



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 11:49 AM GMT

PDB ID : 2ISM  
Title : Crystal structure of the putative oxidoreductase (glucose dehydrogenase) (TTHA0570) from thermus thermophilus HB8  
Authors : Jeyakanthan, J.; Kanaujia, S.P.; Vasuki Ranjani, C.; Sekar, K.; Ebihara, A.; Shinkai, A.; Nakagawa, N.; Shimizu, N.; Yamamoto, M.; Kuramitsu, S.; Shiro, Y.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2006-10-18  
Resolution : 1.90 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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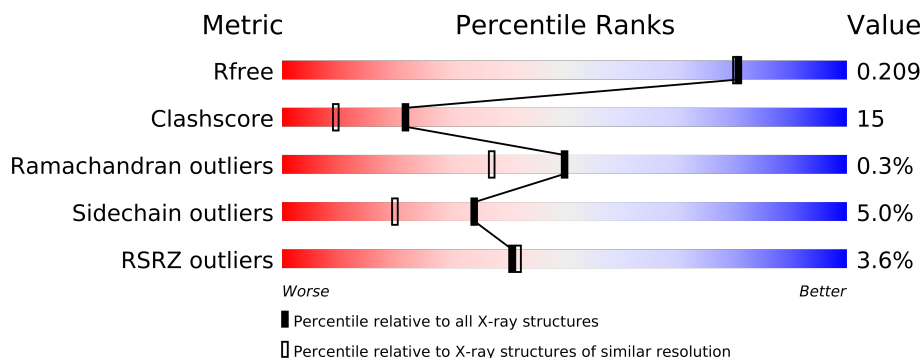
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.90 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	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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	352	
1	B	352	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CA	A	1002	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5815 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 Putative oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2558	1621	488	447	2			
1	B	333	Total	C	N	O	S	0	0	0
			2602	1647	495	458	2			

- 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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

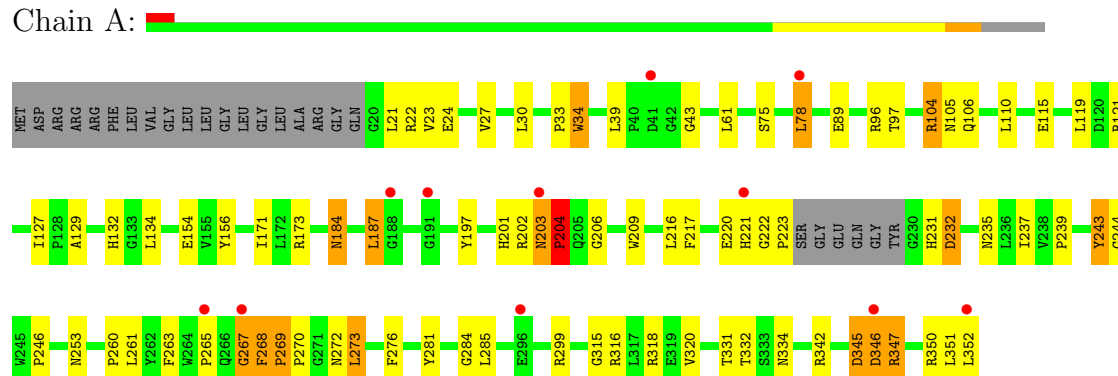
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	350	Total	O	0	0
			350	350		
4	B	301	Total	O	0	0
			301	301		

### 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.

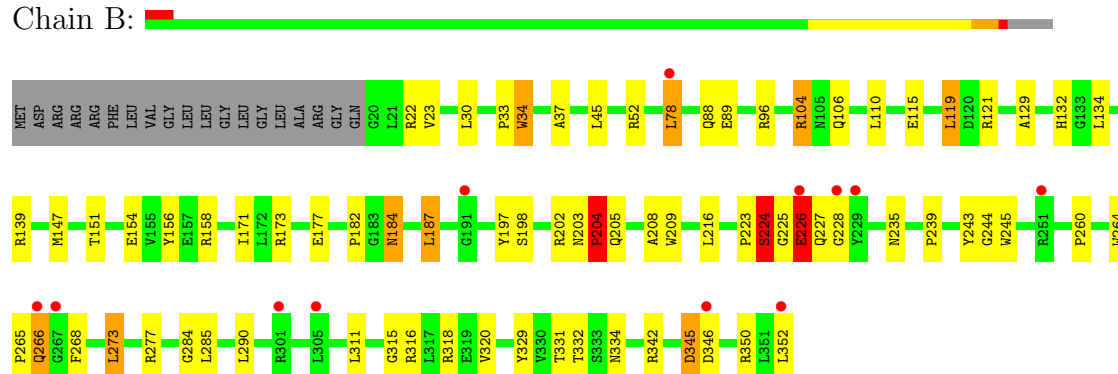
#### • Molecule 1: Putative oxidoreductase

Chain A:



#### • Molecule 1: Putative oxidoreductase

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.90Å 132.96Å 60.78Å 90.00° 97.18° 90.00°	Depositor
Resolution (Å)	36.61 – 1.90 36.61 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (36.61-1.90) 97.9 (36.61-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.181 , 0.208 0.181 , 0.209	Depositor DCC
$R_{free}$ test set	2236 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.9	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 45594 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5815	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CL

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	0.43	1/2625 (0.0%)	0.85	15/3559 (0.4%)
1	B	0.35	1/2671 (0.0%)	0.79	8/3622 (0.2%)
All	All	0.39	2/5296 (0.0%)	0.82	23/7181 (0.3%)

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
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	PRO	N-CD	15.42	1.69	1.47
1	B	204	PRO	N-CD	5.79	1.55	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	GLY	N-CA-C	16.74	154.96	113.10
1	B	78	LEU	N-CA-C	9.82	137.51	111.00
1	A	268	PHE	N-CA-CB	-9.80	92.95	110.60
1	A	78	LEU	N-CA-C	9.10	135.56	111.00
1	A	203	ASN	C-N-CD	-8.44	102.03	120.60
1	A	204	PRO	N-CA-CB	7.65	112.48	103.30
1	B	226	GLU	N-CA-C	-7.61	90.46	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	PRO	CA-N-CD	-7.53	100.95	111.50
1	A	89	GLU	N-CA-C	-6.01	94.77	111.00
1	B	224	SER	N-CA-CB	-6.00	101.50	110.50
1	A	318	ARG	N-CA-C	5.88	126.86	111.00
1	B	203	ASN	N-CA-C	-5.85	95.21	111.00
1	A	244	GLY	N-CA-C	5.81	127.62	113.10
1	B	226	GLU	N-CA-CB	-5.73	100.28	110.60
1	B	244	GLY	N-CA-C	5.54	126.94	113.10
1	B	318	ARG	N-CA-C	5.49	125.83	111.00
1	A	232	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	346	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	345	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	89	GLU	N-CA-C	-5.20	96.97	111.00
1	A	201	HIS	CB-CA-C	5.08	120.56	110.40
1	A	78	LEU	CB-CA-C	-5.03	100.64	110.20
1	A	171	ILE	N-CA-C	-5.01	97.46	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	TYR	Sidechain
1	B	243	TYR	Sidechain

## 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	2558	0	2538	68	0
1	B	2602	0	2573	87	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	350	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	301	0	0	7	0
All	All	5815	0	5111	155	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 15.

All (155) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:204:PRO:N	1:A:204:PRO:CD	1.69	1.38
1:B:266:GLN:HB3	4:B:1053:HOH:O	1.01	1.19
1:A:203:ASN:O	1:A:220:GLU:HB2	1.57	1.03
1:B:223:PRO:HB3	1:B:226:GLU:O	1.57	1.03
1:A:267:GLY:O	1:A:269:PRO:HD3	1.59	1.02
1:B:332:THR:OG1	1:B:346:ASP:HA	1.61	1.01
1:A:332:THR:OG1	1:A:346:ASP:HA	1.63	0.97
1:A:34:TRP:CE3	1:A:78:LEU:O	2.19	0.95
1:A:203:ASN:C	1:A:204:PRO:CD	2.36	0.94
1:A:342:ARG:O	1:A:345:ASP:HB2	1.68	0.93
1:B:132:HIS:HD2	1:B:134:LEU:H	1.16	0.91
1:A:132:HIS:HD2	1:A:134:LEU:H	1.13	0.90
1:B:202:ARG:HH21	1:B:226:GLU:HG2	1.34	0.89
1:B:277:ARG:HH12	1:B:352:LEU:HD12	1.42	0.85
1:A:202:ARG:HD3	1:A:222:GLY:HA2	1.59	0.83
1:B:96:ARG:HE	1:B:106:GLN:HE21	1.27	0.82
1:A:34:TRP:HE3	1:A:78:LEU:O	1.67	0.78
1:A:22:ARG:H	1:A:352:LEU:HG	1.50	0.76
1:A:132:HIS:CD2	1:A:134:LEU:H	2.03	0.75
1:B:173:ARG:HE	1:B:184:ASN:HD21	1.32	0.75
1:B:34:TRP:CE3	1:B:78:LEU:O	2.40	0.75
1:B:265:PRO:HD2	1:B:266:GLN:HE22	1.54	0.72
1:A:285:LEU:O	1:A:316:ARG:HG2	1.89	0.72
1:A:332:THR:HG1	1:A:346:ASP:HA	1.55	0.72
1:B:158:ARG:HH22	1:B:227:GLN:HB2	1.55	0.71
1:B:223:PRO:HB2	1:B:228:GLY:O	1.90	0.71
1:B:225:GLY:HA2	4:B:1299:HOH:O	1.90	0.71
1:B:226:GLU:HG3	1:B:226:GLU:O	1.90	0.71
1:B:285:LEU:O	1:B:316:ARG:HG2	1.90	0.70
1:A:96:ARG:HE	1:A:106:GLN:HE21	1.39	0.69
1:B:147:MET:HE3	1:B:182:PRO:HD2	1.75	0.69
1:A:115:GLU:HG3	4:A:1032:HOH:O	1.93	0.68
1:B:147:MET:CE	1:B:182:PRO:HD2	2.23	0.68
1:B:115:GLU:HG2	4:B:1203:HOH:O	1.93	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:277:ARG:NH1	1:B:352:LEU:HD12	2.09	0.67
1:B:139:ARG:HB2	1:B:205:GLN:O	1.95	0.67
1:B:22:ARG:H	1:B:352:LEU:CD2	2.08	0.66
1:B:227:GLN:O	1:B:227:GLN:HG2	1.94	0.66
1:B:264:TRP:HB3	1:B:266:GLN:HE21	1.62	0.65
1:A:232:ASP:CB	1:A:268:PHE:O	2.47	0.63
1:A:231:HIS:HB3	1:A:263:PHE:CZ	2.34	0.62
1:B:173:ARG:HE	1:B:184:ASN:ND2	1.97	0.62
1:B:266:GLN:NE2	1:B:266:GLN:O	2.30	0.61
1:B:342:ARG:O	1:B:345:ASP:HB2	2.01	0.61
1:A:221:HIS:CD2	1:A:232:ASP:OD1	2.54	0.60
1:A:203:ASN:CA	1:A:204:PRO:CD	2.80	0.60
1:B:96:ARG:HE	1:B:106:GLN:NE2	1.96	0.59
1:A:96:ARG:HE	1:A:106:GLN:NE2	2.00	0.59
1:A:173:ARG:HE	1:A:184:ASN:HD21	1.50	0.59
1:B:224:SER:O	1:B:225:GLY:C	2.39	0.59
1:B:332:THR:HG1	1:B:346:ASP:HA	1.65	0.58
1:B:316:ARG:H	1:B:334:ASN:HD21	1.50	0.58
1:B:264:TRP:HB3	1:B:266:GLN:O	2.04	0.58
1:B:224:SER:C	1:B:226:GLU:N	2.55	0.57
1:B:268:PHE:CZ	1:B:284:GLY:HA3	2.39	0.57
1:A:110:LEU:CD2	1:A:119:LEU:HD23	2.35	0.57
1:B:110:LEU:HD22	1:B:119:LEU:HA	1.86	0.56
1:B:224:SER:O	1:B:226:GLU:HB3	2.05	0.56
1:A:197:TYR:OH	1:A:239:PRO:HG3	2.05	0.56
1:A:173:ARG:HE	1:A:184:ASN:ND2	2.05	0.55
1:B:350:ARG:HD2	4:B:1116:HOH:O	2.06	0.55
1:B:158:ARG:NH2	1:B:227:GLN:HE21	2.03	0.55
1:B:34:TRP:HE3	1:B:78:LEU:O	1.87	0.55
1:B:316:ARG:H	1:B:334:ASN:ND2	2.04	0.55
1:B:30:LEU:O	1:B:346:ASP:HB2	2.07	0.54
1:B:147:MET:HE2	4:B:1082:HOH:O	2.05	0.54
1:A:232:ASP:HB3	1:A:270:PRO:HD3	1.88	0.54
1:A:203:ASN:O	1:A:220:GLU:CB	2.44	0.53
1:A:235:ASN:HD22	1:A:260:PRO:HA	1.73	0.53
1:B:110:LEU:CD2	1:B:119:LEU:HA	2.37	0.53
1:A:263:PHE:O	1:A:265:PRO:HD3	2.09	0.53
1:A:273:LEU:H	1:A:273:LEU:HD12	1.73	0.53
1:B:37:ALA:HB3	1:B:45:LEU:HB2	1.90	0.53
1:A:316:ARG:H	1:A:334:ASN:HD21	1.57	0.52
1:B:158:ARG:HH21	1:B:227:GLN:NE2	2.08	0.52
1:A:217:PHE:HE1	1:A:261:LEU:HD22	1.74	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:202:ARG:NE	1:B:226:GLU:OE2	2.43	0.52
1:B:202:ARG:NH2	1:B:226:GLU:HG2	2.15	0.52
1:A:268:PHE:O	1:A:270:PRO:HD3	2.10	0.52
1:B:277:ARG:HH22	1:B:352:LEU:HD12	1.75	0.51
1:B:158:ARG:HH21	1:B:227:GLN:HE21	1.58	0.51
1:B:52:ARG:HD3	4:B:1156:HOH:O	2.10	0.51
1:B:22:ARG:H	1:B:352:LEU:HD21	1.75	0.51
1:B:197:TYR:OH	1:B:239:PRO:HG3	2.11	0.51
1:B:264:TRP:HB3	1:B:266:GLN:NE2	2.24	0.51
1:B:22:ARG:H	1:B:352:LEU:HD23	1.75	0.50
1:B:224:SER:H	1:B:226:GLU:CG	2.24	0.50
1:A:184:ASN:HB2	1:A:187:LEU:HD13	1.93	0.50
1:A:30:LEU:HB2	1:A:346:ASP:O	2.11	0.50
1:B:235:ASN:HD22	1:B:260:PRO:HA	1.77	0.50
1:A:235:ASN:ND2	1:A:260:PRO:HA	2.26	0.49
1:B:315:GLY:HA3	1:B:334:ASN:HD21	1.77	0.49
1:A:104:ARG:HA	1:A:129:ALA:HB3	1.94	0.49
1:B:173:ARG:HH21	1:B:184:ASN:HD22	1.61	0.49
1:A:21:LEU:HA	1:A:352:LEU:HD12	1.93	0.49
1:A:350:ARG:HD2	4:A:1199:HOH:O	2.13	0.48
1:A:132:HIS:HE1	4:A:1048:HOH:O	1.96	0.48
1:B:132:HIS:CD2	1:B:134:LEU:H	2.09	0.48
1:B:139:ARG:CB	1:B:205:GLN:O	2.62	0.47
1:A:209:TRP:CE2	1:A:216:LEU:HD13	2.49	0.47
1:A:237:ILE:HA	1:A:243:TYR:OH	2.15	0.47
1:A:315:GLY:HA3	1:A:334:ASN:HD21	1.80	0.46
1:A:23:VAL:HG22	1:A:24:GLU:N	2.30	0.46
1:B:151:THR:HB	1:B:204:PRO:HG2	1.98	0.46
1:B:266:GLN:H	1:B:266:GLN:CD	2.18	0.46
1:A:217:PHE:CE1	1:A:261:LEU:HD22	2.49	0.46
1:A:39:LEU:HD12	1:A:43:GLY:HA3	1.97	0.45
1:A:22:ARG:N	1:A:352:LEU:HG	2.27	0.45
1:B:223:PRO:CB	1:B:226:GLU:O	2.46	0.45
1:A:316:ARG:H	1:A:334:ASN:ND2	2.15	0.45
1:A:223:PRO:HB2	1:A:231:HIS:CD2	2.52	0.45
1:B:104:ARG:HA	1:B:129:ALA:HB3	1.98	0.45
1:A:27:VAL:O	1:A:347:ARG:HB3	2.16	0.45
1:B:223:PRO:HG3	1:B:245:TRP:CZ3	2.52	0.45
1:B:273:LEU:HD12	1:B:273:LEU:H	1.82	0.45
1:A:204:PRO:HA	1:A:220:GLU:CB	2.46	0.44
1:B:320:VAL:HA	1:B:329:TYR:O	2.18	0.44
1:A:33:PRO:HG2	1:A:331:THR:HB	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:222:GLY:O	1:A:223:PRO:C	2.54	0.44
1:A:221:HIS:CD2	1:A:222:GLY:O	2.71	0.44
1:B:121:ARG:NH2	1:B:177:GLU:O	2.51	0.43
1:A:351:LEU:HD12	1:A:351:LEU:N	2.33	0.43
1:B:277:ARG:NH2	1:B:352:LEU:HD12	2.33	0.43
1:B:316:ARG:N	1:B:334:ASN:HD21	2.16	0.43
1:B:202:ARG:HH21	1:B:226:GLU:CG	2.19	0.43
1:A:273:LEU:N	1:A:273:LEU:HD12	2.32	0.43
1:A:221:HIS:HD2	1:A:232:ASP:OD1	1.98	0.43
1:A:75:SER:HB3	1:A:97:THR:OG1	2.19	0.42
1:B:208:ALA:CB	1:B:273:LEU:HD13	2.48	0.42
1:B:208:ALA:HB2	1:B:273:LEU:HD13	2.00	0.42
1:A:173:ARG:HH21	1:A:184:ASN:HD22	1.66	0.42
1:B:23:VAL:HG21	1:B:311:LEU:HD11	2.01	0.42
1:B:265:PRO:HD2	1:B:266:GLN:NE2	2.30	0.42
1:B:158:ARG:NH2	1:B:227:GLN:NE2	2.67	0.42
1:B:30:LEU:HB2	1:B:346:ASP:O	2.19	0.42
1:B:96:ARG:HH21	1:B:106:GLN:HE22	1.68	0.42
1:B:33:PRO:HG2	1:B:331:THR:HB	2.01	0.41
1:B:197:TYR:CZ	1:B:239:PRO:HG3	2.55	0.41
1:B:235:ASN:ND2	1:B:260:PRO:HA	2.35	0.41
1:A:75:SER:HB3	1:A:97:THR:HG1	1.85	0.41
1:A:276:PHE:HB3	1:A:281:TYR:CD2	2.55	0.41
1:A:206:GLY:HA2	1:A:272:ASN:OD1	2.20	0.41
1:B:132:HIS:HE1	4:B:1079:HOH:O	2.03	0.41
1:A:268:PHE:CZ	1:A:284:GLY:HA3	2.56	0.41
1:B:171:ILE:HB	1:B:198:SER:OG	2.21	0.41
1:A:299:ARG:HG2	1:A:299:ARG:HH11	1.86	0.41
1:B:173:ARG:HH21	1:B:184:ASN:ND2	2.19	0.41
1:B:290:LEU:HB3	1:B:311:LEU:HB3	2.02	0.41
1:A:320:VAL:O	1:A:320:VAL:HG13	2.21	0.41
1:B:187:LEU:HA	1:B:187:LEU:HD12	1.86	0.41
1:B:34:TRP:HB3	1:B:78:LEU:O	2.21	0.40
1:A:105:ASN:HB2	1:A:127:ILE:HB	2.04	0.40
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.89	0.40
1:A:232:ASP:CG	1:A:268:PHE:O	2.60	0.40
1:B:209:TRP:CE2	1:B:216:LEU:HD13	2.57	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	323/352 (92%)	307 (95%)	15 (5%)	1 (0%)	50	37
1	B	331/352 (94%)	314 (95%)	16 (5%)	1 (0%)	50	37
All	All	654/704 (93%)	621 (95%)	31 (5%)	2 (0%)	50	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	PRO
1	B	204	PRO

### 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	257/275 (94%)	244 (95%)	13 (5%)	33	19
1	B	261/275 (95%)	248 (95%)	13 (5%)	34	20
All	All	518/550 (94%)	492 (95%)	26 (5%)	34	20

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	TRP
1	A	61	LEU
1	A	104	ARG
1	A	121	ARG
1	A	154	GLU
1	A	156	TYR
1	A	184	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	187	LEU
1	A	246	PRO
1	A	253	ASN
1	A	269	PRO
1	A	273	LEU
1	A	347	ARG
1	B	34	TRP
1	B	88	GLN
1	B	104	ARG
1	B	119	LEU
1	B	154	GLU
1	B	156	TYR
1	B	184	ASN
1	B	187	LEU
1	B	224	SER
1	B	226	GLU
1	B	266	GLN
1	B	273	LEU
1	B	345	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	106	GLN
1	A	132	HIS
1	A	184	ASN
1	A	221	HIS
1	A	231	HIS
1	A	235	ASN
1	A	334	ASN
1	B	88	GLN
1	B	105	ASN
1	B	106	GLN
1	B	132	HIS
1	B	184	ASN
1	B	221	HIS
1	B	227	GLN
1	B	235	ASN
1	B	266	GLN
1	B	334	ASN

### 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 ⓘ

Of 4 ligands modelled in this entry, 4 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.

## 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	327/352 (92%)	-0.06	11 (3%) 43 44	9, 20, 46, 72	0
1	B	333/352 (94%)	-0.05	12 (3%) 41 42	9, 19, 45, 79	0
All	All	660/704 (93%)	-0.05	23 (3%) 41 43	9, 19, 46, 79	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	226	GLU	4.7
1	B	266	GLN	4.2
1	A	352	LEU	3.7
1	A	267	GLY	3.7
1	B	228	GLY	3.3
1	B	301	ARG	3.2
1	B	305	LEU	3.2
1	A	346	ASP	2.9
1	A	78	LEU	2.8
1	B	229	TYR	2.7
1	A	203	ASN	2.6
1	A	265	PRO	2.6
1	A	221	HIS	2.6
1	B	191	GLY	2.5
1	A	296	GLU	2.5
1	B	267	GLY	2.3
1	A	188	GLY	2.3
1	B	346	ASP	2.2
1	B	78	LEU	2.2
1	B	251	ARG	2.2
1	B	352	LEU	2.1
1	A	41	ASP	2.1
1	A	191	GLY	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 ⓘ

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<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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	A	1002	1/1	0.30	10.16	82,82,82,82	0
2	CA	B	1001	1/1	0.06	-1.06	21,21,21,21	0
3	CL	A	1003	1/1	0.06	-1.48	24,24,24,24	0
3	CL	B	1004	1/1	0.04	-3.09	23,23,23,23	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.