



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:45 PM UTC

PDB ID : 2R7Q / pdb_00002r7q
Title : Crystal Structure of VP1 apoenzyme of Rotavirus SA11 (C-terminal hexahistidine-tagged)
Authors : Lu, X.; Harrison, S.C.; Tao, Y.J.; Patton, J.T.; Nibert, M.L.
Deposited on : 2007-09-09
Resolution : 2.90 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

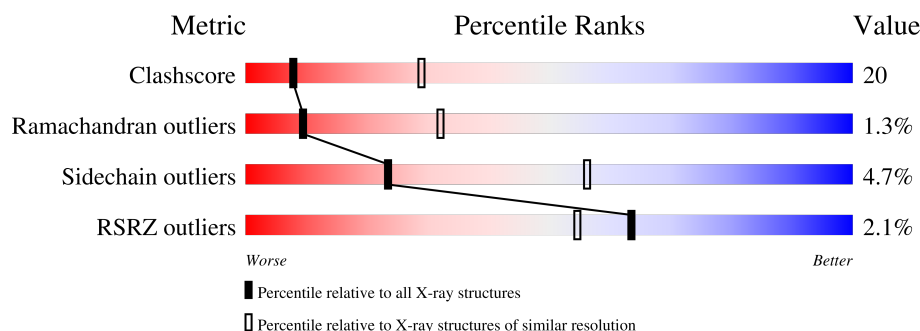
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	1095	2% 56% 37% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8686 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.

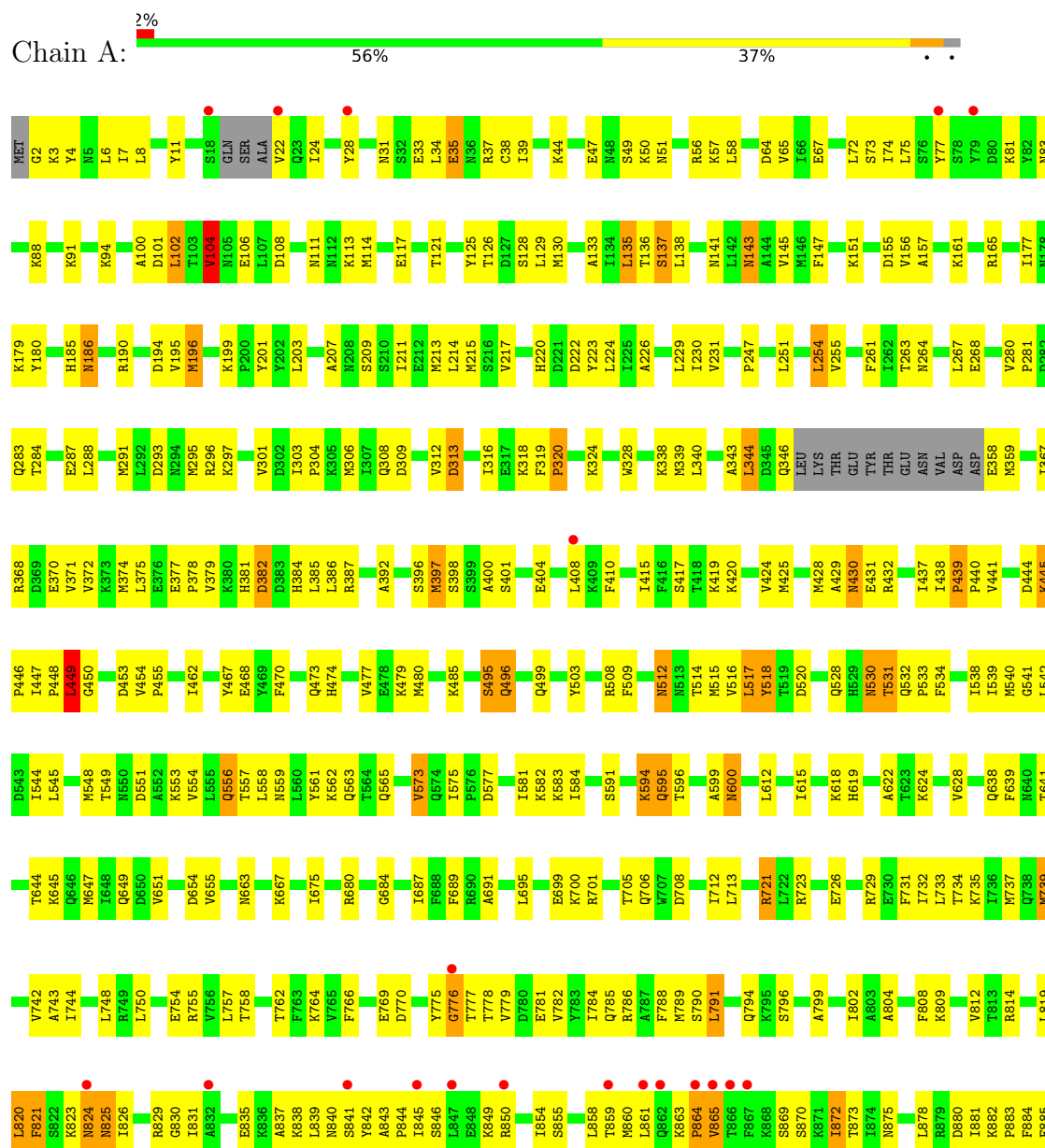
- Molecule 1 is a protein called RNA-dependent RNA polymerase.

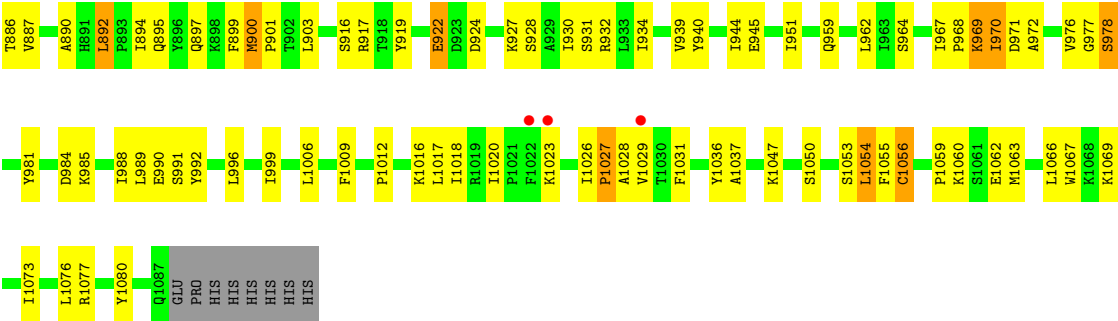
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1072	8686	5571	1446	1631	38	0	0	0

3 Residue-property plots

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: RNA-dependent RNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.38Å 112.47Å 143.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.2 (30.00-2.90) 96.1 (30.00-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.290 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8686	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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

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	0.45	0/8857	0.93	27/11973 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	824	ASN	N-CA-C	14.27	130.18	113.19
1	A	254	LEU	N-CA-C	7.94	119.72	111.14
1	A	900	MET	CA-C-N	7.75	129.53	119.84
1	A	900	MET	C-N-CA	7.75	129.53	119.84
1	A	196	MET	N-CA-C	7.07	120.02	111.82
1	A	449	LEU	N-CA-C	6.60	120.37	108.69
1	A	474	HIS	N-CA-C	6.53	118.05	111.07
1	A	757	LEU	N-CA-C	6.11	118.91	111.82
1	A	881	ILE	N-CA-C	6.08	116.86	110.72
1	A	573	VAL	N-CA-C	5.99	117.10	108.48
1	A	823	LYS	N-CA-C	5.93	119.14	107.98
1	A	594	LYS	N-CA-C	-5.92	105.14	112.90
1	A	67	GLU	N-CA-C	5.86	117.75	111.36
1	A	379	VAL	N-CA-C	5.83	116.01	110.53
1	A	157	ALA	CB-CA-C	-5.78	109.89	116.54
1	A	496	GLN	N-CA-C	-5.59	106.67	112.93
1	A	530	ASN	N-CA-C	5.57	117.43	111.36
1	A	255	VAL	N-CA-C	5.47	116.76	109.37
1	A	231	VAL	N-CA-C	5.45	115.65	110.53
1	A	531	THR	N-CA-C	5.31	117.76	111.33
1	A	344	LEU	N-CA-C	5.29	117.79	111.71
1	A	821	PHE	N-CA-C	-5.18	105.03	112.13
1	A	137	SER	N-CA-C	5.17	118.49	110.17
1	A	445	LYS	CA-C-N	5.17	125.41	119.83
1	A	445	LYS	C-N-CA	5.17	125.41	119.83
1	A	739	MET	N-CA-C	5.04	116.86	111.36
1	A	104	VAL	N-CA-C	5.02	117.37	111.09

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	8686	0	8776	346	0
All	All	8686	0	8776	346	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 20.

All (346) 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:A:81:LYS:HB2	1:A:83:ASN:HD22	1.21	0.98
1:A:556:GLN:HA	1:A:556:GLN:HE21	1.30	0.95
1:A:385:LEU:HD23	1:A:479:LYS:HE2	1.57	0.86
1:A:470:PHE:HE1	1:A:594:LYS:HD3	1.40	0.85
1:A:254:LEU:HD23	1:A:280:VAL:HG21	1.59	0.84
1:A:186:ASN:HD21	1:A:190:ARG:H	1.24	0.84
1:A:705:THR:HB	1:A:850:ARG:NH1	1.94	0.82
1:A:789:MET:HE2	1:A:1076:LEU:HD21	1.63	0.81
1:A:102:LEU:HD22	1:A:102:LEU:H	1.47	0.78
1:A:438:ILE:HD12	1:A:563:GLN:HB3	1.65	0.78
1:A:398:SER:HB2	1:A:838:LYS:HE2	1.68	0.76
1:A:959:GLN:HG2	1:A:976:VAL:HG21	1.68	0.76
1:A:186:ASN:ND2	1:A:190:ARG:H	1.82	0.76
1:A:296:ARG:HH22	1:A:308:GLN:NE2	1.84	0.76
1:A:470:PHE:CE1	1:A:594:LYS:HD3	2.21	0.75
1:A:81:LYS:HB2	1:A:83:ASN:ND2	2.01	0.75
1:A:180:TYR:HB3	1:A:199:LYS:HG2	1.69	0.74
1:A:1059:PRO:HB2	1:A:1062:GLU:HB2	1.70	0.73
1:A:3:LYS:O	1:A:7:ILE:HG12	1.88	0.72
1:A:840:ASN:O	1:A:846:SER:HB3	1.90	0.72
1:A:177:ILE:HD13	1:A:203:LEU:HD11	1.71	0.71
1:A:503:TYR:HB2	1:A:687:ILE:HD13	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:HA	1:A:91:LYS:HE2	1.72	0.71
1:A:972:ALA:O	1:A:976:VAL:HG23	1.92	0.70
1:A:283:GLN:OE1	1:A:649:GLN:HG3	1.92	0.70
1:A:764:LYS:HD3	1:A:1080:TYR:CG	2.27	0.70
1:A:622:ALA:HB3	1:A:638:GLN:HB3	1.74	0.69
1:A:453:ASP:HB2	1:A:699:GLU:HG3	1.73	0.69
1:A:762:THR:HA	1:A:1077:ARG:O	1.93	0.69
1:A:44:LYS:HB3	1:A:58:LEU:HD21	1.74	0.69
1:A:295:MET:HE1	1:A:303:ILE:HG22	1.74	0.68
1:A:473:GLN:HG2	1:A:561:TYR:CE1	2.27	0.68
1:A:556:GLN:HA	1:A:556:GLN:NE2	2.08	0.68
1:A:145:VAL:HG21	1:A:211:ILE:HG23	1.76	0.67
1:A:528:GLN:O	1:A:531:THR:HG22	1.94	0.67
1:A:1023:LYS:HB3	1:A:1060:LYS:HE2	1.75	0.67
1:A:316:ILE:HD13	1:A:684:GLY:HA3	1.75	0.67
1:A:734:THR:HA	1:A:737:MET:HE3	1.77	0.67
1:A:781:GLU:O	1:A:784:ILE:HG22	1.95	0.67
1:A:796:SER:HB2	1:A:849:LYS:HE3	1.77	0.67
1:A:887:VAL:HG22	1:A:1054:LEU:HD11	1.75	0.67
1:A:744:ILE:HD13	1:A:748:LEU:HG	1.77	0.66
1:A:968:PRO:HG2	1:A:971:ASP:HB2	1.78	0.66
1:A:843:ALA:HB3	1:A:844:PRO:HD3	1.78	0.66
1:A:186:ASN:C	1:A:186:ASN:HD22	2.03	0.66
1:A:744:ILE:HD11	1:A:750:LEU:HB2	1.79	0.65
1:A:386:LEU:O	1:A:557:THR:HG21	1.97	0.65
1:A:367:ILE:O	1:A:371:VAL:HG23	1.97	0.64
1:A:1059:PRO:O	1:A:1063:MET:HG3	1.97	0.64
1:A:392:ALA:HB2	1:A:939:VAL:HG21	1.79	0.64
1:A:591:SER:HB2	1:A:596:THR:HG21	1.80	0.63
1:A:449:LEU:HD13	1:A:573:VAL:HG13	1.78	0.63
1:A:309:ASP:O	1:A:312:VAL:HG22	1.99	0.63
1:A:381:HIS:O	1:A:382:ASP:HB2	1.97	0.63
1:A:430:ASN:O	1:A:432:ARG:HG3	1.99	0.63
1:A:735:LYS:O	1:A:739:MET:HG3	1.98	0.63
1:A:864:PRO:O	1:A:865:VAL:HG12	1.98	0.63
1:A:370:GLU:O	1:A:374:MET:HG3	1.98	0.62
1:A:573:VAL:HG12	1:A:575:ILE:HG13	1.80	0.62
1:A:777:THR:HG21	1:A:882:LYS:HE3	1.80	0.62
1:A:296:ARG:HH22	1:A:308:GLN:HE21	1.45	0.62
1:A:324:LYS:O	1:A:328:TRP:HD1	1.82	0.61
1:A:951:ILE:HG12	1:A:985:LYS:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:THR:HG22	1:A:638:GLN:HG3	1.82	0.61
1:A:820:LEU:HD22	1:A:824:ASN:ND2	2.15	0.61
1:A:855:SER:HA	1:A:858:LEU:HD12	1.83	0.61
1:A:530:ASN:O	1:A:533:PRO:HD2	2.01	0.61
1:A:945:GLU:HG2	1:A:992:TYR:HE1	1.66	0.61
1:A:612:LEU:HD23	1:A:615:ILE:HD11	1.83	0.60
1:A:840:ASN:HD21	1:A:849:LYS:NZ	1.99	0.60
1:A:924:ASP:C	1:A:944:ILE:HD13	2.25	0.60
1:A:31:ASN:OD1	1:A:33:GLU:HG2	2.02	0.60
1:A:165:ARG:HD3	1:A:223:TYR:HB2	1.84	0.60
1:A:829:ARG:HG3	1:A:830:GLY:N	2.16	0.60
1:A:721:ARG:HD2	1:A:726:GLU:HG3	1.84	0.60
1:A:769:GLU:HG2	1:A:1047:LYS:HE2	1.84	0.60
1:A:4:TYR:HD1	1:A:733:LEU:HD22	1.66	0.60
1:A:538:ILE:O	1:A:542:LEU:HG	2.01	0.60
1:A:293:ASP:O	1:A:297:LYS:HG2	2.02	0.59
1:A:372:VAL:HA	1:A:545:LEU:HD21	1.83	0.59
1:A:820:LEU:HD13	1:A:824:ASN:HB2	1.83	0.59
1:A:8:LEU:HD23	1:A:74:ILE:HD12	1.85	0.59
1:A:447:ILE:HG22	1:A:448:PRO:O	2.03	0.58
1:A:264:ASN:HD21	1:A:268:GLU:HG3	1.68	0.58
1:A:1029:VAL:HG13	1:A:1066:LEU:HD23	1.86	0.58
1:A:28:TYR:CZ	1:A:784:ILE:HD13	2.38	0.58
1:A:553:LYS:O	1:A:557:THR:HG22	2.02	0.58
1:A:894:ILE:O	1:A:894:ILE:HG13	2.03	0.58
1:A:778:THR:O	1:A:782:VAL:HG23	2.03	0.58
1:A:959:GLN:CG	1:A:976:VAL:HG21	2.34	0.57
1:A:882:LYS:HB3	1:A:883:PRO:HD3	1.86	0.57
1:A:755:ARG:HD2	1:A:781:GLU:HG2	1.86	0.57
1:A:161:LYS:O	1:A:165:ARG:HG3	2.05	0.57
1:A:312:VAL:HG23	1:A:313:ASP:N	2.20	0.57
1:A:930:ILE:O	1:A:934:ILE:HG13	2.03	0.57
1:A:962:LEU:O	1:A:967:ILE:HB	2.05	0.57
1:A:368:ARG:HD3	1:A:540:MET:HE2	1.86	0.56
1:A:446:PRO:HG2	1:A:583:LYS:HD3	1.87	0.56
1:A:24:ILE:HB	1:A:75:LEU:HB3	1.87	0.56
1:A:303:ILE:HB	1:A:304:PRO:HD3	1.86	0.56
1:A:916:SER:HB2	1:A:1006:LEU:O	2.05	0.56
1:A:1018:ILE:HD12	1:A:1037:ALA:HB1	1.86	0.56
1:A:410:PHE:CZ	1:A:425:MET:HE3	2.40	0.56
1:A:705:THR:HB	1:A:850:ARG:HH11	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ILE:O	1:A:548:MET:HG3	2.06	0.55
1:A:900:MET:HE2	1:A:903:LEU:HG	1.89	0.55
1:A:969:LYS:NZ	1:A:969:LYS:HB2	2.21	0.55
1:A:400:ALA:HB2	1:A:470:PHE:CE2	2.42	0.55
1:A:135:LEU:HB3	1:A:706:GLN:HG2	1.90	0.54
1:A:340:LEU:O	1:A:344:LEU:HB2	2.08	0.54
1:A:419:LYS:HE3	1:A:841:SER:OG	2.07	0.54
1:A:824:ASN:O	1:A:826:ILE:N	2.41	0.54
1:A:343:ALA:O	1:A:346:GLN:HG3	2.08	0.54
1:A:368:ARG:HG3	1:A:541:GLY:N	2.23	0.54
1:A:398:SER:HB2	1:A:838:LYS:CE	2.37	0.54
1:A:319:PHE:N	1:A:320:PRO:CD	2.71	0.53
1:A:554:VAL:O	1:A:558:LEU:HB2	2.08	0.53
1:A:596:THR:O	1:A:600:ASN:HB2	2.07	0.53
1:A:75:LEU:HG	1:A:748:LEU:HD11	1.89	0.53
1:A:396:SER:O	1:A:398:SER:N	2.41	0.53
1:A:556:GLN:HE21	1:A:556:GLN:CA	2.04	0.53
1:A:840:ASN:HD21	1:A:849:LYS:HZ1	1.55	0.53
1:A:6:LEU:N	1:A:6:LEU:HD22	2.24	0.53
1:A:301:VAL:C	1:A:304:PRO:HD2	2.33	0.53
1:A:186:ASN:ND2	1:A:186:ASN:C	2.64	0.53
1:A:539:ILE:HG23	1:A:562:LYS:HG3	1.91	0.53
1:A:392:ALA:HB2	1:A:939:VAL:CG2	2.39	0.53
1:A:419:LYS:HE3	1:A:841:SER:CB	2.39	0.53
1:A:102:LEU:HD22	1:A:102:LEU:N	2.22	0.52
1:A:618:LYS:HD3	1:A:654:ASP:OD2	2.09	0.52
1:A:114:MET:HE1	1:A:180:TYR:CE1	2.45	0.52
1:A:1018:ILE:HD12	1:A:1037:ALA:CB	2.40	0.52
1:A:397:MET:HE2	1:A:470:PHE:HD2	1.73	0.52
1:A:551:ASP:HB3	1:A:554:VAL:HB	1.91	0.51
1:A:981:TYR:O	1:A:985:LYS:HG3	2.09	0.51
1:A:44:LYS:CB	1:A:58:LEU:HD21	2.39	0.51
1:A:207:ALA:O	1:A:211:ILE:HG13	2.11	0.51
1:A:791:LEU:HD23	1:A:791:LEU:H	1.75	0.51
1:A:886:THR:OG1	1:A:1055:PHE:HB3	2.11	0.51
1:A:651:VAL:O	1:A:655:VAL:HG23	2.10	0.51
1:A:804:ALA:O	1:A:809:LYS:HE3	2.11	0.51
1:A:820:LEU:HD13	1:A:824:ASN:CB	2.40	0.51
1:A:854:ILE:O	1:A:858:LEU:HG	2.11	0.51
1:A:217:VAL:HG13	1:A:222:ASP:HB2	1.91	0.51
1:A:283:GLN:CD	1:A:649:GLN:HG3	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:THR:HB	1:A:739:MET:HE3	1.92	0.51
1:A:56:ARG:HH12	1:A:57:LYS:HD3	1.76	0.50
1:A:209:SER:O	1:A:213:MET:HG3	2.10	0.50
1:A:644:THR:OG1	1:A:647:MET:HG3	2.11	0.50
1:A:2:GLY:HA2	1:A:754:GLU:OE1	2.12	0.50
1:A:928:SER:O	1:A:932:ARG:HD2	2.11	0.50
1:A:518:TYR:N	1:A:518:TYR:CD2	2.79	0.50
1:A:532:GLN:HB2	1:A:533:PRO:HD3	1.93	0.50
1:A:899:PHE:O	1:A:901:PRO:HD3	2.11	0.50
1:A:359:MET:HE2	1:A:359:MET:HA	1.94	0.50
1:A:375:LEU:C	1:A:378:PRO:HD2	2.37	0.50
1:A:880:ASP:OD2	1:A:1069:LYS:HE2	2.11	0.50
1:A:885:PHE:CE1	1:A:1056:CYS:HB2	2.47	0.50
1:A:485:LYS:HZ2	1:A:495:SER:HA	1.77	0.50
1:A:420:LYS:O	1:A:424:VAL:HG23	2.11	0.49
1:A:860:MET:HA	1:A:860:MET:HE3	1.94	0.49
1:A:138:LEU:HA	1:A:141:ASN:HD22	1.77	0.49
1:A:217:VAL:HG13	1:A:222:ASP:CB	2.42	0.49
1:A:473:GLN:HG2	1:A:561:TYR:CD1	2.48	0.49
1:A:473:GLN:HE21	1:A:594:LYS:HB3	1.76	0.49
1:A:680:ARG:HB3	1:A:689:PHE:CE1	2.47	0.49
1:A:970:ILE:HG23	1:A:971:ASP:OD1	2.13	0.49
1:A:999:ILE:HD11	1:A:1009:PHE:CZ	2.48	0.49
1:A:37:ARG:HH21	1:A:64:ASP:CG	2.20	0.49
1:A:295:MET:HE2	1:A:304:PRO:HG3	1.94	0.49
1:A:882:LYS:HE2	1:A:1036:TYR:OH	2.13	0.49
1:A:324:LYS:O	1:A:328:TRP:CD1	2.64	0.49
1:A:384:HIS:HE1	1:A:939:VAL:HB	1.78	0.49
1:A:428:MET:HE2	1:A:814:ARG:CZ	2.43	0.49
1:A:820:LEU:HD22	1:A:824:ASN:HD22	1.78	0.49
1:A:758:THR:HG22	1:A:766:PHE:O	2.12	0.49
1:A:145:VAL:CG2	1:A:211:ILE:HG23	2.42	0.49
1:A:213:MET:HB3	1:A:328:TRP:HZ3	1.78	0.49
1:A:397:MET:CE	1:A:467:TYR:HB2	2.43	0.49
1:A:515:MET:HE3	1:A:639:PHE:CE2	2.47	0.49
1:A:38:CYS:SG	1:A:65:VAL:HG13	2.53	0.49
1:A:775:TYR:O	1:A:777:THR:HG23	2.13	0.49
1:A:6:LEU:HD22	1:A:6:LEU:H	1.78	0.48
1:A:101:ASP:O	1:A:104:VAL:HG23	2.13	0.48
1:A:226:ALA:O	1:A:230:ILE:HG13	2.13	0.48
1:A:8:LEU:CD2	1:A:74:ILE:HD12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:SER:C	1:A:51:ASN:H	2.21	0.48
1:A:976:VAL:O	1:A:976:VAL:HG12	2.13	0.48
1:A:977:GLY:O	1:A:978:SER:O	2.30	0.48
1:A:137:SER:HB2	1:A:185:HIS:CD2	2.48	0.48
1:A:820:LEU:HD22	1:A:824:ASN:CB	2.44	0.48
1:A:439:PRO:HG2	1:A:468:GLU:OE1	2.13	0.48
1:A:789:MET:HE1	1:A:873:THR:HG21	1.96	0.48
1:A:885:PHE:CZ	1:A:1056:CYS:HB2	2.49	0.48
1:A:509:PHE:CD2	1:A:624:LYS:HB3	2.48	0.48
1:A:860:MET:HE1	1:A:864:PRO:HB3	1.96	0.48
1:A:8:LEU:HA	1:A:737:MET:SD	2.54	0.47
1:A:776:GLY:HA3	1:A:785:GLN:NE2	2.29	0.47
1:A:880:ASP:O	1:A:883:PRO:HD2	2.13	0.47
1:A:892:LEU:HD22	1:A:1017:LEU:HD11	1.96	0.47
1:A:133:ALA:CB	1:A:701:ARG:HG3	2.45	0.47
1:A:559:ASN:O	1:A:562:LYS:HB3	2.14	0.47
1:A:35:GLU:O	1:A:39:ILE:HG13	2.15	0.47
1:A:114:MET:HB2	1:A:117:GLU:HG2	1.95	0.47
1:A:992:TYR:CE2	1:A:996:LEU:HD11	2.50	0.47
1:A:101:ASP:OD1	1:A:101:ASP:C	2.56	0.47
1:A:377:GLU:HB2	1:A:378:PRO:HD3	1.97	0.47
1:A:449:LEU:HD22	1:A:573:VAL:CG1	2.45	0.47
1:A:1012:PRO:O	1:A:1016:LYS:HG3	2.15	0.47
1:A:699:GLU:OE1	1:A:700:LYS:HE3	2.15	0.47
1:A:790:SER:OG	1:A:791:LEU:HD23	2.15	0.47
1:A:808:PHE:O	1:A:812:VAL:HG23	2.14	0.47
1:A:419:LYS:HE3	1:A:841:SER:HB2	1.97	0.47
1:A:539:ILE:CG2	1:A:562:LYS:HE3	2.45	0.47
1:A:708:ASP:O	1:A:712:ILE:HG13	2.14	0.47
1:A:161:LYS:HB3	1:A:165:ARG:NH1	2.30	0.47
1:A:969:LYS:HB2	1:A:969:LYS:HZ2	1.80	0.47
1:A:368:ARG:O	1:A:372:VAL:HG23	2.15	0.46
1:A:534:PHE:HZ	1:A:599:ALA:HB1	1.81	0.46
1:A:165:ARG:HE	1:A:220:HIS:HA	1.79	0.46
1:A:108:ASP:HB2	1:A:113:LYS:NZ	2.31	0.46
1:A:126:THR:HG23	1:A:126:THR:O	2.14	0.46
1:A:247:PRO:O	1:A:251:LEU:HG	2.16	0.46
1:A:794:GLN:O	1:A:849:LYS:HE2	2.14	0.46
1:A:878:LEU:HD22	1:A:1036:TYR:CD1	2.51	0.46
1:A:1028:ALA:HB3	1:A:1067:TRP:HD1	1.80	0.46
1:A:581:ILE:O	1:A:581:ILE:HG22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:ILE:HG21	1:A:839:LEU:HD13	1.97	0.46
1:A:835:GLU:O	1:A:839:LEU:HG	2.15	0.46
1:A:34:LEU:O	1:A:37:ARG:HB2	2.15	0.46
1:A:56:ARG:NH1	1:A:57:LYS:HD3	2.30	0.46
1:A:100:ALA:O	1:A:102:LEU:HD22	2.16	0.46
1:A:224:LEU:HD12	1:A:306:MET:HE3	1.97	0.46
1:A:691:ALA:HB2	1:A:723:ARG:HB2	1.98	0.46
1:A:75:LEU:HD12	1:A:750:LEU:HD13	1.97	0.46
1:A:899:PHE:C	1:A:901:PRO:HD3	2.41	0.46
1:A:917:ARG:HD2	1:A:919:TYR:CE1	2.51	0.46
1:A:729:ARG:HE	1:A:770:ASP:CG	2.23	0.45
1:A:133:ALA:HB1	1:A:701:ARG:HG3	1.97	0.45
1:A:261:PHE:CD2	1:A:899:PHE:HB3	2.51	0.45
1:A:295:MET:HE1	1:A:303:ILE:CG2	2.41	0.45
1:A:517:LEU:C	1:A:517:LEU:HD23	2.41	0.45
1:A:984:ASP:O	1:A:988:ILE:HG12	2.15	0.45
1:A:130:MET:SD	1:A:130:MET:C	2.99	0.45
1:A:437:ILE:O	1:A:439:PRO:HD3	2.15	0.45
1:A:102:LEU:H	1:A:102:LEU:CD2	2.25	0.45
1:A:143:ASN:HD22	1:A:143:ASN:HA	1.56	0.45
1:A:837:ALA:C	1:A:839:LEU:H	2.24	0.45
1:A:147:PHE:O	1:A:151:LYS:HG2	2.17	0.45
1:A:622:ALA:N	1:A:638:GLN:O	2.50	0.45
1:A:415:ILE:HB	1:A:842:TYR:OH	2.15	0.45
1:A:542:LEU:HA	1:A:545:LEU:HD12	1.99	0.45
1:A:641:THR:HG23	1:A:647:MET:HE1	1.99	0.45
1:A:819:LEU:HD11	1:A:940:TYR:HB2	1.99	0.45
1:A:439:PRO:HA	1:A:440:PRO:HD3	1.79	0.44
1:A:397:MET:HE1	1:A:467:TYR:HB2	1.99	0.44
1:A:699:GLU:CD	1:A:700:LYS:HE3	2.43	0.44
1:A:824:ASN:ND2	1:A:964:SER:O	2.50	0.44
1:A:1026:ILE:HA	1:A:1027:PRO:HD2	1.78	0.44
1:A:397:MET:O	1:A:400:ALA:HB3	2.17	0.44
1:A:897:GLN:OE1	1:A:897:GLN:N	2.43	0.44
1:A:75:LEU:CD1	1:A:750:LEU:HD13	2.47	0.44
1:A:786:ARG:HD3	1:A:869:SER:HB2	2.00	0.44
1:A:924:ASP:HA	1:A:944:ILE:HB	2.00	0.44
1:A:1020:ILE:HG12	1:A:1056:CYS:HB3	1.99	0.44
1:A:473:GLN:O	1:A:477:VAL:HG23	2.17	0.44
1:A:111:ASN:O	1:A:113:LYS:N	2.48	0.44
1:A:495:SER:OG	1:A:496:GLN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:GLU:HG3	1:A:991:SER:OG	2.18	0.44
1:A:47:GLU:HA	1:A:50:LYS:HG2	1.99	0.44
1:A:440:PRO:O	1:A:445:LYS:HB3	2.17	0.44
1:A:479:LYS:HD3	1:A:479:LYS:HA	1.86	0.44
1:A:831:ILE:O	1:A:835:GLU:HG2	2.18	0.44
1:A:264:ASN:ND2	1:A:268:GLU:HG3	2.32	0.43
1:A:444:ASP:C	1:A:446:PRO:HD3	2.43	0.43
1:A:129:LEU:HB2	1:A:201:TYR:CE2	2.53	0.43
1:A:1026:ILE:O	1:A:1026:ILE:HG13	2.17	0.43
1:A:129:LEU:HB2	1:A:201:TYR:HE2	1.83	0.43
1:A:534:PHE:CZ	1:A:599:ALA:HB1	2.53	0.43
1:A:872:ILE:HG22	1:A:1073:ILE:HA	2.00	0.43
1:A:50:LYS:O	1:A:50:LYS:HG3	2.19	0.43
1:A:473:GLN:OE1	1:A:595:GLN:HG2	2.18	0.43
1:A:990:GLU:HG3	1:A:1031:PHE:CE1	2.54	0.43
1:A:404:GLU:H	1:A:404:GLU:HG2	1.62	0.43
1:A:967:ILE:HD12	1:A:967:ILE:N	2.34	0.43
1:A:215:MET:HE3	1:A:731:PHE:HB2	2.01	0.43
1:A:385:LEU:HD13	1:A:939:VAL:HG23	2.00	0.43
1:A:577:ASP:OD1	1:A:582:LYS:HE2	2.18	0.43
1:A:784:ILE:HG13	1:A:788:PHE:CE2	2.54	0.43
1:A:989:LEU:C	1:A:989:LEU:HD23	2.44	0.43
1:A:263:THR:HG23	1:A:267:LEU:HA	1.99	0.43
1:A:387:ARG:NH1	1:A:387:ARG:HB3	2.34	0.43
1:A:520:ASP:HB3	1:A:667:LYS:HB3	2.01	0.43
1:A:791:LEU:HD21	1:A:860:MET:SD	2.59	0.43
1:A:821:PHE:N	1:A:821:PHE:HD2	2.17	0.43
1:A:512:ASN:N	1:A:512:ASN:HD22	2.17	0.42
1:A:22:VAL:CG2	1:A:77:TYR:HB3	2.49	0.42
1:A:804:ALA:HA	1:A:809:LYS:HE3	2.00	0.42
1:A:826:ILE:O	1:A:829:ARG:HG2	2.19	0.42
1:A:538:ILE:HD12	1:A:565:GLN:NE2	2.35	0.42
1:A:514:THR:HG22	1:A:638:GLN:HA	2.00	0.42
1:A:516:VAL:HG21	1:A:675:ILE:CG2	2.49	0.42
1:A:863:LYS:HA	1:A:864:PRO:HD3	1.70	0.42
1:A:288:LEU:HD12	1:A:288:LEU:O	2.19	0.42
1:A:454:VAL:HG22	1:A:455:PRO:N	2.35	0.42
1:A:821:PHE:N	1:A:821:PHE:CD2	2.86	0.42
1:A:499:GLN:OE1	1:A:680:ARG:NH1	2.44	0.42
1:A:165:ARG:HD3	1:A:223:TYR:CB	2.48	0.42
1:A:338:LYS:O	1:A:339:MET:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:VAL:HG12	1:A:743:ALA:N	2.34	0.42
1:A:214:LEU:HA	1:A:217:VAL:HG23	2.01	0.42
1:A:73:SER:OG	1:A:750:LEU:HD11	2.20	0.41
1:A:195:VAL:HG23	1:A:196:MET:N	2.35	0.41
1:A:477:VAL:HG21	1:A:594:LYS:HG3	2.02	0.41
1:A:713:LEU:CD2	1:A:732:ILE:HG23	2.50	0.41
1:A:890:ALA:HB2	1:A:1053:SER:HB2	2.02	0.41
1:A:408:LEU:HD12	1:A:417:SER:HB3	2.02	0.41
1:A:799:ALA:HB2	1:A:845:ILE:HG23	2.02	0.41
1:A:1026:ILE:HD11	1:A:1067:TRP:CD1	2.55	0.41
1:A:549:THR:HG21	1:A:554:VAL:HG11	2.02	0.41
1:A:892:LEU:HD13	1:A:1017:LEU:HD21	2.03	0.41
1:A:151:LYS:HA	1:A:151:LYS:HD3	1.88	0.41
1:A:161:LYS:CB	1:A:165:ARG:HH12	2.33	0.41
1:A:179:LYS:HD3	1:A:180:TYR:CE2	2.56	0.41
1:A:542:LEU:HD11	1:A:561:TYR:HD2	1.86	0.41
1:A:441:VAL:HB	1:A:447:ILE:HD11	2.02	0.41
1:A:450:GLY:O	1:A:462:ILE:N	2.48	0.41
1:A:721:ARG:HH11	1:A:721:ARG:CG	2.34	0.41
1:A:58:LEU:HD12	1:A:58:LEU:HA	1.92	0.41
1:A:864:PRO:HB2	1:A:865:VAL:H	1.53	0.41
1:A:951:ILE:HG13	1:A:985:LYS:HG2	2.03	0.41
1:A:11:TYR:HA	1:A:147:PHE:CE1	2.56	0.41
1:A:429:ALA:C	1:A:431:GLU:H	2.29	0.40
1:A:541:GLY:O	1:A:545:LEU:HG	2.21	0.40
1:A:824:ASN:O	1:A:825:ASN:C	2.64	0.40
1:A:72:LEU:HD23	1:A:861:LEU:O	2.21	0.40
1:A:385:LEU:CD1	1:A:939:VAL:HG23	2.51	0.40
1:A:125:TYR:CG	1:A:126:THR:N	2.88	0.40
1:A:287:GLU:O	1:A:291:MET:HG3	2.22	0.40
1:A:430:ASN:OD1	1:A:430:ASN:N	2.55	0.40
1:A:477:VAL:HA	1:A:480:MET:HE3	2.04	0.40
1:A:775:TYR:HD1	1:A:875:ASN:OD1	2.04	0.40
1:A:884:PHE:CD1	1:A:1059:PRO:HD3	2.56	0.40
1:A:281:PRO:HG2	1:A:284:THR:OG1	2.21	0.40
1:A:318:LYS:HB2	1:A:318:LYS:NZ	2.37	0.40
1:A:185:HIS:CD2	1:A:185:HIS:H	2.38	0.40

There are no symmetry-related clashes.

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	1066/1095 (97%)	988 (93%)	64 (6%)	14 (1%)	9	32

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	397	MET
1	A	825	ASN
1	A	864	PRO
1	A	978	SER
1	A	382	ASP
1	A	495	SER
1	A	776	GLY
1	A	128	SER
1	A	430	ASN
1	A	870	SER
1	A	94	LYS
1	A	865	VAL
1	A	439	PRO
1	A	1027	PRO

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	973/996 (98%)	927 (95%)	46 (5%)	23	56

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	102	LEU
1	A	104	VAL
1	A	106	GLU
1	A	121	THR
1	A	135	LEU
1	A	143	ASN
1	A	155	ASP
1	A	156	VAL
1	A	186	ASN
1	A	194	ASP
1	A	229	LEU
1	A	313	ASP
1	A	320	PRO
1	A	358	GLU
1	A	401	SER
1	A	449	LEU
1	A	508	ARG
1	A	512	ASN
1	A	517	LEU
1	A	518	TYR
1	A	556	GLN
1	A	584	ILE
1	A	595	GLN
1	A	600	ASN
1	A	619	HIS
1	A	628	VAL
1	A	645	LYS
1	A	663	ASN
1	A	695	LEU
1	A	721	ARG
1	A	779	VAL
1	A	791	LEU
1	A	820	LEU
1	A	859	THR
1	A	872	ILE
1	A	892	LEU
1	A	895	GLN
1	A	922	GLU
1	A	927	LYS
1	A	931	SER
1	A	969	LYS
1	A	970	ILE

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Mol	Chain	Res	Type
1	A	1050	SER
1	A	1054	LEU
1	A	1056	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	36	ASN
1	A	48	ASN
1	A	83	ASN
1	A	143	ASN
1	A	185	HIS
1	A	186	ASN
1	A	289	ASN
1	A	290	GLN
1	A	308	GLN
1	A	337	GLN
1	A	384	HIS
1	A	423	HIS
1	A	473	GLN
1	A	512	ASN
1	A	528	GLN
1	A	530	ASN
1	A	532	GLN
1	A	556	GLN
1	A	565	GLN
1	A	574	GLN
1	A	579	ASN
1	A	649	GLN
1	A	653	ASN
1	A	698	ASN
1	A	706	GLN
1	A	760	ASN
1	A	810	ASN
1	A	824	ASN
1	A	840	ASN
1	A	853	GLN
1	A	895	GLN
1	A	908	GLN
1	A	912	GLN
1	A	1087	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	1072/1095 (97%)	0.14	23 (2%) 63 54	16, 53, 97, 147	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	861	LEU	4.5
1	A	28	TYR	3.8
1	A	79	TYR	3.3
1	A	18	SER	3.2
1	A	1023	LYS	2.9
1	A	776	GLY	2.7
1	A	865	VAL	2.7
1	A	864	PRO	2.7
1	A	1022	PHE	2.6
1	A	841	SER	2.6
1	A	847	LEU	2.6
1	A	408	LEU	2.5
1	A	866	THR	2.4
1	A	845	ILE	2.4
1	A	832	ALA	2.4
1	A	850	ARG	2.3
1	A	1029	VAL	2.3
1	A	867	PHE	2.3
1	A	77	TYR	2.3
1	A	824	ASN	2.2
1	A	22	VAL	2.2
1	A	862	GLN	2.2
1	A	859	THR	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.