



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:13 PM UTC

PDB ID : 4HBO / pdb_00004hbo
Title : Crystal Structure of Rubella virus capsid protein (residues 127-277)
Authors : Mangala Prasad, V.; Fokine, A.; Rossmann, M.G.
Deposited on : 2012-09-28
Resolution : 3.24 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

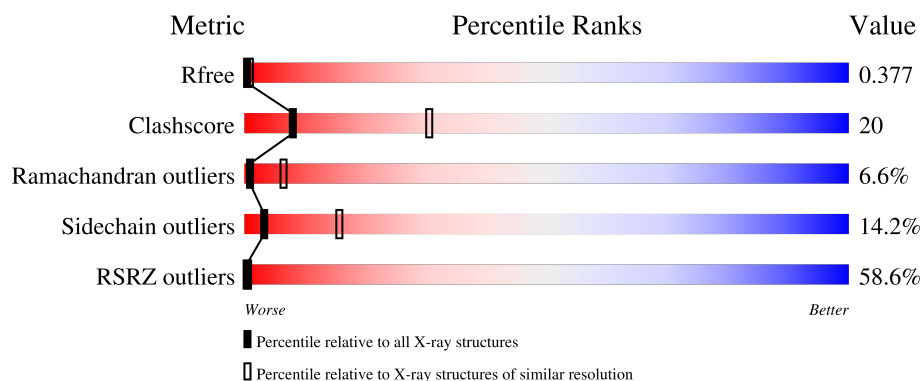
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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	131	44% 25% 23% 10% . 40%
1	B	131	40% 30% 21% 5% . 42%
1	C	131	45% 35% 21% 5% . 37%
1	D	131	19% 45% 15% .. 38%
1	E	131	27% 45% 14% . 38%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3155 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.

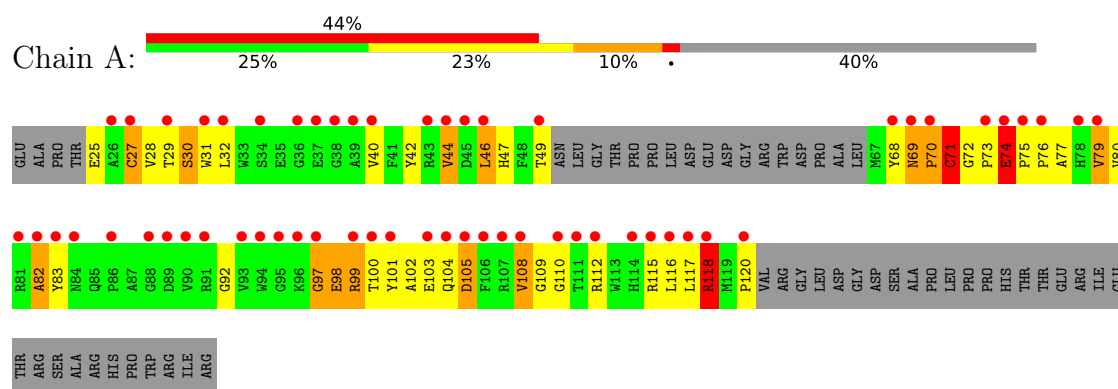
- Molecule 1 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	79	Total	C	N	O	S	Se	0	0	0
			628	397	117	111	2	1			
1	B	76	Total	C	N	O	S		0	0	0
			602	381	114	105	2				
1	C	82	Total	C	N	O	S	Se	0	0	0
			646	410	118	115	2	1			
1	D	81	Total	C	N	O	S	Se	0	0	0
			641	406	120	112	2	1			
1	E	81	Total	C	N	O	S	Se	0	0	0
			638	404	117	114	2	1			

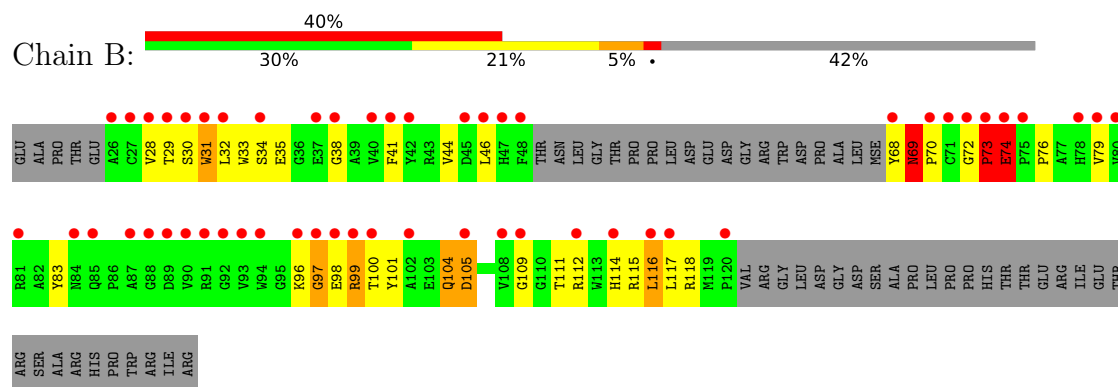
3 Residue-property plots [i](#)

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.

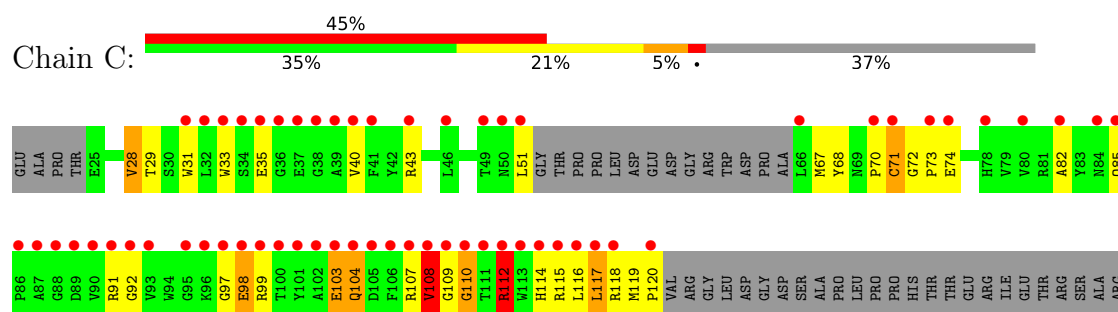
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein

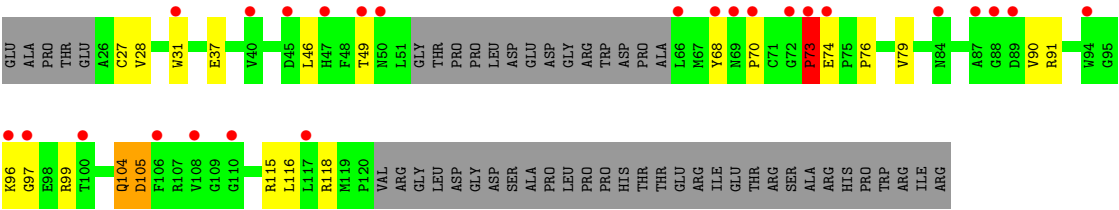


• Molecule 1: Capsid protein

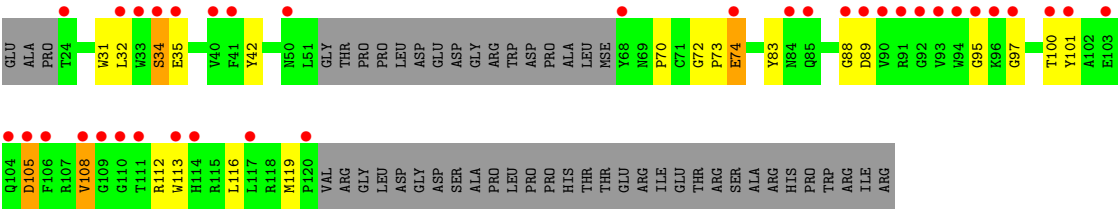


HIS
PRO
TRP
ARG
ILE
ARG

● Molecule 1: Capsid protein



● Molecule 1: Capsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	42.79Å 279.70Å 76.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.62 – 3.24 46.62 – 3.24	Depositor EDS
% Data completeness (in resolution range)	96.7 (46.62-3.24) 98.4 (46.62-3.24)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.340 , 0.368 0.348 , 0.377	Depositor DCC
R_{free} test set	760 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 123.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	3155	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 78.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.2009e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.56	0/647	1.73	15/878 (1.7%)
1	B	0.55	0/621	1.09	9/843 (1.1%)
1	C	0.46	0/664	1.02	2/901 (0.2%)
1	D	0.32	0/658	0.82	1/891 (0.1%)
1	E	0.33	0/657	0.83	2/893 (0.2%)
All	All	0.45	0/3247	1.14	29/4406 (0.7%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	PRO	CB-CA-C	19.11	143.09	111.56
1	A	71	CYS	CB-CA-C	-19.10	72.41	110.42
1	A	73	PRO	N-CA-C	16.27	145.99	112.47
1	A	74	GLU	N-CA-CB	14.39	135.99	110.37
1	A	72	GLY	N-CA-C	12.20	137.22	112.34
1	A	71	CYS	N-CA-C	-10.67	88.07	110.80
1	C	67	MSE	N-CA-C	-9.59	103.69	114.62
1	B	69	ASN	CA-C-N	7.97	129.80	119.84
1	B	69	ASN	C-N-CA	7.97	129.80	119.84
1	D	73	PRO	N-CA-CB	7.70	111.07	102.60
1	A	74	GLU	CA-C-N	6.58	127.16	120.38
1	A	74	GLU	C-N-CA	6.58	127.16	120.38
1	A	99	ARG	NE-CZ-NH1	-6.45	115.05	121.50
1	A	118	ARG	NE-CZ-NH1	6.41	127.91	121.50
1	B	72	GLY	CA-C-N	6.32	127.74	119.84
1	B	72	GLY	C-N-CA	6.32	127.74	119.84
1	B	74	GLU	CA-C-N	6.00	126.56	120.38
1	B	74	GLU	C-N-CA	6.00	126.56	120.38
1	B	38	GLY	N-CA-C	-5.97	107.01	115.43
1	B	73	PRO	CA-N-CD	-5.90	103.74	112.00
1	A	118	ARG	N-CA-CB	5.84	118.62	109.69
1	A	27	CYS	N-CA-C	5.78	118.07	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	ARG	NE-CZ-NH1	-5.65	115.85	121.50
1	E	72	GLY	CA-C-N	5.40	124.58	118.97
1	E	72	GLY	C-N-CA	5.40	124.58	118.97
1	A	97	GLY	N-CA-C	5.37	118.93	110.71
1	A	118	ARG	CD-NE-CZ	5.23	131.73	124.40
1	B	97	GLY	N-CA-C	5.21	119.05	110.77
1	A	118	ARG	NE-CZ-NH2	-5.08	114.62	119.20

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	628	0	581	47	1
1	B	602	0	552	19	0
1	C	646	0	598	25	0
1	D	641	0	597	13	0
1	E	638	0	587	16	0
All	All	3155	0	2915	119	1

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 (119) 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:118:ARG:HG2	1:C:120:PRO:HD3	1.50	0.93
1:A:99:ARG:HE	1:A:118:ARG:HE	1.09	0.93
1:A:99:ARG:NE	1:A:118:ARG:HE	1.78	0.81
1:A:99:ARG:HE	1:A:118:ARG:NE	1.79	0.80
1:A:105:ASP:N	1:A:105:ASP:OD1	2.20	0.74
1:A:71:CYS:SG	1:A:71:CYS:O	2.37	0.73
1:C:31:TRP:HE1	1:C:43:ARG:HG2	1.56	0.70
1:C:31:TRP:NE1	1:C:43:ARG:HG2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:ARG:HB2	1:D:118:ARG:HH12	1.58	0.69
1:A:28:VAL:HB	1:A:46:LEU:HD11	1.75	0.69
1:A:99:ARG:HA	1:A:118:ARG:NH2	2.08	0.68
1:A:30:SER:OG	1:A:83:TYR:OH	2.11	0.68
1:A:97:GLY:HA2	1:A:98:GLU:C	2.19	0.67
1:D:73:PRO:O	1:D:74:GLU:HG3	1.95	0.66
1:A:28:VAL:HG12	1:A:29:THR:H	1.61	0.65
1:A:29:THR:OG1	1:A:44:VAL:O	2.12	0.65
1:D:97:GLY:HA3	1:D:99:ARG:N	2.12	0.65
1:D:91:ARG:NH1	1:D:105:ASP:OD2	2.28	0.64
1:B:105:ASP:OD2	1:B:105:ASP:N	2.31	0.63
1:C:92:GLY:HA2	1:D:96:LYS:HD3	1.79	0.63
1:C:82:ALA:O	1:C:115:ARG:NH2	2.32	0.62
1:A:115:ARG:HG2	1:A:117:LEU:HD11	1.82	0.62
1:A:97:GLY:HA2	1:A:99:ARG:N	2.15	0.61
1:C:103:GLU:HB2	1:C:114:HIS:CE1	2.36	0.61
1:C:114:HIS:ND1	1:C:115:ARG:N	2.47	0.61
1:E:32:LEU:HD22	1:E:83:TYR:HB2	1.83	0.59
1:E:95:GLY:HA3	1:E:100:THR:HA	1.84	0.59
1:A:118:ARG:HG3	1:A:120:PRO:HD3	1.84	0.59
1:C:104:GLN:HG3	1:C:115:ARG:HB3	1.85	0.58
1:C:117:LEU:HD13	1:C:119:MSE:HE2	1.85	0.58
1:C:115:ARG:HG2	1:C:117:LEU:HG	1.85	0.57
1:A:25:GLU:HG3	1:A:49:THR:HA	1.85	0.57
1:E:73:PRO:O	1:E:74:GLU:HB2	2.04	0.57
1:B:101:TYR:HB3	1:B:116:LEU:HD23	1.87	0.57
1:B:73:PRO:O	1:B:74:GLU:HG3	2.05	0.57
1:C:107:ARG:HA	1:C:112:ARG:HA	1.87	0.56
1:B:97:GLY:HA3	1:B:98:GLU:HB2	1.88	0.56
1:A:92:GLY:HA3	1:A:103:GLU:HB3	1.87	0.56
1:A:27:CYS:SG	1:A:47:HIS:ND1	2.46	0.56
1:A:32:LEU:O	1:A:42:TYR:HB2	2.06	0.56
1:C:85:GLN:O	1:C:115:ARG:NH1	2.22	0.55
1:C:103:GLU:CB	1:C:114:HIS:CE1	2.90	0.55
1:A:104:GLN:HG2	1:A:115:ARG:O	2.07	0.55
1:C:97:GLY:HA3	1:C:99:ARG:H	1.71	0.54
1:B:68:TYR:O	1:B:69:ASN:ND2	2.41	0.54
1:A:76:PRO:HB2	1:A:79:VAL:HG23	1.91	0.53
1:C:97:GLY:HA3	1:C:99:ARG:N	2.23	0.53
1:A:30:SER:C	1:A:31:TRP:HD1	2.16	0.52
1:A:99:ARG:CZ	1:A:118:ARG:HE	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:TRP:CD1	1:C:43:ARG:HG2	2.44	0.52
1:A:82:ALA:O	1:A:115:ARG:NH2	2.38	0.52
1:C:28:VAL:HG12	1:C:29:THR:H	1.76	0.51
1:C:35:GLU:HB2	1:C:112:ARG:HE	1.76	0.51
1:D:97:GLY:HA3	1:D:99:ARG:H	1.76	0.50
1:A:77:ALA:HA	1:A:80:VAL:HG12	1.93	0.50
1:E:100:THR:OG1	1:E:119:MSE:O	2.28	0.50
1:A:102:ALA:O	1:A:116:LEU:HA	2.12	0.50
1:A:100:THR:O	1:A:118:ARG:HD3	2.12	0.50
1:D:105:ASP:N	1:D:105:ASP:OD1	2.43	0.50
1:A:42:TYR:CZ	1:A:79:VAL:HG11	2.47	0.49
1:E:108:VAL:CG1	1:E:113:TRP:CD1	2.96	0.49
1:B:33:TRP:HB3	1:B:41:PHE:CD1	2.47	0.49
1:A:30:SER:HG	1:A:83:TYR:HH	1.40	0.49
1:B:32:LEU:HD22	1:B:83:TYR:HB2	1.95	0.49
1:A:28:VAL:HG13	1:A:99:ARG:HH12	1.77	0.49
1:B:31:TRP:CD1	1:B:31:TRP:N	2.81	0.48
1:A:99:ARG:NH2	1:A:118:ARG:HG2	2.28	0.48
1:B:34:SER:OG	1:B:35:GLU:N	2.37	0.48
1:A:68:TYR:O	1:A:69:ASN:HB2	2.14	0.48
1:E:31:TRP:HZ3	1:E:101:TYR:CZ	2.32	0.48
1:B:30:SER:OG	1:B:83:TYR:OH	2.20	0.48
1:B:83:TYR:O	1:B:115:ARG:NH1	2.47	0.48
1:B:104:GLN:HG3	1:B:115:ARG:HB3	1.96	0.47
1:E:105:ASP:N	1:E:105:ASP:OD1	2.47	0.47
1:A:44:VAL:HG21	1:A:83:TYR:CZ	2.50	0.46
1:A:99:ARG:HH21	1:A:118:ARG:NE	2.13	0.46
1:C:107:ARG:NH1	1:C:109:GLY:H	2.14	0.46
1:A:99:ARG:HA	1:A:118:ARG:CZ	2.45	0.46
1:E:32:LEU:O	1:E:42:TYR:HB2	2.16	0.46
1:A:42:TYR:CE1	1:A:79:VAL:HG11	2.51	0.45
1:A:118:ARG:HD2	1:A:120:PRO:HD3	1.98	0.45
1:A:99:ARG:NH2	1:A:118:ARG:HE	2.15	0.45
1:C:103:GLU:CB	1:C:114:HIS:HE1	2.29	0.45
1:D:31:TRP:CE3	1:D:116:LEU:HD23	2.52	0.45
1:E:108:VAL:HG13	1:E:113:TRP:CD1	2.51	0.45
1:A:32:LEU:HD22	1:A:83:TYR:HB2	1.99	0.45
1:C:103:GLU:HB3	1:C:114:HIS:HE1	1.81	0.44
1:C:72:GLY:HA2	1:C:73:PRO:HD3	1.77	0.44
1:B:33:TRP:CE2	1:B:114:HIS:HB2	2.52	0.44
1:D:27:CYS:HA	1:D:46:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:ASP:OD1	1:E:89:ASP:N	2.37	0.44
1:D:104:GLN:HG3	1:D:115:ARG:HB3	1.99	0.44
1:E:34:SER:HA	1:E:112:ARG:O	2.17	0.44
1:E:31:TRP:HB2	1:E:116:LEU:HB2	2.00	0.43
1:A:46:LEU:H	1:A:46:LEU:HG	1.71	0.43
1:B:76:PRO:HB2	1:B:79:VAL:HG23	2.01	0.43
1:C:108:VAL:C	1:C:110:GLY:H	2.26	0.43
1:B:28:VAL:HG12	1:B:46:LEU:HB2	2.00	0.43
1:A:99:ARG:HD3	1:A:101:TYR:CE2	2.54	0.43
1:D:28:VAL:HG13	1:D:46:LEU:HB2	2.00	0.43
1:A:108:VAL:O	1:A:110:GLY:N	2.51	0.43
1:C:91:ARG:CZ	1:C:91:ARG:HB2	2.48	0.42
1:A:99:ARG:HH21	1:A:118:ARG:HE	1.66	0.42
1:D:28:VAL:CG2	1:D:118:ARG:HD3	2.49	0.42
1:D:76:PRO:HB2	1:D:79:VAL:HG23	2.02	0.42
1:A:115:ARG:HG2	1:A:117:LEU:CD1	2.49	0.42
1:C:31:TRP:HB2	1:C:116:LEU:HB3	2.02	0.42
1:B:97:GLY:HA3	1:B:99:ARG:N	2.34	0.42
1:B:97:GLY:CA	1:B:98:GLU:HB2	2.49	0.42
1:A:31:TRP:CD1	1:A:31:TRP:N	2.88	0.42
1:E:108:VAL:CG1	1:E:113:TRP:HD1	2.33	0.41
1:A:116:LEU:C	1:A:117:LEU:HD12	2.45	0.41
1:E:32:LEU:HG	1:E:113:TRP:CE3	2.55	0.41
1:A:118:ARG:HD2	1:A:120:PRO:N	2.36	0.41
1:B:100:THR:H	1:B:118:ARG:NH1	2.19	0.41
1:E:108:VAL:HG13	1:E:113:TRP:HD1	1.86	0.41
1:B:97:GLY:HA3	1:B:99:ARG:H	1.86	0.41
1:E:35:GLU:OE1	1:E:112:ARG:NH1	2.54	0.40
1:A:80:VAL:O	1:A:82:ALA:N	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLU:OE1	1:A:99:ARG:NH2[3_455]	2.13	0.07

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	75/131 (57%)	57 (76%)	10 (13%)	8 (11%)	0	2
1	B	72/131 (55%)	61 (85%)	6 (8%)	5 (7%)	1	6
1	C	78/131 (60%)	60 (77%)	12 (15%)	6 (8%)	1	4
1	D	77/131 (59%)	62 (80%)	13 (17%)	2 (3%)	4	23
1	E	77/131 (59%)	64 (83%)	9 (12%)	4 (5%)	1	10
All	All	379/655 (58%)	304 (80%)	50 (13%)	25 (7%)	1	6

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	PRO
1	A	74	GLU
1	B	70	PRO
1	B	73	PRO
1	D	73	PRO
1	A	98	GLU
1	A	109	GLY
1	B	96	LYS
1	C	108	VAL
1	D	70	PRO
1	E	97	GLY
1	A	82	ALA
1	C	71	CYS
1	E	74	GLU
1	A	71	CYS
1	A	75	PRO
1	C	98	GLU
1	A	69	ASN
1	B	109	GLY
1	C	74	GLU
1	B	74	GLU

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Mol	Chain	Res	Type
1	C	70	PRO
1	E	88	GLY
1	C	110	GLY
1	E	70	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	62/106 (58%)	51 (82%)	11 (18%)	2	9
1	B	58/106 (55%)	46 (79%)	12 (21%)	1	6
1	C	64/106 (60%)	52 (81%)	12 (19%)	1	8
1	D	63/106 (59%)	57 (90%)	6 (10%)	8	30
1	E	63/106 (59%)	60 (95%)	3 (5%)	23	53
All	All	310/530 (58%)	266 (86%)	44 (14%)	3	16

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	SER
1	A	40	VAL
1	A	44	VAL
1	A	46	LEU
1	A	71	CYS
1	A	74	GLU
1	A	79	VAL
1	A	105	ASP
1	A	108	VAL
1	A	112	ARG
1	A	118	ARG
1	B	29	THR
1	B	31	TRP
1	B	44	VAL
1	B	69	ASN

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Mol	Chain	Res	Type
1	B	73	PRO
1	B	99	ARG
1	B	104	GLN
1	B	105	ASP
1	B	111	THR
1	B	112	ARG
1	B	116	LEU
1	B	117	LEU
1	C	28	VAL
1	C	33	TRP
1	C	40	VAL
1	C	51	LEU
1	C	68	TYR
1	C	71	CYS
1	C	98	GLU
1	C	103	GLU
1	C	104	GLN
1	C	108	VAL
1	C	112	ARG
1	C	117	LEU
1	D	37	GLU
1	D	49	THR
1	D	68	TYR
1	D	90	VAL
1	D	104	GLN
1	D	105	ASP
1	E	34	SER
1	E	105	ASP
1	E	108	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	C	69	ASN
1	C	84	ASN
1	D	78	HIS
1	E	78	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](#)

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	77/131 (58%)	2.97	57 (74%) 0 0	52, 119, 166, 207	0
1	B	75/131 (57%)	2.54	52 (69%) 0 0	56, 95, 145, 167	0
1	C	80/131 (61%)	2.89	59 (73%) 0 0	46, 110, 172, 216	0
1	D	79/131 (60%)	1.74	25 (31%) 1 1	41, 70, 113, 131	0
1	E	80/131 (61%)	1.98	36 (45%) 0 1	42, 79, 124, 146	0
All	All	391/655 (59%)	2.42	229 (58%) 0 0	41, 96, 149, 216	0

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	PHE	11.8
1	C	114	HIS	9.4
1	A	100	THR	7.1
1	A	78	HIS	6.3
1	B	73	PRO	6.2
1	C	87	ALA	6.1
1	C	105	ASP	5.9
1	E	90	VAL	5.7
1	A	75	PRO	5.7
1	A	27	CYS	5.5
1	C	100	THR	5.5
1	E	95	GLY	5.4
1	A	114	HIS	5.3
1	B	48	PHE	5.3
1	C	36	GLY	5.3
1	A	74	GLU	5.3
1	E	110	GLY	5.1
1	C	116	LEU	5.1
1	A	73	PRO	4.9
1	C	34	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	84	ASN	4.8
1	E	89	ASP	4.7
1	B	100	THR	4.7
1	C	107	ARG	4.7
1	A	95	GLY	4.6
1	C	106	PHE	4.6
1	C	99	ARG	4.5
1	A	29	THR	4.4
1	B	29	THR	4.4
1	C	104	GLN	4.3
1	C	88	GLY	4.3
1	B	72	GLY	4.3
1	D	50	ASN	4.3
1	E	41	PHE	4.2
1	C	86	PRO	4.2
1	C	43	ARG	4.2
1	D	66	LEU	4.1
1	A	84	ASN	4.1
1	A	94	TRP	4.1
1	B	112	ARG	4.1
1	B	37	GLU	4.0
1	B	47	HIS	4.0
1	C	90	VAL	4.0
1	A	34	SER	4.0
1	A	90	VAL	4.0
1	D	88	GLY	4.0
1	A	68	TYR	4.0
1	B	38	GLY	3.9
1	E	88	GLY	3.9
1	C	78	HIS	3.9
1	E	113	TRP	3.9
1	C	74	GLU	3.8
1	A	26	ALA	3.8
1	D	106	PHE	3.8
1	C	71	CYS	3.8
1	A	99	ARG	3.8
1	C	89	ASP	3.8
1	C	96	LYS	3.8
1	B	70	PRO	3.8
1	D	89	ASP	3.8
1	E	106	PHE	3.7
1	D	74	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	74	GLU	3.6
1	B	26	ALA	3.6
1	D	110	GLY	3.6
1	E	34	SER	3.6
1	B	88	GLY	3.6
1	E	93	VAL	3.6
1	C	109	GLY	3.5
1	B	40	VAL	3.5
1	B	27	CYS	3.5
1	C	38	GLY	3.5
1	C	111	THR	3.4
1	A	81	ARG	3.4
1	A	118	ARG	3.4
1	E	101	TYR	3.4
1	A	36	GLY	3.4
1	D	100	THR	3.4
1	C	120	PRO	3.4
1	B	93	VAL	3.4
1	A	70	PRO	3.4
1	A	107	ARG	3.3
1	D	31	TRP	3.3
1	A	96	LYS	3.3
1	D	97	GLY	3.3
1	A	49	THR	3.2
1	E	94	TRP	3.2
1	E	109	GLY	3.2
1	E	74	GLU	3.2
1	A	89	ASP	3.2
1	B	97	GLY	3.2
1	B	68	TYR	3.2
1	C	110	GLY	3.1
1	B	116	LEU	3.1
1	C	92	GLY	3.1
1	A	82	ALA	3.1
1	A	32	LEU	3.1
1	B	46	LEU	3.1
1	B	99	ARG	3.1
1	E	33	TRP	3.1
1	B	90	VAL	3.0
1	A	120	PRO	3.0
1	C	39	ALA	3.0
1	C	101	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	46	LEU	3.0
1	B	114	HIS	3.0
1	B	84	ASN	3.0
1	C	37	GLU	3.0
1	C	102	ALA	3.0
1	A	40	VAL	2.9
1	C	80	VAL	2.9
1	C	95	GLY	2.9
1	C	97	GLY	2.9
1	A	79	VAL	2.9
1	B	30	SER	2.9
1	B	91	ARG	2.9
1	A	86	PRO	2.9
1	C	103	GLU	2.9
1	D	87	ALA	2.9
1	E	108	VAL	2.9
1	C	35	GLU	2.9
1	B	31	TRP	2.9
1	D	94	TRP	2.9
1	A	38	GLY	2.9
1	A	101	TYR	2.9
1	C	41	PHE	2.9
1	C	33	TRP	2.8
1	C	50	ASN	2.8
1	A	112	ARG	2.8
1	A	108	VAL	2.8
1	E	40	VAL	2.8
1	B	89	ASP	2.8
1	A	31	TRP	2.8
1	B	78	HIS	2.8
1	A	104	GLN	2.8
1	B	81	ARG	2.8
1	D	40	VAL	2.8
1	C	32	LEU	2.8
1	A	110	GLY	2.7
1	B	108	VAL	2.7
1	E	24	THR	2.7
1	A	117	LEU	2.7
1	C	51	LEU	2.7
1	C	70	PRO	2.7
1	D	70	PRO	2.7
1	C	115	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	49	THR	2.7
1	E	105	ASP	2.7
1	C	91	ARG	2.7
1	B	102	ALA	2.7
1	B	41	PHE	2.6
1	B	80	VAL	2.6
1	D	45	ASP	2.6
1	C	112	ARG	2.6
1	D	73	PRO	2.6
1	D	72	GLY	2.6
1	C	40	VAL	2.6
1	E	114	HIS	2.6
1	E	97	GLY	2.6
1	A	44	VAL	2.6
1	B	92	GLY	2.6
1	C	108	VAL	2.6
1	B	96	LYS	2.6
1	B	71	CYS	2.6
1	E	68	TYR	2.6
1	C	73	PRO	2.6
1	A	45	ASP	2.6
1	C	82	ALA	2.6
1	A	115	ARG	2.5
1	E	100	THR	2.5
1	A	43	ARG	2.5
1	C	118	ARG	2.5
1	D	69	ASN	2.5
1	C	113	TRP	2.5
1	E	96	LYS	2.5
1	E	32	LEU	2.5
1	A	93	VAL	2.5
1	C	66	LEU	2.4
1	D	68	TYR	2.4
1	A	97	GLY	2.4
1	B	28	VAL	2.4
1	B	98	GLU	2.4
1	E	103	GLU	2.4
1	A	105	ASP	2.4
1	B	45	ASP	2.4
1	A	83	TYR	2.4
1	E	104	GLN	2.4
1	C	117	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	39	ALA	2.4
1	E	120	PRO	2.4
1	E	50	ASN	2.3
1	D	47	HIS	2.3
1	E	91	ARG	2.3
1	C	31	TRP	2.3
1	C	98	GLU	2.3
1	D	96	LYS	2.2
1	D	108	VAL	2.2
1	E	92	GLY	2.2
1	E	84	ASN	2.2
1	A	111	THR	2.2
1	B	34	SER	2.2
1	B	117	LEU	2.1
1	B	87	ALA	2.1
1	E	111	THR	2.1
1	A	91	ARG	2.1
1	E	35	GLU	2.1
1	B	94	TRP	2.1
1	A	116	LEU	2.1
1	A	103	GLU	2.1
1	B	109	GLY	2.1
1	A	69	ASN	2.1
1	D	84	ASN	2.1
1	B	32	LEU	2.1
1	B	105	ASP	2.1
1	E	117	LEU	2.1
1	A	88	GLY	2.1
1	A	76	PRO	2.1
1	B	75	PRO	2.1
1	E	85	GLN	2.1
1	A	37	GLU	2.1
1	C	93	VAL	2.0
1	D	117	LEU	2.0
1	C	85	GLN	2.0
1	B	120	PRO	2.0
1	B	42	TYR	2.0
1	C	49	THR	2.0
1	B	85	GLN	2.0
1	B	79	VAL	2.0
1	C	46	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.