



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:25 AM GMT

PDB ID : 3IDD
Title : Cofactor-Independent Phosphoglycerate Mutase from *Thermoplasma acidophilum* DSM 1728
Authors : Joachimiak, A.; Duke, N.E.C.; Marshall, N.; Buck, K.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2009-07-20
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

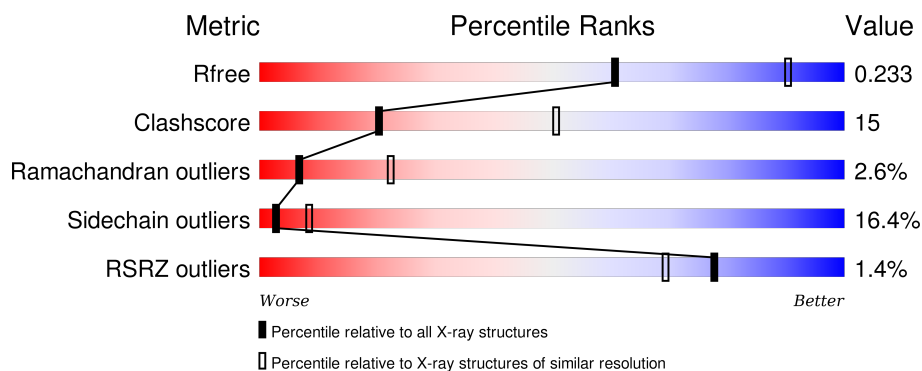
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

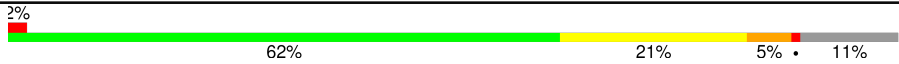

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	407	 2% 62% 21% 5% 11%
1	B	407	 1% 57% 26% 6% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5667 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	364	Total	C	N	O	S	Se	0	0	0
			2806	1752	507	532	3	12			
1	B	361	Total	C	N	O	S	Se	0	0	0
			2777	1735	502	524	3	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9HL27
A	-1	ASN	-	expression tag	UNP Q9HL27
A	0	ALA	-	expression tag	UNP Q9HL27
B	-2	SER	-	expression tag	UNP Q9HL27
B	-1	ASN	-	expression tag	UNP Q9HL27
B	0	ALA	-	expression tag	UNP Q9HL27

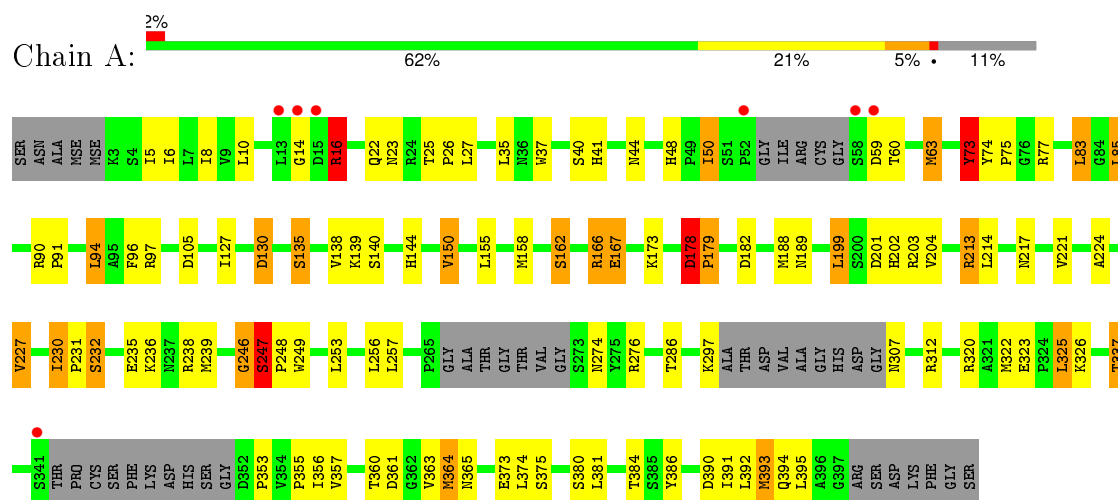
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	50	Total	O	0	0
			50	50		
2	B	34	Total	O	0	0
			34	34		

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: 2,3-bisphosphoglycerate-independent phosphoglycerate mutase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.61Å 136.74Å 63.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.36 – 2.80 51.50 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (74.36-2.80) 99.0 (51.50-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.230 , 0.311 0.235 , 0.233	Depositor DCC
R_{free} test set	1005 reflections (5.44%)	DCC
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 32.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 24160 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5667	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.67	0/2846	0.79	1/3826 (0.0%)
1	B	0.64	0/2815	0.76	0/3782
All	All	0.65	0/5661	0.78	1/7608 (0.0%)

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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	246	GLY	N-CA-C	-5.58	99.16	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	73	TYR	Peptide

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	2806	0	2788	72	0
1	B	2777	0	2766	92	0
2	A	50	0	0	3	0
2	B	34	0	0	1	0
All	All	5667	0	5554	162	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 15.

All (162) 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:B:352:ASP:HB3	1:B:353:PRO:CD	1.44	1.41
1:B:352:ASP:CB	1:B:353:PRO:HD3	1.60	1.30
1:A:150:VAL:HG11	1:A:188:MSE:HE1	1.17	1.15
1:B:297:LYS:HD3	1:B:298:ALA:H	1.13	1.13
1:B:245:VAL:HG11	1:B:250:LEU:HB3	1.34	1.04
1:A:246:GLY:O	1:A:247:SER:HB3	1.61	0.99
1:B:176:PRO:O	1:B:177:THR:HB	1.71	0.89
1:B:188:MSE:HA	1:B:188:MSE:CE	2.02	0.89
1:A:232:SER:HB2	1:A:235:GLU:H	1.37	0.88
1:B:297:LYS:CD	1:B:298:ALA:H	1.86	0.88
1:B:246:GLY:O	1:B:247:SER:HB3	1.72	0.88
1:B:322:MSE:HG3	1:B:325:LEU:HD23	1.56	0.87
1:B:136:PHE:HE2	1:B:188:MSE:HE1	1.46	0.79
1:B:352:ASP:CB	1:B:353:PRO:CD	2.30	0.78
1:A:150:VAL:CG1	1:A:188:MSE:HE1	2.09	0.78
1:B:352:ASP:HB3	1:B:353:PRO:HD2	1.62	0.74
1:B:296:ILE:HG23	1:B:297:LYS:N	2.01	0.74
1:A:213:ARG:HH11	1:A:213:ARG:CG	2.01	0.74
1:B:64:SER:HB2	1:B:385:SER:HB3	1.70	0.73
1:B:352:ASP:HB3	1:B:353:PRO:HD3	0.75	0.73
1:B:297:LYS:HD3	1:B:298:ALA:N	1.97	0.72
1:B:188:MSE:HA	1:B:188:MSE:HE3	1.71	0.72
1:A:74:TYR:CD2	1:A:75:PRO:HD2	2.26	0.70
1:A:360:THR:O	1:A:363:VAL:HG12	1.92	0.70
1:A:162:SER:HB3	1:A:221:VAL:HG22	1.73	0.70
1:B:13:LEU:HD13	1:B:27:LEU:HD22	1.73	0.69
1:B:384:THR:HG22	1:B:386:TYR:H	1.57	0.69
1:B:142:VAL:HG12	1:B:143:GLU:HG3	1.75	0.69
1:A:90:ARG:NH1	2:A:439:HOH:O	2.26	0.68
1:B:296:ILE:CG2	1:B:297:LYS:N	2.57	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:MSE:HA	1:B:188:MSE:HE2	1.75	0.68
1:A:395:LEU:O	1:A:395:LEU:HD23	1.95	0.67
1:B:127:ILE:HG21	1:B:199:LEU:HD13	1.76	0.67
1:B:90:ARG:NH2	1:B:256:LEU:O	2.28	0.67
1:B:251:LYS:HD3	1:B:255:ARG:HH12	1.60	0.67
1:B:144:HIS:CD2	1:B:144:HIS:H	2.13	0.67
1:B:158:MSE:O	1:B:176:PRO:O	2.13	0.66
1:B:60:THR:HG22	1:B:63:MSE:H	1.61	0.65
1:B:238:ARG:HH11	1:B:238:ARG:CG	2.08	0.65
1:A:150:VAL:HG11	1:A:188:MSE:CE	2.11	0.64
1:A:91:PRO:HA	1:A:227:VAL:HG22	1.80	0.64
1:A:166:ARG:HG3	1:A:166:ARG:HH11	1.63	0.63
1:B:296:ILE:CG2	1:B:297:LYS:H	2.12	0.62
1:B:246:GLY:O	1:B:247:SER:CB	2.46	0.62
1:B:74:TYR:CD1	1:B:75:PRO:HD2	2.34	0.62
1:B:196:ARG:CD	1:B:218:GLU:OE2	2.48	0.61
1:B:188:MSE:CA	1:B:188:MSE:HE3	2.29	0.61
1:B:91:PRO:HB3	1:B:228:PRO:O	2.01	0.60
1:B:238:ARG:NH1	1:B:238:ARG:HG2	2.15	0.60
1:B:323:GLU:N	1:B:324:PRO:HD2	2.15	0.60
1:A:179:PRO:HA	1:A:182:ASP:OD1	2.02	0.60
1:B:283:VAL:O	1:B:286:THR:HB	2.02	0.60
1:B:44:ASN:N	1:B:366:ASP:OD2	2.30	0.59
1:A:213:ARG:HH11	1:A:213:ARG:HG2	1.68	0.58
1:A:158:MSE:HG3	1:A:178:ASP:OD1	2.04	0.58
1:A:355:PRO:HG3	1:A:373:GLU:HA	1.85	0.58
1:A:232:SER:HB2	1:A:235:GLU:HB2	1.85	0.58
1:A:363:VAL:O	1:A:364:MSE:HB2	2.04	0.58
1:B:238:ARG:HH11	1:B:238:ARG:HG2	1.68	0.57
1:A:96:PHE:CE2	1:A:224:ALA:HB2	2.40	0.56
1:B:155:LEU:O	1:B:226:LYS:NZ	2.37	0.56
1:B:5:ILE:HG21	1:B:392:LEU:HD13	1.86	0.56
1:A:6:ILE:HD11	1:A:286:THR:HG21	1.88	0.56
1:A:202:HIS:ND1	1:A:204:VAL:HG13	2.21	0.56
1:B:196:ARG:HD2	1:B:218:GLU:OE2	2.06	0.56
1:A:130:ASP:CB	1:B:331:HIS:CD2	2.89	0.56
1:A:40:SER:O	1:A:365:ASN:CG	2.45	0.56
1:A:144:HIS:CD2	1:A:144:HIS:H	2.25	0.55
1:B:136:PHE:HE2	1:B:188:MSE:CE	2.18	0.55
1:A:16:ARG:HE	1:A:16:ARG:HA	1.71	0.55
1:B:251:LYS:HD3	1:B:255:ARG:NH1	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LEU:HB2	1:B:319:ASP:OD2	2.08	0.54
1:B:356:ILE:HD13	1:B:383:ILE:HD11	1.89	0.54
1:A:246:GLY:O	1:A:247:SER:CB	2.41	0.54
1:B:176:PRO:O	1:B:177:THR:CB	2.46	0.53
1:B:296:ILE:HG23	1:B:297:LYS:HG3	1.91	0.53
1:A:337:THR:HG23	1:A:356:ILE:HB	1.91	0.53
1:B:119:GLY:HA3	1:B:204:VAL:HG11	1.91	0.52
1:A:230:ILE:O	1:A:230:ILE:HG23	2.08	0.52
1:B:230:ILE:O	1:B:230:ILE:HG22	2.08	0.52
1:B:127:ILE:CG2	1:B:199:LEU:HD13	2.40	0.52
1:A:130:ASP:HB3	1:B:331:HIS:CD2	2.45	0.52
1:A:166:ARG:HH11	1:A:166:ARG:CG	2.22	0.52
1:B:178:ASP:C	1:B:178:ASP:OD1	2.48	0.52
1:A:320:ARG:NH2	2:A:450:HOH:O	2.42	0.51
1:A:63:MSE:HE3	1:A:253:LEU:HD11	1.92	0.51
1:B:296:ILE:HG23	1:B:297:LYS:H	1.71	0.51
1:A:25:THR:HG22	1:A:27:LEU:H	1.76	0.51
1:A:5:ILE:HG23	1:A:392:LEU:HD22	1.94	0.50
1:B:328:ILE:HG13	1:B:334:ILE:HD11	1.94	0.49
1:B:89:ILE:HG13	1:B:227:VAL:HG21	1.94	0.49
1:B:25:THR:OG1	1:B:28:GLN:HG3	2.12	0.49
1:A:213:ARG:HG3	1:A:213:ARG:HH11	1.75	0.49
1:B:83:LEU:HD13	1:B:89:ILE:HD12	1.95	0.48
1:B:108:ILE:HD11	1:B:171:PRO:HG3	1.96	0.48
1:A:232:SER:HB2	1:A:235:GLU:N	2.19	0.48
1:A:85:LEU:O	1:A:139:LYS:HE2	2.14	0.48
1:B:325:LEU:HD12	1:B:328:ILE:HD11	1.96	0.48
1:A:391:ILE:O	1:A:395:LEU:HB2	2.14	0.47
1:B:258:ARG:HG2	1:B:258:ARG:HH11	1.80	0.47
1:A:247:SER:HB2	1:A:297:LYS:NZ	2.29	0.47
1:A:363:VAL:O	1:A:364:MSE:CB	2.62	0.47
1:B:83:LEU:CD1	1:B:89:ILE:CD1	2.93	0.47
1:A:322:MSE:HG2	1:A:325:LEU:HD22	1.97	0.47
1:B:69:ASP:HB3	1:B:72:VAL:HG13	1.97	0.46
1:A:307:ASN:OD1	1:A:307:ASN:C	2.54	0.46
1:B:136:PHE:CE2	1:B:188:MSE:HE1	2.37	0.46
1:A:73:TYR:HB2	1:A:230:ILE:HD12	1.96	0.46
1:A:135:SER:O	1:A:150:VAL:HA	2.15	0.46
1:B:13:LEU:HD21	1:B:315:ILE:HD11	1.97	0.46
1:A:22:GLN:NE2	2:A:405:HOH:O	2.45	0.46
1:B:120:ASN:HA	1:B:123:LEU:HD12	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:HD12	1:A:83:LEU:HA	1.76	0.45
1:A:77:ARG:HB2	1:A:97:ARG:HH11	1.79	0.45
1:A:50:ILE:HD13	1:A:50:ILE:HA	1.73	0.45
1:A:202:HIS:CE1	1:A:204:VAL:HG13	2.51	0.45
1:B:8:ILE:HG12	1:B:294:VAL:HG13	1.99	0.45
1:B:70:PRO:O	1:B:71:LYS:CB	2.64	0.45
1:A:6:ILE:HD11	1:A:286:THR:CG2	2.47	0.45
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.88	0.44
1:A:127:ILE:HD12	1:A:138:VAL:HG21	1.98	0.44
1:B:246:GLY:O	2:B:413:HOH:O	2.21	0.44
1:A:25:THR:HG22	1:A:26:PRO:N	2.32	0.44
1:A:393:MSE:HE2	1:A:394:GLN:HG3	1.99	0.44
1:B:352:ASP:CG	1:B:353:PRO:HD3	2.32	0.44
1:A:213:ARG:NH1	1:A:213:ARG:CG	2.70	0.44
1:B:264:VAL:HG12	1:B:274:ASN:ND2	2.32	0.44
1:A:94:LEU:HD13	1:A:96:PHE:CE1	2.53	0.44
1:A:386:TYR:C	1:A:386:TYR:CD2	2.91	0.44
1:B:83:LEU:HD11	1:B:89:ILE:CD1	2.48	0.43
1:A:231:PRO:HB3	1:A:235:GLU:HB3	2.01	0.43
1:B:330:ASP:OD2	1:B:331:HIS:CD2	2.72	0.43
1:B:8:ILE:HD13	1:B:322:MSE:HE2	1.99	0.43
1:B:115:ARG:HD3	1:B:143:GLU:OE1	2.18	0.43
1:A:16:ARG:HA	1:A:16:ARG:NE	2.32	0.43
1:B:73:TYR:CE2	1:B:231:PRO:HD3	2.54	0.43
1:B:296:ILE:HD12	1:B:296:ILE:HA	1.84	0.42
1:B:196:ARG:NH1	1:B:218:GLU:OE2	2.53	0.42
1:A:173:LYS:HG2	1:A:189:ASN:ND2	2.35	0.42
1:B:193:GLU:O	1:B:196:ARG:HB3	2.20	0.42
1:B:199:LEU:HB3	1:B:217:ASN:HA	2.01	0.42
1:B:33:PRO:HD2	1:B:319:ASP:OD1	2.20	0.42
1:A:37:TRP:CE2	1:A:41:HIS:CD2	3.07	0.42
1:A:48:HIS:CD2	1:A:353:PRO:HB3	2.55	0.42
1:A:357:VAL:O	1:A:357:VAL:HG13	2.20	0.42
1:A:360:THR:HG22	1:A:395:LEU:HD21	2.01	0.42
1:A:230:ILE:O	1:A:230:ILE:CG2	2.68	0.42
1:A:360:THR:O	1:A:363:VAL:CG1	2.66	0.41
1:A:247:SER:HA	1:A:248:PRO:HD2	1.83	0.41
1:A:199:LEU:HB3	1:A:217:ASN:HA	2.02	0.41
1:B:114:GLY:O	1:B:115:ARG:HB2	2.21	0.41
1:B:366:ASP:OD1	1:B:380:SER:HB3	2.20	0.41
1:B:131:MSE:HG2	1:B:136:PHE:HE1	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ARG:HD2	1:B:163:ASP:OD1	2.20	0.41
1:B:82:ALA:O	1:B:87:MSE:HB3	2.21	0.41
1:A:390:ASP:O	1:A:394:GLN:HB2	2.21	0.41
1:B:92:GLY:HA2	1:B:226:LYS:HE3	2.03	0.41
1:A:44:ASN:OD1	1:A:357:VAL:HG23	2.21	0.41
1:B:111:ARG:NH1	1:B:163:ASP:OD2	2.53	0.41
1:B:255:ARG:CZ	1:B:261:VAL:HG21	2.50	0.40
1:A:167:GLU:H	1:A:167:GLU:HG2	1.32	0.40
1:B:218:GLU:HB3	1:B:220:LEU:HD13	2.03	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	354/407 (87%)	317 (90%)	27 (8%)	10 (3%)	6	21
1	B	351/407 (86%)	319 (91%)	24 (7%)	8 (2%)	8	26
All	All	705/814 (87%)	636 (90%)	51 (7%)	18 (3%)	7	22

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	MSE
1	B	247	SER
1	A	247	SER
1	B	232	SER
1	B	385	SER
1	A	14	GLY
1	A	232	SER
1	B	177	THR
1	A	16	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	105	ASP
1	A	179	PRO
1	A	230	ILE
1	B	71	LYS
1	B	87	MSE
1	B	230	ILE
1	B	296	ILE
1	A	73	TYR
1	A	178	ASP

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	308/324 (95%)	259 (84%)	49 (16%)	3	9
1	B	302/324 (93%)	251 (83%)	51 (17%)	2	7
All	All	610/648 (94%)	510 (84%)	100 (16%)	3	8

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	10	LEU
1	A	16	ARG
1	A	23	ASN
1	A	35	LEU
1	A	50	ILE
1	A	59	ASP
1	A	60	THR
1	A	63	MSE
1	A	73	TYR
1	A	83	LEU
1	A	85	LEU
1	A	94	LEU
1	A	130	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	135	SER
1	A	140	SER
1	A	150	VAL
1	A	155	LEU
1	A	162	SER
1	A	166	ARG
1	A	167	GLU
1	A	178	ASP
1	A	199	LEU
1	A	201	ASP
1	A	203	ARG
1	A	213	ARG
1	A	214	LEU
1	A	227	VAL
1	A	236	LYS
1	A	238	ARG
1	A	239	MSE
1	A	247	SER
1	A	249	TRP
1	A	256	LEU
1	A	257	LEU
1	A	274	ASN
1	A	276	ARG
1	A	312	ARG
1	A	323	GLU
1	A	325	LEU
1	A	326	LYS
1	A	337	THR
1	A	361	ASP
1	A	374	LEU
1	A	375	SER
1	A	380	SER
1	A	381	LEU
1	A	384	THR
1	A	393	MSE
1	B	2	MSE
1	B	28	GLN
1	B	35	LEU
1	B	38	LEU
1	B	40	SER
1	B	64	SER
1	B	72	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	77	ARG
1	B	83	LEU
1	B	85	LEU
1	B	87	MSE
1	B	89	ILE
1	B	117	ASN
1	B	118	LYS
1	B	135	SER
1	B	137	ARG
1	B	140	SER
1	B	173	LYS
1	B	178	ASP
1	B	182	ASP
1	B	186	GLU
1	B	188	MSE
1	B	192	LEU
1	B	197	ARG
1	B	199	LEU
1	B	203	ARG
1	B	213	ARG
1	B	232	SER
1	B	238	ARG
1	B	247	SER
1	B	260	ASP
1	B	276	ARG
1	B	281	LYS
1	B	286	THR
1	B	294	VAL
1	B	297	LYS
1	B	312	ARG
1	B	320	ARG
1	B	322	MSE
1	B	325	LEU
1	B	327	SER
1	B	339	ASP
1	B	361	ASP
1	B	366	ASP
1	B	370	LEU
1	B	381	LEU
1	B	382	ARG
1	B	386	TYR
1	B	393	MSE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	394	GLN
1	B	395	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	23	ASN
1	A	41	HIS
1	A	48	HIS
1	A	144	HIS
1	A	274	ASN
1	A	365	ASN
1	A	387	ASN
1	B	144	HIS
1	B	237	ASN
1	B	331	HIS
1	B	394	GLN

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 ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	352/407 (86%)	-0.33	7 (1%) 68 58	15, 31, 50, 68	0
1	B	348/407 (85%)	-0.31	3 (0%) 85 79	16, 35, 52, 69	0
All	All	700/814 (85%)	-0.32	10 (1%) 78 69	15, 32, 52, 69	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	GLY	4.5
1	A	58	SER	4.1
1	B	266	GLY	3.8
1	B	267	ALA	3.4
1	A	15	ASP	2.9
1	A	59	ASP	2.9
1	A	13	LEU	2.6
1	A	341	SER	2.6
1	B	298	ALA	2.6
1	A	52	PRO	2.4

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.