



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:50 PM UTC

PDB ID : 7YPF / pdb_00007ypf
Title : Crystal structure of AsfvPCNA in space group of P1
Authors : Shao, Z.W.; Gan, J.H.
Deposited on : 2022-08-03
Resolution : 2.50 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

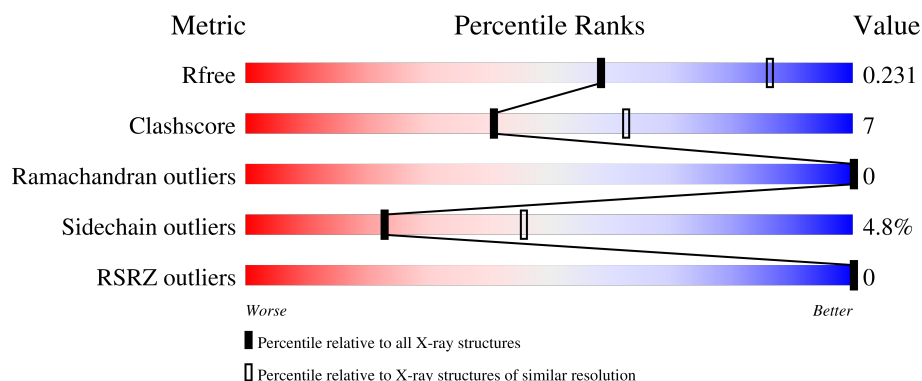
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	303	
1	B	303	
1	C	303	
1	D	303	
1	E	303	

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Mol	Chain	Length	Quality of chain
1	F	303	74% 18% • 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13935 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 E301R.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	Se	0	0	0
			2299	1479	377	433	3	7			
1	B	282	Total	C	N	O	S	Se	0	0	0
			2305	1485	377	433	3	7			
1	C	282	Total	C	N	O	S	Se	0	0	0
			2305	1484	377	433	3	8			
1	D	282	Total	C	N	O	S	Se	0	0	0
			2302	1482	377	433	3	7			
1	E	282	Total	C	N	O	S	Se	0	0	0
			2302	1482	377	433	3	7			
1	F	282	Total	C	N	O	S	Se	0	0	0
			2312	1489	377	435	3	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A0A1E3R5
A	0	SER	-	expression tag	UNP A0A0A1E3R5
B	-1	GLY	-	expression tag	UNP A0A0A1E3R5
B	0	SER	-	expression tag	UNP A0A0A1E3R5
C	-1	GLY	-	expression tag	UNP A0A0A1E3R5
C	0	SER	-	expression tag	UNP A0A0A1E3R5
D	-1	GLY	-	expression tag	UNP A0A0A1E3R5
D	0	SER	-	expression tag	UNP A0A0A1E3R5
E	-1	GLY	-	expression tag	UNP A0A0A1E3R5
E	0	SER	-	expression tag	UNP A0A0A1E3R5
F	-1	GLY	-	expression tag	UNP A0A0A1E3R5
F	0	SER	-	expression tag	UNP A0A0A1E3R5

- Molecule 2 is water.

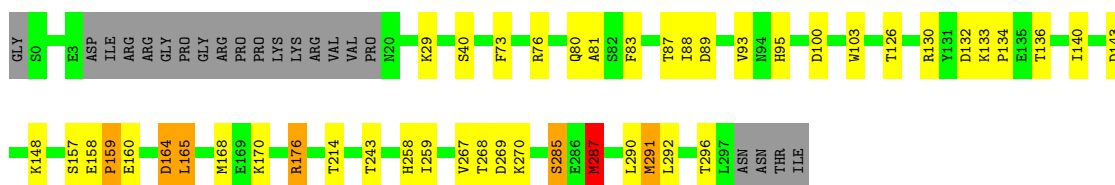
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	16	Total 16	O 16	0	0
2	B	23	Total 23	O 23	0	0
2	C	21	Total 21	O 21	0	0
2	D	14	Total 14	O 14	0	0
2	E	19	Total 19	O 19	0	0
2	F	17	Total 17	O 17	0	0

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: E301R

Chain A: 



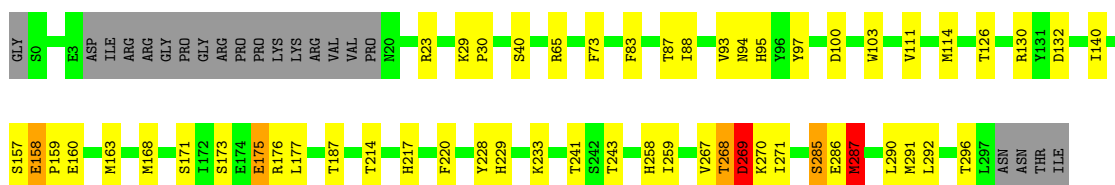
• Molecule 1: E301R

Chain B: 



• Molecule 1: E301R

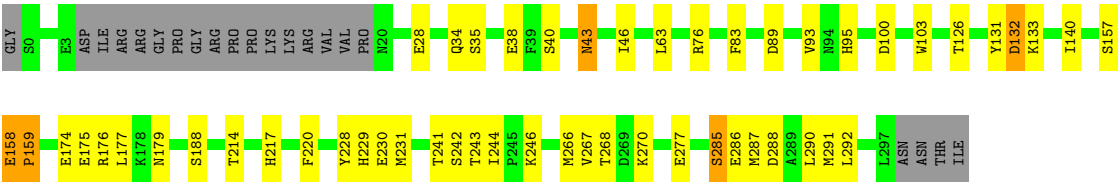
Chain C: 



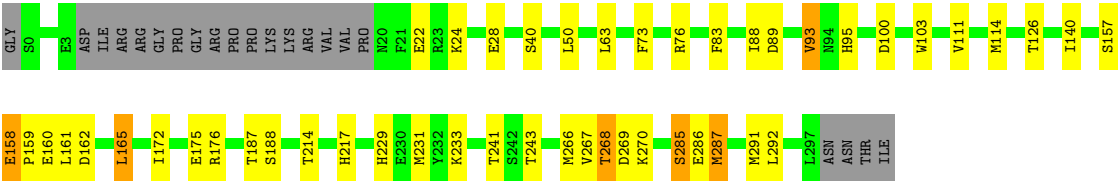
• Molecule 1: E301R

Chain D: 

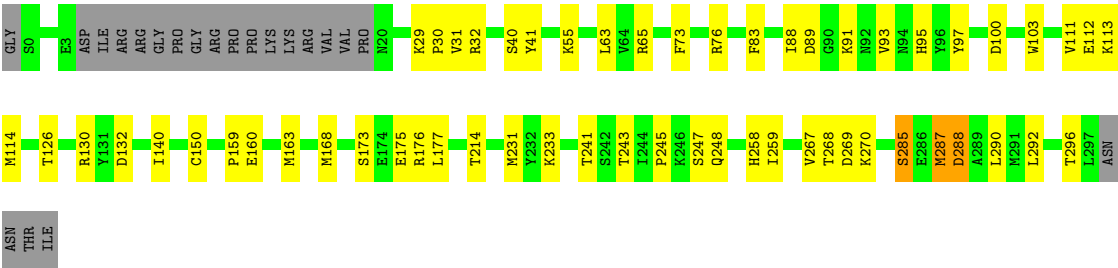




• Molecule 1: E301R



• Molecule 1: E301R



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.66Å 118.87Å 118.84Å 60.03° 89.98° 89.96°	Depositor
Resolution (Å)	29.73 – 2.50 29.73 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.5 (29.73-2.50) 93.4 (29.73-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.19.1_4122: ???)	Depositor
R, R_{free}	0.208 , 0.233 0.211 , 0.231	Depositor DCC
R_{free} test set	4429 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 9.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.477 for h,k-l,k 0.477 for h,l,-k+l 0.469 for h,-l,k-l 0.469 for h,-k+l,-k 0.477 for h,-k,-l 0.030 for -h,-k+l,l 0.029 for -h,k,k-l 0.030 for -h,l,k 0.031 for -h,-l,-k 0.031 for -h,k-l,-l 0.030 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13935	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.42% 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	0.60	1/2338 (0.0%)	0.70	11/3140 (0.4%)
1	B	0.59	2/2344 (0.1%)	0.63	4/3148 (0.1%)
1	C	0.50	2/2344 (0.1%)	0.67	8/3147 (0.3%)
1	D	0.54	1/2341 (0.0%)	0.64	9/3144 (0.3%)
1	E	0.55	0/2341	0.65	4/3144 (0.1%)
1	F	0.46	1/2351 (0.0%)	0.60	4/3156 (0.1%)
All	All	0.54	7/14059 (0.0%)	0.65	40/18879 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	124	LYS	C-O	-5.25	1.17	1.23
1	B	289	ALA	C-O	-5.24	1.17	1.24
1	A	136	THR	C-O	-5.22	1.17	1.23
1	C	87	THR	C-O	-5.19	1.17	1.24
1	F	288	ASP	C-O	-5.17	1.19	1.24
1	C	271	ILE	C-O	-5.12	1.18	1.24
1	D	288	ASP	C-O	-5.11	1.20	1.24

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	GLU	N-CA-C	-8.30	99.19	109.65
1	E	158	GLU	N-CA-C	-7.87	99.84	109.83
1	D	158	GLU	N-CA-C	-7.68	100.41	109.93
1	D	176	ARG	N-CA-C	7.66	119.70	111.36
1	C	29	LYS	CA-C-N	7.24	127.81	120.14
1	C	29	LYS	C-N-CA	7.24	127.81	120.14
1	F	176	ARG	N-CA-C	7.00	118.99	111.36
1	C	269	ASP	N-CA-C	6.91	118.89	111.36
1	D	159	PRO	N-CA-C	6.60	121.88	111.38
1	C	268	THR	N-CA-C	6.37	118.62	109.14
1	A	158	GLU	CA-C-N	6.36	126.33	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	GLU	C-N-CA	6.36	126.33	119.78
1	B	176	ARG	N-CA-C	6.32	119.47	111.69
1	E	268	THR	N-CA-C	6.22	118.87	109.41
1	A	176	ARG	N-CA-C	6.02	117.92	111.36
1	C	175	GLU	N-CA-C	-5.99	104.83	111.36
1	F	290	LEU	N-CA-C	5.91	119.27	109.46
1	A	290	LEU	N-CA-C	5.79	119.07	109.46
1	F	29	LYS	CA-C-N	5.75	125.94	120.31
1	F	29	LYS	C-N-CA	5.75	125.94	120.31
1	A	159	PRO	N-CA-C	5.55	120.03	111.21
1	A	160	GLU	N-CA-C	-5.49	101.73	109.96
1	E	176	ARG	N-CA-C	5.46	117.32	111.36
1	C	287	MSE	N-CA-CB	-5.46	102.19	110.77
1	E	286	GLU	N-CA-C	5.32	117.40	107.99
1	A	164	ASP	N-CA-C	5.30	118.85	112.38
1	A	287	MSE	N-CA-CB	-5.25	102.86	110.84
1	D	133	LYS	CA-C-N	5.23	124.89	119.56
1	D	133	LYS	C-N-CA	5.23	124.89	119.56
1	D	290	LEU	N-CA-C	5.20	117.71	109.24
1	D	131	TYR	CA-C-N	5.19	127.23	120.28
1	D	131	TYR	C-N-CA	5.19	127.23	120.28
1	B	29	LYS	CA-C-N	5.17	125.62	120.14
1	B	29	LYS	C-N-CA	5.17	125.62	120.14
1	B	290	LEU	N-CA-C	5.15	117.63	109.24
1	C	290	LEU	N-CA-C	5.11	117.57	109.24
1	A	81	ALA	N-CA-C	5.09	116.91	111.36
1	D	286	GLU	N-CA-C	5.02	116.80	108.02
1	A	29	LYS	CA-C-N	5.00	125.44	120.14
1	A	29	LYS	C-N-CA	5.00	125.44	120.14

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	2299	0	2282	26	0
1	B	2305	0	2300	36	0
1	C	2305	0	2298	35	0
1	D	2302	0	2291	25	0
1	E	2302	0	2291	28	0
1	F	2312	0	2311	32	0
2	A	16	0	0	0	0
2	B	23	0	0	1	0
2	C	21	0	0	0	0
2	D	14	0	0	0	0
2	E	19	0	0	0	0
2	F	17	0	0	0	0
All	All	13935	0	13773	180	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 7.

All (180) 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:268:THR:HG22	1:E:287:MSE:HB2	1.41	1.00
1:E:268:THR:HG22	1:E:287:MSE:CB	1.98	0.92
1:F:231:MSE:HE3	1:F:233:LYS:HD3	1.52	0.91
1:C:103:TRP:HB3	1:C:159:PRO:HG2	1.58	0.85
1:C:268:THR:HG22	1:C:287:MSE:CB	2.10	0.81
1:A:103:TRP:HB3	1:A:159:PRO:HG3	1.65	0.78
1:D:103:TRP:HB3	1:D:159:PRO:HG2	1.66	0.77
1:E:103:TRP:HB3	1:E:159:PRO:HG3	1.65	0.77
1:E:268:THR:OG1	1:E:285:SER:HB3	1.84	0.77
1:A:269:ASP:CG	1:A:287:MSE:HE1	2.10	0.77
1:C:176:ARG:HH21	1:C:176:ARG:HG3	1.50	0.76
1:C:268:THR:HG22	1:C:287:MSE:HB2	1.67	0.76
1:A:76:ARG:HG3	1:A:83:PHE:CD1	2.28	0.69
1:F:76:ARG:HG2	1:F:83:PHE:HD1	1.59	0.68
1:B:231:MSE:HE3	1:B:233:LYS:HD3	1.76	0.68
1:A:76:ARG:HG3	1:A:83:PHE:HD1	1.59	0.67
1:C:268:THR:OG1	1:C:285:SER:HB3	1.94	0.67
1:A:269:ASP:OD2	1:A:287:MSE:HE1	1.95	0.66
1:C:268:THR:HG22	1:C:287:MSE:HB3	1.78	0.65
1:B:103:TRP:HB3	1:B:159:PRO:HG2	1.78	0.65
1:D:229:HIS:HE1	1:D:231:MSE:HE3	1.61	0.64
1:C:160:GLU:O	1:C:160:GLU:HG3	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ARG:NH2	1:B:132:ASP:OD2	2.32	0.61
1:C:103:TRP:CB	1:C:159:PRO:HG2	2.29	0.61
1:A:132:ASP:O	1:A:134:PRO:HD3	2.02	0.59
1:D:229:HIS:CE1	1:D:231:MSE:HE3	2.37	0.59
1:E:268:THR:CG2	1:E:287:MSE:HB2	2.25	0.59
1:E:160:GLU:O	1:E:160:GLU:HG3	2.03	0.58
1:B:246:LYS:NZ	2:B:402:HOH:O	2.35	0.58
1:E:217:HIS:HD2	1:E:229:HIS:NE2	2.01	0.58
1:C:171:SER:HA	1:C:176:ARG:HD2	1.86	0.58
1:C:267:VAL:HG11	1:C:292:LEU:HD23	1.85	0.58
1:F:267:VAL:HG11	1:F:292:LEU:HD23	1.86	0.58
1:C:173:SER:O	1:C:177:LEU:HG	2.04	0.57
1:F:231:MSE:CE	1:F:233:LYS:HD3	2.31	0.57
1:F:83:PHE:HB2	1:F:168:MSE:HE3	1.87	0.57
1:C:268:THR:CG2	1:C:287:MSE:HB2	2.33	0.56
1:E:268:THR:HG22	1:E:287:MSE:HB3	1.82	0.56
1:F:31:VAL:HG12	1:F:32:ARG:HD2	1.88	0.56
1:F:103:TRP:HB3	1:F:159:PRO:HG2	1.88	0.56
1:A:258:HIS:CE1	1:A:296:THR:HG21	2.42	0.55
1:B:267:VAL:HG11	1:B:292:LEU:HD23	1.89	0.55
1:A:269:ASP:CG	1:A:287:MSE:CE	2.79	0.55
1:D:103:TRP:CB	1:D:159:PRO:HG2	2.36	0.55
1:A:267:VAL:HG11	1:A:292:LEU:HD23	1.89	0.54
1:B:83:PHE:HB2	1:B:168:MSE:HE3	1.88	0.54
1:D:63:LEU:HD22	1:D:159:PRO:HB3	1.90	0.54
1:E:291:MSE:HA	1:E:291:MSE:HE3	1.88	0.54
1:E:187:THR:HG22	1:E:270:LYS:HD3	1.90	0.54
1:C:130:ARG:NH1	1:C:132:ASP:OD2	2.41	0.54
1:F:268:THR:HG22	1:F:287:MSE:HB2	1.91	0.53
1:C:269:ASP:HB2	1:C:287:MSE:HE1	1.90	0.52
1:F:173:SER:O	1:F:177:LEU:HG	2.09	0.52
1:C:40:SER:HB3	1:C:95:HIS:HB3	1.91	0.52
1:B:149:GLU:OE2	1:C:233:LYS:NZ	2.33	0.52
1:C:176:ARG:HG3	1:C:176:ARG:NH2	2.23	0.52
1:B:76:ARG:HD3	1:B:80:GLN:HG2	1.92	0.51
1:B:258:HIS:CE1	1:B:259:ILE:HG13	2.45	0.51
1:B:188:SER:HB2	1:B:266:MSE:SE	2.61	0.51
1:E:165:LEU:C	1:E:165:LEU:HD12	2.36	0.51
1:E:76:ARG:HG2	1:E:83:PHE:CD1	2.47	0.50
1:F:231:MSE:HE3	1:F:233:LYS:CD	2.35	0.50
1:A:76:ARG:HH12	1:A:164:ASP:HB2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:258:HIS:CE1	1:F:259:ILE:HG13	2.47	0.49
1:B:89:ASP:OD2	1:B:91:LYS:HG2	2.12	0.49
1:E:111:VAL:HB	1:E:114:MSE:HE2	1.93	0.49
1:E:103:TRP:CB	1:E:159:PRO:HG3	2.39	0.49
1:A:170:LYS:O	1:A:176:ARG:HD3	2.13	0.48
1:B:76:ARG:HG3	1:B:83:PHE:HD1	1.77	0.48
1:B:166:ILE:O	1:B:170:LYS:HD2	2.13	0.48
1:F:268:THR:OG1	1:F:285:SER:HB3	2.12	0.48
1:C:286:GLU:HB2	1:C:291:MSE:SE	2.64	0.48
1:D:268:THR:OG1	1:D:285:SER:HB3	2.13	0.48
1:C:83:PHE:HB2	1:C:168:MSE:HE3	1.96	0.48
1:D:126:THR:HB	1:D:140:ILE:HB	1.95	0.48
1:A:83:PHE:HB2	1:A:168:MSE:HE3	1.95	0.48
1:F:30:PRO:HB3	1:F:97:TYR:CD2	2.49	0.48
1:C:126:THR:HB	1:C:140:ILE:HB	1.95	0.48
1:D:267:VAL:HG11	1:D:292:LEU:HD23	1.95	0.48
1:E:267:VAL:HG11	1:E:292:LEU:HD23	1.95	0.48
1:F:258:HIS:CE1	1:F:296:THR:HG21	2.48	0.48
1:E:76:ARG:HG2	1:E:83:PHE:CE1	2.49	0.47
1:A:258:HIS:CE1	1:A:259:ILE:HG13	2.49	0.47
1:C:291:MSE:HE3	1:C:291:MSE:HA	1.96	0.47
1:D:40:SER:HB3	1:D:95:HIS:HB3	1.96	0.47
1:E:126:THR:HB	1:E:140:ILE:HB	1.96	0.47
1:C:217:HIS:HD2	1:C:229:HIS:NE2	2.13	0.47
1:A:268:THR:OG1	1:A:285:SER:HB3	2.15	0.47
1:A:40:SER:HB3	1:A:95:HIS:HB3	1.97	0.47
1:B:111:VAL:HB	1:B:114:MSE:HE2	1.96	0.47
1:C:291:MSE:HE3	1:C:292:LEU:H	1.80	0.47
1:A:291:MSE:HE3	1:A:291:MSE:HA	1.97	0.47
1:B:100:ASP:OD1	1:B:100:ASP:N	2.48	0.47
1:E:22:GLU:HB3	1:E:24:LYS:HD3	1.97	0.46
1:B:268:THR:HG22	1:B:287:MSE:HB2	1.97	0.46
1:C:258:HIS:CE1	1:C:296:THR:HG21	2.51	0.46
1:B:268:THR:OG1	1:B:285:SER:HB3	2.15	0.46
1:C:111:VAL:HB	1:C:114:MSE:HE2	1.97	0.46
1:F:89:ASP:OD2	1:F:91:LYS:HE3	2.15	0.46
1:E:188:SER:HB2	1:E:266:MSE:SE	2.66	0.46
1:E:231:MSE:HE3	1:E:233:LYS:HD3	1.97	0.46
1:F:40:SER:HB3	1:F:95:HIS:HB3	1.98	0.46
1:D:100:ASP:N	1:D:100:ASP:OD1	2.49	0.46
1:C:100:ASP:OD1	1:C:100:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:SER:HB3	1:E:95:HIS:HB3	1.98	0.45
1:B:286:GLU:HB2	1:B:291:MSE:SE	2.67	0.45
1:F:100:ASP:N	1:F:100:ASP:OD1	2.48	0.45
1:B:63:LEU:HD22	1:B:159:PRO:HB3	1.98	0.45
1:F:130:ARG:NH1	1:F:132:ASP:OD2	2.49	0.45
1:A:269:ASP:OD1	1:A:269:ASP:N	2.49	0.45
1:B:40:SER:HB3	1:B:95:HIS:HB3	1.99	0.45
1:A:270:LYS:HA	1:A:270:LYS:HD2	1.85	0.44
1:A:100:ASP:N	1:A:100:ASP:OD1	2.49	0.44
1:D:177:LEU:C	1:D:179:ASN:H	2.26	0.44
1:B:76:ARG:CD	1:B:80:GLN:HG2	2.47	0.44
1:A:83:PHE:CG	1:A:168:MSE:HE3	2.52	0.44
1:D:217:HIS:CD2	1:D:231:MSE:HE2	2.53	0.44
1:F:73:PHE:HE1	1:F:88:ILE:HD12	1.83	0.44
1:F:83:PHE:CB	1:F:168:MSE:HE3	2.47	0.44
1:E:100:ASP:N	1:E:100:ASP:OD1	2.49	0.44
1:B:126:THR:HB	1:B:140:ILE:HB	1.99	0.44
1:B:284:GLN:HG2	1:B:293:ASN:OD1	2.17	0.44
1:C:187:THR:HG22	1:C:270:LYS:HD3	2.00	0.44
1:D:242:SER:OG	1:D:244:ILE:HD12	2.18	0.44
1:E:40:SER:O	1:E:93:VAL:HG13	2.18	0.44
1:E:63:LEU:HD21	1:E:160:GLU:O	2.18	0.43
1:F:111:VAL:HB	1:F:114:MSE:HE2	1.99	0.43
1:D:220:PHE:CE2	1:D:228:TYR:HB3	2.53	0.43
1:B:31:VAL:HG12	1:B:32:ARG:HD2	1.99	0.43
1:E:73:PHE:HE1	1:E:88:ILE:HD12	1.84	0.43
1:F:55:LYS:HE2	1:F:112:GLU:CD	2.44	0.43
1:F:126:THR:HB	1:F:140:ILE:HB	2.00	0.43
1:B:103:TRP:HB3	1:B:159:PRO:CG	2.48	0.43
1:A:165:LEU:HD12	1:A:165:LEU:O	2.19	0.43
1:B:46:ILE:HD13	1:B:46:ILE:HA	1.88	0.43
1:D:188:SER:HB2	1:D:266:MSE:SE	2.69	0.43
1:F:270:LYS:HD2	1:F:270:LYS:HA	1.81	0.43
1:F:41:TYR:OH	1:F:288:ASP:OD2	2.27	0.43
1:F:245:PRO:HG2	1:F:248:GLN:OE1	2.18	0.43
1:B:269:ASP:OD1	1:B:269:ASP:N	2.46	0.43
1:C:30:PRO:HB3	1:C:97:TYR:CD2	2.54	0.42
1:C:268:THR:OG1	1:C:285:SER:CB	2.63	0.42
1:B:30:PRO:HB3	1:B:97:TYR:CD2	2.54	0.42
1:C:65:ARG:HD3	1:C:103:TRP:CZ2	2.54	0.42
1:D:230:GLU:HG3	1:F:150:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:ARG:HG2	1:F:83:PHE:CD1	2.46	0.42
1:C:258:HIS:CE1	1:C:259:ILE:HG13	2.55	0.42
1:A:73:PHE:HE1	1:A:88:ILE:HD12	1.84	0.42
1:A:83:PHE:CB	1:A:168:MSE:HE3	2.48	0.42
1:B:185:GLU:HG2	1:B:272:ARG:HG3	2.02	0.42
1:D:277:GLU:H	1:D:277:GLU:HG2	1.67	0.42
1:B:23:ARG:HA	1:B:94:ASN:HA	2.02	0.42
1:D:76:ARG:HG3	1:D:83:PHE:CE1	2.55	0.42
1:E:269:ASP:OD1	1:E:287:MSE:SE	2.88	0.41
1:F:269:ASP:OD1	1:F:269:ASP:N	2.45	0.41
1:C:83:PHE:CB	1:C:168:MSE:HE3	2.49	0.41
1:D:43:ASN:HD22	1:D:43:ASN:HA	1.64	0.41
1:A:126:THR:HB	1:A:140:ILE:HB	2.03	0.41
1:D:46:ILE:HD13	1:D:46:ILE:HA	1.88	0.41
1:D:177:LEU:C	1:D:179:ASN:N	2.79	0.41
1:A:170:LYS:O	1:A:176:ARG:CD	2.68	0.41
1:C:23:ARG:HA	1:C:94:ASN:HA	2.03	0.41
1:E:291:MSE:HE3	1:E:292:LEU:H	1.85	0.41
1:A:143:ASP:HB3	1:A:148:LYS:HB3	2.03	0.41
1:B:65:ARG:HD3	1:B:103:TRP:CZ2	2.56	0.41
1:B:143:ASP:HB3	1:B:148:LYS:HB3	2.02	0.41
1:C:220:PHE:CE2	1:C:228:TYR:HB3	2.56	0.41
1:F:103:TRP:HB3	1:F:159:PRO:CG	2.49	0.41
1:B:30:PRO:HD3	1:B:97:TYR:CZ	2.56	0.41
1:C:73:PHE:HE1	1:C:88:ILE:HD12	1.86	0.41
1:B:270:LYS:HD2	1:B:270:LYS:HA	1.82	0.40
1:B:158:GLU:HA	1:B:159:PRO:HD3	1.92	0.40
1:D:270:LYS:HD2	1:D:270:LYS:HA	1.83	0.40
1:D:291:MSE:HE3	1:D:292:LEU:H	1.86	0.40
1:D:34:GLN:HG2	1:D:132:ASP:CG	2.47	0.40
1:F:63:LEU:HD21	1:F:160:GLU:O	2.22	0.40
1:E:50:LEU:O	1:E:50:LEU:HD12	2.21	0.40
1:B:245:PRO:HG2	1:B:248:GLN:OE1	2.20	0.40
1:D:35:SER:HB3	1:D:38:GLU:HG3	2.03	0.40
1:F:65:ARG:HD3	1:F:103:TRP:CZ2	2.57	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	278/303 (92%)	273 (98%)	5 (2%)	0	100	100
1	B	278/303 (92%)	270 (97%)	8 (3%)	0	100	100
1	C	278/303 (92%)	270 (97%)	8 (3%)	0	100	100
1	D	278/303 (92%)	269 (97%)	9 (3%)	0	100	100
1	E	278/303 (92%)	274 (99%)	4 (1%)	0	100	100
1	F	278/303 (92%)	272 (98%)	6 (2%)	0	100	100
All	All	1668/1818 (92%)	1628 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	260/279 (93%)	247 (95%)	13 (5%)	22	44
1	B	262/279 (94%)	251 (96%)	11 (4%)	26	52
1	C	262/279 (94%)	251 (96%)	11 (4%)	26	52
1	D	261/279 (94%)	246 (94%)	15 (6%)	18	39
1	E	261/279 (94%)	246 (94%)	15 (6%)	18	39
1	F	264/279 (95%)	254 (96%)	10 (4%)	29	56
All	All	1570/1674 (94%)	1495 (95%)	75 (5%)	23	46

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	87	THR
1	A	89	ASP
1	A	93	VAL
1	A	130	ARG
1	A	133	LYS
1	A	157	SER
1	A	165	LEU
1	A	214	THR
1	A	243	THR
1	A	285	SER
1	A	287	MSE
1	A	291	MSE
1	B	28	GLU
1	B	76	ARG
1	B	89	ASP
1	B	93	VAL
1	B	170	LYS
1	B	175	GLU
1	B	214	THR
1	B	243	THR
1	B	247	SER
1	B	285	SER
1	B	287	MSE
1	C	93	VAL
1	C	157	SER
1	C	158	GLU
1	C	163	MSE
1	C	175	GLU
1	C	214	THR
1	C	241	THR
1	C	243	THR
1	C	269	ASP
1	C	285	SER
1	C	287	MSE
1	D	28	GLU
1	D	43	ASN
1	D	89	ASP
1	D	93	VAL
1	D	132	ASP
1	D	157	SER
1	D	158	GLU

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Mol	Chain	Res	Type
1	D	174	GLU
1	D	175	GLU
1	D	214	THR
1	D	241	THR
1	D	243	THR
1	D	246	LYS
1	D	285	SER
1	D	287	MSE
1	E	28	GLU
1	E	89	ASP
1	E	93	VAL
1	E	157	SER
1	E	158	GLU
1	E	161	LEU
1	E	162	ASP
1	E	165	LEU
1	E	172	ILE
1	E	175	GLU
1	E	214	THR
1	E	241	THR
1	E	243	THR
1	E	285	SER
1	E	287	MSE
1	F	93	VAL
1	F	113	LYS
1	F	163	MSE
1	F	175	GLU
1	F	214	THR
1	F	241	THR
1	F	243	THR
1	F	247	SER
1	F	285	SER
1	F	287	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	179	ASN
1	A	258	HIS
1	B	80	GLN
1	B	179	ASN

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Mol	Chain	Res	Type
1	B	217	HIS
1	B	258	HIS
1	B	278	ASN
1	C	61	ASN
1	C	217	HIS
1	C	258	HIS
1	D	43	ASN
1	D	217	HIS
1	E	34	GLN
1	E	179	ASN
1	E	217	HIS
1	F	43	ASN
1	F	78	GLN
1	F	179	ASN
1	F	217	HIS
1	F	258	HIS
1	F	278	ASN

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 ⓘ

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(Å ²)	Q<0.9
1	A	274/303 (90%)	-1.33	0 100 100	18, 33, 70, 88	0
1	B	274/303 (90%)	-1.30	0 100 100	18, 33, 71, 104	0
1	C	274/303 (90%)	-1.32	0 100 100	18, 33, 71, 85	0
1	D	274/303 (90%)	-1.34	0 100 100	18, 33, 71, 93	0
1	E	274/303 (90%)	-1.30	0 100 100	17, 33, 69, 88	0
1	F	274/303 (90%)	-1.27	0 100 100	18, 33, 72, 88	0
All	All	1644/1818 (90%)	-1.31	0 100 100	17, 33, 71, 104	0

There are no RSRZ outliers to report.

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.