



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:41 PM UTC

PDB ID : 5LV9 / pdb_00005lv9
Title : Crystal structure of thermophilic tryptophan halogenase (Th-Hal) enzyme from *Streptomyces violaceusniger*.
Authors : Dunstan, M.S.; Menon, B.
Deposited on : 2016-09-13
Resolution : 2.33 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)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

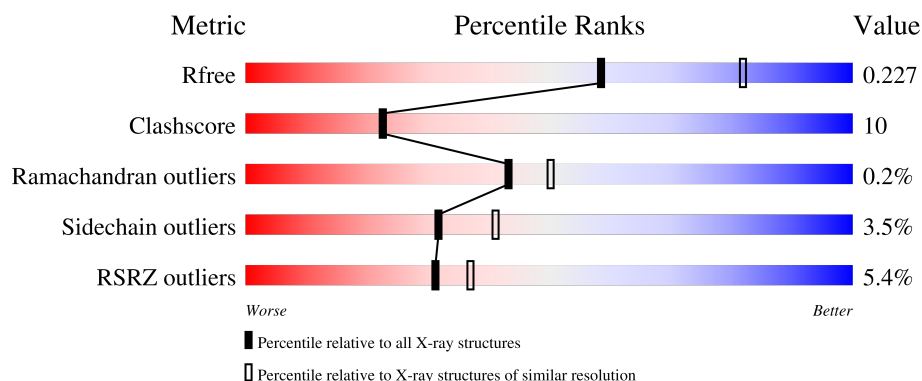
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	513	6% 76% 21% ..
1	B	513	4% 80% 17% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8510 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 thermophilic tryptophan halogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			4047	2579	696	753	19			
1	B	513	Total	C	N	O	S	0	0	0
			4086	2606	701	760	19			

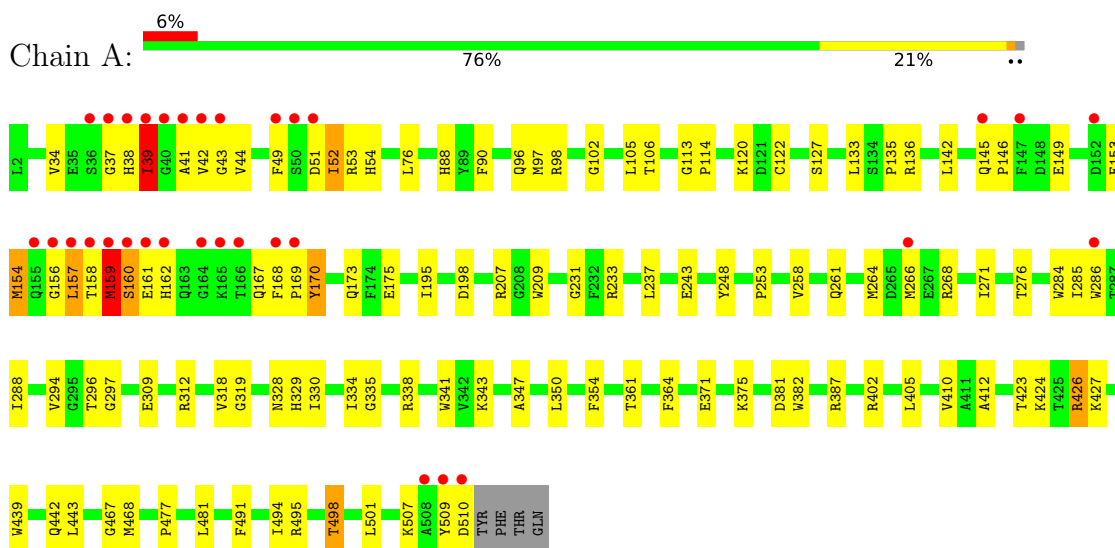
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	170	Total	O	0	0
			170	170		
2	B	207	Total	O	0	0
			207	207		

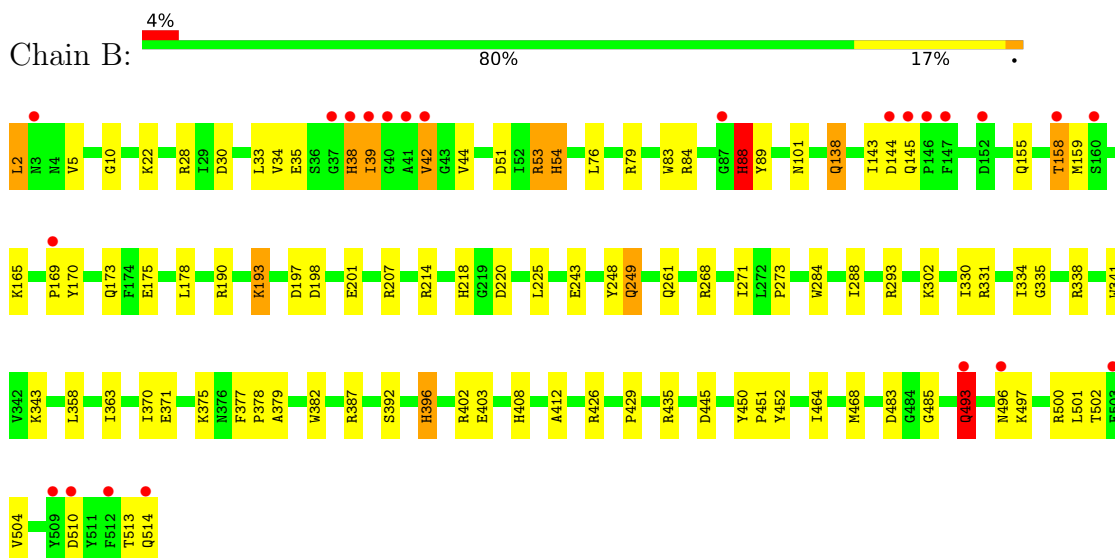
3 Residue-property plots

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: thermophilic tryptophan halogenase



- Molecule 1: thermophilic tryptophan halogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	67.14Å 67.14Å 477.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.49 – 2.33 56.49 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.7 (56.49-2.33) 99.7 (56.49-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.179 , 0.224 0.185 , 0.227	Depositor DCC
R_{free} test set	2547 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.073 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8510	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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	0.55	0/4154	0.88	10/5639 (0.2%)
1	B	0.54	1/4195 (0.0%)	0.90	9/5695 (0.2%)
All	All	0.54	1/8349 (0.0%)	0.89	19/11334 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	54	HIS	CE1-NE2	-5.32	1.27	1.32

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	HIS	N-CA-C	7.73	122.06	109.85
1	B	38	HIS	CA-C-N	7.17	131.79	120.47
1	B	38	HIS	C-N-CA	7.17	131.79	120.47
1	A	170	TYR	N-CA-C	6.97	118.78	108.60
1	B	170	TYR	N-CA-C	6.97	118.77	108.60
1	A	157	LEU	CA-CB-CG	6.74	139.89	116.30
1	B	504	VAL	N-CA-C	6.14	116.88	111.90
1	B	493	GLN	CA-CB-CG	6.07	126.24	114.10
1	A	157	LEU	CB-CA-C	6.07	118.90	110.16
1	B	42	VAL	N-CA-C	-5.92	107.52	113.20
1	A	443	LEU	CA-C-N	5.70	126.96	119.84
1	A	443	LEU	C-N-CA	5.70	126.96	119.84
1	A	319	GLY	CA-C-N	5.63	126.00	119.47
1	A	319	GLY	C-N-CA	5.63	126.00	119.47
1	A	159	MET	N-CA-C	5.48	118.02	111.71
1	B	396	HIS	N-CA-CB	5.26	118.40	110.30
1	A	39	ILE	N-CA-C	-5.18	108.79	113.71
1	B	39	ILE	N-CA-C	5.17	117.51	111.05
1	A	37	GLY	N-CA-C	5.04	117.39	110.58

There are no chirality outliers.

There are no planarity outliers.

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	4047	0	3915	98	0
1	B	4086	0	3948	74	0
2	A	170	0	0	15	1
2	B	207	0	0	11	1
All	All	8510	0	7863	168	1

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 10.

All (168) 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:198:ASP:OD2	2:A:601:HOH:O	1.82	0.95
1:B:53:ARG:NH1	2:B:601:HOH:O	1.99	0.95
1:A:382:TRP:O	2:A:602:HOH:O	1.89	0.89
1:A:157:LEU:HG	1:A:162:HIS:CE1	2.12	0.84
1:A:97:MET:HE1	1:A:106:THR:H	1.44	0.83
1:B:145:GLN:NE2	1:B:169:PRO:HB3	1.95	0.81
1:A:136:ARG:NH1	1:A:170:TYR:OH	2.13	0.80
1:A:145:GLN:HG2	1:A:146:PRO:HD2	1.65	0.77
1:A:157:LEU:HG	1:A:162:HIS:NE2	2.00	0.76
1:A:39:ILE:HG13	1:A:41:ALA:H	1.50	0.76
1:A:49:PHE:HB2	1:A:51:ASP:OD1	1.84	0.75
1:A:276:THR:OG1	2:A:604:HOH:O	2.05	0.73
1:B:403:GLU:OE1	2:B:603:HOH:O	2.07	0.73
1:B:343:LYS:O	1:B:387:ARG:NH1	2.21	0.72
1:A:381:ASP:OD1	2:A:605:HOH:O	2.07	0.71
1:B:84:ARG:HD2	1:B:88:HIS:CD2	2.25	0.71
1:B:371:GLU:OE2	2:B:602:HOH:O	2.07	0.71
1:A:42:VAL:HG23	1:A:43:GLY:H	1.56	0.71
1:A:207:ARG:NH1	2:A:606:HOH:O	2.24	0.69
1:A:154:MET:HB2	1:A:157:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLU:OE2	1:A:312:ARG:NH2	2.27	0.68
1:A:97:MET:CE	1:A:106:THR:H	2.05	0.68
1:B:218:HIS:O	2:B:604:HOH:O	2.12	0.68
1:B:392:SER:O	1:B:396:HIS:HD2	1.78	0.67
1:A:481:LEU:O	1:B:28:ARG:NH1	2.27	0.67
1:B:201:GLU:OE1	1:B:214:ARG:NH1	2.29	0.66
1:A:105:LEU:HD23	1:A:122:CYS:SG	2.36	0.66
1:B:268:ARG:HD3	1:B:271:ILE:HD13	1.77	0.65
1:B:83:TRP:CE3	1:B:468:MET:HE1	2.31	0.65
1:A:296:THR:HG21	1:A:318:VAL:HG21	1.79	0.64
1:B:249:GLN:OE1	2:B:605:HOH:O	2.15	0.64
1:A:156:GLY:HA3	1:B:101:ASN:HA	1.80	0.64
1:B:248:TYR:HB2	1:B:334:ILE:HG22	1.79	0.64
1:A:410:VAL:O	1:A:424:LYS:NZ	2.31	0.64
1:B:214:ARG:HG2	1:B:220:ASP:OD1	1.98	0.63
1:A:412:ALA:HA	1:A:468:MET:HB3	1.79	0.63
1:A:495:ARG:O	1:A:498:THR:HG22	1.98	0.63
1:A:96:GLN:OE1	1:A:167:GLN:HB2	1.99	0.63
1:B:83:TRP:HB3	1:B:468:MET:HE1	1.81	0.62
1:B:54:HIS:HD2	2:B:627:HOH:O	1.83	0.62
1:A:54:HIS:CE1	1:A:162:HIS:HD1	2.17	0.62
1:B:83:TRP:HE3	1:B:468:MET:HE1	1.65	0.61
1:A:97:MET:HE1	1:A:106:THR:N	2.14	0.61
1:B:426:ARG:O	2:B:606:HOH:O	2.16	0.61
1:A:120:LYS:NZ	1:A:127:SER:OG	2.34	0.61
1:A:268:ARG:O	1:A:271:ILE:HG12	2.01	0.60
1:A:136:ARG:NH2	1:A:149:GLU:OE1	2.35	0.60
1:B:30:ASP:OD1	1:B:193:LYS:NZ	2.36	0.59
1:A:233:ARG:NH2	2:A:603:HOH:O	1.99	0.59
1:A:49:PHE:CZ	1:A:361:THR:HG22	2.38	0.59
1:A:53:ARG:NH2	1:A:153:GLU:OE1	2.36	0.58
1:A:161:GLU:OE1	1:A:161:GLU:N	2.37	0.58
1:A:412:ALA:O	1:A:424:LYS:NZ	2.36	0.58
1:A:158:THR:O	1:A:162:HIS:CE1	2.58	0.56
1:B:408:HIS:O	1:B:468:MET:HE2	2.06	0.56
1:B:387:ARG:NH2	2:B:617:HOH:O	2.38	0.56
1:B:138:GLN:O	1:B:138:GLN:HG3	2.05	0.56
1:A:264:MET:HE3	1:A:268:ARG:HG2	1.88	0.55
1:B:173:GLN:HG2	1:B:288:ILE:HG23	1.90	0.54
1:A:51:ASP:HB2	1:A:159:MET:HG3	1.89	0.54
1:B:83:TRP:HB3	1:B:468:MET:CE	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:TRP:CG	1:B:387:ARG:HG3	2.42	0.54
1:A:154:MET:H	1:A:157:LEU:HD13	1.73	0.54
1:A:142:LEU:HD11	1:A:169:PRO:HG2	1.89	0.53
1:B:51:ASP:OD1	2:B:607:HOH:O	2.18	0.53
1:A:76:LEU:HD21	1:A:135:PRO:HG3	1.91	0.53
1:A:158:THR:O	1:A:162:HIS:NE2	2.42	0.53
1:B:84:ARG:CZ	1:B:88:HIS:HE2	2.22	0.52
1:B:2:LEU:HD21	1:B:382:TRP:CE2	2.45	0.51
1:A:258:VAL:HG23	1:A:329:HIS:CD2	2.45	0.51
1:A:402:ARG:HD3	2:A:633:HOH:O	2.10	0.51
1:B:412:ALA:HA	1:B:468:MET:HE3	1.93	0.51
1:A:53:ARG:HH22	1:A:153:GLU:CD	2.19	0.50
1:A:160:SER:OG	1:A:371:GLU:OE2	2.20	0.50
1:A:423:THR:OG1	1:A:424:LYS:HE2	2.12	0.50
1:A:102:GLY:O	1:B:375:LYS:NZ	2.45	0.49
1:A:509:TYR:HD2	1:A:510:ASP:OD1	1.95	0.49
1:A:43:GLY:HA3	1:A:286:TRP:HH2	1.77	0.49
1:A:98:ARG:HD2	1:A:494:ILE:HD11	1.94	0.49
1:A:97:MET:HE3	1:A:105:LEU:N	2.28	0.49
1:A:231:GLY:HA2	1:A:350:LEU:HB2	1.95	0.49
1:A:54:HIS:CE1	1:A:162:HIS:ND1	2.81	0.48
1:A:44:VAL:HG23	2:A:609:HOH:O	2.12	0.48
1:B:158:THR:HG23	1:B:371:GLU:OE1	2.14	0.48
1:B:341:TRP:CD2	1:B:387:ARG:HG3	2.49	0.48
1:A:88:HIS:HE1	2:A:756:HOH:O	1.97	0.48
1:B:79:ARG:HD2	1:B:89:TYR:CD1	2.49	0.48
1:B:248:TYR:CD2	1:B:335:GLY:HA2	2.49	0.47
1:B:435:ARG:NH2	1:B:451:PRO:HD3	2.29	0.47
1:B:155:GLN:NE2	2:B:625:HOH:O	2.44	0.47
1:B:44:VAL:HG22	1:B:175:GLU:HG3	1.96	0.47
1:B:145:GLN:HE21	1:B:169:PRO:HB3	1.74	0.47
1:B:396:HIS:HB3	1:B:450:TYR:HE1	1.79	0.47
1:B:284:TRP:CE2	1:B:358:LEU:HD13	2.50	0.47
1:B:331:ARG:HD3	2:B:718:HOH:O	2.14	0.47
1:A:157:LEU:CG	1:A:162:HIS:CE1	2.93	0.47
1:A:154:MET:O	1:A:157:LEU:HB2	2.15	0.46
1:B:158:THR:HG23	1:B:371:GLU:CD	2.41	0.46
1:B:302:LYS:HD3	1:B:331:ARG:NH1	2.30	0.46
1:A:159:MET:HE3	1:A:159:MET:HB3	1.62	0.46
1:B:261:GLN:NE2	1:B:293:ARG:HD3	2.31	0.46
1:A:173:GLN:HG2	1:A:288:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:MET:HE2	1:B:159:MET:HB3	1.75	0.46
1:A:477:PRO:HB3	1:B:379:ALA:HB2	1.98	0.45
1:B:138:GLN:HE22	1:B:514:GLN:HB3	1.81	0.45
1:A:375:LYS:NZ	2:A:618:HOH:O	2.49	0.45
1:A:439:TRP:HA	1:A:442:GLN:O	2.15	0.45
1:A:49:PHE:HZ	1:A:361:THR:HG22	1.80	0.45
1:B:144:ASP:O	1:B:497:LYS:HE2	2.16	0.45
1:B:5:VAL:HG22	1:B:225:LEU:HB3	1.98	0.45
1:A:157:LEU:C	1:A:162:HIS:CE1	2.95	0.45
1:B:396:HIS:CE1	1:B:452:TYR:CD2	3.04	0.45
1:A:209:TRP:CD1	1:A:343:LYS:HD3	2.52	0.44
1:A:237:LEU:HD22	1:A:347:ALA:HB2	1.99	0.44
1:A:350:LEU:HD22	1:A:354:PHE:HD1	1.82	0.44
1:B:88:HIS:ND1	1:B:89:TYR:N	2.65	0.44
1:A:154:MET:N	1:A:157:LEU:HD13	2.32	0.44
1:A:361:THR:O	1:A:364:PHE:HB3	2.17	0.44
1:B:22:LYS:HE3	1:B:190:ARG:O	2.17	0.44
1:A:127:SER:HB2	1:A:498:THR:OG1	2.18	0.44
1:A:266:MET:HB3	2:A:634:HOH:O	2.17	0.44
1:A:286:TRP:CE2	1:A:297:GLY:HA3	2.53	0.44
1:B:268:ARG:O	1:B:271:ILE:HG12	2.18	0.44
1:B:468:MET:HE3	1:B:468:MET:HB3	1.67	0.44
1:A:285:ILE:HA	1:A:297:GLY:O	2.17	0.44
1:A:90:PHE:HZ	1:A:468:MET:HE3	1.83	0.44
1:A:248:TYR:HB2	1:A:334:ILE:HG22	2.00	0.43
1:A:268:ARG:NH2	2:A:620:HOH:O	2.50	0.43
1:A:330:ILE:HD12	1:A:330:ILE:HA	1.83	0.43
1:B:268:ARG:HH11	1:B:271:ILE:HG21	1.83	0.43
2:A:708:HOH:O	1:B:158:THR:HG21	2.18	0.43
1:B:42:VAL:HG13	1:B:330:ILE:HG21	1.99	0.43
1:B:496:ASN:O	1:B:500:ARG:HG3	2.19	0.43
1:A:160:SER:HB3	2:A:747:HOH:O	2.18	0.43
1:A:44:VAL:HG22	1:A:175:GLU:HG3	2.00	0.43
1:B:10:GLY:HA3	1:B:35:GLU:OE1	2.19	0.42
1:B:197:ASP:OD1	1:B:198:ASP:N	2.48	0.42
1:A:341:TRP:NE1	1:A:387:ARG:HH11	2.17	0.42
1:B:143:ILE:HD11	1:B:501:LEU:HD13	1.99	0.42
1:A:105:LEU:HD21	1:A:491:PHE:CE1	2.53	0.42
1:A:158:THR:O	1:A:162:HIS:CD2	2.72	0.42
1:A:162:HIS:CD2	1:A:162:HIS:N	2.88	0.42
1:A:113:GLY:HA2	1:A:114:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:TYR:CD1	1:B:402:ARG:HD2	2.55	0.42
1:A:142:LEU:HD21	1:A:169:PRO:HG2	2.02	0.41
1:A:136:ARG:HG2	1:A:142:LEU:HA	2.01	0.41
1:B:330:ILE:HD12	1:B:330:ILE:HA	1.89	0.41
1:A:168:PHE:HA	1:A:169:PRO:HD3	1.79	0.41
1:A:248:TYR:CD2	1:A:335:GLY:HA2	2.56	0.41
1:B:377:PHE:HA	1:B:378:PRO:HD3	1.88	0.41
1:A:52:ILE:HD12	1:A:52:ILE:HA	1.78	0.41
1:B:464:ILE:O	1:B:468:MET:HG2	2.21	0.41
1:A:328:ASN:HB3	2:A:741:HOH:O	2.21	0.41
1:B:178:LEU:HA	1:B:178:LEU:HD23	1.83	0.41
1:B:493:GLN:C	1:B:493:GLN:OE1	2.64	0.41
1:A:243:GLU:OE2	1:A:338:ARG:HB3	2.21	0.40
1:B:243:GLU:OE2	1:B:338:ARG:HB3	2.21	0.40
1:B:402:ARG:NH2	1:B:429:PRO:HG3	2.36	0.40
1:A:90:PHE:CZ	1:A:467:GLY:HA3	2.56	0.40
1:A:501:LEU:HD23	1:A:501:LEU:HA	1.86	0.40
1:A:34:VAL:HA	1:A:195:ILE:O	2.22	0.40
1:A:253:PRO:HG3	1:A:426:ARG:CZ	2.50	0.40
1:B:76:LEU:HD13	1:B:273:PRO:HB2	2.03	0.40
1:A:160:SER:N	1:A:371:GLU:OE2	2.45	0.40
1:B:33:LEU:C	1:B:33:LEU:HD23	2.46	0.40
1:B:483:ASP:C	1:B:485:GLY:H	2.30	0.40
1:A:284:TRP:CZ3	1:A:286:TRP:HB3	2.57	0.40
1:A:405:LEU:HD23	1:A:405:LEU:HA	1.89	0.40

All (1) 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)
2:A:648:HOH:O	2:B:749:HOH:O[6_544]	2.11	0.09

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	507/513 (99%)	488 (96%)	18 (4%)	1 (0%)	43	50
1	B	511/513 (100%)	489 (96%)	21 (4%)	1 (0%)	43	50
All	All	1018/1026 (99%)	977 (96%)	39 (4%)	2 (0%)	43	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	B	510	ASP

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	424/428 (99%)	412 (97%)	12 (3%)	38	50
1	B	428/428 (100%)	410 (96%)	18 (4%)	26	34
All	All	852/856 (100%)	822 (96%)	30 (4%)	32	41

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ILE
1	A	52	ILE
1	A	133	LEU
1	A	154	MET
1	A	159	MET
1	A	160	SER
1	A	261	GLN
1	A	294	VAL
1	A	426	ARG
1	A	427	LYS
1	A	498	THR

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Mol	Chain	Res	Type
1	A	507	LYS
1	B	2	LEU
1	B	34	VAL
1	B	38	HIS
1	B	39	ILE
1	B	53	ARG
1	B	88	HIS
1	B	138	GLN
1	B	158	THR
1	B	165	LYS
1	B	193	LYS
1	B	207	ARG
1	B	249	GLN
1	B	363	ILE
1	B	370	ILE
1	B	445	ASP
1	B	493	GLN
1	B	502	THR
1	B	513	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	GLN
1	A	254	ASN
1	A	376	ASN
1	A	386	HIS
1	B	3	ASN
1	B	54	HIS
1	B	145	GLN
1	B	396	HIS

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 [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	509/513 (99%)	0.11	32 (6%) 26 31	25, 40, 74, 117	0
1	B	513/513 (100%)	-0.04	23 (4%) 38 44	22, 37, 71, 106	0
All	All	1022/1026 (99%)	0.03	55 (5%) 31 37	22, 38, 73, 117	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	ILE	6.9
1	A	42	VAL	6.6
1	A	39	ILE	6.4
1	B	41	ALA	5.9
1	A	41	ALA	5.3
1	A	157	LEU	5.3
1	A	162	HIS	5.1
1	A	37	GLY	5.0
1	A	40	GLY	4.9
1	A	38	HIS	4.9
1	B	38	HIS	4.9
1	B	37	GLY	4.8
1	B	42	VAL	4.7
1	A	50	SER	4.5
1	A	161	GLU	4.5
1	B	514	GLN	4.2
1	B	509	TYR	4.1
1	A	169	PRO	4.1
1	A	164	GLY	3.8
1	A	155	GLN	3.7
1	A	160	SER	3.6
1	B	40	GLY	3.5
1	A	159	MET	3.5
1	A	156	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	509	TYR	3.3
1	A	152	ASP	3.1
1	B	169	PRO	3.1
1	A	158	THR	3.1
1	A	145	GLN	2.9
1	B	144	ASP	2.9
1	A	51	ASP	2.9
1	A	286	TRP	2.8
1	B	145	GLN	2.7
1	B	87	GLY	2.6
1	A	165	LYS	2.6
1	A	266	MET	2.5
1	B	496	ASN	2.5
1	A	43	GLY	2.5
1	A	36	SER	2.5
1	B	510	ASP	2.5
1	B	503	GLU	2.4
1	A	168	PHE	2.4
1	A	147	PHE	2.4
1	A	510	ASP	2.4
1	A	166	THR	2.3
1	B	493	GLN	2.3
1	B	3	ASN	2.3
1	B	160	SER	2.2
1	B	146	PRO	2.1
1	B	147	PHE	2.1
1	A	508	ALA	2.1
1	B	158	THR	2.1
1	A	49	PHE	2.1
1	B	152	ASP	2.0
1	B	512	PHE	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.