



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 11:52 AM GMT

PDB ID : 2GP4  
Title : Structure of [FeS]cluster-free Apo Form of 6-Phosphogluconate Dehydratase from *Shewanella oneidensis*  
Authors : Schormann, N.; Symersky, J.; Southeast Collaboratory for Structural Genomics (SECSG)  
Deposited on : 2006-04-16  
Resolution : 2.49 Å(reported)

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

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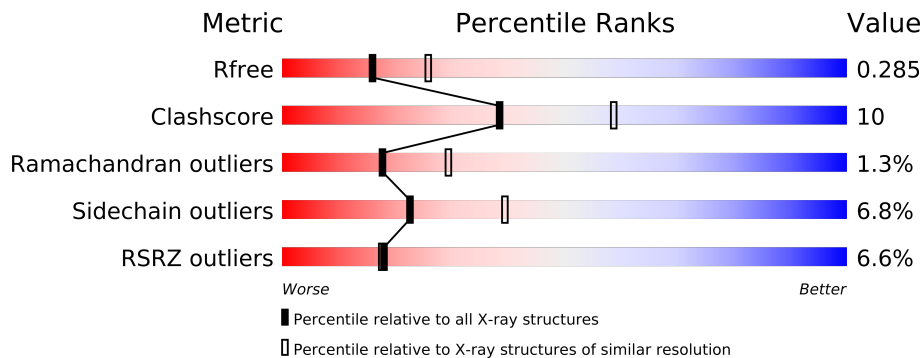
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.49 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	628	
1	B	628	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8116 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 6-phosphogluconate dehydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	523	Total	C	N	O	S	Se	0	0	0
			3892	2445	685	743	5	14			
1	B	495	Total	C	N	O	S	Se	0	0	0
			3671	2307	649	697	4	14			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	EXPRESSION TAG	GB 24348501
A	-18	GLY	-	EXPRESSION TAG	GB 24348501
A	-17	SER	-	EXPRESSION TAG	GB 24348501
A	-16	SER	-	EXPRESSION TAG	GB 24348501
A	-15	HIS	-	EXPRESSION TAG	GB 24348501
A	-14	HIS	-	EXPRESSION TAG	GB 24348501
A	-13	HIS	-	EXPRESSION TAG	GB 24348501
A	-12	HIS	-	EXPRESSION TAG	GB 24348501
A	-11	HIS	-	EXPRESSION TAG	GB 24348501
A	-10	HIS	-	EXPRESSION TAG	GB 24348501
A	-9	SER	-	EXPRESSION TAG	GB 24348501
A	-8	SER	-	EXPRESSION TAG	GB 24348501
A	-7	GLY	-	EXPRESSION TAG	GB 24348501
A	-6	LEU	-	EXPRESSION TAG	GB 24348501
A	-5	VAL	-	EXPRESSION TAG	GB 24348501
A	-4	PRO	-	EXPRESSION TAG	GB 24348501
A	-3	ARG	-	EXPRESSION TAG	GB 24348501
A	-2	GLY	-	EXPRESSION TAG	GB 24348501
A	-1	SER	-	EXPRESSION TAG	GB 24348501
A	0	HIS	-	EXPRESSION TAG	GB 24348501
A	1	MSE	MET	MODIFIED RESIDUE	GB 24348501
A	77	MSE	MET	MODIFIED RESIDUE	GB 24348501
A	111	MSE	MET	MODIFIED RESIDUE	GB 24348501
A	122	MSE	MET	MODIFIED RESIDUE	GB 24348501
A	134	MSE	MET	MODIFIED RESIDUE	GB 24348501

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Chain	Residue	Modelled	Actual	Comment	Reference
A	144	MSE	MET	MODIFIED RESIDUE	GB 24348501
A	173	MSE	MET	MODIFIED RESIDUE	GB 24348501
A	181	MSE	MET	MODIFIED RESIDUE	GB 24348501
A	233	MSE	MET	MODIFIED RESIDUE	GB 24348501
A	237	MSE	MET	MODIFIED RESIDUE	GB 24348501
A	260	MSE	MET	MODIFIED RESIDUE	GB 24348501
A	305	MSE	MET	MODIFIED RESIDUE	GB 24348501
A	353	MSE	MET	MODIFIED RESIDUE	GB 24348501
A	484	MSE	MET	MODIFIED RESIDUE	GB 24348501
A	507	MSE	MET	MODIFIED RESIDUE	GB 24348501
A	512	MSE	MET	MODIFIED RESIDUE	GB 24348501
A	579	MSE	MET	MODIFIED RESIDUE	GB 24348501
B	-19	MSE	-	EXPRESSION TAG	GB 24348501
B	-18	GLY	-	EXPRESSION TAG	GB 24348501
B	-17	SER	-	EXPRESSION TAG	GB 24348501
B	-16	SER	-	EXPRESSION TAG	GB 24348501
B	-15	HIS	-	EXPRESSION TAG	GB 24348501
B	-14	HIS	-	EXPRESSION TAG	GB 24348501
B	-13	HIS	-	EXPRESSION TAG	GB 24348501
B	-12	HIS	-	EXPRESSION TAG	GB 24348501
B	-11	HIS	-	EXPRESSION TAG	GB 24348501
B	-10	HIS	-	EXPRESSION TAG	GB 24348501
B	-9	SER	-	EXPRESSION TAG	GB 24348501
B	-8	SER	-	EXPRESSION TAG	GB 24348501
B	-7	GLY	-	EXPRESSION TAG	GB 24348501
B	-6	LEU	-	EXPRESSION TAG	GB 24348501
B	-5	VAL	-	EXPRESSION TAG	GB 24348501
B	-4	PRO	-	EXPRESSION TAG	GB 24348501
B	-3	ARG	-	EXPRESSION TAG	GB 24348501
B	-2	GLY	-	EXPRESSION TAG	GB 24348501
B	-1	SER	-	EXPRESSION TAG	GB 24348501
B	0	HIS	-	EXPRESSION TAG	GB 24348501
B	1	MSE	MET	MODIFIED RESIDUE	GB 24348501
B	77	MSE	MET	MODIFIED RESIDUE	GB 24348501
B	111	MSE	MET	MODIFIED RESIDUE	GB 24348501
B	122	MSE	MET	MODIFIED RESIDUE	GB 24348501
B	134	MSE	MET	MODIFIED RESIDUE	GB 24348501
B	144	MSE	MET	MODIFIED RESIDUE	GB 24348501
B	173	MSE	MET	MODIFIED RESIDUE	GB 24348501
B	181	MSE	MET	MODIFIED RESIDUE	GB 24348501
B	233	MSE	MET	MODIFIED RESIDUE	GB 24348501
B	237	MSE	MET	MODIFIED RESIDUE	GB 24348501

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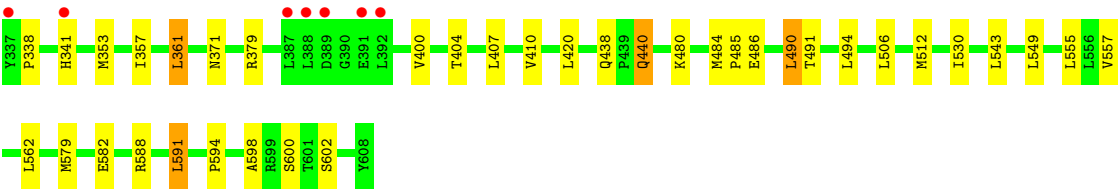
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Chain	Residue	Modelled	Actual	Comment	Reference
B	260	MSE	MET	MODIFIED RESIDUE	GB 24348501
B	305	MSE	MET	MODIFIED RESIDUE	GB 24348501
B	353	MSE	MET	MODIFIED RESIDUE	GB 24348501
B	484	MSE	MET	MODIFIED RESIDUE	GB 24348501
B	507	MSE	MET	MODIFIED RESIDUE	GB 24348501
B	512	MSE	MET	MODIFIED RESIDUE	GB 24348501
B	579	MSE	MET	MODIFIED RESIDUE	GB 24348501

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	292	Total 292	O 292	0	0
2	B	261	Total 261	O 261	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.36Å 118.65Å 160.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.68 – 2.49 47.65 – 2.49	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.68-2.49) 99.6 (47.65-2.49)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.39 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.230 , 0.291 0.226 , 0.285	Depositor DCC
$R_{free}$ test set	2086 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 35.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 41472 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8116	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.37	0/3934	0.55	0/5304
1	B	0.36	0/3710	0.56	0/5003
All	All	0.37	0/7644	0.55	0/10307

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3892	0	3949	85	0
1	B	3671	0	3735	65	0
2	A	292	0	0	7	0
2	B	261	0	0	2	0
All	All	8116	0	7684	150	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (150) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:122:MSE:HE2	1:B:486:GLU:H	1.17	1.08

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:305:MSE:HE2	1:B:598:ALA:HB2	1.34	1.05
1:A:119:GLN:HB2	1:A:120:PRO:HD3	1.40	1.04
1:B:305:MSE:CE	1:B:598:ALA:HB2	1.89	1.02
1:B:305:MSE:HE2	1:B:598:ALA:CB	1.97	0.94
1:A:122:MSE:HE2	1:A:486:GLU:H	1.31	0.93
1:A:158:VAL:HG11	1:A:234:LEU:HD21	1.48	0.93
1:B:440:GLN:H	1:B:440:GLN:HE21	1.19	0.87
1:B:158:VAL:HG11	1:B:234:LEU:HD21	1.57	0.86
1:A:507:MSE:HE1	1:A:544:ILE:HG21	1.58	0.86
1:B:122:MSE:HE2	1:B:486:GLU:N	1.94	0.81
1:A:507:MSE:CE	1:A:544:ILE:HG21	2.12	0.80
1:A:158:VAL:CG1	1:A:234:LEU:HD21	2.13	0.79
1:A:507:MSE:HE1	1:A:544:ILE:CG2	2.12	0.78
1:B:119:GLN:HB2	1:B:120:PRO:HD3	1.68	0.73
1:B:353:MSE:O	1:B:357:ILE:HG12	1.88	0.73
1:A:209:GLU:OE1	1:A:251:ASP:HB3	1.89	0.72
1:A:210:ALA:O	1:A:211:GLU:HB3	1.89	0.72
1:A:379:ARG:HD2	2:A:712:HOH:O	1.90	0.72
1:A:305:MSE:SE	1:A:484:MSE:HE1	2.40	0.72
1:A:269:THR:HG22	1:A:271:LEU:H	1.56	0.70
1:B:588:ARG:HA	1:B:591:LEU:HD22	1.73	0.70
1:A:214:SER:HB2	1:A:216:HIS:ND1	2.06	0.70
1:B:555:LEU:HG	1:B:557:VAL:HG22	1.73	0.70
1:A:96:GLN:O	1:A:97:GLU:HB2	1.91	0.69
1:A:206:GLN:O	1:A:209:GLU:HG2	1.91	0.69
1:B:122:MSE:CE	1:B:486:GLU:H	2.02	0.68
1:A:571:ASP:OD1	1:A:573:ARG:HD3	1.94	0.68
1:A:119:GLN:HB2	1:A:120:PRO:CD	2.20	0.67
1:B:122:MSE:HE3	1:B:122:MSE:O	1.95	0.67
1:A:103:GLN:HG3	1:A:145:PHE:CE1	2.30	0.66
1:B:440:GLN:H	1:B:440:GLN:NE2	1.94	0.65
1:B:353:MSE:HE3	1:B:357:ILE:HD11	1.78	0.64
1:A:156:LYS:HA	2:A:879:HOH:O	1.97	0.64
1:A:211:GLU:HB2	1:A:388:LEU:HD22	1.79	0.64
1:A:174:LEU:HD13	1:A:265:VAL:HG22	1.79	0.63
1:B:305:MSE:HE3	1:B:594:PRO:HA	1.82	0.62
1:A:255:GLU:O	1:A:259:LYS:HG2	2.01	0.61
1:A:216:HIS:O	1:A:220:THR:HG22	2.00	0.61
1:A:123:GLU:HG3	2:A:781:HOH:O	2.01	0.60
1:A:204:ARG:HG3	1:A:221:CYS:SG	2.41	0.60
1:B:357:ILE:HG22	1:B:361:LEU:HD22	1.82	0.60
1:B:15:ARG:NH2	1:B:322:ASP:OD2	2.34	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:103:GLN:HG2	1:A:108:VAL:O	2.02	0.59
1:B:174:LEU:HD13	1:B:265:VAL:HG13	1.83	0.59
1:A:96:GLN:N	2:A:658:HOH:O	2.35	0.59
1:A:149:LEU:HD21	1:A:265:VAL:HG21	1.85	0.59
1:A:333:LEU:HD21	1:A:410:VAL:HG12	1.83	0.59
1:B:440:GLN:HE21	1:B:440:GLN:N	1.98	0.58
1:A:236:VAL:HG11	1:A:293:ALA:HB2	1.83	0.58
1:A:534:LEU:HD11	1:A:562:LEU:HD13	1.86	0.58
1:A:388:LEU:HD12	1:A:393:ARG:HD3	1.86	0.58
1:A:588:ARG:HA	1:A:591:LEU:HD22	1.87	0.57
1:A:261:ALA:O	1:A:265:VAL:HG23	2.03	0.57
1:B:236:VAL:HG11	1:B:293:ALA:HB2	1.86	0.56
1:A:157:ILE:O	1:A:158:VAL:HB	2.05	0.56
1:A:361:LEU:HD13	1:A:366:LEU:HB2	1.87	0.56
1:B:116:THR:CG2	1:B:125:SER:HA	2.36	0.55
1:B:305:MSE:SE	1:B:484:MSE:HE1	2.55	0.55
1:A:211:GLU:HB2	1:A:388:LEU:CD2	2.37	0.55
1:B:319:ASN:C	1:B:319:ASN:HD22	2.10	0.55
1:A:116:THR:HG23	1:A:125:SER:HA	1.87	0.55
1:B:244:SER:O	1:B:254:ARG:NH2	2.40	0.55
1:B:490:LEU:CB	1:B:512:MSE:HE1	2.36	0.54
1:A:153:ILE:HD13	1:A:157:ILE:HD12	1.89	0.54
1:A:507:MSE:HE2	1:A:553:LEU:HD11	1.89	0.53
1:B:122:MSE:HE2	1:B:485:PRO:HA	1.89	0.53
1:A:103:GLN:HB2	1:A:145:PHE:CD1	2.43	0.53
1:B:494:LEU:HD22	1:B:506:LEU:HD22	1.91	0.52
1:B:490:LEU:HB2	1:B:512:MSE:HE1	1.91	0.52
1:A:337:TYR:O	1:A:338:PRO:C	2.46	0.52
1:A:507:MSE:HE1	1:A:544:ILE:HG23	1.93	0.51
1:B:103:GLN:HB3	1:B:145:PHE:CD2	2.46	0.51
1:A:216:HIS:CD2	1:A:217:SER:HG	2.28	0.51
1:B:116:THR:HG23	1:B:125:SER:HA	1.92	0.51
1:A:231:GLN:HA	1:A:234:LEU:HD23	1.93	0.51
1:A:204:ARG:HA	1:A:207:LEU:HD12	1.92	0.51
1:A:240:GLN:HE22	1:A:245:SER:HB3	1.76	0.50
1:B:294:LEU:HD22	1:B:299:GLY:HA3	1.93	0.50
1:B:15:ARG:HD3	2:B:847:HOH:O	2.12	0.50
1:B:120:PRO:HB2	1:B:579:MSE:HG3	1.94	0.50
1:A:97:GLU:CG	1:A:114:GLY:HA3	2.42	0.50
1:B:237:MSE:HE3	1:B:239:LEU:CD2	2.42	0.49
1:A:215:TYR:CG	1:A:402:LEU:HD11	2.47	0.49
1:A:337:TYR:O	1:A:340:GLY:O	2.30	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:404:THR:HA	1:B:407:LEU:O	2.13	0.49
1:A:319:ASN:C	1:A:319:ASN:HD22	2.15	0.49
1:B:122:MSE:CE	1:B:485:PRO:HA	2.43	0.49
1:B:491:THR:HG23	1:B:512:MSE:HE2	1.95	0.48
1:B:357:ILE:HG22	1:B:361:LEU:CD2	2.42	0.48
1:B:231:GLN:HE21	1:B:245:SER:HB2	1.78	0.48
1:A:494:LEU:HD13	1:A:506:LEU:HD21	1.96	0.48
1:A:158:VAL:HB	1:A:159:PRO:HD3	1.96	0.47
1:B:169:GLY:O	1:B:277:PRO:HB2	2.14	0.47
1:A:149:LEU:CD2	1:A:265:VAL:HG21	2.45	0.47
1:A:211:GLU:HG2	1:A:211:GLU:O	2.15	0.47
1:A:148:ALA:HB3	1:A:173:MSE:HG2	1.96	0.47
1:A:122:MSE:HE2	1:A:486:GLU:N	2.14	0.47
1:A:97:GLU:HG3	1:A:114:GLY:HA3	1.97	0.47
1:A:530:ILE:HG21	1:A:572:LEU:HD11	1.96	0.47
1:B:288:VAL:O	1:B:292:VAL:HG12	2.14	0.47
1:A:348:HIS:HD2	2:A:687:HOH:O	1.98	0.46
1:A:408:THR:HG21	1:A:413:PRO:HA	1.97	0.45
1:B:237:MSE:HE3	1:B:239:LEU:HD22	1.99	0.45
1:B:484:MSE:HE2	1:B:484:MSE:HB3	1.86	0.45
1:A:359:GLU:HB3	1:A:410:VAL:HG13	1.99	0.45
1:B:240:GLN:NE2	1:B:245:SER:HB3	2.32	0.45
1:A:170:HIS:CD2	1:A:170:HIS:H	2.35	0.45
1:A:582:GLU:CD	1:A:582:GLU:H	2.18	0.44
1:B:305:MSE:HE2	1:B:598:ALA:HB3	1.90	0.44
1:B:240:GLN:HE22	1:B:245:SER:HB3	1.83	0.44
1:B:269:THR:HG22	1:B:270:GLU:N	2.33	0.44
1:B:582:GLU:H	1:B:582:GLU:CD	2.21	0.44
1:B:170:HIS:H	1:B:170:HIS:CD2	2.34	0.44
1:A:408:THR:CG2	1:A:413:PRO:HA	2.48	0.44
1:A:358:LYS:HE3	1:A:399:THR:HG22	1.99	0.44
1:B:480:LYS:HB3	1:B:530:ILE:HD11	2.00	0.44
1:A:487:LEU:O	1:A:512:MSE:HG3	2.18	0.43
1:A:448:ALA:HB2	1:A:544:ILE:HD12	2.00	0.43
1:B:153:ILE:HG13	1:B:153:ILE:H	1.58	0.43
1:B:156:LYS:HA	2:B:739:HOH:O	2.17	0.43
1:B:591:LEU:HD13	1:B:600:SER:HB3	2.01	0.43
1:B:101:VAL:HG13	1:B:150:LEU:HD23	2.00	0.43
1:A:215:TYR:CD2	1:A:402:LEU:HD11	2.54	0.43
1:B:153:ILE:HD12	1:B:157:ILE:HG13	2.01	0.43
1:A:201:LYS:O	1:A:204:ARG:HD3	2.18	0.42
1:A:268:LEU:HG	1:A:276:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:294:LEU:HD22	1:A:299:GLY:HA3	2.00	0.42
1:A:427:LEU:HD13	1:A:507:MSE:SE	2.70	0.42
1:A:288:VAL:O	1:A:292:VAL:HG13	2.20	0.42
1:A:149:LEU:HD21	1:A:265:VAL:CG2	2.47	0.42
1:A:204:ARG:HG2	1:A:205:ALA:N	2.35	0.42
1:B:103:GLN:CB	1:B:145:PHE:CD2	3.02	0.42
1:A:466:LEU:HB3	1:A:497:LEU:HD21	2.02	0.42
1:A:99:GLY:N	2:A:852:HOH:O	2.51	0.41
1:A:555:LEU:HG	1:A:557:VAL:HG22	2.02	0.41
1:B:336:VAL:HG13	1:B:338:PRO:HD2	2.02	0.41
1:A:219:GLY:HA2	1:A:349:ALA:HB1	2.03	0.41
1:B:438:GLN:HB3	1:B:440:GLN:NE2	2.36	0.41
1:A:592:SER:O	1:A:598:ALA:HA	2.20	0.41
1:A:578:GLY:N	1:A:582:GLU:OE2	2.50	0.41
1:A:117:GLN:HB2	2:A:883:HOH:O	2.20	0.41
1:B:116:THR:HG21	1:B:125:SER:HA	2.02	0.40
1:A:154:CYS:SG	1:A:155:ASP:N	2.94	0.40
1:B:146:ASP:O	1:B:172:PRO:HD2	2.22	0.40
1:B:557:VAL:HG21	1:B:562:LEU:HD21	2.04	0.40
1:B:115:VAL:HG12	1:B:157:ILE:HD11	2.03	0.40
1:A:204:ARG:HG2	1:A:205:ALA:H	1.86	0.40
1:B:371:ASN:HD22	1:B:371:ASN:HA	1.75	0.40
1:B:379:ARG:HA	1:B:379:ARG:HD3	1.90	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/628 (81%)	486 (96%)	16 (3%)	7 (1%)	16	27
1	B	483/628 (77%)	461 (95%)	16 (3%)	6 (1%)	19	32
All	All	992/1256 (79%)	947 (96%)	32 (3%)	13 (1%)	18	29

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	GLU
1	A	158	VAL
1	B	98	VAL
1	B	153	ILE
1	A	153	ILE
1	A	155	ASP
1	B	97	GLU
1	B	273	THR
1	A	119	GLN
1	A	337	TYR
1	B	119	GLN
1	B	271	LEU
1	A	202	VAL

### 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	416/482 (86%)	385 (92%)	31 (8%)	19	34
1	B	392/482 (81%)	368 (94%)	24 (6%)	26	46
All	All	808/964 (84%)	753 (93%)	55 (7%)	22	39

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LYS
1	A	103	GLN
1	A	116	THR
1	A	117	GLN
1	A	126	LEU
1	A	156	LYS
1	A	162	LEU
1	A	203	ASP
1	A	204	ARG
1	A	211	GLU
1	A	215	TYR
1	A	220	THR
1	A	239	LEU

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Mol	Chain	Res	Type
1	A	241	LEU
1	A	271	LEU
1	A	292	VAL
1	A	303	LEU
1	A	319	ASN
1	A	333	LEU
1	A	356	LEU
1	A	361	LEU
1	A	410	VAL
1	A	420	LEU
1	A	468	ARG
1	A	490	LEU
1	A	494	LEU
1	A	497	LEU
1	A	512	MSE
1	A	543	LEU
1	A	549	LEU
1	A	591	LEU
1	B	103	GLN
1	B	116	THR
1	B	122	MSE
1	B	126	LEU
1	B	157	ILE
1	B	162	LEU
1	B	239	LEU
1	B	241	LEU
1	B	250	ASP
1	B	265	VAL
1	B	292	VAL
1	B	319	ASN
1	B	333	LEU
1	B	341	HIS
1	B	361	LEU
1	B	400	VAL
1	B	410	VAL
1	B	420	LEU
1	B	440	GLN
1	B	490	LEU
1	B	543	LEU
1	B	549	LEU
1	B	591	LEU
1	B	602	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	142	HIS
1	A	170	HIS
1	A	231	GLN
1	A	240	GLN
1	A	319	ASN
1	A	438	GLN
1	B	6	GLN
1	B	96	GLN
1	B	142	HIS
1	B	170	HIS
1	B	231	GLN
1	B	240	GLN
1	B	248	ASN
1	B	319	ASN
1	B	371	ASN
1	B	440	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	523/628 (83%)	0.19	35 (6%) 17 17	16, 26, 49, 70	0
1	B	495/628 (78%)	0.17	32 (6%) 18 18	16, 25, 48, 62	0
All	All	1018/1256 (81%)	0.18	67 (6%) 18 17	16, 26, 49, 70	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	215	TYR	6.5
1	B	271	LEU	6.2
1	B	273	THR	6.1
1	A	91	LEU	5.9
1	B	389	ASP	5.5
1	B	116	THR	5.5
1	B	391	GLU	4.7
1	B	144	MSE	4.5
1	A	144	MSE	4.4
1	A	116	THR	4.3
1	B	95	CYS	4.2
1	B	272	GLY	4.1
1	B	388	LEU	4.0
1	B	112	CYS	3.9
1	A	271	LEU	3.9
1	A	103	GLN	3.8
1	B	103	GLN	3.8
1	A	155	ASP	3.6
1	A	233	MSE	3.6
1	A	273	THR	3.6
1	B	96	GLN	3.5
1	A	114	GLY	3.5
1	A	98	VAL	3.5
1	B	265	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	154	CYS	3.5
1	A	153	ILE	3.3
1	A	202	VAL	3.3
1	B	274	GLN	3.3
1	A	113	ASP	3.3
1	A	0	HIS	3.2
1	A	90	LEU	3.2
1	B	117	GLN	3.2
1	B	387	LEU	3.1
1	B	153	ILE	2.9
1	B	154	CYS	2.9
1	A	118	GLY	2.9
1	B	115	VAL	2.9
1	A	97	GLU	2.9
1	A	112	CYS	2.9
1	A	117	GLN	2.8
1	A	223	PHE	2.8
1	B	113	ASP	2.7
1	A	337	TYR	2.7
1	B	0	HIS	2.7
1	A	272	GLY	2.7
1	A	224	TYR	2.7
1	A	557	VAL	2.6
1	B	392	LEU	2.6
1	B	337	TYR	2.6
1	A	115	VAL	2.6
1	B	267	ARG	2.6
1	A	216	HIS	2.6
1	A	221	CYS	2.6
1	A	203	ASP	2.5
1	A	96	GLN	2.5
1	A	102	ALA	2.5
1	B	266	CYS	2.3
1	B	105	ALA	2.3
1	B	252	PRO	2.3
1	B	341	HIS	2.3
1	A	341	HIS	2.2
1	A	201	LYS	2.2
1	B	269	THR	2.2
1	B	270	GLU	2.1
1	A	250	ASP	2.1
1	B	250	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	264	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.