



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:52 AM UTC

PDB ID : 3IDD / pdb_00003idd
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

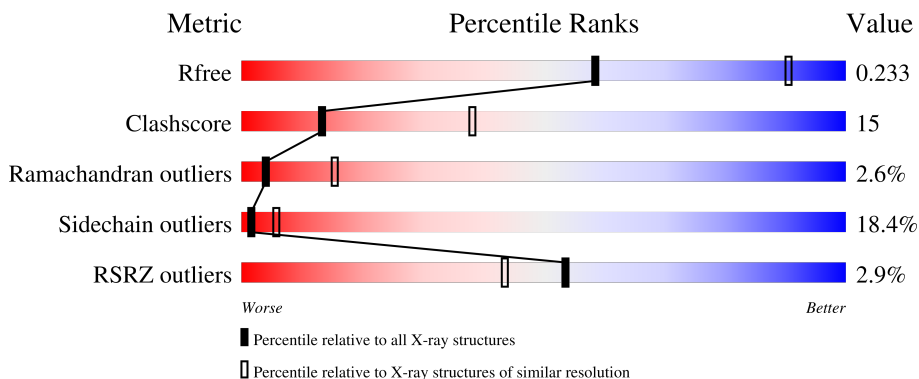
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	407	 3% 60% 22% 6% • 11%
1	B	407	 2% 57% 25% 6% • 11%

2 Entry composition [i](#)

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	
			Total	C	N	O	S				Se
1	A	364	2806	1752	507	532	3	12	0	0	0
1	B	361	2777	1735	502	524	3	13	0	0	0

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

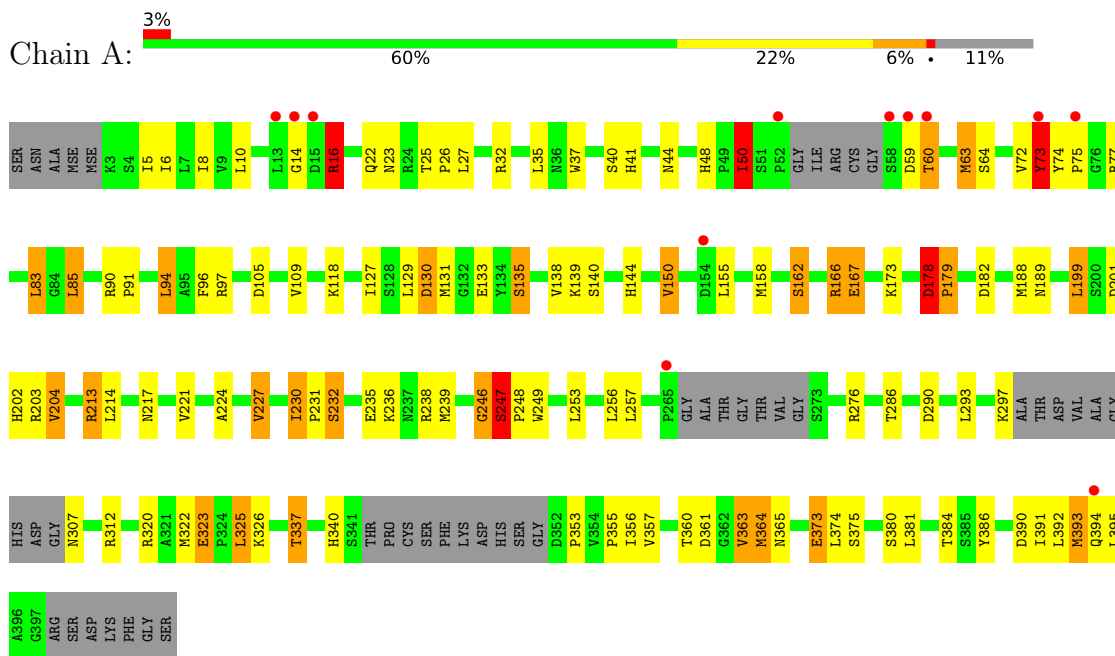
- Molecule 2 is water.

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

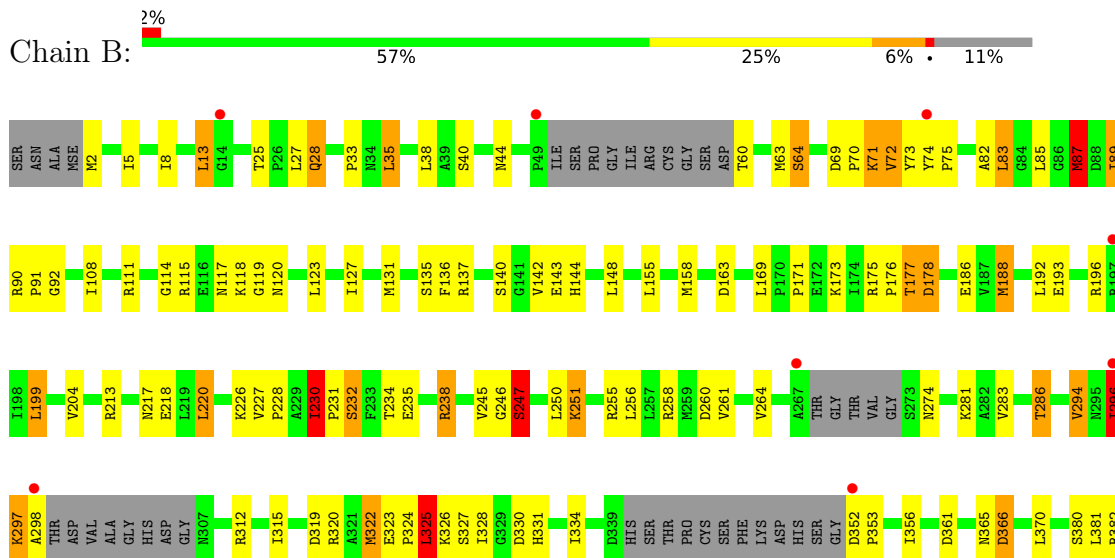
3 Residue-property plots i

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



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



I383	L392	ARG
T384	M393	SER
S385	Q394	ASP
Y386	L395	LYS
	A396	PHE
	G397	GLY
		SER

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 74.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (74.36-2.80) 99.3 (74.36-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.230 , 0.311 0.235 , 0.233	Depositor DCC
R_{free} test set	1226 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtrriage
Anisotropy	0.123	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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	0.82	0/2846	1.06	8/3826 (0.2%)
1	B	0.80	0/2815	1.04	7/3782 (0.2%)
All	All	0.81	0/5661	1.05	15/7608 (0.2%)

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 (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	GLY	N-CA-C	-7.11	99.16	112.10
1	A	60	THR	N-CA-C	7.11	120.90	108.75
1	A	178	ASP	CA-C-N	7.09	128.71	119.84
1	A	178	ASP	C-N-CA	7.09	128.71	119.84
1	B	365	ASN	CA-C-N	6.66	130.10	120.38
1	B	365	ASN	C-N-CA	6.66	130.10	120.38
1	A	340	HIS	N-CA-C	6.56	120.22	109.72
1	A	323	GLU	CA-C-N	-6.04	112.64	119.28
1	A	323	GLU	C-N-CA	-6.04	112.64	119.28
1	B	325	LEU	N-CA-C	5.68	119.02	111.75
1	B	169	LEU	CA-C-N	-5.44	114.77	120.38
1	B	169	LEU	C-N-CA	-5.44	114.77	120.38
1	B	175	ARG	CA-C-N	5.17	126.30	119.84
1	B	175	ARG	C-N-CA	5.17	126.30	119.84
1	A	50	ILE	N-CA-C	5.12	117.01	109.63

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2806	0	2788	73	0
1	B	2777	0	2766	94	0
2	A	50	0	0	3	0
2	B	34	0	0	1	0
All	All	5667	0	5554	165	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 (165) 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:296:ILE:HG23	1:B:297:LYS:N	2.01	0.74
1:B:352:ASP:HB3	1:B:353:PRO:HD2	1.62	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:142:VAL:HG12	1:B:143:GLU:HG3	1.75	0.69
1:B:384:THR:HG22	1:B:386:TYR:H	1.57	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
1:B:188:MSE:HA	1:B:188:MSE:HE2	1.75	0.68
1:A:395:LEU:HD23	1:A:395:LEU:O	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:H	1:B:144:HIS:CD2	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:74:TYR:CD1	1:B:75:PRO:HD2	2.34	0.62
1:B:246:GLY:O	1:B:247:SER:CB	2.46	0.62
1:B:196:ARG:CD	1:B:218:GLU:OE2	2.48	0.61
1:B:188:MSE:HE3	1:B:188:MSE:CA	2.29	0.61
1:B:91:PRO:HB3	1:B:228:PRO:O	2.01	0.60
1:A:40:SER:O	1:A:365:ASN:CG	2.45	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:158:MSE:HG3	1:A:178:ASP:OD1	2.04	0.58
1:A:213:ARG:HH11	1:A:213:ARG:HG2	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:178:ASP:C	1:B:178:ASP:OD1	2.48	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:A:130:ASP:CB	1:B:331:HIS:CD2	2.89	0.56
1:B:196:ARG:HD2	1:B:218:GLU:OE2	2.06	0.56
1:A:144:HIS:CD2	1:A:144:HIS:H	2.25	0.55
1:A:16:ARG:HE	1:A:16:ARG:HA	1.71	0.55
1:B:136:PHE:HE2	1:B:188:MSE:CE	2.18	0.55
1:B:251:LYS:HD3	1:B:255:ARG:NH1	2.22	0.54
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:HG22	1:B:230:ILE:O	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:A:63:MSE:HE3	1:A:253:LEU:HD11	1.92	0.51
1:A:320:ARG:NH2	2:A:450:HOH:O	2.42	0.51
1:A:307:ASN:C	1:A:307:ASN:OD1	2.54	0.51
1:A:25:THR:HG22	1:A:27:LEU:H	1.76	0.51
1:B:296:ILE:HG23	1:B:297:LYS:H	1.71	0.51
1:A:5:ILE:HG23	1:A:392:LEU:HD22	1.94	0.50
1:B:89:ILE:HG13	1:B:227:VAL:HG21	1.94	0.49
1:B:328:ILE:HG13	1:B:334:ILE:HD11	1.94	0.49
1:B:25:THR:OG1	1:B:28:GLN:HG3	2.12	0.49
1:A:213:ARG:HH11	1:A:213:ARG:HG3	1.75	0.49
1:B:352:ASP:CG	1:B:353:PRO:HD3	2.32	0.48
1:B:83:LEU:HD13	1:B:89:ILE:HD12	1.95	0.48
1:A:386:TYR:CD2	1:A:386:TYR:C	2.91	0.48
1:B:108:ILE:HD11	1:B:171:PRO:HG3	1.96	0.48
1:A:85:LEU:O	1:A:139:LYS:HE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:SER:HB2	1:A:235:GLU:N	2.19	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:A:322:MSE:HG2	1:A:325:LEU:HD22	1.97	0.47
1:B:83:LEU:CD1	1:B:89:ILE:CD1	2.93	0.47
1:B:69:ASP:HB3	1:B:72:VAL:HG13	1.97	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:A:83:LEU:HD12	1:A:83:LEU:HA	1.76	0.45
1:B:120:ASN:HA	1:B:123:LEU:HD12	1.97	0.45
1:A:50:ILE:HD13	1:A:50:ILE:HA	1.73	0.45
1:A:77:ARG:HB2	1:A:97:ARG:HH11	1.79	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:A:25:THR:HG22	1:A:26:PRO:N	2.32	0.44
1:B:246:GLY:O	2:B:413:HOH:O	2.21	0.44
1:A:393:MSE:HE2	1:A:394:GLN:HG3	1.99	0.44
1:A:373:GLU:H	1:A:373:GLU:CD	2.26	0.44
1:A:213:ARG:CG	1:A:213:ARG:NH1	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: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:A:16:ARG:HA	1:A:16:ARG:NE	2.32	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:GLU:O	1:B:196:ARG:HB3	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:B:33:PRO:HD2	1:B:319:ASP:OD1	2.20	0.42
1:B:199:LEU:HB3	1:B:217:ASN:HA	2.01	0.42
1:B:384:THR:O	1:B:385:SER:C	2.62	0.42
1:A:357:VAL:O	1:A:357:VAL:HG13	2.20	0.42
1:A:230:ILE:O	1:A:230:ILE:CG2	2.68	0.42
1:A:360:THR:HG22	1:A:395:LEU:HD21	2.01	0.42
1:A:360:THR:O	1:A:363:VAL:CG1	2.66	0.41
1:A:199:LEU:HB3	1:A:217:ASN:HA	2.02	0.41
1:A:247:SER:HA	1:A:248:PRO:HD2	1.83	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
1:B:234:THR:O	1:B:235:GLU:C	2.63	0.41
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:A:44:ASN:OD1	1:A:357:VAL:HG23	2.21	0.41
1:B:92:GLY:HA2	1:B:226:LYS:HE3	2.03	0.41
1:B:111:ARG:NH1	1:B:163:ASP:OD2	2.53	0.41
1:A:167:GLU:H	1:A:167:GLU:HG2	1.32	0.40
1:B:255:ARG:CZ	1:B:261:VAL:HG21	2.50	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%)	4 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	351/407 (86%)	319 (91%)	24 (7%)	8 (2%)	5	18
All	All	705/814 (87%)	636 (90%)	51 (7%)	18 (3%)	4	15

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
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 [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	308/324 (95%)	248 (80%)	60 (20%)	1	5
1	B	302/324 (93%)	250 (83%)	52 (17%)	2	7
All	All	610/648 (94%)	498 (82%)	112 (18%)	1	6

All (112) 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	32	ARG
1	A	35	LEU
1	A	50	ILE
1	A	59	ASP
1	A	60	THR
1	A	63	MSE
1	A	64	SER
1	A	72	VAL
1	A	83	LEU
1	A	85	LEU
1	A	94	LEU
1	A	109	VAL
1	A	118	LYS
1	A	129	LEU
1	A	130	ASP
1	A	131	MSE
1	A	133	GLU
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	204	VAL
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

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Mol	Chain	Res	Type
1	A	276	ARG
1	A	290	ASP
1	A	293	LEU
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	363	VAL
1	A	373	GLU
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	13	LEU
1	B	28	GLN
1	B	35	LEU
1	B	38	LEU
1	B	40	SER
1	B	64	SER
1	B	72	VAL
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	148	LEU
1	B	173	LYS
1	B	178	ASP
1	B	186	GLU
1	B	188	MSE
1	B	192	LEU
1	B	199	LEU
1	B	213	ARG

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Mol	Chain	Res	Type
1	B	220	LEU
1	B	230	ILE
1	B	232	SER
1	B	238	ARG
1	B	247	SER
1	B	251	LYS
1	B	260	ASP
1	B	281	LYS
1	B	286	THR
1	B	294	VAL
1	B	296	ILE
1	B	297	LYS
1	B	312	ARG
1	B	320	ARG
1	B	322	MSE
1	B	325	LEU
1	B	326	LYS
1	B	327	SER
1	B	361	ASP
1	B	366	ASP
1	B	370	LEU
1	B	381	LEU
1	B	382	ARG
1	B	384	THR
1	B	393	MSE
1	B	394	GLN
1	B	395	LEU

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	41	HIS
1	A	48	HIS
1	A	144	HIS
1	A	274	ASN
1	A	387	ASN
1	B	44	ASN
1	B	62	HIS
1	B	144	HIS
1	B	237	ASN
1	B	331	HIS
1	B	394	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	352/407 (86%)	0.09	12 (3%) 48 39	15, 31, 50, 68	0
1	B	348/407 (85%)	0.12	8 (2%) 61 51	16, 35, 52, 69	0
All	All	700/814 (85%)	0.11	20 (2%) 53 43	15, 32, 52, 69	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	GLY	6.2
1	B	267	ALA	3.7
1	B	352	ASP	3.5
1	A	52	PRO	3.2
1	A	13	LEU	3.1
1	A	59	ASP	2.6
1	A	73	TYR	2.5
1	B	14	GLY	2.4
1	A	58	SER	2.4
1	A	15	ASP	2.4
1	A	60	THR	2.4
1	B	298	ALA	2.3
1	A	265	PRO	2.3
1	B	49	PRO	2.2
1	A	394	GLN	2.2
1	B	197	ARG	2.2
1	B	296	ILE	2.2
1	A	75	PRO	2.1
1	A	154	ASP	2.1
1	B	74	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.