Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:07 AM GMT

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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

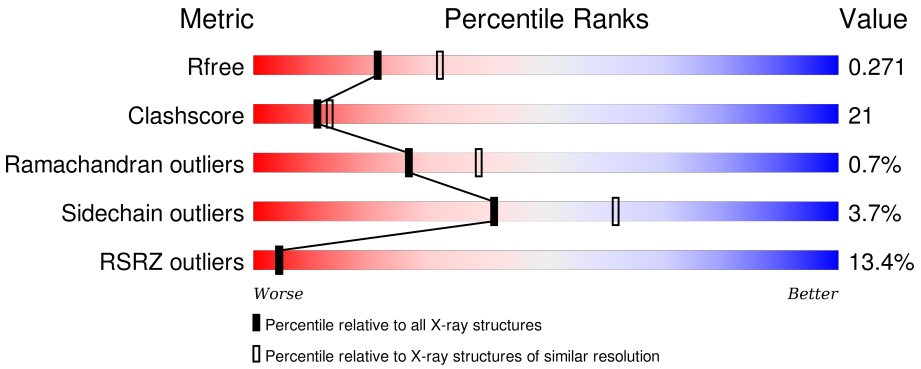
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	12% 57% 22% • 20%
1	B	412	11% 62% 29% • 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	A	414	-	-	-	X
3	ZN	B	414	-	-	-	X

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
1	A	330	Total	C	N	O	S	0	0	0
			2540	1613	435	480	12			
1	B	381	Total	C	N	O	S	0	0	0
			2953	1876	517	549	11			

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

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

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

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

- Molecule 4 is water.

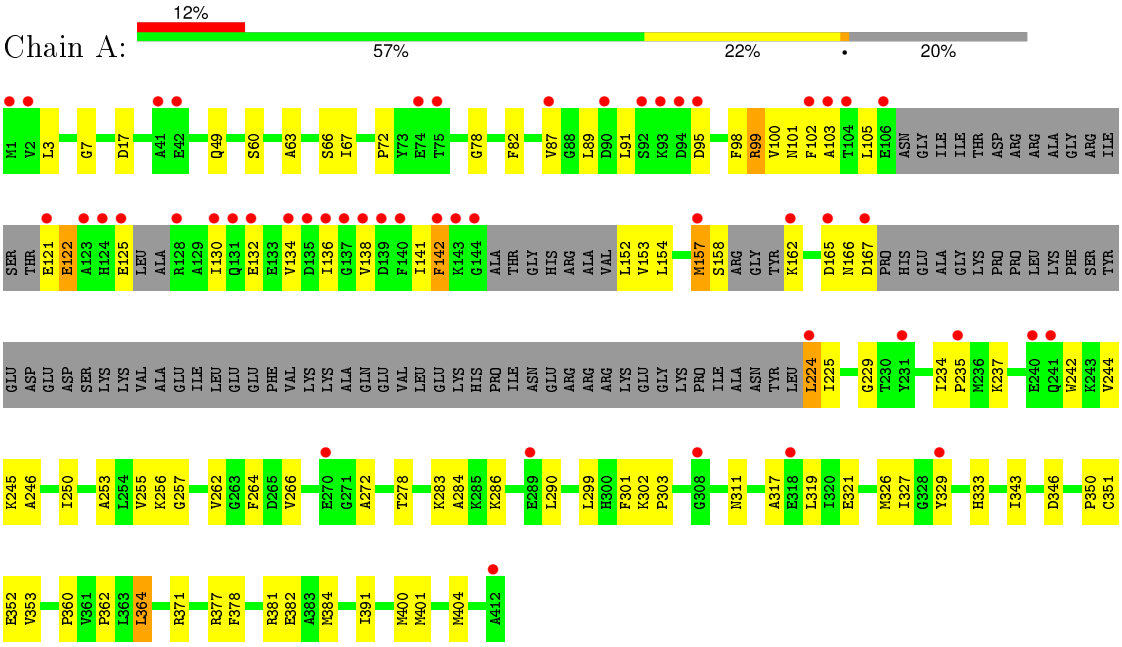
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	106	Total	O	0	0
			106	106		
4	B	115	Total	O	0	0
			115	115		

3 Residue-property plots (i)

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.

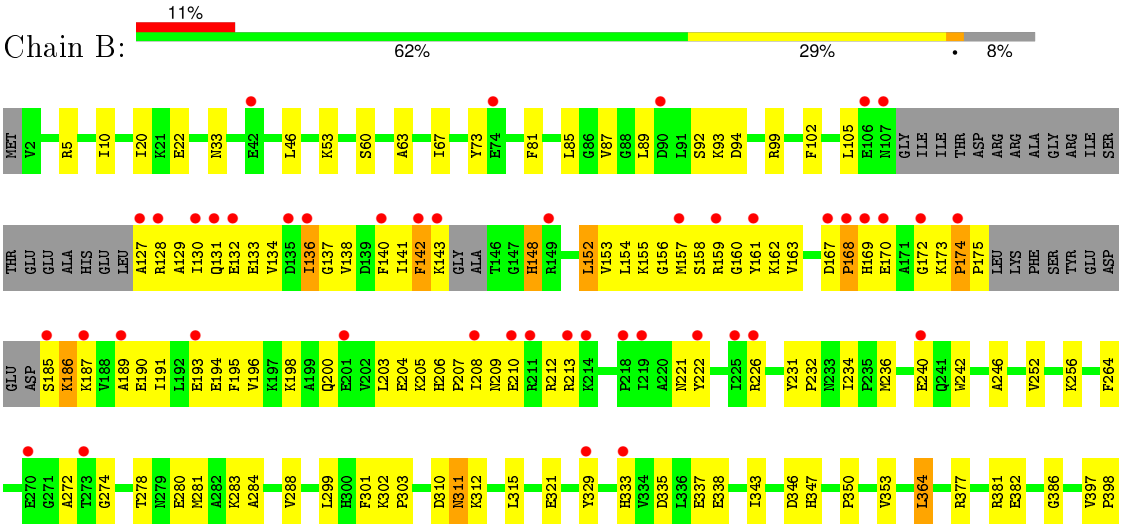
- Molecule 1: 2,3-bisphosphoglycerate-independent phosphoglycerate mutase

Chain A:



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

Chain B:




M401
A412

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	3.80 (at 2.41Å)	Xtriage
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 (5.33%)	DCC
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 70.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 41580 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5720	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: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:A:283:LYS:HB3	1:A:299:LEU:HD11	1.72	0.70
1:B:127:ALA:O	1:B:128:ARG:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ASP:HA	1:B:170:GLU:HG2	1.74	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:400:MET:HB3	1:A:404:MET:HE3	1.79	0.64
1:A:7:GLY:HA3	1:A:404:MET:HE1	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:131:GLN:HG3	1:B:158:SER:HA	1.80	0.64
1:B:105:LEU:HD23	1:B:200:GLN:OE1	1.97	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:HD12	1:B:364:LEU:C	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:HD22	1:B:152:LEU:C	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:242:TRP:O	1:A:244:VAL:HG13	2.06	0.55
1:A:95:ASP:OD1	1:A:167:ASP:HA	2.07	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: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:81:PHE:HE1	1:B:85:LEU:HD11	1.74	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:343:ILE:HB	1:A:364:LEU:HG	1.92	0.52
1:A:301:PHE:CE2	1:A:303:PRO:HG2	2.45	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:381:ARG:O	1:A:384:MET:HB2	2.12	0.50
1:A:91:LEU:HG	1:A:165:ASP:OD2	2.12	0.50
1:B:346:ASP:OD1	1:B:346:ASP:N	2.45	0.50
1:B:10:ILE:HB	1:B:343:ILE:HG12	1.94	0.50
1:A:360:PRO:HD3	4:A:486:HOH:O	2.12	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:B:142:PHE:CE1	1:B:152:LEU:O	2.67	0.48
1:B:138:VAL:HG21	1:B:156:GLY:CA	2.43	0.48
1:A:105:LEU:HD12	1:A:121:GLU:O	2.13	0.48
1:B:154:LEU:HG	1:B:162:LYS:HD2	1.95	0.48
1:B:283:LYS:HB3	1:B:299:LEU:HD11	1.94	0.47
1:A:250:ILE:HD13	1:A:255:VAL:HG12	1.96	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:B:170:GLU:O	1:B:173:LYS:HB3	2.14	0.47
1:A:346:ASP:OD1	1:A:346:ASP:N	2.43	0.47
1:A:256:LYS:HE3	1:A:266:VAL:CG1	2.45	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:B:157:MET:HG3	1:B:158:SER:N	2.26	0.45
1:A:286:LYS:HE3	1:A:290:LEU:HD21	1.98	0.45
1:B:350:PRO:HB2	1:B:353:VAL:HG23	1.98	0.45
1:B:142:PHE:CE2	1:B:153:VAL:HG13	2.51	0.45
1:B:138:VAL:HG22	1:B:162:LYS:HD2	1.98	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:100:VAL:CG1	1:A:162:LYS:HG3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:98:PHE:HE2	1:A:166:ASN:HD22	1.64	0.45
1:A:246:ALA:HB1	1:A:264:PHE:CE2	2.52	0.45
1:A:132:GLU:CD	1:A:132:GLU:H	2.21	0.44
1:A:152:LEU:HD12	1:A:152:LEU:C	2.37	0.44
1:B:81:PHE:CE1	1:B:85:LEU:HD11	2.52	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: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:148:HIS:ND1	1:B:148:HIS:N	2.56	0.44
1:B:142:PHE:HE1	1:B:152:LEU:O	2.00	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:B:136:ILE:O	1:B:136:ILE:HD12	2.17	0.44
1:A:242:TRP:CE3	1:A:401:MET:HG3	2.53	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:B:329:TYR:CZ	1:B:333:HIS:CE1	3.06	0.43
1:A:377:ARG:NH1	1:B:377:ARG:HD3	2.33	0.43
1:B:397:VAL:HB	1:B:398:PRO:HD3	2.00	0.43
1:B:234:ILE:HG13	1:B:234:ILE:O	2.18	0.43
1:B:136:ILE:CG2	1:B:137:GLY:H	2.31	0.43
1:B:92:SER:HB2	1:B:94:ASP:OD1	2.18	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: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:B:46:LEU:O	1:B:386:GLY:HA3	2.19	0.42
1:A:245:LYS:HE3	1:A:245:LYS:HB3	1.78	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:HD12	1:A:91:LEU:N	2.35	0.41
1:B:154:LEU:HD13	1:B:195:PHE:HZ	1.85	0.41
1:A:303:PRO:HB2	1:A:319:LEU:HD22	2.02	0.41
1:A:234:ILE:O	1:A:234:ILE:HG13	2.18	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:B:142:PHE:CZ	1:B:153:VAL:HG13	2.56	0.41
1:A:362:PRO:HB2	1:A:378:PHE:CE1	2.55	0.41
1:A:49:GLN:HA	1:A:391:ILE:O	2.19	0.41
1:A:301:PHE:CZ	1:A:303:PRO:HG2	2.56	0.41
1:A:66:SER:OG	1:A:72:PRO:CG	2.68	0.41
1:A:17:ASP:CG	1:A:350:PRO:HA	2.41	0.41
1:B:209:ASN:O	1:B:212:ARG:HB2	2.21	0.41
1:A:103:ALA:HB2	1:A:125:GLU:HA	1.97	0.41
1:B:301:PHE:CE2	1:B:303:PRO:HG2	2.56	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:207:PRO:CA	1:B:210:GLU:HB2	2.48	0.40
1:B:134:VAL:HG11	1:B:161:TYR:O	2.21	0.40
1:B:134:VAL:O	1:B:138:VAL:CG2	2.68	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%)	46 63
1	B	373/412 (90%)	354 (95%)	15 (4%)	4 (1%)	17 25
All	All	691/824 (84%)	654 (95%)	32 (5%)	5 (1%)	26 38

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%)	40 60
1	B	308/333 (92%)	297 (96%)	11 (4%)	42 63
All	All	573/666 (86%)	552 (96%)	21 (4%)	41 62

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

Some 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 carbohydrates 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^{th} 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	330/412 (80%)	0.68	49 (14%)	3	3	34, 52, 77, 91	0
1	B	381/412 (92%)	0.60	46 (12%)	6	5	34, 53, 76, 88	0
All	All	711/824 (86%)	0.64	95 (13%)	4	4	34, 53, 77, 91	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	PHE	13.4
1	B	168	PRO	10.2
1	B	140	PHE	7.7
1	A	1	MET	7.7
1	A	412	ALA	6.6
1	B	107	ASN	6.3
1	B	157	MET	6.2
1	B	130	ILE	5.8
1	A	131	GLN	5.2
1	A	130	ILE	5.0
1	B	412	ALA	4.9
1	A	157	MET	4.8
1	A	135	ASP	4.8
1	B	159	ARG	4.7
1	B	149	ARG	4.7
1	B	210	GLU	4.7
1	A	94	ASP	4.4
1	A	128	ARG	4.4
1	A	90	ASP	4.3
1	B	131	GLN	4.2
1	B	211	ARG	4.1
1	A	138	VAL	4.1
1	A	162	LYS	3.9
1	A	74	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	167	ASP	3.8
1	A	42	GLU	3.8
1	A	143	LYS	3.7
1	A	136	ILE	3.6
1	A	103	ALA	3.6
1	B	128	ARG	3.6
1	A	289	GLU	3.4
1	A	134	VAL	3.4
1	B	106	GLU	3.4
1	A	121	GLU	3.4
1	B	193	GLU	3.4
1	A	139	ASP	3.4
1	A	142	PHE	3.3
1	A	93	LYS	3.3
1	B	42	GLU	3.3
1	B	273	THR	3.2
1	B	132	GLU	3.1
1	A	231	TYR	3.1
1	B	208	ILE	3.0
1	B	214	LYS	2.9
1	B	225	ILE	2.9
1	A	165	ASP	2.8
1	A	132	GLU	2.7
1	A	125	GLU	2.7
1	A	75	THR	2.7
1	A	318	GLU	2.7
1	B	329	TYR	2.7
1	B	143	LYS	2.7
1	B	213	ARG	2.6
1	B	201	GLU	2.6
1	B	127	ALA	2.6
1	B	142	PHE	2.6
1	A	235	PRO	2.6
1	A	329	TYR	2.6
1	B	90	ASP	2.5
1	A	87	VAL	2.5
1	A	224	LEU	2.5
1	B	185	SER	2.5
1	B	170	GLU	2.5
1	B	161	TYR	2.5
1	A	2	VAL	2.5
1	B	218	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	333	HIS	2.5
1	B	222	TYR	2.5
1	A	308	GLY	2.4
1	B	187	LYS	2.4
1	A	104	THR	2.3
1	A	137	GLY	2.3
1	B	167	ASP	2.3
1	B	226	ARG	2.3
1	B	172	GLY	2.3
1	B	189	ALA	2.3
1	A	241	GLN	2.2
1	B	270	GLU	2.2
1	A	92	SER	2.2
1	A	102	PHE	2.2
1	A	124	HIS	2.2
1	B	136	ILE	2.2
1	A	144	GLY	2.2
1	B	135	ASP	2.1
1	A	270	GLU	2.1
1	A	41	ALA	2.1
1	B	174	PRO	2.1
1	A	95	ASP	2.1
1	A	240	GLU	2.1
1	B	74	GLU	2.0
1	A	123	ALA	2.0
1	A	106	GLU	2.0
1	B	169	HIS	2.0
1	B	219	ILE	2.0
1	B	240	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 carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	A	414	1/1	0.93	0.30	5.64	50,50,50,50	0
3	ZN	B	414	1/1	0.95	0.27	3.67	55,55,55,55	0
3	ZN	A	415	1/1	0.97	0.22	1.94	52,52,52,52	0
2	CA	B	413	1/1	0.88	0.15	-0.45	46,46,46,46	0
3	ZN	B	415	1/1	0.99	0.16	-0.65	61,61,61,61	0
2	CA	A	413	1/1	0.95	0.15	-1.07	49,49,49,49	0

6.5 Other polymers

There are no such residues in this entry.