



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:24 AM UTC

PDB ID : 5IY4 / pdb_00005iy4
Title : Crystal structure of human PCNA in complex with the PIP box of DVC1
Authors : Jiang, T.; Xu, M.; Wang, Y.
Deposited on : 2016-03-24
Resolution : 2.94 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

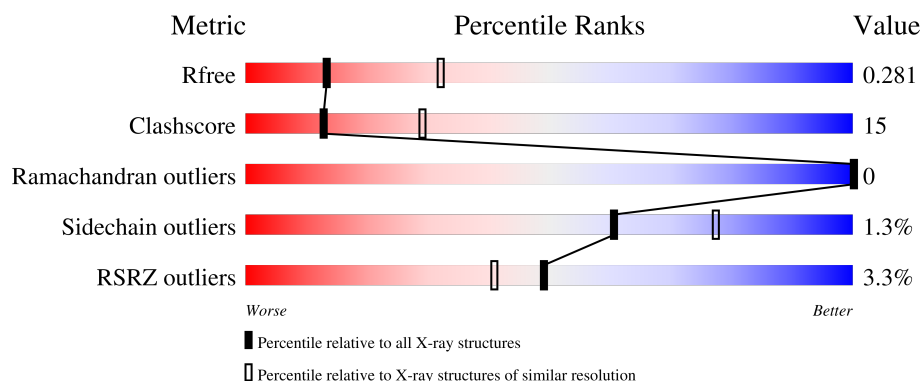
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	270	0% 69% 23% 7%
1	C	270	3% 70% 22% 7%
1	E	270	4% 70% 21% 7%
2	B	16	6% 81% 6% 12%
2	D	16	56% 31% 12%

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Mol	Chain	Length	Quality of chain
2	F	16	19%19%50%31%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6099 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 Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1922	1209	315	382	16			
1	C	251	Total	C	N	O	S	0	0	0
			1931	1214	316	385	16			
1	E	250	Total	C	N	O	S	0	0	0
			1922	1209	315	382	16			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	262	LEU	-	expression tag	UNP P12004
A	263	GLU	-	expression tag	UNP P12004
A	264	HIS	-	expression tag	UNP P12004
A	265	HIS	-	expression tag	UNP P12004
A	266	HIS	-	expression tag	UNP P12004
A	267	HIS	-	expression tag	UNP P12004
A	268	HIS	-	expression tag	UNP P12004
A	269	HIS	-	expression tag	UNP P12004
A	270	HIS	-	expression tag	UNP P12004
C	262	LEU	-	expression tag	UNP P12004
C	263	GLU	-	expression tag	UNP P12004
C	264	HIS	-	expression tag	UNP P12004
C	265	HIS	-	expression tag	UNP P12004
C	266	HIS	-	expression tag	UNP P12004
C	267	HIS	-	expression tag	UNP P12004
C	268	HIS	-	expression tag	UNP P12004
C	269	HIS	-	expression tag	UNP P12004
C	270	HIS	-	expression tag	UNP P12004
E	262	LEU	-	expression tag	UNP P12004
E	263	GLU	-	expression tag	UNP P12004
E	264	HIS	-	expression tag	UNP P12004
E	265	HIS	-	expression tag	UNP P12004
E	266	HIS	-	expression tag	UNP P12004

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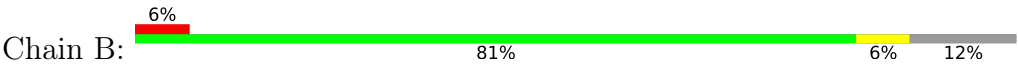
Chain	Residue	Modelled	Actual	Comment	Reference
E	267	HIS	-	expression tag	UNP P12004
E	268	HIS	-	expression tag	UNP P12004
E	269	HIS	-	expression tag	UNP P12004
E	270	HIS	-	expression tag	UNP P12004

- Molecule 2 is a protein called DVC1 PIP box.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	0	0	0
			116	73	22	21			
2	D	14	Total	C	N	O	0	0	0
			116	73	22	21			
2	F	11	Total	C	N	O	0	0	0
			92	59	16	17			

ASP	GLU	GLY	SER	LEU	GLU	HIS	HIS	HIS	HIS	HIS
GLU	GLY	SER	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS

● Molecule 2: DVC1 PIP box



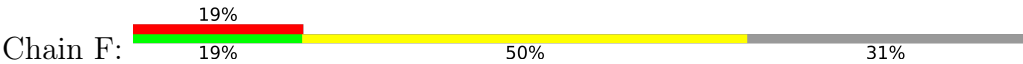
SER	ASN	R334	V335	S336
SER	ASN	R334	V335	S336

● Molecule 2: DVC1 PIP box



SER	ASN	S323	V327	L328	S329	V335	S336
SER	ASN	S323	V327	L328	S329	V335	S336

● Molecule 2: DVC1 PIP box



SER	ASN	H324	Q325	N326	V327	L328	S329	N330	Y331	F332	F333	ARG	VAL	SER
SER	ASN	H324	Q325	N326	V327	L328	S329	N330	Y331	F332	F333	ARG	VAL	SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	71.65Å 71.65Å 322.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.33 – 2.94 48.33 – 2.94	Depositor EDS
% Data completeness (in resolution range)	94.6 (48.33-2.94) 94.6 (48.33-2.94)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.207 , 0.270 0.224 , 0.281	Depositor DCC
R_{free} test set	919 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6099	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.77	0/1947	1.01	4/2629 (0.2%)
1	C	0.83	0/1956	1.04	3/2641 (0.1%)
1	E	0.77	1/1947 (0.1%)	1.03	8/2629 (0.3%)
2	B	0.53	0/119	0.87	0/161
2	D	0.53	0/119	1.04	0/161
2	F	0.55	0/95	0.75	0/129
All	All	0.78	1/6183 (0.0%)	1.02	15/8350 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	129	PRO	N-CD	5.82	1.55	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	VAL	N-CA-C	6.40	116.62	106.32
1	E	185	THR	N-CA-C	6.33	120.17	110.36
1	C	41	ASP	N-CA-C	-6.29	101.47	110.59
1	A	109	GLU	N-CA-C	-5.67	105.95	112.92
1	E	131	GLN	N-CA-C	5.66	117.84	109.69
1	E	176	GLY	N-CA-C	-5.61	103.11	110.29
1	E	219	THR	CA-C-N	-5.46	114.06	120.12
1	E	219	THR	C-N-CA	-5.46	114.06	120.12
1	E	65	ASN	N-CA-C	5.45	117.76	110.35
1	A	147	ILE	CB-CA-C	-5.44	104.92	111.88
1	A	137	VAL	N-CA-C	5.20	115.39	108.11
1	E	149	ARG	N-CA-C	-5.16	105.35	111.69
1	E	96	ALA	N-CA-C	-5.16	105.64	112.24
1	A	73	THR	N-CA-C	-5.05	105.68	111.14
1	C	123	VAL	CB-CA-C	-5.04	106.20	112.45

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	1922	0	1932	60	1
1	C	1931	0	1938	57	1
1	E	1922	0	1934	69	0
2	B	116	0	108	1	0
2	D	116	0	108	5	0
2	F	92	0	81	15	0
All	All	6099	0	6101	184	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 15.

All (184) 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:47:LEU:CD2	1:E:128:ILE:HD11	1.42	1.45
1:E:44:HIS:O	2:F:327:VAL:HG13	1.33	1.25
1:E:216:THR:O	1:E:219:THR:HG23	1.45	1.15
1:E:47:LEU:HD22	1:E:128:ILE:HD11	1.23	1.12
1:C:16:LEU:HD22	1:C:79:LEU:HD12	1.30	1.10
1:E:47:LEU:HD21	1:E:128:ILE:HD11	1.21	1.10
1:A:16:LEU:CD1	1:A:79:LEU:HD12	1.80	1.09
1:A:16:LEU:HD12	1:A:79:LEU:HD12	1.31	1.06
1:E:47:LEU:CD2	1:E:128:ILE:CD1	2.36	1.03
1:E:128:ILE:HG21	1:E:250:TYR:CZ	1.97	0.98
1:E:44:HIS:O	2:F:327:VAL:CG1	2.18	0.92
2:F:327:VAL:HG12	2:F:328:LEU:N	1.84	0.92
1:E:127:GLY:O	1:E:129:PRO:HD3	1.70	0.90
1:A:166:GLY:HA2	1:A:197:ILE:HD13	1.52	0.90
2:F:327:VAL:HG12	2:F:328:LEU:H	1.38	0.88
1:A:74:SER:HA	1:E:175:LEU:HD21	1.56	0.87
1:C:16:LEU:CD2	1:C:79:LEU:HD12	2.03	0.87
1:C:16:LEU:HD13	1:C:79:LEU:CD1	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLY:HA2	1:A:121:LEU:HD12	1.60	0.83
1:A:195:VAL:HG23	1:C:109:GLU:OE1	1.78	0.83
1:C:56:GLY:HA3	1:C:244:MET:HG2	1.61	0.83
1:E:255:ILE:HA	2:F:324:HIS:HB3	1.62	0.82
1:E:138:LYS:HE2	1:E:226:THR:CG2	2.10	0.81
2:F:327:VAL:CG1	2:F:328:LEU:H	1.95	0.79
1:E:47:LEU:HD21	1:E:128:ILE:CD1	2.07	0.77
1:E:47:LEU:HD22	1:E:128:ILE:CD1	2.04	0.76
1:E:216:THR:O	1:E:219:THR:CG2	2.32	0.76
1:A:16:LEU:HD11	1:A:75:MET:HG2	1.69	0.74
1:E:192:GLU:HG3	1:E:193:GLU:H	1.50	0.74
1:A:16:LEU:HD12	1:A:79:LEU:CD1	2.17	0.73
1:E:138:LYS:CE	1:E:226:THR:CG2	2.66	0.72
2:F:327:VAL:CG1	2:F:328:LEU:N	2.50	0.72
1:C:191:GLU:HG2	1:C:192:GLU:H	1.55	0.72
2:F:326:ASN:HD21	2:F:331:TYR:HE2	1.38	0.72
1:C:23:ILE:HG13	1:C:72:LEU:HD12	1.70	0.72
1:A:69:GLY:HA2	1:A:121:LEU:CD1	2.20	0.70
1:E:168:LYS:HD3	1:E:181:LYS:HE2	1.74	0.70
1:C:184:GLN:HE21	1:C:197:ILE:HB	1.55	0.70
1:A:175:LEU:HD12	1:A:175:LEU:H	1.56	0.69
1:C:175:LEU:H	1:C:175:LEU:HD12	1.58	0.69
1:C:16:LEU:HD23	1:C:76:SER:HA	1.73	0.69
1:A:74:SER:HB3	1:E:175:LEU:HG	1.75	0.69
1:C:192:GLU:HG3	1:C:193:GLU:HG3	1.75	0.68
1:A:74:SER:HA	1:E:175:LEU:CD2	2.23	0.68
1:E:107:ASN:O	1:E:108:GLN:HB2	1.95	0.68
1:E:75:MET:HG3	1:E:116:MET:HE1	1.76	0.67
1:A:74:SER:CB	1:E:175:LEU:HG	2.24	0.67
1:A:195:VAL:CG2	1:C:109:GLU:OE1	2.42	0.67
1:E:138:LYS:CE	1:E:226:THR:HG22	2.23	0.66
1:A:105:ALA:O	1:A:108:GLN:HG3	1.96	0.66
1:C:191:GLU:HG2	1:C:192:GLU:N	2.11	0.66
1:A:64:ARG:HD2	1:A:65:ASN:H	1.61	0.65
1:A:56:GLY:HA3	1:A:244:MET:HG2	1.78	0.64
1:E:56:GLY:HA3	1:E:244:MET:HG2	1.81	0.63
1:C:23:ILE:HD13	1:C:48:VAL:HG11	1.81	0.63
1:E:138:LYS:HE3	1:E:226:THR:HG22	1.80	0.63
1:A:124:GLU:HG3	2:B:334:ARG:HE	1.64	0.62
1:C:255:ILE:HB	2:D:323:SER:HA	1.81	0.62
1:C:44:HIS:O	2:D:327:VAL:HG13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:LEU:HD23	1:C:76:SER:CA	2.29	0.62
1:A:117:LYS:HE3	1:E:176:GLY:HA2	1.81	0.61
1:A:64:ARG:HD2	1:A:65:ASN:N	2.15	0.61
1:A:182:LEU:HA	1:C:109:GLU:O	1.99	0.61
1:E:192:GLU:HG3	1:E:193:GLU:N	2.16	0.60
1:A:75:MET:HG3	1:A:116:MET:HE1	1.83	0.60
1:E:5:ARG:HB3	1:E:59:THR:HB	1.84	0.60
1:E:44:HIS:C	2:F:327:VAL:HG13	2.21	0.60
1:C:191:GLU:CG	1:C:192:GLU:H	2.15	0.59
1:A:16:LEU:CG	1:A:79:LEU:HD12	2.31	0.58
1:A:185:THR:HG23	1:A:195:VAL:H	1.68	0.58
1:E:52:LEU:HD22	1:E:244:MET:HE2	1.83	0.58
1:E:53:ARG:NH1	1:E:245:GLY:HA2	2.18	0.58
1:C:16:LEU:HD21	1:C:75:MET:HG2	1.84	0.58
1:C:123:VAL:HG12	1:C:125:GLN:HG2	1.86	0.58
1:A:143:GLU:O	1:A:147:ILE:HG12	2.04	0.57
1:C:9:GLY:HA3	1:C:88:ILE:HG13	1.85	0.57
1:A:78:ILE:HD12	1:A:116:MET:HE2	1.85	0.57
1:C:16:LEU:CD2	1:C:76:SER:HA	2.35	0.56
1:A:109:GLU:HA	1:A:109:GLU:OE1	2.06	0.56
1:C:16:LEU:HD13	1:C:79:LEU:HD12	1.85	0.56
1:E:69:GLY:HA2	1:E:121:LEU:HD12	1.87	0.56
1:E:129:PRO:HD2	2:F:332:PHE:CD1	2.40	0.56
1:E:143:GLU:O	1:E:147:ILE:HG12	2.05	0.56
1:E:40:MET:HG3	1:E:47:LEU:HD12	1.88	0.56
1:E:128:ILE:CG2	1:E:250:TYR:CZ	2.83	0.56
1:C:30:ILE:HG13	1:C:68:MET:HE2	1.88	0.55
1:A:166:GLY:HA2	1:A:197:ILE:CD1	2.33	0.55
1:A:7:VAL:HA	1:A:87:ILE:HG23	1.90	0.54
1:C:143:GLU:O	1:C:147:ILE:HG12	2.07	0.54
1:E:133:TYR:HA	1:E:230:SER:OG	2.08	0.53
1:E:128:ILE:HD13	1:E:250:TYR:CE1	2.44	0.53
1:A:27:CYS:HB2	1:A:123:VAL:HG21	1.91	0.53
1:A:242:ALA:O	1:A:243:ASP:HB2	2.08	0.53
1:E:23:ILE:HG13	1:E:72:LEU:HD12	1.91	0.52
1:A:16:LEU:CD1	1:A:79:LEU:CD1	2.72	0.52
1:A:105:ALA:O	1:A:108:GLN:CG	2.57	0.52
1:C:114:TYR:C	1:C:115:GLU:HG3	2.32	0.52
1:C:7:VAL:HA	1:C:87:ILE:HG23	1.90	0.52
1:E:219:THR:OG1	1:E:220:PRO:HD3	2.09	0.52
1:A:185:THR:CG2	1:A:195:VAL:H	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:PRO:HD2	2:F:332:PHE:HD1	1.75	0.51
2:D:327:VAL:HG12	2:D:329:SER:H	1.75	0.51
1:C:5:ARG:HB3	1:C:59:THR:HB	1.93	0.51
1:C:70:VAL:HG12	1:C:72:LEU:HD23	1.93	0.50
1:C:53:ARG:HG3	1:C:244:MET:O	2.12	0.50
1:C:64:ARG:HG2	1:C:65:ASN:N	2.27	0.50
1:C:191:GLU:CG	1:C:192:GLU:N	2.74	0.50
1:C:16:LEU:CD1	1:C:79:LEU:HD12	2.42	0.49
1:A:23:ILE:HD12	1:A:39:SER:HB3	1.93	0.49
1:A:31:SER:O	1:A:60:TYR:OH	2.26	0.49
1:C:75:MET:HG3	1:C:116:MET:HE1	1.93	0.49
1:E:114:TYR:C	1:E:115:GLU:HG3	2.37	0.49
1:E:7:VAL:HG22	1:E:87:ILE:HD13	1.95	0.48
1:E:107:ASN:OD1	1:E:108:GLN:N	2.47	0.48
1:E:138:LYS:CE	1:E:226:THR:HG21	2.44	0.48
1:C:203:VAL:CG1	1:C:205:LEU:HG	2.44	0.47
1:E:216:THR:C	1:E:219:THR:HG23	2.30	0.47
1:E:254:LYS:O	1:E:255:ILE:HG12	2.14	0.47
1:E:78:ILE:HD12	1:E:116:MET:HE2	1.97	0.47
1:E:127:GLY:O	2:F:332:PHE:HB3	2.15	0.47
2:D:327:VAL:HG12	2:D:328:LEU:N	2.30	0.47
1:E:2:PHE:O	1:E:91:ARG:HA	2.15	0.47
2:F:328:LEU:HD12	2:F:328:LEU:HA	1.75	0.46
1:C:11:ILE:O	1:C:15:VAL:HG23	2.15	0.46
1:C:16:LEU:CD1	1:C:79:LEU:CD1	2.87	0.46
1:C:146:ARG:NH1	1:E:110:LYS:HZ1	2.13	0.46
1:E:1:MET:HB3	1:E:63:ASP:OD2	2.16	0.46
1:A:212:LEU:O	1:A:216:THR:HG23	2.15	0.46
1:A:74:SER:CA	1:E:175:LEU:CD2	2.93	0.46
1:C:230:SER:HB2	1:C:233:VAL:CG2	2.46	0.46
1:E:127:GLY:C	1:E:129:PRO:HD3	2.41	0.46
1:E:138:LYS:HE2	1:E:226:THR:HG22	1.87	0.46
1:A:133:TYR:HA	1:A:230:SER:OG	2.16	0.46
1:A:70:VAL:HG12	1:A:72:LEU:HD23	1.98	0.45
1:A:5:ARG:HB3	1:A:59:THR:HB	1.96	0.45
1:E:89:THR:HB	1:E:102:VAL:HB	1.98	0.45
1:E:128:ILE:HG21	1:E:250:TYR:OH	2.13	0.45
1:A:192:GLU:HB3	1:A:193:GLU:H	1.48	0.45
1:C:16:LEU:HD13	1:C:79:LEU:HD11	1.91	0.45
1:C:242:ALA:O	1:C:243:ASP:HB2	2.16	0.45
1:C:246:HIS:CD2	1:C:248:LYS:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:SER:OG	1:E:175:LEU:HG	2.17	0.45
1:E:192:GLU:CG	1:E:193:GLU:H	2.24	0.45
1:A:96:ALA:O	1:A:118:LEU:HD12	2.16	0.45
1:A:184:GLN:HG3	1:A:195:VAL:O	2.17	0.45
1:A:27:CYS:SG	1:A:67:ALA:HB1	2.57	0.45
1:C:184:GLN:NE2	1:C:197:ILE:HB	2.28	0.44
1:C:230:SER:HB2	1:C:233:VAL:HG22	1.99	0.44
1:C:31:SER:O	1:C:60:TYR:OH	2.33	0.44
1:C:101:LEU:HD11	1:C:116:MET:HE3	1.99	0.44
1:A:23:ILE:HG13	1:A:72:LEU:HD12	1.98	0.44
1:E:138:LYS:HE3	1:E:226:THR:CG2	2.39	0.43
1:A:16:LEU:HD13	1:A:76:SER:HA	1.99	0.43
1:A:179:ASN:ND2	1:C:113:ASP:OD2	2.43	0.43
1:C:107:ASN:OD1	1:C:108:GLN:N	2.51	0.43
1:A:89:THR:HB	1:A:102:VAL:HB	2.01	0.43
1:A:130:GLU:O	1:A:130:GLU:HG3	2.19	0.43
1:C:107:ASN:O	1:C:108:GLN:HB2	2.18	0.43
1:A:40:MET:HE3	1:A:40:MET:HB2	1.88	0.43
2:F:324:HIS:O	2:F:325:GLN:HB2	2.17	0.43
1:C:125:GLN:O	1:C:126:LEU:HD12	2.19	0.42
1:A:16:LEU:HG	1:A:79:LEU:HD12	2.00	0.42
1:E:230:SER:HB2	1:E:233:VAL:HG22	2.00	0.42
1:C:64:ARG:CZ	1:C:66:LEU:HD21	2.49	0.42
1:E:140:PRO:HG3	1:E:193:GLU:HA	2.01	0.42
1:A:38:GLN:NE2	1:A:126:LEU:H	2.18	0.42
1:E:75:MET:HA	1:E:116:MET:HE1	2.02	0.42
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.88	0.42
1:E:107:ASN:O	1:E:108:GLN:CB	2.65	0.42
1:E:219:THR:OG1	1:E:220:PRO:CD	2.68	0.42
1:A:52:LEU:HD22	1:A:244:MET:HE2	2.02	0.41
1:A:199:MET:HE3	1:A:201:GLU:N	2.35	0.41
1:C:60:TYR:C	1:C:61:ARG:HG2	2.45	0.41
2:F:327:VAL:HG12	2:F:329:SER:H	1.85	0.41
1:A:5:ARG:NH2	1:A:104:GLU:OE1	2.54	0.41
1:C:125:GLN:HB2	2:D:335:VAL:O	2.20	0.41
1:C:244:MET:HE2	1:C:244:MET:HB3	1.89	0.41
1:C:212:LEU:O	1:C:216:THR:HG23	2.21	0.41
1:A:12:LEU:HA	1:A:12:LEU:HD12	1.87	0.41
1:E:79:LEU:HA	1:E:79:LEU:HD23	1.90	0.41
1:C:23:ILE:HG22	1:C:41:ASP:HA	2.03	0.41
1:E:138:LYS:HE3	1:E:138:LYS:HB2	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:SER:CB	1:E:177:ASN:HB3	2.51	0.40
1:A:74:SER:O	1:A:78:ILE:HG13	2.21	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:5:ARG:NH1	1:C:95:ASN:ND2[5_454]	2.15	0.05

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	246/270 (91%)	243 (99%)	3 (1%)	0	100	100
1	C	247/270 (92%)	238 (96%)	9 (4%)	0	100	100
1	E	246/270 (91%)	242 (98%)	4 (2%)	0	100	100
2	B	12/16 (75%)	12 (100%)	0	0	100	100
2	D	12/16 (75%)	11 (92%)	1 (8%)	0	100	100
2	F	9/16 (56%)	4 (44%)	5 (56%)	0	100	100
All	All	772/858 (90%)	750 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	218/237 (92%)	216 (99%)	2 (1%)	70	82
1	C	219/237 (92%)	215 (98%)	4 (2%)	51	72
1	E	218/237 (92%)	215 (99%)	3 (1%)	59	76
2	B	14/16 (88%)	14 (100%)	0	100	100
2	D	14/16 (88%)	14 (100%)	0	100	100
2	F	11/16 (69%)	11 (100%)	0	100	100
All	All	694/759 (91%)	685 (99%)	9 (1%)	61	77

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ILE
1	A	107	ASN
1	C	16	LEU
1	C	78	ILE
1	C	108	GLN
1	C	226	THR
1	E	16	LEU
1	E	78	ILE
1	E	115	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	200	ASN
1	A	246	HIS
2	B	325	GLN
2	B	330	ASN
1	C	177	ASN
1	C	184	GLN
2	D	324	HIS
1	E	36	ASN
1	E	177	ASN

5.3.3 RNA ⓘ

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	250/270 (92%)	-0.02	4 (1%) 70 62	23, 38, 64, 78	0
1	C	251/270 (92%)	0.03	7 (2%) 55 46	23, 40, 65, 85	0
1	E	250/270 (92%)	0.31	11 (4%) 39 31	30, 50, 77, 90	0
2	B	14/16 (87%)	0.69	1 (7%) 22 19	39, 50, 60, 70	0
2	D	14/16 (87%)	0.58	0 100 100	46, 52, 72, 74	0
2	F	11/16 (68%)	1.43	3 (27%) 1 1	58, 71, 79, 84	0
All	All	790/858 (92%)	0.14	26 (3%) 49 41	23, 43, 72, 90	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	109	GLU	4.0
1	E	128	ILE	3.8
1	E	124	GLU	3.5
1	E	126	LEU	3.1
1	A	165	ASP	3.0
1	E	175	LEU	3.0
1	C	123	VAL	3.0
1	E	123	VAL	2.9
1	C	255	ILE	2.7
1	E	125	GLN	2.7
1	C	63	ASP	2.6
1	E	95	ASN	2.5
1	E	193	GLU	2.4
2	F	333	PRO	2.4
1	E	96	ALA	2.4
1	C	1	MET	2.4
2	B	336	SER	2.3
1	A	177	ASN	2.3
1	E	132	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	8	GLN	2.2
1	A	232	ASP	2.2
2	F	324	HIS	2.2
1	E	255	ILE	2.1
1	A	123	VAL	2.1
1	C	107	ASN	2.1
2	F	325	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.