Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:52 am BST

PDB ID	:	1X0L
Title	:	Crystal structure of tetrameric homoisocitrate dehydrogenase from an extreme thermophile, Thermus thermophilus
Authors	:	Miyazaki, J.; Asada, K.; Fushinobu, S.; Kuzuyama, T.; Nishiyama, M.
Deposited on	:	2005-03-24
Resolution	:	1.85 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 following versions of software and data (see references ⓘ) were used in the production of this report:

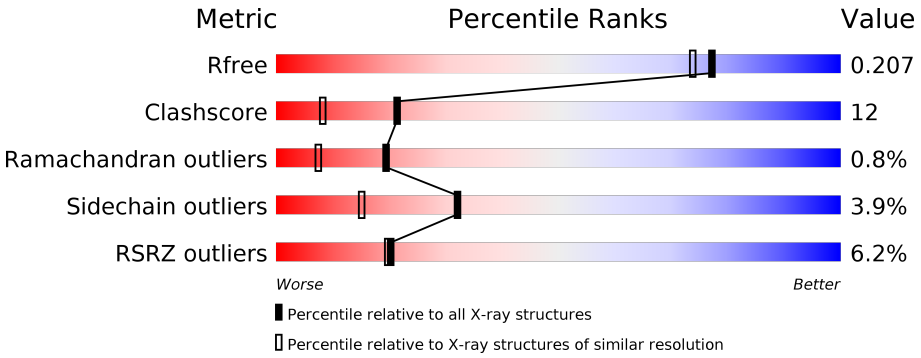
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.85 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}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 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 <=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	333	2% 82% 15%
1	B	333	11% 72% 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5361 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 Homoisocitrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2519	1590	448	474	7			
1	B	326	Total	C	N	O	S	0	0	0
			2464	1557	437	463	7			

- Molecule 2 is water.

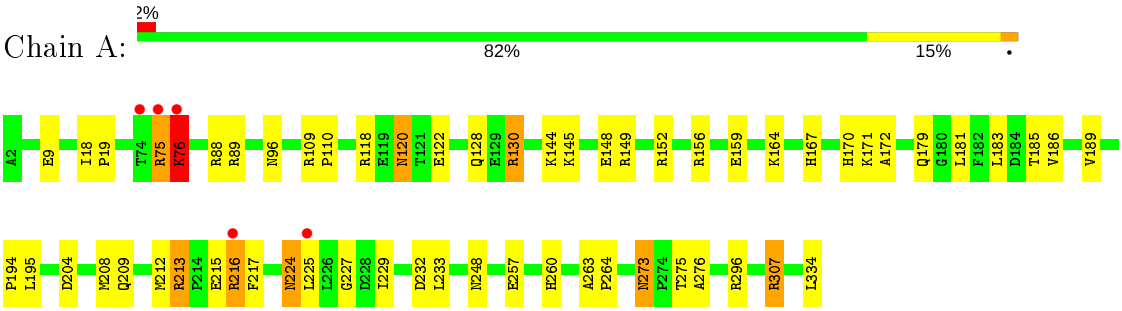
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	250	Total	O	0	0
			250	250		
2	B	128	Total	O	0	0
			128	128		

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 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.

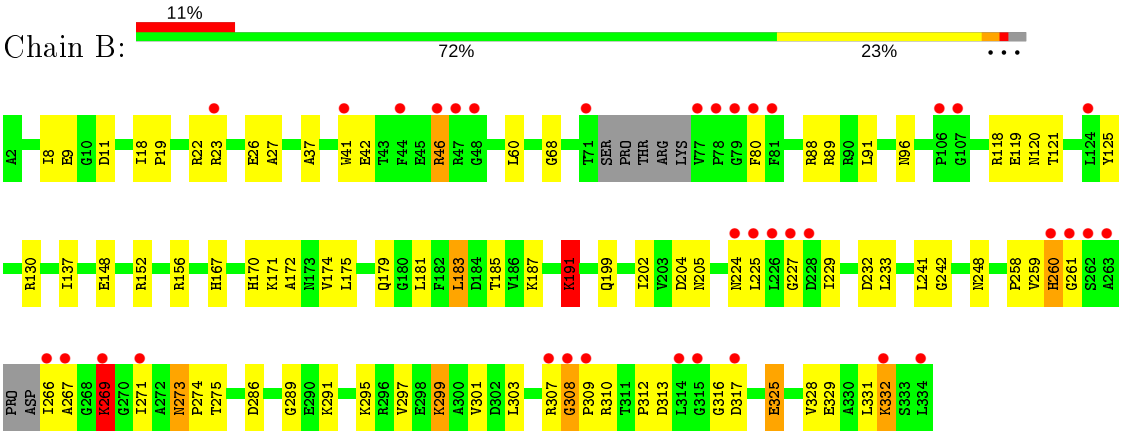
- Molecule 1: Homoisocitrate dehydrogenase

Chain A:



- Molecule 1: Homoisocitrate dehydrogenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	60.96Å 143.24Å 177.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.44 – 1.85 47.44 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.44-1.85) 99.8 (47.44-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.05 (at 1.86Å)	Xtriage
Refinement program	CNS 1.1, XTALVIEW	Depositor
R, R_{free}	0.216 , 0.248 0.215 , 0.207	Depositor DCC
R_{free} test set	3370 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5361	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.74	4/2560 (0.2%)	0.82	10/3474 (0.3%)
1	B	0.27	0/2501	0.64	9/3390 (0.3%)
All	All	0.56	4/5061 (0.1%)	0.74	19/6864 (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	1	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	ARG	CA-CB	-25.65	0.97	1.53
1	A	75	ARG	CZ-NH1	-16.57	1.11	1.33
1	A	75	ARG	NE-CZ	-11.73	1.17	1.33
1	A	75	ARG	CG-CD	-9.17	1.29	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	75	ARG	NE-CZ-NH1	-21.46	109.57	120.30
1	A	75	ARG	NE-CZ-NH2	14.22	127.41	120.30
1	A	76	LYS	CB-CA-C	10.01	130.42	110.40
1	B	191	LYS	CB-CA-C	9.97	130.34	110.40
1	A	75	ARG	CB-CA-C	7.64	125.68	110.40
1	A	75	ARG	N-CA-CB	6.91	123.03	110.60
1	A	75	ARG	CA-CB-CG	6.62	127.97	113.40
1	B	269	LYS	CB-CA-C	-6.45	97.50	110.40
1	A	213	ARG	CB-CA-C	-6.45	97.51	110.40
1	A	120	ASN	N-CA-C	-6.04	94.69	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	310	ARG	CB-CA-C	5.35	121.09	110.40
1	A	307	ARG	CB-CA-C	5.34	121.08	110.40
1	B	89	ARG	CB-CA-C	5.33	121.06	110.40
1	B	46	ARG	CB-CA-C	5.32	121.04	110.40
1	B	299	LYS	CB-CA-C	5.31	121.03	110.40
1	B	295	LYS	CB-CA-C	5.31	121.02	110.40
1	B	332	LYS	CB-CA-C	5.29	120.99	110.40
1	B	120	ASN	N-CA-C	-5.20	96.97	111.00
1	A	75	ARG	CD-NE-CZ	5.09	130.73	123.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	75	ARG	CA

There are no planarity outliers.

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	2519	0	2581	61	3
1	B	2464	0	2524	71	4
2	A	250	0	0	4	0
2	B	128	0	0	2	0
All	All	5361	0	5105	121	4

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 12.

All (121) 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:209:GLN:HB3	1:A:216:ARG:NH2	1.24	1.43
1:B:269:LYS:HB3	1:B:269:LYS:NZ	1.56	1.06
1:A:209:GLN:CB	1:A:216:ARG:NH2	2.19	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ARG:HD2	1:A:217:PHE:CZ	1.99	0.96
1:B:266:ILE:HG22	1:B:267:ALA:H	1.40	0.86
1:B:269:LYS:HB3	1:B:269:LYS:HZ3	1.36	0.85
1:A:209:GLN:HB3	1:A:216:ARG:HH22	1.06	0.85
1:A:209:GLN:CB	1:A:216:ARG:HH22	1.86	0.85
1:B:269:LYS:HB3	1:B:269:LYS:HZ2	1.39	0.85
1:A:170:HIS:HD2	1:A:172:ALA:H	1.27	0.82
1:B:170:HIS:HD2	1:B:172:ALA:H	1.33	0.76
1:A:208:MET:HE1	1:B:241:LEU:HG	1.67	0.75
1:A:209:GLN:HB3	1:A:216:ARG:CZ	2.15	0.74
1:B:171:LYS:HG3	1:B:174:VAL:HG22	1.71	0.72
1:A:225:LEU:HD12	1:B:171:LYS:HE2	1.71	0.72
1:A:216:ARG:HD2	1:A:217:PHE:CE1	2.24	0.72
1:B:269:LYS:CB	1:B:269:LYS:NZ	2.45	0.72
1:A:204:ASP:HB3	1:B:232:ASP:OD1	1.92	0.70
1:A:213:ARG:CZ	1:A:216:ARG:NH1	2.54	0.70
1:B:88:ARG:HE	1:B:248:ASN:ND2	1.90	0.69
1:B:118:ARG:HD3	1:B:227:GLY:HA3	1.76	0.67
1:A:171:LYS:HE2	1:B:225:LEU:HD22	1.79	0.65
1:B:152:ARG:HG2	1:B:156:ARG:NH1	2.11	0.65
1:B:156:ARG:HG3	1:B:156:ARG:HH11	1.62	0.64
1:B:266:ILE:HG22	1:B:267:ALA:N	2.13	0.63
1:A:88:ARG:HE	1:A:248:ASN:ND2	1.99	0.61
1:B:303:LEU:O	1:B:307:ARG:HG2	2.00	0.61
1:A:170:HIS:CD2	1:A:172:ALA:H	2.15	0.60
1:B:328:VAL:HG12	1:B:332:LYS:HD2	1.82	0.60
1:A:229:ILE:HG21	1:B:229:ILE:HD13	1.84	0.60
1:B:266:ILE:O	1:B:267:ALA:HB3	2.03	0.59
1:A:120:ASN:HD21	1:A:248:ASN:HD22	1.50	0.57
1:B:273:ASN:ND2	1:B:275:THR:H	2.02	0.57
1:B:170:HIS:CD2	1:B:172:ALA:H	2.18	0.57
1:B:9:GLU:HA	1:B:18:ILE:HG13	1.86	0.57
1:B:22:ARG:O	1:B:26:GLU:HG3	2.06	0.56
1:B:171:LYS:HB3	1:B:179:GLN:HG3	1.89	0.55
1:A:225:LEU:H	1:A:225:LEU:HD22	1.70	0.55
1:B:271:ILE:HB	1:B:312:PRO:HG2	1.87	0.55
1:A:224:ASN:HB3	1:A:225:LEU:HD22	1.89	0.55
1:B:23:ARG:HG3	1:B:23:ARG:HH21	1.70	0.55
1:A:208:MET:CE	1:B:241:LEU:HG	2.35	0.54
1:A:229:ILE:HD13	1:B:229:ILE:HG21	1.89	0.54
1:A:145:LYS:O	1:A:149:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ARG:HG2	1:A:109:ARG:HH21	1.74	0.53
1:A:195:LEU:HD22	1:A:195:LEU:N	2.23	0.53
1:A:215:GLU:CD	1:A:215:GLU:H	2.11	0.53
1:B:289:GLY:HA2	1:B:291:LYS:NZ	2.24	0.53
1:B:41:TRP:HA	1:B:80:PHE:HE2	1.75	0.52
1:B:11:ASP:OD1	1:B:42:GLU:HG3	2.09	0.52
1:B:8:ILE:HG12	1:B:37:ALA:HB3	1.92	0.51
1:B:286:ASP:OD1	1:B:291:LYS:HE3	2.10	0.51
1:A:229:ILE:CG2	1:B:229:ILE:HD13	2.40	0.51
1:A:273:ASN:ND2	1:A:275:THR:H	2.09	0.51
1:B:241:LEU:HD22	1:B:259:VAL:HG11	1.93	0.50
1:A:194:PRO:HG2	1:A:195:LEU:HD22	1.94	0.50
1:B:273:ASN:C	1:B:273:ASN:HD22	2.15	0.50
1:B:273:ASN:HD22	1:B:274:PRO:N	2.09	0.50
1:A:118:ARG:HD3	1:A:227:GLY:HA3	1.94	0.50
1:B:289:GLY:HA2	1:B:291:LYS:HZ3	1.76	0.49
1:B:307:ARG:HG3	1:B:308:GLY:N	2.27	0.49
1:B:19:PRO:O	1:B:23:ARG:HG2	2.12	0.49
1:B:167:HIS:HD2	2:B:346:HOH:O	1.94	0.49
1:A:225:LEU:N	1:A:225:LEU:HD22	2.28	0.49
1:A:148:GLU:HG3	1:A:185:THR:CG2	2.43	0.48
1:B:267:ALA:O	1:B:269:LYS:HG2	2.13	0.48
1:B:174:VAL:HG23	1:B:175:LEU:HG	1.96	0.47
1:B:233:LEU:C	1:B:233:LEU:HD23	2.35	0.47
1:A:167:HIS:HD2	2:A:343:HOH:O	1.96	0.47
1:A:216:ARG:HG3	1:A:217:PHE:CD1	2.49	0.47
1:B:202:ILE:HB	1:B:205:ASN:HD22	1.79	0.46
1:B:23:ARG:HG3	1:B:23:ARG:NH2	2.30	0.46
1:A:296:ARG:NH1	2:A:440:HOH:O	2.49	0.46
1:A:229:ILE:HD13	1:B:229:ILE:CG2	2.44	0.46
1:B:312:PRO:HA	1:B:316:GLY:O	2.15	0.46
1:B:88:ARG:HH21	1:B:248:ASN:HD21	1.63	0.46
1:A:144:LYS:HE2	2:A:452:HOH:O	2.15	0.46
1:A:273:ASN:C	1:A:273:ASN:HD22	2.19	0.45
1:B:18:ILE:HB	1:B:19:PRO:HD3	1.97	0.45
1:A:76:LYS:HE2	1:A:76:LYS:HB2	1.67	0.45
1:A:233:LEU:HD23	1:A:233:LEU:C	2.37	0.45
1:B:148:GLU:HG3	1:B:185:THR:CG2	2.47	0.45
1:B:18:ILE:HD11	1:B:68:GLY:HA2	1.99	0.45
1:A:128:GLN:HB2	2:A:458:HOH:O	2.16	0.45
1:B:152:ARG:CG	1:B:156:ARG:NH1	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLY:O	1:B:258:PRO:HD2	2.17	0.44
1:B:325:GLU:O	1:B:329:GLU:HG3	2.17	0.44
1:B:60:LEU:HD21	1:B:91:LEU:HD22	1.99	0.44
1:B:242:GLY:HA2	1:B:260:HIS:ND1	2.33	0.44
1:A:109:ARG:NH2	1:A:110:PRO:O	2.51	0.44
1:A:296:ARG:HD2	1:A:334:LEU:O	2.17	0.44
1:A:263:ALA:N	1:A:264:PRO:HD3	2.32	0.43
1:A:9:GLU:HA	1:A:18:ILE:HG13	2.00	0.43
1:A:208:MET:HE1	1:B:241:LEU:CG	2.43	0.43
1:A:89:ARG:HG3	1:A:122:GLU:O	2.18	0.43
1:A:208:MET:HG2	1:A:212:MET:CE	2.49	0.43
1:B:130:ARG:HH21	1:B:137:ILE:CG2	2.32	0.43
1:A:18:ILE:HB	1:A:19:PRO:HD3	2.00	0.42
1:A:186:VAL:O	1:A:189:VAL:HG22	2.19	0.42
1:B:266:ILE:O	1:B:267:ALA:CB	2.66	0.42
1:B:297:VAL:O	1:B:301:VAL:HG23	2.19	0.42
1:A:128:GLN:HG2	1:A:130:ARG:HD2	2.01	0.42
1:A:159:GLU:O	1:A:164:LYS:HE3	2.19	0.42
1:A:89:ARG:HG2	1:A:89:ARG:HH11	1.83	0.42
1:B:241:LEU:HD22	1:B:259:VAL:CG1	2.49	0.42
1:A:260:HIS:CE1	1:A:276:ALA:HB3	2.54	0.42
1:B:273:ASN:HB2	1:B:313:ASP:OD1	2.20	0.42
1:A:195:LEU:N	1:A:195:LEU:CD2	2.83	0.42
1:A:213:ARG:CZ	1:A:216:ARG:CZ	2.97	0.42
1:A:171:LYS:HB2	1:A:179:GLN:HG3	2.02	0.41
1:B:119:GLU:CD	1:B:121:THR:HG22	2.40	0.41
1:B:27:ALA:HB3	1:B:331:LEU:HD23	2.02	0.41
1:B:183:LEU:HD22	1:B:187:LYS:HD2	2.03	0.41
1:A:194:PRO:HG2	1:A:195:LEU:CD2	2.49	0.41
1:A:224:ASN:HB3	1:A:225:LEU:H	1.69	0.41
1:B:266:ILE:CG2	1:B:267:ALA:H	2.13	0.41
1:A:18:ILE:HD13	1:A:18:ILE:HA	1.97	0.40
1:B:191:LYS:HB3	1:B:191:LYS:HE3	1.83	0.40
1:A:152:ARG:O	1:A:156:ARG:HG3	2.22	0.40
1:B:156:ARG:HD2	2:B:409:HOH:O	2.20	0.40
1:A:232:ASP:OD2	1:B:204:ASP:HB3	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ARG:NH2	1:B:199:GLN:NE2[3_555]	1.17	1.03
1:A:307:ARG:NH2	1:B:199:GLN:CD[3_555]	1.67	0.53
1:B:317:ASP:OD2	1:B:317:ASP:OD2[3_555]	2.01	0.19
1:A:307:ARG:NH2	1:B:199:GLN:OE1[3_555]	2.17	0.03

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	331/333 (99%)	321 (97%)	9 (3%)	1 (0%)	41 26
1	B	320/333 (96%)	302 (94%)	14 (4%)	4 (1%)	12 3
All	All	651/666 (98%)	623 (96%)	23 (4%)	5 (1%)	19 7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ASN
1	B	224	ASN
1	B	308	GLY
1	B	309	PRO
1	B	261	GLY

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	263/263 (100%)	254 (97%)	9 (3%)	37 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	256/263 (97%)	245 (96%)	11 (4%)	29 12
All	All	519/526 (99%)	499 (96%)	20 (4%)	32 15

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ARG
1	A	76	LYS
1	A	96	ASN
1	A	130	ARG
1	A	181	LEU
1	A	183	LEU
1	A	216	ARG
1	A	257	GLU
1	A	273	ASN
1	B	46	ARG
1	B	96	ASN
1	B	125	TYR
1	B	181	LEU
1	B	183	LEU
1	B	191	LYS
1	B	260	HIS
1	B	269	LYS
1	B	273	ASN
1	B	299	LYS
1	B	325	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	167	HIS
1	A	170	HIS
1	A	248	ASN
1	A	260	HIS
1	A	273	ASN
1	B	96	ASN
1	B	120	ASN
1	B	167	HIS
1	B	170	HIS
1	B	205	ASN

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Mol	Chain	Res	Type
1	B	209	GLN
1	B	248	ASN
1	B	273	ASN

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

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	333/333 (100%)	0.07	5 (1%) 73 74	11, 20, 36, 56	0
1	B	326/333 (97%)	0.67	36 (11%) 5 5	14, 30, 59, 75	0
All	All	659/666 (98%)	0.36	41 (6%) 20 20	11, 25, 54, 75	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	SER	10.0
1	B	261	GLY	8.1
1	B	260	HIS	7.1
1	B	334	LEU	6.7
1	B	315	GLY	6.4
1	B	267	ALA	5.6
1	B	46	ARG	4.7
1	B	263	ALA	4.5
1	B	44	PHE	4.4
1	B	266	ILE	4.4
1	B	225	LEU	4.1
1	B	80	PHE	4.1
1	B	106	PRO	4.0
1	A	75	ARG	4.0
1	B	77	VAL	3.9
1	B	78	PRO	3.8
1	B	81	PHE	3.7
1	B	48	GLY	3.6
1	B	227	GLY	3.5
1	B	226	LEU	3.4
1	B	79	GLY	3.4
1	B	317	ASP	3.4
1	A	216	ARG	3.2
1	B	41	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	308	GLY	3.0
1	B	271	ILE	3.0
1	A	74	THR	2.9
1	B	307	ARG	2.7
1	B	23	ARG	2.7
1	A	225	LEU	2.5
1	B	71	THR	2.3
1	B	269	LYS	2.3
1	B	332	LYS	2.2
1	B	228	ASP	2.2
1	B	314	LEU	2.2
1	B	309	PRO	2.2
1	A	76	LYS	2.2
1	B	224	ASN	2.2
1	B	107	GLY	2.1
1	B	124	LEU	2.1
1	B	47	ARG	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.