



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:25 PM EDT

PDB ID : 3MWT / pdb_00003mwt
Title : Crystal structure of Lassa fever virus nucleoprotein in complex with Mn²⁺
Authors : Qi, X.; Lan, S.; Wang, W.; Schelde, L.M.; Dong, H.; Wallat, G.; Liang, Y.;
Ly, H.; Dong, C.; Scottish Structural Proteomics Facility (SSPF)
Deposited on : 2010-05-06
Resolution : 1.98 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
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

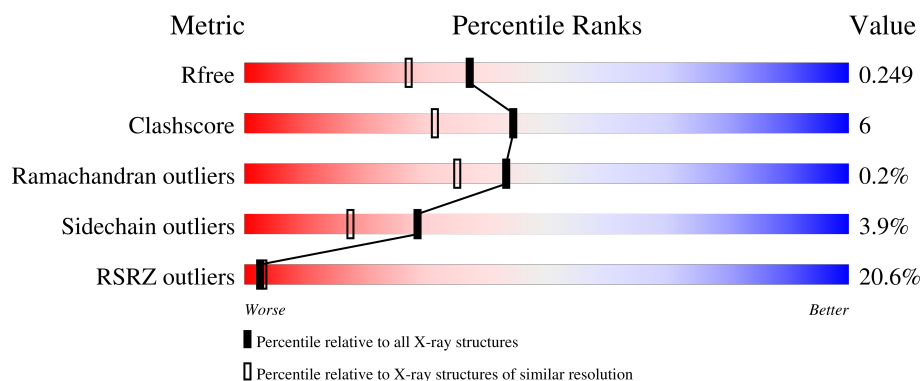
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	577	20% 76% 11% 11%
1	B	577	15% 72% 15% 11%
1	C	577	19% 72% 13% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12279 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	513	Total	C	N	O	S	0	0	0
			4012	2521	697	767	27			
1	B	512	Total	C	N	O	S	0	0	0
			4001	2510	696	768	27			
1	C	500	Total	C	N	O	S	0	0	0
			3918	2463	681	747	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 MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

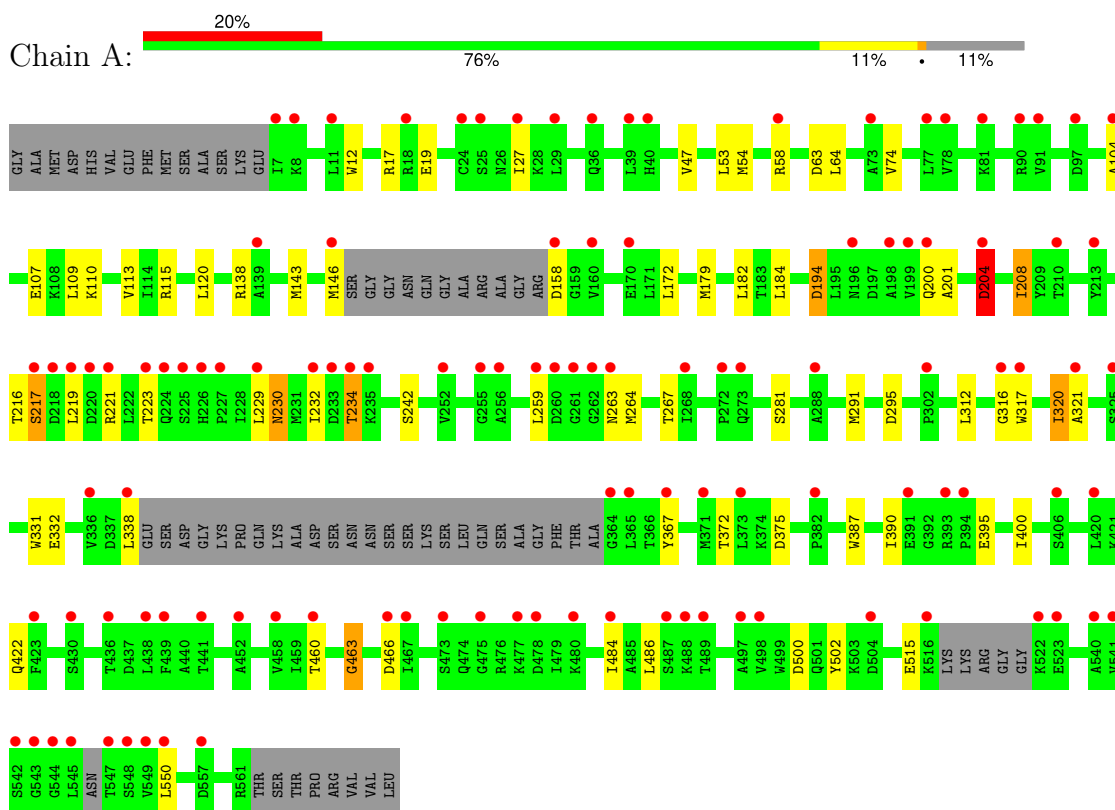
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total	O	0	0
			135	135		
4	B	158	Total	O	0	0
			158	158		
4	C	49	Total	O	0	0
			49	49		

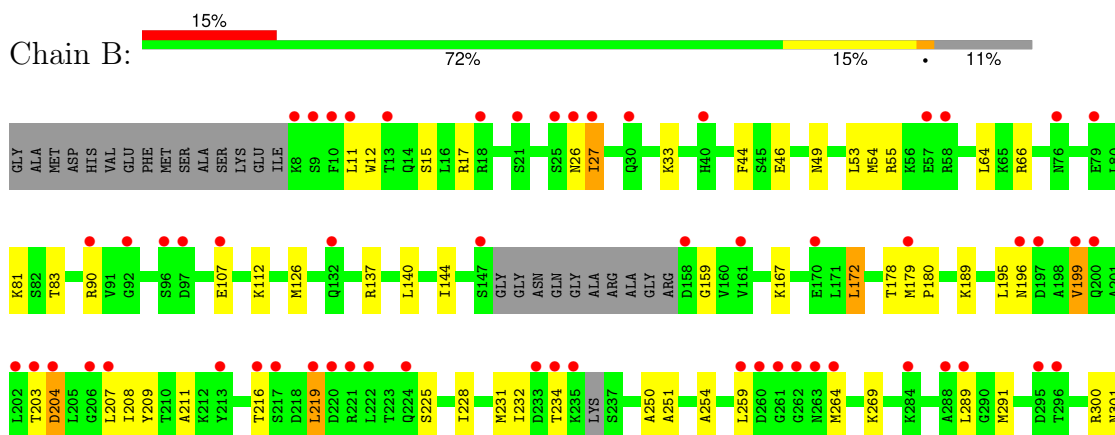
3 Residue-property plots [i](#)

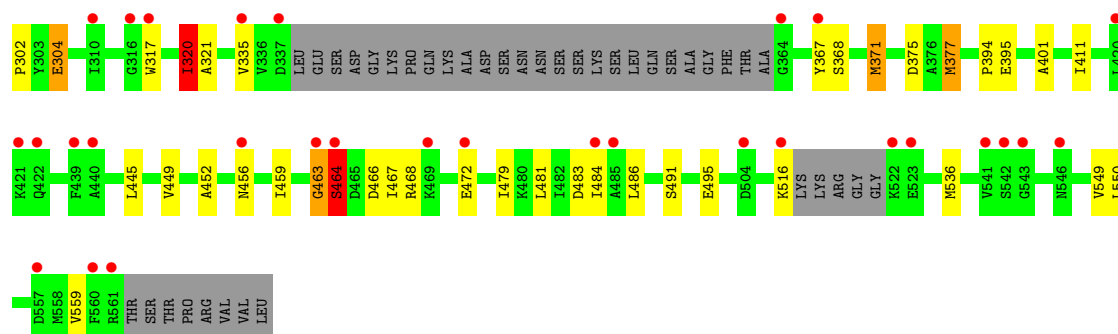
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Nucleoprotein

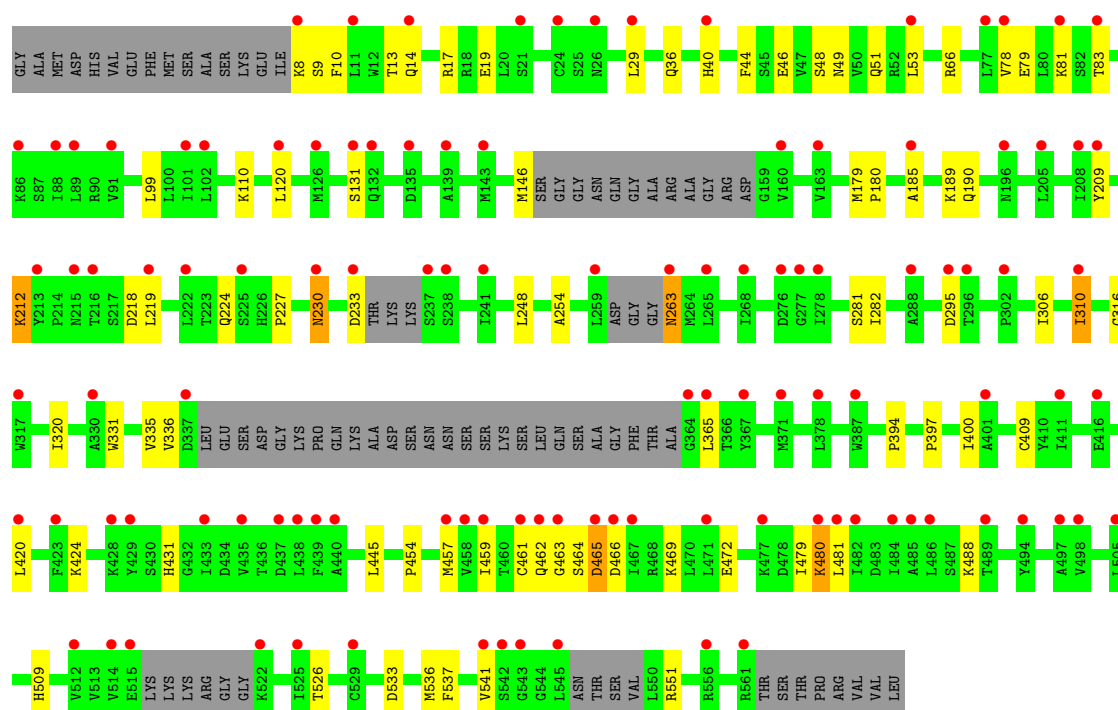
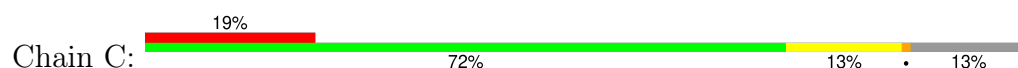


• Molecule 1: Nucleoprotein





● Molecule 1: Nucleoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	176.88Å 176.88Å 56.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	153.18 – 1.98 153.18 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.5 (153.18-1.98) 99.8 (153.18-1.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.181 , 0.218 0.211 , 0.249	Depositor DCC
R_{free} test set	6843 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.069 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.553 for H, K, L 0.447 for K, H, -L	Depositor
Outliers	0 of 136770 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12279	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 2.85% 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: ZN, MN

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	0.97	3/4068 (0.1%)	1.06	5/5491 (0.1%)
1	B	1.15	3/4057 (0.1%)	1.17	10/5477 (0.2%)
1	C	0.92	1/3972 (0.0%)	1.06	4/5360 (0.1%)
All	All	1.02	7/12097 (0.1%)	1.10	19/16328 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	449	VAL	CA-CB	6.72	1.62	1.54
1	A	204	ASP	CA-C	5.97	1.61	1.52
1	A	104	ALA	CA-CB	5.50	1.61	1.53
1	B	204	ASP	CA-CB	5.27	1.61	1.53
1	B	559	VAL	CA-CB	5.21	1.60	1.54
1	C	185	ALA	CA-CB	5.17	1.61	1.53
1	A	204	ASP	CA-CB	5.02	1.62	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	MET	CG-SD-CE	-7.99	83.32	100.90
1	C	316	GLY	N-CA-C	6.87	119.39	110.45
1	B	27	ILE	N-CA-C	6.46	118.37	112.43
1	A	316	GLY	N-CA-C	6.14	118.87	110.58
1	B	259	LEU	N-CA-C	6.12	119.21	109.24
1	B	172	LEU	N-CA-C	-5.96	105.84	113.23
1	C	526	THR	N-CA-C	-5.88	102.24	109.65
1	B	320	ILE	N-CA-C	5.79	119.32	113.47
1	C	295	ASP	N-CA-C	-5.59	105.14	112.41
1	A	204	ASP	CB-CA-C	5.58	122.09	110.32
1	A	332	GLU	N-CA-C	-5.36	106.42	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	GLU	N-CA-C	-5.32	105.48	111.28
1	B	179	MET	CB-CA-C	-5.29	103.12	110.16
1	A	47	VAL	N-CA-C	-5.13	105.50	110.42
1	B	368	SER	CB-CA-C	-5.13	102.61	110.81
1	C	310	ILE	N-CA-C	5.10	115.32	110.42
1	B	464	SER	N-CA-C	5.10	116.92	111.36
1	B	55	ARG	N-CA-C	5.09	118.58	112.38
1	A	320	ILE	N-CA-C	5.01	119.76	109.34

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	4012	0	4084	51	0
1	B	4001	0	4060	56	0
1	C	3918	0	3980	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	135	0	0	4	0
4	B	158	0	0	3	2
4	C	49	0	0	2	0
All	All	12279	0	12124	144	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 6.

All (144) 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:464:SER:HB3	1:B:483:ASP:OD2	1.85	0.77
1:A:502:TYR:CE1	1:A:550:LEU:HD13	2.21	0.75
1:B:459:ILE:HD12	1:B:479:ILE:HG21	1.69	0.75
1:A:74:VAL:CG1	1:A:179:MET:HE1	2.18	0.73
1:A:216:THR:OG1	1:A:234:THR:CG2	2.40	0.69
1:C:46:GLU:OE2	1:C:66:ARG:HD2	1.94	0.68
1:B:463:GLY:O	1:B:467:ILE:HG12	1.95	0.66
1:A:500:ASP:OD2	4:A:572:HOH:O	2.14	0.65
1:C:51:GLN:HE22	1:C:190:GLN:HE22	1.43	0.65
1:C:397:PRO:HB2	1:C:400:ILE:HD11	1.80	0.64
1:A:208:ILE:HD11	1:B:208:ILE:HD13	1.81	0.63
1:C:120:LEU:HD23	1:C:146:MET:HG3	1.80	0.63
1:A:216:THR:OG1	1:A:234:THR:HG23	1.99	0.61
1:C:219:LEU:HD22	1:C:248:LEU:HD13	1.82	0.61
1:A:115:ARG:HD2	1:A:375:ASP:OD2	2.00	0.61
1:C:454:PRO:O	1:C:457:MET:HG3	2.00	0.60
1:B:81:LYS:HA	1:B:321:ALA:HB1	1.83	0.60
1:A:58:ARG:NH2	4:A:669:HOH:O	2.35	0.60
1:A:259:LEU:HD12	1:A:264:MET:HE3	1.84	0.59
1:B:367:TYR:CZ	1:B:371:MET:SD	2.96	0.58
1:A:208:ILE:CD1	1:B:208:ILE:HD13	2.34	0.58
1:A:317:TRP:HB2	1:A:321:ALA:HB2	1.86	0.58
1:A:19:GLU:HG3	1:A:281:SER:HB3	1.87	0.56
1:C:282:ILE:HD11	1:C:310:ILE:CD1	2.35	0.56
1:B:196:ASN:HA	1:B:199:VAL:HG13	1.88	0.56
1:C:99:LEU:HD22	1:C:336:VAL:HG13	1.87	0.56
1:C:431:HIS:O	1:C:509:HIS:ND1	2.35	0.56
1:B:216:THR:HG22	1:B:234:THR:HB	1.88	0.55
1:C:365:LEU:HD12	1:C:365:LEU:H	1.72	0.55
1:C:537:PHE:O	1:C:541:VAL:HG23	2.06	0.55
1:C:44:PHE:CD2	1:C:189:LYS:HG2	2.43	0.54
1:A:17:ARG:HG2	1:A:263:ASN:O	2.07	0.54
1:B:300:ARG:CZ	4:B:657:HOH:O	2.56	0.54
1:B:107:GLU:HG2	4:B:580:HOH:O	2.08	0.54
1:A:120:LEU:HD23	1:A:146:MET:SD	2.49	0.53
1:C:36:GLN:O	1:C:40:HIS:ND1	2.41	0.53
1:B:180:PRO:HB3	1:B:254:ALA:HA	1.90	0.52
1:B:269:LYS:HD2	1:B:317:TRP:CE2	2.44	0.52
1:B:232:ILE:HD13	1:B:251:ALA:CB	2.39	0.52
1:A:223:THR:HG21	1:A:230:ASN:HB3	1.91	0.52
1:C:36:GLN:HG2	4:C:595:HOH:O	2.09	0.52
1:C:461:CYS:SG	1:C:464:SER:HA	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:MET:HG3	1:C:320:ILE:O	2.10	0.52
1:C:120:LEU:HD23	1:C:146:MET:CG	2.40	0.52
1:A:216:THR:OG1	1:A:234:THR:HG21	2.09	0.52
1:B:463:GLY:O	1:B:466:ASP:OD1	2.28	0.52
1:C:110:LYS:HG3	1:C:331:TRP:CE2	2.45	0.52
1:B:301:ASN:OD1	1:B:304:GLU:HG3	2.10	0.52
1:A:390:ILE:HG22	1:A:400:ILE:HD12	1.92	0.51
1:A:390:ILE:HG22	1:A:400:ILE:CD1	2.40	0.51
1:C:209:TYR:HA	1:C:212:LYS:O	2.10	0.51
1:A:194:ASP:N	1:A:194:ASP:OD1	2.44	0.51
1:B:204:ASP:HA	1:B:207:LEU:HD12	1.92	0.51
1:C:365:LEU:HD12	1:C:365:LEU:N	2.26	0.51
1:B:371:MET:HA	1:B:371:MET:HE2	1.93	0.50
1:A:259:LEU:CD1	1:A:264:MET:HE3	2.42	0.49
1:C:394:PRO:HG3	1:C:466:ASP:HB2	1.94	0.49
1:A:74:VAL:HG11	1:A:179:MET:HE1	1.91	0.49
1:A:74:VAL:HG12	1:A:179:MET:HE1	1.92	0.49
1:A:200:GLN:HG2	1:B:225:SER:HB3	1.94	0.49
1:B:367:TYR:O	1:B:371:MET:HG2	2.13	0.49
1:A:109:LEU:O	1:A:113:VAL:HG23	2.12	0.49
1:B:216:THR:HG22	1:B:234:THR:CB	2.43	0.49
1:B:377:MET:CE	1:B:452:ALA:HB3	2.42	0.49
1:B:140:LEU:O	1:B:144:ILE:HG12	2.13	0.49
1:A:312:LEU:HD22	4:A:684:HOH:O	2.13	0.48
1:C:409:CYS:HA	1:C:551:ARG:O	2.13	0.48
1:A:216:THR:HG23	1:A:234:THR:HG21	1.96	0.48
1:A:64:LEU:HD13	1:A:172:LEU:HD23	1.95	0.48
1:C:480:LYS:HE3	1:C:481:LEU:O	2.14	0.48
1:A:53:LEU:HD22	1:A:63:ASP:OD1	2.13	0.48
1:A:158:ASP:N	4:A:696:HOH:O	2.46	0.47
1:C:10:PHE:CE2	1:C:14:GLN:HG3	2.49	0.47
1:C:19:GLU:HG3	1:C:281:SER:HB3	1.96	0.47
1:B:459:ILE:HD12	1:B:479:ILE:CG2	2.42	0.47
1:A:463:GLY:O	1:A:466:ASP:OD1	2.32	0.47
1:A:484:ILE:HG22	1:A:486:LEU:HG	1.97	0.47
1:B:15:SER:OG	1:B:289:LEU:HD11	2.15	0.47
1:A:208:ILE:CD1	1:B:208:ILE:CD1	2.93	0.47
1:A:27:ILE:HD11	1:A:267:THR:HG22	1.97	0.47
1:C:13:THR:O	1:C:17:ARG:HG3	2.15	0.47
1:C:78:VAL:O	1:C:81:LYS:HE3	2.14	0.47
1:C:533:ASP:OD1	1:C:536:MET:HE3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:MET:HE2	1:A:242:SER:HB3	1.97	0.46
1:A:179:MET:HE2	1:A:182:LEU:HB2	1.96	0.46
1:B:178:THR:HG21	1:B:250:ALA:HB2	1.97	0.46
1:A:208:ILE:HD13	1:B:208:ILE:CD1	2.46	0.46
1:B:126:MET:N	1:B:159:GLY:O	2.36	0.46
1:B:495:GLU:HG3	1:B:536:MET:HE1	1.98	0.46
1:B:12:TRP:CZ2	1:B:291:MET:HA	2.52	0.45
1:B:317:TRP:HB3	1:B:320:ILE:HG13	1.98	0.45
1:B:375:ASP:HB3	4:B:586:HOH:O	2.16	0.45
1:C:212:LYS:NZ	1:C:218:ASP:OD2	2.50	0.45
1:C:263:ASN:N	4:C:603:HOH:O	2.49	0.45
1:A:387:TRP:CH2	1:A:484:ILE:HG13	2.52	0.45
1:B:203:THR:O	1:B:207:LEU:HG	2.17	0.44
1:B:445:LEU:HD23	1:B:445:LEU:HA	1.77	0.44
1:A:219:LEU:HD21	1:A:232:ILE:HB	1.98	0.44
1:B:46:GLU:OE2	1:B:66:ARG:HD2	2.17	0.44
1:B:401:ALA:HA	1:B:411:ILE:O	2.17	0.44
1:A:12:TRP:CZ2	1:A:291:MET:HA	2.53	0.44
1:C:465:ASP:O	1:C:469:LYS:HD3	2.17	0.44
1:C:120:LEU:CD2	1:C:146:MET:HG3	2.47	0.44
1:C:488:LYS:N	1:C:488:LYS:HD2	2.33	0.44
1:B:17:ARG:CZ	1:B:264:MET:HE1	2.47	0.44
1:B:228:ILE:O	1:B:231:MET:HG3	2.18	0.44
1:C:48:SER:HA	1:C:51:GLN:NE2	2.32	0.44
1:C:365:LEU:HD21	1:C:445:LEU:HD23	1.99	0.43
1:B:468:ARG:HB2	1:B:481:LEU:CD1	2.49	0.43
1:A:115:ARG:HD3	1:A:372:THR:HA	2.00	0.43
1:C:282:ILE:CD1	1:C:310:ILE:CD1	2.96	0.43
1:A:208:ILE:HD13	1:B:208:ILE:HD12	2.01	0.43
1:B:44:PHE:CG	1:B:189:LYS:HG2	2.54	0.43
1:B:468:ARG:O	1:B:472:GLU:HG3	2.19	0.43
1:C:488:LYS:HE3	1:C:488:LYS:HA	2.01	0.43
1:A:201:ALA:HB1	1:A:229:LEU:HD11	2.01	0.42
1:A:221:ARG:HB3	1:B:207:LEU:CD2	2.49	0.42
1:B:195:LEU:O	1:B:199:VAL:HG12	2.19	0.42
1:C:19:GLU:CG	1:C:281:SER:HB3	2.49	0.42
1:C:49:ASN:O	1:C:53:LEU:HG	2.20	0.42
1:B:486:LEU:HD13	1:B:491:SER:HA	2.02	0.42
1:B:49:ASN:O	1:B:53:LEU:HG	2.20	0.42
1:A:110:LYS:HA	1:A:331:TRP:CZ3	2.55	0.42
1:A:204:ASP:OD2	1:B:204:ASP:OD2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ILE:HD12	1:A:320:ILE:C	2.45	0.42
1:A:502:TYR:CZ	1:A:550:LEU:HD13	2.55	0.42
1:C:306:ILE:HG12	1:C:310:ILE:HD12	2.02	0.41
1:A:295:ASP:OD2	1:A:367:TYR:OH	2.37	0.41
1:B:219:LEU:HD22	1:B:234:THR:HG23	2.02	0.41
1:C:420:LEU:O	1:C:424:LYS:HG2	2.21	0.41
1:C:227:PRO:O	1:C:230:ASN:ND2	2.53	0.41
1:A:387:TRP:HA	1:A:460:THR:O	2.20	0.41
1:C:180:PRO:HB3	1:C:254:ALA:HA	2.02	0.41
1:C:457:MET:HB2	1:C:479:ILE:HG12	2.03	0.41
1:A:217:SER:OG	1:A:221:ARG:NH1	2.54	0.41
1:B:126:MET:SD	1:B:137:ARG:HB3	2.61	0.41
1:B:209:TYR:C	1:B:211:ALA:H	2.28	0.41
1:B:64:LEU:HD13	1:B:172:LEU:HD23	2.02	0.40
1:C:48:SER:HA	1:C:51:GLN:HE21	1.85	0.40
1:B:394:PRO:HB3	1:B:466:ASP:O	2.21	0.40
1:B:289:LEU:HD23	1:B:289:LEU:HA	1.68	0.40
1:B:46:GLU:OE1	1:B:66:ARG:NH1	2.54	0.40
1:B:54:MET:HE3	1:B:54:MET:HB3	1.94	0.40
1:A:466:ASP:OD1	1:A:466:ASP:N	2.54	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)
4:B:573:HOH:O	4:B:727:HOH:O[2_455]	1.78	0.42
4:B:623:HOH:O	4:B:679:HOH:O[3_445]	2.18	0.02

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	503/577 (87%)	494 (98%)	8 (2%)	1 (0%)	43	35
1	B	502/577 (87%)	490 (98%)	11 (2%)	1 (0%)	43	35
1	C	486/577 (84%)	478 (98%)	7 (1%)	1 (0%)	43	35
All	All	1491/1731 (86%)	1462 (98%)	26 (2%)	3 (0%)	43	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	463	GLY
1	C	463	GLY
1	A	463	GLY

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%)	436 (97%)	14 (3%)	35	26
1	B	449/498 (90%)	428 (95%)	21 (5%)	23	12
1	C	439/498 (88%)	422 (96%)	17 (4%)	28	17
All	All	1338/1494 (90%)	1286 (96%)	52 (4%)	28	17

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	GLU
1	A	138	ARG
1	A	143	MET
1	A	184	LEU
1	A	194	ASP
1	A	204	ASP
1	A	208	ILE
1	A	217	SER
1	A	230	ASN
1	A	234	THR

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Mol	Chain	Res	Type
1	A	338	LEU
1	A	395	GLU
1	A	422	GLN
1	A	515	GLU
1	B	11	LEU
1	B	26	ASN
1	B	27	ILE
1	B	33	LYS
1	B	83	THR
1	B	90	ARG
1	B	112	LYS
1	B	167	LYS
1	B	199	VAL
1	B	219	LEU
1	B	302	PRO
1	B	320	ILE
1	B	335	VAL
1	B	371	MET
1	B	395	GLU
1	B	456	ASN
1	B	464	SER
1	B	484	ILE
1	B	516	LYS
1	B	549	VAL
1	B	550	LEU
1	C	8	LYS
1	C	9	SER
1	C	29	LEU
1	C	79	GLU
1	C	83	THR
1	C	131	SER
1	C	212	LYS
1	C	224	GLN
1	C	230	ASN
1	C	233	ASP
1	C	263	ASN
1	C	335	VAL
1	C	459	ILE
1	C	462	GLN
1	C	465	ASP
1	C	472	GLU
1	C	480	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	30	GLN
1	A	71	ASN
1	A	72	GLN
1	A	175	GLN
1	A	230	ASN
1	A	383	ASN
1	A	474	GLN
1	A	507	HIS
1	B	30	GLN
1	B	383	ASN
1	B	507	HIS
1	B	528	HIS
1	C	14	GLN
1	C	51	GLN
1	C	72	GLN
1	C	132	GLN
1	C	200	GLN
1	C	383	ASN
1	C	528	HIS

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 6 ligands modelled in this entry, 6 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	513/577 (88%)	1.39	114 (22%)  	25, 40, 58, 83	1 (0%)
1	B	512/577 (88%)	1.10	88 (17%)  	24, 34, 51, 79	0
1	C	500/577 (86%)	1.41	112 (22%)  	32, 44, 64, 76	0
All	All	1525/1731 (88%)	1.30	314 (20%)  	24, 40, 59, 83	1 (0%)

All (314) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	463	GLY	7.5
1	A	7	ILE	7.5
1	A	439	PHE	6.2
1	B	207	LEU	6.1
1	A	234	THR	6.0
1	A	484	ILE	5.9
1	A	338	LEU	5.7
1	B	259	LEU	5.5
1	B	262	GLY	5.2
1	B	147	SER	5.1
1	C	439	PHE	5.1
1	C	88	ILE	4.7
1	A	213	TYR	4.6
1	A	545	LEU	4.5
1	C	485	ALA	4.5
1	B	27	ILE	4.5
1	A	261	GLY	4.3
1	C	91	VAL	4.2
1	A	224	GLN	4.2
1	B	25	SER	4.2
1	C	365	LEU	4.2
1	C	83	THR	4.1
1	B	234	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	420	LEU	3.9
1	A	365	LEU	3.8
1	C	277	GLY	3.8
1	B	263	ASN	3.8
1	A	504	ASP	3.8
1	A	557	ASP	3.8
1	B	261	GLY	3.8
1	C	463	GLY	3.8
1	C	545	LEU	3.8
1	B	235	LYS	3.7
1	A	219	LEU	3.7
1	A	548	SER	3.7
1	C	259	LEU	3.6
1	B	260	ASP	3.6
1	B	26	ASN	3.6
1	B	557	ASP	3.6
1	A	480	LYS	3.6
1	C	477	LYS	3.6
1	B	216	THR	3.6
1	B	439	PHE	3.6
1	B	337	ASP	3.5
1	C	542	SER	3.5
1	B	224	GLN	3.5
1	A	367	TYR	3.5
1	C	458	VAL	3.5
1	B	202	LEU	3.4
1	C	471	LEU	3.4
1	C	263	ASN	3.4
1	A	478	ASP	3.4
1	C	440	ALA	3.4
1	B	9	SER	3.4
1	C	486	LEU	3.4
1	A	488	LYS	3.4
1	B	97	ASP	3.4
1	B	92	GLY	3.4
1	B	543	GLY	3.4
1	A	549	VAL	3.4
1	A	288	ALA	3.4
1	C	233	ASP	3.3
1	A	198	ALA	3.3
1	C	219	LEU	3.3
1	B	516	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	364	GLY	3.3
1	C	29	LEU	3.3
1	C	241	ILE	3.3
1	A	547	THR	3.3
1	A	73	ALA	3.2
1	A	160	VAL	3.2
1	A	302	PRO	3.2
1	B	196	ASN	3.2
1	A	158	ASP	3.2
1	B	504	ASP	3.2
1	A	223	THR	3.2
1	B	560	PHE	3.2
1	C	120	LEU	3.1
1	A	235	LYS	3.1
1	B	132	GLN	3.1
1	C	143	MET	3.1
1	C	24	CYS	3.1
1	A	220	ASP	3.0
1	A	232	ILE	3.0
1	C	467	ILE	3.0
1	C	11	LEU	3.0
1	B	213	TYR	3.0
1	C	367	TYR	3.0
1	B	523	GLU	3.0
1	A	420	LEU	3.0
1	A	77	LEU	3.0
1	A	40	HIS	3.0
1	B	21	SER	3.0
1	B	421	LYS	3.0
1	A	423	PHE	2.9
1	B	11	LEU	2.9
1	C	160	VAL	2.9
1	B	206	GLY	2.9
1	B	288	ALA	2.9
1	B	440	ALA	2.9
1	B	233	ASP	2.9
1	C	276	ASP	2.9
1	C	420	LEU	2.9
1	B	485	ALA	2.9
1	A	210	THR	2.8
1	A	8	LYS	2.8
1	C	21	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	255	GLY	2.8
1	A	393	ARG	2.8
1	A	477	LYS	2.8
1	C	522	LYS	2.8
1	B	204	ASP	2.8
1	C	457	MET	2.8
1	C	132	GLN	2.8
1	B	222	LEU	2.8
1	C	438	LEU	2.8
1	C	482	ILE	2.8
1	A	97	ASP	2.8
1	A	233	ASP	2.8
1	B	179	MET	2.8
1	B	546	ASN	2.7
1	B	472	GLU	2.7
1	A	436	THR	2.7
1	C	265	LEU	2.7
1	A	196	ASN	2.7
1	A	516	LYS	2.7
1	C	86	LYS	2.7
1	A	316	GLY	2.7
1	A	543	GLY	2.7
1	C	222	LEU	2.7
1	B	484	ILE	2.7
1	A	225	SER	2.7
1	B	18	ARG	2.7
1	B	30	GLN	2.7
1	B	58	ARG	2.7
1	B	284	LYS	2.7
1	A	541	VAL	2.7
1	C	288	ALA	2.7
1	C	216	THR	2.7
1	A	259	LEU	2.7
1	A	373	LEU	2.7
1	A	252	VAL	2.7
1	A	204	ASP	2.6
1	C	429	TYR	2.6
1	A	217	SER	2.6
1	A	550	LEU	2.6
1	C	378	LEU	2.6
1	B	161	VAL	2.6
1	B	217	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	90	ARG	2.6
1	C	387	TRP	2.6
1	B	200	GLN	2.6
1	C	480	LYS	2.6
1	B	561	ARG	2.5
1	A	39	LEU	2.5
1	C	135	ASP	2.5
1	C	310	ILE	2.5
1	A	263	ASN	2.5
1	A	452	ALA	2.5
1	B	40	HIS	2.5
1	C	541	VAL	2.5
1	A	441	THR	2.5
1	B	367	TYR	2.5
1	B	10	PHE	2.5
1	A	544	GLY	2.5
1	B	317	TRP	2.5
1	C	433	ILE	2.5
1	B	79	GLU	2.5
1	B	107	GLU	2.5
1	B	296	THR	2.5
1	A	394	PRO	2.5
1	A	262	GLY	2.5
1	A	27	ILE	2.5
1	C	208	ILE	2.5
1	C	237	SER	2.5
1	C	14	GLN	2.5
1	A	256	ALA	2.5
1	A	497	ALA	2.5
1	C	401	ALA	2.5
1	A	364	GLY	2.4
1	B	221	ARG	2.4
1	A	104	ALA	2.4
1	A	139	ALA	2.4
1	B	158	ASP	2.4
1	C	437	ASP	2.4
1	A	78	VAL	2.4
1	C	78	VAL	2.4
1	A	221	ARG	2.4
1	C	461	CYS	2.4
1	A	438	LEU	2.4
1	B	96	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	219	LEU	2.4
1	C	126	MET	2.4
1	C	225	SER	2.4
1	B	8	LYS	2.4
1	C	278	ILE	2.4
1	A	58	ARG	2.4
1	A	227	PRO	2.4
1	C	515	GLU	2.4
1	C	131	SER	2.4
1	C	89	LEU	2.4
1	C	494	TYR	2.4
1	A	260	ASP	2.4
1	C	295	ASP	2.4
1	A	460	THR	2.4
1	A	466	ASP	2.3
1	C	209	TYR	2.3
1	A	523	GLU	2.3
1	C	139	ALA	2.3
1	C	185	ALA	2.3
1	C	497	ALA	2.3
1	B	456	ASN	2.3
1	C	40	HIS	2.3
1	C	543	GLY	2.3
1	A	336	VAL	2.3
1	B	541	VAL	2.3
1	C	512	VAL	2.3
1	B	295	ASP	2.3
1	A	24	CYS	2.3
1	C	416	GLU	2.3
1	C	53	LEU	2.3
1	C	481	LEU	2.3
1	C	196	ASN	2.3
1	C	371	MET	2.3
1	C	459	ILE	2.3
1	A	475	GLY	2.3
1	B	522	LYS	2.3
1	C	428	LYS	2.3
1	A	200	GLN	2.3
1	B	310	ILE	2.3
1	A	473	SER	2.3
1	C	498	VAL	2.3
1	C	230	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	529	CYS	2.3
1	C	296	THR	2.3
1	A	36	GLN	2.2
1	C	77	LEU	2.2
1	C	505	LEU	2.2
1	B	364	GLY	2.2
1	C	337	ASP	2.2
1	C	465	ASP	2.2
1	A	317	TRP	2.2
1	A	467	ILE	2.2
1	A	146	MET	2.2
1	C	556	ARG	2.2
1	A	489	THR	2.2
1	B	13	THR	2.2
1	A	29	LEU	2.2
1	A	229	LEU	2.2
1	A	273	GLN	2.2
1	C	102	LEU	2.2
1	C	462	GLN	2.2
1	C	466	ASP	2.2
1	A	540	ALA	2.2
1	C	411	ILE	2.2
1	C	484	ILE	2.2
1	C	317	TRP	2.2
1	A	458	VAL	2.2
1	B	199	VAL	2.2
1	C	435	VAL	2.2
1	C	514	VAL	2.2
1	A	542	SER	2.2
1	B	464	SER	2.2
1	A	382	PRO	2.2
1	C	330	ALA	2.2
1	A	18	ARG	2.2
1	B	335	VAL	2.1
1	C	489	THR	2.1
1	A	11	LEU	2.1
1	A	90	ARG	2.1
1	A	272	PRO	2.1
1	B	469	LYS	2.1
1	C	525	ILE	2.1
1	B	220	ASP	2.1
1	A	406	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	203	THR	2.1
1	C	163	VAL	2.1
1	C	81	LYS	2.1
1	B	289	LEU	2.1
1	B	422	GLN	2.1
1	C	423	PHE	2.1
1	B	197	ASP	2.1
1	A	25	SER	2.1
1	A	487	SER	2.1
1	A	391	GLU	2.1
1	A	522	LYS	2.1
1	B	170	GLU	2.1
1	C	8	LYS	2.1
1	B	316	GLY	2.1
1	B	264	MET	2.1
1	A	226	HIS	2.1
1	A	91	VAL	2.1
1	C	302	PRO	2.1
1	A	218	ASP	2.1
1	A	268	ILE	2.0
1	B	57	GLU	2.0
1	B	542	SER	2.0
1	C	213	TYR	2.0
1	A	371	MET	2.0
1	B	76	ASN	2.0
1	C	26	ASN	2.0
1	A	498	VAL	2.0
1	C	205	LEU	2.0
1	A	321	ALA	2.0
1	A	170	GLU	2.0
1	A	81	LYS	2.0
1	A	325	SER	2.0
1	A	430	SER	2.0
1	C	238	SER	2.0
1	C	101	ILE	2.0
1	C	268	ILE	2.0
1	C	215	ASN	2.0
1	A	199	VAL	2.0
1	C	561	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	A	680	1/1	0.83	0.20	76,76,76,76	0
2	MN	C	680	1/1	0.91	0.12	87,87,87,87	0
2	MN	B	680	1/1	0.94	0.10	54,54,54,54	0
3	ZN	A	690	1/1	0.94	0.12	57,57,57,57	0
3	ZN	C	690	1/1	0.94	0.09	61,61,61,61	0
3	ZN	B	690	1/1	0.97	0.10	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.