



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:43 AM GMT

PDB ID : 3MWP
Title : Nucleoprotein structure of lassa fever virus
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Deposited on : 2010-05-06
Resolution : 1.79 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

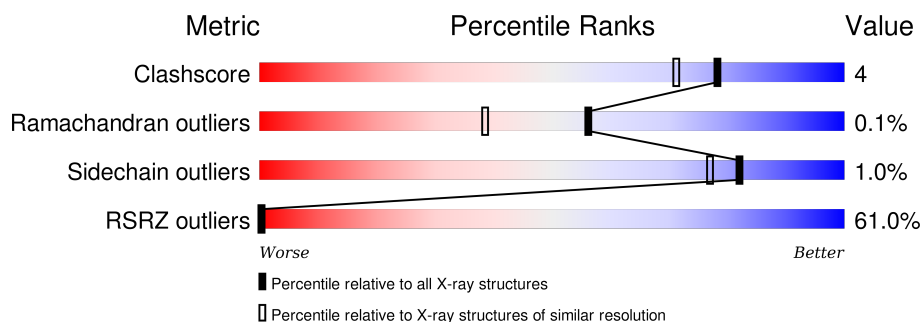
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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))
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 $\leq 5\%$. 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	577	<div> <div>52%</div> <div> <div></div> <div>83%</div> <div>5%</div> <div>11%</div> </div> </div>
1	B	577	<div> <div>52%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>11%</div> </div> </div>
1	C	577	<div> <div>58%</div> <div> <div></div> <div>77%</div> <div>10%</div> <div>12%</div> </div> </div>

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	ZN	B	570	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12477 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	1	0
			4011	2521	697	766	27			
1	B	515	Total	C	N	O	S	0	0	0
			4027	2528	701	771	27			
1	C	506	Total	C	N	O	S	0	0	0
			3961	2488	688	758	27			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP P13699
A	-6	ALA	-	EXPRESSION TAG	UNP P13699
A	-5	MET	-	EXPRESSION TAG	UNP P13699
A	-4	ASP	-	EXPRESSION TAG	UNP P13699
A	-3	HIS	-	EXPRESSION TAG	UNP P13699
A	-2	VAL	-	EXPRESSION TAG	UNP P13699
A	-1	GLU	-	EXPRESSION TAG	UNP P13699
A	0	PHE	-	EXPRESSION TAG	UNP P13699
B	-7	GLY	-	EXPRESSION TAG	UNP P13699
B	-6	ALA	-	EXPRESSION TAG	UNP P13699
B	-5	MET	-	EXPRESSION TAG	UNP P13699
B	-4	ASP	-	EXPRESSION TAG	UNP P13699
B	-3	HIS	-	EXPRESSION TAG	UNP P13699
B	-2	VAL	-	EXPRESSION TAG	UNP P13699
B	-1	GLU	-	EXPRESSION TAG	UNP P13699
B	0	PHE	-	EXPRESSION TAG	UNP P13699
C	-7	GLY	-	EXPRESSION TAG	UNP P13699
C	-6	ALA	-	EXPRESSION TAG	UNP P13699
C	-5	MET	-	EXPRESSION TAG	UNP P13699
C	-4	ASP	-	EXPRESSION TAG	UNP P13699
C	-3	HIS	-	EXPRESSION TAG	UNP P13699
C	-2	VAL	-	EXPRESSION TAG	UNP P13699
C	-1	GLU	-	EXPRESSION TAG	UNP P13699

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	PHE	-	EXPRESSION TAG	UNP P13699

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

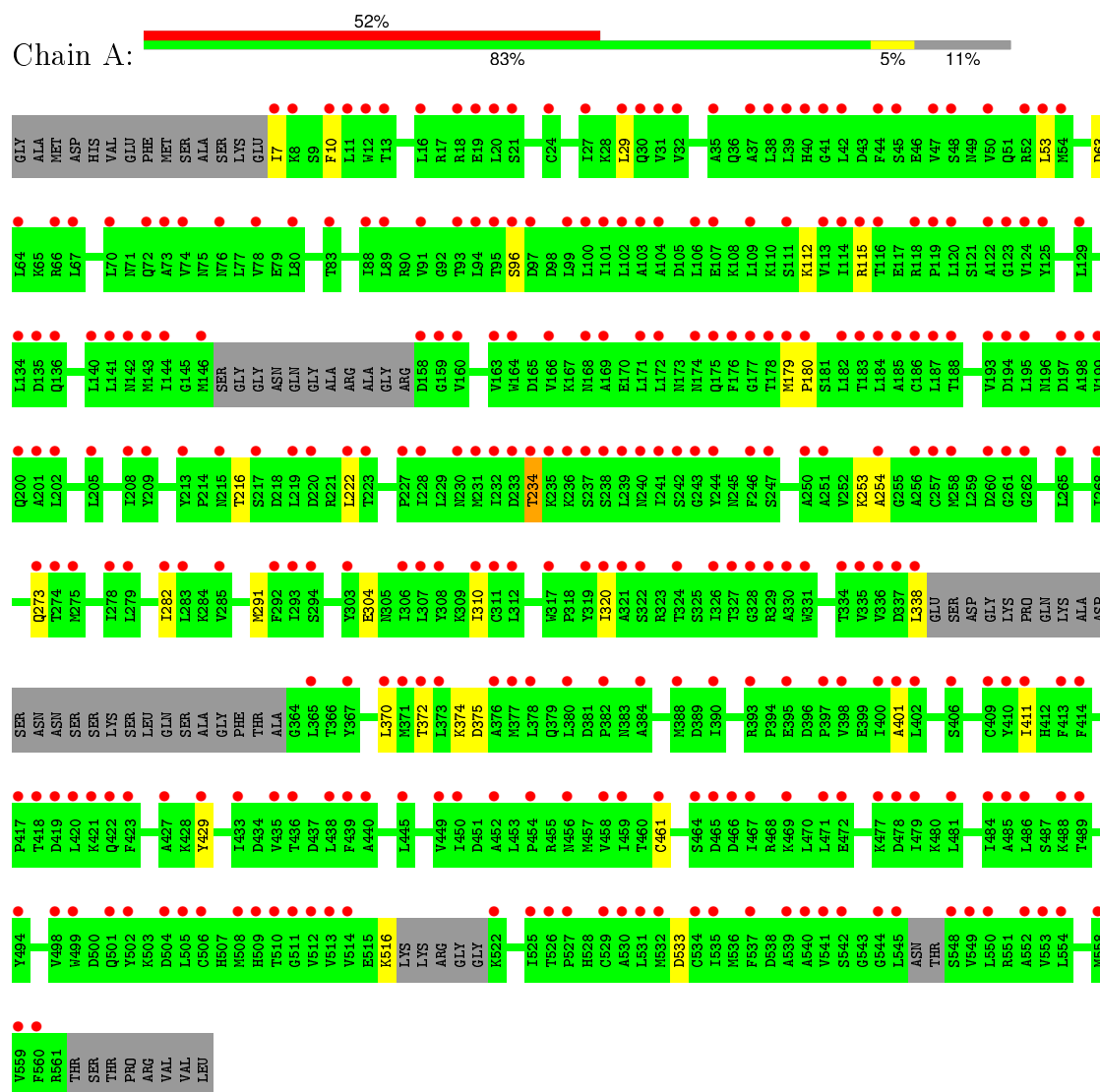
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	175	Total	O	0	0
			175	175		
3	B	192	Total	O	0	0
			192	192		
3	C	108	Total	O	0	0
			108	108		

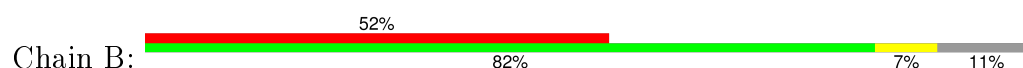
3 Residue-property plots

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: Nucleoprotein



• Molecule 1: Nucleoprotein







4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	176.82Å 176.82Å 56.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	153.18 – 1.79 47.59 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (153.18-1.79) 99.9 (47.59-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.6.0081	Depositor
R, R_{free}	0.178 , 0.196 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.2	EDS
Estimated twinning fraction	0.348 for H, K, L 0.652 for K, H, -L 0.008 for -h,-k,l 0.021 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.348 for H, K, L 0.652 for K, H, -L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 184177 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12477	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.61	1/4070 (0.0%)	0.71	1/5493 (0.0%)
1	B	0.64	0/4084	0.76	4/5513 (0.1%)
1	C	0.57	0/4015	0.68	1/5418 (0.0%)
All	All	0.61	1/12169 (0.0%)	0.72	6/16424 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	461	CYS	CB-SG	-8.33	1.68	1.82

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	MET	CG-SD-CE	-13.53	78.55	100.20
1	B	115	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	B	115	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	461	CYS	CB-CA-C	-5.73	98.95	110.40
1	B	500	ASP	CB-CG-OD1	5.07	122.87	118.30
1	C	500	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

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	4011	0	4085	22	0
1	B	4027	0	4098	28	0
1	C	3961	0	4019	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	175	0	0	3	0
3	B	192	0	0	2	0
3	C	108	0	0	2	0
All	All	12477	0	12202	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 4.

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:C:219:LEU:HD23	1:C:234:THR:HG22	1.37	1.01
1:C:24:CYS:SG	1:C:268:ILE:HG12	2.17	0.85
1:B:502:TYR:CE1	1:B:550:LEU:HD13	2.16	0.80
1:C:265:LEU:O	1:C:268:ILE:HG13	1.82	0.78
1:C:408:GLY:O	1:C:550:LEU:HA	1.83	0.78
1:C:533:ASP:OD2	3:C:655:HOH:O	2.01	0.78
1:C:397:PRO:HB2	1:C:400:ILE:HD11	1.75	0.69
1:C:219:LEU:HD23	1:C:234:THR:CG2	2.19	0.66
1:B:502:TYR:CE1	1:B:550:LEU:CD1	2.79	0.66
1:A:533:ASP:OD2	3:A:728:HOH:O	2.13	0.65
1:C:219:LEU:CD2	1:C:234:THR:HG22	2.22	0.63
1:A:7:ILE:HG23	1:A:10:PHE:H	1.65	0.62
1:C:112:LYS:HE3	1:C:304:GLU:OE1	2.00	0.61
1:C:515:GLU:HG3	1:C:525:ILE:HD13	1.82	0.61
1:A:216:THR:HG23	1:A:234:THR:HG21	1.86	0.57
1:C:365:LEU:HD22	1:C:370:LEU:HD23	1.86	0.57
1:C:387:TRP:CH2	1:C:484:ILE:HG12	2.41	0.56
1:C:389:ASP:OD1	3:C:655:HOH:O	2.18	0.56
1:B:212:LYS:HE3	1:B:218:ASP:OD2	2.07	0.54
1:A:115:ARG:HD2	1:A:375:ASP:OD2	2.08	0.54
1:B:49:ASN:O	1:B:53:LEU:HG	2.08	0.53
1:B:365:LEU:HD22	1:B:370:LEU:HD23	1.88	0.53
1:B:78:VAL:O	1:B:81:LYS:HE2	2.09	0.52
1:A:179:MET:HG3	1:A:320:ILE:O	2.10	0.52
1:B:215:ASN:HB2	3:B:681:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:LYS:NZ	1:C:298:GLY:O	2.44	0.50
1:C:442:GLN:NE2	1:C:443:PRO:HD2	2.25	0.50
1:C:306:ILE:HG12	1:C:310:ILE:HD12	1.94	0.50
1:C:179:MET:HG3	1:C:320:ILE:O	2.10	0.50
1:C:386:THR:HB	1:C:459:ILE:HD13	1.93	0.50
1:C:265:LEU:HD22	1:C:268:ILE:HD11	1.92	0.50
1:A:216:THR:HA	1:A:234:THR:HG21	1.94	0.50
1:A:370:LEU:HG	1:A:374:LYS:HE3	1.92	0.49
1:B:484:ILE:CG2	1:B:486:LEU:HG	2.42	0.49
1:A:273:GLN:HG2	3:A:646:HOH:O	2.12	0.49
1:B:502:TYR:HE1	1:B:550:LEU:HD13	1.71	0.49
1:C:219:LEU:HD21	1:C:232:ILE:HB	1.96	0.48
1:B:216:THR:HG22	1:B:234:THR:CB	2.43	0.48
1:B:126:MET:CE	1:B:138:ARG:HG3	2.44	0.47
1:C:10:PHE:CE2	1:C:14:GLN:HG3	2.49	0.47
1:B:216:THR:HG22	1:B:234:THR:HB	1.95	0.47
1:C:399:GLU:O	1:C:400:ILE:HD13	2.15	0.46
1:C:454:PRO:HD2	1:C:457:MET:SD	2.55	0.46
1:C:212:LYS:HE2	1:C:218:ASP:OD2	2.16	0.46
1:C:112:LYS:HE2	1:C:296:THR:O	2.16	0.46
1:A:222:LEU:HD23	1:B:207:LEU:HD13	1.98	0.46
1:A:96:SER:OG	1:A:338:LEU:HD21	2.16	0.45
1:C:380:LEU:HD11	1:C:411:ILE:HD11	1.98	0.45
1:A:429:TYR:CZ	1:A:516:LYS:HE2	2.52	0.45
1:C:462:GLN:HB2	1:C:484:ILE:HD11	1.98	0.45
1:C:484:ILE:HG13	1:C:484:ILE:H	1.71	0.44
1:C:209:TYR:HA	1:C:212:LYS:O	2.18	0.44
1:B:180:PRO:HB3	1:B:254:ALA:HA	1.99	0.44
1:A:53:LEU:HD22	1:A:63:ASP:OD1	2.18	0.44
1:A:115:ARG:HD3	1:A:372:THR:HA	2.00	0.44
1:A:338:LEU:HD11	3:A:654:HOH:O	2.18	0.44
1:B:484:ILE:HG22	1:B:486:LEU:HG	2.00	0.44
1:B:282:ILE:HD11	1:B:310:ILE:CD1	2.48	0.43
1:C:443:PRO:HG3	1:C:561:ARG:HH21	1.83	0.43
1:B:110:LYS:NZ	3:B:695:HOH:O	2.51	0.43
1:C:387:TRP:HH2	1:C:484:ILE:HG12	1.84	0.42
1:B:387:TRP:CH2	1:B:484:ILE:HG13	2.54	0.42
1:B:502:TYR:CZ	1:B:550:LEU:HD11	2.54	0.42
1:A:180:PRO:HG3	1:A:253:LYS:HG2	2.01	0.42
1:A:216:THR:CB	1:A:234:THR:HG21	2.50	0.42
1:B:460:THR:CG2	1:B:484:ILE:HG12	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:PRO:HB3	1:A:254:ALA:HA	2.01	0.42
1:B:484:ILE:HD13	1:B:484:ILE:HA	1.80	0.42
1:A:112:LYS:HD2	1:A:304:GLU:OE2	2.19	0.42
1:A:401:ALA:HA	1:A:411:ILE:O	2.20	0.41
1:A:29:LEU:HD23	1:A:29:LEU:C	2.41	0.41
1:C:32:VAL:O	1:C:36:GLN:HG3	2.21	0.41
1:B:487:SER:O	1:B:491:SER:HB2	2.20	0.41
1:A:282:ILE:HD11	1:A:310:ILE:CD1	2.51	0.41
1:A:291:MET:O	1:C:477:LYS:NZ	2.53	0.41
1:C:488:LYS:HD3	1:C:488:LYS:HA	1.80	0.41
1:C:53:LEU:HD22	1:C:63:ASP:OD1	2.20	0.41
1:B:8:LYS:HB2	1:B:9:SER:H	1.68	0.41
1:C:46:GLU:OE2	1:C:66:ARG:HD2	2.21	0.41
1:B:44:PHE:CG	1:B:189:LYS:HG2	2.56	0.41
1:B:221:ARG:HD3	1:B:221:ARG:HA	1.91	0.41
1:B:235:LYS:HG3	1:B:236:LYS:N	2.36	0.41
1:B:15:SER:CB	1:B:289:LEU:HD11	2.51	0.40
1:B:550:LEU:N	1:B:550:LEU:HD12	2.35	0.40
1:C:78:VAL:O	1:C:81:LYS:HE3	2.21	0.40
1:C:158:ASP:HB3	1:C:159:GLY:H	1.67	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	503/577 (87%)	496 (99%)	7 (1%)	0	100	100
1	B	507/577 (88%)	502 (99%)	5 (1%)	0	100	100
1	C	492/577 (85%)	483 (98%)	8 (2%)	1 (0%)	52	35
All	All	1502/1731 (87%)	1481 (99%)	20 (1%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	550	LEU

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	450/498 (90%)	449 (100%)	1 (0%)	95	94
1	B	452/498 (91%)	448 (99%)	4 (1%)	84	80
1	C	444/498 (89%)	436 (98%)	8 (2%)	66	54
All	All	1346/1494 (90%)	1333 (99%)	13 (1%)	82	77

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	THR
1	B	8	LYS
1	B	158	ASP
1	B	464	SER
1	B	484	ILE
1	C	11	LEU
1	C	212	LYS
1	C	224	GLN
1	C	233	ASP
1	C	263	ASN
1	C	464	SER
1	C	473	SER
1	C	549	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	501	GLN
1	B	132	GLN

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 3 ligands modelled in this entry, 3 are 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 [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	512/577 (88%)	2.33	298 (58%) 0 0	31, 33, 45, 66	0
1	B	515/577 (89%)	2.43	300 (58%) 0 0	31, 33, 45, 58	0
1	C	506/577 (87%)	2.57	337 (66%) 0 0	32, 36, 49, 65	0
All	All	1533/1731 (88%)	2.44	935 (60%) 0 0	31, 34, 47, 66	0

All (935) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	547	THR	8.9
1	A	7	ILE	8.2
1	C	88	ILE	7.2
1	C	549	VAL	7.1
1	B	338	LEU	7.0
1	C	260	ASP	6.8
1	A	338	LEU	6.8
1	C	439	PHE	6.7
1	B	548	SER	6.5
1	C	219	LEU	6.3
1	B	549	VAL	6.2
1	B	546	ASN	6.1
1	A	467	ILE	6.1
1	A	114	ILE	5.9
1	C	473	SER	5.7
1	B	147	SER	5.6
1	A	236	LYS	5.5
1	C	223	THR	5.5
1	C	132	GLN	5.5
1	A	548	SER	5.4
1	B	456	ASN	5.3
1	C	556	ARG	5.3
1	B	542	SER	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	158	ASP	5.3
1	B	262	GLY	5.3
1	B	172	LEU	5.2
1	C	367	TYR	5.2
1	C	516	LYS	5.1
1	C	465	ASP	5.0
1	C	413	PHE	5.0
1	B	421	LYS	5.0
1	C	225	SER	5.0
1	A	549	VAL	5.0
1	C	486	LEU	5.0
1	C	467	ILE	4.9
1	C	83	THR	4.9
1	B	484	ILE	4.9
1	B	260	ASP	4.8
1	B	47	VAL	4.8
1	B	114	ILE	4.8
1	B	411	ILE	4.8
1	C	259	LEU	4.7
1	B	311	CYS	4.7
1	B	109	LEU	4.7
1	A	484	ILE	4.7
1	C	539	ALA	4.7
1	A	42	LEU	4.7
1	C	464	SER	4.7
1	B	176	PHE	4.7
1	A	439	PHE	4.6
1	B	233	ASP	4.6
1	C	100	LEU	4.6
1	C	370	LEU	4.6
1	C	545	LEU	4.6
1	B	120	LEU	4.6
1	C	186	CYS	4.6
1	B	171	LEU	4.5
1	A	529	CYS	4.5
1	A	113	VAL	4.5
1	C	224	GLN	4.5
1	C	32	VAL	4.4
1	C	91	VAL	4.4
1	C	24	CYS	4.4
1	A	235	LYS	4.4
1	A	234	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	250	ALA	4.4
1	C	470	LEU	4.4
1	C	131	SER	4.4
1	A	320	ILE	4.4
1	B	39	LEU	4.3
1	B	42	LEU	4.3
1	B	106	LEU	4.3
1	C	285	VAL	4.3
1	A	186	CYS	4.3
1	B	50	VAL	4.3
1	B	124	VAL	4.3
1	B	183	THR	4.3
1	C	233	ASP	4.3
1	B	307	LEU	4.3
1	C	447	SER	4.2
1	A	102	LEU	4.2
1	A	244	TYR	4.2
1	B	378	LEU	4.2
1	B	529	CYS	4.2
1	B	27	ILE	4.2
1	B	517	LYS	4.2
1	C	402	LEU	4.2
1	C	550	LEU	4.2
1	B	559	VAL	4.2
1	C	271	SER	4.2
1	C	230	ASN	4.2
1	A	331	TRP	4.1
1	C	232	ILE	4.1
1	A	24	CYS	4.1
1	A	38	LEU	4.1
1	A	172	LEU	4.1
1	B	11	LEU	4.1
1	B	70	LEU	4.1
1	B	370	LEU	4.1
1	C	427	ALA	4.1
1	C	12	TRP	4.1
1	B	373	LEU	4.1
1	C	461	CYS	4.1
1	A	227	PRO	4.1
1	B	525	ILE	4.1
1	A	445	LEU	4.1
1	B	534	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	227	PRO	4.0
1	B	64	LEU	4.0
1	B	182	LEU	4.0
1	C	196	ASN	4.0
1	C	144	ILE	4.0
1	C	365	LEU	4.0
1	C	40	HIS	4.0
1	B	512	VAL	4.0
1	A	311	CYS	4.0
1	A	109	LEU	4.0
1	A	47	VAL	4.0
1	B	449	VAL	4.0
1	C	78	VAL	4.0
1	C	386	THR	4.0
1	A	471	LEU	4.0
1	B	122	ALA	4.0
1	A	559	VAL	3.9
1	C	25	SER	3.9
1	C	178	THR	3.9
1	B	413	PHE	3.9
1	B	535	ILE	3.9
1	C	335	VAL	3.9
1	C	541	VAL	3.9
1	B	164	TRP	3.9
1	C	397	PRO	3.9
1	B	186	CYS	3.9
1	A	144	ILE	3.9
1	B	244	TYR	3.9
1	B	236	LYS	3.9
1	C	429	TYR	3.8
1	A	106	LEU	3.8
1	B	179	MET	3.8
1	B	331	TRP	3.8
1	C	226	HIS	3.8
1	B	140	LEU	3.8
1	B	312	LEU	3.8
1	B	241	ILE	3.8
1	A	261	GLY	3.8
1	B	166	VAL	3.8
1	B	439	PHE	3.8
1	C	23	TYR	3.8
1	A	456	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	44	PHE	3.8
1	A	176	PHE	3.8
1	C	529	CYS	3.8
1	B	401	ALA	3.7
1	B	530	ALA	3.7
1	B	223	THR	3.7
1	B	489	THR	3.7
1	C	241	ILE	3.7
1	B	463	GLY	3.7
1	C	44	PHE	3.7
1	C	409	CYS	3.7
1	B	499	TRP	3.7
1	C	213	TYR	3.7
1	A	120	LEU	3.7
1	A	531	LEU	3.7
1	C	449	VAL	3.7
1	A	254	ALA	3.7
1	A	140	LEU	3.7
1	B	187	LEU	3.7
1	C	484	ILE	3.7
1	C	480	LYS	3.7
1	B	158	ASP	3.7
1	A	485	ALA	3.7
1	C	201	ALA	3.7
1	C	257	CYS	3.7
1	C	474	GLN	3.7
1	C	557	ASP	3.7
1	B	184	LEU	3.7
1	A	88	ILE	3.7
1	C	208	ILE	3.7
1	A	213	TYR	3.6
1	B	367	TYR	3.6
1	C	140	LEU	3.6
1	C	435	VAL	3.6
1	A	232	ILE	3.6
1	B	393	ARG	3.6
1	A	371	MET	3.6
1	C	421	LYS	3.6
1	B	216	THR	3.6
1	C	489	THR	3.6
1	B	445	LEU	3.6
1	C	487	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	505	LEU	3.6
1	B	113	VAL	3.6
1	B	376	ALA	3.6
1	C	199	VAL	3.6
1	B	144	ILE	3.6
1	B	293	ILE	3.6
1	B	467	ILE	3.6
1	C	263	ASN	3.6
1	A	499	TRP	3.6
1	C	387	TRP	3.6
1	B	410	TYR	3.6
1	C	26	ASN	3.6
1	A	486	LEU	3.6
1	B	74	VAL	3.6
1	C	534	CYS	3.6
1	B	400	ILE	3.6
1	C	469	LYS	3.6
1	A	418	THR	3.6
1	B	372	THR	3.6
1	B	44	PHE	3.6
1	A	146	MET	3.6
1	A	440	ALA	3.6
1	A	303	TYR	3.6
1	B	38	LEU	3.6
1	B	243	GLY	3.6
1	B	101	ILE	3.6
1	C	311	CYS	3.6
1	C	414	PHE	3.5
1	C	200	GLN	3.5
1	B	531	LEU	3.5
1	C	270	VAL	3.5
1	C	471	LEU	3.5
1	A	158	ASP	3.5
1	C	278	ILE	3.5
1	A	250	ALA	3.5
1	B	35	ALA	3.5
1	C	485	ALA	3.5
1	A	239	LEU	3.5
1	A	307	LEU	3.5
1	B	398	VAL	3.5
1	B	554	LEU	3.5
1	C	113	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	183	THR	3.5
1	C	265	LEU	3.5
1	C	107	GLU	3.5
1	B	461	CYS	3.5
1	A	545	LEU	3.5
1	B	53	LEU	3.5
1	C	229	LEU	3.5
1	C	512	VAL	3.5
1	C	96	SER	3.5
1	A	27	ILE	3.5
1	A	241	ILE	3.5
1	C	185	ALA	3.5
1	C	504	ASP	3.5
1	C	239	LEU	3.5
1	B	477	LYS	3.4
1	B	433	ILE	3.4
1	A	163	VAL	3.4
1	A	438	LEU	3.4
1	B	207	LEU	3.4
1	C	250	ALA	3.4
1	B	246	PHE	3.4
1	B	308	TYR	3.4
1	B	282	ILE	3.4
1	A	285	VAL	3.4
1	A	398	VAL	3.4
1	B	514	VAL	3.4
1	A	182	LEU	3.4
1	B	471	LEU	3.4
1	C	159	GLY	3.4
1	C	244	TYR	3.4
1	A	12	TRP	3.4
1	B	217	SER	3.4
1	A	91	VAL	3.4
1	A	53	LEU	3.4
1	A	409	CYS	3.4
1	B	279	LEU	3.4
1	B	224	GLN	3.4
1	A	400	ILE	3.4
1	B	310	ILE	3.4
1	B	320	ILE	3.4
1	C	390	ILE	3.4
1	C	459	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	122	ALA	3.4
1	C	287	LYS	3.4
1	B	526	THR	3.4
1	A	32	VAL	3.3
1	A	74	VAL	3.3
1	B	67	LEU	3.3
1	B	283	LEU	3.3
1	C	184	LEU	3.3
1	B	257	CYS	3.3
1	C	310	ILE	3.3
1	C	463	GLY	3.3
1	C	448	ALA	3.3
1	A	116	THR	3.3
1	C	336	VAL	3.3
1	A	21	SER	3.3
1	A	365	LEU	3.3
1	B	129	LEU	3.3
1	C	202	LEU	3.3
1	A	539	ALA	3.3
1	C	530	ALA	3.3
1	A	525	ILE	3.3
1	C	411	ILE	3.3
1	C	274	THR	3.3
1	C	407	SER	3.3
1	A	64	LEU	3.3
1	A	219	LEU	3.3
1	B	319	TYR	3.3
1	A	413	PHE	3.3
1	A	526	THR	3.3
1	B	116	THR	3.3
1	B	465	ASP	3.3
1	A	370	LEU	3.3
1	B	89	LEU	3.3
1	C	67	LEU	3.3
1	A	95	THR	3.3
1	C	296	THR	3.3
1	A	101	ILE	3.3
1	C	320	ILE	3.3
1	A	50	VAL	3.2
1	B	427	ALA	3.2
1	A	11	LEU	3.2
1	B	402	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	209	TYR	3.2
1	B	268	ILE	3.2
1	C	228	ILE	3.2
1	C	433	ILE	3.2
1	A	237	SER	3.2
1	B	103	ALA	3.2
1	C	552	ALA	3.2
1	A	335	VAL	3.2
1	C	163	VAL	3.2
1	C	455	ARG	3.2
1	B	453	LEU	3.2
1	A	410	TYR	3.2
1	C	317	TRP	3.2
1	C	403	TYR	3.2
1	C	237	SER	3.2
1	A	292	PHE	3.2
1	A	306	ILE	3.2
1	A	310	ILE	3.2
1	A	326	ILE	3.2
1	C	101	ILE	3.2
1	C	292	PHE	3.2
1	C	423	PHE	3.2
1	A	8	LYS	3.2
1	B	24	CYS	3.2
1	A	449	VAL	3.2
1	A	67	LEU	3.2
1	B	102	LEU	3.2
1	C	283	LEU	3.2
1	C	325	SER	3.2
1	C	542	SER	3.2
1	B	303	TYR	3.2
1	B	552	ALA	3.2
1	A	230	ASN	3.2
1	B	10	PHE	3.2
1	C	456	ASN	3.2
1	C	130	SER	3.2
1	C	368	SER	3.2
1	A	80	LEU	3.2
1	A	141	LEU	3.2
1	A	378	LEU	3.2
1	B	239	LEU	3.2
1	B	365	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	94	LEU	3.2
1	C	182	LEU	3.2
1	B	263	ASN	3.2
1	B	235	LYS	3.2
1	A	228	ILE	3.2
1	A	164	TRP	3.1
1	A	414	PHE	3.1
1	C	57	GLU	3.1
1	A	177	GLY	3.1
1	A	124	VAL	3.1
1	A	240	ASN	3.1
1	B	409	CYS	3.1
1	A	312	LEU	3.1
1	B	229	LEU	3.1
1	B	104	ALA	3.1
1	B	48	SER	3.1
1	B	96	SER	3.1
1	C	451	ASP	3.1
1	A	282	ILE	3.1
1	C	75	ASN	3.1
1	C	92	GLY	3.1
1	C	543	GLY	3.1
1	C	164	TRP	3.1
1	C	499	TRP	3.1
1	B	371	MET	3.1
1	B	324	THR	3.1
1	C	116	THR	3.1
1	C	366	THR	3.1
1	A	89	LEU	3.1
1	B	94	LEU	3.1
1	B	380	LEU	3.1
1	B	505	LEU	3.1
1	C	307	LEU	3.1
1	A	238	SER	3.1
1	B	469	LYS	3.1
1	C	477	LYS	3.1
1	B	49	ASN	3.1
1	A	278	ILE	3.1
1	C	258	MET	3.1
1	C	327	THR	3.1
1	C	560	PHE	3.1
1	A	512	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	376	ALA	3.1
1	A	427	ALA	3.1
1	A	171	LEU	3.1
1	C	29	LEU	3.1
1	B	208	ILE	3.1
1	C	326	ILE	3.1
1	C	272	PRO	3.1
1	A	35	ALA	3.1
1	A	552	ALA	3.1
1	C	10	PHE	3.1
1	C	31	VAL	3.1
1	C	124	VAL	3.1
1	C	252	VAL	3.1
1	C	458	VAL	3.1
1	A	194	ASP	3.1
1	A	465	ASP	3.1
1	B	516	LYS	3.1
1	A	317	TRP	3.1
1	C	11	LEU	3.1
1	B	111	SER	3.1
1	C	231	MET	3.1
1	C	62	ASN	3.1
1	A	308	TYR	3.0
1	C	319	TYR	3.0
1	A	293	ILE	3.0
1	B	553	VAL	3.0
1	B	464	SER	3.0
1	A	178	THR	3.0
1	C	34	ASP	3.0
1	A	321	ALA	3.0
1	B	330	ALA	3.0
1	C	114	ILE	3.0
1	C	400	ILE	3.0
1	A	553	VAL	3.0
1	B	513	VAL	3.0
1	C	47	VAL	3.0
1	C	160	VAL	3.0
1	A	550	LEU	3.0
1	C	16	LEU	3.0
1	C	324	THR	3.0
1	B	201	ALA	3.0
1	C	406	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	433	ILE	3.0
1	B	450	ILE	3.0
1	C	393	ARG	3.0
1	A	31	VAL	3.0
1	B	328	GLY	3.0
1	A	246	PHE	3.0
1	A	99	LEU	3.0
1	C	187	LEU	3.0
1	C	438	LEU	3.0
1	A	111	SER	3.0
1	A	275	MET	3.0
1	A	422	GLN	3.0
1	B	200	GLN	3.0
1	B	125	TYR	3.0
1	A	257	CYS	3.0
1	C	97	ASP	3.0
1	B	161	VAL	3.0
1	B	199	VAL	3.0
1	B	121	SER	3.0
1	C	90	ARG	3.0
1	C	109	LEU	3.0
1	A	384	ALA	3.0
1	C	35	ALA	3.0
1	C	234	THR	2.9
1	B	12	TRP	2.9
1	C	450	ILE	2.9
1	C	424	LYS	2.9
1	A	200	GLN	2.9
1	B	458	VAL	2.9
1	C	506	CYS	2.9
1	A	29	LEU	2.9
1	A	202	LEU	2.9
1	A	279	LEU	2.9
1	C	378	LEU	2.9
1	C	452	ALA	2.9
1	C	481	LEU	2.9
1	A	10	PHE	2.9
1	B	210	THR	2.9
1	C	410	TYR	2.9
1	C	27	ILE	2.9
1	A	251	ALA	2.9
1	A	530	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	485	ALA	2.9
1	A	477	LYS	2.9
1	A	70	LEU	2.9
1	C	95	THR	2.9
1	B	543	GLY	2.9
1	B	429	TYR	2.9
1	A	397	PRO	2.9
1	A	401	ALA	2.9
1	B	37	ALA	2.9
1	C	540	ALA	2.9
1	B	510	THR	2.9
1	C	120	LEU	2.9
1	C	141	LEU	2.9
1	B	414	PHE	2.9
1	B	169	ALA	2.9
1	A	45	SER	2.9
1	B	252	VAL	2.9
1	C	559	VAL	2.9
1	A	188	THR	2.9
1	A	100	LEU	2.8
1	B	248	LEU	2.8
1	C	215	ASN	2.8
1	C	553	VAL	2.8
1	C	328	GLY	2.8
1	C	466	ASP	2.8
1	A	195	LEU	2.8
1	C	106	LEU	2.8
1	C	373	LEU	2.8
1	C	331	TRP	2.8
1	A	185	ALA	2.8
1	B	198	ALA	2.8
1	A	233	ASP	2.8
1	C	418	THR	2.8
1	C	206	GLY	2.8
1	A	513	VAL	2.8
1	B	232	ILE	2.8
1	A	134	LEU	2.8
1	A	554	LEU	2.8
1	B	29	LEU	2.8
1	B	420	LEU	2.8
1	B	45	SER	2.8
1	A	472	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	335	VAL	2.8
1	A	450	ILE	2.8
1	C	282	ILE	2.8
1	C	179	MET	2.8
1	A	540	ALA	2.8
1	B	177	GLY	2.8
1	B	202	LEU	2.8
1	C	38	LEU	2.8
1	B	273	GLN	2.8
1	A	327	THR	2.8
1	C	203	THR	2.8
1	B	21	SER	2.8
1	A	143	MET	2.8
1	B	213	TYR	2.7
1	B	403	TYR	2.7
1	B	185	ALA	2.7
1	B	211	ALA	2.7
1	A	510	THR	2.7
1	B	486	LEU	2.7
1	C	89	LEU	2.7
1	C	171	LEU	2.7
1	C	242	SER	2.7
1	B	32	VAL	2.7
1	B	274	THR	2.7
1	C	104	ALA	2.7
1	C	181	SER	2.7
1	C	268	ILE	2.7
1	C	502	TYR	2.7
1	A	393	ARG	2.7
1	A	560	PHE	2.7
1	A	489	THR	2.7
1	A	166	VAL	2.7
1	A	187	LEU	2.7
1	A	205	LEU	2.7
1	A	179	MET	2.7
1	A	328	GLY	2.7
1	A	377	MET	2.7
1	B	249	GLY	2.7
1	A	522	LYS	2.7
1	A	382	PRO	2.7
1	B	327	THR	2.7
1	B	436	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	510	THR	2.7
1	B	193	VAL	2.7
1	A	411	ILE	2.7
1	A	479	ILE	2.7
1	A	373	LEU	2.7
1	A	420	LEU	2.7
1	B	141	LEU	2.7
1	B	205	LEU	2.7
1	A	260	ASP	2.7
1	A	395	GLU	2.7
1	C	419	ASP	2.7
1	A	73	ALA	2.7
1	B	497	ALA	2.7
1	C	251	ALA	2.7
1	A	30	GLN	2.7
1	A	136	GLN	2.7
1	A	262	GLY	2.6
1	B	511	GLY	2.6
1	C	21	SER	2.6
1	A	220	ASP	2.6
1	C	535	ILE	2.6
1	A	319	TYR	2.6
1	B	494	TYR	2.6
1	B	52	ARG	2.6
1	C	58	ARG	2.6
1	A	506	CYS	2.6
1	A	534	CYS	2.6
1	C	119	PRO	2.6
1	C	177	GLY	2.6
1	A	322	SER	2.6
1	C	322	SER	2.6
1	B	8	LYS	2.6
1	A	336	VAL	2.6
1	C	50	VAL	2.6
1	B	537	PHE	2.6
1	C	303	TYR	2.6
1	B	251	ALA	2.6
1	A	464	SER	2.6
1	B	447	SER	2.6
1	C	238	SER	2.6
1	A	558	MET	2.6
1	A	273	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	183	THR	2.6
1	A	243	GLY	2.6
1	A	478	ASP	2.6
1	B	83	THR	2.6
1	A	104	ALA	2.6
1	B	390	ILE	2.6
1	B	479	ILE	2.6
1	C	401	ALA	2.6
1	A	39	LEU	2.6
1	A	454	PRO	2.6
1	A	160	VAL	2.6
1	A	435	VAL	2.6
1	C	87	SER	2.6
1	C	513	VAL	2.6
1	A	330	ALA	2.6
1	C	384	ALA	2.6
1	A	54	MET	2.6
1	A	535	ILE	2.6
1	C	371	MET	2.6
1	A	367	TYR	2.6
1	B	195	LEU	2.6
1	C	42	LEU	2.6
1	B	66	ARG	2.6
1	B	523	GLU	2.6
1	A	37	ALA	2.5
1	A	498	VAL	2.5
1	A	541	VAL	2.5
1	C	166	VAL	2.5
1	C	443	PRO	2.5
1	A	123	GLY	2.5
1	A	283	LEU	2.5
1	A	481	LEU	2.5
1	A	505	LEU	2.5
1	B	20	LEU	2.5
1	B	209	TYR	2.5
1	C	554	LEU	2.5
1	A	406	SER	2.5
1	B	247	SER	2.5
1	A	372	THR	2.5
1	A	419	ASP	2.5
1	B	18	ARG	2.5
1	B	115	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	169	ALA	2.5
1	A	461	CYS	2.5
1	C	73	ALA	2.5
1	C	139	ALA	2.5
1	A	199	VAL	2.5
1	A	514	VAL	2.5
1	C	302	PRO	2.5
1	A	19	GLU	2.5
1	B	305	ASN	2.5
1	B	278	ILE	2.5
1	B	326	ILE	2.5
1	C	483	ASP	2.5
1	B	545	LEU	2.5
1	A	125	TYR	2.5
1	C	93	THR	2.5
1	A	198	ALA	2.5
1	B	73	ALA	2.5
1	C	180	PRO	2.5
1	A	13	THR	2.5
1	B	77	LEU	2.5
1	B	134	LEU	2.5
1	C	207	LEU	2.5
1	A	231	MET	2.5
1	B	54	MET	2.5
1	B	119	PRO	2.5
1	B	557	ASP	2.5
1	C	217	SER	2.5
1	A	469	LYS	2.5
1	B	163	VAL	2.5
1	C	74	VAL	2.5
1	A	223	THR	2.5
1	B	366	THR	2.5
1	B	506	CYS	2.5
1	A	142	ASN	2.5
1	A	115	ARG	2.5
1	B	118	ARG	2.5
1	B	466	ASP	2.5
1	C	555	PRO	2.5
1	A	129	LEU	2.5
1	A	390	ILE	2.5
1	B	228	ILE	2.5
1	B	508	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	39	LEU	2.5
1	C	172	LEU	2.5
1	C	531	LEU	2.5
1	A	96	SER	2.5
1	A	494	TYR	2.4
1	B	448	ALA	2.5
1	B	539	ALA	2.5
1	C	494	TYR	2.4
1	A	97	ASP	2.4
1	A	324	THR	2.4
1	C	460	THR	2.4
1	A	193	VAL	2.4
1	A	94	LEU	2.4
1	A	222	LEU	2.4
1	B	438	LEU	2.4
1	C	53	LEU	2.4
1	B	504	ASP	2.4
1	C	66	ARG	2.4
1	C	125	TYR	2.4
1	C	176	PHE	2.4
1	B	142	ASN	2.4
1	C	561	ARG	2.4
1	B	387	TRP	2.4
1	C	273	GLN	2.4
1	C	422	GLN	2.4
1	B	227	PRO	2.4
1	C	527	PRO	2.4
1	B	242	SER	2.4
1	A	508	MET	2.4
1	A	103	ALA	2.4
1	C	142	ASN	2.4
1	C	440	ALA	2.4
1	A	175	GLN	2.4
1	A	380	LEU	2.4
1	C	306	ILE	2.4
1	C	420	LEU	2.4
1	B	318	PRO	2.4
1	C	290	GLY	2.4
1	A	135	ASP	2.4
1	A	532	MET	2.4
1	C	143	MET	2.4
1	B	215	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	514	VAL	2.4
1	A	256	ALA	2.4
1	A	421	LYS	2.4
1	C	334	THR	2.4
1	C	430	SER	2.4
1	C	446	THR	2.4
1	A	268	ILE	2.4
1	B	306	ILE	2.4
1	C	135	ASP	2.4
1	C	126	MET	2.4
1	C	508	MET	2.4
1	C	537	PHE	2.4
1	C	133	GLN	2.4
1	B	498	VAL	2.4
1	C	161	VAL	2.4
1	A	197	ASP	2.4
1	A	215	ASN	2.4
1	A	209	TYR	2.3
1	A	537	PHE	2.3
1	A	242	SER	2.3
1	B	9	SER	2.3
1	B	51	GLN	2.3
1	B	496	ASN	2.3
1	B	317	TRP	2.3
1	C	210	THR	2.3
1	B	220	ASP	2.3
1	B	265	LEU	2.3
1	C	205	LEU	2.3
1	A	107	GLU	2.3
1	A	72	GLN	2.3
1	B	261	GLY	2.3
1	B	406	SER	2.3
1	A	423	PHE	2.3
1	B	527	PRO	2.3
1	C	246	PHE	2.3
1	B	93	THR	2.3
1	A	458	VAL	2.3
1	C	193	VAL	2.3
1	C	457	MET	2.3
1	A	217	SER	2.3
1	A	184	LEU	2.3
1	C	70	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	289	LEU	2.3
1	C	318	PRO	2.3
1	C	54	MET	2.3
1	C	398	VAL	2.3
1	A	159	GLY	2.3
1	B	191	GLY	2.3
1	B	444	GLY	2.3
1	C	243	GLY	2.3
1	C	515	GLU	2.3
1	C	18	ARG	2.3
1	B	419	ASP	2.3
1	A	452	ALA	2.3
1	B	540	ALA	2.3
1	C	497	ALA	2.3
1	A	208	ILE	2.3
1	B	65	LYS	2.3
1	B	178	THR	2.3
1	A	258	MET	2.3
1	B	231	MET	2.3
1	C	305	ASN	2.3
1	A	18	ARG	2.3
1	B	123	GLY	2.3
1	B	423	PHE	2.3
1	C	262	GLY	2.3
1	A	180	PRO	2.3
1	C	436	THR	2.2
1	B	99	LEU	2.2
1	C	76	ASN	2.2
1	C	195	LEU	2.2
1	C	380	LEU	2.2
1	C	468	ARG	2.2
1	B	558	MET	2.2
1	A	542	SER	2.2
1	B	451	ASP	2.2
1	C	490	ASP	2.2
1	B	23	TYR	2.2
1	B	285	VAL	2.2
1	B	292	PHE	2.2
1	A	93	THR	2.2
1	A	436	THR	2.2
1	B	254	ALA	2.2
1	B	321	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	446	THR	2.2
1	A	294	SER	2.2
1	B	258	MET	2.2
1	B	377	MET	2.2
1	C	8	LYS	2.2
1	A	16	LEU	2.2
1	A	265	LEU	2.2
1	A	511	GLY	2.2
1	A	544	GLY	2.2
1	B	299	GLU	2.2
1	B	472	GLU	2.2
1	C	22	GLY	2.2
1	C	79	GLU	2.2
1	C	425	GLN	2.2
1	A	174	ASN	2.2
1	A	502	TYR	2.2
1	B	336	VAL	2.2
1	B	188	THR	2.2
1	B	296	THR	2.2
1	B	532	MET	2.2
1	B	536	MET	2.2
1	A	168	ASN	2.2
1	B	412	HIS	2.2
1	C	20	LEU	2.2
1	C	64	LEU	2.2
1	C	77	LEU	2.2
1	A	466	ASP	2.2
1	C	167	LYS	2.2
1	C	479	ILE	2.2
1	C	121	SER	2.2
1	B	291	MET	2.2
1	C	98	ASP	2.2
1	A	119	PRO	2.2
1	B	470	LEU	2.2
1	C	248	LEU	2.2
1	A	247	SER	2.2
1	B	368	SER	2.2
1	A	66	ARG	2.2
1	B	79	GLU	2.2
1	C	316	GLY	2.2
1	C	525	ILE	2.2
1	C	13	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	201	ALA	2.2
1	B	218	ASP	2.2
1	C	194	ASP	2.2
1	C	198	ALA	2.2
1	C	442	GLN	2.2
1	B	560	PHE	2.1
1	A	48	SER	2.1
1	B	87	SER	2.1
1	B	271	SER	2.1
1	A	488	LYS	2.1
1	B	100	LEU	2.1
1	C	134	LEU	2.1
1	C	240	ASN	2.1
1	C	523	GLU	2.1
1	B	430	SER	2.1
1	A	388	MET	2.1
1	B	550	LEU	2.1
1	A	504	ASP	2.1
1	C	295	ASP	2.1
1	C	396	ASP	2.1
1	C	294	SER	2.1
1	A	41	GLY	2.1
1	C	173	ASN	2.1
1	C	308	TYR	2.1
1	C	509	HIS	2.1
1	A	274	THR	2.1
1	C	188	THR	2.1
1	C	103	ALA	2.1
1	C	220	ASP	2.1
1	A	20	LEU	2.1
1	A	501	GLN	2.1
1	C	222	LEU	2.1
1	C	445	LEU	2.1
1	B	333	ASN	2.1
1	B	88	ILE	2.1
1	C	293	ILE	2.1
1	C	544	GLY	2.1
1	A	509	HIS	2.1
1	A	78	VAL	2.1
1	B	541	VAL	2.1
1	A	334	THR	2.1
1	A	429	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	204	ASP	2.1
1	C	136	GLN	2.1
1	A	118	ARG	2.1
1	A	329	ARG	2.1
1	B	55	ARG	2.1
1	B	221	ARG	2.1
1	A	417	PRO	2.0
1	A	527	PRO	2.0
1	C	498	VAL	2.0
1	C	536	MET	2.0
1	A	76	ASN	2.0
1	B	483	ASP	2.0
1	A	402	LEU	2.0
1	C	112	LYS	2.0
1	C	382	PRO	2.0
1	A	459	ILE	2.0
1	C	437	ASP	2.0
1	B	139	ALA	2.0
1	B	384	ALA	2.0
1	C	37	ALA	2.0
1	C	256	ALA	2.0
1	B	36	GLN	2.0
1	A	52	ARG	2.0
1	A	83	THR	2.0
1	A	337	ASP	2.0
1	B	13	THR	2.0
1	B	146	MET	2.0
1	B	219	LEU	2.0
1	B	426	ASP	2.0
1	A	40	HIS	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 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	B	570	1/1	0.84	0.30	3.96	103,103,103,103	0
2	ZN	A	570	1/1	0.97	0.12	-4.24	33,33,33,33	0
2	ZN	C	570	1/1	0.96	0.12	-5.47	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.