



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:05 PM UTC

PDB ID : 1WD7 / pdb_00001wd7
Title : Crystal Structure of Uroporphyrinogen III Synthase from an Extremely Thermophilic Bacterium *Thermus thermophilus* HB8 (Wild type, Native, Form-2 crystal)
Authors : Mizohata, E.; Matsuura, T.; Sakai, H.; Murayama, K.; Terada, T.; Shirouzu, M.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2004-05-12
Resolution : 1.60 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
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)	:	Engl & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

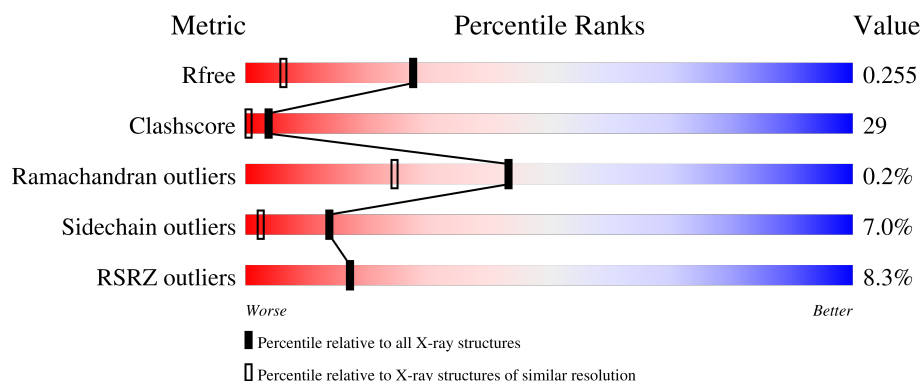
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	261	7% 65% 26% 6% ..
1	B	261	9% 69% 23% 5% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4357 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 Uroporphyrinogen III Synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1943	1252	348	342	1			
1	B	255	Total	C	N	O	S	0	0	0
			1951	1256	349	345	1			

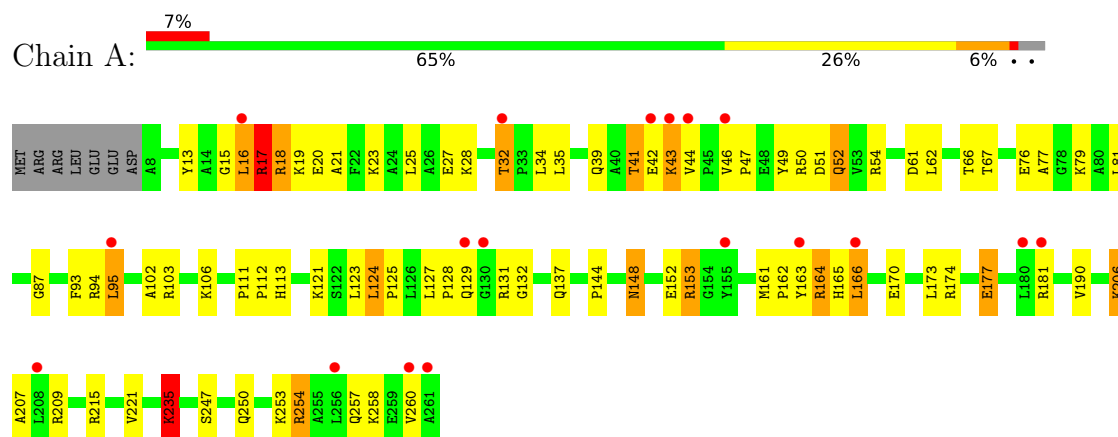
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	235	Total	O	0	0
			235	235		
2	B	228	Total	O	0	0
			228	228		

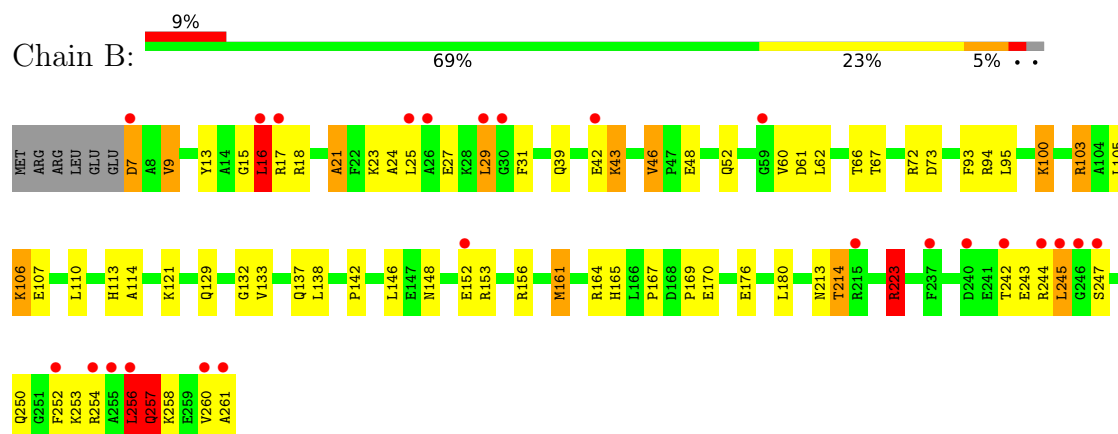
3 Residue-property plots [i](#)

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: Uroporphyrinogen III Synthase



• Molecule 1: Uroporphyrinogen III Synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	37.90Å 84.88Å 73.95Å 90.00° 91.25° 90.00°	Depositor
Resolution (Å)	37.89 – 1.60 37.89 – 1.60	Depositor EDS
% Data completeness (in resolution range)	86.7 (37.89-1.60) 86.7 (37.89-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.59Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.255 0.224 , 0.255	Depositor DCC
R_{free} test set	2710 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.056 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4357	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.38% 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	0.84	2/1979 (0.1%)	1.12	17/2678 (0.6%)
1	B	0.96	10/1987 (0.5%)	1.27	23/2689 (0.9%)
All	All	0.90	12/3966 (0.3%)	1.20	40/5367 (0.7%)

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	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	257	GLN	CA-C	12.32	1.69	1.52
1	B	257	GLN	C-O	8.09	1.34	1.24
1	B	252	PHE	N-CA	-7.63	1.36	1.46
1	B	258	LYS	CA-C	-7.62	1.42	1.52
1	B	252	PHE	CA-C	6.37	1.61	1.52
1	B	252	PHE	CB-CG	-6.18	1.36	1.50
1	B	257	GLN	CA-CB	6.00	1.63	1.53
1	B	214	THR	CA-C	5.55	1.60	1.52
1	B	256	LEU	N-CA	-5.51	1.39	1.46
1	A	52	GLN	CA-C	5.44	1.59	1.52
1	A	32	THR	CA-CB	5.25	1.60	1.53
1	B	43	LYS	CA-CB	-5.09	1.45	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	LEU	N-CA-C	-15.85	93.48	111.71
1	B	214	THR	N-CA-CB	-13.30	88.00	110.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	ARG	N-CA-C	12.01	128.63	112.90
1	B	256	LEU	CA-C-N	-11.90	100.44	120.68
1	B	256	LEU	C-N-CA	-11.90	100.44	120.68
1	B	257	GLN	CA-C-O	9.84	131.40	119.79
1	A	32	THR	CB-CA-C	9.37	119.89	110.33
1	B	257	GLN	CB-CA-C	9.14	129.02	110.38
1	A	235	LYS	CD-CE-NZ	8.82	140.13	111.90
1	A	164	ARG	NE-CZ-NH1	-8.73	112.77	121.50
1	A	164	ARG	NE-CZ-NH2	8.23	126.61	119.20
1	B	214	THR	CB-CA-C	7.97	126.27	110.42
1	B	43	LYS	N-CA-CB	-7.67	97.64	109.92
1	A	46	VAL	CA-C-N	6.64	128.15	119.84
1	A	46	VAL	C-N-CA	6.64	128.15	119.84
1	A	207	ALA	N-CA-C	-6.63	104.14	111.36
1	A	124	LEU	CA-C-N	6.59	126.53	119.28
1	A	124	LEU	C-N-CA	6.59	126.53	119.28
1	A	166	LEU	CA-C-N	-6.54	113.21	120.14
1	A	166	LEU	C-N-CA	-6.54	113.21	120.14
1	B	245	LEU	N-CA-C	-6.52	104.36	112.90
1	B	258	LYS	CA-C-N	-6.45	114.15	122.79
1	B	258	LYS	C-N-CA	-6.45	114.15	122.79
1	B	9	VAL	N-CA-C	6.10	117.16	108.93
1	B	256	LEU	O-C-N	-6.04	115.16	122.22
1	A	44	VAL	CA-C-N	6.03	125.97	119.76
1	A	44	VAL	C-N-CA	6.03	125.97	119.76
1	B	21	ALA	N-CA-C	-6.00	104.82	111.36
1	A	52	GLN	N-CA-C	-5.68	105.00	111.14
1	B	16	LEU	CA-CB-CG	5.62	135.98	116.30
1	A	235	LYS	CA-CB-CG	-5.47	103.16	114.10
1	B	257	GLN	N-CA-C	5.39	119.03	112.23
1	B	214	THR	CA-CB-CG2	5.22	119.38	110.50
1	A	166	LEU	N-CA-C	5.22	117.87	109.15
1	B	93	PHE	N-CA-C	-5.14	101.58	109.76
1	A	16	LEU	N-CA-C	-5.13	107.67	114.04
1	B	223	ARG	CG-CD-NE	5.11	123.23	112.00
1	B	46	VAL	CA-C-N	5.06	125.09	119.32
1	B	46	VAL	C-N-CA	5.06	125.09	119.32
1	B	258	LYS	N-CA-C	-5.01	107.00	113.01

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ARG	Sidechain
1	A	153	ARG	Sidechain
1	A	164	ARG	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	1943	0	2042	139	6
1	B	1951	0	2044	97	3
2	A	235	0	0	24	5
2	B	228	0	0	13	0
All	All	4357	0	4086	229	7

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 29.

All (229) 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:17:ARG:HB2	1:A:18:ARG:NE	1.42	1.33
1:B:260:VAL:CG1	1:B:261:ALA:H	1.48	1.20
1:B:244:ARG:NH2	1:B:247:SER:OG	1.79	1.15
1:A:121:LYS:NZ	2:A:494:HOH:O	1.75	1.14
1:A:177:GLU:HG2	1:A:181:ARG:HH11	1.04	1.14
1:A:173:LEU:HD21	2:A:476:HOH:O	1.46	1.10
1:B:260:VAL:HG12	1:B:261:ALA:N	1.62	1.08
1:A:17:ARG:HB2	1:A:18:ARG:CZ	1.86	1.04
1:B:94:ARG:H	1:B:113:HIS:HD2	1.06	1.03
1:B:260:VAL:HG12	1:B:261:ALA:H	0.85	1.02
1:A:18:ARG:HD2	2:A:486:HOH:O	1.61	1.01
1:B:244:ARG:CZ	1:B:247:SER:OG	2.11	0.98
1:A:173:LEU:CD2	2:A:476:HOH:O	2.04	0.97
1:A:17:ARG:CB	1:A:18:ARG:HE	1.78	0.97
1:B:129:GLN:NE2	1:B:153:ARG:HD3	1.80	0.96
1:A:17:ARG:HB3	1:A:18:ARG:HH11	1.31	0.96
1:B:29:LEU:HD23	1:B:253:LYS:HD2	1.48	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:HG2	1:A:181:ARG:NH1	1.81	0.94
1:B:244:ARG:NH1	1:B:247:SER:OG	2.01	0.93
1:A:174:ARG:NH2	2:A:267:HOH:O	2.01	0.93
1:B:25:LEU:CD2	2:B:475:HOH:O	2.15	0.93
1:A:129:GLN:HG3	1:A:153:ARG:HH21	1.34	0.91
1:A:129:GLN:CG	1:A:153:ARG:HH21	1.84	0.90
1:A:153:ARG:NH1	2:A:439:HOH:O	2.03	0.90
1:A:131:ARG:HB3	1:B:223:ARG:NH2	1.85	0.89
1:B:254:ARG:O	1:B:257:GLN:N	2.04	0.89
1:A:17:ARG:HB2	1:A:18:ARG:HE	1.11	0.88
1:A:94:ARG:H	1:A:113:HIS:HD2	1.21	0.88
1:B:25:LEU:HD22	2:B:475:HOH:O	1.74	0.88
1:A:17:ARG:CB	1:A:18:ARG:NE	2.33	0.86
1:A:19:LYS:HG2	1:A:35:LEU:HD23	1.58	0.85
1:B:129:GLN:CD	1:B:153:ARG:HD3	2.00	0.85
1:B:107:GLU:HG2	2:B:397:HOH:O	1.75	0.84
1:A:106:LYS:HD2	1:A:112:PRO:HD2	1.59	0.84
1:B:164:ARG:NH2	2:B:336:HOH:O	2.07	0.83
1:B:29:LEU:HD23	1:B:253:LYS:CD	2.09	0.83
1:A:102:ALA:HB1	1:A:106:LYS:HZ2	1.43	0.82
1:A:206:LYS:HG2	1:A:209:ARG:NH2	1.94	0.82
1:B:261:ALA:O	2:B:398:HOH:O	1.96	0.82
1:A:177:GLU:CG	1:A:181:ARG:HH11	1.92	0.80
1:B:94:ARG:H	1:B:113:HIS:CD2	1.98	0.79
1:A:94:ARG:H	1:A:113:HIS:CD2	2.01	0.79
1:B:260:VAL:CG1	1:B:261:ALA:N	2.28	0.79
1:A:39:GLN:NE2	1:A:165:HIS:HD2	1.80	0.78
1:A:67:THR:H	1:A:137:GLN:HE22	1.31	0.77
1:A:17:ARG:CB	1:A:18:ARG:NH1	2.46	0.77
1:B:129:GLN:NE2	1:B:153:ARG:CD	2.47	0.77
1:B:213:ASN:C	1:B:214:THR:OG1	2.18	0.77
1:B:29:LEU:CD2	1:B:253:LYS:HD2	2.16	0.76
1:B:254:ARG:C	1:B:257:GLN:H	1.93	0.76
1:A:17:ARG:CB	1:A:18:ARG:HH11	1.98	0.75
1:A:39:GLN:HE22	1:A:165:HIS:HD2	1.32	0.74
1:A:28:LYS:HD3	1:A:28:LYS:C	2.13	0.74
1:A:50:ARG:NE	1:A:54:ARG:HH12	1.85	0.74
1:A:17:ARG:CB	1:A:18:ARG:CZ	2.66	0.73
1:A:43:LYS:HD3	1:A:43:LYS:H	1.54	0.73
1:A:247:SER:HA	1:A:250:GLN:HE21	1.55	0.72
1:B:46:VAL:HG12	1:B:48:GLU:OE1	1.89	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:HD12	1:A:35:LEU:N	2.05	0.71
1:B:21:ALA:O	1:B:25:LEU:HD23	1.92	0.70
1:B:95:LEU:CD2	1:B:114:ALA:HB3	2.22	0.70
1:A:131:ARG:NH2	1:A:131:ARG:HB2	2.07	0.69
1:B:100:LYS:NZ	1:B:100:LYS:HB2	2.08	0.69
1:B:67:THR:H	1:B:137:GLN:HE22	1.42	0.68
1:A:28:LYS:HD3	1:A:28:LYS:O	1.92	0.68
1:A:106:LYS:HD2	1:A:112:PRO:CD	2.24	0.67
1:A:95:LEU:CD2	1:A:123:LEU:HD22	2.25	0.67
1:A:49:TYR:HA	1:A:52:GLN:HE21	1.59	0.66
1:B:73:ASP:HB3	2:B:444:HOH:O	1.94	0.66
1:A:129:GLN:HG3	1:A:153:ARG:NH2	2.11	0.66
1:A:16:LEU:HD11	1:A:39:GLN:O	1.96	0.66
1:A:13:TYR:OH	1:A:17:ARG:HG3	1.96	0.65
1:A:129:GLN:HE22	1:B:72:ARG:NH1	1.95	0.65
1:A:50:ARG:NE	1:A:54:ARG:NH1	2.44	0.65
1:A:17:ARG:HB2	1:A:18:ARG:NH1	2.12	0.64
1:A:129:GLN:CG	1:A:153:ARG:NH2	2.60	0.64
1:B:244:ARG:HH22	1:B:247:SER:HG	1.42	0.63
1:A:129:GLN:O	2:A:454:HOH:O	2.15	0.63
1:A:129:GLN:HG2	1:A:153:ARG:HH21	1.64	0.62
1:A:50:ARG:O	1:A:54:ARG:HG3	1.99	0.62
1:A:173:LEU:CD2	2:A:452:HOH:O	2.48	0.62
1:A:170:GLU:H	1:A:170:GLU:CD	2.07	0.62
1:A:131:ARG:CB	1:B:223:ARG:NH2	2.61	0.62
1:A:206:LYS:HG2	1:A:209:ARG:HH21	1.63	0.62
1:A:102:ALA:HB1	1:A:106:LYS:NZ	2.15	0.62
1:B:138:LEU:HB2	1:B:161:MET:HG3	1.81	0.62
1:B:244:ARG:HH12	1:B:247:SER:HG	1.47	0.61
1:A:131:ARG:HG2	1:B:223:ARG:HH22	1.66	0.61
1:B:167:PRO:O	1:B:169:PRO:HD3	2.01	0.61
1:B:244:ARG:CZ	1:B:244:ARG:HB2	2.30	0.60
1:A:17:ARG:NE	1:A:190:VAL:HG21	2.16	0.60
1:A:39:GLN:NE2	1:A:165:HIS:CD2	2.68	0.59
1:A:87:GLY:HA3	1:B:254:ARG:HH12	1.67	0.59
1:A:50:ARG:HB3	2:A:487:HOH:O	2.02	0.59
1:A:106:LYS:HE3	2:A:326:HOH:O	2.03	0.59
1:A:95:LEU:HD22	1:A:123:LEU:HD22	1.84	0.59
1:A:173:LEU:HD23	2:A:452:HOH:O	2.02	0.59
1:A:17:ARG:HB3	1:A:18:ARG:NH1	2.04	0.58
1:B:24:ALA:HB3	2:B:475:HOH:O	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:PRO:CG	1:B:164:ARG:HH22	2.17	0.58
1:B:242:THR:OG1	1:B:247:SER:HB2	2.03	0.58
1:A:87:GLY:HA3	1:B:254:ARG:NH1	2.19	0.58
1:B:39:GLN:NE2	1:B:165:HIS:ND1	2.51	0.58
1:A:124:LEU:CB	1:A:125:PRO:HD3	2.34	0.57
1:B:176:GLU:O	1:B:180:LEU:HD13	2.05	0.57
1:A:50:ARG:HG2	1:A:54:ARG:NH1	2.20	0.57
1:A:177:GLU:CG	1:A:181:ARG:NH1	2.59	0.56
1:A:177:GLU:O	1:A:181:ARG:HB2	2.05	0.56
1:A:39:GLN:HE22	1:A:165:HIS:CD2	2.19	0.56
1:A:62:LEU:HD12	1:A:93:PHE:O	2.05	0.56
1:A:18:ARG:HA	2:A:448:HOH:O	2.06	0.56
1:A:177:GLU:OE2	2:A:374:HOH:O	2.18	0.56
1:A:124:LEU:HB2	1:A:125:PRO:HD3	1.87	0.56
1:B:23:LYS:O	1:B:27:GLU:HG3	2.05	0.55
1:B:100:LYS:NZ	1:B:100:LYS:CB	2.69	0.55
1:A:260:VAL:HG23	2:A:496:HOH:O	2.05	0.55
1:A:131:ARG:HB2	1:A:131:ARG:HH21	1.70	0.55
1:A:19:LYS:CG	1:A:35:LEU:HD23	2.34	0.54
1:B:148:ASN:O	1:B:152:GLU:HG3	2.07	0.54
1:A:21:ALA:O	1:A:25:LEU:HD23	2.08	0.54
1:A:43:LYS:HD2	2:A:443:HOH:O	2.07	0.54
1:B:257:GLN:HE21	1:B:257:GLN:CA	2.21	0.53
1:B:66:THR:H	1:B:137:GLN:NE2	2.06	0.53
1:A:17:ARG:CG	1:A:18:ARG:HE	2.22	0.53
1:B:257:GLN:NE2	1:B:257:GLN:HA	2.23	0.53
1:B:100:LYS:HB2	1:B:100:LYS:HZ3	1.73	0.53
1:A:247:SER:HA	1:A:250:GLN:NE2	2.22	0.52
1:B:46:VAL:CG1	1:B:48:GLU:OE1	2.56	0.52
1:A:95:LEU:HD23	1:A:123:LEU:HD22	1.92	0.52
1:B:244:ARG:CZ	1:B:244:ARG:CB	2.87	0.51
1:B:257:GLN:HE21	1:B:257:GLN:HA	1.75	0.51
1:A:13:TYR:OH	1:A:17:ARG:CG	2.58	0.51
1:A:52:GLN:NE2	2:A:331:HOH:O	2.43	0.51
1:B:42:GLU:N	1:B:42:GLU:OE2	2.41	0.51
1:B:73:ASP:CB	2:B:444:HOH:O	2.54	0.50
1:A:129:GLN:HG2	1:A:153:ARG:NH2	2.26	0.50
1:A:66:THR:H	1:A:137:GLN:NE2	2.10	0.50
1:A:106:LYS:CD	1:A:112:PRO:HD2	2.35	0.50
1:B:170:GLU:H	1:B:170:GLU:CD	2.20	0.50
1:B:16:LEU:HD13	1:B:42:GLU:OE1	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:THR:HG23	1:A:42:GLU:H	1.76	0.49
1:A:54:ARG:NH2	2:A:429:HOH:O	2.45	0.49
1:B:29:LEU:HD23	1:B:253:LYS:HD3	1.94	0.49
1:B:9:VAL:HB	1:B:31:PHE:CD2	2.48	0.48
1:B:133:VAL:CG2	1:B:156:ARG:NH1	2.76	0.48
1:A:144:PRO:O	1:A:148:ASN:HB2	2.14	0.48
1:A:34:LEU:C	1:A:35:LEU:HD12	2.38	0.48
1:A:50:ARG:CD	1:A:54:ARG:NH1	2.76	0.48
1:B:39:GLN:OE1	1:B:165:HIS:ND1	2.46	0.48
1:B:95:LEU:HD22	1:B:114:ALA:HB3	1.92	0.48
1:B:113:HIS:HE1	2:B:487:HOH:O	1.95	0.48
1:A:42:GLU:HG3	1:A:43:LYS:N	2.29	0.48
1:A:79:LYS:HE2	2:A:470:HOH:O	2.14	0.48
1:B:61:ASP:OD2	1:B:132:GLY:HA3	2.14	0.48
1:B:129:GLN:CG	1:B:153:ARG:HD3	2.43	0.47
1:B:164:ARG:CZ	2:B:464:HOH:O	2.62	0.47
1:A:173:LEU:HD22	1:A:173:LEU:N	2.29	0.47
1:B:39:GLN:CD	1:B:165:HIS:ND1	2.72	0.47
1:A:41:THR:HG23	1:A:42:GLU:N	2.29	0.47
1:A:28:LYS:C	1:A:28:LYS:CD	2.84	0.47
1:A:253:LYS:O	1:A:257:GLN:HG3	2.16	0.46
1:B:260:VAL:HG12	1:B:261:ALA:CA	2.43	0.46
1:A:260:VAL:CG2	2:A:496:HOH:O	2.62	0.46
1:A:165:HIS:HE1	2:A:368:HOH:O	1.99	0.46
1:A:206:LYS:HE2	1:A:209:ARG:HD2	1.96	0.46
1:A:43:LYS:HB2	1:A:43:LYS:NZ	2.30	0.46
1:A:50:ARG:NE	1:A:81:LEU:CD2	2.79	0.46
1:A:50:ARG:HG2	1:A:54:ARG:CZ	2.46	0.46
1:B:152:GLU:HG3	2:B:466:HOH:O	2.15	0.46
1:A:50:ARG:HE	1:A:54:ARG:HH12	1.60	0.46
1:B:142:PRO:HG3	1:B:164:ARG:HH22	1.81	0.46
1:A:102:ALA:O	1:A:106:LYS:HD3	2.16	0.45
1:B:242:THR:C	1:B:243:GLU:HG3	2.41	0.45
1:A:206:LYS:HG2	1:A:209:ARG:HH22	1.75	0.45
1:A:23:LYS:O	1:A:27:GLU:HG3	2.17	0.45
1:B:213:ASN:O	1:B:214:THR:OG1	2.34	0.45
1:B:13:TYR:CZ	1:B:15:GLY:HA3	2.52	0.45
1:B:103:ARG:HE	1:B:103:ARG:HB2	1.47	0.45
1:B:142:PRO:CG	1:B:164:ARG:NH2	2.80	0.45
1:B:60:VAL:HG12	1:B:133:VAL:CG1	2.47	0.45
1:A:93:PHE:HE2	1:A:95:LEU:HD11	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:PRO:O	1:A:153:ARG:NE	2.42	0.45
1:A:93:PHE:CE2	1:A:95:LEU:HD12	2.52	0.44
1:A:206:LYS:HE2	1:A:209:ARG:HH21	1.80	0.44
1:A:76:GLU:HG2	1:A:77:ALA:N	2.31	0.44
1:A:41:THR:CG2	1:A:42:GLU:N	2.81	0.44
1:A:51:ASP:HA	1:A:54:ARG:HG3	2.00	0.44
1:A:61:ASP:OD2	1:A:132:GLY:HA3	2.17	0.44
1:B:52:GLN:NE2	2:B:340:HOH:O	2.50	0.44
1:A:170:GLU:CD	1:A:170:GLU:N	2.74	0.44
1:B:9:VAL:HB	1:B:31:PHE:HD2	1.83	0.43
1:B:25:LEU:O	1:B:29:LEU:HD12	2.17	0.43
1:A:106:LYS:NZ	2:A:286:HOH:O	2.47	0.43
1:A:15:GLY:HA3	1:A:17:ARG:HD3	2.00	0.43
1:B:213:ASN:C	1:B:214:THR:HG1	2.25	0.43
1:A:190:VAL:HA	1:A:221:VAL:HB	1.99	0.43
1:B:105:LEU:HB3	1:B:110:LEU:O	2.19	0.43
1:A:131:ARG:CG	1:B:223:ARG:HH22	2.31	0.43
1:A:17:ARG:CG	1:A:18:ARG:H	2.32	0.42
1:A:127:LEU:O	1:A:153:ARG:CZ	2.67	0.42
1:B:60:VAL:HG12	1:B:133:VAL:HG11	2.01	0.42
1:B:16:LEU:CD1	1:B:42:GLU:CD	2.92	0.42
1:A:50:ARG:HE	1:A:54:ARG:NH1	2.16	0.42
1:A:173:LEU:CD1	2:A:476:HOH:O	2.67	0.42
1:A:62:LEU:HD13	1:A:93:PHE:HD2	1.83	0.42
1:A:161:MET:HG2	1:A:163:TYR:O	2.19	0.42
1:B:62:LEU:C	1:B:62:LEU:HD23	2.44	0.42
1:B:142:PRO:HG3	1:B:164:ARG:NH2	2.35	0.42
1:B:7:ASP:O	1:B:7:ASP:CG	2.63	0.42
1:A:52:GLN:CD	2:A:331:HOH:O	2.62	0.42
1:A:93:PHE:CE2	1:A:95:LEU:CD1	3.03	0.42
1:A:20:GLU:OE2	1:A:20:GLU:HA	2.20	0.41
1:A:106:LYS:CE	2:A:326:HOH:O	2.65	0.41
1:A:127:LEU:HA	1:A:128:PRO:HD3	1.81	0.41
1:A:76:GLU:CG	1:A:77:ALA:N	2.83	0.41
1:B:106:LYS:NZ	1:B:106:LYS:CB	2.84	0.41
1:B:133:VAL:HG22	1:B:156:ARG:NH1	2.36	0.41
1:A:93:PHE:HE2	1:A:95:LEU:CD1	2.33	0.41
1:A:161:MET:HA	1:A:162:PRO:HD2	1.95	0.41
1:A:43:LYS:HD3	1:A:43:LYS:N	2.29	0.41
1:A:235:LYS:HD2	1:A:235:LYS:HA	1.56	0.41
1:B:7:ASP:O	1:B:7:ASP:OD2	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LYS:HE3	2:B:481:HOH:O	2.21	0.41
1:B:170:GLU:CD	1:B:170:GLU:N	2.79	0.41
1:B:244:ARG:NH1	1:B:247:SER:HG	2.08	0.41
1:A:106:LYS:HG3	1:A:111:PRO:HB3	2.02	0.40
1:A:166:LEU:HA	1:A:166:LEU:HD23	1.85	0.40
1:B:18:ARG:NH2	1:B:245:LEU:HD12	2.36	0.40
1:B:256:LEU:O	1:B:257:GLN:C	2.61	0.40

All (7) 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:20:GLU:OE1	1:B:254:ARG:CZ[2_645]	1.72	0.48
1:B:106:LYS:NZ	2:A:282:HOH:O[1_455]	1.82	0.38
1:A:258:LYS:NZ	2:A:464:HOH:O[1_655]	1.91	0.29
1:A:28:LYS:CE	2:A:457:HOH:O[1_655]	1.95	0.25
1:A:28:LYS:NZ	2:A:457:HOH:O[1_655]	1.96	0.24
1:A:20:GLU:OE1	1:B:254:ARG:NH1[2_645]	1.98	0.22
1:A:254:ARG:NH2	2:A:475:HOH:O[1_655]	1.99	0.21

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	252/261 (97%)	247 (98%)	4 (2%)	1 (0%)	30	14
1	B	253/261 (97%)	248 (98%)	5 (2%)	0	100	100
All	All	505/522 (97%)	495 (98%)	9 (2%)	1 (0%)	43	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ARG

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	192/199 (96%)	178 (93%)	14 (7%)	13	2
1	B	193/199 (97%)	180 (93%)	13 (7%)	15	3
All	All	385/398 (97%)	358 (93%)	27 (7%)	14	2

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

Mol	Chain	Res	Type
1	A	17	ARG
1	A	18	ARG
1	A	32	THR
1	A	41	THR
1	A	43	LYS
1	A	47	PRO
1	A	95	LEU
1	A	148	ASN
1	A	152	GLU
1	A	177	GLU
1	A	206	LYS
1	A	215	ARG
1	A	235	LYS
1	A	254	ARG
1	B	7	ASP
1	B	16	LEU
1	B	29	LEU
1	B	43	LYS
1	B	100	LYS
1	B	103	ARG
1	B	106	LYS
1	B	146	LEU
1	B	161	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	223	ARG
1	B	250	GLN
1	B	256	LEU
1	B	257	GLN

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

Mol	Chain	Res	Type
1	A	39	GLN
1	A	52	GLN
1	A	113	HIS
1	A	129	GLN
1	A	137	GLN
1	A	148	ASN
1	A	165	HIS
1	A	250	GLN
1	A	257	GLN
1	B	39	GLN
1	B	52	GLN
1	B	113	HIS
1	B	137	GLN
1	B	257	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	254/261 (97%)	0.60	18 (7%)	22 22	13, 25, 46, 59	0
1	B	255/261 (97%)	0.66	24 (9%)	14 14	15, 26, 48, 73	0
All	All	509/522 (97%)	0.63	42 (8%)	17 17	13, 26, 47, 73	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	LEU	5.2
1	B	256	LEU	4.8
1	A	130	GLY	4.0
1	B	255	ALA	4.0
1	A	260	VAL	3.7
1	A	163	TYR	3.5
1	A	155	TYR	3.2
1	B	237	PHE	3.1
1	A	43	LYS	3.0
1	B	260	VAL	3.0
1	A	166	LEU	3.0
1	A	129	GLN	2.9
1	A	180	LEU	2.9
1	B	252	PHE	2.9
1	A	46	VAL	2.9
1	A	256	LEU	2.9
1	B	152	GLU	2.9
1	B	261	ALA	2.8
1	B	16	LEU	2.8
1	A	181	ARG	2.7
1	B	242	THR	2.6
1	A	44	VAL	2.6
1	B	25	LEU	2.6
1	B	17	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	215	ARG	2.5
1	B	29	LEU	2.4
1	A	32	THR	2.4
1	A	95	LEU	2.4
1	A	42	GLU	2.4
1	B	30	GLY	2.3
1	B	246	GLY	2.3
1	A	208	LEU	2.3
1	B	254	ARG	2.3
1	B	26	ALA	2.3
1	B	244	ARG	2.3
1	B	240	ASP	2.2
1	B	245	LEU	2.2
1	B	247	SER	2.2
1	B	42	GLU	2.2
1	B	59	GLY	2.1
1	B	7	ASP	2.1
1	A	261	ALA	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.