



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 08:44 AM EST

PDB ID : 2ZKT  
Title : Structure of PH0037 protein from *Pyrococcus horikoshii*  
Authors : Lokanath, N.K.; Pampa, K.J.; Kunishima, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2008-03-29  
Resolution : 2.40 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](mailto: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>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

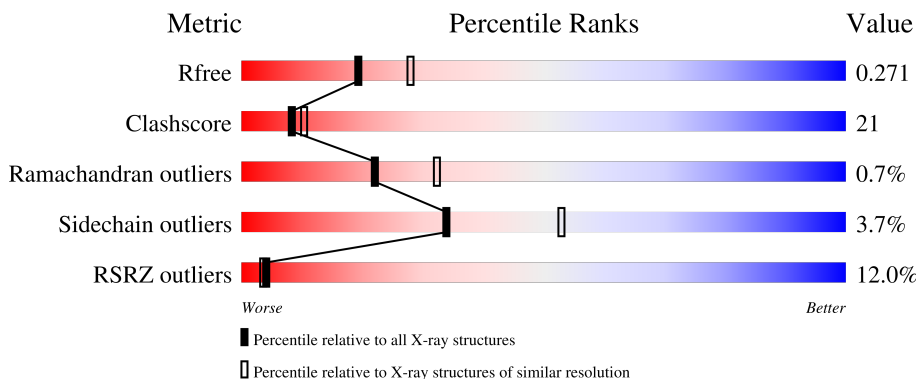
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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	412	 11% 57% 22% 20%
1	B	412	 10% 62% 29% 8%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5720 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 2,3-bisphosphoglycerate-independent phosphoglycerate mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	2540	1613	435	480	12	0	0	0
1	B	381	2953	1876	517	549	11	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

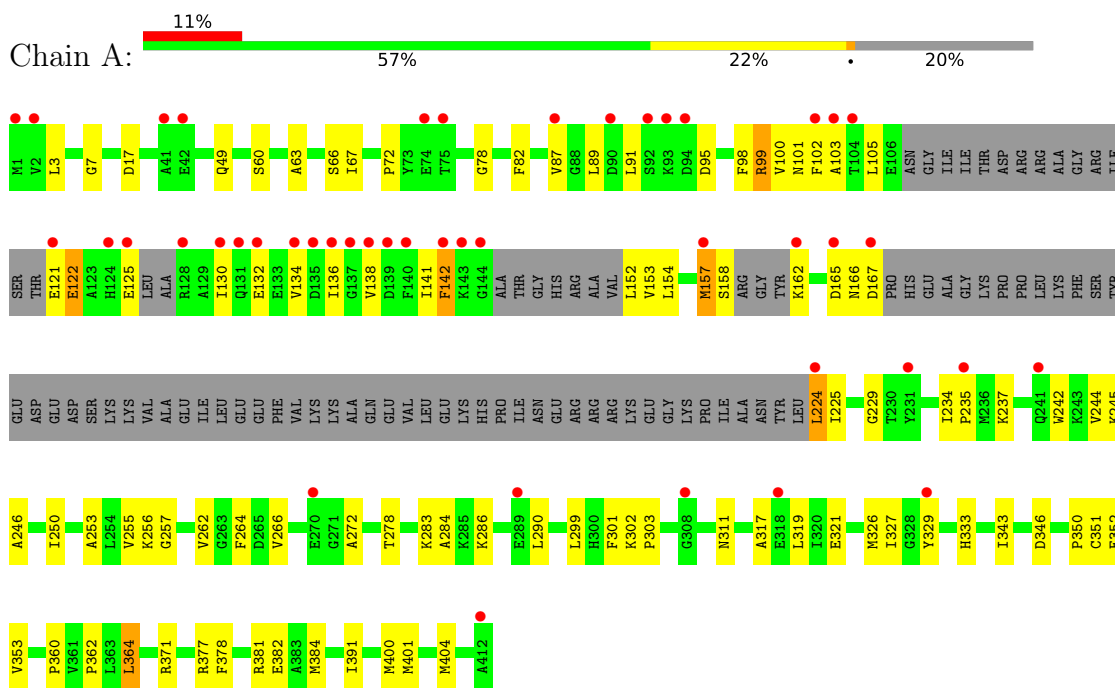
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	106	Total 106	O 106	0	0
4	B	115	Total 115	O 115	0	0

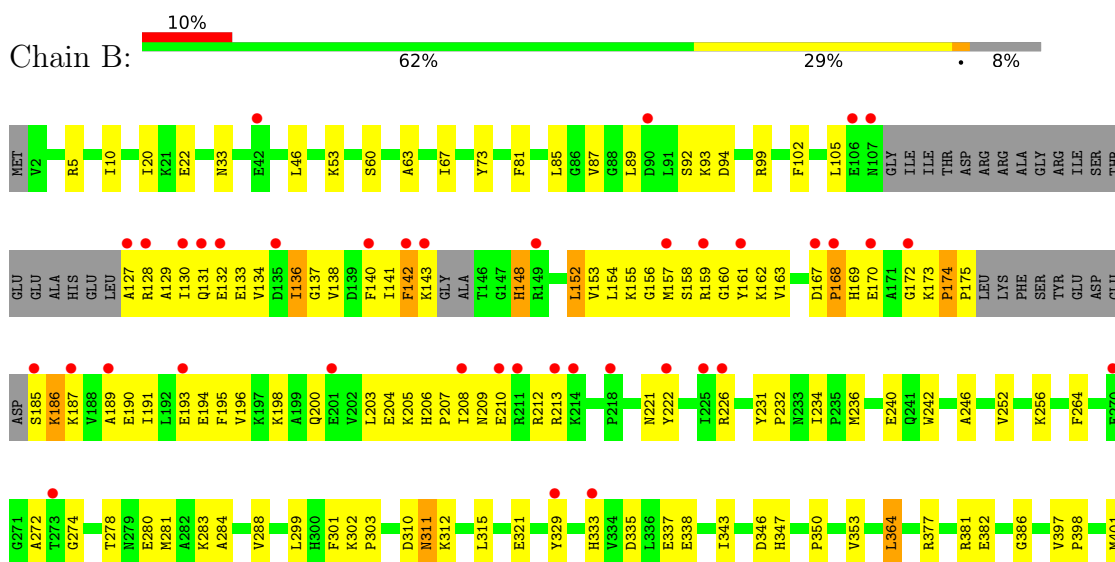
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 2,3-bisphosphoglycerate-independent phosphoglycerate mutase



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## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.90Å 155.90Å 230.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.40 10.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (10.00-2.40) 99.9 (10.00-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.80 (at 2.41Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.277 , 0.286 0.271 , 0.271	Depositor DCC
$R_{free}$ test set	2104 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtrriage
Anisotropy	0.073	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 70.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5720	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3604e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical 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: ZN, CA

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	0.52	0/2583	0.67	0/3475
1	B	0.58	0/3008	0.71	0/4050
All	All	0.55	0/5591	0.69	0/7525

There are no bond length outliers.

There are no bond angle outliers.

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	2540	0	2543	94	0
1	B	2953	0	2984	139	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	106	0	0	4	0
4	B	115	0	0	4	0
All	All	5720	0	5527	232	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 21.

All (232) 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:87:VAL:HG12	1:A:157:MET:HG2	1.21	1.15
1:A:154:LEU:HD11	1:A:162:LYS:HE3	1.26	1.09
1:B:136:ILE:HG21	1:B:208:ILE:CD1	1.84	1.08
1:A:100:VAL:HG11	1:A:162:LYS:HE2	1.08	1.07
1:A:141:ILE:HG21	1:A:154:LEU:HD22	1.37	1.06
1:A:100:VAL:CG1	1:A:162:LYS:HE2	1.85	1.05
1:B:142:PHE:CZ	1:B:153:VAL:HA	1.91	1.05
1:A:100:VAL:HG11	1:A:162:LYS:CE	1.86	1.03
1:A:87:VAL:CG1	1:A:157:MET:HG2	1.89	1.03
1:A:100:VAL:HB	1:A:162:LYS:HG3	1.38	1.03
1:A:141:ILE:HG21	1:A:154:LEU:CD2	1.94	0.98
1:B:127:ALA:HB1	1:B:212:ARG:HH21	1.30	0.96
1:B:136:ILE:HG21	1:B:208:ILE:HD11	1.47	0.94
1:B:148:HIS:HE1	1:B:152:LEU:HD12	1.33	0.94
1:B:141:ILE:HG21	1:B:154:LEU:HD22	1.48	0.94
1:B:127:ALA:HB1	1:B:212:ARG:NH2	1.82	0.93
1:A:103:ALA:HB1	1:A:125:GLU:HA	1.51	0.90
1:B:310:ASP:HB2	1:B:312:LYS:HE2	1.52	0.90
1:A:100:VAL:HB	1:A:162:LYS:CG	2.04	0.88
1:B:102:PHE:CD2	1:B:134:VAL:HG22	2.09	0.87
1:B:167:ASP:HB3	1:B:168:PRO:HD2	1.57	0.87
1:B:102:PHE:HE2	1:B:134:VAL:HG13	1.40	0.86
1:B:141:ILE:CG2	1:B:154:LEU:HD22	2.06	0.85
1:A:103:ALA:CB	1:A:125:GLU:HA	2.08	0.82
1:A:154:LEU:CD1	1:A:162:LYS:HE3	2.08	0.82
1:B:148:HIS:CE1	1:B:152:LEU:HD12	2.16	0.79
1:A:100:VAL:CB	1:A:162:LYS:HG3	2.13	0.77
1:B:102:PHE:CE2	1:B:134:VAL:HG22	2.19	0.77
1:A:3:LEU:HD12	4:A:464:HOH:O	1.85	0.77
1:B:157:MET:HG3	1:B:158:SER:H	1.52	0.75
1:A:134:VAL:O	1:A:138:VAL:HG23	1.87	0.73
1:A:103:ALA:HB3	1:A:224:LEU:HD13	1.71	0.72
1:A:154:LEU:HD11	1:A:162:LYS:CE	2.14	0.72
1:A:122:GLU:OE2	1:A:224:LEU:HD21	1.90	0.71
1:A:284:ALA:HB2	1:A:326:MET:HG3	1.73	0.70
1:B:283:LYS:NZ	4:B:517:HOH:O	2.24	0.70
1:A:283:LYS:HB3	1:A:299:LEU:HD11	1.72	0.70
1:B:136:ILE:CG2	1:B:208:ILE:CD1	2.67	0.70
1:B:142:PHE:HZ	1:B:153:VAL:HA	1.54	0.70
1:B:94:ASP:HA	1:B:170:GLU:HG2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ALA:O	1:B:128:ARG:HB2	1.93	0.68
1:B:138:VAL:HG22	1:B:162:LYS:CD	2.23	0.68
1:B:133:GLU:O	1:B:136:ILE:HG22	1.93	0.68
1:B:136:ILE:HG13	1:B:206:HIS:CE1	2.29	0.67
1:B:310:ASP:CB	1:B:312:LYS:HE2	2.24	0.67
1:B:134:VAL:HG21	1:B:159:ARG:O	1.93	0.67
1:A:311:ASN:HD22	1:A:351:CYS:HB3	1.58	0.67
1:B:154:LEU:HD21	1:B:162:LYS:NZ	2.09	0.67
1:B:207:PRO:HA	1:B:210:GLU:HB2	1.78	0.66
1:A:400:MET:HB3	1:A:404:MET:CE	2.25	0.66
1:B:127:ALA:CB	1:B:212:ARG:HH21	2.06	0.66
1:A:364:LEU:HD12	1:A:364:LEU:C	2.17	0.65
1:B:329:TYR:CE1	1:B:333:HIS:HE1	2.14	0.65
1:B:173:LYS:N	1:B:174:PRO:HD3	2.12	0.65
1:A:7:GLY:HA3	1:A:404:MET:HE1	1.79	0.64
1:A:400:MET:HB3	1:A:404:MET:HE3	1.79	0.64
1:A:87:VAL:HG23	1:A:89:LEU:HG	1.79	0.64
1:B:312:LYS:HE3	1:B:315:LEU:HD23	1.77	0.64
1:B:105:LEU:HD23	1:B:200:GLN:OE1	1.97	0.64
1:B:131:GLN:HG3	1:B:158:SER:HA	1.80	0.64
1:B:329:TYR:CE1	1:B:333:HIS:CE1	2.87	0.63
1:B:136:ILE:HG23	1:B:137:GLY:N	2.11	0.63
1:B:134:VAL:O	1:B:138:VAL:HG23	1.98	0.63
1:A:317:ALA:O	1:A:321:GLU:HG3	1.99	0.63
1:B:377:ARG:O	1:B:382:GLU:HG2	1.98	0.63
1:A:302:LYS:N	1:A:303:PRO:HD2	2.13	0.63
1:A:102:PHE:CE2	1:A:134:VAL:HG13	2.33	0.62
1:B:154:LEU:HD21	1:B:162:LYS:HZ2	1.64	0.62
1:A:141:ILE:CG2	1:A:154:LEU:CD2	2.72	0.61
1:A:63:ALA:O	1:A:67:ILE:HG12	2.01	0.61
1:A:132:GLU:O	1:A:136:ILE:HG12	2.01	0.60
1:B:131:GLN:HG3	1:B:159:ARG:H	1.67	0.60
1:B:138:VAL:HG22	1:B:162:LYS:HD3	1.84	0.59
1:B:136:ILE:CG2	1:B:137:GLY:N	2.66	0.59
1:B:302:LYS:N	1:B:303:PRO:HD2	2.17	0.59
1:A:66:SER:OG	1:A:72:PRO:HG3	2.02	0.59
1:A:234:ILE:HD11	1:A:237:LYS:HD3	1.85	0.58
1:B:136:ILE:HG21	1:B:208:ILE:HD12	1.80	0.58
1:B:136:ILE:CG2	1:B:208:ILE:HD12	2.35	0.57
1:B:311:ASN:C	1:B:311:ASN:HD22	2.07	0.57
1:B:364:LEU:C	1:B:364:LEU:HD12	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LEU:O	1:B:209:ASN:ND2	2.38	0.57
1:A:142:PHE:CZ	1:A:153:VAL:HA	2.40	0.56
1:B:173:LYS:N	1:B:174:PRO:CD	2.67	0.56
1:B:152:LEU:C	1:B:152:LEU:HD22	2.25	0.56
1:A:329:TYR:CE1	1:A:333:HIS:CE1	2.94	0.56
1:A:141:ILE:CG2	1:A:154:LEU:HD23	2.35	0.55
1:A:95:ASP:OD1	1:A:167:ASP:HA	2.07	0.55
1:A:242:TRP:O	1:A:244:VAL:HG13	2.06	0.55
1:B:274:GLY:HA2	4:B:517:HOH:O	2.07	0.55
1:B:102:PHE:CE2	1:B:134:VAL:HG13	2.32	0.54
1:B:196:VAL:HG11	1:B:222:TYR:CZ	2.43	0.54
1:B:172:GLY:O	1:B:175:PRO:HD3	2.08	0.54
1:A:103:ALA:HB3	1:A:224:LEU:CD1	2.37	0.54
1:B:196:VAL:CG1	1:B:222:TYR:CE1	2.91	0.54
1:A:141:ILE:HG21	1:A:154:LEU:HD23	1.87	0.54
1:B:133:GLU:HG2	1:B:208:ILE:HG21	1.89	0.54
1:B:173:LYS:C	1:B:175:PRO:HD3	2.28	0.54
1:B:138:VAL:HG11	1:B:155:LYS:HA	1.89	0.53
1:B:301:PHE:CZ	1:B:303:PRO:HG2	2.44	0.53
1:B:236:MET:HB2	1:B:240:GLU:CD	2.29	0.53
1:A:100:VAL:CB	1:A:162:LYS:CG	2.82	0.53
1:A:122:GLU:OE2	1:A:125:GLU:HB3	2.09	0.53
1:B:81:PHE:HE1	1:B:85:LEU:HD11	1.74	0.53
1:B:162:LYS:HG2	1:B:163:VAL:N	2.24	0.53
1:B:172:GLY:C	1:B:174:PRO:CD	2.77	0.53
1:B:209:ASN:HA	1:B:212:ARG:HB2	1.91	0.53
1:B:272:ALA:HA	1:B:278:THR:HG23	1.90	0.52
1:B:154:LEU:HD11	1:B:162:LYS:HZ1	1.75	0.52
1:A:102:PHE:HE2	1:A:134:VAL:HG13	1.74	0.52
1:B:136:ILE:HG13	1:B:206:HIS:HE1	1.73	0.52
1:B:207:PRO:O	1:B:210:GLU:HB2	2.10	0.52
1:A:301:PHE:CE2	1:A:303:PRO:HG2	2.45	0.52
1:A:343:ILE:HB	1:A:364:LEU:HG	1.92	0.52
1:A:381:ARG:NH2	4:A:427:HOH:O	2.35	0.52
1:B:5:ARG:HD3	1:B:337:GLU:O	2.10	0.51
1:B:53:LYS:HE2	1:B:73:TYR:OH	2.11	0.51
1:A:311:ASN:ND2	1:A:351:CYS:HB3	2.25	0.51
1:A:130:ILE:HG22	1:A:132:GLU:OE1	2.11	0.51
1:B:252:VAL:O	1:B:256:LYS:HG3	2.10	0.51
1:B:99:ARG:NH1	1:B:226:ARG:HD3	2.26	0.50
1:A:87:VAL:HG12	1:A:157:MET:CG	2.16	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ARG:O	1:A:225:ILE:HA	2.10	0.50
1:A:91:LEU:HG	1:A:165:ASP:OD2	2.12	0.50
1:A:381:ARG:O	1:A:384:MET:HB2	2.12	0.50
1:B:346:ASP:OD1	1:B:346:ASP:N	2.45	0.50
1:A:360:PRO:HD3	4:A:486:HOH:O	2.12	0.50
1:B:10:ILE:HB	1:B:343:ILE:HG12	1.94	0.50
1:B:203:LEU:C	1:B:205:LYS:H	2.16	0.49
1:A:141:ILE:CG2	1:A:154:LEU:HD22	2.27	0.49
1:B:167:ASP:CB	1:B:168:PRO:HD2	2.37	0.49
1:B:148:HIS:HE1	1:B:152:LEU:CD1	2.15	0.49
1:B:130:ILE:HG22	1:B:132:GLU:H	1.78	0.48
1:B:167:ASP:O	1:B:169:HIS:ND1	2.34	0.48
1:A:82:PHE:O	1:A:257:GLY:HA3	2.14	0.48
1:A:105:LEU:HD12	1:A:121:GLU:O	2.13	0.48
1:B:138:VAL:HG21	1:B:156:GLY:CA	2.43	0.48
1:B:142:PHE:CE1	1:B:152:LEU:O	2.67	0.48
1:B:154:LEU:HG	1:B:162:LYS:HD2	1.95	0.48
1:A:250:ILE:HD13	1:A:255:VAL:HG12	1.96	0.47
1:B:283:LYS:HB3	1:B:299:LEU:HD11	1.94	0.47
1:B:33:ASN:O	1:B:321:GLU:HG2	2.14	0.47
1:A:100:VAL:CG1	1:A:162:LYS:CG	2.93	0.47
1:A:256:LYS:HE3	1:A:266:VAL:CG1	2.45	0.47
1:A:346:ASP:OD1	1:A:346:ASP:N	2.43	0.47
1:B:170:GLU:O	1:B:173:LYS:HB3	2.14	0.47
1:A:327:ILE:HD13	1:A:343:ILE:HD13	1.97	0.47
1:B:87:VAL:HG23	1:B:89:LEU:HG	1.96	0.47
1:B:63:ALA:O	1:B:67:ILE:HG12	2.15	0.46
1:B:204:GLU:HG3	1:B:221:ASN:HB2	1.98	0.46
1:B:160:GLY:HA3	4:B:514:HOH:O	2.15	0.46
1:B:284:ALA:O	1:B:288:VAL:HG23	2.15	0.46
1:B:206:HIS:CG	1:B:207:PRO:HD2	2.51	0.46
1:B:140:PHE:CD1	1:B:206:HIS:NE2	2.84	0.45
1:A:286:LYS:HE3	1:A:290:LEU:HD21	1.98	0.45
1:B:157:MET:HG3	1:B:158:SER:N	2.26	0.45
1:B:350:PRO:HB2	1:B:353:VAL:HG23	1.98	0.45
1:B:138:VAL:HG22	1:B:162:LYS:HD2	1.98	0.45
1:B:142:PHE:CE2	1:B:153:VAL:HG13	2.51	0.45
1:B:174:PRO:N	1:B:175:PRO:HD3	2.31	0.45
1:A:87:VAL:CG1	1:A:157:MET:CG	2.79	0.45
1:A:99:ARG:HG2	1:A:99:ARG:HH11	1.81	0.45
1:A:98:PHE:HE2	1:A:166:ASN:HD22	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:VAL:CG1	1:A:162:LYS:HG3	2.46	0.45
1:A:246:ALA:HB1	1:A:264:PHE:CE2	2.52	0.45
1:B:172:GLY:C	1:B:174:PRO:HD2	2.37	0.45
1:B:311:ASN:O	1:B:311:ASN:ND2	2.48	0.45
1:A:132:GLU:H	1:A:132:GLU:CD	2.21	0.44
1:A:152:LEU:HD12	1:A:152:LEU:C	2.37	0.44
1:A:98:PHE:HB3	1:A:225:ILE:CG1	2.47	0.44
1:A:272:ALA:HA	1:A:278:THR:OG1	2.16	0.44
1:B:81:PHE:CE1	1:B:85:LEU:HD11	2.52	0.44
1:B:194:GLU:CG	1:B:198:LYS:HE3	2.47	0.44
1:B:154:LEU:CD2	1:B:162:LYS:HD2	2.48	0.44
1:B:142:PHE:HE1	1:B:152:LEU:O	2.00	0.44
1:B:148:HIS:ND1	1:B:148:HIS:N	2.56	0.44
1:B:173:LYS:C	1:B:175:PRO:CD	2.85	0.44
1:B:246:ALA:HB1	1:B:264:PHE:CE2	2.52	0.44
1:A:242:TRP:CE3	1:A:401:MET:HG3	2.53	0.44
1:B:136:ILE:O	1:B:136:ILE:HD12	2.17	0.44
1:B:102:PHE:HD2	1:B:134:VAL:HG22	1.72	0.44
1:A:103:ALA:HB2	1:A:224:LEU:HD22	2.00	0.43
1:A:377:ARG:NH1	1:B:377:ARG:HD3	2.33	0.43
1:B:234:ILE:O	1:B:234:ILE:HG13	2.18	0.43
1:B:329:TYR:CZ	1:B:333:HIS:CE1	3.06	0.43
1:B:397:VAL:HB	1:B:398:PRO:HD3	2.00	0.43
1:B:92:SER:HB2	1:B:94:ASP:OD1	2.18	0.43
1:B:136:ILE:CG2	1:B:137:GLY:H	2.31	0.43
1:B:346:ASP:O	1:B:347:HIS:HB3	2.17	0.43
1:B:154:LEU:HD11	1:B:162:LYS:HE3	2.00	0.43
1:B:231:TYR:CD1	1:B:232:PRO:HD2	2.53	0.43
1:B:130:ILE:HG12	1:B:133:GLU:OE1	2.18	0.43
1:B:148:HIS:CE1	1:B:152:LEU:CD1	2.95	0.43
1:A:262:VAL:HG23	1:A:264:PHE:HD1	1.84	0.43
1:A:352:GLU:HG3	1:A:353:VAL:HG23	2.01	0.43
1:B:189:ALA:O	1:B:193:GLU:CG	2.66	0.43
1:A:245:LYS:HB3	1:A:245:LYS:HE3	1.78	0.42
1:B:46:LEU:O	1:B:386:GLY:HA3	2.19	0.42
1:B:196:VAL:HG11	1:B:222:TYR:OH	2.19	0.42
1:B:280:GLU:HG2	1:B:281:MET:N	2.33	0.42
1:A:78:GLY:HA3	1:A:229:GLY:HA2	2.01	0.42
1:A:371:ARG:HG3	4:A:421:HOH:O	2.18	0.42
1:B:335:ASP:OD2	1:B:338:GLU:HG3	2.19	0.42
1:B:242:TRP:CD2	1:B:401:MET:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:VAL:HB	1:A:162:LYS:HG2	1.95	0.42
1:B:186:LYS:O	1:B:190:GLU:HG3	2.20	0.42
1:B:187:LYS:O	1:B:191:ILE:HG13	2.19	0.42
1:A:91:LEU:N	1:A:91:LEU:HD12	2.35	0.41
1:A:234:ILE:O	1:A:234:ILE:HG13	2.18	0.41
1:A:303:PRO:HB2	1:A:319:LEU:HD22	2.02	0.41
1:B:154:LEU:HD13	1:B:195:PHE:HZ	1.85	0.41
1:B:189:ALA:O	1:B:193:GLU:HG3	2.20	0.41
1:B:213:ARG:HH11	1:B:213:ARG:HD3	1.69	0.41
1:A:49:GLN:HA	1:A:391:ILE:O	2.19	0.41
1:A:362:PRO:HB2	1:A:378:PHE:CE1	2.55	0.41
1:B:142:PHE:CZ	1:B:153:VAL:HG13	2.56	0.41
1:A:17:ASP:CG	1:A:350:PRO:HA	2.41	0.41
1:A:66:SER:OG	1:A:72:PRO:CG	2.68	0.41
1:A:301:PHE:CZ	1:A:303:PRO:HG2	2.56	0.41
1:A:103:ALA:HB2	1:A:125:GLU:HA	1.97	0.41
1:A:329:TYR:CE1	1:A:333:HIS:HE1	2.38	0.41
1:B:20:ILE:HG22	1:B:22:GLU:HG2	2.01	0.41
1:B:209:ASN:O	1:B:212:ARG:HB2	2.21	0.41
1:B:301:PHE:CE2	1:B:303:PRO:HG2	2.56	0.41
1:B:207:PRO:CA	1:B:210:GLU:HB2	2.48	0.40
1:B:134:VAL:O	1:B:138:VAL:CG2	2.68	0.40
1:B:134:VAL:HG11	1:B:161:TYR:O	2.21	0.40
1:B:167:ASP:HB3	1:B:168:PRO:CD	2.40	0.40
1:B:231:TYR:N	4:B:510:HOH:O	2.25	0.40
1:A:102:PHE:CD2	1:A:134:VAL:HG13	2.57	0.40
1:B:242:TRP:CE3	1:B:401:MET:HG3	2.57	0.40
1:A:157:MET:SD	1:A:253:ALA:HB2	2.62	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	318/412 (77%)	300 (94%)	17 (5%)	1 (0%)	41	55
1	B	373/412 (90%)	354 (95%)	15 (4%)	4 (1%)	14	20
All	All	691/824 (84%)	654 (95%)	32 (5%)	5 (1%)	22	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	168	PRO
1	B	129	ALA
1	A	235	PRO
1	B	174	PRO
1	B	93	LYS

### 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	265/333 (80%)	255 (96%)	10 (4%)	33	51
1	B	308/333 (92%)	297 (96%)	11 (4%)	35	54
All	All	573/666 (86%)	552 (96%)	21 (4%)	34	53

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	SER
1	A	99	ARG
1	A	101	ASN
1	A	122	GLU
1	A	142	PHE
1	A	157	MET
1	A	158	SER
1	A	224	LEU
1	A	364	LEU
1	A	382	GLU
1	B	60	SER

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Mol	Chain	Res	Type
1	B	136	ILE
1	B	142	PHE
1	B	143	LYS
1	B	148	HIS
1	B	152	LEU
1	B	185	SER
1	B	186	LYS
1	B	311	ASN
1	B	364	LEU
1	B	381	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	241	GLN
1	A	311	ASN
1	A	333	HIS
1	B	101	ASN
1	B	131	GLN
1	B	233	ASN
1	B	241	GLN
1	B	311	ASN
1	B	333	HIS
1	B	347	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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

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	330/412 (80%)	0.60	45 (13%) <b>3</b> <b>2</b>	34, 52, 77, 91	0
1	B	381/412 (92%)	0.54	40 (10%) <b>6</b> <b>5</b>	34, 53, 76, 88	0
All	All	711/824 (86%)	0.57	85 (11%) <b>4</b> <b>3</b>	34, 53, 77, 91	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	PHE	13.0
1	B	168	PRO	9.7
1	B	140	PHE	7.5
1	A	1	MET	7.3
1	A	412	ALA	6.2
1	B	107	ASN	6.1
1	B	157	MET	5.9
1	B	130	ILE	5.5
1	A	131	GLN	5.0
1	B	412	ALA	4.8
1	A	135	ASP	4.6
1	A	130	ILE	4.6
1	A	157	MET	4.6
1	B	149	ARG	4.5
1	B	159	ARG	4.5
1	B	210	GLU	4.5
1	A	128	ARG	4.2
1	A	94	ASP	4.1
1	A	90	ASP	4.1
1	B	131	GLN	4.0
1	B	211	ARG	4.0
1	A	138	VAL	3.8
1	A	162	LYS	3.7
1	A	74	GLU	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	42	GLU	3.6
1	A	167	ASP	3.6
1	A	143	LYS	3.5
1	A	136	ILE	3.5
1	B	128	ARG	3.4
1	A	103	ALA	3.4
1	A	134	VAL	3.4
1	B	193	GLU	3.3
1	A	142	PHE	3.3
1	A	289	GLU	3.3
1	B	106	GLU	3.3
1	A	121	GLU	3.2
1	A	139	ASP	3.2
1	B	42	GLU	3.1
1	A	93	LYS	3.1
1	B	132	GLU	3.0
1	B	273	THR	3.0
1	A	231	TYR	2.9
1	B	214	LYS	2.9
1	B	208	ILE	2.8
1	B	225	ILE	2.8
1	A	165	ASP	2.7
1	A	132	GLU	2.6
1	A	318	GLU	2.6
1	A	125	GLU	2.6
1	B	329	TYR	2.6
1	A	329	TYR	2.5
1	A	75	THR	2.5
1	B	143	LYS	2.5
1	B	213	ARG	2.5
1	B	201	GLU	2.5
1	B	142	PHE	2.5
1	B	222	TYR	2.4
1	B	218	PRO	2.4
1	B	90	ASP	2.4
1	B	161	TYR	2.4
1	A	235	PRO	2.4
1	B	170	GLU	2.4
1	A	224	LEU	2.4
1	A	2	VAL	2.4
1	A	87	VAL	2.4
1	B	185	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	127	ALA	2.4
1	B	333	HIS	2.3
1	B	187	LYS	2.3
1	B	226	ARG	2.2
1	A	308	GLY	2.2
1	A	137	GLY	2.2
1	B	172	GLY	2.2
1	B	167	ASP	2.1
1	A	124	HIS	2.1
1	A	241	GLN	2.1
1	B	270	GLU	2.1
1	A	104	THR	2.1
1	A	92	SER	2.1
1	B	189	ALA	2.1
1	A	102	PHE	2.1
1	A	41	ALA	2.0
1	A	270	GLU	2.0
1	A	144	GLY	2.0
1	B	135	ASP	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 monosaccharides 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	CA	B	413	1/1	0.88	0.15	46,46,46,46	0
3	ZN	A	414	1/1	0.93	0.30	50,50,50,50	0
2	CA	A	413	1/1	0.95	0.15	49,49,49,49	0
3	ZN	B	414	1/1	0.95	0.27	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	A	415	1/1	0.97	0.22	52,52,52,52	0
3	ZN	B	415	1/1	0.99	0.16	61,61,61,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.