



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 12:19 AM GMT

PDB ID : 2CSU  
Title : Crystal structure of PH0766 from *Pyrococcus horikoshii* OT3  
Authors : Sugahara, M.; Kunishima, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2005-05-23  
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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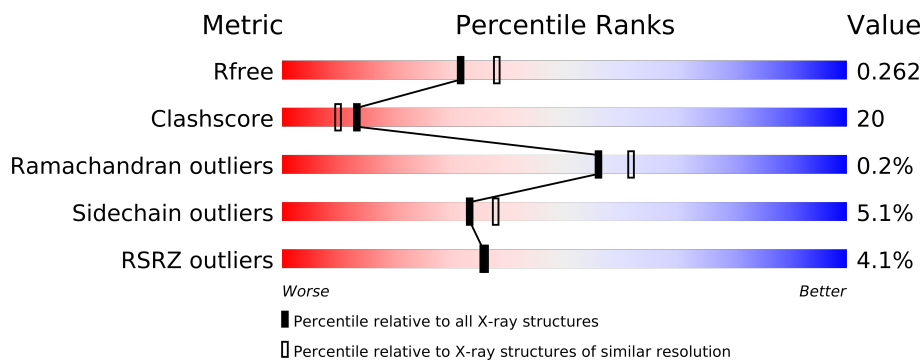
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	457	
1	B	457	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7131 atoms, of which 0 are hydrogen and 0 are deuterium.

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 457aa long hypothetical protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	Se	0	0	0
			3341	2143	553	627	3	15			
1	B	434	Total	C	N	O	S	Se	0	0	0
			3330	2135	552	625	3	15			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP O58493
A	122	MSE	MET	MODIFIED RESIDUE	UNP O58493
A	133	MSE	MET	MODIFIED RESIDUE	UNP O58493
A	185	MSE	MET	MODIFIED RESIDUE	UNP O58493
A	194	MSE	MET	MODIFIED RESIDUE	UNP O58493
A	220	MSE	MET	MODIFIED RESIDUE	UNP O58493
A	279	MSE	MET	MODIFIED RESIDUE	UNP O58493
A	282	MSE	MET	MODIFIED RESIDUE	UNP O58493
A	299	MSE	MET	MODIFIED RESIDUE	UNP O58493
A	338	MSE	MET	MODIFIED RESIDUE	UNP O58493
A	347	MSE	MET	MODIFIED RESIDUE	UNP O58493
A	371	MSE	MET	MODIFIED RESIDUE	UNP O58493
A	384	MSE	MET	MODIFIED RESIDUE	UNP O58493
A	409	MSE	MET	MODIFIED RESIDUE	UNP O58493
A	411	MSE	MET	MODIFIED RESIDUE	UNP O58493
B	1	MSE	MET	MODIFIED RESIDUE	UNP O58493
B	122	MSE	MET	MODIFIED RESIDUE	UNP O58493
B	133	MSE	MET	MODIFIED RESIDUE	UNP O58493
B	185	MSE	MET	MODIFIED RESIDUE	UNP O58493
B	194	MSE	MET	MODIFIED RESIDUE	UNP O58493
B	220	MSE	MET	MODIFIED RESIDUE	UNP O58493
B	279	MSE	MET	MODIFIED RESIDUE	UNP O58493
B	282	MSE	MET	MODIFIED RESIDUE	UNP O58493
B	299	MSE	MET	MODIFIED RESIDUE	UNP O58493
B	338	MSE	MET	MODIFIED RESIDUE	UNP O58493

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Chain	Residue	Modelled	Actual	Comment	Reference
B	347	MSE	MET	MODIFIED RESIDUE	UNP O58493
B	371	MSE	MET	MODIFIED RESIDUE	UNP O58493
B	384	MSE	MET	MODIFIED RESIDUE	UNP O58493
B	409	MSE	MET	MODIFIED RESIDUE	UNP O58493
B	411	MSE	MET	MODIFIED RESIDUE	UNP O58493

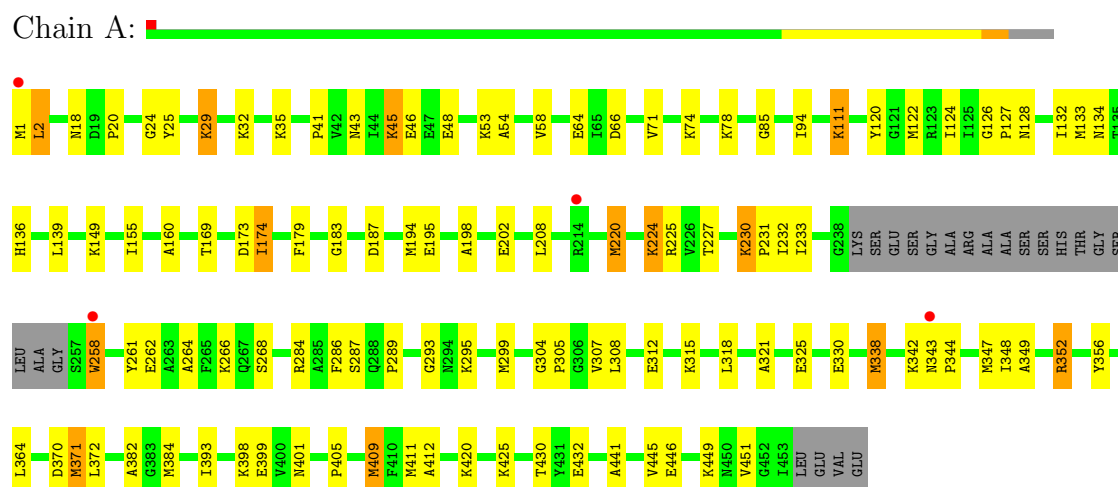
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	287	Total O 287 287	0	0
2	B	173	Total O 173 173	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 457aa long hypothetical protein



- Molecule 1: 457aa long hypothetical protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.46Å 70.59Å 88.51Å 90.00° 90.66° 90.00°	Depositor
Resolution (Å)	19.85 – 2.20 19.85 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.85-2.20) 96.1 (19.85-2.19)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.246 , 0.261 0.246 , 0.262	Depositor DCC
$R_{free}$ test set	2244 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 33.8	EDS
Estimated twinning fraction	0.135 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 45198 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7131	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.64	3/3379 (0.1%)	0.82	5/4528 (0.1%)
1	B	0.59	2/3366 (0.1%)	0.70	0/4508
All	All	0.62	5/6745 (0.1%)	0.76	5/9036 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	TRP	NE1-CE2	8.74	1.49	1.37
1	A	194	MSE	SE-CE	-6.31	1.58	1.95
1	A	371	MSE	SE-CE	-5.85	1.60	1.95
1	B	194	MSE	CG-SE	-5.21	1.77	1.95
1	B	371	MSE	CG-SE	-5.05	1.78	1.95

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	GLU	CA-CB-CG	6.07	126.75	113.40
1	A	330	GLU	CG-CD-OE1	5.87	130.03	118.30
1	A	330	GLU	CG-CD-OE2	-5.71	106.88	118.30
1	A	225	ARG	CD-NE-CZ	-5.20	116.32	123.60
1	A	352	ARG	CD-NE-CZ	-5.04	116.55	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	214	ARG	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3341	0	3460	102	0
1	B	3330	0	3458	181	0
2	A	287	0	0	6	0
2	B	173	0	0	8	0
All	All	7131	0	6918	278	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (278) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:409:MSE:HE1	1:A:411:MSE:SE	2.16	0.95
1:B:156:SER:HB2	1:B:209:TYR:HB3	1.48	0.95
1:B:411:MSE:HB3	1:B:412:ALA:HB2	1.49	0.95
1:A:343:ASN:HB2	1:A:344:PRO:HD3	1.58	0.86
1:B:136:HIS:HA	1:B:149:LYS:HE2	1.59	0.85
1:B:411:MSE:CB	1:B:412:ALA:HB2	2.08	0.83
1:B:130:VAL:HG12	1:B:142:THR:HG23	1.60	0.82
1:B:343:ASN:CB	1:B:344:PRO:HD3	2.09	0.82
1:B:133:MSE:HB2	1:B:179:PHE:HB3	1.60	0.81
1:B:49:VAL:HG23	1:B:54:ALA:HB2	1.63	0.81
1:A:318:LEU:HD21	1:A:445:VAL:HG21	1.63	0.80
1:A:371:MSE:HE1	1:A:441:ALA:HB1	1.64	0.80
1:B:142:THR:HG21	1:B:144:ILE:HG12	1.64	0.80
1:B:292:ARG:HG2	1:B:453:ILE:CG2	2.13	0.79
1:B:292:ARG:HD3	1:B:292:ARG:C	2.04	0.78
1:B:280:LEU:O	1:B:284:ARG:HG3	1.85	0.77
1:A:411:MSE:CB	1:A:412:ALA:HB2	2.15	0.77
1:B:292:ARG:HG2	1:B:453:ILE:HG22	1.67	0.76
1:B:41:PRO:CG	1:B:49:VAL:HG21	2.16	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:29:LYS:O	1:B:32:LYS:HB2	1.86	0.74
1:B:343:ASN:HB2	1:B:344:PRO:HD3	1.67	0.73
1:A:371:MSE:HE1	1:A:441:ALA:CB	2.17	0.73
1:B:41:PRO:CB	1:B:49:VAL:HG21	2.18	0.73
1:B:41:PRO:HB2	1:B:49:VAL:HG21	1.71	0.73
1:A:411:MSE:CA	1:A:412:ALA:HB2	2.18	0.72
1:A:173:ASP:HB2	2:A:672:HOH:O	1.91	0.71
1:B:340:ALA:HB3	1:B:346:ASP:HB3	1.73	0.71
1:A:411:MSE:HB3	1:A:412:ALA:HB2	1.73	0.70
1:A:231:PRO:HG3	1:A:286:PHE:CE1	2.27	0.70
1:B:299:MSE:HE1	1:B:360:ALA:HB2	1.74	0.69
1:B:119:LYS:O	1:B:119:LYS:HD2	1.93	0.69
1:A:348:ILE:HG22	1:A:349:ALA:H	1.59	0.68
1:B:233:ILE:HD12	1:B:233:ILE:N	2.08	0.68
1:B:142:THR:HG22	1:B:143:PHE:N	2.09	0.67
1:B:142:THR:CG2	1:B:144:ILE:HG12	2.25	0.67
1:B:11:ILE:HG22	1:B:67:LEU:HB3	1.77	0.67
1:A:364:LEU:HG	1:A:372:LEU:HD22	1.76	0.67
1:A:233:ILE:N	1:A:233:ILE:HD12	2.11	0.66
1:B:285:ALA:HB2	1:B:440:ALA:HB1	1.77	0.66
1:A:45:LYS:HG2	1:A:45:LYS:O	1.94	0.66
1:B:411:MSE:CA	1:B:412:ALA:HB2	2.26	0.66
1:B:291:PRO:HB3	1:B:405:PRO:HG3	1.77	0.66
1:A:304:GLY:O	1:A:307:VAL:HG22	1.97	0.65
1:B:288:GLN:HB3	1:B:289:PRO:HD2	1.79	0.65
1:B:149:LYS:NZ	2:B:567:HOH:O	2.30	0.65
1:B:142:THR:HG22	1:B:144:ILE:H	1.62	0.65
1:A:348:ILE:HG22	1:A:349:ALA:N	2.12	0.64
1:B:11:ILE:HG13	1:B:39:VAL:HG13	1.79	0.64
1:B:18:ASN:ND2	2:B:621:HOH:O	2.24	0.64
1:A:409:MSE:HE2	1:A:411:MSE:HG3	1.79	0.63
1:A:409:MSE:CE	1:A:411:MSE:HG3	2.28	0.63
1:A:409:MSE:HE3	1:A:432:GLU:C	2.19	0.63
1:B:214:ARG:HG3	1:B:215:ASN:N	2.15	0.62
1:A:425:LYS:O	1:A:425:LYS:HG2	1.99	0.62
1:B:12:ALA:HB2	1:B:65:ILE:HG21	1.81	0.62
1:A:169:THR:HG22	1:A:174:ILE:HG13	1.82	0.61
1:A:411:MSE:HA	1:A:412:ALA:HB2	1.82	0.61
1:B:134:ASN:HB3	1:B:139:LEU:HB3	1.81	0.61
1:B:68:ALA:HB3	1:B:92:VAL:HG22	1.82	0.61
1:B:55:TYR:CD2	1:B:61:ILE:HG12	2.35	0.60
1:B:169:THR:HB	1:B:174:ILE:O	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:124:ILE:O	1:A:187:ASP:HB3	2.00	0.60
1:B:295:LYS:HB3	1:B:321:ALA:HB2	1.83	0.59
1:B:343:ASN:CB	1:B:344:PRO:CD	2.80	0.59
1:B:50:GLN:O	1:B:50:GLN:HG3	2.03	0.59
1:A:94:ILE:CG2	1:A:127:PRO:HB3	2.32	0.58
1:A:409:MSE:HE1	1:A:411:MSE:CG	2.33	0.58
1:A:231:PRO:HG3	1:A:286:PHE:CZ	2.39	0.58
1:B:71:VAL:O	1:B:71:VAL:HG22	2.03	0.57
1:A:133:MSE:HG3	1:A:179:PHE:HB3	1.86	0.57
1:B:223:ALA:HB3	1:B:268:SER:OG	2.04	0.57
1:B:12:ALA:CB	1:B:65:ILE:HG21	2.34	0.57
1:A:43:ASN:HB3	1:A:46:GLU:HB2	1.85	0.57
1:B:300:THR:HB	1:B:375:ILE:HB	1.86	0.57
1:A:411:MSE:HA	1:A:412:ALA:CB	2.34	0.57
1:B:340:ALA:HB3	1:B:346:ASP:CB	2.35	0.57
1:A:231:PRO:HG3	1:A:286:PHE:CD1	2.40	0.57
1:B:5:PHE:CE1	1:B:125:ILE:HG13	2.39	0.57
1:A:371:MSE:HG3	1:A:405:PRO:HG2	1.86	0.57
1:A:451:VAL:HG12	1:A:451:VAL:O	2.06	0.55
1:A:299:MSE:HE3	1:A:347:MSE:HE1	1.87	0.55
1:B:72:VAL:HB	1:B:73:PRO:HD2	1.89	0.55
1:B:195:GLU:HG3	1:B:222:VAL:HG13	1.89	0.55
1:B:292:ARG:HD3	1:B:292:ARG:O	2.06	0.55
1:B:231:PRO:HG3	1:B:286:PHE:CD1	2.42	0.55
1:B:50:GLN:O	1:B:50:GLN:CG	2.54	0.55
1:A:85:GLY:HA2	1:A:122:MSE:SE	2.57	0.55
1:B:59:LYS:HE2	1:B:83:GLN:HG2	1.87	0.55
1:B:36:LYS:HG2	1:B:137:VAL:HB	1.89	0.54
1:B:130:VAL:HG12	1:B:142:THR:CG2	2.34	0.54
1:B:300:THR:HA	1:B:375:ILE:O	2.07	0.54
1:A:343:ASN:CB	1:A:344:PRO:HD3	2.35	0.54
1:B:4:TYR:O	1:B:8:PRO:HB3	2.08	0.54
1:B:18:ASN:HD22	1:B:18:ASN:C	2.11	0.54
1:B:222:VAL:O	1:B:226:VAL:HG23	2.08	0.54
1:A:352:ARG:HG2	1:A:384:MSE:SE	2.58	0.53
1:B:336:PRO:HG2	1:B:348:ILE:CG1	2.38	0.53
1:A:25:TYR:HE2	1:A:29:LYS:HZ3	1.55	0.53
1:A:41:PRO:HG2	1:A:54:ALA:HA	1.90	0.53
1:A:295:LYS:HB3	1:A:321:ALA:HB2	1.90	0.53
1:B:155:ILE:HG12	1:B:180:ILE:HD12	1.91	0.53
1:B:14:ILE:HD13	1:B:80:THR:HG23	1.90	0.53
1:B:55:TYR:CE1	1:B:62:PRO:HD3	2.44	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:69:ILE:HD13	1:B:93:VAL:HB	1.90	0.53
1:B:14:ILE:HA	1:B:42:VAL:HB	1.91	0.53
1:B:294:ASN:HB2	1:B:318:LEU:HD22	1.89	0.53
1:B:142:THR:HG22	1:B:143:PHE:H	1.74	0.52
1:B:6:PHE:O	1:B:134:ASN:ND2	2.42	0.52
1:B:145:THR:HG22	2:B:499:HOH:O	2.09	0.52
1:B:265:PHE:HB3	1:B:270:VAL:CG2	2.40	0.52
1:B:265:PHE:CD1	1:B:270:VAL:HG21	2.44	0.52
1:B:301:ASN:HA	1:B:347:MSE:O	2.10	0.52
1:B:174:ILE:CD1	1:B:284:ARG:HD2	2.40	0.52
1:B:215:ASN:HB3	1:B:218:LYS:HB3	1.91	0.52
1:A:46:GLU:HA	1:A:46:GLU:OE2	2.10	0.51
1:B:231:PRO:HG3	1:B:286:PHE:CE1	2.44	0.51
1:B:420:LYS:NZ	1:B:430:THR:O	2.44	0.51
1:A:409:MSE:CE	1:A:411:MSE:CG	2.87	0.51
1:B:18:ASN:HB3	1:B:49:VAL:O	2.11	0.51
1:B:408:ALA:O	1:B:430:THR:HA	2.10	0.51
1:A:232:ILE:C	1:A:233:ILE:HD12	2.31	0.51
1:A:258:TRP:O	1:A:262:GLU:HG2	2.11	0.51
1:B:343:ASN:HB3	1:B:344:PRO:HD3	1.91	0.51
1:A:169:THR:HB	1:A:174:ILE:O	2.10	0.51
1:B:347:MSE:HB3	1:B:351:ALA:HB2	1.92	0.51
1:A:111:LYS:HD3	2:A:566:HOH:O	2.10	0.51
1:B:411:MSE:HB3	1:B:412:ALA:CB	2.33	0.51
1:A:136:HIS:HA	1:A:149:LYS:HE2	1.92	0.51
1:B:124:ILE:O	1:B:187:ASP:HB3	2.11	0.51
1:A:318:LEU:CD2	1:A:445:VAL:HG21	2.38	0.50
1:A:356:TYR:HD2	1:A:393:ILE:HD11	1.76	0.50
1:B:412:ALA:N	1:B:416:SER:HB3	2.27	0.50
1:A:53:LYS:NZ	2:A:650:HOH:O	2.35	0.50
1:B:18:ASN:C	1:B:18:ASN:ND2	2.65	0.50
1:B:385:THR:OG1	1:B:388:GLU:HB2	2.10	0.50
1:B:123:ARG:NH2	1:B:192:GLU:OE1	2.42	0.50
1:B:408:ALA:HB3	1:B:430:THR:OG1	2.12	0.50
1:B:148:LYS:HE3	1:B:170:ILE:HG23	1.94	0.49
1:B:198:ALA:HA	1:B:230:LYS:HD2	1.93	0.49
1:B:142:THR:CG2	1:B:143:PHE:N	2.75	0.49
1:A:227:THR:HG21	1:A:268:SER:O	2.13	0.49
1:B:214:ARG:HG3	1:B:215:ASN:H	1.77	0.49
1:B:59:LYS:HA	1:B:87:LYS:HG3	1.94	0.49
1:A:420:LYS:HG3	1:A:430:THR:HB	1.93	0.49
1:A:289:PRO:O	1:A:405:PRO:HB3	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:312:GLU:HA	1:A:315:LYS:HD3	1.95	0.48
1:B:130:VAL:O	1:B:142:THR:HG23	2.13	0.48
1:B:5:PHE:CZ	1:B:125:ILE:HG12	2.49	0.48
1:B:340:ALA:O	1:B:346:ASP:N	2.47	0.48
1:B:213:VAL:HG12	1:B:214:ARG:N	2.27	0.48
1:B:61:ILE:HB	1:B:87:LYS:HZ2	1.78	0.48
1:B:133:MSE:CB	1:B:179:PHE:HB3	2.37	0.48
1:B:125:ILE:HD13	1:B:188:VAL:HB	1.96	0.48
1:A:94:ILE:HG21	1:A:127:PRO:HB3	1.95	0.48
1:A:371:MSE:HE1	1:A:441:ALA:CA	2.42	0.48
1:A:352:ARG:NH2	1:A:382:ALA:O	2.42	0.48
1:A:25:TYR:HE2	1:A:29:LYS:NZ	2.12	0.48
1:B:356:TYR:OH	1:B:376:CYS:HB2	2.13	0.48
1:A:220:MSE:HE3	1:A:264:ALA:HB1	1.95	0.47
1:B:61:ILE:HD12	1:B:65:ILE:HG13	1.95	0.47
1:A:409:MSE:HE3	1:A:432:GLU:O	2.14	0.47
1:B:174:ILE:O	1:B:174:ILE:HG13	2.14	0.47
1:A:1:MSE:O	1:A:2:LEU:HB2	2.13	0.47
1:A:348:ILE:CG2	1:A:349:ALA:H	2.26	0.47
1:B:6:PHE:HB3	1:B:134:ASN:HD22	1.78	0.47
1:B:5:PHE:CE1	1:B:125:ILE:CG1	2.98	0.47
1:B:151:ASN:HB3	1:B:204:LYS:HG3	1.96	0.47
1:B:233:ILE:N	1:B:233:ILE:CD1	2.78	0.47
1:A:71:VAL:O	1:A:71:VAL:HG22	2.15	0.47
1:B:407:LEU:CD2	1:B:429:PRO:HG2	2.44	0.47
1:B:119:LYS:O	1:B:119:LYS:CD	2.63	0.46
1:B:11:ILE:HG12	1:B:39:VAL:HG22	1.97	0.46
1:B:232:ILE:O	1:B:271:LEU:N	2.48	0.46
1:B:198:ALA:O	1:B:230:LYS:HE3	2.15	0.46
1:B:324:GLU:O	1:B:327:THR:HB	2.15	0.46
1:B:194:MSE:HE3	1:B:232:ILE:HD13	1.98	0.46
1:B:447:GLN:OE1	1:B:447:GLN:HA	2.16	0.46
1:B:29:LYS:HA	1:B:50:GLN:HE22	1.80	0.46
1:A:134:ASN:HB3	1:A:139:LEU:HB3	1.97	0.46
1:A:18:ASN:O	1:A:20:PRO:HD3	2.16	0.46
1:A:293:GLY:HA3	1:A:370:ASP:OD1	2.16	0.46
1:B:11:ILE:HD12	1:B:31:LEU:HD13	1.98	0.46
1:B:348:ILE:HG22	1:B:349:ALA:N	2.30	0.46
1:B:282:MSE:HG2	1:B:443:ALA:HB2	1.98	0.46
1:A:401:ASN:HB3	2:A:513:HOH:O	2.15	0.46
1:A:132:ILE:HA	1:A:179:PHE:O	2.16	0.46
1:B:71:VAL:O	1:B:71:VAL:HG13	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:8:PRO:HB2	1:B:11:ILE:HG22	1.97	0.45
1:A:169:THR:CG2	1:A:174:ILE:HG13	2.46	0.45
1:B:336:PRO:HG2	1:B:348:ILE:HG12	1.97	0.45
1:B:156:SER:CB	1:B:209:TYR:HB3	2.34	0.45
1:A:202:GLU:N	1:A:202:GLU:OE1	2.49	0.45
1:A:307:VAL:HG23	1:A:308:LEU:N	2.30	0.45
1:A:195:GLU:HG2	2:A:533:HOH:O	2.16	0.45
1:A:446:GLU:O	1:A:449:LYS:HB2	2.16	0.45
1:A:348:ILE:CG2	1:A:349:ALA:N	2.79	0.45
1:A:233:ILE:N	1:A:233:ILE:CD1	2.78	0.45
1:B:299:MSE:SE	1:B:372:LEU:HD11	2.67	0.45
1:B:61:ILE:HG22	1:B:63:ASP:H	1.82	0.45
1:B:120:TYR:HB2	1:B:122:MSE:HG3	1.99	0.45
1:A:284:ARG:HD2	2:A:550:HOH:O	2.15	0.45
1:B:411:MSE:HA	1:B:412:ALA:HB2	1.99	0.45
1:B:7:ASN:N	1:B:8:PRO:CD	2.79	0.45
1:B:210:ILE:HG21	1:B:213:VAL:HG23	1.98	0.45
1:B:69:ILE:CD1	1:B:93:VAL:HB	2.47	0.44
1:B:130:VAL:HG12	1:B:130:VAL:O	2.18	0.44
1:B:49:VAL:CG2	1:B:54:ALA:HB2	2.41	0.44
1:B:11:ILE:CD1	1:B:31:LEU:HD13	2.47	0.44
1:A:128:ASN:O	1:A:183:GLY:HA3	2.16	0.44
1:B:447:GLN:O	1:B:450:ASN:HB2	2.17	0.44
1:B:312:GLU:HG3	1:B:435:GLU:HA	2.00	0.44
1:A:343:ASN:HB2	1:A:344:PRO:CD	2.40	0.44
1:A:262:GLU:O	1:A:266:LYS:HG2	2.17	0.44
1:A:224:LYS:O	1:A:227:THR:HG22	2.17	0.44
1:B:40:TYR:HD2	1:B:65:ILE:HD11	1.83	0.43
1:A:284:ARG:HD2	1:A:284:ARG:HH11	1.65	0.43
1:A:371:MSE:HE1	1:A:441:ALA:HA	2.00	0.43
1:B:126:GLY:HA3	1:B:127:PRO:HA	1.79	0.43
1:B:394:ILE:CD1	1:B:422:LEU:HG	2.48	0.43
1:A:126:GLY:HA3	1:A:127:PRO:HA	1.84	0.43
1:A:338:MSE:SE	1:B:102:THR:HA	2.68	0.43
1:A:71:VAL:O	1:A:71:VAL:HG13	2.18	0.43
1:B:391:GLU:HG3	1:B:422:LEU:HD21	2.00	0.43
1:B:31:LEU:C	1:B:33:GLU:H	2.21	0.43
1:B:409:MSE:HE3	1:B:432:GLU:C	2.39	0.43
1:B:108:ARG:HG2	1:B:108:ARG:HH11	1.82	0.43
1:B:217:LYS:HA	1:B:217:LYS:HD2	1.73	0.43
1:A:32:LYS:O	1:A:35:LYS:NZ	2.47	0.43
1:B:53:LYS:NZ	2:B:608:HOH:O	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:41:PRO:HG3	1:B:49:VAL:HG21	1.96	0.42
1:A:120:TYR:HB2	1:A:122:MSE:HG3	2.01	0.42
1:B:407:LEU:HD22	1:B:429:PRO:HG2	1.99	0.42
1:B:409:MSE:HA	1:B:431:TYR:O	2.19	0.42
1:B:341:VAL:HG23	1:B:341:VAL:O	2.19	0.42
1:B:174:ILE:HD13	1:B:284:ARG:HD2	2.01	0.42
1:B:32:LYS:HD2	1:B:50:GLN:HE21	1.85	0.42
1:B:2:LEU:HB3	1:B:5:PHE:HD2	1.83	0.42
1:A:307:VAL:CG2	1:A:308:LEU:N	2.82	0.42
1:B:11:ILE:CG1	1:B:39:VAL:HG13	2.46	0.42
1:A:24:GLY:HA2	1:A:71:VAL:HG11	2.02	0.42
1:A:305:PRO:HG3	1:B:161:LEU:HD13	2.02	0.42
1:A:155:ILE:HB	1:A:208:LEU:HD23	2.02	0.42
1:B:7:ASN:ND2	2:B:592:HOH:O	2.53	0.42
1:B:5:PHE:CZ	1:B:125:ILE:CG1	3.03	0.42
1:B:174:ILE:HD12	1:B:284:ARG:HD2	2.01	0.42
1:A:58:VAL:O	1:A:58:VAL:HG22	2.20	0.42
1:B:133:MSE:HB2	1:B:179:PHE:CB	2.40	0.41
1:B:340:ALA:O	1:B:345:VAL:HA	2.20	0.41
1:A:307:VAL:HG23	1:B:237:ALA:HB1	2.02	0.41
1:B:190:PHE:HB3	1:B:219:PHE:HE1	1.85	0.41
1:A:398:LYS:O	1:A:401:ASN:ND2	2.53	0.41
1:A:111:LYS:HG2	1:A:111:LYS:O	2.20	0.41
1:A:133:MSE:CG	1:A:179:PHE:HB3	2.50	0.41
1:B:142:THR:CG2	1:B:143:PHE:H	2.34	0.41
1:A:198:ALA:O	1:A:230:LYS:HE3	2.20	0.41
1:B:27:VAL:HA	1:B:142:THR:O	2.20	0.41
1:A:307:VAL:CG2	1:B:237:ALA:HB1	2.50	0.41
1:B:368:ASN:HB3	2:B:494:HOH:O	2.21	0.41
1:A:160:ALA:CB	1:B:302:ALA:HB1	2.51	0.41
1:B:27:VAL:HG23	1:B:143:PHE:HB3	2.02	0.41
1:A:318:LEU:HD21	1:A:445:VAL:CG2	2.44	0.41
1:B:93:VAL:HG22	1:B:125:ILE:HB	2.01	0.41
1:B:188:VAL:O	2:B:490:HOH:O	2.22	0.41
1:A:20:PRO:HA	1:A:25:TYR:CD2	2.56	0.41
1:B:100:GLY:N	1:B:110:GLU:OE1	2.47	0.41
1:A:342:LYS:HB2	1:A:343:ASN:H	1.69	0.41
1:B:61:ILE:HA	1:B:62:PRO:HD3	1.94	0.41
1:B:120:TYR:HB2	1:B:122:MSE:SE	2.71	0.41
1:B:321:ALA:HB1	1:B:368:ASN:O	2.21	0.41
1:B:66:ASP:HB2	1:B:90:LYS:HD2	2.03	0.41
1:B:271:LEU:HD13	1:B:443:ALA:HB1	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:325:GLU:HB2	2:B:477:HOH:O	2.21	0.40
1:B:155:ILE:HB	1:B:208:LEU:CD2	2.51	0.40
1:B:284:ARG:HD3	1:B:284:ARG:HH11	1.72	0.40
1:A:66:ASP:OD1	1:A:66:ASP:N	2.55	0.40
1:B:347:MSE:SE	1:B:359:THR:HG21	2.72	0.40
1:B:407:LEU:HD11	1:B:444:LEU:HD12	2.04	0.40
1:B:410:PHE:N	1:B:410:PHE:CD1	2.90	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	431/457 (94%)	410 (95%)	21 (5%)	0	100	100
1	B	430/457 (94%)	394 (92%)	34 (8%)	2 (0%)	38	38
All	All	861/914 (94%)	804 (93%)	55 (6%)	2 (0%)	56	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	TYR
1	B	262	GLU

### 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	354/354 (100%)	336 (95%)	18 (5%)	33	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	353/354 (100%)	335 (95%)	18 (5%)	33	38
All	All	707/708 (100%)	671 (95%)	36 (5%)	33	38

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	29	LYS
1	A	45	LYS
1	A	48	GLU
1	A	64	GLU
1	A	74	LYS
1	A	78	LYS
1	A	111	LYS
1	A	174	ILE
1	A	220	MSE
1	A	224	LYS
1	A	230	LYS
1	A	261	TYR
1	A	287	SER
1	A	325	GLU
1	A	338	MSE
1	A	399	GLU
1	A	409	MSE
1	B	18	ASN
1	B	32	LYS
1	B	36	LYS
1	B	47	GLU
1	B	48	GLU
1	B	53	LYS
1	B	59	LYS
1	B	87	LYS
1	B	149	LYS
1	B	217	LYS
1	B	267	GLN
1	B	292	ARG
1	B	295	LYS
1	B	338	MSE
1	B	343	ASN
1	B	347	MSE
1	B	403	GLU
1	B	409	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	343	ASN
1	A	365	GLN
1	A	401	ASN
1	B	18	ASN
1	B	50	GLN
1	B	343	ASN
1	B	365	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	435/457 (95%)	-0.10	4 (0%) 81 82	19, 33, 50, 69	0
1	B	434/457 (94%)	0.54	32 (7%) 14 14	28, 53, 83, 88	0
All	All	869/914 (95%)	0.22	36 (4%) 35 36	19, 42, 74, 88	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	62	PRO	5.2
1	B	63	ASP	5.1
1	B	49	VAL	4.8
1	B	453	ILE	4.5
1	B	451	VAL	4.2
1	B	45	LYS	4.1
1	A	1	MSE	4.1
1	B	56	LYS	4.0
1	B	1	MSE	3.9
1	B	54	ALA	3.8
1	B	292	ARG	3.6
1	B	214	ARG	3.4
1	B	259	LYS	3.3
1	B	347	MSE	3.2
1	B	28	PHE	3.0
1	B	260	ILE	2.9
1	B	216	GLY	2.8
1	B	40	TYR	2.8
1	B	267	GLN	2.7
1	B	227	THR	2.7
1	B	118	HIS	2.6
1	B	269	GLY	2.5
1	A	214	ARG	2.4
1	B	217	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	25	TYR	2.4
1	A	258	TRP	2.4
1	A	343	ASN	2.3
1	B	18	ASN	2.2
1	B	239	LYS	2.2
1	B	20	PRO	2.2
1	B	42	VAL	2.1
1	B	44	ILE	2.1
1	B	21	LYS	2.1
1	B	65	ILE	2.1
1	B	58	VAL	2.0
1	B	36	LYS	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.