



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:48 AM UTC

PDB ID : 3P83 / pdb_00003p83
Title : Structure of the PCNA:RNase HII complex from *Archaeoglobus fulgidus*.
Authors : Bubeck, D.; Reijns, M.A.; Graham, S.C.; Astell, K.R.; Jones, E.Y.; Jackson, A.P.
Deposited on : 2010-10-13
Resolution : 3.05 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

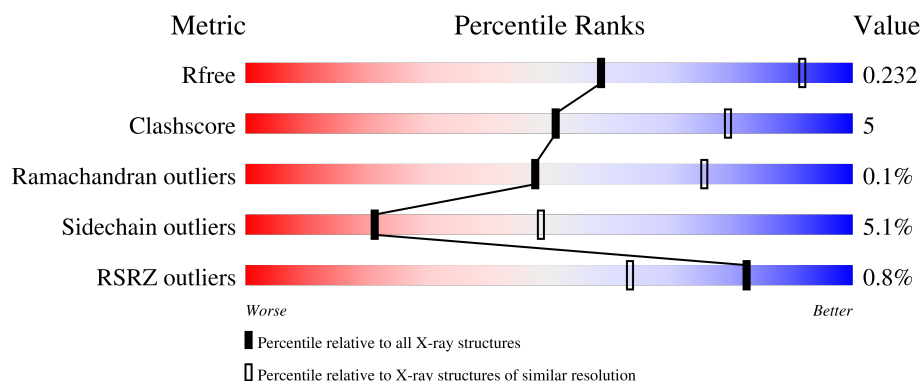
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	245	 82% 17% .
1	B	245	 80% 18% .
1	C	245	 82% 17% ..
2	D	217	 85% 12% . .
2	E	217	 79% 12% . 7%

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Mol	Chain	Length	Quality of chain
2	F	217	3% 76% 16% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10465 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 DNA polymerase sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1895	1214	311	362	8			
1	B	244	Total	C	N	O	S	0	0	0
			1894	1214	306	366	8			
1	C	243	Total	C	N	O	S	0	0	0
			1881	1206	305	362	8			

- Molecule 2 is a protein called Ribonuclease HII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	213	Total	C	N	O	S	0	0	0
			1665	1043	302	312	8			
2	E	202	Total	C	N	O	S	0	0	0
			1564	977	277	302	8			
2	F	205	Total	C	N	O	S	0	0	0
			1566	978	284	297	7			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	GLY	-	expression tag	UNP O29634
D	-10	PRO	-	expression tag	UNP O29634
D	-9	LEU	-	expression tag	UNP O29634
D	-8	GLY	-	expression tag	UNP O29634
D	-7	SER	-	expression tag	UNP O29634
D	-6	PRO	-	expression tag	UNP O29634
D	-5	GLU	-	expression tag	UNP O29634
D	-4	PHE	-	expression tag	UNP O29634
D	-3	PRO	-	expression tag	UNP O29634
D	-2	GLY	-	expression tag	UNP O29634
D	-1	ARG	-	expression tag	UNP O29634
D	0	LEU	-	expression tag	UNP O29634

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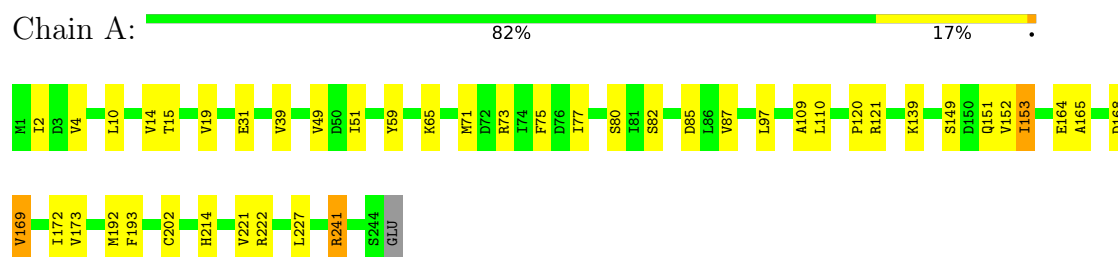
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	GLY	-	expression tag	UNP O29634
E	-10	PRO	-	expression tag	UNP O29634
E	-9	LEU	-	expression tag	UNP O29634
E	-8	GLY	-	expression tag	UNP O29634
E	-7	SER	-	expression tag	UNP O29634
E	-6	PRO	-	expression tag	UNP O29634
E	-5	GLU	-	expression tag	UNP O29634
E	-4	PHE	-	expression tag	UNP O29634
E	-3	PRO	-	expression tag	UNP O29634
E	-2	GLY	-	expression tag	UNP O29634
E	-1	ARG	-	expression tag	UNP O29634
E	0	LEU	-	expression tag	UNP O29634
F	-11	GLY	-	expression tag	UNP O29634
F	-10	PRO	-	expression tag	UNP O29634
F	-9	LEU	-	expression tag	UNP O29634
F	-8	GLY	-	expression tag	UNP O29634
F	-7	SER	-	expression tag	UNP O29634
F	-6	PRO	-	expression tag	UNP O29634
F	-5	GLU	-	expression tag	UNP O29634
F	-4	PHE	-	expression tag	UNP O29634
F	-3	PRO	-	expression tag	UNP O29634
F	-2	GLY	-	expression tag	UNP O29634
F	-1	ARG	-	expression tag	UNP O29634
F	0	LEU	-	expression tag	UNP O29634

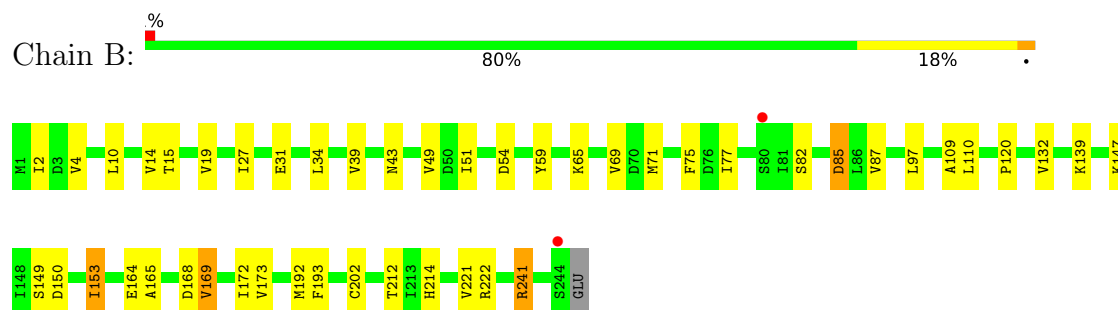
3 Residue-property plots [i](#)

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.

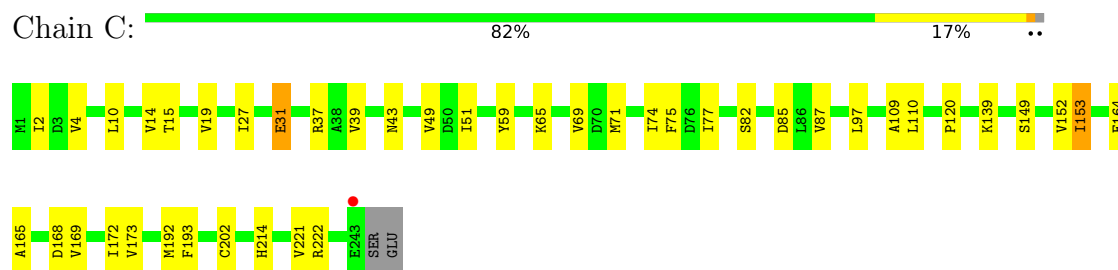
- Molecule 1: DNA polymerase sliding clamp



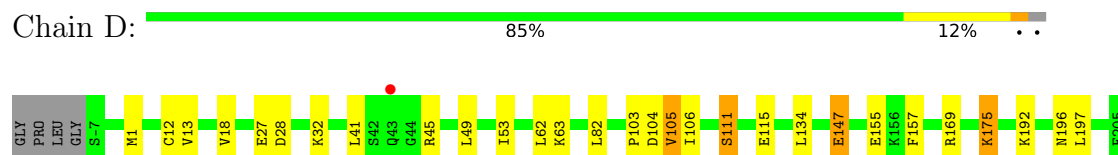
- Molecule 1: DNA polymerase sliding clamp



- Molecule 1: DNA polymerase sliding clamp

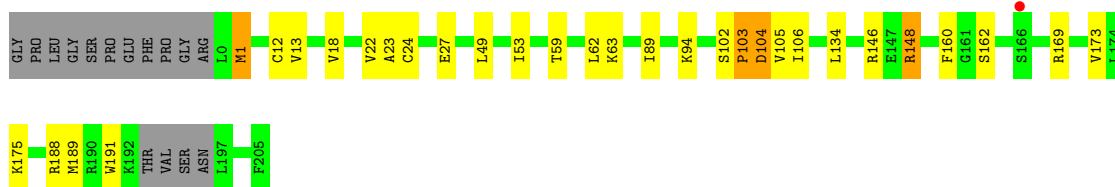


- Molecule 2: Ribonuclease HII



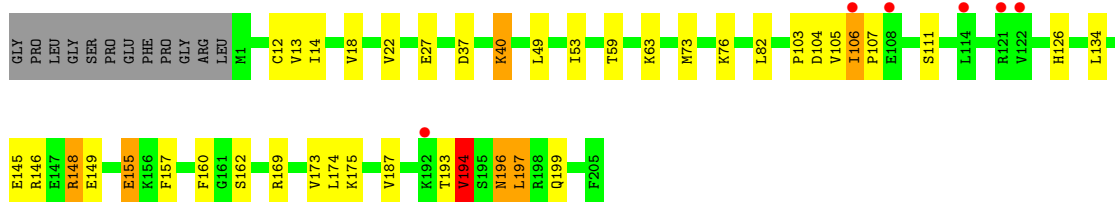
- Molecule 2: Ribonuclease HII

Chain E: 



- Molecule 2: Ribonuclease HII

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	149.67Å 152.03Å 90.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.54 – 3.05 44.54 – 3.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (44.54-3.05) 99.6 (44.54-3.05)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.07Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.187 , 0.216 0.198 , 0.232	Depositor DCC
R_{free} test set	1996 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	72.8	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 76.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10465	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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	0.68	0/1923	1.09	3/2595 (0.1%)
1	B	0.70	0/1922	1.13	5/2594 (0.2%)
1	C	0.68	0/1909	1.13	2/2577 (0.1%)
2	D	0.78	0/1687	1.26	10/2268 (0.4%)
2	E	0.78	0/1582	1.30	7/2127 (0.3%)
2	F	0.76	0/1585	1.34	12/2135 (0.6%)
All	All	0.73	0/10608	1.20	39/14296 (0.3%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	13	VAL	N-CA-C	-8.16	104.79	111.81
1	C	31	GLU	CA-C-N	7.92	130.89	120.28
1	C	31	GLU	C-N-CA	7.92	130.89	120.28
1	A	31	GLU	CA-C-N	7.52	132.11	120.82
1	A	31	GLU	C-N-CA	7.52	132.11	120.82
2	F	155	GLU	CB-CG-CD	7.27	124.95	112.60
2	E	104	ASP	N-CA-C	7.05	119.41	110.24
2	E	13	VAL	N-CA-C	-7.03	105.76	111.81
2	D	13	VAL	N-CA-C	-6.88	105.89	111.81
2	E	94	LYS	CB-CA-C	6.77	116.01	111.20
2	F	194	VAL	CB-CA-C	6.65	118.41	111.23
2	F	194	VAL	N-CA-CB	6.62	119.07	111.39
1	B	31	GLU	CA-C-N	6.62	129.45	120.38
1	B	31	GLU	C-N-CA	6.62	129.45	120.38
2	F	157	PHE	N-CA-C	6.26	121.08	113.38
2	E	103	PRO	CA-C-N	5.96	129.58	120.82
2	E	103	PRO	C-N-CA	5.96	129.58	120.82
2	D	111	SER	CA-C-N	5.79	127.97	120.44
2	D	111	SER	C-N-CA	5.79	127.97	120.44
2	F	149	GLU	CB-CG-CD	5.76	122.39	112.60
2	D	157	PHE	N-CA-C	5.71	120.36	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	ASP	CA-CB-CG	5.51	118.11	112.60
2	D	105	VAL	N-CA-CB	-5.43	101.29	111.62
2	D	147	GLU	CB-CG-CD	5.40	121.78	112.60
2	F	106	ILE	N-CA-CB	5.39	118.76	111.21
2	F	196	ASN	CA-C-N	5.39	129.31	120.63
2	F	196	ASN	C-N-CA	5.39	129.31	120.63
2	F	105	VAL	N-CA-C	5.38	116.11	110.62
1	B	169	VAL	N-CA-CB	-5.32	106.00	112.33
2	D	104	ASP	CA-C-N	5.27	129.82	122.23
2	D	104	ASP	C-N-CA	5.27	129.82	122.23
2	D	196	ASN	CA-CB-CG	5.20	117.80	112.60
2	E	104	ASP	CA-C-N	5.18	127.56	120.46
2	E	104	ASP	C-N-CA	5.18	127.56	120.46
1	A	169	VAL	N-CA-CB	-5.13	106.22	112.33
1	B	31	GLU	N-CA-C	-5.12	105.70	111.28
2	D	1	MET	N-CA-C	5.09	118.31	110.42
2	F	111	SER	CA-C-N	5.07	127.08	120.28
2	F	111	SER	C-N-CA	5.07	127.08	120.28

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	1895	0	1941	24	0
1	B	1894	0	1936	28	0
1	C	1881	0	1918	24	0
2	D	1665	0	1715	11	0
2	E	1564	0	1576	15	0
2	F	1566	0	1574	14	0
All	All	10465	0	10660	107	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 5.

All (107) 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:19:VAL:HG12	2:E:106:ILE:HG13	1.46	0.97
2:F:82:LEU:HD23	2:F:103:PRO:HG3	1.61	0.82
1:A:214:HIS:HB2	1:A:222:ARG:HB2	1.61	0.81
1:B:109:ALA:HB3	1:C:169:VAL:HG22	1.65	0.79
2:E:1:MET:HE2	2:E:23:ALA:HB1	1.65	0.77
1:C:214:HIS:HB2	1:C:222:ARG:HB2	1.67	0.77
1:B:214:HIS:HB2	1:B:222:ARG:HB2	1.66	0.77
1:A:82:SER:HB3	1:A:85:ASP:HB2	1.68	0.74
1:B:82:SER:HB3	1:B:85:ASP:HB2	1.70	0.74
1:C:82:SER:HB3	1:C:85:ASP:HB2	1.73	0.71
2:D:41:LEU:HD22	2:D:45:ARG:HG2	1.76	0.68
1:A:151:GLN:OE1	1:A:241:ARG:NH1	2.28	0.66
1:B:19:VAL:HG21	1:B:75:PHE:HB2	1.78	0.65
2:D:41:LEU:HD13	2:D:45:ARG:HG3	1.79	0.64
1:B:15:THR:O	1:B:19:VAL:HG23	2.00	0.61
1:C:19:VAL:HG21	1:C:75:PHE:HB2	1.82	0.61
1:C:15:THR:O	1:C:19:VAL:HG23	2.00	0.61
1:A:15:THR:O	1:A:19:VAL:HG23	2.02	0.60
1:A:19:VAL:HG21	1:A:75:PHE:HB2	1.84	0.59
1:C:153:ILE:HG13	1:C:192:MET:HE3	1.85	0.59
1:B:153:ILE:HG13	1:B:192:MET:HE3	1.85	0.58
1:A:153:ILE:HG13	1:A:192:MET:HE3	1.86	0.57
2:F:14:ILE:HG12	2:F:187:VAL:HG22	1.87	0.56
2:D:111:SER:O	2:D:115:GLU:HG3	2.04	0.56
1:C:2:ILE:HD11	1:C:65:LYS:HB3	1.90	0.54
1:B:2:ILE:HD11	1:B:65:LYS:HB3	1.90	0.53
1:A:2:ILE:HD11	1:A:65:LYS:HB3	1.90	0.52
1:A:139:LYS:HG3	1:A:202:CYS:HB3	1.92	0.51
1:B:19:VAL:CG1	2:E:106:ILE:HG13	2.29	0.51
1:A:14:VAL:HG23	1:A:49:VAL:HG11	1.93	0.51
2:D:28:ASP:O	2:D:32:LYS:HG2	2.11	0.50
1:C:139:LYS:HG3	1:C:202:CYS:HB3	1.93	0.50
2:E:49:LEU:O	2:E:53:ILE:HG12	2.11	0.50
1:C:37:ARG:HG3	1:C:120:PRO:HG2	1.94	0.49
1:C:39:VAL:HG23	1:C:120:PRO:HB3	1.93	0.49
2:D:82:LEU:HD23	2:D:103:PRO:HG3	1.93	0.49
1:A:39:VAL:HG23	1:A:120:PRO:HB3	1.95	0.49
2:D:49:LEU:O	2:D:53:ILE:HG12	2.13	0.49
1:B:150:ASP:OD2	1:B:241:ARG:NH2	2.44	0.49
1:A:19:VAL:HG22	1:A:71:MET:HB3	1.93	0.49
1:B:39:VAL:HG23	1:B:120:PRO:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:175:LYS:HG3	2:D:197:LEU:HD22	1.95	0.49
2:E:18:VAL:HG22	2:E:63:LYS:HG2	1.94	0.48
1:B:139:LYS:HG3	1:B:202:CYS:HB3	1.95	0.48
2:E:188:ARG:O	2:E:191:TRP:HD1	1.97	0.48
1:C:19:VAL:HG22	1:C:71:MET:HB3	1.95	0.48
1:A:4:VAL:HG12	1:A:59:TYR:HA	1.96	0.47
1:A:97:LEU:HB2	1:A:110:LEU:HD21	1.96	0.47
1:B:19:VAL:HG22	1:B:71:MET:HB3	1.97	0.47
2:F:40:LYS:HE3	2:F:40:LYS:HB3	1.64	0.47
2:F:49:LEU:O	2:F:53:ILE:HG12	2.13	0.47
2:F:194:VAL:HG13	2:F:197:LEU:HD22	1.96	0.47
1:A:14:VAL:HB	1:A:51:ILE:HD11	1.97	0.47
1:B:14:VAL:HG23	1:B:49:VAL:HG11	1.96	0.47
1:B:4:VAL:HG12	1:B:59:TYR:HA	1.97	0.46
1:C:193:PHE:CZ	1:C:221:VAL:HB	2.50	0.46
2:D:106:ILE:HG12	2:E:148:ARG:HB2	1.96	0.46
1:C:14:VAL:HG23	1:C:49:VAL:HG11	1.96	0.46
2:F:106:ILE:HA	2:F:107:PRO:HD3	1.76	0.46
1:B:193:PHE:CZ	1:B:221:VAL:HB	2.50	0.46
1:B:164:GLU:HB3	1:B:173:VAL:HG22	1.98	0.46
1:A:80:SER:OG	1:B:147:LYS:HE3	2.16	0.46
2:F:18:VAL:HG22	2:F:63:LYS:HG2	1.96	0.45
1:C:165:ALA:HB3	1:C:172:ILE:HG22	1.99	0.45
2:D:18:VAL:HG22	2:D:63:LYS:HG2	1.98	0.45
1:A:39:VAL:CG2	1:A:120:PRO:HB3	2.46	0.45
1:C:39:VAL:CG2	1:C:120:PRO:HB3	2.46	0.45
2:E:160:PHE:HA	2:E:173:VAL:HG21	1.99	0.45
1:A:169:VAL:HG22	1:C:109:ALA:HB3	1.98	0.44
1:B:14:VAL:HB	1:B:51:ILE:HD11	1.98	0.44
2:E:146:ARG:NH2	2:E:162:SER:O	2.43	0.44
1:B:27:ILE:HD12	1:B:69:VAL:HG21	1.98	0.44
1:C:14:VAL:HB	1:C:51:ILE:HD11	1.99	0.44
1:A:193:PHE:CZ	1:A:221:VAL:HB	2.53	0.44
1:B:165:ALA:HB3	1:B:172:ILE:HG22	1.99	0.44
2:F:22:VAL:HG22	2:F:59:THR:HG22	1.99	0.44
1:C:164:GLU:HB3	1:C:173:VAL:HG22	1.99	0.44
1:A:152:VAL:HG12	1:A:165:ALA:HB2	1.99	0.44
1:C:27:ILE:HD12	1:C:69:VAL:HG21	1.99	0.44
1:A:164:GLU:HB3	1:A:173:VAL:HG22	1.99	0.44
1:A:165:ALA:HB3	1:A:172:ILE:HG22	1.99	0.44
1:C:152:VAL:HG12	1:C:165:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:41:LEU:HD22	2:D:45:ARG:CG	2.46	0.44
1:C:4:VAL:HG12	1:C:59:TYR:HA	2.00	0.43
2:E:22:VAL:HG22	2:E:59:THR:HG22	2.00	0.43
2:F:146:ARG:NH2	2:F:162:SER:O	2.48	0.43
2:F:160:PHE:HA	2:F:173:VAL:HG21	2.00	0.43
1:A:109:ALA:HB3	1:B:169:VAL:HG22	2.01	0.42
2:E:105:VAL:HG12	2:E:106:ILE:HG12	2.01	0.42
1:B:97:LEU:HB2	1:B:110:LEU:HD21	2.00	0.42
1:C:39:VAL:CG1	1:C:43:ASN:HA	2.48	0.42
1:C:97:LEU:HB2	1:C:110:LEU:HD21	2.01	0.42
1:B:39:VAL:CG2	1:B:120:PRO:HB3	2.50	0.42
1:A:192:MET:HG2	1:A:241:ARG:HG3	2.01	0.42
1:B:241:ARG:HG3	2:F:199:GLN:HA	2.02	0.41
2:E:102:SER:HA	2:E:103:PRO:HD3	1.96	0.41
2:E:1:MET:CE	2:E:23:ALA:HB1	2.45	0.41
2:F:145:GLU:O	2:F:148:ARG:HG2	2.20	0.41
1:B:132:VAL:HG22	1:B:212:THR:HG23	2.03	0.41
2:F:174:LEU:HD13	2:F:197:LEU:HD21	2.03	0.41
1:A:73:ARG:NH2	1:B:147:LYS:O	2.54	0.40
2:E:62:LEU:HB2	2:E:89:ILE:HD11	2.03	0.40
1:B:34:LEU:HB3	1:B:51:ILE:HB	2.04	0.40
2:D:62:LEU:C	2:D:62:LEU:HD23	2.46	0.40
2:E:1:MET:HE1	2:E:24:CYS:N	2.36	0.40
2:F:73:MET:HA	2:F:76:LYS:O	2.22	0.40
1:C:15:THR:HG21	1:C:74:ILE:HG22	2.04	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	242/245 (99%)	235 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	242/245 (99%)	236 (98%)	6 (2%)	0	100	100
1	C	241/245 (98%)	234 (97%)	7 (3%)	0	100	100
2	D	211/217 (97%)	207 (98%)	4 (2%)	0	100	100
2	E	198/217 (91%)	191 (96%)	6 (3%)	1 (0%)	24	52
2	F	203/217 (94%)	199 (98%)	4 (2%)	0	100	100
All	All	1337/1386 (96%)	1302 (97%)	34 (2%)	1 (0%)	48	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	1	MET

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	208/212 (98%)	199 (96%)	9 (4%)	26	53
1	B	209/212 (99%)	200 (96%)	9 (4%)	26	53
1	C	206/212 (97%)	199 (97%)	7 (3%)	32	59
2	D	177/185 (96%)	168 (95%)	9 (5%)	21	48
2	E	164/185 (89%)	156 (95%)	8 (5%)	22	50
2	F	161/185 (87%)	146 (91%)	15 (9%)	8	28
All	All	1125/1191 (94%)	1068 (95%)	57 (5%)	21	48

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	77	ILE
1	A	87	VAL
1	A	121	ARG
1	A	149	SER

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Mol	Chain	Res	Type
1	A	153	ILE
1	A	168	ASP
1	A	227	LEU
1	A	241	ARG
1	B	10	LEU
1	B	43	ASN
1	B	54	ASP
1	B	77	ILE
1	B	87	VAL
1	B	149	SER
1	B	153	ILE
1	B	168	ASP
1	B	241	ARG
1	C	10	LEU
1	C	31	GLU
1	C	77	ILE
1	C	87	VAL
1	C	149	SER
1	C	153	ILE
1	C	168	ASP
2	D	12	CYS
2	D	27	GLU
2	D	105	VAL
2	D	134	LEU
2	D	147	GLU
2	D	155	GLU
2	D	169	ARG
2	D	175	LYS
2	D	192	LYS
2	E	12	CYS
2	E	27	GLU
2	E	104	ASP
2	E	134	LEU
2	E	148	ARG
2	E	169	ARG
2	E	175	LYS
2	E	189	MET
2	F	12	CYS
2	F	27	GLU
2	F	37	ASP
2	F	40	LYS
2	F	104	ASP

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Mol	Chain	Res	Type
2	F	126	HIS
2	F	134	LEU
2	F	148	ARG
2	F	155	GLU
2	F	169	ARG
2	F	175	LYS
2	F	193	THR
2	F	194	VAL
2	F	196	ASN
2	F	197	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	43	ASN
2	D	68	ASN
2	D	199	GLN
2	E	68	ASN
2	E	79	ASN
2	F	68	ASN
2	F	79	ASN
2	F	199	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å²)	Q<0.9	
1	A	244/245 (99%)	-0.47	0	100	100	34, 59, 90, 102	0
1	B	244/245 (99%)	-0.21	2 (0%)	82	63	50, 75, 110, 128	0
1	C	243/245 (99%)	-0.17	1 (0%)	88	75	58, 85, 113, 139	0
2	D	213/217 (98%)	-0.43	1 (0%)	87	72	38, 57, 100, 140	0
2	E	202/217 (93%)	-0.16	1 (0%)	87	72	43, 74, 129, 146	0
2	F	205/217 (94%)	0.14	6 (2%)	53	31	41, 90, 145, 170	0
All	All	1351/1386 (97%)	-0.22	11 (0%)	82	63	34, 72, 126, 170	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	106	ILE	2.6
2	F	114	LEU	2.6
1	B	244	SER	2.5
2	F	108	GLU	2.4
2	F	192	LYS	2.2
2	F	121	ARG	2.2
1	C	243	GLU	2.1
2	F	122	VAL	2.1
1	B	80	SER	2.1
2	E	166	SER	2.1
2	D	43	GLN	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.