



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:38 PM UTC

PDB ID : 8XMS / pdb_00008xms
Title : Crystal structure of Porcine Circovirus type II Rep ATPase domain
Authors : Guan, S.Y.; Song, Y.F.
Deposited on : 2023-12-28
Resolution : 2.20 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

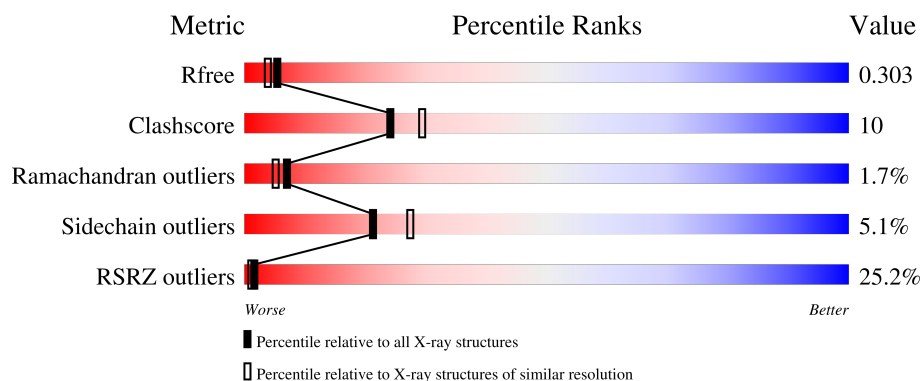
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	163	16% 69% 15% •• 13%
1	B	163	24% 71% 15% •• 12%
1	C	163	21% 72% 11% • 14%
1	D	163	21% 66% 19% • 13%
1	E	163	21% 71% 15% • 13%

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Mol	Chain	Length	Quality of chain
1	F	163	27% 66% 16% •• 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7076 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 Replication-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1154	749	191	210	4			
1	B	144	Total	C	N	O	S	0	0	0
			1166	756	193	213	4			
1	C	140	Total	C	N	O	S	0	0	0
			1141	742	189	206	4			
1	D	142	Total	C	N	O	S	0	0	0
			1153	749	190	210	4			
1	E	141	Total	C	N	O	S	0	0	0
			1149	747	189	209	4			
1	F	139	Total	C	N	O	S	0	0	0
			1135	739	188	204	4			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8BB16
A	154	GLY	-	expression tag	UNP Q8BB16
A	155	SER	-	expression tag	UNP Q8BB16
A	156	LEU	-	expression tag	UNP Q8BB16
A	157	GLU	-	expression tag	UNP Q8BB16
A	158	HIS	-	expression tag	UNP Q8BB16
A	159	HIS	-	expression tag	UNP Q8BB16
A	160	HIS	-	expression tag	UNP Q8BB16
A	161	HIS	-	expression tag	UNP Q8BB16
A	162	HIS	-	expression tag	UNP Q8BB16
A	163	HIS	-	expression tag	UNP Q8BB16
B	1	MET	-	initiating methionine	UNP Q8BB16
B	154	GLY	-	expression tag	UNP Q8BB16
B	155	SER	-	expression tag	UNP Q8BB16
B	156	LEU	-	expression tag	UNP Q8BB16
B	157	GLU	-	expression tag	UNP Q8BB16
B	158	HIS	-	expression tag	UNP Q8BB16

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Chain	Residue	Modelled	Actual	Comment	Reference
B	159	HIS	-	expression tag	UNP Q8BB16
B	160	HIS	-	expression tag	UNP Q8BB16
B	161	HIS	-	expression tag	UNP Q8BB16
B	162	HIS	-	expression tag	UNP Q8BB16
B	163	HIS	-	expression tag	UNP Q8BB16
C	1	MET	-	initiating methionine	UNP Q8BB16
C	154	GLY	-	expression tag	UNP Q8BB16
C	155	SER	-	expression tag	UNP Q8BB16
C	156	LEU	-	expression tag	UNP Q8BB16
C	157	GLU	-	expression tag	UNP Q8BB16
C	158	HIS	-	expression tag	UNP Q8BB16
C	159	HIS	-	expression tag	UNP Q8BB16
C	160	HIS	-	expression tag	UNP Q8BB16
C	161	HIS	-	expression tag	UNP Q8BB16
C	162	HIS	-	expression tag	UNP Q8BB16
C	163	HIS	-	expression tag	UNP Q8BB16
D	1	MET	-	initiating methionine	UNP Q8BB16
D	154	GLY	-	expression tag	UNP Q8BB16
D	155	SER	-	expression tag	UNP Q8BB16
D	156	LEU	-	expression tag	UNP Q8BB16
D	157	GLU	-	expression tag	UNP Q8BB16
D	158	HIS	-	expression tag	UNP Q8BB16
D	159	HIS	-	expression tag	UNP Q8BB16
D	160	HIS	-	expression tag	UNP Q8BB16
D	161	HIS	-	expression tag	UNP Q8BB16
D	162	HIS	-	expression tag	UNP Q8BB16
D	163	HIS	-	expression tag	UNP Q8BB16
E	1	MET	-	initiating methionine	UNP Q8BB16
E	154	GLY	-	expression tag	UNP Q8BB16
E	155	SER	-	expression tag	UNP Q8BB16
E	156	LEU	-	expression tag	UNP Q8BB16
E	157	GLU	-	expression tag	UNP Q8BB16
E	158	HIS	-	expression tag	UNP Q8BB16
E	159	HIS	-	expression tag	UNP Q8BB16
E	160	HIS	-	expression tag	UNP Q8BB16
E	161	HIS	-	expression tag	UNP Q8BB16
E	162	HIS	-	expression tag	UNP Q8BB16
E	163	HIS	-	expression tag	UNP Q8BB16
F	1	MET	-	initiating methionine	UNP Q8BB16
F	154	GLY	-	expression tag	UNP Q8BB16
F	155	SER	-	expression tag	UNP Q8BB16
F	156	LEU	-	expression tag	UNP Q8BB16

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Chain	Residue	Modelled	Actual	Comment	Reference
F	157	GLU	-	expression tag	UNP Q8BB16
F	158	HIS	-	expression tag	UNP Q8BB16
F	159	HIS	-	expression tag	UNP Q8BB16
F	160	HIS	-	expression tag	UNP Q8BB16
F	161	HIS	-	expression tag	UNP Q8BB16
F	162	HIS	-	expression tag	UNP Q8BB16
F	163	HIS	-	expression tag	UNP Q8BB16

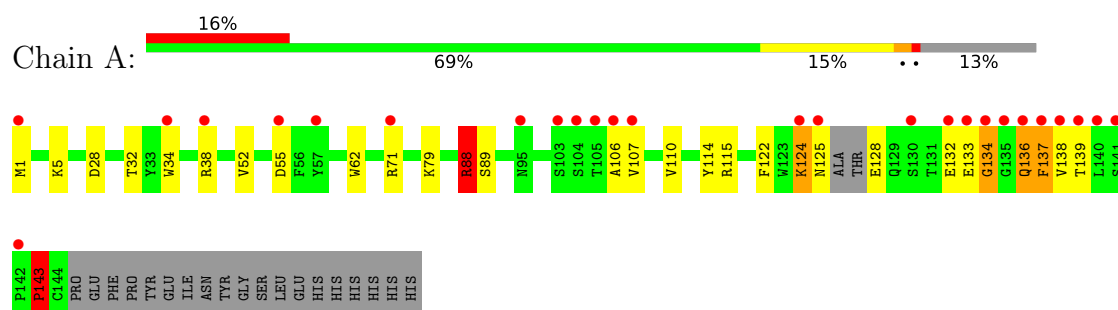
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	44	Total O 44 44	0	0
2	B	35	Total O 35 35	0	0
2	C	27	Total O 27 27	0	0
2	D	25	Total O 25 25	0	0
2	E	26	Total O 26 26	0	0
2	F	21	Total O 21 21	0	0

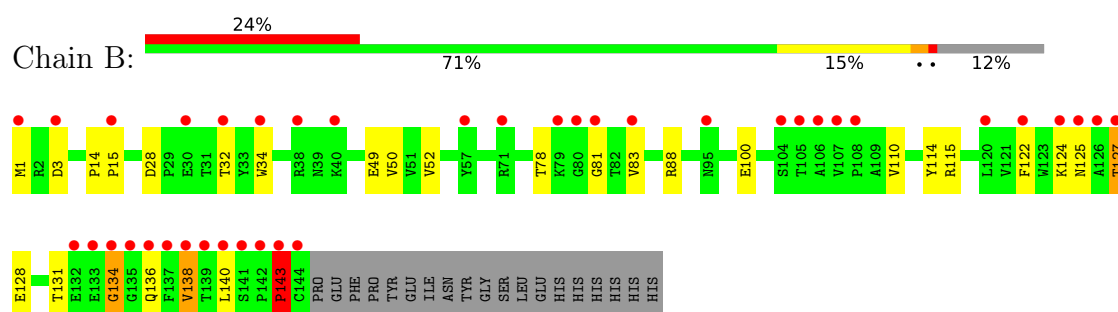
3 Residue-property plots [i](#)

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.

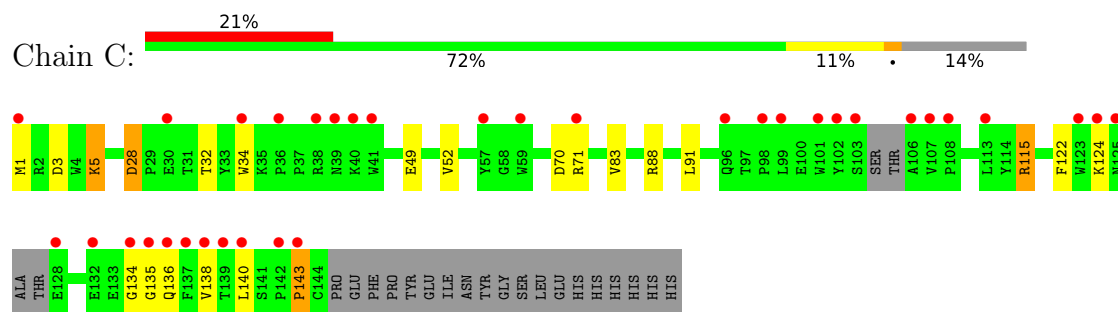
• Molecule 1: Replication-associated protein



• Molecule 1: Replication-associated protein

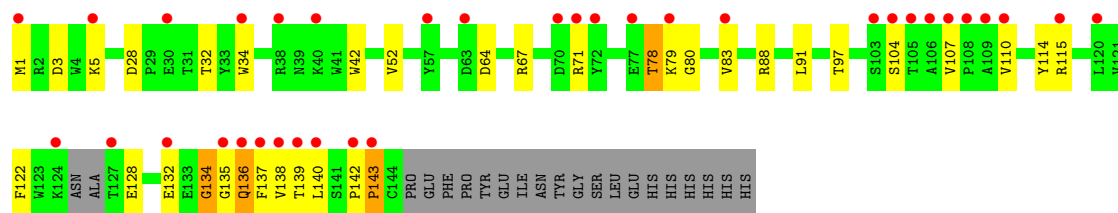


• Molecule 1: Replication-associated protein

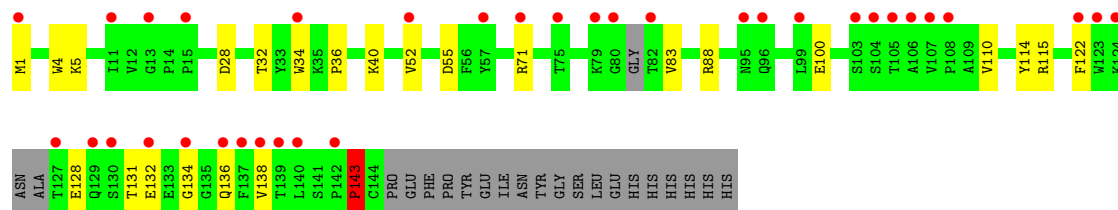


• Molecule 1: Replication-associated protein

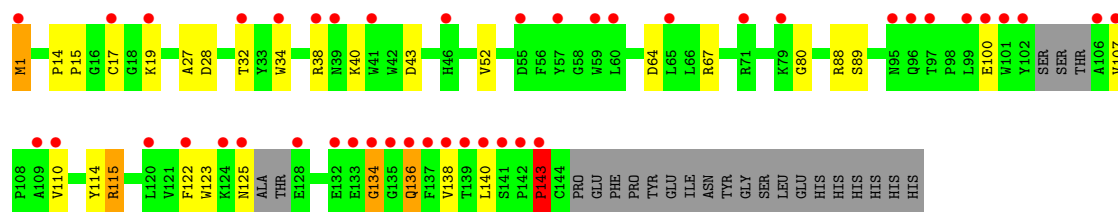




● Molecule 1: Replication-associated protein



● Molecule 1: Replication-associated protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.92Å 103.93Å 76.85Å 90.00° 109.90° 90.00°	Depositor
Resolution (Å)	59.33 – 2.20 59.33 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (59.33-2.20) 100.0 (59.33-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.289 , 0.319 0.283 , 0.303	Depositor DCC
R_{free} test set	2491 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7076	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.85% 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

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	0.74	0/1195	1.10	3/1638 (0.2%)
1	B	0.81	2/1208 (0.2%)	1.14	4/1658 (0.2%)
1	C	0.68	0/1181	1.08	6/1617 (0.4%)
1	D	0.72	0/1194	1.15	7/1637 (0.4%)
1	E	0.68	0/1189	1.15	7/1629 (0.4%)
1	F	0.69	0/1175	1.09	1/1609 (0.1%)
All	All	0.72	2/7142 (0.0%)	1.12	28/9788 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	125	ASN	CA-C	-6.50	1.46	1.53
1	B	127	THR	CA-C	-5.72	1.45	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	88	ARG	N-CA-C	-9.07	102.72	113.88
1	F	88	ARG	N-CA-C	-7.84	103.94	113.97
1	E	88	ARG	N-CA-C	-7.80	104.28	113.88
1	A	88	ARG	N-CA-C	-7.69	104.13	113.97
1	E	36	PRO	CA-C-N	-7.68	112.78	120.31
1	E	36	PRO	C-N-CA	-7.68	112.78	120.31
1	A	38	ARG	N-CA-C	7.61	121.98	112.24
1	C	88	ARG	N-CA-C	-7.42	104.48	113.97
1	B	128	GLU	N-CA-C	6.81	118.55	108.60
1	B	88	ARG	N-CA-C	-6.80	105.11	113.41
1	D	128	GLU	N-CA-C	6.71	119.37	108.76
1	E	128	GLU	N-CA-C	6.23	118.60	108.76
1	E	131	THR	CA-CB-OG1	-5.59	101.21	109.60
1	C	83	VAL	CB-CA-C	5.46	114.68	109.33
1	E	83	VAL	O-C-N	-5.40	118.29	121.69
1	B	143	PRO	N-CA-CB	-5.39	97.59	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	78	THR	N-CA-C	5.33	116.84	110.44
1	A	143	PRO	N-CA-CB	-5.18	97.81	103.25
1	D	83	VAL	O-C-N	-5.16	118.44	121.69
1	C	5	LYS	CA-C-N	-5.14	114.26	121.72
1	C	5	LYS	C-N-CA	-5.14	114.26	121.72
1	C	28	ASP	CA-CB-CG	5.11	117.71	112.60
1	D	83	VAL	CB-CA-C	5.07	114.30	109.33
1	B	83	VAL	CB-CA-C	5.07	114.30	109.33
1	C	135	GLY	N-CA-C	-5.05	101.22	113.18
1	D	97	THR	N-CA-CB	5.04	117.30	110.05
1	E	143	PRO	N-CA-CB	-5.04	97.96	103.25
1	D	135	GLY	N-CA-C	-5.02	101.28	113.18

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	1154	0	1107	30	0
1	B	1166	0	1120	16	0
1	C	1141	0	1094	17	0
1	D	1153	0	1108	25	0
1	E	1149	0	1104	30	0
1	F	1135	0	1089	24	0
2	A	44	0	0	2	0
2	B	35	0	0	1	0
2	C	27	0	0	4	0
2	D	25	0	0	3	0
2	E	26	0	0	2	0
2	F	21	0	0	6	0
All	All	7076	0	6622	135	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 10.

All (135) 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:E:5:LYS:HA	1:E:71:ARG:HG2	1.17	1.14
1:D:5:LYS:HA	1:D:71:ARG:HG2	1.16	1.12
1:C:5:LYS:HA	1:C:71:ARG:HG2	1.35	1.08
1:E:132:GLU:HB3	1:E:136:GLN:OE1	1.54	1.06
1:E:132:GLU:HB3	1:E:136:GLN:CD	1.93	0.92
1:E:5:LYS:CA	1:E:71:ARG:HG2	2.00	0.92
1:E:122:PHE:CE2	1:E:138:VAL:HG11	2.08	0.89
1:B:3:ASP:OD2	1:F:1:MET:HG2	1.71	0.88
1:C:122:PHE:CE1	1:C:138:VAL:HG11	2.10	0.85
1:D:5:LYS:CA	1:D:71:ARG:HG2	2.05	0.84
1:A:122:PHE:CE1	1:A:138:VAL:HG11	2.16	0.80
1:E:132:GLU:HB3	1:E:136:GLN:NE2	1.96	0.79
1:B:28:ASP:O	1:B:32:THR:HG23	1.83	0.79
1:D:122:PHE:CE2	1:D:138:VAL:HG11	2.18	0.79
1:F:122:PHE:CE2	1:F:138:VAL:HG11	2.18	0.78
1:D:34:TRP:HZ3	2:D:205:HOH:O	1.67	0.77
1:A:34:TRP:CE2	1:A:52:VAL:HG21	2.18	0.77
1:D:134:GLY:HA3	1:D:143:PRO:HD3	1.68	0.75
1:B:34:TRP:CE2	1:B:52:VAL:HG21	2.21	0.75
1:E:34:TRP:CE2	1:E:52:VAL:HG21	2.23	0.73
1:F:28:ASP:O	1:F:32:THR:HG23	1.89	0.72
1:E:28:ASP:O	1:E:32:THR:HG23	1.91	0.71
1:A:28:ASP:O	1:A:32:THR:HG23	1.91	0.70
1:E:132:GLU:CB	1:E:136:GLN:HE22	2.05	0.70
1:C:28:ASP:O	1:C:32:THR:HG23	1.92	0.70
1:D:28:ASP:O	1:D:32:THR:HG23	1.91	0.70
1:F:34:TRP:CE2	1:F:52:VAL:HG21	2.28	0.69
1:C:5:LYS:CA	1:C:71:ARG:HG2	2.18	0.69
1:C:34:TRP:CE2	1:C:52:VAL:HG21	2.27	0.69
1:E:122:PHE:CZ	1:E:138:VAL:HG11	2.29	0.68
1:D:52:VAL:HG22	1:D:91:LEU:HB2	1.76	0.67
1:A:1:MET:N	2:A:202:HOH:O	2.28	0.67
1:E:138:VAL:O	1:E:138:VAL:HG12	1.94	0.66
1:A:136:GLN:HE21	1:A:139:THR:HB	1.60	0.66
1:A:34:TRP:CD1	1:A:52:VAL:HG23	2.31	0.66
1:B:49:GLU:HG3	2:B:215:HOH:O	1.96	0.66
1:F:1:MET:N	2:F:203:HOH:O	2.27	0.65
1:E:132:GLU:HB3	1:E:136:GLN:HE22	1.59	0.65
1:E:5:LYS:HB2	1:E:71:ARG:NE	2.13	0.63
1:E:34:TRP:CD2	1:E:52:VAL:HG21	2.34	0.62
1:B:34:TRP:CD2	1:B:52:VAL:HG21	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:LYS:HB2	1:D:71:ARG:NE	2.15	0.62
1:F:122:PHE:CZ	1:F:138:VAL:HG11	2.36	0.60
1:E:132:GLU:CB	1:E:136:GLN:NE2	2.65	0.60
1:A:55:ASP:OD2	1:E:55:ASP:OD2	2.20	0.59
1:A:34:TRP:CD1	1:A:52:VAL:CG2	2.86	0.59
1:A:62:TRP:CZ2	1:A:107:VAL:HG11	2.38	0.58
1:A:62:TRP:CE2	1:A:107:VAL:CG1	2.87	0.58
1:B:122:PHE:CZ	1:B:138:VAL:HG11	2.39	0.57
1:F:17:CYS:SG	1:F:19:LYS:HG3	2.45	0.57
1:F:125:ASN:N	2:F:202:HOH:O	2.24	0.57
1:F:115:ARG:NH1	2:F:204:HOH:O	2.29	0.57
1:D:136:GLN:HE21	1:D:139:THR:HB	1.70	0.57
1:A:62:TRP:CE2	1:A:107:VAL:HG13	2.40	0.57
1:B:34:TRP:CG	1:B:52:VAL:CG2	2.88	0.56
1:C:34:TRP:CG	1:C:52:VAL:CG2	2.88	0.56
1:D:78:THR:O	1:F:80:GLY:HA3	2.05	0.56
1:E:1:MET:N	2:E:204:HOH:O	2.38	0.56
1:D:122:PHE:CZ	1:D:138:VAL:HG11	2.41	0.56
1:E:138:VAL:O	1:E:138:VAL:CG1	2.53	0.56
1:A:34:TRP:CD2	1:A:52:VAL:HG21	2.42	0.55
1:E:34:TRP:CG	1:E:52:VAL:CG2	2.89	0.55
1:A:132:GLU:HB3	1:A:136:GLN:OE1	2.06	0.55
1:C:34:TRP:CD2	1:C:52:VAL:HG21	2.41	0.55
1:E:40:LYS:NZ	2:E:202:HOH:O	2.23	0.55
1:C:34:TRP:CD1	1:C:52:VAL:CG2	2.92	0.53
1:D:110:VAL:HG22	1:D:114:TYR:CZ	2.44	0.53
1:A:122:PHE:CZ	1:A:138:VAL:HG11	2.44	0.52
1:C:1:MET:N	2:C:203:HOH:O	2.41	0.52
1:A:34:TRP:CG	1:A:52:VAL:CG2	2.93	0.52
1:A:136:GLN:HG2	1:A:139:THR:H	1.74	0.52
1:C:122:PHE:CZ	1:C:138:VAL:HG11	2.44	0.51
1:C:34:TRP:CD1	1:C:52:VAL:HG23	2.44	0.51
1:D:138:VAL:HG12	1:D:138:VAL:O	2.10	0.51
1:F:27:ALA:O	2:F:201:HOH:O	2.20	0.51
1:A:110:VAL:HG22	1:A:114:TYR:CZ	2.46	0.51
1:D:34:TRP:CZ3	2:D:205:HOH:O	2.50	0.50
1:E:110:VAL:HG22	1:E:114:TYR:CZ	2.46	0.50
1:F:115:ARG:NH1	2:F:206:HOH:O	2.44	0.50
1:F:136:GLN:HG3	2:F:213:HOH:O	2.12	0.50
1:B:34:TRP:CD1	1:B:52:VAL:CG2	2.95	0.49
1:E:132:GLU:CB	1:E:136:GLN:OE1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:TRP:CD2	1:F:52:VAL:HG21	2.47	0.49
1:E:34:TRP:CD1	1:E:52:VAL:HG23	2.48	0.49
1:B:134:GLY:HA3	1:B:143:PRO:HD3	1.94	0.49
1:E:34:TRP:CD1	1:E:52:VAL:CG2	2.97	0.48
1:D:136:GLN:HG2	1:D:139:THR:H	1.79	0.48
1:C:70:ASP:HB3	2:C:218:HOH:O	2.14	0.48
1:C:3:ASP:OD2	1:F:89:SER:OG	2.27	0.47
1:A:79:LYS:NZ	2:A:208:HOH:O	2.48	0.47
1:B:34:TRP:CD1	1:B:52:VAL:HG23	2.50	0.47
1:D:132:GLU:HB3	1:D:136:GLN:OE1	2.13	0.47
1:C:52:VAL:HG12	1:C:91:LEU:HD12	1.97	0.46
1:F:110:VAL:HG22	1:F:114:TYR:CZ	2.51	0.46
1:B:34:TRP:CD2	1:B:52:VAL:CG2	2.99	0.46
1:D:80:GLY:HA2	1:F:43:ASP:OD2	2.16	0.46
1:E:34:TRP:CD2	1:E:52:VAL:CG2	2.99	0.46
1:D:134:GLY:HA3	1:D:143:PRO:CD	2.44	0.45
1:A:134:GLY:HA3	1:A:143:PRO:HD3	1.98	0.45
1:A:88:ARG:HE	1:A:88:ARG:HB3	1.64	0.45
1:D:42:TRP:HB2	1:D:78:THR:HG22	1.99	0.45
1:A:34:TRP:NE1	1:A:52:VAL:HG21	2.32	0.45
1:B:110:VAL:HG22	1:B:114:TYR:CZ	2.52	0.45
1:F:34:TRP:CD1	1:F:52:VAL:HG23	2.52	0.44
1:E:132:GLU:CD	1:E:136:GLN:NE2	2.75	0.44
1:E:134:GLY:HA3	1:E:143:PRO:HD3	1.99	0.44
1:F:34:TRP:CG	1:F:52:VAL:CG2	3.01	0.43
1:A:89:SER:OG	1:D:3:ASP:OD2	2.31	0.43
1:D:142:PRO:HA	1:D:143:PRO:HD3	1.91	0.43
1:C:49:GLU:HG3	2:C:215:HOH:O	2.18	0.43
1:D:64:ASP:OD1	1:D:67:ARG:NH2	2.52	0.43
1:A:62:TRP:CE2	1:A:107:VAL:HG11	2.52	0.43
1:D:1:MET:N	2:D:201:HOH:O	2.51	0.43
1:D:138:VAL:O	1:D:138:VAL:CG1	2.67	0.42
1:E:5:LYS:HB2	1:E:71:ARG:CD	2.49	0.42
1:F:134:GLY:HA3	1:F:143:PRO:HD3	2.02	0.42
1:A:106:ALA:C	1:A:107:VAL:HG23	2.44	0.42
1:B:78:THR:OG1	1:B:81:GLY:O	2.32	0.42
1:F:14:PRO:O	1:F:15:PRO:C	2.61	0.42
1:A:5:LYS:HA	1:A:71:ARG:HB3	2.03	0.41
1:C:115:ARG:NH1	2:C:201:HOH:O	2.33	0.41
1:E:5:LYS:HD3	1:E:71:ARG:CG	2.51	0.41
1:F:34:TRP:CD1	1:F:52:VAL:CG2	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ARG:HH22	1:B:131:THR:HG23	1.85	0.41
1:D:5:LYS:HD3	1:D:71:ARG:CG	2.50	0.41
1:C:34:TRP:CD2	1:C:52:VAL:CG2	3.04	0.41
1:A:136:GLN:NE2	1:A:139:THR:HB	2.31	0.41
1:E:4:TRP:O	1:E:71:ARG:HA	2.20	0.41
1:B:14:PRO:O	1:B:15:PRO:C	2.63	0.41
1:F:64:ASP:OD1	1:F:67:ARG:NH2	2.54	0.41
1:A:62:TRP:NE1	1:A:107:VAL:HG13	2.37	0.40
1:B:32:THR:HA	1:B:50:VAL:O	2.20	0.40
1:A:34:TRP:CD2	1:A:52:VAL:CG2	3.04	0.40
1:A:137:PHE:HD1	1:A:138:VAL:HG23	1.87	0.40
1:F:17:CYS:HB2	1:F:123:TRP:CD2	2.57	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	138/163 (85%)	129 (94%)	6 (4%)	3 (2%)	5	3
1	B	142/163 (87%)	131 (92%)	8 (6%)	3 (2%)	5	3
1	C	134/163 (82%)	125 (93%)	6 (4%)	3 (2%)	5	3
1	D	138/163 (85%)	130 (94%)	6 (4%)	2 (1%)	9	7
1	E	135/163 (83%)	127 (94%)	7 (5%)	1 (1%)	18	19
1	F	133/163 (82%)	124 (93%)	7 (5%)	2 (2%)	8	6
All	All	820/978 (84%)	766 (93%)	40 (5%)	14 (2%)	7	5

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	GLY

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Mol	Chain	Res	Type
1	B	134	GLY
1	C	124	LYS
1	C	134	GLY
1	F	134	GLY
1	A	143	PRO
1	B	143	PRO
1	C	143	PRO
1	E	143	PRO
1	F	143	PRO
1	D	134	GLY
1	D	143	PRO
1	B	124	LYS
1	A	124	LYS

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	125/144 (87%)	116 (93%)	9 (7%)	13	15
1	B	126/144 (88%)	119 (94%)	7 (6%)	19	24
1	C	123/144 (85%)	119 (97%)	4 (3%)	33	45
1	D	125/144 (87%)	118 (94%)	7 (6%)	19	24
1	E	125/144 (87%)	123 (98%)	2 (2%)	55	71
1	F	122/144 (85%)	113 (93%)	9 (7%)	13	14
All	All	746/864 (86%)	708 (95%)	38 (5%)	21	27

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ARG
1	A	115	ARG
1	A	124	LYS
1	A	125	ASN
1	A	128	GLU

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Mol	Chain	Res	Type
1	A	133	GLU
1	A	136	GLN
1	A	137	PHE
1	A	143	PRO
1	B	1	MET
1	B	100	GLU
1	B	115	ARG
1	B	127	THR
1	B	136	GLN
1	B	138	VAL
1	B	140	LEU
1	C	115	ARG
1	C	136	GLN
1	C	140	LEU
1	C	143	PRO
1	D	79	LYS
1	D	104	SER
1	D	107	VAL
1	D	115	ARG
1	D	136	GLN
1	D	137	PHE
1	D	140	LEU
1	E	100	GLU
1	E	115	ARG
1	F	1	MET
1	F	38	ARG
1	F	40	LYS
1	F	100	GLU
1	F	107	VAL
1	F	115	ARG
1	F	136	GLN
1	F	140	LEU
1	F	143	PRO

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

Mol	Chain	Res	Type
1	A	125	ASN
1	C	129	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	142/163 (87%)	1.06	26 (18%) 3 2	22, 35, 55, 82	0
1	B	144/163 (88%)	1.21	39 (27%) 1 1	19, 35, 69, 97	0
1	C	140/163 (85%)	1.48	35 (25%) 2 1	25, 42, 74, 120	0
1	D	142/163 (87%)	1.32	35 (24%) 2 1	25, 40, 81, 96	0
1	E	141/163 (86%)	1.40	35 (24%) 2 1	26, 40, 78, 107	0
1	F	139/163 (85%)	1.67	44 (31%) 1 1	31, 46, 72, 102	0
All	All	848/978 (86%)	1.36	214 (25%) 1 1	19, 40, 74, 120	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	140	LEU	7.9
1	C	140	LEU	7.6
1	C	106	ALA	7.5
1	A	140	LEU	7.2
1	B	137	PHE	7.2
1	A	137	PHE	7.0
1	F	139	THR	6.9
1	E	140	LEU	6.8
1	F	106	ALA	6.6
1	E	137	PHE	6.5
1	C	103	SER	6.3
1	D	140	LEU	6.2
1	D	57	TYR	6.2
1	B	126	ALA	6.2
1	A	57	TYR	6.1
1	D	127	THR	5.8
1	C	137	PHE	5.8
1	E	57	TYR	5.6
1	F	137	PHE	5.6

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Mol	Chain	Res	Type	RSRZ
1	F	57	TYR	5.5
1	D	137	PHE	5.5
1	B	57	TYR	5.5
1	B	1	MET	5.5
1	C	125	ASN	5.4
1	B	127	THR	5.3
1	E	127	THR	5.3
1	B	138	VAL	5.3
1	F	102	TYR	5.2
1	F	125	ASN	5.1
1	F	138	VAL	5.1
1	C	1	MET	5.0
1	D	109	ALA	4.9
1	F	136	GLN	4.9
1	E	1	MET	4.8
1	B	106	ALA	4.8
1	C	57	TYR	4.7
1	E	103	SER	4.6
1	A	1	MET	4.6
1	B	140	LEU	4.6
1	B	139	THR	4.5
1	D	139	THR	4.5
1	A	138	VAL	4.5
1	F	38	ARG	4.5
1	E	105	THR	4.4
1	B	105	THR	4.4
1	B	38	ARG	4.4
1	D	107	VAL	4.4
1	E	104	SER	4.3
1	F	120	LEU	4.3
1	B	143	PRO	4.2
1	F	1	MET	4.2
1	D	105	THR	4.2
1	F	124	LYS	4.2
1	C	38	ARG	4.2
1	E	139	THR	4.2
1	D	106	ALA	4.1
1	E	138	VAL	4.1
1	E	106	ALA	4.0
1	A	139	THR	4.0
1	F	142	PRO	4.0
1	C	99	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	138	VAL	4.0
1	F	39	ASN	4.0
1	D	104	SER	4.0
1	D	124	LYS	3.9
1	B	135	GLY	3.9
1	D	1	MET	3.9
1	B	80	GLY	3.8
1	E	71	ARG	3.7
1	B	136	GLN	3.7
1	E	130	SER	3.6
1	C	136	GLN	3.6
1	A	71	ARG	3.6
1	D	136	GLN	3.6
1	F	101	TRP	3.6
1	A	38	ARG	3.5
1	F	122	PHE	3.5
1	C	139	THR	3.5
1	A	125	ASN	3.5
1	D	38	ARG	3.5
1	C	101	TRP	3.5
1	F	34	TRP	3.5
1	C	107	VAL	3.4
1	E	13	GLY	3.4
1	D	132	GLU	3.4
1	A	136	GLN	3.4
1	F	79	LYS	3.4
1	C	59	TRP	3.3
1	F	128	GLU	3.3
1	A	130	SER	3.3
1	D	110	VAL	3.3
1	C	102	TYR	3.3
1	D	5	LYS	3.3
1	B	132	GLU	3.2
1	C	34	TRP	3.2
1	D	72	TYR	3.2
1	F	135	GLY	3.2
1	F	141	SER	3.2
1	B	40	LYS	3.1
1	D	79	LYS	3.1
1	E	124	LYS	3.1
1	D	71	ARG	3.1
1	F	133	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	124	LYS	3.1
1	A	142	PRO	3.1
1	D	108	PRO	3.1
1	C	40	LYS	3.0
1	D	143	PRO	3.0
1	B	104	SER	3.0
1	D	142	PRO	3.0
1	E	79	LYS	3.0
1	E	123	TRP	3.0
1	A	106	ALA	3.0
1	A	132	GLU	3.0
1	E	15	PRO	2.9
1	B	122	PHE	2.9
1	E	99	LEU	2.9
1	F	95	ASN	2.9
1	B	107	VAL	2.9
1	E	108	PRO	2.9
1	F	71	ARG	2.9
1	C	96	GLN	2.9
1	D	103	SER	2.8
1	B	108	PRO	2.8
1	C	143	PRO	2.8
1	C	138	VAL	2.8
1	C	41	TRP	2.8
1	C	128	GLU	2.8
1	C	134	GLY	2.8
1	A	134	GLY	2.8
1	C	132	GLU	2.8
1	E	107	VAL	2.8
1	D	135	GLY	2.7
1	E	134	GLY	2.7
1	C	142	PRO	2.7
1	E	52	VAL	2.7
1	F	143	PRO	2.7
1	B	133	GLU	2.7
1	D	34	TRP	2.7
1	F	107	VAL	2.7
1	B	79	LYS	2.7
1	F	65	LEU	2.7
1	B	3	ASP	2.7
1	F	110	VAL	2.7
1	E	82	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	15	PRO	2.7
1	B	34	TRP	2.7
1	F	41	TRP	2.6
1	C	123	TRP	2.5
1	A	107	VAL	2.5
1	E	80	GLY	2.5
1	A	141	SER	2.5
1	B	141	SER	2.5
1	F	59	TRP	2.5
1	D	120	LEU	2.5
1	F	60	LEU	2.5
1	A	95	ASN	2.5
1	B	142	PRO	2.5
1	C	108	PRO	2.5
1	E	142	PRO	2.5
1	F	134	GLY	2.5
1	F	100	GLU	2.4
1	F	132	GLU	2.4
1	A	34	TRP	2.4
1	C	113	LEU	2.4
1	B	125	ASN	2.4
1	A	55	ASP	2.4
1	E	132	GLU	2.4
1	F	32	THR	2.4
1	C	98	PRO	2.4
1	F	109	ALA	2.4
1	C	30	GLU	2.4
1	B	134	GLY	2.3
1	D	77	GLU	2.3
1	E	34	TRP	2.3
1	F	99	LEU	2.3
1	D	70	ASP	2.3
1	B	71	ARG	2.3
1	E	136	GLN	2.3
1	D	40	LYS	2.3
1	B	81	GLY	2.3
1	A	104	SER	2.3
1	B	144	CYS	2.2
1	C	71	ARG	2.2
1	D	63	ASP	2.2
1	C	36	PRO	2.2
1	A	133	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	124	LYS	2.2
1	B	30	GLU	2.2
1	E	96	GLN	2.2
1	C	124	LYS	2.1
1	F	46	HIS	2.1
1	A	135	GLY	2.1
1	C	135	GLY	2.1
1	F	17	CYS	2.1
1	A	105	THR	2.1
1	E	75	THR	2.1
1	D	30	GLU	2.1
1	E	11	ILE	2.1
1	E	95	ASN	2.1
1	B	83	VAL	2.1
1	F	97	THR	2.1
1	B	120	LEU	2.1
1	C	39	ASN	2.1
1	E	129	GLN	2.1
1	F	55	ASP	2.1
1	F	96	GLN	2.1
1	D	83	VAL	2.1
1	B	32	THR	2.0
1	B	95	ASN	2.0
1	E	122	PHE	2.0
1	A	103	SER	2.0
1	D	115	ARG	2.0
1	F	19	LYS	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.