



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:54 PM EDT

PDB ID : 2YZG / pdb_00002yzg
Title : Crystal structure of D-ALA:D-ALA Ligase from *Thermus thermophilus* HB8
Authors : Kitamura, Y.; Yokoyama, S.; Kuramitsu, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-05-05
Resolution : 2.30 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)
Xtriage (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

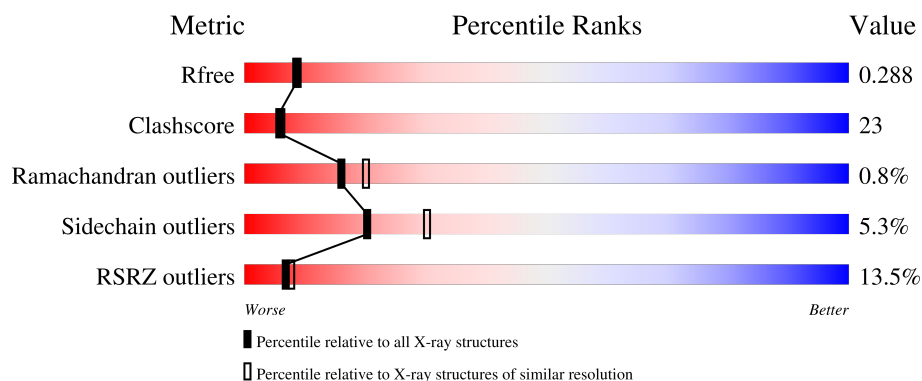
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	319	8% 66% 30% .
1	B	319	12% 60% 31% 6% .
1	C	319	20% 63% 31% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7393 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 D-alanine–D-alanine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	Se	0	0	0
			2453	1593	406	449	1	4			
1	B	311	Total	C	N	O	S	Se	0	0	0
			2377	1543	397	432	1	4			
1	C	309	Total	C	N	O	S	Se	0	0	0
			2359	1529	395	430	1	4			

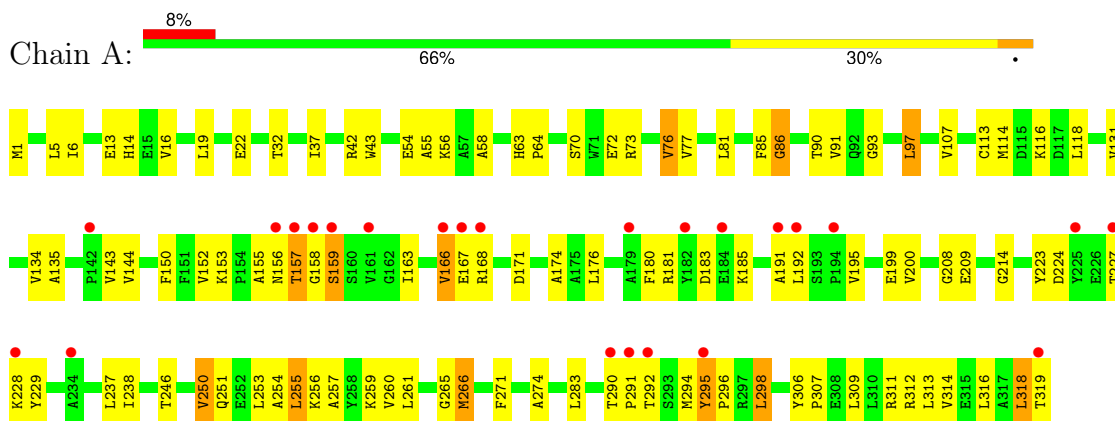
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	85	Total	O	0	0
			85	85		
2	B	57	Total	O	0	0
			57	57		
2	C	62	Total	O	0	0
			62	62		

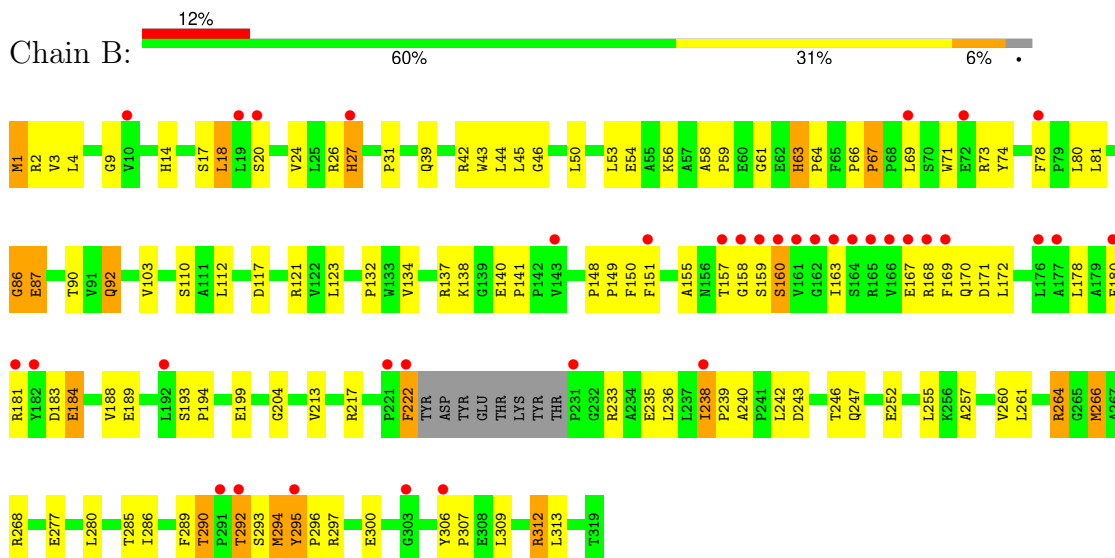
3 Residue-property plots

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.

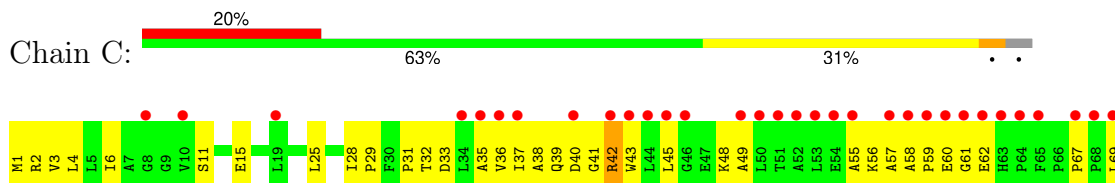
• Molecule 1: D-alanine–D-alanine ligase

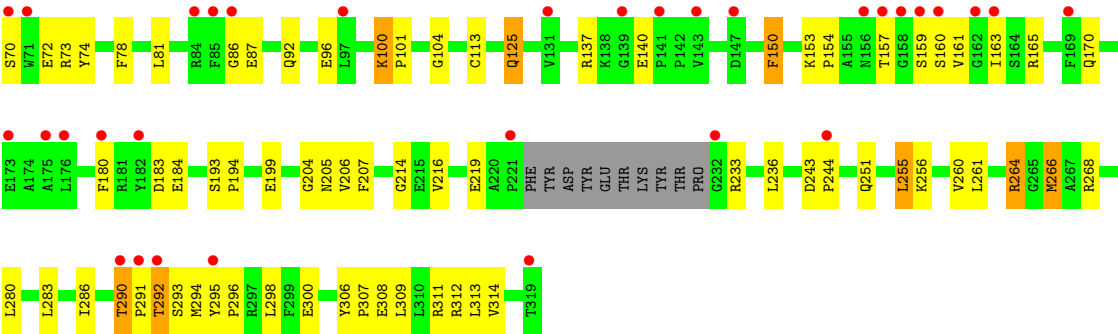


• Molecule 1: D-alanine–D-alanine ligase



• Molecule 1: D-alanine–D-alanine ligase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.22Å 56.41Å 142.21Å 90.00° 109.08° 90.00°	Depositor
Resolution (Å)	44.09 – 2.30 44.09 – 2.31	Depositor EDS
% Data completeness (in resolution range)	96.4 (44.09-2.30) 96.5 (44.09-2.31)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.27 (at 2.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.290 0.242 , 0.288	Depositor DCC
R_{free} test set	5573 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7393	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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

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	0.48	0/2515	0.96	8/3425 (0.2%)
1	B	0.43	0/2435	0.98	11/3313 (0.3%)
1	C	0.49	0/2415	0.94	6/3286 (0.2%)
All	All	0.47	0/7365	0.96	25/10024 (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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	264	ARG	N-CA-C	8.05	123.16	112.13
1	C	264	ARG	N-CA-C	7.71	123.27	113.55
1	B	66	PRO	CA-C-N	7.53	125.16	119.66
1	B	66	PRO	C-N-CA	7.53	125.16	119.66
1	B	155	ALA	N-CA-C	7.48	119.22	111.14
1	C	268	ARG	N-CA-C	-6.66	98.34	109.07
1	B	290	THR	N-CA-C	-6.58	101.78	109.93
1	B	160	SER	N-CA-C	-6.36	105.17	114.39
1	A	144	VAL	CA-C-N	6.26	126.38	119.87
1	A	144	VAL	C-N-CA	6.26	126.38	119.87
1	B	63	HIS	N-CA-C	6.21	117.48	109.72
1	C	300	GLU	N-CA-C	-6.00	104.82	111.36
1	A	209	GLU	N-CA-C	-5.78	100.29	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	TYR	N-CA-C	5.66	118.53	110.10
1	A	107	VAL	N-CA-C	5.50	115.70	110.42
1	B	58	ALA	CA-C-N	5.48	125.13	119.05
1	B	58	ALA	C-N-CA	5.48	125.13	119.05
1	B	300	GLU	N-CA-C	-5.44	105.25	111.07
1	B	67	PRO	N-CA-C	5.40	115.65	110.47
1	C	32	THR	N-CA-C	5.21	117.56	108.76
1	A	208	GLY	N-CA-C	5.19	120.78	112.58
1	A	318	LEU	N-CA-C	-5.14	106.85	113.02
1	A	63	HIS	N-CA-C	5.12	117.70	109.15
1	C	104	GLY	N-CA-C	5.09	119.30	112.17
1	C	41	GLY	N-CA-C	-5.01	108.21	115.27

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	295	TYR	Sidechain
1	B	295	TYR	Sidechain

5.2 Too-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 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	2453	0	2470	114	0
1	B	2377	0	2406	118	0
1	C	2359	0	2389	105	0
2	A	85	0	0	3	0
2	B	57	0	0	2	0
2	C	62	0	0	1	0
All	All	7393	0	7265	335	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 23.

All (335) 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:266:MSE:SE	1:A:295:TYR:HE1	1.83	1.11
1:B:266:MSE:SE	1:B:295:TYR:HE1	1.84	1.08
1:A:266:MSE:SE	1:A:295:TYR:CE1	2.56	1.07
1:A:266:MSE:HG3	1:A:313:LEU:HD21	1.31	1.07
1:C:266:MSE:HG3	1:C:313:LEU:HD21	1.31	1.07
1:B:266:MSE:SE	1:B:295:TYR:CE1	2.61	1.04
1:B:266:MSE:HG3	1:B:313:LEU:HD21	1.45	0.97
1:C:1:MSE:HE1	1:C:314:VAL:HG11	1.43	0.97
1:C:266:MSE:SE	1:C:295:TYR:OH	2.39	0.90
1:B:26:ARG:HH21	1:B:26:ARG:HB3	1.36	0.89
1:C:266:MSE:SE	1:C:295:TYR:CE1	2.76	0.88
1:B:260:VAL:HG23	1:B:261:LEU:HD22	1.54	0.88
1:A:266:MSE:HE2	1:A:309:LEU:HD11	1.53	0.88
1:B:312:ARG:HH11	1:B:312:ARG:HB3	1.40	0.86
1:C:266:MSE:CE	1:C:295:TYR:HE1	1.88	0.84
1:A:251:GLN:O	1:A:255:LEU:HD22	1.80	0.82
1:C:205:ASN:O	1:C:206:VAL:HG22	1.80	0.81
1:C:290:THR:HG22	1:C:292:THR:H	1.45	0.81
1:C:87:GLU:HB3	1:C:286:ILE:HD12	1.63	0.80
1:C:266:MSE:SE	1:C:295:TYR:HE1	2.13	0.79
1:A:195:VAL:HG12	1:A:274:ALA:HB2	1.63	0.79
1:C:199:GLU:HB2	1:C:294:MSE:HE2	1.62	0.79
1:A:55:ALA:O	1:A:56:LYS:HG3	1.83	0.79
1:B:306:TYR:HB3	1:B:307:PRO:HD3	1.65	0.78
1:C:74:TYR:O	1:C:100:LYS:HE2	1.84	0.78
1:B:123:LEU:HD21	1:B:261:LEU:HD21	1.65	0.77
1:B:26:ARG:HB3	1:B:26:ARG:NH2	1.99	0.76
1:C:266:MSE:CE	1:C:309:LEU:HD11	2.14	0.76
1:B:266:MSE:HE1	1:B:309:LEU:HD21	1.68	0.75
1:B:290:THR:OG1	1:B:292:THR:HG23	1.87	0.75
1:C:1:MSE:CE	1:C:314:VAL:HG11	2.16	0.74
1:B:50:LEU:O	1:B:54:GLU:HG3	1.88	0.74
1:B:148:PRO:HD3	1:B:169:PHE:CE1	2.23	0.73
1:A:246:THR:O	1:A:250:VAL:HG12	1.88	0.73
1:C:266:MSE:SE	1:C:295:TYR:CZ	2.92	0.73
1:A:266:MSE:CE	1:A:295:TYR:HE1	2.01	0.72
1:B:233:ARG:HB3	1:B:233:ARG:NH1	2.05	0.72
1:A:113:CYS:SG	1:A:261:LEU:HD23	2.30	0.72
1:A:266:MSE:HE1	1:A:309:LEU:HD21	1.71	0.72
1:A:266:MSE:CE	1:A:309:LEU:HD11	2.19	0.72
1:C:36:VAL:HG23	1:C:49:ALA:HB1	1.71	0.72
1:C:290:THR:CG2	1:C:292:THR:H	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:SER:C	1:C:163:ILE:HD13	2.16	0.71
1:C:290:THR:HG23	1:C:291:PRO:HD2	1.71	0.71
1:B:168:ARG:HH21	1:B:170:GLN:NE2	1.89	0.70
1:B:92:GLN:H	1:B:92:GLN:NE2	1.88	0.70
1:B:39:GLN:HE21	1:B:59:PRO:HA	1.55	0.70
1:B:238:ILE:HD12	1:B:239:PRO:CA	2.21	0.70
1:B:285:THR:C	1:B:286:ILE:HD12	2.16	0.70
1:C:55:ALA:O	1:C:56:LYS:HB2	1.91	0.70
1:A:266:MSE:SE	1:A:295:TYR:OH	2.59	0.70
1:A:266:MSE:CE	1:A:295:TYR:CE1	2.75	0.69
1:A:266:MSE:SE	1:A:295:TYR:CZ	2.95	0.68
1:B:297:ARG:HH21	1:B:297:ARG:HG2	1.58	0.68
1:C:206:VAL:HG23	1:C:207:PHE:CD1	2.27	0.68
1:A:6:ILE:HG22	1:A:81:LEU:HD21	1.74	0.68
1:A:290:THR:CG2	1:A:292:THR:HG22	2.24	0.68
1:B:39:GLN:NE2	1:B:59:PRO:HA	2.08	0.68
1:A:42:ARG:NH2	1:A:64:PRO:HG3	2.10	0.67
1:B:238:ILE:HD12	1:B:239:PRO:HA	1.77	0.67
1:A:199:GLU:HB2	1:A:294:MSE:CE	2.25	0.67
1:A:290:THR:HG21	1:A:292:THR:HG22	1.77	0.67
1:A:152:VAL:HG11	1:A:176:LEU:HD12	1.77	0.66
1:B:285:THR:O	1:B:286:ILE:HD12	1.95	0.66
1:A:116:LYS:HE2	1:A:153:LYS:HE2	1.75	0.66
1:A:156:ASN:HD21	1:A:159:SER:HB2	1.61	0.66
1:C:266:MSE:HE2	1:C:313:LEU:HD11	1.78	0.66
1:A:70:SER:HB2	1:A:73:ARG:HD3	1.78	0.65
1:B:1:MSE:HE3	1:B:2:ARG:N	2.11	0.65
1:C:199:GLU:HB2	1:C:294:MSE:CE	2.26	0.65
1:C:290:THR:HG21	1:C:292:THR:HG22	1.78	0.65
1:B:20:SER:HB2	1:B:289:PHE:HB2	1.79	0.64
1:C:39:GLN:NE2	1:C:59:PRO:HA	2.13	0.64
1:A:157:THR:HG22	1:A:158:GLY:N	2.12	0.64
1:A:156:ASN:ND2	1:A:159:SER:HB2	2.13	0.64
1:C:266:MSE:HE1	1:C:309:LEU:HD21	1.80	0.64
1:C:295:TYR:HB3	1:C:296:PRO:CD	2.28	0.63
1:B:295:TYR:HB2	2:B:320:HOH:O	2.00	0.62
1:A:1:MSE:HE1	1:A:318:LEU:HD11	1.81	0.62
1:A:1:MSE:CE	1:A:318:LEU:HD11	2.29	0.62
1:A:214:GLY:HA3	1:A:294:MSE:HE1	1.81	0.62
1:A:290:THR:HG22	1:A:292:THR:H	1.65	0.62
1:C:2:ARG:HG2	1:C:73:ARG:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LYS:HB3	1:A:163:ILE:HG12	1.81	0.62
1:A:157:THR:HG22	1:A:158:GLY:H	1.65	0.62
1:C:1:MSE:O	1:C:31:PRO:HD2	2.00	0.62
1:B:1:MSE:HE3	1:B:1:MSE:C	2.25	0.61
1:B:236:LEU:HG	1:B:294:MSE:HG2	1.81	0.61
1:C:266:MSE:CE	1:C:313:LEU:HD11	2.31	0.61
1:C:48:LYS:HE2	1:C:62:GLU:OE1	2.01	0.61
1:B:26:ARG:HH21	1:B:26:ARG:CB	2.11	0.61
1:C:4:LEU:HB2	1:C:74:TYR:CD2	2.35	0.61
1:B:92:GLN:H	1:B:92:GLN:HE21	1.48	0.60
1:C:243:ASP:HB3	1:C:244:PRO:HD2	1.83	0.60
1:A:266:MSE:CG	1:A:313:LEU:HD21	2.20	0.60
1:A:294:MSE:SE	1:A:298:LEU:HD13	2.51	0.60
1:B:312:ARG:HH11	1:B:312:ARG:CB	2.13	0.60
1:B:242:LEU:HB3	1:B:246:THR:HG23	1.83	0.60
1:B:257:ALA:O	1:B:261:LEU:HD23	2.01	0.60
1:B:178:LEU:HA	1:B:181:ARG:HH21	1.67	0.60
1:B:44:LEU:HD21	1:B:61:GLY:HA2	1.84	0.59
1:C:113:CYS:SG	1:C:261:LEU:HD13	2.43	0.59
1:C:153:LYS:HB3	1:C:163:ILE:HG13	1.83	0.59
1:A:81:LEU:HB2	1:A:86:GLY:HA2	1.85	0.59
1:B:236:LEU:HB3	1:B:294:MSE:HE2	1.84	0.59
1:B:2:ARG:HG2	1:B:73:ARG:O	2.02	0.58
1:B:1:MSE:O	1:B:31:PRO:HD2	2.03	0.58
1:C:40:ASP:OD1	1:C:60:GLU:HA	2.02	0.58
1:C:236:LEU:HG	1:C:294:MSE:HG2	1.84	0.58
1:A:97:LEU:HD22	1:B:90:THR:HB	1.85	0.58
1:A:306:TYR:HB3	1:A:307:PRO:HD3	1.84	0.58
1:C:290:THR:HG22	1:C:292:THR:N	2.18	0.58
1:A:228:LYS:HB3	1:A:228:LYS:NZ	2.19	0.58
1:B:160:SER:HA	1:B:163:ILE:HD12	1.86	0.58
1:C:70:SER:HB3	1:C:72:GLU:OE2	2.04	0.57
1:C:160:SER:O	1:C:163:ILE:HD13	2.02	0.57
1:C:42:ARG:HH11	1:C:42:ARG:HB2	1.67	0.57
1:A:295:TYR:HB3	1:A:296:PRO:CD	2.35	0.56
1:A:56:LYS:C	1:A:56:LYS:HD2	2.30	0.56
1:A:5:LEU:HD13	1:A:32:THR:HG21	1.87	0.56
1:A:70:SER:HB3	1:A:72:GLU:OE2	2.05	0.56
1:C:199:GLU:OE1	1:C:294:MSE:HG3	2.06	0.56
1:B:14:HIS:O	1:B:18:LEU:HD22	2.06	0.56
1:A:290:THR:HG23	1:A:291:PRO:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:THR:HG23	1:C:291:PRO:CD	2.34	0.55
1:B:148:PRO:HD3	1:B:169:PHE:HE1	1.66	0.55
1:B:45:LEU:HD22	1:B:69:LEU:HD13	1.89	0.55
1:B:236:LEU:CB	1:B:294:MSE:HE2	2.36	0.55
1:B:157:THR:O	1:B:159:SER:N	2.40	0.55
1:C:163:ILE:HD12	1:C:163:ILE:N	2.22	0.55
1:C:205:ASN:OD1	1:C:264:ARG:O	2.25	0.54
1:B:233:ARG:HB3	1:B:233:ARG:HH11	1.73	0.54
1:A:311:ARG:HG2	1:A:311:ARG:HH11	1.72	0.54
1:B:204:GLY:O	1:B:264:ARG:O	2.25	0.54
1:C:33:ASP:HB2	1:C:74:TYR:HE2	1.71	0.54
1:C:293:SER:HB2	1:C:296:PRO:HD2	1.90	0.54
1:A:237:LEU:C	1:A:238:ILE:HD12	2.32	0.54
1:A:238:ILE:HD12	1:A:238:ILE:N	2.23	0.54
1:B:81:LEU:N	1:B:81:LEU:HD22	2.22	0.54
1:B:266:MSE:CE	1:B:295:TYR:CE1	2.90	0.54
1:C:48:LYS:HE2	1:C:62:GLU:CD	2.33	0.54
1:A:143:VAL:HG13	1:A:143:VAL:O	2.07	0.54
1:B:266:MSE:CE	1:B:295:TYR:HE1	2.21	0.53
1:B:14:HIS:CE1	1:B:18:LEU:HD21	2.43	0.53
1:C:69:LEU:HD23	1:C:70:SER:N	2.24	0.53
1:A:290:THR:CG2	1:A:291:PRO:HD2	2.38	0.53
1:B:295:TYR:HB3	1:B:296:PRO:CD	2.39	0.53
1:C:290:THR:CG2	1:C:292:THR:HG22	2.38	0.53
1:B:236:LEU:CD2	1:B:294:MSE:HG2	2.39	0.53
1:C:280:LEU:C	1:C:280:LEU:HD23	2.33	0.53
1:C:137:ARG:O	1:C:140:GLU:HB2	2.08	0.53
1:B:266:MSE:SE	1:B:295:TYR:CZ	3.11	0.53
1:C:157:THR:HG21	1:C:161:VAL:HG22	1.91	0.53
1:A:14:HIS:HE1	1:A:58:ALA:H	1.57	0.53
1:A:199:GLU:HB2	1:A:294:MSE:HE2	1.90	0.52
1:C:38:ALA:HB1	1:C:58:ALA:O	2.10	0.52
1:C:43:TRP:CD2	1:C:67:PRO:HG3	2.44	0.52
1:A:260:VAL:HG13	1:A:261:LEU:HD13	1.92	0.52
1:A:283:LEU:C	1:A:283:LEU:HD23	2.35	0.52
1:A:153:LYS:CB	1:A:163:ILE:HG12	2.40	0.52
1:C:39:GLN:HE21	1:C:59:PRO:HA	1.73	0.52
1:B:9:GLY:O	1:B:14:HIS:HD2	1.92	0.52
1:A:6:ILE:HD13	1:A:77:VAL:CG1	2.40	0.51
1:A:72:GLU:CD	1:A:72:GLU:H	2.18	0.51
1:C:266:MSE:HE1	1:C:309:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ALA:HB2	1:A:185:LYS:HG2	1.93	0.51
1:B:233:ARG:HH11	1:B:233:ARG:CB	2.24	0.51
1:B:266:MSE:CE	1:B:309:LEU:HD21	2.39	0.51
1:A:228:LYS:HB3	1:A:228:LYS:HZ3	1.76	0.51
1:A:54:GLU:O	1:A:54:GLU:HG2	2.10	0.51
1:B:69:LEU:HD23	1:B:71:TRP:CZ2	2.45	0.51
1:A:158:GLY:O	1:A:159:SER:C	2.53	0.51
1:B:20:SER:O	1:B:24:VAL:HG23	2.11	0.51
1:C:266:MSE:CE	1:C:295:TYR:CE1	2.80	0.51
1:B:243:ASP:HB2	1:B:246:THR:HG22	1.92	0.50
1:B:149:PRO:HB3	1:B:167:GLU:OE2	2.11	0.50
1:B:14:HIS:O	1:B:17:SER:HB3	2.12	0.50
1:B:103:VAL:HG13	2:B:329:HOH:O	2.12	0.50
1:B:193:SER:HA	1:B:194:PRO:C	2.37	0.50
1:B:290:THR:C	1:B:292:THR:N	2.69	0.50
1:C:236:LEU:CD2	1:C:294:MSE:HG2	2.42	0.50
1:A:199:GLU:HB2	1:A:294:MSE:HE3	1.94	0.49
1:A:199:GLU:OE1	1:A:294:MSE:HG3	2.12	0.49
1:A:295:TYR:HB3	1:A:296:PRO:HD3	1.93	0.49
1:C:180:PHE:HA	1:C:183:ASP:O	2.12	0.49
1:C:251:GLN:O	1:C:255:LEU:HD22	2.12	0.49
1:B:117:ASP:O	1:B:121:ARG:HG3	2.12	0.49
1:A:76:VAL:HG21	1:A:314:VAL:HG13	1.95	0.49
1:B:290:THR:C	1:B:292:THR:H	2.20	0.49
1:B:1:MSE:CE	1:B:3:VAL:HG23	2.42	0.49
1:B:235:GLU:C	1:B:236:LEU:HD12	2.37	0.49
1:C:6:ILE:HD12	1:C:43:TRP:CZ3	2.48	0.49
1:C:157:THR:HG21	1:C:161:VAL:CG2	2.42	0.49
1:C:214:GLY:HA3	1:C:294:MSE:HE1	1.93	0.49
1:B:4:LEU:HB2	1:B:74:TYR:CD2	2.48	0.49
1:A:19:LEU:O	1:A:22:GLU:HB3	2.13	0.48
1:B:277:GLU:HA	1:B:277:GLU:OE2	2.12	0.48
1:A:311:ARG:HG2	1:A:311:ARG:NH1	2.28	0.48
1:B:137:ARG:O	1:B:140:GLU:HG2	2.14	0.48
1:A:42:ARG:HH21	1:A:64:PRO:HG3	1.76	0.48
1:C:153:LYS:CB	1:C:163:ILE:HG13	2.42	0.48
1:A:116:LYS:NZ	1:A:156:ASN:O	2.46	0.48
1:A:266:MSE:CE	1:A:309:LEU:HD21	2.42	0.48
1:B:168:ARG:HH21	1:B:170:GLN:HE21	1.61	0.48
1:B:42:ARG:NH1	1:B:64:PRO:HG3	2.29	0.47
1:C:311:ARG:HD3	1:C:311:ARG:C	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:TRP:CE3	1:C:67:PRO:HG3	2.49	0.47
1:C:266:MSE:HE2	1:C:309:LEU:HD11	1.95	0.47
1:B:236:LEU:CG	1:B:294:MSE:HG2	2.44	0.47
1:C:28:ILE:HG13	1:C:29:PRO:HD2	1.96	0.47
1:A:55:ALA:O	1:A:56:LYS:CG	2.60	0.47
1:B:240:ALA:HB3	1:B:242:LEU:CD2	2.44	0.47
1:C:6:ILE:HD13	1:C:35:ALA:HB3	1.95	0.47
1:A:13:GLU:O	1:A:16:VAL:HG12	2.15	0.47
1:A:93:GLY:O	1:A:97:LEU:HD22	2.14	0.47
1:A:70:SER:CB	1:A:73:ARG:HD3	2.43	0.47
1:C:56:LYS:O	1:C:57:ALA:HB2	2.15	0.47
1:A:181:ARG:HG2	1:A:181:ARG:HH11	1.79	0.47
1:C:256:LYS:O	1:C:260:VAL:HG23	2.15	0.47
1:B:81:LEU:HB2	1:B:86:GLY:HA2	1.97	0.47
1:B:138:LYS:HA	1:B:180:PHE:CE1	2.50	0.47
1:A:180:PHE:HA	1:A:183:ASP:O	2.14	0.47
1:B:53:LEU:O	1:B:56:LYS:HD2	2.15	0.47
1:C:42:ARG:HB2	1:C:42:ARG:NH1	2.28	0.47
1:A:260:VAL:HG13	1:A:261:LEU:CD1	2.45	0.46
1:A:266:MSE:HE1	1:A:295:TYR:CE1	2.50	0.46
1:C:236:LEU:HD23	1:C:294:MSE:HA	1.97	0.46
1:B:280:LEU:C	1:B:280:LEU:HD23	2.40	0.46
1:B:238:ILE:HD12	1:B:239:PRO:N	2.29	0.46
1:C:42:ARG:HH11	1:C:42:ARG:CB	2.28	0.46
1:B:268:ARG:HB2	1:B:295:TYR:CD2	2.51	0.45
1:B:268:ARG:CA	1:B:295:TYR:HE2	2.29	0.45
1:C:295:TYR:HB3	1:C:296:PRO:HD3	1.98	0.45
1:A:81:LEU:HD12	1:A:91:VAL:HG21	1.99	0.45
1:A:257:ALA:HA	1:A:260:VAL:HG12	1.97	0.45
1:B:290:THR:CB	1:B:292:THR:HG23	2.46	0.45
1:A:295:TYR:HB2	2:A:320:HOH:O	2.17	0.45
1:B:233:ARG:NH1	1:B:233:ARG:CB	2.79	0.45
1:B:286:ILE:HG22	1:B:286:ILE:O	2.16	0.45
1:C:33:ASP:HB2	1:C:74:TYR:CE2	2.50	0.45
1:C:61:GLY:O	1:C:62:GLU:HG3	2.16	0.45
1:C:92:GLN:O	1:C:96:GLU:HG2	2.16	0.45
1:B:170:GLN:HG3	1:B:171:ASP:OD1	2.16	0.45
1:A:14:HIS:CE1	1:A:58:ALA:H	2.34	0.45
1:A:266:MSE:HE1	1:A:295:TYR:HE1	1.81	0.45
1:C:204:GLY:O	1:C:264:ARG:O	2.34	0.45
1:B:199:GLU:OE2	1:B:294:MSE:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:MSE:HA	1:A:157:THR:HB	1.98	0.44
1:B:213:VAL:CG2	1:B:247:GLN:HG3	2.47	0.44
1:A:192:LEU:HD12	1:A:192:LEU:N	2.32	0.44
1:A:256:LYS:O	1:A:260:VAL:HG12	2.17	0.44
1:C:170:GLN:OE1	1:C:170:GLN:N	2.48	0.44
1:A:42:ARG:HH21	1:A:42:ARG:HG2	1.82	0.44
1:B:266:MSE:SE	1:B:295:TYR:OH	2.85	0.44
1:C:261:LEU:HD12	1:C:283:LEU:HD13	1.99	0.44
1:B:151:PHE:O	1:B:188:VAL:HA	2.17	0.44
1:C:39:GLN:HE21	1:C:39:GLN:HB2	1.56	0.44
1:C:236:LEU:CG	1:C:294:MSE:HG2	2.48	0.44
1:C:290:THR:HB	1:C:293:SER:OG	2.18	0.44
1:A:224:ASP:HB3	1:A:227:THR:HG22	2.00	0.44
1:B:123:LEU:CD2	1:B:261:LEU:HD21	2.41	0.44
1:B:160:SER:HA	1:B:163:ILE:CD1	2.48	0.43
1:B:222:PHE:CD1	1:B:222:PHE:N	2.86	0.43
1:C:306:TYR:HB3	1:C:307:PRO:HD3	2.00	0.43
1:C:78:PHE:CD1	1:C:78:PHE:C	2.94	0.43
1:C:165:ARG:HG2	1:C:165:ARG:HH21	1.83	0.43
1:B:268:ARG:HA	1:B:295:TYR:HE2	1.82	0.43
1:C:154:PRO:HG2	1:C:157:THR:HB	1.99	0.43
1:C:295:TYR:HB2	2:C:320:HOH:O	2.17	0.43
1:A:6:ILE:HG23	1:A:37:ILE:HD13	1.99	0.43
1:A:157:THR:CG2	1:A:158:GLY:N	2.79	0.43
1:C:159:SER:OG	1:C:161:VAL:HG22	2.18	0.43
1:A:191:ALA:C	1:A:192:LEU:HD12	2.43	0.43
1:A:259:LYS:HD3	1:A:259:LYS:C	2.43	0.43
1:B:26:ARG:O	1:B:27:HIS:CG	2.72	0.43
1:B:63:HIS:HA	1:B:64:PRO:HD3	1.82	0.43
1:B:87:GLU:O	1:B:110:SER:HB3	2.18	0.43
1:B:78:PHE:CE1	1:B:80:LEU:HD13	2.54	0.43
1:B:184:GLU:OE1	1:B:184:GLU:HA	2.19	0.43
1:B:297:ARG:HH21	1:B:297:ARG:CG	2.30	0.43
1:A:1:MSE:HE3	1:A:318:LEU:HD11	2.01	0.43
1:A:85:PHE:HA	1:A:90:THR:OG1	2.19	0.43
1:C:2:ARG:HG3	1:C:74:TYR:CD2	2.52	0.43
1:C:150:PHE:HD2	1:C:150:PHE:O	2.02	0.43
1:A:167:GLU:HB3	1:A:168:ARG:HD3	2.00	0.43
1:A:312:ARG:HD2	2:A:332:HOH:O	2.19	0.43
1:B:150:PHE:HB2	1:B:189:GLU:O	2.19	0.43
1:A:5:LEU:HD13	1:A:32:THR:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:VAL:HG13	1:A:192:LEU:HD11	2.00	0.42
1:C:36:VAL:HG12	1:C:37:ILE:N	2.34	0.42
1:B:81:LEU:HD22	1:B:81:LEU:H	1.84	0.42
1:B:183:ASP:OD2	1:B:184:GLU:N	2.52	0.42
1:A:312:ARG:NH2	2:A:332:HOH:O	2.52	0.42
1:B:297:ARG:HG2	1:B:297:ARG:NH2	2.30	0.42
1:C:1:MSE:HE1	1:C:3:VAL:CG2	2.50	0.42
1:B:42:ARG:HH11	1:B:42:ARG:HG2	1.85	0.42
1:A:55:ALA:C	1:A:56:LYS:HG3	2.45	0.42
1:A:250:VAL:HG23	1:A:271:PHE:CD1	2.55	0.42
1:A:265:GLY:O	1:A:266:MSE:HG2	2.20	0.42
1:A:150:PHE:CE1	1:A:166:VAL:CG2	3.03	0.41
1:A:150:PHE:CE1	1:A:166:VAL:HG22	2.55	0.41
1:B:159:SER:OG	1:B:160:SER:N	2.50	0.41
1:B:312:ARG:HH11	1:B:312:ARG:CG	2.32	0.41
1:C:125:GLN:CD	1:C:125:GLN:C	2.88	0.41
1:C:219:GLU:OE1	1:C:233:ARG:HB3	2.20	0.41
1:B:39:GLN:HE21	1:B:39:GLN:HB2	1.62	0.41
1:B:242:LEU:N	1:B:242:LEU:HD22	2.35	0.41
1:B:293:SER:HB2	1:B:296:PRO:HD2	2.02	0.41
1:C:100:LYS:HA	1:C:101:PRO:HD3	1.87	0.41
1:C:308:GLU:O	1:C:312:ARG:HG3	2.20	0.41
1:C:45:LEU:CD2	1:C:69:LEU:HD12	2.49	0.41
1:C:163:ILE:N	1:C:163:ILE:CD1	2.84	0.41
1:A:114:MSE:HE3	1:A:114:MSE:HB3	1.85	0.41
1:C:36:VAL:HG23	1:C:49:ALA:CB	2.46	0.41
1:A:316:LEU:O	1:A:319:THR:N	2.50	0.41
1:A:6:ILE:CD1	1:A:77:VAL:HG13	2.51	0.41
1:A:37:ILE:HD11	1:A:43:TRP:CH2	2.56	0.41
1:B:46:GLY:O	1:B:50:LEU:HD23	2.21	0.41
1:A:171:ASP:O	1:A:174:ALA:HB3	2.20	0.41
1:B:2:ARG:NH1	1:B:73:ARG:NH2	2.68	0.41
1:C:45:LEU:HD22	1:C:69:LEU:HD12	2.02	0.41
1:A:6:ILE:HG23	1:A:37:ILE:CD1	2.51	0.40
1:A:81:LEU:HB2	1:A:86:GLY:CA	2.51	0.40
1:B:20:SER:HB3	1:B:289:PHE:H	1.86	0.40
1:B:43:TRP:CE3	1:B:67:PRO:HG3	2.55	0.40
1:B:123:LEU:HD21	1:B:261:LEU:CD2	2.40	0.40
1:C:193:SER:HA	1:C:194:PRO:C	2.46	0.40
1:A:157:THR:CG2	1:A:158:GLY:H	2.30	0.40
1:A:200:VAL:HG11	1:A:254:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ALA:HA	1:A:260:VAL:CG1	2.51	0.40
1:C:183:ASP:OD2	1:C:184:GLU:N	2.54	0.40
1:B:140:GLU:HA	1:B:141:PRO:HD3	1.85	0.40
1:A:118:LEU:HD13	1:B:112:LEU:CD1	2.52	0.40
1:A:134:VAL:HG12	1:A:135:ALA:N	2.36	0.40
1:C:78:PHE:C	1:C:78:PHE:HD1	2.28	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	317/319 (99%)	303 (96%)	11 (4%)	3 (1%)	14	17
1	B	307/319 (96%)	283 (92%)	21 (7%)	3 (1%)	12	15
1	C	305/319 (96%)	282 (92%)	22 (7%)	1 (0%)	36	46
All	All	929/957 (97%)	868 (93%)	54 (6%)	7 (1%)	16	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	SER
1	B	158	GLY
1	B	86	GLY
1	A	86	GLY
1	A	157	THR
1	B	27	HIS
1	C	86	GLY

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	256/252 (102%)	247 (96%)	9 (4%)	32	48
1	B	248/252 (98%)	231 (93%)	17 (7%)	14	20
1	C	246/252 (98%)	232 (94%)	14 (6%)	18	27
All	All	750/756 (99%)	710 (95%)	40 (5%)	20	30

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	VAL
1	A	97	LEU
1	A	166	VAL
1	A	223	TYR
1	A	250	VAL
1	A	253	LEU
1	A	255	LEU
1	A	266	MSE
1	A	298	LEU
1	B	1	MSE
1	B	18	LEU
1	B	87	GLU
1	B	92	GLN
1	B	132	PRO
1	B	134	VAL
1	B	172	LEU
1	B	184	GLU
1	B	217	ARG
1	B	222	PHE
1	B	238	ILE
1	B	252	GLU
1	B	255	LEU
1	B	266	MSE
1	B	292	THR
1	B	294	MSE
1	B	312	ARG

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Mol	Chain	Res	Type
1	C	11	SER
1	C	15	GLU
1	C	25	LEU
1	C	42	ARG
1	C	81	LEU
1	C	100	LYS
1	C	125	GLN
1	C	150	PHE
1	C	216	VAL
1	C	255	LEU
1	C	266	MSE
1	C	290	THR
1	C	292	THR
1	C	298	LEU

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

Mol	Chain	Res	Type
1	A	14	HIS
1	A	156	ASN
1	A	247	GLN
1	A	251	GLN
1	A	281	ASN
1	A	284	ASN
1	B	14	HIS
1	B	39	GLN
1	B	63	HIS
1	B	82	HIS
1	B	92	GLN
1	B	156	ASN
1	B	170	GLN
1	B	281	ASN
1	C	39	GLN
1	C	205	ASN
1	C	247	GLN
1	C	251	GLN

5.3.3 RNA ⓘ

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	315/319 (98%)	0.48	24 (7%) 20 21	23, 36, 63, 82	0
1	B	307/319 (96%)	0.90	37 (12%) 8 9	26, 47, 75, 90	0
1	C	305/319 (95%)	0.89	64 (20%) 2 3	20, 42, 73, 82	0
All	All	927/957 (96%)	0.75	125 (13%) 7 8	20, 42, 72, 90	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	THR	6.3
1	A	161	VAL	5.8
1	B	295	TYR	4.9
1	A	158	GLY	4.7
1	B	161	VAL	4.7
1	B	222	PHE	4.7
1	B	231	PRO	4.3
1	B	158	GLY	4.2
1	B	160	SER	4.1
1	C	232	GLY	4.0
1	C	59	PRO	4.0
1	A	156	ASN	4.0
1	C	50	LEU	3.9
1	A	319	THR	3.9
1	A	159	SER	3.8
1	B	164	SER	3.8
1	C	62	GLU	3.8
1	A	227	THR	3.6
1	B	163	ILE	3.6
1	C	55	ALA	3.5
1	A	292	THR	3.5
1	A	291	PRO	3.5
1	C	51	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	166	VAL	3.4
1	A	295	TYR	3.4
1	C	84	ARG	3.4
1	C	69	LEU	3.3
1	C	60	GLU	3.3
1	B	182	TYR	3.2
1	B	238	ILE	3.2
1	C	64	PRO	3.2
1	B	169	PHE	3.2
1	A	225	TYR	3.1
1	C	43	TRP	3.1
1	C	159	SER	3.1
1	B	306	TYR	3.0
1	C	139	GLY	3.0
1	C	58	ALA	3.0
1	C	163	ILE	3.0
1	B	159	SER	3.0
1	C	68	PRO	3.0
1	C	162	GLY	3.0
1	C	44	LEU	2.9
1	C	182	TYR	2.9
1	C	158	GLY	2.9
1	C	143	VAL	2.9
1	B	72	GLU	2.9
1	B	221	PRO	2.9
1	A	192	LEU	2.9
1	B	162	GLY	2.8
1	C	61	GLY	2.8
1	C	46	GLY	2.8
1	C	131	VAL	2.8
1	A	184	GLU	2.8
1	A	182	TYR	2.7
1	C	34	LEU	2.7
1	B	27	HIS	2.6
1	C	85	PHE	2.6
1	C	295	TYR	2.6
1	B	165	ARG	2.5
1	B	143	VAL	2.5
1	A	142	PRO	2.5
1	B	291	PRO	2.5
1	C	319	THR	2.5
1	C	156	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	157	THR	2.4
1	B	292	THR	2.4
1	B	166	VAL	2.4
1	C	63	HIS	2.4
1	C	175	ALA	2.4
1	C	169	PHE	2.4
1	B	176	LEU	2.4
1	C	52	ALA	2.3
1	C	292	THR	2.3
1	C	40	ASP	2.3
1	C	67	PRO	2.3
1	C	291	PRO	2.3
1	B	177	ALA	2.3
1	C	65	PHE	2.3
1	C	53	LEU	2.3
1	C	8	GLY	2.3
1	C	221	PRO	2.3
1	C	45	LEU	2.2
1	A	194	PRO	2.2
1	C	42	ARG	2.2
1	A	234	ALA	2.2
1	C	71	TRP	2.2
1	B	69	LEU	2.2
1	C	10	VAL	2.2
1	B	303	GLY	2.2
1	A	179	ALA	2.2
1	C	36	VAL	2.2
1	C	147	ASP	2.2
1	C	244	PRO	2.2
1	C	97	LEU	2.2
1	B	78	PHE	2.2
1	C	54	GLU	2.2
1	C	173	GLU	2.2
1	A	191	ALA	2.2
1	C	70	SER	2.2
1	B	10	VAL	2.1
1	A	228	LYS	2.1
1	B	151	PHE	2.1
1	B	167	GLU	2.1
1	C	141	PRO	2.1
1	A	290	THR	2.1
1	B	19	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	37	ILE	2.1
1	C	176	LEU	2.1
1	B	180	PHE	2.1
1	B	20	SER	2.1
1	C	157	THR	2.1
1	C	160	SER	2.1
1	C	290	THR	2.1
1	C	35	ALA	2.1
1	B	192	LEU	2.1
1	C	19	LEU	2.1
1	C	180	PHE	2.1
1	B	181	ARG	2.1
1	C	57	ALA	2.0
1	B	168	ARG	2.0
1	C	86	GLY	2.0
1	A	167	GLU	2.0
1	C	49	ALA	2.0
1	A	168	ARG	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.