



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:58 AM UTC

PDB ID : 4W8Y / pdb_00004w8y
Title : Structure of full length Cmr2 from *Pyrococcus furiosus* (Manganese bound form)
Authors : Benda, C.; Ebert, J.; Baumgaertner, M.; Conti, E.
Deposited on : 2014-08-26
Resolution : 3.00 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

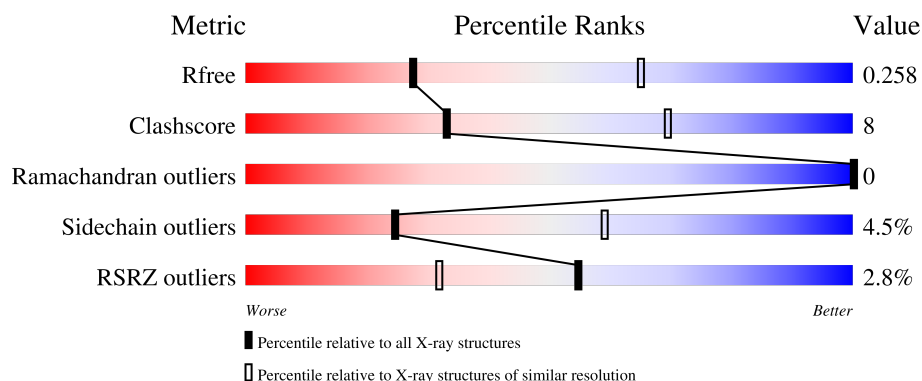
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

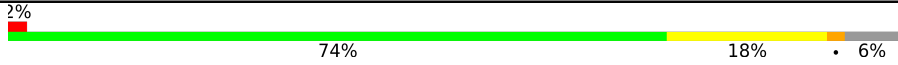
The reported resolution of this entry is 3.00 Å.

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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	888	 2% 74% 18% • 6%
1	B	888	 3% 72% 20% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13055 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 Cmr2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	835	Total	C	N	O	S	0	0	0
			6498	4211	1076	1198	13			
1	B	828	Total	C	N	O	S	0	0	0
			6517	4235	1069	1199	14			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP Q8U1S6
A	-15	HIS	-	expression tag	UNP Q8U1S6
A	-14	HIS	-	expression tag	UNP Q8U1S6
A	-13	HIS	-	expression tag	UNP Q8U1S6
A	-12	HIS	-	expression tag	UNP Q8U1S6
A	-11	HIS	-	expression tag	UNP Q8U1S6
A	-10	HIS	-	expression tag	UNP Q8U1S6
A	-9	GLU	-	expression tag	UNP Q8U1S6
A	-8	ASN	-	expression tag	UNP Q8U1S6
A	-7	LEU	-	expression tag	UNP Q8U1S6
A	-6	TYR	-	expression tag	UNP Q8U1S6
A	-5	PHE	-	expression tag	UNP Q8U1S6
A	-4	GLN	-	expression tag	UNP Q8U1S6
A	-3	GLY	-	expression tag	UNP Q8U1S6
A	-2	ALA	-	expression tag	UNP Q8U1S6
A	-1	ALA	-	expression tag	UNP Q8U1S6
A	0	SER	-	expression tag	UNP Q8U1S6
B	-16	MET	-	initiating methionine	UNP Q8U1S6
B	-15	HIS	-	expression tag	UNP Q8U1S6
B	-14	HIS	-	expression tag	UNP Q8U1S6
B	-13	HIS	-	expression tag	UNP Q8U1S6
B	-12	HIS	-	expression tag	UNP Q8U1S6
B	-11	HIS	-	expression tag	UNP Q8U1S6
B	-10	HIS	-	expression tag	UNP Q8U1S6
B	-9	GLU	-	expression tag	UNP Q8U1S6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	ASN	-	expression tag	UNP Q8U1S6
B	-7	LEU	-	expression tag	UNP Q8U1S6
B	-6	TYR	-	expression tag	UNP Q8U1S6
B	-5	PHE	-	expression tag	UNP Q8U1S6
B	-4	GLN	-	expression tag	UNP Q8U1S6
B	-3	GLY	-	expression tag	UNP Q8U1S6
B	-2	ALA	-	expression tag	UNP Q8U1S6
B	-1	ALA	-	expression tag	UNP Q8U1S6
B	0	SER	-	expression tag	UNP Q8U1S6

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

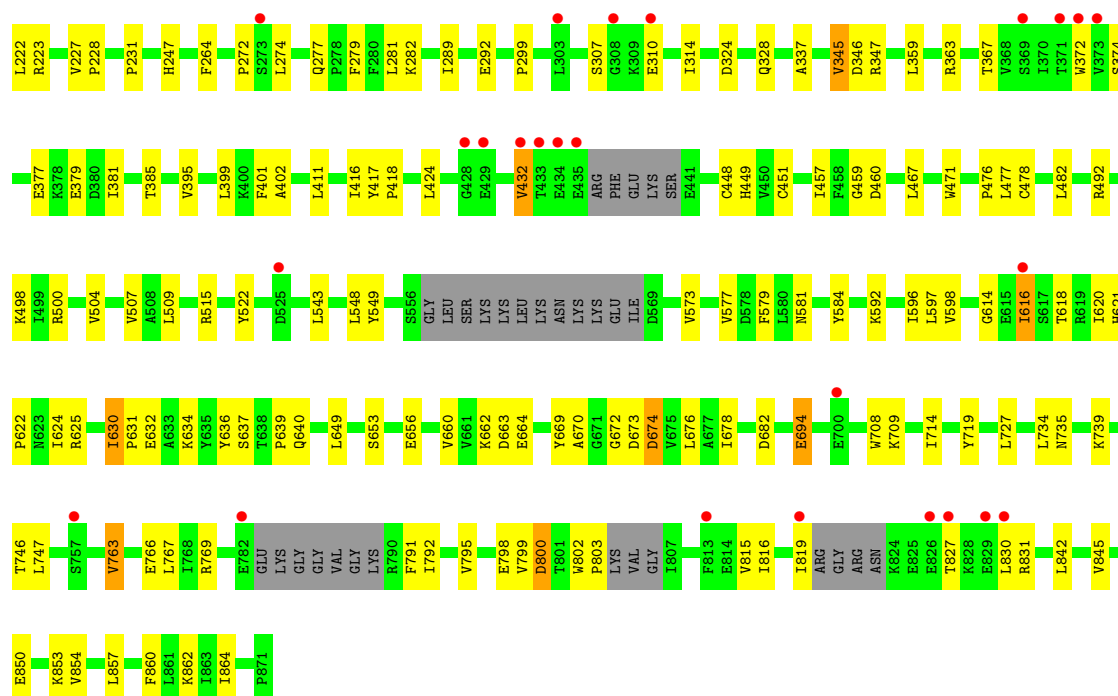
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mn	0	0
			4	4		
3	B	4	Total	Mn	0	0
			4	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	14	Total	O	0	0
			14	14		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.40Å 167.93Å 100.91Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	85.72 – 3.00 85.72 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (85.72-3.00) 98.4 (85.72-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1678)	Depositor
R, R_{free}	0.223 , 0.259 0.228 , 0.258	Depositor DCC
R_{free} test set	2017 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	90.0	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13055	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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](#)

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

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	0.30	0/6634	0.75	1/9002 (0.0%)
1	B	0.30	0/6656	0.74	1/9024 (0.0%)
All	All	0.30	0/13290	0.74	2/18026 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	662	LYS	CB-CA-C	-5.83	109.83	116.54
1	A	662	LYS	CB-CA-C	-5.45	110.27	116.54

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	6498	0	6297	95	0
1	B	6517	0	6365	105	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	16	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	0	2	0
All	All	13055	0	12662	200	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 8.

All (200) 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:A:360:LYS:NZ	1:A:440:SER:OG	2.07	0.86
1:A:210:LEU:HD11	1:A:639:PRO:HB2	1.63	0.80
1:B:21:LYS:O	1:B:28:ARG:NH2	2.19	0.73
1:A:21:LYS:O	1:A:28:ARG:NH2	2.21	0.72
1:B:656:GLU:HB3	1:B:694:GLU:HG2	1.71	0.71
1:B:17:ASP:OD2	1:B:28:ARG:NH1	2.26	0.68
1:A:656:GLU:HB3	1:A:694:GLU:HG2	1.76	0.68
1:A:381:ILE:HD11	1:A:411:LEU:HD12	1.75	0.67
1:A:790:ARG:O	1:A:794:HIS:ND1	2.27	0.67
1:A:529:LYS:HB3	1:A:576:VAL:HG22	1.78	0.66
1:B:800:ASP:N	1:B:800:ASP:OD1	2.30	0.64
1:A:228:PRO:HB2	1:A:231:PRO:HD2	1.80	0.63
1:B:381:ILE:HD11	1:B:411:LEU:HD12	1.79	0.63
1:B:9:PHE:HB2	1:B:38:ILE:HG21	1.81	0.62
1:B:620:ILE:HD11	1:B:630:ILE:HD12	1.80	0.62
1:B:795:VAL:O	1:B:799:VAL:HG23	1.99	0.62
1:A:845:VAL:HG21	1:A:857:LEU:HB2	1.82	0.62
1:B:227:VAL:HG21	1:B:432:VAL:HG23	1.82	0.61
1:A:394:ASP:OD2	1:A:634:LYS:N	2.33	0.61
1:B:4:ILE:HD11	1:B:156:ILE:HD12	1.82	0.61
1:B:74:LEU:HD11	1:B:107:ILE:HD12	1.84	0.59
1:B:735:ASN:OD1	1:B:739:LYS:NZ	2.36	0.59
1:A:222:LEU:HD12	1:A:372:TRP:HB3	1.85	0.59
1:B:592:LYS:NZ	4:B:1010:HOH:O	2.35	0.59
1:A:125:ARG:NH2	1:A:175:GLU:OE1	2.35	0.58
1:A:28:ARG:O	1:A:32:ILE:HG12	2.04	0.58
1:B:28:ARG:O	1:B:32:ILE:HG12	2.04	0.57
1:A:418:PRO:HG2	1:A:636:TYR:HB3	1.87	0.57
1:B:845:VAL:HG21	1:B:857:LEU:HB2	1.86	0.57
1:A:377:GLU:OE1	1:A:413:ARG:NH1	2.38	0.57
1:B:281:LEU:HB2	1:B:289:ILE:HD11	1.87	0.57
1:B:222:LEU:HD12	1:B:372:TRP:HB3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:THR:OG1	1:A:831:ARG:NH1	2.38	0.56
1:A:617:SER:O	1:A:625:ARG:NH2	2.39	0.56
1:A:220:THR:HG22	1:A:374:SER:HA	1.87	0.56
1:A:735:ASN:OD1	1:A:739:LYS:NZ	2.39	0.55
1:B:228:PRO:HB2	1:B:231:PRO:HD2	1.88	0.55
1:A:2:VAL:HG13	1:A:7:LYS:HD2	1.88	0.55
1:A:708:TRP:CG	1:A:709:LYS:H	2.25	0.55
1:B:195:ALA:HB2	1:B:204:ILE:HA	1.87	0.55
1:B:708:TRP:CG	1:B:709:LYS:H	2.25	0.55
1:B:674:ASP:OD1	1:B:674:ASP:N	2.36	0.55
1:A:816:ILE:HA	1:A:831:ARG:HE	1.72	0.55
1:B:395:VAL:O	1:B:399:LEU:HG	2.07	0.55
1:A:195:ALA:HB2	1:A:204:ILE:HA	1.89	0.54
1:B:381:ILE:HG22	1:B:399:LEU:HD13	1.90	0.54
1:A:714:ILE:HG13	1:A:747:LEU:HD11	1.90	0.54
1:A:860:PHE:CZ	1:A:864:ILE:HD11	2.42	0.54
1:A:448:CYS:HB2	1:A:478:CYS:HB3	1.90	0.54
1:B:507:VAL:HG11	1:B:678:ILE:HG22	1.90	0.54
1:B:418:PRO:HG3	1:B:637:SER:O	2.07	0.53
1:A:401:PHE:HB2	1:A:631:PRO:HB3	1.89	0.53
1:A:500:ARG:NH1	1:A:663:ASP:OD1	2.41	0.53
1:A:443:LEU:HB2	1:A:455:LEU:HD22	1.89	0.53
1:A:91:HIS:HB3	1:A:94:SER:HB2	1.90	0.53
1:B:448:CYS:HB3	1:B:451:CYS:SG	2.49	0.52
1:A:379:GLU:OE2	1:A:413:ARG:NH2	2.43	0.52
1:A:459:GLY:HA2	1:A:467:LEU:HD22	1.92	0.52
1:A:395:VAL:O	1:A:399:LEU:HG	2.09	0.52
1:B:220:THR:HG22	1:B:374:SER:HA	1.90	0.52
1:A:330:TYR:HB2	1:A:483:ILE:HD11	1.92	0.52
1:B:7:LYS:HE2	1:B:264:PHE:O	2.09	0.52
1:A:460:ASP:N	1:A:460:ASP:OD1	2.37	0.52
1:A:791:PHE:O	1:A:795:VAL:HG23	2.09	0.52
1:A:346:ASP:HB2	1:A:347:ARG:HE	1.75	0.51
1:B:142:SER:HA	1:B:152:GLN:HE21	1.76	0.51
1:A:649:LEU:HB3	1:A:672:GLY:HA2	1.93	0.51
1:B:210:LEU:HD12	1:B:640:GLN:HG3	1.92	0.51
1:B:792:ILE:HG21	1:B:862:LYS:HB2	1.91	0.51
1:A:74:LEU:HG	1:A:119:VAL:HG13	1.93	0.51
1:A:607:VAL:HG13	1:A:613:LEU:HD21	1.93	0.51
1:B:460:ASP:OD1	1:B:460:ASP:N	2.38	0.51
1:B:247:HIS:CD2	1:B:279:PHE:HZ	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:714:ILE:HG13	1:B:747:LEU:HD11	1.94	0.50
1:A:148:GLU:HG3	1:A:151:LYS:HG3	1.93	0.50
1:A:674:ASP:OD1	1:A:674:ASP:N	2.32	0.50
1:B:477:LEU:HD23	1:B:482:LEU:HA	1.94	0.50
1:B:500:ARG:NH1	1:B:663:ASP:OD1	2.45	0.49
1:A:227:VAL:HG21	1:A:432:VAL:HG13	1.95	0.49
1:B:73:PHE:CE2	1:B:87:PRO:HG2	2.48	0.49
1:B:114:ARG:HB2	1:B:118:PHE:HB2	1.94	0.49
1:A:100:TYR:HD1	1:A:189:GLU:HB3	1.78	0.48
1:B:103:LEU:O	1:B:107:ILE:HG12	2.13	0.48
1:B:815:VAL:O	1:B:819:ILE:HG22	2.13	0.48
1:B:682:ASP:OD1	1:B:682:ASP:N	2.47	0.48
1:A:73:PHE:CE2	1:A:87:PRO:HG2	2.48	0.48
1:A:247:HIS:CD2	1:A:279:PHE:HZ	2.31	0.48
1:B:860:PHE:CZ	1:B:864:ILE:HD11	2.48	0.48
1:A:746:THR:HG22	1:A:846:ARG:HE	1.78	0.48
1:A:385:THR:HG21	1:A:399:LEU:HD11	1.95	0.48
1:B:769:ARG:NH1	4:B:1004:HOH:O	2.46	0.48
1:A:545:ASP:OD1	4:A:1003:HOH:O	2.20	0.48
1:A:850:GLU:O	1:A:854:VAL:HG23	2.14	0.48
1:B:791:PHE:O	1:B:795:VAL:HG23	2.13	0.48
1:B:272:PRO:HG3	1:B:299:PRO:HD2	1.96	0.47
1:B:282:LYS:HB2	1:B:289:ILE:HD12	1.95	0.47
1:B:448:CYS:HB2	1:B:478:CYS:HB3	1.95	0.47
1:A:457:ILE:HB	1:A:471:TRP:HZ2	1.79	0.47
1:B:53:SER:O	1:B:56:THR:OG1	2.28	0.47
1:B:842:LEU:O	1:B:853:LYS:HD3	2.15	0.47
1:A:771:PHE:CE2	1:A:777:ARG:HG3	2.50	0.47
1:A:815:VAL:HG13	1:A:819:ILE:HD12	1.97	0.47
1:B:142:SER:HA	1:B:152:GLN:NE2	2.30	0.47
1:A:272:PRO:HG3	1:A:299:PRO:HD2	1.97	0.47
1:A:86:TYR:CD2	1:A:104:GLU:HG3	2.50	0.47
1:B:45:LYS:HB3	1:B:215:SER:HB2	1.97	0.47
1:B:596:ILE:HD13	1:B:727:LEU:HD23	1.97	0.47
1:B:766:GLU:H	1:B:766:GLU:CD	2.23	0.47
1:A:84:VAL:HG12	1:A:623:ASN:HB3	1.96	0.46
1:A:160:TYR:HB3	1:A:161:PRO:HD3	1.96	0.46
1:B:160:TYR:HB3	1:B:161:PRO:HD3	1.98	0.46
1:B:543:LEU:HB3	1:B:548:LEU:HD12	1.97	0.46
1:A:842:LEU:O	1:A:853:LYS:HD3	2.14	0.46
1:B:614:GLY:HA2	1:B:634:LYS:HE2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:GLU:O	1:A:413:ARG:HD2	2.16	0.46
1:B:165:LYS:HB2	1:B:191:VAL:HG21	1.97	0.46
1:A:507:VAL:HG11	1:A:678:ILE:HG22	1.97	0.46
1:B:417:TYR:CG	1:B:639:PRO:HG3	2.51	0.46
1:A:245:SER:OG	1:A:484:LYS:HD2	2.16	0.46
1:A:446:TRP:CZ2	1:A:464:HIS:HB2	2.51	0.46
1:A:673:ASP:OD1	1:A:673:ASP:N	2.48	0.45
1:B:850:GLU:O	1:B:854:VAL:HG23	2.16	0.45
1:B:816:ILE:HA	1:B:831:ARG:HE	1.81	0.45
1:A:511:TYR:HB3	1:A:591:PRO:HG3	1.99	0.45
1:A:792:ILE:O	1:A:796:LEU:HD22	2.17	0.45
1:A:841:LEU:O	1:A:845:VAL:HG23	2.17	0.45
1:B:449:HIS:CG	1:B:476:PRO:HD2	2.52	0.44
1:B:543:LEU:HD13	1:B:548:LEU:HB2	1.99	0.44
1:B:597:LEU:HD13	1:B:714:ILE:HG12	1.99	0.44
1:A:807:ILE:HA	1:A:810:MET:HB3	2.00	0.44
1:B:110:GLY:HA3	1:B:118:PHE:CE2	2.53	0.44
1:B:598:VAL:HG12	1:B:734:LEU:HD22	1.99	0.44
1:B:673:ASP:OD1	1:B:673:ASP:N	2.45	0.44
1:A:73:PHE:C	1:A:74:LEU:HD13	2.42	0.44
1:A:74:LEU:HD23	1:A:123:LEU:HD21	2.00	0.44
1:B:359:LEU:O	1:B:363:ARG:HB2	2.18	0.44
1:B:58:ARG:CZ	1:B:402:ALA:HB2	2.48	0.44
1:B:310:GLU:O	1:B:314:ILE:HG13	2.18	0.44
1:B:324:ASP:O	1:B:328:GLN:HG3	2.18	0.44
1:B:337:ALA:HB2	1:B:482:LEU:HD11	2.00	0.44
1:B:424:LEU:HD12	1:B:424:LEU:HA	1.85	0.44
1:B:549:TYR:O	1:B:584:TYR:OH	2.35	0.44
1:B:577:VAL:O	1:B:581:ASN:ND2	2.47	0.44
1:B:792:ILE:HD12	1:B:792:ILE:H	1.83	0.44
1:A:356:GLU:O	1:A:360:LYS:HB2	2.17	0.43
1:B:385:THR:HG21	1:B:399:LEU:HD11	2.00	0.43
1:B:649:LEU:HB3	1:B:672:GLY:HA2	1.99	0.43
1:A:839:LYS:HA	1:A:839:LYS:HE2	2.00	0.43
1:B:459:GLY:HA2	1:B:467:LEU:HD22	2.00	0.43
1:B:592:LYS:HD3	1:B:719:TYR:HE2	1.83	0.43
1:B:653:SER:HB2	1:B:670:ALA:O	2.18	0.43
1:A:624:ILE:O	1:A:628:VAL:HG12	2.18	0.43
1:B:227:VAL:HG21	1:B:432:VAL:CG2	2.48	0.43
1:B:457:ILE:HB	1:B:471:TRP:HZ2	1.83	0.43
1:A:4:ILE:HD11	1:A:156:ILE:HD12	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:LEU:HA	1:B:277:GLN:HG3	2.01	0.43
1:B:91:HIS:HB3	1:B:94:SER:HB2	2.00	0.43
1:A:324:ASP:O	1:A:328:GLN:HG3	2.18	0.43
1:B:622:PRO:HA	1:B:625:ARG:HG3	2.01	0.43
1:A:23:GLU:HG2	1:A:23:GLU:O	2.18	0.43
1:A:310:GLU:O	1:A:314:ILE:HG13	2.19	0.43
1:B:3:ASN:OD1	1:B:3:ASN:N	2.51	0.43
1:B:763:VAL:HG22	1:B:767:LEU:HD13	2.00	0.43
1:A:416:ILE:HG22	1:A:419:LEU:HB2	2.00	0.42
1:A:51:ALA:O	1:A:55:LYS:HG2	2.20	0.42
1:A:274:LEU:HA	1:A:277:GLN:HG3	2.01	0.42
1:A:291:ASP:OD2	1:A:291:ASP:N	2.52	0.42
1:B:418:PRO:HG2	1:B:636:TYR:HB3	2.01	0.42
1:B:492:ARG:NH1	1:B:498:LYS:HD3	2.35	0.42
1:A:32:ILE:HD12	1:A:130:GLU:HB2	2.00	0.42
1:A:420:LEU:HD12	1:A:420:LEU:HA	1.93	0.42
1:B:621:HIS:HA	1:B:622:PRO:HD3	1.92	0.42
1:A:270:ILE:HD11	1:A:305:ILE:HD11	2.00	0.42
1:A:145:PHE:O	1:A:152:GLN:NE2	2.53	0.42
1:B:802:TRP:HA	1:B:803:PRO:HD3	1.90	0.42
1:A:827:THR:O	1:A:831:ARG:HG3	2.20	0.42
1:B:345:VAL:HG13	1:B:346:ASP:O	2.19	0.42
1:B:798:GLU:O	1:B:802:TRP:N	2.52	0.42
1:A:145:PHE:HB2	1:A:152:GLN:HG3	2.01	0.41
1:B:401:PHE:HB2	1:B:631:PRO:HB3	2.02	0.41
1:B:819:ILE:HD12	1:B:819:ILE:HA	1.94	0.41
1:A:558:LEU:HD12	1:A:558:LEU:HA	1.90	0.41
1:B:509:LEU:HB3	1:B:515:ARG:HB2	2.02	0.41
1:A:573:VAL:O	1:A:577:VAL:HG23	2.20	0.41
1:B:616:ILE:HG12	1:B:630:ILE:HD13	2.02	0.41
1:B:573:VAL:O	1:B:577:VAL:HG23	2.21	0.41
1:A:763:VAL:HG11	1:A:767:LEU:HD22	2.02	0.41
1:B:669:TYR:HB3	1:B:676:LEU:HB3	2.03	0.41
1:B:20:LEU:HD23	1:B:73:PHE:CD2	2.56	0.41
1:A:369:SER:HB3	1:A:431:LYS:HD3	2.02	0.41
1:A:603:ASP:O	1:A:607:VAL:HG23	2.21	0.41
1:B:9:PHE:HE2	1:B:43:THR:HG21	1.85	0.41
1:B:137:VAL:HG12	1:B:156:ILE:HG12	2.03	0.41
1:B:227:VAL:HG23	1:B:367:THR:HB	2.02	0.41
1:B:522:TYR:HB3	1:B:579:PHE:HZ	1.86	0.41
1:B:656:GLU:O	1:B:660:VAL:HG23	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:VAL:HG12	1:A:734:LEU:HD22	2.03	0.40
1:A:603:ASP:OD1	1:A:744:LYS:NZ	2.48	0.40
1:A:523:GLY:O	1:A:527:VAL:HG23	2.21	0.40
1:A:223:ARG:NH1	1:A:225:LYS:HB2	2.36	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	819/888 (92%)	797 (97%)	22 (3%)	0	100	100
1	B	810/888 (91%)	789 (97%)	21 (3%)	0	100	100
All	All	1629/1776 (92%)	1586 (97%)	43 (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	666/795 (84%)	634 (95%)	32 (5%)	23	57
1	B	677/795 (85%)	648 (96%)	29 (4%)	26	60
All	All	1343/1590 (84%)	1282 (96%)	61 (4%)	24	59

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ILE
1	A	74	LEU
1	A	84	VAL
1	A	148	GLU
1	A	210	LEU
1	A	223	ARG
1	A	282	LYS
1	A	345	VAL
1	A	347	ARG
1	A	379	GLU
1	A	394	ASP
1	A	413	ARG
1	A	416	ILE
1	A	436	ARG
1	A	443	LEU
1	A	504	VAL
1	A	532	GLU
1	A	541	ASN
1	A	575	GLU
1	A	616	ILE
1	A	624	ILE
1	A	626	ASP
1	A	630	ILE
1	A	634	LYS
1	A	674	ASP
1	A	681	VAL
1	A	746	THR
1	A	763	VAL
1	A	796	LEU
1	A	800	ASP
1	A	801	THR
1	A	810	MET
1	B	1	MET
1	B	74	LEU
1	B	84	VAL
1	B	148	GLU
1	B	175	GLU
1	B	216	VAL
1	B	223	ARG
1	B	292	GLU
1	B	307	SER
1	B	345	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	347	ARG
1	B	377	GLU
1	B	379	GLU
1	B	416	ILE
1	B	432	VAL
1	B	504	VAL
1	B	616	ILE
1	B	618	THR
1	B	624	ILE
1	B	630	ILE
1	B	632	GLU
1	B	664	GLU
1	B	674	ASP
1	B	694	GLU
1	B	746	THR
1	B	763	VAL
1	B	800	ASP
1	B	827	THR
1	B	830	LEU

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	207	HIS
1	A	230	GLN
1	B	152	GLN
1	B	230	GLN
1	B	300	ASN
1	B	340	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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	835/888 (94%)	0.10	17 (2%)	65 41	53, 89, 134, 213	0
1	B	828/888 (93%)	0.21	30 (3%)	46 26	58, 92, 129, 192	0
All	All	1663/1776 (93%)	0.16	47 (2%)	55 32	53, 91, 131, 213	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	435	GLU	4.7
1	B	432	VAL	4.4
1	A	305	ILE	3.4
1	B	434	GLU	3.2
1	A	613	LEU	3.2
1	A	185	LYS	3.2
1	B	829	GLU	3.0
1	B	525	ASP	3.0
1	B	813	PHE	2.9
1	B	373	VAL	2.8
1	A	113	ASN	2.7
1	B	119	VAL	2.7
1	B	757	SER	2.7
1	B	616	ILE	2.7
1	A	39	GLN	2.6
1	A	181	GLU	2.6
1	A	184	GLU	2.5
1	A	219	PRO	2.5
1	B	308	GLY	2.5
1	B	428	GLY	2.5
1	B	830	LEU	2.4
1	A	635	TYR	2.4
1	A	559	SER	2.4
1	B	433	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	221	LEU	2.3
1	A	188	GLU	2.3
1	B	782	GLU	2.3
1	B	372	TRP	2.3
1	B	310	GLU	2.3
1	A	36	GLY	2.3
1	B	371	THR	2.3
1	B	273	SER	2.2
1	A	573	VAL	2.2
1	A	180	GLU	2.2
1	A	112	SER	2.2
1	B	218	ASP	2.2
1	A	117	ARG	2.2
1	B	48	GLN	2.1
1	B	429	GLU	2.1
1	B	819	ILE	2.1
1	A	62	ARG	2.1
1	B	369	SER	2.1
1	B	303	LEU	2.1
1	B	77	SER	2.0
1	B	827	THR	2.0
1	B	700	GLU	2.0
1	B	826	GLU	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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MN	B	903	1/1	0.69	0.17	168,168,168,168	0
3	MN	A	905	1/1	0.85	0.09	132,132,132,132	0
3	MN	B	905	1/1	0.86	0.11	191,191,191,191	0
3	MN	B	902	1/1	0.90	0.10	143,143,143,143	0
3	MN	A	902	1/1	0.91	0.15	172,172,172,172	0
3	MN	A	903	1/1	0.92	0.13	153,153,153,153	0
3	MN	B	904	1/1	0.96	0.06	82,82,82,82	0
3	MN	A	904	1/1	0.98	0.06	76,76,76,76	0
2	ZN	B	901	1/1	0.99	0.04	85,85,85,85	0
2	ZN	A	901	1/1	1.00	0.01	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.