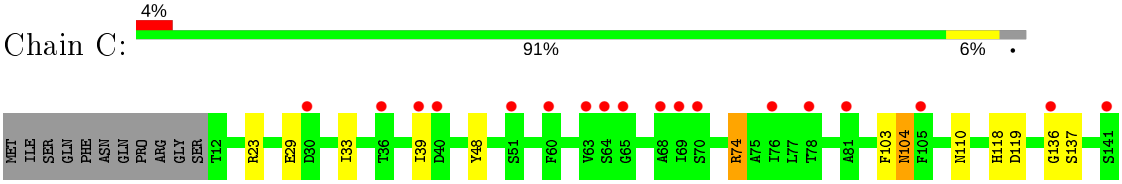
- Molecule 1: tailspike protein 3

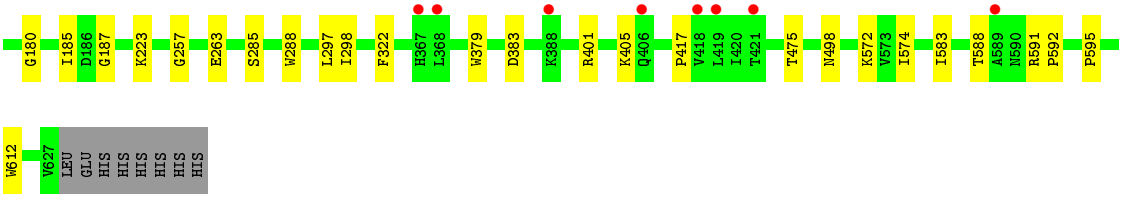
Chain B:



- Molecule 1: tailspike protein 3

Chain C:




G180
I185
D186
G187
K223
G257
E263
S285
W288
L297
I298
F322
H367
L368
W379
D383
K388
R401
K405
Q406
P417
V418
L419
I420
T421
T475
N498
K572
V573
I574
I583
T588
A589
N590
R591
P592
P595

W612
V627
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.58Å 66.78Å 161.99Å 90.00° 105.86° 90.00°	Depositor
Resolution (Å)	49.48 – 2.18 49.48 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.48-2.18) 97.3 (49.48-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.180 , 0.219 0.183 , 0.210	Depositor DCC
R_{free} test set	6959 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	32.6	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.007 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15366	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: 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	0.24	0/4823	0.46	0/6552
1	B	0.25	0/4820	0.47	0/6547
1	C	0.24	0/4803	0.46	0/6525
All	All	0.24	0/14446	0.46	0/19624

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	4719	0	4587	25	0
1	B	4717	0	4585	43	0
1	C	4700	0	4569	28	0
2	C	1	0	0	0	0
3	A	429	0	0	4	0
3	B	375	0	0	3	0
3	C	425	0	0	2	0
All	All	15366	0	13741	86	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 3.

All (86) 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:74:ARG:NH2	1:B:110:ASN:O	2.08	0.85
1:A:570:ARG:NH1	3:A:701:HOH:O	2.18	0.76
1:B:233[B]:ARG:NH1	3:B:702:HOH:O	2.26	0.69
1:B:74:ARG:HD3	1:B:129:LEU:HD22	1.80	0.64
1:A:223:LYS:HD3	1:C:187:GLY:HA3	1.81	0.62
1:C:74:ARG:NH2	1:C:110:ASN:OD1	2.31	0.62
3:A:706:HOH:O	1:B:233[B]:ARG:NH2	2.30	0.60
1:C:405:LYS:NZ	3:C:805:HOH:O	2.34	0.60
1:B:63:VAL:O	1:B:66:THR:OG1	2.16	0.60
1:A:320:ARG:NH2	3:A:709:HOH:O	2.36	0.57
1:A:620:LYS:NZ	3:A:702:HOH:O	2.25	0.57
1:C:298:ILE:HG12	1:C:322:PHE:HB3	1.87	0.56
1:A:104:ASN:O	1:A:136:GLY:N	2.32	0.56
1:B:73:GLU:OE2	1:B:74:ARG:NH1	2.40	0.55
1:C:285:SER:HA	1:C:288:TRP:CD2	2.42	0.55
1:C:285:SER:HA	1:C:288:TRP:CE2	2.44	0.53
1:A:187:GLY:HA3	1:B:223:LYS:HD3	1.90	0.53
1:B:103:PHE:CD1	1:B:118:HIS:HB2	2.44	0.53
1:C:104:ASN:O	1:C:136:GLY:N	2.37	0.53
1:B:285:SER:HA	1:B:288:TRP:CE2	2.43	0.52
1:C:33:ILE:HD11	1:C:39:ILE:HD12	1.91	0.52
1:A:180:GLY:HA3	1:A:185:ILE:HD12	1.93	0.51
1:B:404:GLN:NE2	1:B:406:GLN:HB3	2.25	0.51
1:C:103:PHE:CD1	1:C:118:HIS:HB2	2.46	0.51
1:C:257:GLY:HA3	1:C:297:LEU:HB3	1.92	0.51
1:A:379:TRP:CD1	1:A:401:ARG:HB2	2.46	0.51
1:A:138:THR:H	1:A:141:SER:HB3	1.77	0.49
1:C:23:ARG:NH1	1:C:29:GLU:OE2	2.45	0.49
1:B:526:ARG:NH2	3:B:709:HOH:O	2.33	0.49
1:B:257:GLY:HA3	1:B:297:LEU:HB3	1.94	0.49
1:A:285:SER:HA	1:A:288:TRP:CD2	2.48	0.49
1:B:18:LYS:HG2	1:B:32:VAL:HB	1.95	0.48
1:A:285:SER:HA	1:A:288:TRP:CE2	2.48	0.48
1:B:493:VAL:HG12	1:B:516:VAL:HB	1.96	0.48
1:A:263:GLU:HG2	1:A:298:ILE:HB	1.96	0.48
1:C:572:LYS:HE2	1:C:572:LYS:HB3	1.63	0.47
1:B:23:ARG:NH2	1:B:29:GLU:OE2	2.48	0.47
1:C:475:THR:HA	1:C:498:ASN:O	2.15	0.47
1:B:407:VAL:HG11	1:B:413:PHE:N	2.30	0.46
1:C:595:PRO:HG2	1:C:612:TRP:CG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ASP:OD1	1:A:417:PRO:HG2	2.15	0.46
1:B:379:TRP:CD1	1:B:401:ARG:HB2	2.50	0.46
1:B:79:HIS:CE1	1:B:81:ALA:HB3	2.50	0.46
1:B:602:TYR:OH	3:B:701:HOH:O	2.19	0.46
1:C:263:GLU:HG2	1:C:298:ILE:HB	1.97	0.46
1:B:109:ILE:HD11	1:B:116:LEU:HD22	1.99	0.45
1:B:285:SER:HA	1:B:288:TRP:CD2	2.51	0.45
1:B:187:GLY:HA3	1:C:223:LYS:HD3	1.99	0.45
1:A:223:LYS:HD3	1:C:187:GLY:CA	2.47	0.45
1:A:23:ARG:NH1	1:B:48:TYR:OH	2.50	0.45
1:C:180:GLY:HA3	1:C:185:ILE:HD12	1.99	0.45
1:A:199:ASP:OD1	1:B:235:ARG:HD2	2.18	0.44
1:B:521:GLY:HA3	1:B:554:ASP:HB2	1.99	0.44
1:B:23:ARG:NH2	1:C:48:TYR:OH	2.50	0.44
1:B:592:PRO:HG2	1:B:599:TYR:CE1	2.53	0.44
1:B:407:VAL:HB	1:B:411:ASP:HB2	2.00	0.44
1:C:23:ARG:HA	1:C:23:ARG:HD3	1.86	0.44
1:B:383:ASP:OD1	1:B:417:PRO:HG2	2.18	0.44
1:A:103:PHE:CD1	1:A:118:HIS:HB2	2.52	0.43
1:A:23:ARG:HD3	1:A:23:ARG:HA	1.82	0.43
1:B:72:ASP:OD2	1:B:76:ILE:HB	2.18	0.43
1:C:588:THR:HG23	1:C:591:ARG:CZ	2.47	0.43
1:A:475:THR:HA	1:A:498:ASN:O	2.18	0.43
1:B:23:ARG:HD3	1:B:23:ARG:HA	1.81	0.43
1:A:588:THR:HG23	1:A:591:ARG:CZ	2.49	0.43
1:B:180:GLY:HA3	1:B:185:ILE:HD12	2.01	0.43
1:B:75:ALA:HB1	1:B:86:LEU:HB2	2.01	0.43
1:B:74:ARG:HD3	1:B:129:LEU:CD2	2.49	0.42
1:C:103:PHE:HB3	1:C:137:SER:O	2.20	0.42
1:C:572:LYS:HD2	3:C:1200:HOH:O	2.19	0.42
1:C:383:ASP:OD1	1:C:417:PRO:HG2	2.20	0.42
1:B:597:ALA:O	1:C:583:ILE:HD11	2.19	0.41
1:A:575:ASN:HD22	1:C:574:ILE:HG22	1.84	0.41
1:B:475:THR:HA	1:B:498:ASN:O	2.20	0.41
1:A:439:VAL:HG11	1:B:525:VAL:HG11	2.01	0.41
1:B:588:THR:HG23	1:B:591:ARG:CZ	2.51	0.41
1:A:493:VAL:HG12	1:A:516:VAL:HB	2.02	0.41
1:B:404:GLN:OE1	1:B:404:GLN:HA	2.21	0.41
1:B:111:VAL:HB	1:B:114:GLU:HG3	2.02	0.41
1:B:404:GLN:HE21	1:B:406:GLN:HB3	1.86	0.41
1:B:263:GLU:HG2	1:B:298:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:TRP:CD1	1:C:401:ARG:HB2	2.56	0.41
1:C:591:ARG:HA	1:C:592:PRO:HD3	1.96	0.41
1:B:125:TRP:CE2	1:B:131:LYS:HD3	2.56	0.40
1:A:258:ASN:HB3	1:A:262:PRO:HD3	2.03	0.40
1:A:298:ILE:HG12	1:A:322:PHE:HB3	2.02	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	616/635 (97%)	600 (97%)	16 (3%)	0	100	100
1	B	616/635 (97%)	599 (97%)	17 (3%)	0	100	100
1	C	614/635 (97%)	598 (97%)	16 (3%)	0	100	100
All	All	1846/1905 (97%)	1797 (97%)	49 (3%)	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	504/520 (97%)	504 (100%)	0	100	100
1	B	504/520 (97%)	502 (100%)	2 (0%)	91	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	502/520 (96%)	499 (99%)	3 (1%)	86 92
All	All	1510/1560 (97%)	1505 (100%)	5 (0%)	92 96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	15	GLU
1	B	131	LYS
1	C	74	ARG
1	C	104	ASN
1	C	119	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

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	616/635 (97%)	0.18	21 (3%) 45 46	20, 32, 63, 113	0
1	B	616/635 (97%)	0.55	69 (11%) 5 5	23, 39, 97, 119	0
1	C	616/635 (97%)	0.25	26 (4%) 36 37	21, 34, 69, 93	0
All	All	1848/1905 (97%)	0.33	116 (6%) 20 21	20, 36, 76, 119	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	75	ALA	7.1
1	B	147	LEU	6.5
1	B	44	PHE	6.0
1	B	143	GLY	5.9
1	B	82	GLY	5.9
1	B	64	SER	5.9
1	A	12	THR	5.8
1	B	61	GLY	5.6
1	B	81	ALA	5.6
1	B	70	SER	5.4
1	B	40	ASP	5.1
1	B	84	VAL	5.0
1	B	68	ALA	5.0
1	B	67	THR	4.9
1	C	65	GLY	4.8
1	A	82	GLY	4.7
1	B	136	GLY	4.7
1	B	17	ASN	4.7
1	B	43	GLY	4.6
1	B	127	GLY	4.5
1	B	35	PHE	4.5
1	B	77	LEU	4.4
1	C	406	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	149	ALA	4.3
1	B	79	HIS	4.2
1	B	83	SER	4.1
1	B	39	ILE	4.0
1	B	76	ILE	4.0
1	A	128	SER	4.0
1	C	70	SER	4.0
1	B	627	VAL	3.9
1	B	12	THR	3.9
1	B	41	LEU	3.9
1	B	141	SER	3.7
1	B	73	GLU	3.6
1	B	66	THR	3.6
1	B	14	ILE	3.6
1	A	64	SER	3.5
1	B	36	THR	3.5
1	B	144	GLY	3.4
1	B	80	SER	3.4
1	B	63	VAL	3.3
1	B	135	ALA	3.3
1	B	129	LEU	3.2
1	B	38	GLY	3.2
1	B	139	PRO	3.1
1	C	39	ILE	3.1
1	B	69	ILE	3.1
1	A	105	PHE	3.0
1	B	593	ALA	3.0
1	B	34	TYR	3.0
1	B	13	SER	3.0
1	B	145	VAL	2.9
1	A	368	LEU	2.9
1	A	132	VAL	2.9
1	A	184	VAL	2.9
1	A	81	ALA	2.9
1	B	62	ILE	2.8
1	C	69	ILE	2.8
1	A	134	ALA	2.8
1	B	594	ASN	2.8
1	C	81	ALA	2.8
1	C	63	VAL	2.7
1	A	618	THR	2.7
1	C	141	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	150	TRP	2.7
1	A	44	PHE	2.7
1	C	136	GLY	2.7
1	B	148	GLY	2.6
1	C	60	PHE	2.6
1	C	36	THR	2.6
1	C	51	SER	2.6
1	C	368	LEU	2.6
1	C	76	ILE	2.6
1	B	404	GLN	2.6
1	C	78	THR	2.5
1	A	617	GLY	2.5
1	B	625	ALA	2.5
1	B	406	GLN	2.5
1	A	593	ALA	2.5
1	C	105	PHE	2.5
1	C	64	SER	2.4
1	B	130	PRO	2.4
1	B	60	PHE	2.4
1	A	147	LEU	2.4
1	B	42	SER	2.3
1	B	125	TRP	2.3
1	B	368	LEU	2.3
1	C	40	ASP	2.3
1	C	388	LYS	2.3
1	B	110	ASN	2.3
1	B	105	PHE	2.3
1	A	13	SER	2.3
1	B	623	ALA	2.3
1	C	589	ALA	2.2
1	A	133	VAL	2.2
1	A	386	ILE	2.2
1	B	33	ILE	2.2
1	B	71	LEU	2.2
1	C	419	LEU	2.2
1	A	74	ARG	2.2
1	B	142	SER	2.2
1	C	421	THR	2.2
1	C	367	HIS	2.1
1	B	78	THR	2.1
1	C	30	ASP	2.1
1	A	135	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	68	ALA	2.1
1	B	407	VAL	2.1
1	A	616	SER	2.0
1	B	403	THR	2.0
1	B	321	VAL	2.0
1	C	418	VAL	2.0
1	B	419	LEU	2.0
1	B	111	VAL	2.0
1	B	133	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. 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	CL	C	701	1/1	0.98	0.06	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.