



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:17 PM GMT

PDB ID : 1X1Q
Title : Crystal structure of tryptophan synthase beta chain from *Thermus thermophilus* HB8
Authors : Asada, Y.; Kunishima, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-04-11
Resolution : 2.50 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

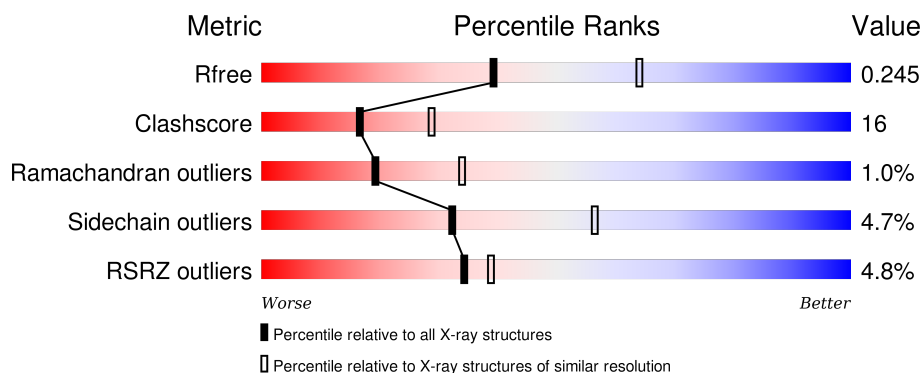
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 ≥ 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	418	<div> <div>3%</div> <div>64%</div> <div>25%</div> <div>8%</div> </div>
1	B	418	<div> <div>6%</div> <div>57%</div> <div>25%</div> <div>15%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5984 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 tryptophan synthase beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	Se	8	0	0
			2953	1882	521	541	1	8			
1	B	354	Total	C	N	O	S	Se	5	0	0
			2728	1742	476	502	1	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P16609
A	15	MSE	MET	MODIFIED RESIDUE	UNP P16609
A	123	MSE	MET	MODIFIED RESIDUE	UNP P16609
A	156	MSE	MET	MODIFIED RESIDUE	UNP P16609
A	171	MSE	MET	MODIFIED RESIDUE	UNP P16609
A	221	MSE	MET	MODIFIED RESIDUE	UNP P16609
A	222	MSE	MET	MODIFIED RESIDUE	UNP P16609
A	308	MSE	MET	MODIFIED RESIDUE	UNP P16609
A	389	MSE	MET	MODIFIED RESIDUE	UNP P16609
A	411	MSE	MET	MODIFIED RESIDUE	UNP P16609
B	1	MSE	MET	MODIFIED RESIDUE	UNP P16609
B	15	MSE	MET	MODIFIED RESIDUE	UNP P16609
B	123	MSE	MET	MODIFIED RESIDUE	UNP P16609
B	156	MSE	MET	MODIFIED RESIDUE	UNP P16609
B	171	MSE	MET	MODIFIED RESIDUE	UNP P16609
B	221	MSE	MET	MODIFIED RESIDUE	UNP P16609
B	222	MSE	MET	MODIFIED RESIDUE	UNP P16609
B	308	MSE	MET	MODIFIED RESIDUE	UNP P16609
B	389	MSE	MET	MODIFIED RESIDUE	UNP P16609
B	411	MSE	MET	MODIFIED RESIDUE	UNP P16609

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Cl 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	174	Total 174	O 174	0	0
3	B	128	Total 128	O 128	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	92.19 Å 109.99 Å 74.67 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 2.50 29.60 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.60-2.50) 98.9 (29.60-2.49)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.48 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.201 , 0.245 0.202 , 0.245	Depositor DCC
R_{free} test set	1364 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 26955 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5984	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 4.36% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.40	1/3009 (0.0%)	0.62	0/4062
1	B	0.40	1/2779 (0.0%)	0.62	0/3755
All	All	0.40	2/5788 (0.0%)	0.62	0/7817

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	TRP	NE1-CE2	9.12	1.49	1.37
1	A	199	TRP	NE1-CE2	8.94	1.49	1.37

There are no bond angle outliers.

There are no chirality outliers.

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	2953	0	2955	103	0
1	B	2728	0	2732	92	0
2	A	1	0	0	0	0
3	A	174	0	0	6	0
3	B	128	0	0	5	0
All	All	5984	0	5687	187	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 16.

All (187) 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:127:ARG:HH11	1:A:206:THR:HG21	1.10	1.13
1:A:42:LEU:HD23	1:A:200:ILE:HD11	1.06	1.04
1:A:42:LEU:CD2	1:A:200:ILE:HD11	1.88	1.02
1:A:127:ARG:NH1	1:A:206:THR:HG21	1.80	0.97
1:B:386:VAL:HA	1:B:389:MSE:HE3	1.43	0.97
1:A:42:LEU:HD23	1:A:200:ILE:CD1	1.94	0.96
1:A:271:GLU:HG3	1:A:272:GLY:H	1.44	0.82
1:A:409:GLU:HG3	1:A:412:ARG:HH22	1.48	0.78
1:A:290:ARG:HH11	1:A:290:ARG:HB3	1.48	0.77
1:A:127:ARG:HH11	1:A:206:THR:CG2	1.94	0.77
1:A:308:MSE:HE1	1:A:333:VAL:N	2.00	0.76
1:A:308:MSE:CE	1:A:334:GLY:H	1.98	0.75
1:B:188:LEU:H	1:B:188:LEU:HD23	1.52	0.75
1:B:156:MSE:O	1:B:180:PRO:HA	1.90	0.72
1:A:290:ARG:HA	1:A:311:LEU:HD12	1.71	0.71
1:A:78:THR:OG1	1:A:98:LYS:HE2	1.90	0.71
1:B:386:VAL:CA	1:B:389:MSE:HE3	2.22	0.69
1:B:258:ASN:HB3	3:B:483:HOH:O	1.94	0.67
1:B:166:LEU:HD21	1:B:170:ARG:NH2	2.10	0.67
1:A:384:LYS:HE2	3:A:1062:HOH:O	1.96	0.66
1:B:275:LYS:HD2	1:B:347:GLU:OE2	1.97	0.64
1:B:357:LEU:HD11	1:B:410:VAL:HG13	1.80	0.64
1:A:196:ILE:O	1:A:200:ILE:HG12	1.98	0.63
1:A:212:SER:OG	1:A:214:VAL:HG13	1.99	0.63
1:A:290:ARG:HB3	1:A:290:ARG:NH1	2.12	0.62
1:A:104:HIS:C	1:A:106:GLY:H	2.02	0.62
1:B:166:LEU:HD21	1:B:170:ARG:HH21	1.64	0.61
1:B:257:SER:O	1:B:260:ILE:HG22	2.00	0.61
1:A:271:GLU:HG3	1:A:272:GLY:N	2.14	0.61
1:B:352:THR:OG1	1:B:355:GLU:HG3	2.01	0.60
1:B:128:VAL:CG2	1:B:209:ILE:HG13	2.32	0.59
1:B:192:THR:HG22	1:B:327:GLY:HA3	1.84	0.59
1:A:354:GLU:O	1:A:358:GLU:HG3	2.02	0.59
1:A:409:GLU:HG3	1:A:412:ARG:NH2	2.16	0.59
1:A:164:GLN:O	1:A:168:VAL:HG23	2.03	0.59
1:B:17:THR:HA	1:B:63:LEU:HD13	1.85	0.58
1:A:308:MSE:HE3	1:A:334:GLY:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLU:HB2	1:A:399:LEU:O	2.04	0.57
1:B:155:TYR:CE2	1:B:179:ARG:HD2	2.40	0.57
1:B:357:LEU:HD21	1:B:414:LEU:HD21	1.85	0.57
1:B:116:GLN:HG2	1:B:222:MSE:HE3	1.86	0.56
1:B:163:ARG:HG3	1:B:164:GLN:HG2	1.87	0.56
1:B:406:ASP:O	1:B:410:VAL:HG23	2.06	0.56
1:A:390:ASP:HB2	1:A:393:GLN:HG3	1.88	0.56
1:B:386:VAL:N	1:B:387:PRO:HD2	2.21	0.55
1:A:224:ARG:HD3	1:A:336:GLU:OE1	2.06	0.55
1:A:257:SER:O	1:A:260:ILE:HG22	2.06	0.55
1:B:92:GLY:HA3	1:B:386:VAL:O	2.06	0.55
1:A:50:GLU:OE2	1:A:217:HIS:NE2	2.40	0.55
1:B:365:ARG:NH1	3:B:521:HOH:O	2.33	0.54
1:B:164:GLN:O	1:B:168:VAL:HG23	2.08	0.54
1:A:308:MSE:HE1	1:A:334:GLY:H	1.73	0.53
1:A:411:MSE:HE3	1:B:169:PHE:CD1	2.44	0.53
1:A:391:LYS:HD3	3:A:1107:HOH:O	2.07	0.53
1:B:42:LEU:HD21	1:B:199:TRP:CZ3	2.44	0.53
1:B:188:LEU:H	1:B:188:LEU:CD2	2.21	0.53
1:A:158:GLU:O	1:A:162:ARG:HD2	2.08	0.52
1:B:125:LYS:HE3	1:B:203:VAL:O	2.09	0.52
1:B:188:LEU:HD23	1:B:188:LEU:N	2.23	0.52
1:B:385:VAL:O	1:B:389:MSE:HG3	2.10	0.52
1:B:44:PRO:HG2	3:B:468:HOH:O	2.09	0.51
1:A:170:ARG:O	1:A:174:LEU:HD22	2.10	0.51
1:A:258:ASN:HB3	3:A:1092:HOH:O	2.10	0.51
1:A:277:ILE:HG21	1:A:381:TYR:CE2	2.46	0.51
1:B:156:MSE:HE2	1:B:160:ASP:HB3	1.93	0.51
1:B:219:TYR:O	1:B:223:VAL:HG23	2.10	0.51
1:B:196:ILE:O	1:B:200:ILE:HG12	2.11	0.51
1:A:113:THR:HG21	1:A:140:SER:OG	2.11	0.50
1:B:123:MSE:HE2	1:B:125:LYS:NZ	2.27	0.50
1:A:291:HIS:O	1:A:295:ILE:HG13	2.11	0.50
1:B:116:GLN:CG	1:B:222:MSE:HE3	2.41	0.50
1:B:42:LEU:HG	1:B:200:ILE:HD11	1.94	0.50
1:B:81:TYR:O	1:B:96:PHE:HA	2.11	0.50
1:A:24:PRO:HG3	1:A:221:MSE:HB2	1.94	0.50
1:A:308:MSE:HE1	1:A:333:VAL:H	1.77	0.50
1:B:217:HIS:ND1	1:B:218:PRO:HA	2.26	0.50
1:A:290:ARG:HH11	1:A:290:ARG:CB	2.20	0.49
1:B:42:LEU:CD1	1:B:328:LEU:HD21	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HD11	1:B:407:VAL:HG13	1.94	0.49
1:A:252:ALA:O	1:A:258:ASN:ND2	2.46	0.49
1:B:402:ARG:HD2	1:B:404:ASP:OD2	2.13	0.49
1:A:246:PRO:O	1:A:274:PRO:HB3	2.12	0.49
1:A:178:VAL:O	1:A:180:PRO:HD3	2.12	0.49
1:A:414:LEU:HD12	1:A:415:GLY:N	2.28	0.49
1:B:218:PRO:HB2	1:B:221:MSE:HE2	1.94	0.49
1:B:85:ARG:HD3	1:B:366:LEU:O	2.13	0.49
1:A:308:MSE:CE	1:A:332:GLY:HA3	2.43	0.49
1:A:214:VAL:HG22	1:A:214:VAL:O	2.12	0.49
1:A:155:TYR:CE2	1:A:194:GLU:HG3	2.47	0.49
1:B:277:ILE:HG21	1:B:381:TYR:CE2	2.48	0.49
1:A:414:LEU:HD12	1:A:415:GLY:H	1.78	0.49
1:A:308:MSE:CE	1:A:333:VAL:H	2.25	0.49
1:B:38:VAL:CG1	1:B:42:LEU:HB3	2.43	0.48
1:A:255:GLY:N	3:A:1163:HOH:O	2.45	0.48
1:B:129:ILE:HD11	1:B:199:TRP:HB2	1.95	0.48
1:B:410:VAL:HG12	1:B:414:LEU:HD12	1.94	0.48
1:A:411:MSE:HB2	1:B:169:PHE:CD2	2.49	0.48
1:A:330:TYR:CD2	1:A:331:PRO:HD2	2.48	0.48
1:B:409:GLU:HG3	1:B:412:ARG:NH2	2.27	0.48
1:B:116:GLN:CD	1:B:222:MSE:HE3	2.34	0.48
1:B:48:GLU:OE2	1:B:48:GLU:HA	2.13	0.48
1:A:308:MSE:HE1	1:A:332:GLY:C	2.34	0.48
1:B:224:ARG:HG3	1:B:336:GLU:OE1	2.13	0.48
1:A:217:HIS:ND1	1:A:218:PRO:HA	2.29	0.48
1:B:390:ASP:HB3	1:B:392:ASP:OD1	2.14	0.48
1:A:411:MSE:SE	1:B:169:PHE:HB2	2.63	0.47
1:B:42:LEU:HD11	1:B:328:LEU:HD21	1.96	0.47
1:B:197:ARG:HH11	1:B:197:ARG:HG3	1.79	0.47
1:B:103:LEU:HD12	1:B:108:HIS:HA	1.95	0.47
1:B:271:GLU:HA	1:B:271:GLU:OE1	2.13	0.47
1:A:104:HIS:C	1:A:106:GLY:N	2.67	0.47
1:B:340:TYR:HB3	1:B:346:ALA:HB3	1.97	0.47
1:B:405:LYS:HG3	1:B:406:ASP:N	2.29	0.47
1:A:262:LEU:HD22	1:A:398:ASN:HB2	1.96	0.47
1:B:98:LYS:HE2	1:B:234:VAL:HG23	1.97	0.46
1:A:368:GLY:HA2	1:B:174:LEU:HD12	1.96	0.46
1:B:128:VAL:HG21	1:B:209:ILE:CD1	2.45	0.46
1:A:98:LYS:HD2	1:A:98:LYS:HA	1.61	0.45
1:B:160:ASP:HA	1:B:163:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ARG:HB3	1:A:206:THR:HG22	1.99	0.45
1:B:409:GLU:HG3	1:B:412:ARG:HH22	1.80	0.45
1:B:141:VAL:HG13	1:B:209:ILE:HD12	1.99	0.45
1:B:131:GLU:OE1	1:B:208:TYR:OH	2.31	0.45
1:A:374:GLU:O	1:A:377:HIS:HB2	2.17	0.45
1:B:231:GLY:HA3	1:B:265:PRO:CG	2.48	0.44
1:A:412:ARG:C	1:A:414:LEU:H	2.20	0.44
1:A:184:GLY:HA3	1:A:190:ASP:OD2	2.18	0.44
1:A:308:MSE:HE1	1:A:332:GLY:HA3	2.00	0.44
1:A:386:VAL:N	1:A:387:PRO:CD	2.81	0.44
1:A:37:TYR:HB2	1:A:305:GLY:HA2	2.00	0.44
1:A:78:THR:O	1:A:98:LYS:HE3	2.18	0.43
1:A:330:TYR:CG	1:A:331:PRO:HD2	2.53	0.43
1:A:59:ASP:OD1	1:A:61:ALA:HB3	2.18	0.43
1:B:156:MSE:HB3	1:B:161:VAL:CG2	2.48	0.43
1:A:358:GLU:HB2	3:A:1039:HOH:O	2.18	0.43
1:B:212:SER:OG	1:B:214:VAL:HG22	2.18	0.43
1:A:146:ALA:O	1:B:85:ARG:NH1	2.46	0.43
1:B:18:LEU:HD22	1:B:19:PRO:HD2	2.00	0.43
1:A:308:MSE:HE1	1:A:332:GLY:CA	2.49	0.43
1:A:260:ILE:CG2	1:A:261:GLY:N	2.82	0.43
1:B:129:ILE:HG13	1:B:208:TYR:HD1	1.84	0.43
1:B:380:ALA:O	1:B:383:ALA:HB3	2.19	0.43
1:A:169:PHE:CZ	1:B:411:MSE:HA	2.53	0.43
1:B:260:ILE:HD11	1:B:336:GLU:HG2	2.01	0.43
1:A:273:ARG:HG2	1:A:274:PRO:O	2.19	0.43
1:A:333:VAL:O	1:A:333:VAL:CG1	2.67	0.42
1:A:241:LEU:HD23	1:A:242:PHE:CE2	2.54	0.42
1:A:158:GLU:HB3	1:A:162:ARG:HH11	1.84	0.42
1:A:24:PRO:HB3	1:A:30:PHE:CE1	2.54	0.42
1:A:406:ASP:O	1:A:410:VAL:HG23	2.19	0.42
1:B:249:LEU:HD23	1:B:396:VAL:HB	2.02	0.42
1:B:224:ARG:HG2	1:B:260:ILE:HG13	2.02	0.42
1:A:125:LYS:HE2	3:A:1099:HOH:O	2.18	0.42
1:A:203:VAL:HG13	1:A:204:ARG:N	2.34	0.42
1:A:28:GLY:HA3	1:A:217:HIS:CG	2.55	0.42
1:A:50:GLU:OE2	1:A:54:ARG:NH1	2.52	0.42
1:A:411:MSE:CE	1:B:169:PHE:HB2	2.49	0.42
1:B:233:GLU:O	1:B:237:GLN:HG3	2.20	0.42
1:A:181:VAL:HG21	1:A:191:ALA:HA	2.02	0.42
1:A:110:ILE:HA	1:A:113:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:VAL:HG12	1:B:334:GLY:CA	2.50	0.41
1:B:371:PRO:O	1:B:403:GLY:HA3	2.20	0.41
1:B:50:GLU:OE2	1:B:54:ARG:NH1	2.52	0.41
1:A:37:TYR:HE1	1:A:307:TYR:HB2	1.86	0.41
1:A:303:LEU:HB2	1:A:310:LEU:HD21	2.02	0.41
1:A:162:ARG:HD2	1:A:162:ARG:N	2.35	0.41
1:A:308:MSE:CE	1:A:333:VAL:N	2.75	0.41
1:B:170:ARG:O	1:B:174:LEU:CD2	2.68	0.41
1:B:413:LEU:HD12	1:B:414:LEU:HG	2.02	0.41
1:A:92:GLY:HA3	1:A:386:VAL:O	2.21	0.41
1:B:54:ARG:HG3	3:B:467:HOH:O	2.19	0.41
1:A:19:PRO:O	1:A:57:LYS:NZ	2.51	0.41
1:B:37:TYR:C	1:B:37:TYR:CD1	2.94	0.41
1:A:33:TYR:CD2	1:A:308:MSE:HA	2.55	0.41
1:B:132:THR:HG23	1:B:156:MSE:HG3	2.02	0.41
1:B:66:LEU:O	1:B:70:LEU:HG	2.21	0.41
1:A:36:ARG:HG3	1:A:36:ARG:O	2.21	0.41
1:B:258:ASN:OD1	1:B:398:ASN:ND2	2.54	0.41
1:A:168:VAL:HG12	1:A:172:LYS:HE3	2.03	0.40
1:A:29:ARG:NH2	1:A:37:TYR:OH	2.49	0.40
1:A:59:ASP:HA	1:A:60:PRO:HD3	1.97	0.40
1:B:273:ARG:HG2	1:B:274:PRO:O	2.20	0.40
1:A:164:GLN:NE2	1:A:164:GLN:HA	2.36	0.40
1:A:43:ILE:O	1:A:47:GLU:HG2	2.22	0.40
1:B:36:ARG:HG2	3:B:443:HOH:O	2.21	0.40
1:A:168:VAL:HA	1:A:171:MSE:HE3	2.02	0.40
1:A:369:ILE:O	1:A:371:PRO:HD3	2.22	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	381/418 (91%)	361 (95%)	15 (4%)	5 (1%)	15	26
1	B	348/418 (83%)	332 (95%)	14 (4%)	2 (1%)	30	50
All	All	729/836 (87%)	693 (95%)	29 (4%)	7 (1%)	19	34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	GLU
1	A	257	SER
1	A	105	THR
1	A	183	ALA
1	A	254	GLY
1	B	413	LEU
1	B	389	MSE

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	296/311 (95%)	281 (95%)	15 (5%)	29	52
1	B	277/311 (89%)	265 (96%)	12 (4%)	35	61
All	All	573/622 (92%)	546 (95%)	27 (5%)	32	56

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	54	ARG
1	A	118	LEU
1	A	162	ARG
1	A	174	LEU
1	A	197	ARG
1	A	213	VAL
1	A	214	VAL
1	A	218	PRO

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Mol	Chain	Res	Type
1	A	258	ASN
1	A	273	ARG
1	A	310	LEU
1	A	330	TYR
1	A	371	PRO
1	A	399	LEU
1	B	36	ARG
1	B	42	LEU
1	B	54	ARG
1	B	131	GLU
1	B	136	GLN
1	B	190	ASP
1	B	218	PRO
1	B	236	ARG
1	B	258	ASN
1	B	271	GLU
1	B	354	GLU
1	B	398	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	164	GLN
1	A	291	HIS
1	A	304	HIS
1	A	398	ASN
1	B	94	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

Of 1 ligands modelled in this entry, 1 is 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.

No monomer is involved in short contacts.

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, 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	377/418 (90%)	-0.12	12 (3%) 51 56	15, 29, 55, 79	2 (0%)
1	B	347/418 (83%)	0.04	23 (6%) 22 24	15, 31, 68, 90	1 (0%)
All	All	724/836 (86%)	-0.04	35 (4%) 34 39	15, 30, 62, 90	3 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	190	ASP	7.8
1	A	285	GLY	6.2
1	B	189	LYS	6.0
1	B	282	ALA	5.8
1	B	188	LEU	5.3
1	A	286	LEU	4.5
1	B	191	ALA	4.1
1	B	272	GLY	4.1
1	A	187	THR	3.9
1	B	187	THR	3.9
1	A	414	LEU	3.8
1	A	284	GLU	3.6
1	B	270	PRO	3.5
1	B	271	GLU	3.4
1	B	281	ALA	3.2
1	B	357	LEU	3.2
1	B	255	GLY	2.8
1	A	312	TYR	2.8
1	B	162	ARG	2.8
1	B	325	SER	2.8
1	B	412	ARG	2.6
1	A	311	LEU	2.4
1	A	42	LEU	2.4
1	B	178	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	399	LEU	2.3
1	A	255	GLY	2.3
1	B	414	LEU	2.3
1	B	323	SER	2.2
1	A	412	ARG	2.2
1	A	283	GLY	2.2
1	B	413	LEU	2.2
1	A	185	SER	2.2
1	B	259	ALA	2.1
1	B	324	VAL	2.1
1	B	163	ARG	2.1

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](#)

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, 95th 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CL	A	1001	1/1	0.99	0.18	-0.09	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.