



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:04 PM UTC

PDB ID : 4W8W / pdb_00004w8w
Title : Crystal structure of oligomeric Cmr4 from *Pyrococcus furiosus*
Authors : Benda, C.; Ebert, J.; Baumgaertner, M.; Conti, E.
Deposited on : 2014-08-26
Resolution : 2.80 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

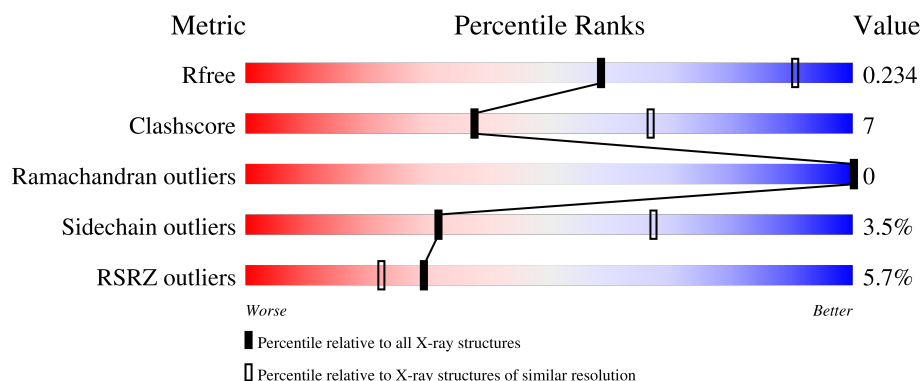
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	312	4% 65%15%20%
1	B	312	5% 63%18%19%
1	C	312	4% 64%17%18%
1	D	312	6% 66%16%18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8024 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 CRISPR system Cmr subunit Cmr4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1957	1270	319	366	2			
1	B	254	Total	C	N	O	S	0	0	0
			1982	1284	322	373	3			
1	C	255	Total	C	N	O	S	0	0	0
			1996	1295	324	374	3			
1	D	257	Total	C	N	O	S	0	0	0
			2007	1300	325	379	3			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP Q8U1S9
A	-15	HIS	-	expression tag	UNP Q8U1S9
A	-14	HIS	-	expression tag	UNP Q8U1S9
A	-13	HIS	-	expression tag	UNP Q8U1S9
A	-12	HIS	-	expression tag	UNP Q8U1S9
A	-11	HIS	-	expression tag	UNP Q8U1S9
A	-10	HIS	-	expression tag	UNP Q8U1S9
A	-9	GLU	-	expression tag	UNP Q8U1S9
A	-8	ASN	-	expression tag	UNP Q8U1S9
A	-7	LEU	-	expression tag	UNP Q8U1S9
A	-6	TYR	-	expression tag	UNP Q8U1S9
A	-5	PHE	-	expression tag	UNP Q8U1S9
A	-4	GLN	-	expression tag	UNP Q8U1S9
A	-3	GLY	-	expression tag	UNP Q8U1S9
A	-2	ALA	-	expression tag	UNP Q8U1S9
A	-1	ALA	-	expression tag	UNP Q8U1S9
A	0	SER	-	expression tag	UNP Q8U1S9
B	-16	MET	-	initiating methionine	UNP Q8U1S9
B	-15	HIS	-	expression tag	UNP Q8U1S9
B	-14	HIS	-	expression tag	UNP Q8U1S9
B	-13	HIS	-	expression tag	UNP Q8U1S9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP Q8U1S9
B	-11	HIS	-	expression tag	UNP Q8U1S9
B	-10	HIS	-	expression tag	UNP Q8U1S9
B	-9	GLU	-	expression tag	UNP Q8U1S9
B	-8	ASN	-	expression tag	UNP Q8U1S9
B	-7	LEU	-	expression tag	UNP Q8U1S9
B	-6	TYR	-	expression tag	UNP Q8U1S9
B	-5	PHE	-	expression tag	UNP Q8U1S9
B	-4	GLN	-	expression tag	UNP Q8U1S9
B	-3	GLY	-	expression tag	UNP Q8U1S9
B	-2	ALA	-	expression tag	UNP Q8U1S9
B	-1	ALA	-	expression tag	UNP Q8U1S9
B	0	SER	-	expression tag	UNP Q8U1S9
C	-16	MET	-	initiating methionine	UNP Q8U1S9
C	-15	HIS	-	expression tag	UNP Q8U1S9
C	-14	HIS	-	expression tag	UNP Q8U1S9
C	-13	HIS	-	expression tag	UNP Q8U1S9
C	-12	HIS	-	expression tag	UNP Q8U1S9
C	-11	HIS	-	expression tag	UNP Q8U1S9
C	-10	HIS	-	expression tag	UNP Q8U1S9
C	-9	GLU	-	expression tag	UNP Q8U1S9
C	-8	ASN	-	expression tag	UNP Q8U1S9
C	-7	LEU	-	expression tag	UNP Q8U1S9
C	-6	TYR	-	expression tag	UNP Q8U1S9
C	-5	PHE	-	expression tag	UNP Q8U1S9
C	-4	GLN	-	expression tag	UNP Q8U1S9
C	-3	GLY	-	expression tag	UNP Q8U1S9
C	-2	ALA	-	expression tag	UNP Q8U1S9
C	-1	ALA	-	expression tag	UNP Q8U1S9
C	0	SER	-	expression tag	UNP Q8U1S9
D	-16	MET	-	initiating methionine	UNP Q8U1S9
D	-15	HIS	-	expression tag	UNP Q8U1S9
D	-14	HIS	-	expression tag	UNP Q8U1S9
D	-13	HIS	-	expression tag	UNP Q8U1S9
D	-12	HIS	-	expression tag	UNP Q8U1S9
D	-11	HIS	-	expression tag	UNP Q8U1S9
D	-10	HIS	-	expression tag	UNP Q8U1S9
D	-9	GLU	-	expression tag	UNP Q8U1S9
D	-8	ASN	-	expression tag	UNP Q8U1S9
D	-7	LEU	-	expression tag	UNP Q8U1S9
D	-6	TYR	-	expression tag	UNP Q8U1S9
D	-5	PHE	-	expression tag	UNP Q8U1S9

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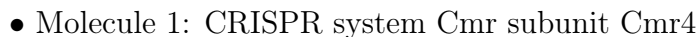
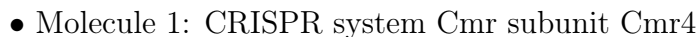
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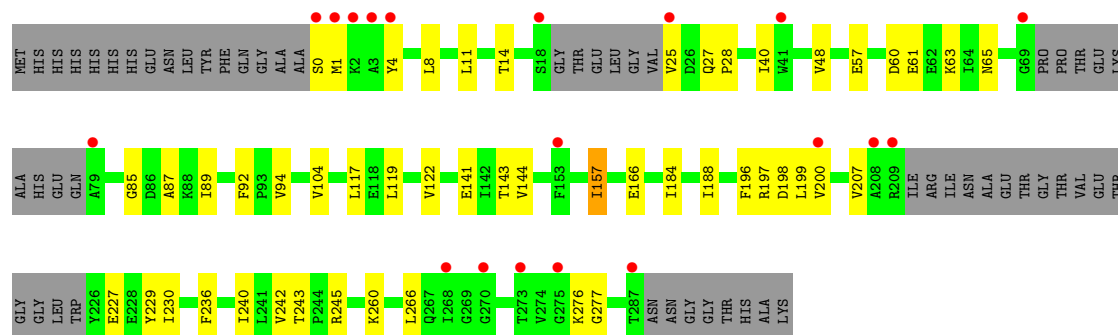
Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	GLN	-	expression tag	UNP Q8U1S9
D	-3	GLY	-	expression tag	UNP Q8U1S9
D	-2	ALA	-	expression tag	UNP Q8U1S9
D	-1	ALA	-	expression tag	UNP Q8U1S9
D	0	SER	-	expression tag	UNP Q8U1S9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	18	Total O 18 18	0	0
2	B	29	Total O 29 29	0	0
2	C	25	Total O 25 25	0	0
2	D	10	Total O 10 10	0	0

- Molecule 1: CRISPR system Cmr subunit Cmr4





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.71Å 129.51Å 195.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 2.80 49.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.38-2.80) 99.8 (49.38-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1678)	Depositor
R, R_{free}	0.197 , 0.230 0.198 , 0.234	Depositor DCC
R_{free} test set	2035 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	64.8	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 74.1	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	0.95	EDS
Total number of atoms	8024	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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	0.28	0/1988	0.71	0/2688
1	B	0.29	0/2012	0.75	4/2719 (0.1%)
1	C	0.30	0/2028	0.71	0/2741
1	D	0.32	0/2037	0.74	0/2753
All	All	0.30	0/8065	0.73	4/10901 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	GLN	CA-C-N	-6.66	113.66	120.85
1	B	27	GLN	C-N-CA	-6.66	113.66	120.85
1	B	15	HIS	CA-C-N	5.31	124.77	119.24
1	B	15	HIS	C-N-CA	5.31	124.77	119.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1957	0	2018	26	0
1	B	1982	0	2042	36	0
1	C	1996	0	2061	30	0
1	D	2007	0	2068	30	0
2	A	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	29	0	0	2	0
2	C	25	0	0	1	0
2	D	10	0	0	0	0
All	All	8024	0	8189	113	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 (113) 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:D:0:SER:N	1:D:242:VAL:O	2.16	0.77
1:D:117:LEU:HB3	1:D:122:VAL:HB	1.72	0.71
1:D:61:GLU:HG3	1:D:65:ASN:HD21	1.58	0.68
1:B:29:ILE:HD13	1:B:230:ILE:HG13	1.76	0.67
1:C:4:TYR:HB2	1:C:240:ILE:HB	1.77	0.67
1:B:230:ILE:HD13	1:B:236:PHE:HZ	1.61	0.65
1:C:97:LEU:O	1:D:197:ARG:NH1	2.30	0.65
1:C:8:LEU:HB2	1:C:236:PHE:HB2	1.79	0.65
1:A:8:LEU:HB2	1:A:236:PHE:HB2	1.79	0.64
1:C:48:VAL:HG12	1:C:266:LEU:HD23	1.81	0.63
1:B:25:VAL:HG12	1:B:26:ASP:H	1.63	0.62
1:B:115:ARG:NH2	2:B:328:HOH:O	2.32	0.61
1:D:61:GLU:O	1:D:65:ASN:ND2	2.32	0.61
1:D:40:ILE:HB	1:D:87:ALA:HB3	1.82	0.60
1:D:197:ARG:NH2	1:D:198:ASP:OD1	2.35	0.60
1:D:141:GLU:N	1:D:141:GLU:OE1	2.36	0.58
1:A:95:ARG:NH2	1:B:201:GLU:OE2	2.35	0.58
1:A:230:ILE:HD13	1:A:236:PHE:HZ	1.69	0.58
1:D:8:LEU:HB2	1:D:236:PHE:HB2	1.85	0.58
1:B:184:ILE:HG22	1:B:188:ILE:HG12	1.86	0.58
1:B:8:LEU:HB2	1:B:236:PHE:HB2	1.84	0.57
1:D:184:ILE:HG22	1:D:188:ILE:HG12	1.86	0.57
1:C:229:TYR:OH	1:C:271:ASN:ND2	2.36	0.57
1:A:48:VAL:HG12	1:A:266:LEU:HD23	1.87	0.56
1:B:25:VAL:O	1:B:27:GLN:NE2	2.37	0.56
1:B:229:TYR:OH	1:B:271:ASN:ND2	2.33	0.56
1:D:143:THR:HG21	1:D:157:ILE:HD12	1.86	0.56
1:C:275:GLY:HA3	1:D:85:GLY:HA2	1.88	0.55
1:C:99:GLY:O	1:C:187:ARG:NH2	2.31	0.55
1:D:48:VAL:HG12	1:D:266:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:ASP:HB3	1:D:63:LYS:HG3	1.90	0.54
1:B:57:GLU:HG2	1:B:260:LYS:HB3	1.90	0.53
1:B:95:ARG:NH2	1:C:201:GLU:OE2	2.41	0.53
1:A:275:GLY:HA3	1:B:85:GLY:HA2	1.90	0.53
1:B:275:GLY:HA3	1:C:85:GLY:HA2	1.90	0.53
1:A:94:VAL:HG21	1:A:199:LEU:HD13	1.90	0.53
1:C:13:PRO:HB2	1:C:276:LYS:HD2	1.91	0.53
1:B:10:THR:HA	1:B:279:VAL:HG12	1.90	0.53
1:A:40:ILE:HB	1:A:87:ALA:HB3	1.92	0.52
1:A:117:LEU:HB3	1:A:122:VAL:HB	1.90	0.52
1:A:184:ILE:HG22	1:A:188:ILE:HG12	1.90	0.52
1:B:40:ILE:HB	1:B:87:ALA:HB3	1.92	0.52
1:A:196:PHE:O	1:A:200:VAL:HG23	2.11	0.51
1:B:267:GLN:NE2	1:B:269:GLY:O	2.42	0.51
1:D:166:GLU:OE1	1:D:166:GLU:N	2.35	0.51
1:B:115:ARG:NH1	2:B:315:HOH:O	2.41	0.51
1:C:230:ILE:HD13	1:C:236:PHE:HZ	1.77	0.49
1:A:138:ALA:HB1	1:A:142:ILE:HD11	1.95	0.49
1:D:230:ILE:HD13	1:D:236:PHE:HZ	1.78	0.49
1:C:49:LEU:HD22	1:C:261:ILE:HD13	1.95	0.48
1:A:63:LYS:HD3	1:A:253:LEU:HD11	1.94	0.48
1:C:2:LYS:HB3	1:C:242:VAL:HB	1.94	0.48
1:D:196:PHE:O	1:D:200:VAL:HG23	2.14	0.48
1:B:94:VAL:HG21	1:B:199:LEU:HD13	1.95	0.48
1:D:104:VAL:HG12	1:D:196:PHE:HD2	1.78	0.48
1:B:48:VAL:HG12	1:B:266:LEU:HD23	1.96	0.48
1:C:9:TYR:CZ	1:C:233:ASP:HA	2.49	0.48
1:A:4:TYR:HB2	1:A:240:ILE:HB	1.94	0.47
1:C:184:ILE:HG22	1:C:188:ILE:HG12	1.96	0.47
1:B:15:HIS:O	1:B:269:GLY:HA3	2.14	0.47
1:D:14:THR:HG23	1:D:277:GLY:HA2	1.95	0.47
1:B:117:LEU:HB3	1:B:122:VAL:HB	1.97	0.47
1:A:104:VAL:HG12	1:A:196:PHE:HD2	1.79	0.47
1:C:197:ARG:NH2	1:C:198:ASP:OD1	2.47	0.47
1:A:141:GLU:OE1	1:A:141:GLU:N	2.42	0.47
1:D:27:GLN:HB3	1:D:28:PRO:HD2	1.96	0.47
1:D:92:PHE:CD2	1:D:200:VAL:HG13	2.51	0.46
1:B:29:ILE:O	1:B:31:ARG:HG3	2.16	0.46
1:A:143:THR:HG21	1:A:157:ILE:HD12	1.98	0.46
1:C:14:THR:HG23	1:C:277:GLY:HA2	1.97	0.46
1:B:104:VAL:HG12	1:B:196:PHE:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:LYS:NZ	2:C:324:HOH:O	2.40	0.45
1:D:61:GLU:HG3	1:D:65:ASN:ND2	2.26	0.45
1:C:94:VAL:HG21	1:C:199:LEU:HD13	1.99	0.45
1:B:9:TYR:CZ	1:B:233:ASP:HA	2.52	0.45
1:C:57:GLU:HG2	1:C:260:LYS:HB3	1.99	0.45
1:D:207:VAL:HG22	1:D:227:GLU:HB2	1.97	0.45
1:C:67:ILE:HD11	1:C:253:LEU:HG	1.98	0.45
1:C:196:PHE:O	1:C:200:VAL:HG23	2.16	0.44
1:A:14:THR:HG23	1:A:277:GLY:HA2	1.99	0.44
1:C:10:THR:HA	1:C:279:VAL:HG12	1.99	0.44
1:B:229:TYR:CE1	1:B:276:LYS:HD3	2.53	0.44
1:D:94:VAL:HG21	1:D:199:LEU:HD13	2.00	0.44
1:B:266:LEU:HD22	1:B:281:VAL:HG21	2.00	0.44
1:B:93:PRO:HG3	1:B:232:SER:O	2.17	0.44
1:A:50:ARG:NH2	1:A:69:GLY:O	2.51	0.43
1:A:53:LEU:HD11	1:A:261:ILE:HD11	2.00	0.43
1:A:273:THR:HB	1:B:46:LYS:NZ	2.33	0.43
1:D:229:TYR:CE1	1:D:276:LYS:HD3	2.53	0.43
1:A:9:TYR:CZ	1:A:233:ASP:HA	2.54	0.43
1:B:230:ILE:HD13	1:B:236:PHE:CZ	2.49	0.43
1:A:193:ASP:N	1:A:193:ASP:OD1	2.50	0.43
1:B:53:LEU:HD11	1:B:261:ILE:HD11	1.99	0.43
1:B:135:THR:OG1	1:B:158:GLN:OE1	2.30	0.43
1:C:40:ILE:HB	1:C:87:ALA:HB3	2.00	0.43
1:C:93:PRO:HG3	1:C:232:SER:O	2.18	0.43
1:D:57:GLU:HG2	1:D:260:LYS:HD3	2.00	0.43
1:C:117:LEU:HB3	1:C:122:VAL:HB	2.00	0.42
1:B:229:TYR:CZ	1:B:276:LYS:HD3	2.54	0.42
1:A:273:THR:HG21	1:B:80:GLY:H	1.85	0.42
1:D:4:TYR:HB2	1:D:240:ILE:HB	2.00	0.42
1:B:135:THR:HB	1:B:158:GLN:HG3	2.01	0.42
1:C:137:ILE:HD11	1:C:158:GLN:HE21	1.84	0.42
1:D:243:THR:OG1	1:D:245:ARG:NH1	2.52	0.42
1:A:93:PRO:HG3	1:A:232:SER:O	2.20	0.42
1:C:168:VAL:O	1:C:172:ILE:HG12	2.19	0.42
1:C:11:LEU:HD23	1:D:119:LEU:HD22	2.02	0.41
1:B:173:GLU:HG3	1:B:178:ASN:HA	2.01	0.41
1:A:168:VAL:O	1:A:172:ILE:HG13	2.20	0.41
1:C:54:LYS:HE3	1:C:54:LYS:HB2	1.91	0.41
1:D:196:PHE:CZ	1:D:200:VAL:HG21	2.56	0.41
1:B:114:LYS:HD2	1:B:129:ILE:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:HB2	1:A:147:LYS:HE3	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	243/312 (78%)	239 (98%)	4 (2%)	0	100	100
1	B	246/312 (79%)	241 (98%)	5 (2%)	0	100	100
1	C	247/312 (79%)	244 (99%)	3 (1%)	0	100	100
1	D	249/312 (80%)	240 (96%)	9 (4%)	0	100	100
All	All	985/1248 (79%)	964 (98%)	21 (2%)	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	213/265 (80%)	205 (96%)	8 (4%)	29	64
1	B	216/265 (82%)	206 (95%)	10 (5%)	24	58
1	C	218/265 (82%)	212 (97%)	6 (3%)	38	73
1	D	219/265 (83%)	213 (97%)	6 (3%)	39	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	866/1060 (82%)	836 (96%)	30 (4%)	32	67

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	30	GLN
1	A	82	ILE
1	A	133	THR
1	A	144	VAL
1	A	150	LEU
1	A	157	ILE
1	A	249	ASN
1	B	11	LEU
1	B	25	VAL
1	B	65	ASN
1	B	141	GLU
1	B	144	VAL
1	B	148	VAL
1	B	150	LEU
1	B	157	ILE
1	B	197	ARG
1	B	200	VAL
1	C	11	LEU
1	C	137	ILE
1	C	144	VAL
1	C	146	ASN
1	C	150	LEU
1	C	157	ILE
1	D	1	MET
1	D	11	LEU
1	D	25	VAL
1	D	89	ILE
1	D	144	VAL
1	D	157	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
1	B	267	GLN

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Mol	Chain	Res	Type
1	C	124	ASN
1	D	65	ASN
1	D	178	ASN
1	D	267	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	251/312 (80%)	0.21	12 (4%) 35 28	45, 76, 138, 177	0
1	B	254/312 (81%)	-0.06	15 (5%) 28 21	35, 63, 120, 162	0
1	C	255/312 (81%)	-0.14	12 (4%) 36 29	36, 61, 115, 146	0
1	D	257/312 (82%)	0.36	19 (7%) 20 15	48, 83, 146, 178	0
All	All	1017/1248 (81%)	0.09	58 (5%) 29 22	35, 71, 134, 178	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	287	THR	6.0
1	D	69	GLY	5.7
1	D	209	ARG	4.6
1	C	226	TYR	4.5
1	D	0	SER	4.5
1	B	18	SER	4.0
1	D	153	PHE	3.9
1	A	153	PHE	3.8
1	D	287	THR	3.5
1	A	287	THR	3.5
1	D	3	ALA	3.5
1	B	0	SER	3.4
1	D	18	SER	3.4
1	C	26	ASP	3.3
1	D	270	GLY	3.2
1	C	27	GLN	3.1
1	D	1	MET	3.0
1	B	153	PHE	3.0
1	C	1	MET	3.0
1	D	275	GLY	2.9
1	B	272	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	41	TRP	2.8
1	C	124	ASN	2.7
1	C	0	SER	2.7
1	B	79	ALA	2.7
1	C	71	PRO	2.7
1	C	269	GLY	2.7
1	A	72	THR	2.6
1	A	206	ILE	2.5
1	C	288	ASN	2.5
1	B	123	LYS	2.5
1	A	2	LYS	2.5
1	A	274	VAL	2.4
1	A	275	GLY	2.4
1	A	268	ILE	2.4
1	D	268	ILE	2.4
1	D	2	LYS	2.3
1	C	123	LYS	2.3
1	D	41	TRP	2.3
1	D	208	ALA	2.3
1	B	227	GLU	2.3
1	B	206	ILE	2.3
1	A	227	GLU	2.2
1	D	273	THR	2.2
1	C	276	LYS	2.2
1	D	4	TYR	2.2
1	D	79	ALA	2.1
1	B	17	GLY	2.1
1	B	275	GLY	2.1
1	A	79	ALA	2.1
1	C	271	ASN	2.1
1	D	200	VAL	2.1
1	B	16	PRO	2.1
1	A	134	ASP	2.1
1	B	1	MET	2.0
1	B	44	SER	2.0
1	B	273	THR	2.0
1	D	25	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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.