



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:18 AM UTC

PDB ID : 7O1F / pdb_00007o1f
Title : PCNA from Chaetomium thermophilum in complex with PolD4 PIP peptide
Authors : Alpey, M.A.; MacNeill, S.; Yang, D.
Deposited on : 2021-03-29
Resolution : 2.45 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

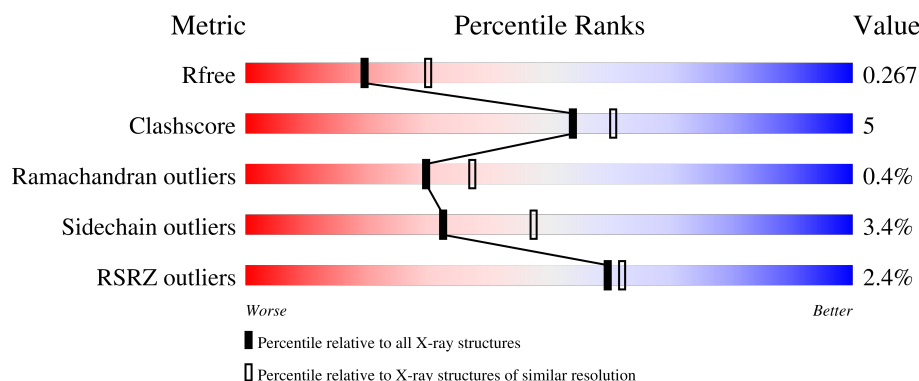
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	261	
1	B	261	
1	C	261	
1	D	261	
1	E	261	

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Mol	Chain	Length	Quality of chain
1	F	261	3% 82% 15% • •
2	J	15	47% 7% 47%
2	K	15	7% 53% 47%
2	M	15	47% 7% 47%
2	O	15	7% 47% 53%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11613 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	253	Total	C	N	O	S	0	0	0
			1889	1195	312	369	13			
1	B	250	Total	C	N	O	S	0	0	0
			1884	1187	309	375	13			
1	C	238	Total	C	N	O	S	0	0	0
			1774	1116	293	352	13			
1	D	254	Total	C	N	O	S	0	0	0
			1894	1195	314	372	13			
1	E	246	Total	C	N	O	S	0	0	0
			1852	1169	306	364	13			
1	F	253	Total	C	N	O	S	0	0	0
			1899	1197	315	374	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP G0SF70
A	0	MET	-	expression tag	UNP G0SF70
A	1	ALA	-	expression tag	UNP G0SF70
B	-1	ALA	-	expression tag	UNP G0SF70
B	0	MET	-	expression tag	UNP G0SF70
B	1	ALA	-	expression tag	UNP G0SF70
C	-1	ALA	-	expression tag	UNP G0SF70
C	0	MET	-	expression tag	UNP G0SF70
C	1	ALA	-	expression tag	UNP G0SF70
D	-1	ALA	-	expression tag	UNP G0SF70
D	0	MET	-	expression tag	UNP G0SF70
D	1	ALA	-	expression tag	UNP G0SF70
E	-1	ALA	-	expression tag	UNP G0SF70
E	0	MET	-	expression tag	UNP G0SF70
E	1	ALA	-	expression tag	UNP G0SF70
F	-1	ALA	-	expression tag	UNP G0SF70
F	0	MET	-	expression tag	UNP G0SF70

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	ALA	-	expression tag	UNP G0SF70

- Molecule 2 is a protein called Peptide fragment from PolD4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	8	Total	C	N	O	0	0	0
			64	40	12	12			
2	K	8	Total	C	N	O	0	0	0
			64	40	12	12			
2	M	8	Total	C	N	O	0	0	0
			64	40	12	12			
2	O	7	Total	C	N	O	0	0	0
			51	33	8	10			

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Na	0	0
			3	3		
3	B	2	Total	Na	0	0
			2	2		
3	C	3	Total	Na	0	0
			3	3		
3	D	4	Total	Na	0	0
			4	4		
3	E	4	Total	Na	0	0
			4	4		
3	F	2	Total	Na	0	0
			2	2		

- Molecule 4 is water.

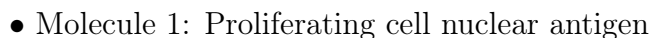
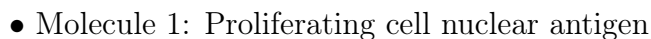
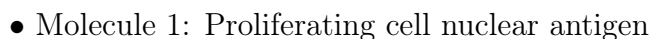
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	32	Total	O	0	0
			32	32		
4	C	27	Total	O	0	0
			27	27		
4	D	34	Total	O	0	0
			34	34		

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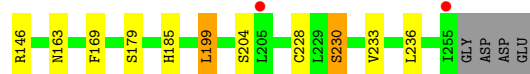
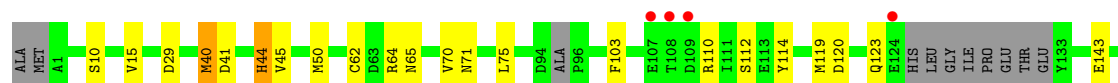
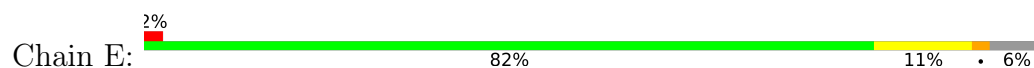
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	20	Total 20	O 20	0	0
4	F	20	Total 20	O 20	0	0
4	M	3	Total 3	O 3	0	0

- Molecule 1: Proliferating cell nuclear antigen

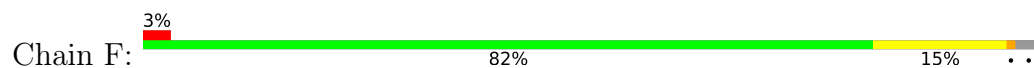




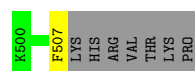
- Molecule 1: Proliferating cell nuclear antigen



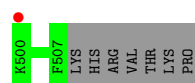
- Molecule 1: Proliferating cell nuclear antigen



- Molecule 2: Peptide fragment from PolD4



- Molecule 2: Peptide fragment from PolD4



- Molecule 2: Peptide fragment from PolD4



- Molecule 2: Peptide fragment from PolD4





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.89Å 84.71Å 84.89Å 60.94° 89.60° 81.22°	Depositor
Resolution (Å)	30.39 – 2.45 30.39 – 2.45	Depositor EDS
% Data completeness (in resolution range)	94.2 (30.39-2.45) 94.2 (30.39-2.45)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.220 , 0.262 0.226 , 0.267	Depositor DCC
R_{free} test set	2829 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,-k+l,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11613	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.35% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	1.04	0/1913	1.35	3/2594 (0.1%)
1	B	1.03	0/1905	1.34	4/2579 (0.2%)
1	C	1.02	1/1791 (0.1%)	1.33	0/2422
1	D	1.05	0/1916	1.36	5/2597 (0.2%)
1	E	1.04	1/1873 (0.1%)	1.33	0/2535
1	F	1.02	0/1922	1.36	4/2605 (0.2%)
2	J	0.97	0/65	1.26	0/87
2	K	1.04	0/65	1.21	0/87
2	M	1.03	0/65	1.18	0/87
2	O	1.07	0/51	1.27	0/68
All	All	1.03	2/11566 (0.0%)	1.34	16/15661 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	45	VAL	C-O	7.66	1.31	1.24
1	C	45	VAL	C-O	5.68	1.29	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	0	MET	CA-C-N	7.45	130.60	120.54
1	F	0	MET	C-N-CA	7.45	130.60	120.54
1	B	122	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	177	ASN	CA-C-N	5.46	125.36	121.65
1	A	177	ASN	C-N-CA	5.46	125.36	121.65
1	F	177	ASN	CA-C-N	5.25	125.22	121.65
1	F	177	ASN	C-N-CA	5.25	125.22	121.65
1	A	45	VAL	N-CA-C	-5.20	107.76	112.96
1	D	45	VAL	N-CA-C	-5.18	107.78	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	0	MET	CA-C-N	5.16	127.46	120.44
1	D	0	MET	C-N-CA	5.16	127.46	120.44
1	B	8	GLN	CA-C-N	5.10	127.12	120.28
1	B	8	GLN	C-N-CA	5.10	127.12	120.28
1	B	45	VAL	N-CA-C	-5.03	107.93	112.96
1	D	8	GLN	CA-C-N	5.00	126.98	120.28
1	D	8	GLN	C-N-CA	5.00	126.98	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	1889	0	1879	15	0
1	B	1884	0	1876	23	0
1	C	1774	0	1734	23	0
1	D	1894	0	1873	21	0
1	E	1852	0	1846	16	0
1	F	1899	0	1888	21	0
2	J	64	0	54	1	0
2	K	64	0	54	0	0
2	M	64	0	54	0	0
2	O	51	0	43	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	3	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	2	0	0	0	0
4	A	24	0	0	0	0
4	B	32	0	0	0	0
4	C	27	0	0	0	0
4	D	34	0	0	0	0
4	E	20	0	0	0	0
4	F	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	3	0	0	0	0
All	All	11613	0	11301	111	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 (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:MET:HE3	1:C:121:ILE:HD11	1.67	0.77
1:B:119:MET:HE3	1:B:121:ILE:HD11	1.70	0.72
1:A:119:MET:HE3	1:A:121:ILE:HD11	1.72	0.72
1:E:71:ASN:HB2	1:E:119:MET:HE1	1.72	0.72
1:E:230:SER:OG	1:E:233:VAL:HG22	1.89	0.72
1:A:25:ASP:OD1	1:A:119:MET:HE1	1.93	0.69
1:D:22:LEU:HG	1:D:214:ASN:ND2	2.08	0.69
1:E:29:ASP:OD1	1:E:123:GLN:NE2	2.28	0.67
1:E:40:MET:HE2	1:E:44:HIS:HA	1.78	0.66
1:C:25:ASP:OD1	1:C:119:MET:HE1	1.96	0.65
1:D:29:ASP:OD1	1:D:123:GLN:NE2	2.27	0.64
1:C:51:MET:HE3	1:C:53:LYS:HE3	1.80	0.63
1:B:25:ASP:OD1	1:B:119:MET:HE1	1.97	0.63
1:D:131:THR:HG21	1:D:233:VAL:HG21	1.81	0.62
1:B:131:THR:HG21	1:B:233:VAL:HG21	1.83	0.60
1:C:51:MET:HE3	1:C:53:LYS:CE	2.31	0.60
1:D:51:MET:HE3	1:D:53:LYS:HE3	1.83	0.60
1:F:131:THR:HG21	1:F:233:VAL:HG21	1.83	0.60
1:A:131:THR:HG21	1:A:233:VAL:HG21	1.84	0.60
1:B:51:MET:HE3	1:B:53:LYS:CE	2.32	0.59
1:B:51:MET:HE3	1:B:53:LYS:HE3	1.84	0.59
1:D:51:MET:HE3	1:D:53:LYS:CE	2.33	0.59
1:E:64:ARG:HD3	1:E:65:ASN:O	2.05	0.56
1:A:109:ASP:OD2	1:B:183:ARG:NH1	2.39	0.56
1:D:64:ARG:HD3	1:D:65:ASN:O	2.06	0.56
1:D:22:LEU:HG	1:D:214:ASN:HD22	1.70	0.55
1:D:103:PHE:HB2	1:D:112:SER:HB2	1.88	0.55
1:C:64:ARG:HD3	1:C:65:ASN:O	2.06	0.55
1:C:103:PHE:HB2	1:C:112:SER:HB2	1.89	0.54
1:E:103:PHE:HB2	1:E:112:SER:HB2	1.89	0.54
1:A:103:PHE:HB2	1:A:112:SER:HB2	1.89	0.54
1:C:40:MET:HE2	1:C:44:HIS:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:PHE:HB2	1:B:112:SER:HB2	1.88	0.54
1:F:103:PHE:HB2	1:F:112:SER:HB2	1.89	0.53
1:B:140:PRO:HG3	1:B:193:GLU:HA	1.93	0.51
1:E:114:TYR:CE2	1:F:154:MET:HE1	2.45	0.51
1:B:119:MET:CE	1:B:121:ILE:HD11	2.40	0.51
1:B:15:VAL:HG11	1:B:50:MET:SD	2.52	0.50
1:B:114:TYR:CE1	1:C:154:MET:HE1	2.47	0.50
1:F:40:MET:HE3	1:F:44:HIS:CE1	2.46	0.49
1:D:161:GLU:HG2	1:D:204:SER:HB2	1.95	0.49
1:E:163:ASN:HA	1:E:199:LEU:HD11	1.95	0.49
1:A:70:VAL:HG11	1:A:75:LEU:HD22	1.94	0.48
1:A:119:MET:CE	1:A:121:ILE:HD11	2.42	0.48
1:E:15:VAL:HG11	1:E:50:MET:SD	2.54	0.48
1:F:28:PHE:CE1	1:F:70:VAL:HG21	2.48	0.47
1:B:28:PHE:CE1	1:B:70:VAL:HG21	2.50	0.47
1:E:70:VAL:HG11	1:E:75:LEU:HD22	1.97	0.47
1:D:174:ASP:O	1:F:117:LYS:HD2	2.15	0.47
1:D:64:ARG:NH1	1:D:65:ASN:O	2.47	0.47
1:F:40:MET:HG2	1:F:44:HIS:HA	1.97	0.46
1:E:169:PHE:O	1:E:179:SER:HA	2.16	0.46
1:A:163:ASN:HA	1:A:199:LEU:CD1	2.45	0.46
1:C:15:VAL:HG11	1:C:50:MET:SD	2.55	0.46
1:C:70:VAL:HG11	1:C:75:LEU:HD22	1.98	0.46
1:C:140:PRO:HG3	1:C:193:GLU:HA	1.98	0.46
1:D:15:VAL:HG11	1:D:50:MET:SD	2.55	0.46
1:D:169:PHE:O	1:D:179:SER:HA	2.16	0.46
1:F:15:VAL:HG11	1:F:50:MET:SD	2.57	0.45
1:C:119:MET:CE	1:C:121:ILE:HD11	2.41	0.45
1:F:169:PHE:O	1:F:179:SER:HA	2.17	0.45
1:B:169:PHE:O	1:B:179:SER:HA	2.16	0.45
1:C:64:ARG:NH1	1:C:65:ASN:O	2.45	0.45
1:A:163:ASN:HA	1:A:199:LEU:HD11	1.99	0.45
1:A:169:PHE:O	1:A:179:SER:HA	2.17	0.45
1:E:64:ARG:NH1	1:E:65:ASN:O	2.48	0.44
1:F:163:ASN:HA	1:F:199:LEU:HD11	1.98	0.44
1:B:110:ARG:HG3	1:C:182:LEU:HD23	1.99	0.44
1:C:169:PHE:O	1:C:179:SER:HA	2.16	0.44
1:E:163:ASN:HA	1:E:199:LEU:CD1	2.48	0.44
1:D:228:CYS:HB2	1:D:236:LEU:HB3	2.00	0.44
1:A:57:PHE:HB2	1:A:60:TYR:HB2	2.00	0.44
1:F:28:PHE:HE1	1:F:70:VAL:HG21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:LEU:HD11	1:C:215:PHE:CE1	2.53	0.43
1:E:110:ARG:HG3	1:F:182:LEU:HD23	2.00	0.43
1:F:143:GLU:OE1	1:F:146:ARG:NH1	2.52	0.43
1:F:163:ASN:HA	1:F:199:LEU:CD1	2.49	0.43
1:B:228:CYS:HB2	1:B:236:LEU:HB3	2.00	0.43
1:B:143:GLU:OE1	1:B:146:ARG:NH1	2.51	0.43
1:A:128:ILE:HG23	2:J:507:PHE:CD1	2.54	0.43
1:C:57:PHE:HB2	1:C:60:TYR:HB2	2.00	0.43
1:D:143:GLU:OE1	1:D:146:ARG:NH1	2.52	0.43
1:D:230:SER:HB2	1:D:233:VAL:HG22	2.01	0.43
1:C:192:ASN:HD22	1:C:223:ASN:HB3	1.85	0.42
1:C:228:CYS:HB2	1:C:236:LEU:HB3	2.01	0.42
1:D:70:VAL:HG11	1:D:75:LEU:HD22	2.00	0.42
1:A:143:GLU:OE1	1:A:146:ARG:NH1	2.52	0.42
1:B:161:GLU:HG2	1:B:204:SER:HB2	2.01	0.42
1:D:57:PHE:HB2	1:D:60:TYR:HB2	2.01	0.42
1:F:57:PHE:HB2	1:F:60:TYR:HB2	2.01	0.42
1:F:228:CYS:HB2	1:F:236:LEU:HB3	2.00	0.42
1:B:76:THR:O	1:B:80:ARG:HG3	2.19	0.42
1:D:163:ASN:HA	1:D:199:LEU:CD1	2.50	0.42
1:B:28:PHE:HE1	1:B:70:VAL:HG21	1.85	0.42
1:C:26:CYS:SG	1:C:37:LEU:HD11	2.60	0.42
1:D:154:MET:HE1	1:F:114:TYR:CE2	2.55	0.42
1:A:228:CYS:HB2	1:A:236:LEU:HB3	2.01	0.42
1:F:22:LEU:HD11	1:F:215:PHE:CE1	2.55	0.42
1:E:143:GLU:OE1	1:E:146:ARG:NH1	2.52	0.42
1:B:81:ALA:HA	1:C:150:ASP:OD2	2.20	0.41
1:E:228:CYS:HB2	1:E:236:LEU:HB3	2.02	0.41
1:F:19:ILE:HG22	1:F:72:LEU:CD1	2.51	0.41
1:B:126:LEU:C	1:B:126:LEU:HD23	2.45	0.41
1:B:57:PHE:HB2	1:B:60:TYR:HB2	2.01	0.41
1:D:22:LEU:HD11	1:D:215:PHE:CE1	2.56	0.41
1:A:19:ILE:HG22	1:A:72:LEU:CD1	2.50	0.41
1:F:161:GLU:HG2	1:F:204:SER:OG	2.22	0.40
1:C:166:GLY:HA2	1:C:197:ILE:HD12	2.04	0.40
1:C:105:SER:OG	1:C:108:THR:N	2.55	0.40
1:F:40:MET:HE2	1:F:40:MET:HB2	1.94	0.40
1:B:40:MET:HE2	1:B:126:LEU:CD1	2.51	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	249/261 (95%)	243 (98%)	5 (2%)	1 (0%)	30	37
1	B	242/261 (93%)	239 (99%)	2 (1%)	1 (0%)	30	37
1	C	226/261 (87%)	222 (98%)	3 (1%)	1 (0%)	30	37
1	D	248/261 (95%)	243 (98%)	4 (2%)	1 (0%)	30	37
1	E	240/261 (92%)	234 (98%)	5 (2%)	1 (0%)	30	37
1	F	249/261 (95%)	243 (98%)	5 (2%)	1 (0%)	30	37
2	J	6/15 (40%)	6 (100%)	0	0	100	100
2	K	6/15 (40%)	6 (100%)	0	0	100	100
2	M	6/15 (40%)	6 (100%)	0	0	100	100
2	O	5/15 (33%)	5 (100%)	0	0	100	100
All	All	1477/1626 (91%)	1447 (98%)	24 (2%)	6 (0%)	30	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	10	SER
1	E	10	SER
1	F	10	SER
1	A	10	SER
1	C	10	SER
1	D	10	SER

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	207/229 (90%)	202 (98%)	5 (2%)	43	58
1	B	210/229 (92%)	203 (97%)	7 (3%)	33	48
1	C	192/229 (84%)	186 (97%)	6 (3%)	35	50
1	D	206/229 (90%)	200 (97%)	6 (3%)	37	52
1	E	204/229 (89%)	195 (96%)	9 (4%)	25	37
1	F	209/229 (91%)	200 (96%)	9 (4%)	26	38
2	J	7/15 (47%)	7 (100%)	0	100	100
2	K	7/15 (47%)	7 (100%)	0	100	100
2	M	7/15 (47%)	6 (86%)	1 (14%)	3	2
2	O	5/15 (33%)	5 (100%)	0	100	100
All	All	1254/1434 (87%)	1211 (97%)	43 (3%)	32	47

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	62	CYS
1	A	105	SER
1	A	199	LEU
1	A	230	SER
1	B	40	MET
1	B	62	CYS
1	B	83	GLN
1	B	108	THR
1	B	185	HIS
1	B	204	SER
1	B	230	SER
1	C	40	MET
1	C	62	CYS
1	C	108	THR
1	C	120	ASP
1	C	185	HIS
1	C	230	SER
1	D	62	CYS
1	D	119	MET
1	D	199	LEU
1	D	200	SER
1	D	204	SER
1	D	230	SER

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Mol	Chain	Res	Type
1	E	40	MET
1	E	41	ASP
1	E	44	HIS
1	E	62	CYS
1	E	120	ASP
1	E	185	HIS
1	E	199	LEU
1	E	204	SER
1	E	230	SER
1	F	38	GLN
1	F	40	MET
1	F	62	CYS
1	F	105	SER
1	F	108	THR
1	F	119	MET
1	F	185	HIS
1	F	199	LEU
1	F	230	SER
2	M	506	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	27	ASN
1	A	65	ASN
1	A	100	ASN
1	A	184	GLN
1	A	231	ASN
1	B	24	GLN
1	B	65	ASN
1	B	100	ASN
1	B	184	GLN
1	C	27	ASN
1	C	65	ASN
1	C	192	ASN
1	D	24	GLN
1	D	65	ASN
1	D	84	ASN
1	D	100	ASN
1	D	184	GLN
1	E	24	GLN

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Mol	Chain	Res	Type
1	E	65	ASN
1	E	84	ASN
1	E	100	ASN
1	E	184	GLN
1	E	214	ASN
1	E	231	ASN
1	F	24	GLN
1	F	27	ASN
1	F	44	HIS
1	F	84	ASN
1	F	100	ASN
1	F	184	GLN
2	J	501	HIS
2	M	501	HIS
2	O	502	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 ⓘ

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	253/261 (96%)	0.11	3 (1%) 76 78	30, 43, 67, 81	0
1	B	250/261 (95%)	0.11	2 (0%) 82 83	27, 44, 72, 95	0
1	C	238/261 (91%)	0.35	11 (4%) 37 36	36, 52, 78, 96	0
1	D	254/261 (97%)	0.13	4 (1%) 70 73	29, 43, 69, 100	0
1	E	246/261 (94%)	0.17	6 (2%) 59 62	29, 45, 69, 84	0
1	F	253/261 (96%)	0.35	9 (3%) 46 46	35, 51, 81, 98	0
2	J	8/15 (53%)	0.39	0 100 100	37, 41, 57, 78	0
2	K	8/15 (53%)	0.55	1 (12%) 8 6	30, 47, 70, 78	0
2	M	8/15 (53%)	0.42	0 100 100	41, 48, 62, 67	0
2	O	7/15 (46%)	1.36	1 (14%) 6 4	67, 68, 79, 80	0
All	All	1525/1626 (93%)	0.21	37 (2%) 59 62	27, 47, 75, 100	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	108	THR	4.3
1	F	122	ASP	3.6
1	F	123	GLN	3.1
1	E	109	ASP	3.0
1	F	120	ASP	2.9
1	C	204	SER	2.9
1	A	165	ASP	2.8
1	A	107	GLU	2.8
1	F	23	VAL	2.8
1	D	108	THR	2.8
1	C	107	GLU	2.7
1	D	165	ASP	2.7
1	A	108	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	124	GLU	2.6
1	E	124	GLU	2.6
1	E	255	ILE	2.5
1	B	123	GLN	2.5
1	F	128	ILE	2.5
1	F	255	ILE	2.5
1	C	166	GLY	2.5
1	C	125	HIS	2.5
1	E	107	GLU	2.4
1	C	188	VAL	2.4
2	K	500	LYS	2.3
1	C	43	SER	2.3
1	B	124	GLU	2.3
1	F	121	ILE	2.2
1	C	131	THR	2.2
1	E	205	LEU	2.2
1	C	42	ASN	2.1
1	D	94	ASP	2.1
1	D	0	MET	2.1
1	F	107	GLU	2.1
1	C	45	VAL	2.1
1	C	232	GLU	2.1
1	C	108	THR	2.1
2	O	506	ASN	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	A	303	1/1	0.78	0.20	66,66,66,66	0
3	NA	C	302	1/1	0.80	0.13	59,59,59,59	0
3	NA	E	304	1/1	0.80	0.14	38,38,38,38	0
3	NA	E	302	1/1	0.81	0.10	57,57,57,57	0
3	NA	E	303	1/1	0.84	0.16	40,40,40,40	0
3	NA	C	303	1/1	0.84	0.11	41,41,41,41	0
3	NA	E	301	1/1	0.86	0.17	47,47,47,47	0
3	NA	D	304	1/1	0.86	0.12	41,41,41,41	0
3	NA	A	301	1/1	0.87	0.14	39,39,39,39	0
3	NA	D	302	1/1	0.89	0.07	48,48,48,48	0
3	NA	B	302	1/1	0.90	0.18	45,45,45,45	0
3	NA	F	301	1/1	0.90	0.15	47,47,47,47	0
3	NA	B	301	1/1	0.92	0.13	50,50,50,50	0
3	NA	D	303	1/1	0.92	0.08	34,34,34,34	0
3	NA	F	302	1/1	0.92	0.07	56,56,56,56	0
3	NA	A	302	1/1	0.93	0.06	49,49,49,49	0
3	NA	D	301	1/1	0.97	0.05	42,42,42,42	0
3	NA	C	301	1/1	0.97	0.04	37,37,37,37	0

6.5 Other polymers ⓘ

There are no such residues in this entry.