



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:02 AM UTC

PDB ID : 6LHX / pdb_00006lhx
Title : Crystal structure of ThsA
Authors : Bae, E.; Ka, D.; Oh, H.
Deposited on : 2019-12-10
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

<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

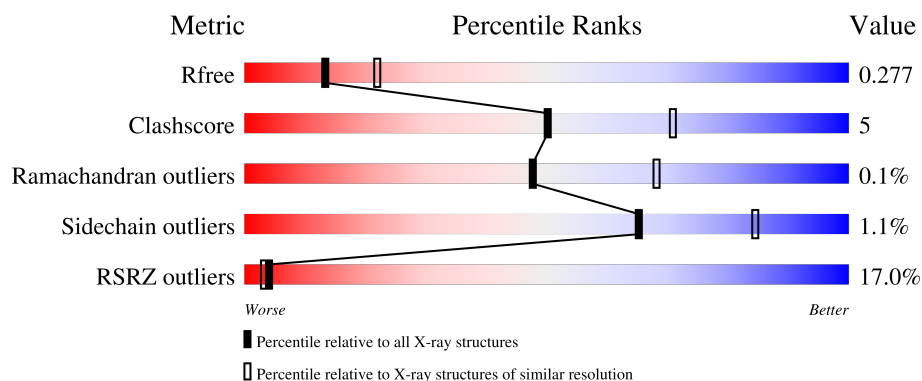
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	476	16% 83% 14% .
1	B	476	13% 75% 10% . 15%
1	C	476	14% 83% 13% .
1	D	476	17% 72% 12% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13332 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 ThsA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	Se	0	0	0
			3556	2273	597	677	2	7			
1	B	406	Total	C	N	O	S	Se	0	0	0
			3170	2034	531	596	1	8			
1	C	458	Total	C	N	O	S	Se	0	0	0
			3535	2262	587	677	2	7			
1	D	401	Total	C	N	O	S	Se	0	0	0
			3035	1944	514	569	1	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP J8G6Z1
A	2	HIS	-	expression tag	UNP J8G6Z1
B	1	GLY	-	expression tag	UNP J8G6Z1
B	2	HIS	-	expression tag	UNP J8G6Z1
C	1	GLY	-	expression tag	UNP J8G6Z1
C	2	HIS	-	expression tag	UNP J8G6Z1
D	1	GLY	-	expression tag	UNP J8G6Z1
D	2	HIS	-	expression tag	UNP J8G6Z1

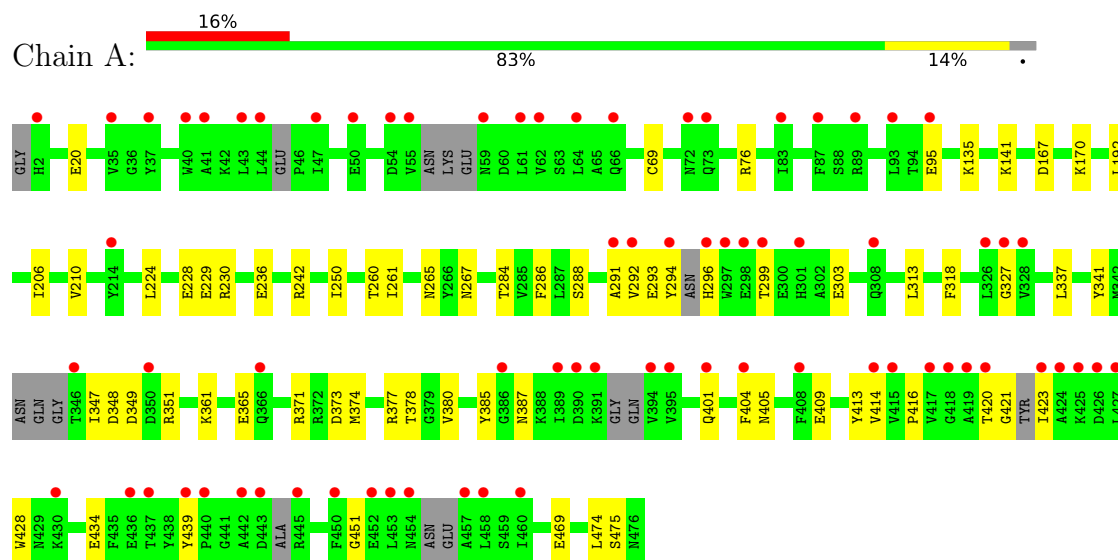
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	O	0	0
			15	15		
2	B	9	Total	O	0	0
			9	9		
2	C	7	Total	O	0	0
			7	7		
2	D	5	Total	O	0	0
			5	5		

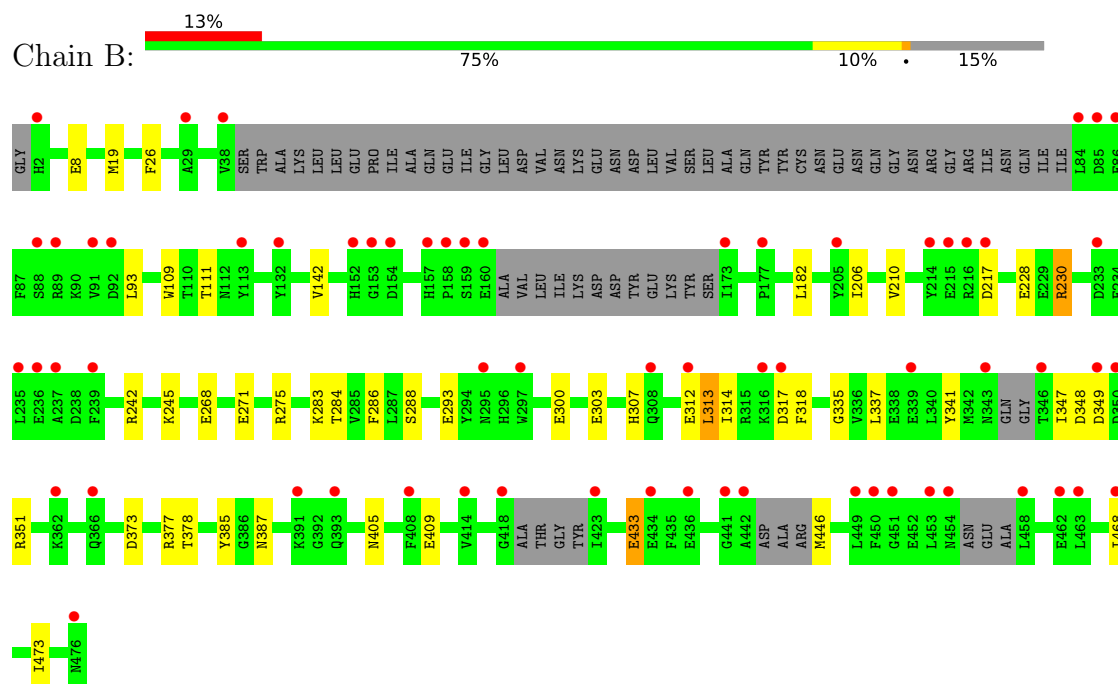
3 Residue-property plots [i](#)

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.

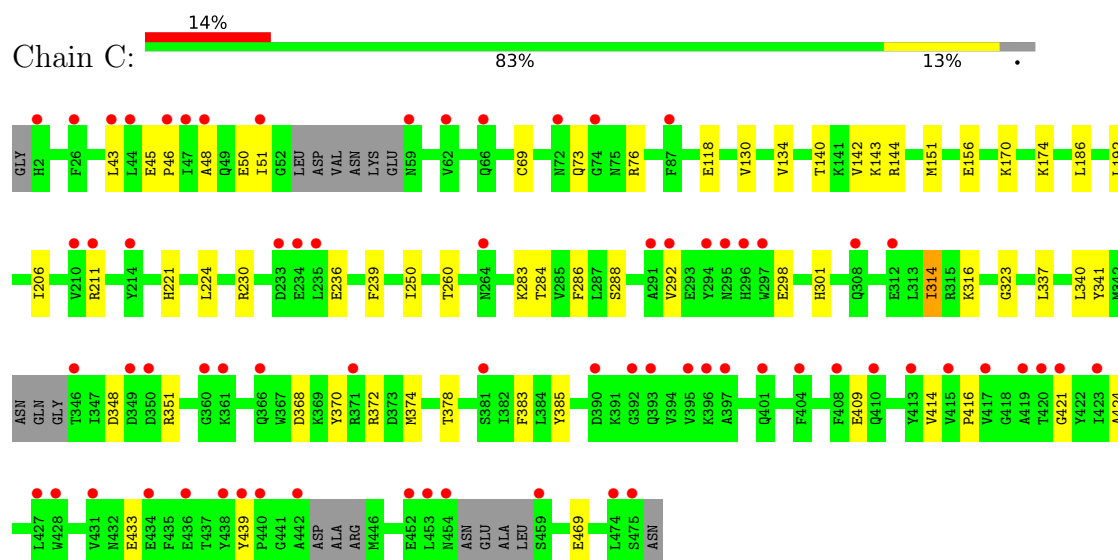
• Molecule 1: TbsA



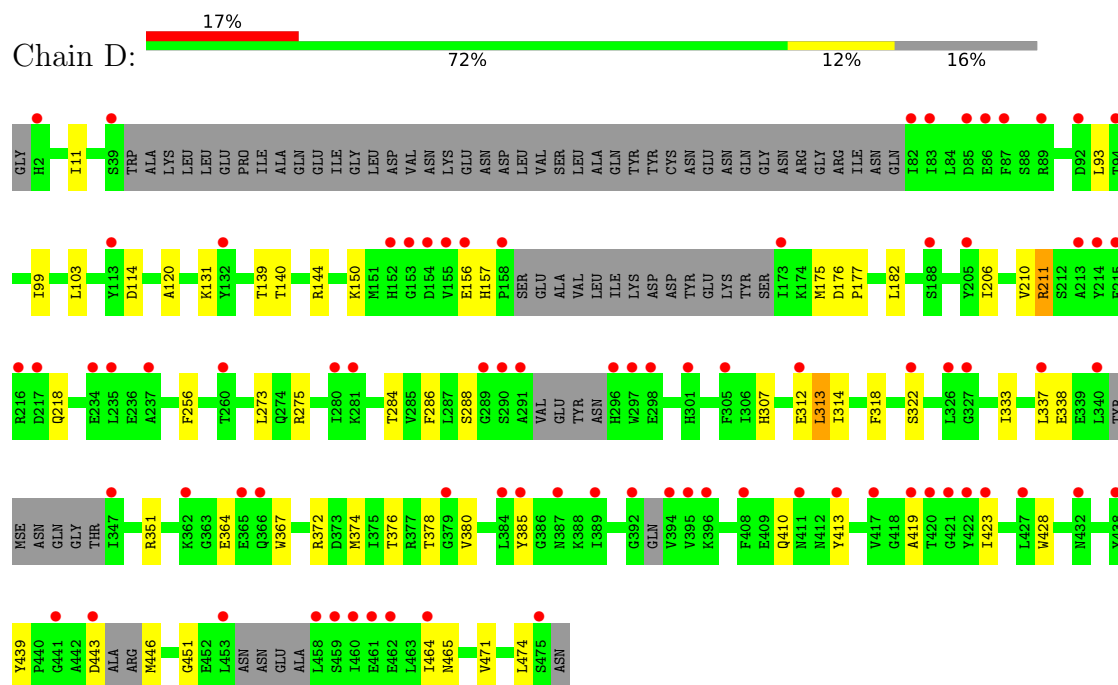
• Molecule 1: TbsA



• Molecule 1: ThsA



• Molecule 1: ThsA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	180.42Å 168.58Å 93.61Å 90.00° 106.71° 90.00°	Depositor
Resolution (Å)	31.64 – 2.50 31.64 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (31.64-2.50) 88.5 (31.64-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.43 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.242 , 0.273 0.246 , 0.277	Depositor DCC
R_{free} test set	1996 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13332	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.56% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.28	0/3610	0.77	1/4874 (0.0%)
1	B	0.30	0/3219	0.80	3/4339 (0.1%)
1	C	0.29	0/3594	0.76	1/4867 (0.0%)
1	D	0.30	0/3083	0.80	2/4172 (0.0%)
All	All	0.29	0/13506	0.78	7/18252 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	292	VAL	N-CA-C	-6.86	106.35	111.90
1	A	292	VAL	N-CA-C	-5.68	107.28	112.96
1	D	313	LEU	N-CA-C	-5.68	105.17	111.36
1	B	93	LEU	N-CA-C	5.60	118.57	110.28
1	B	385	TYR	CB-CA-C	-5.47	109.80	117.23
1	B	313	LEU	N-CA-C	-5.36	105.52	111.36
1	D	385	TYR	CB-CA-C	-5.08	110.32	117.23

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	3556	0	3330	42	0
1	B	3170	0	3017	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3535	0	3298	36	0
1	D	3035	0	2793	32	0
2	A	15	0	0	0	0
2	B	9	0	0	0	0
2	C	7	0	0	0	0
2	D	5	0	0	0	0
All	All	13332	0	12438	136	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 5.

All (136) 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:C:142:VAL:HG12	1:C:143:LYS:HG2	1.65	0.77
1:A:76:ARG:NH2	1:A:167:ASP:OD1	2.20	0.74
1:A:69:CYS:SG	1:A:170:LYS:NZ	2.63	0.72
1:B:283:LYS:NZ	1:B:317:ASP:O	2.23	0.71
1:A:228:GLU:HG2	1:A:242:ARG:HB3	1.72	0.71
1:C:230:ARG:NH1	1:C:236:GLU:OE2	2.23	0.71
1:C:385:TYR:HA	1:C:421:GLY:HA2	1.73	0.71
1:D:99:ILE:HG21	1:D:273:LEU:HB3	1.75	0.69
1:C:69:CYS:SG	1:C:170:LYS:NZ	2.65	0.69
1:C:186:LEU:O	1:C:211:ARG:NH2	2.26	0.68
1:A:230:ARG:NE	1:A:236:GLU:OE2	2.25	0.68
1:A:414:VAL:HG12	1:A:416:PRO:HD3	1.74	0.67
1:D:284:THR:HG22	1:D:378:THR:HG22	1.80	0.63
1:D:11:ILE:HD13	1:D:275:ARG:HG2	1.80	0.63
1:C:348:ASP:HB3	1:C:351:ARG:HG2	1.81	0.62
1:B:312:GLU:HG2	1:B:468:ILE:HD13	1.82	0.61
1:B:284:THR:HG22	1:B:378:THR:HG22	1.82	0.61
1:A:380:VAL:HG22	1:A:413:TYR:HB2	1.83	0.60
1:A:284:THR:HG22	1:A:378:THR:HG22	1.84	0.60
1:B:228:GLU:HG3	1:B:242:ARG:HH21	1.67	0.60
1:A:428:TRP:HZ2	1:A:451:GLY:HA2	1.68	0.59
1:D:380:VAL:HG22	1:D:413:TYR:HB2	1.83	0.59
1:C:433:GLU:N	1:C:433:GLU:OE1	2.36	0.58
1:A:475:SER:O	1:A:475:SER:OG	2.21	0.58
1:A:377:ARG:NH2	1:B:349:ASP:OD2	2.36	0.58
1:B:286:PHE:HB2	1:B:378:THR:HG21	1.86	0.57
1:C:421:GLY:HA3	1:C:424:ALA:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:PHE:HE2	1:A:414:VAL:HG11	1.68	0.57
1:A:405:ASN:O	1:A:409:GLU:HG3	2.04	0.57
1:C:211:ARG:HH21	1:C:221:HIS:HE2	1.53	0.57
1:A:404:PHE:CE2	1:A:414:VAL:HG11	2.40	0.56
1:A:439:TYR:HE2	1:A:474:LEU:HD21	1.70	0.56
1:A:371:ARG:HA	1:A:374:MSE:HE3	1.86	0.56
1:D:286:PHE:HB2	1:D:378:THR:HG21	1.88	0.56
1:C:283:LYS:NZ	1:C:316:LYS:O	2.38	0.56
1:A:141:LYS:NZ	1:C:156:GLU:OE2	2.33	0.55
1:A:286:PHE:HB2	1:A:378:THR:HG21	1.88	0.55
1:A:361:LYS:O	1:A:365:GLU:HG3	2.07	0.55
1:A:294:TYR:O	1:A:296:HIS:N	2.40	0.54
1:B:182:LEU:HD23	1:B:210:VAL:HG11	1.88	0.54
1:B:433:GLU:N	1:B:433:GLU:OE1	2.41	0.54
1:B:446:MSE:HG3	1:B:473:ILE:HG21	1.90	0.53
1:D:443:ASP:HA	1:D:446:MSE:HB3	1.91	0.53
1:C:151:MSE:HE1	1:C:206:ILE:HD13	1.89	0.53
1:D:428:TRP:HZ2	1:D:451:GLY:HA2	1.74	0.53
1:C:211:ARG:NH2	1:C:221:HIS:HE2	2.08	0.52
1:B:19:MSE:SE	1:B:283:LYS:HE2	2.59	0.52
1:C:250:ILE:HG12	1:C:260:THR:HG21	1.91	0.51
1:B:230:ARG:CG	1:B:230:ARG:HH11	2.24	0.51
1:C:414:VAL:O	1:C:439:TYR:OH	2.20	0.51
1:B:268:GLU:HA	1:B:271:GLU:HG3	1.93	0.51
1:B:293:GLU:O	1:B:387:ASN:ND2	2.40	0.51
1:D:182:LEU:HD23	1:D:210:VAL:HG11	1.93	0.51
1:D:439:TYR:HE1	1:D:474:LEU:HD21	1.75	0.51
1:D:206:ILE:O	1:D:210:VAL:HG22	2.10	0.51
1:B:206:ILE:O	1:B:210:VAL:HG22	2.11	0.50
1:C:230:ARG:HG2	1:C:239:PHE:CG	2.47	0.50
1:C:45:GLU:HA	1:C:48:ALA:HB3	1.95	0.49
1:A:291:ALA:O	1:A:327:GLY:HA3	2.12	0.49
1:B:26:PHE:HA	1:B:109:TRP:O	2.12	0.49
1:C:73:GLN:HE21	1:C:76:ARG:HD2	1.78	0.48
1:A:349:ASP:OD1	1:B:377:ARG:NH1	2.46	0.48
1:B:26:PHE:HZ	1:B:111:THR:HG23	1.78	0.48
1:D:286:PHE:CE2	1:D:288:SER:HB2	2.48	0.48
1:D:333:ILE:O	1:D:337:LEU:HD12	2.13	0.48
1:A:348:ASP:HB3	1:A:351:ARG:HG2	1.95	0.48
1:A:349:ASP:OD1	1:B:377:ARG:NH2	2.46	0.48
1:D:314:ILE:O	1:D:351:ARG:NH2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:PHE:CE2	1:A:288:SER:HB2	2.48	0.47
1:A:135:LYS:HG2	1:B:217:ASP:HB3	1.95	0.47
1:A:192:LEU:HD11	1:A:224:LEU:HG	1.96	0.47
1:B:307:HIS:CE1	1:B:335:GLY:HA2	2.50	0.47
1:B:313:LEU:O	1:B:318:PHE:HB2	2.15	0.47
1:C:284:THR:HG22	1:C:378:THR:HG22	1.95	0.47
1:D:114:ASP:O	1:D:150:LYS:NZ	2.48	0.47
1:A:421:GLY:O	1:A:423:ILE:N	2.47	0.47
1:C:337:LEU:HD22	1:C:341:TYR:CE2	2.50	0.47
1:B:230:ARG:HH11	1:B:230:ARG:HG3	1.80	0.46
1:B:286:PHE:CE2	1:B:288:SER:HB2	2.50	0.46
1:C:368:ASP:O	1:C:372:ARG:HG3	2.14	0.46
1:B:337:LEU:HD21	1:B:347:ILE:HD11	1.96	0.46
1:C:134:VAL:HG21	1:C:174:LYS:HA	1.98	0.46
1:D:372:ARG:O	1:D:376:THR:OG1	2.27	0.46
1:D:211:ARG:NH1	1:D:256:PHE:O	2.45	0.46
1:D:374:MSE:HE2	1:D:374:MSE:HB3	1.92	0.46
1:C:286:PHE:CE2	1:C:288:SER:HB2	2.51	0.46
1:A:265:ASN:ND2	1:A:267:ASN:HB2	2.31	0.46
1:B:314:ILE:HG23	1:B:351:ARG:HH21	1.80	0.46
1:B:26:PHE:CZ	1:B:111:THR:HG23	2.51	0.45
1:C:50:GLU:HG2	1:C:51:ILE:H	1.81	0.45
1:C:286:PHE:HB2	1:C:378:THR:HG21	1.98	0.45
1:C:43:LEU:O	1:C:46:PRO:HD2	2.17	0.45
1:A:250:ILE:HG12	1:A:260:THR:HG21	1.99	0.45
1:B:405:ASN:O	1:B:409:GLU:HG3	2.17	0.45
1:A:385:TYR:CD1	1:A:420:THR:HB	2.52	0.44
1:D:322:SER:C	1:D:374:MSE:HE1	2.43	0.44
1:A:337:LEU:HD22	1:A:341:TYR:CE2	2.53	0.44
1:B:348:ASP:HB3	1:B:351:ARG:HG2	1.99	0.44
1:A:206:ILE:O	1:A:210:VAL:HG22	2.18	0.44
1:D:376:THR:HA	1:D:410:GLN:NE2	2.32	0.44
1:D:364:GLU:HA	1:D:367:TRP:CG	2.53	0.43
1:A:293:GLU:O	1:A:387:ASN:ND2	2.40	0.43
1:C:383:PHE:HB2	1:C:416:PRO:HA	2.01	0.43
1:A:373:ASP:OD2	1:B:347:ILE:HG13	2.19	0.43
1:D:464:ILE:HG13	1:D:465:ASN:N	2.33	0.43
1:B:337:LEU:HD22	1:B:341:TYR:CZ	2.54	0.43
1:C:370:TYR:O	1:C:374:MSE:HG3	2.18	0.43
1:D:313:LEU:O	1:D:318:PHE:HB2	2.18	0.42
1:D:140:THR:HG23	1:D:144:ARG:CZ	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:THR:HG23	1:C:144:ARG:CZ	2.50	0.42
1:C:323:GLY:N	1:C:374:MSE:HE1	2.34	0.42
1:A:347:ILE:HG13	1:B:373:ASP:OD2	2.20	0.42
1:D:156:GLU:O	1:D:157:HIS:CG	2.72	0.42
1:D:471:VAL:O	1:D:474:LEU:HB2	2.20	0.42
1:A:299:THR:O	1:A:303:GLU:HG3	2.20	0.42
1:C:374:MSE:HE2	1:C:374:MSE:HB3	1.81	0.42
1:A:224:LEU:HD23	1:A:261:ILE:HB	2.03	0.41
1:A:313:LEU:O	1:A:318:PHE:HB2	2.19	0.41
1:D:307:HIS:NE2	1:D:338:GLU:OE2	2.34	0.41
1:A:20:GLU:OE1	1:B:142:VAL:HG13	2.19	0.41
1:C:192:LEU:HD11	1:C:224:LEU:HG	2.02	0.41
1:A:385:TYR:CE1	1:A:420:THR:HB	2.55	0.41
1:C:314:ILE:HG23	1:C:351:ARG:NH2	2.35	0.41
1:A:401:GLN:O	1:A:404:PHE:HB3	2.20	0.41
1:B:300:GLU:O	1:B:303:GLU:HB2	2.19	0.41
1:D:93:LEU:HD11	1:D:120:ALA:HB2	2.03	0.41
1:C:314:ILE:HG21	1:C:340:LEU:CD1	2.50	0.41
1:D:176:ASP:HB3	1:D:177:PRO:HD3	2.02	0.41
1:C:118:GLU:HG2	1:C:130:VAL:CG2	2.50	0.41
1:D:99:ILE:O	1:D:103:LEU:HG	2.21	0.40
1:C:298:GLU:HG3	1:C:301:HIS:HB2	2.02	0.40
1:D:131:LYS:NZ	1:D:139:THR:O	2.53	0.40
1:D:211:ARG:NH2	1:D:218:GLN:HB3	2.36	0.40
1:A:337:LEU:HD21	1:A:347:ILE:HD11	2.03	0.40
1:B:8:GLU:CD	1:B:275:ARG:HH12	2.29	0.40
1:D:471:VAL:HA	1:D:474:LEU:HD12	2.03	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	443/476 (93%)	430 (97%)	13 (3%)	0	100	100
1	B	392/476 (82%)	377 (96%)	15 (4%)	0	100	100
1	C	448/476 (94%)	431 (96%)	17 (4%)	0	100	100
1	D	385/476 (81%)	371 (96%)	13 (3%)	1 (0%)	36	55
All	All	1668/1904 (88%)	1609 (96%)	58 (4%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	419	ALA

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	356/417 (85%)	352 (99%)	4 (1%)	65	84
1	B	323/417 (78%)	320 (99%)	3 (1%)	70	87
1	C	355/417 (85%)	352 (99%)	3 (1%)	73	88
1	D	293/417 (70%)	289 (99%)	4 (1%)	59	81
All	All	1327/1668 (80%)	1313 (99%)	14 (1%)	65	84

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	GLU
1	A	229	GLU
1	A	434	GLU
1	A	469	GLU
1	B	230	ARG
1	B	245	LYS
1	B	433	GLU
1	C	314	ILE
1	C	409	GLU
1	C	469	GLU

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Mol	Chain	Res	Type
1	D	175	MSE
1	D	211	ARG
1	D	312	GLU
1	D	423	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	366	GLN
1	A	429	ASN
1	A	476	ASN
1	B	246	GLN
1	B	267	ASN
1	B	432	ASN
1	C	73	GLN
1	C	432	ASN
1	D	2	HIS
1	D	218	GLN
1	D	265	ASN
1	D	267	ASN
1	D	411	ASN

5.3.3 RNA [i](#)

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

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	453/476 (95%)	1.06	74 (16%) 4 3	45, 77, 119, 138	0
1	B	398/476 (83%)	1.00	64 (16%) 4 4	44, 78, 114, 135	0
1	C	450/476 (94%)	1.09	69 (15%) 5 4	44, 82, 121, 145	0
1	D	394/476 (82%)	1.23	81 (20%) 2 2	51, 88, 128, 160	0
All	All	1695/1904 (89%)	1.09	288 (16%) 4 3	44, 81, 121, 160	0

All (288) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	457	ALA	6.6
1	C	453	LEU	5.9
1	D	458	LEU	5.8
1	B	442	ALA	5.6
1	B	458	LEU	5.3
1	B	423	ILE	5.1
1	A	454	ASN	4.9
1	D	113	TYR	4.9
1	D	420	THR	4.8
1	C	454	ASN	4.8
1	C	459	SER	4.8
1	A	391	LYS	4.7
1	D	82	ILE	4.6
1	A	66	GLN	4.5
1	D	39	SER	4.4
1	C	420	THR	4.4
1	B	451	GLY	4.4
1	A	423	ILE	4.4
1	C	475	SER	4.4
1	A	87	PHE	4.3
1	A	453	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	349	ASP	4.3
1	D	443	ASP	4.3
1	D	205	TYR	4.3
1	D	475	SER	4.3
1	A	443	ASP	4.2
1	A	299	THR	4.2
1	B	215	GLU	4.2
1	D	453	LEU	4.1
1	D	387	ASN	4.1
1	B	343	ASN	4.0
1	C	47	ILE	4.0
1	D	155	VAL	4.0
1	A	292	VAL	3.9
1	D	217	ASP	3.9
1	A	458	LEU	3.9
1	B	84	LEU	3.9
1	C	346	THR	3.9
1	D	154	ASP	3.9
1	A	296	HIS	3.8
1	B	418	GLY	3.8
1	B	391	LYS	3.8
1	B	2	HIS	3.8
1	B	454	ASN	3.8
1	B	476	ASN	3.8
1	C	452	GLU	3.8
1	D	301	HIS	3.7
1	D	347	ILE	3.7
1	C	214	TYR	3.7
1	B	88	SER	3.7
1	C	48	ALA	3.7
1	D	153	GLY	3.7
1	A	436	GLU	3.6
1	A	442	ALA	3.6
1	C	46	PRO	3.6
1	D	441	GLY	3.6
1	B	217	ASP	3.6
1	C	436	GLU	3.6
1	A	417	VAL	3.5
1	D	422	TYR	3.5
1	D	2	HIS	3.5
1	D	462	GLU	3.4
1	C	415	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	441	GLY	3.4
1	B	85	ASP	3.4
1	C	294	TYR	3.4
1	D	173	ILE	3.4
1	D	413	TYR	3.4
1	C	442	ALA	3.3
1	C	410	GLN	3.3
1	C	434	GLU	3.3
1	D	156	GLU	3.3
1	B	317	ASP	3.3
1	B	29	ALA	3.3
1	A	386	GLY	3.3
1	B	393	GLN	3.2
1	C	66	GLN	3.2
1	C	393	GLN	3.2
1	D	427	LEU	3.2
1	B	132	TYR	3.2
1	D	419	ALA	3.2
1	C	350	ASP	3.2
1	A	59	ASN	3.2
1	B	214	TYR	3.2
1	D	327	GLY	3.2
1	A	43	LEU	3.2
1	D	337	LEU	3.2
1	B	89	ARG	3.1
1	C	404	PHE	3.1
1	A	326	LEU	3.1
1	A	427	LEU	3.1
1	D	85	ASP	3.1
1	B	205	TYR	3.1
1	A	452	GLU	3.1
1	B	154	ASP	3.1
1	B	233	ASP	3.1
1	D	459	SER	3.1
1	C	428	TRP	3.1
1	C	440	PRO	3.0
1	B	295	ASN	3.0
1	B	113	TYR	3.0
1	B	177	PRO	3.0
1	C	408	PHE	3.0
1	A	47	ILE	3.0
1	C	235	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	87	PHE	3.0
1	C	59	ASN	3.0
1	D	291	ALA	2.9
1	A	390	ASP	2.9
1	D	411	ASN	2.9
1	B	236	GLU	2.9
1	B	434	GLU	2.9
1	B	436	GLU	2.9
1	D	365	GLU	2.9
1	A	346	THR	2.9
1	D	385	TYR	2.9
1	B	160	GLU	2.9
1	C	360	GLY	2.9
1	D	289	GLY	2.9
1	A	2	HIS	2.8
1	D	216	ARG	2.8
1	A	291	ALA	2.8
1	B	449	LEU	2.8
1	C	43	LEU	2.8
1	A	294	TYR	2.8
1	A	301	HIS	2.8
1	C	264	ASN	2.8
1	D	340	LEU	2.8
1	A	327	GLY	2.8
1	D	460	ILE	2.8
1	A	93	LEU	2.8
1	A	419	ALA	2.8
1	A	308	GLN	2.8
1	D	215	GLU	2.8
1	A	54	ASP	2.8
1	C	296	HIS	2.8
1	C	292	VAL	2.8
1	C	417	VAL	2.8
1	B	173	ILE	2.7
1	D	297	TRP	2.7
1	A	55	VAL	2.7
1	B	38	VAL	2.7
1	C	396	LYS	2.7
1	C	308	GLN	2.7
1	C	44	LEU	2.7
1	A	298	GLU	2.7
1	B	92	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	440	PRO	2.7
1	A	72	ASN	2.7
1	C	419	ALA	2.7
1	C	233	ASP	2.7
1	A	62	VAL	2.7
1	D	298	GLU	2.7
1	B	159	SER	2.6
1	B	462	GLU	2.6
1	B	235	LEU	2.6
1	D	86	GLU	2.6
1	D	94	THR	2.6
1	A	40	TRP	2.6
1	B	350	ASP	2.6
1	A	460	ILE	2.6
1	B	297	TRP	2.6
1	D	326	LEU	2.6
1	A	414	VAL	2.6
1	B	308	GLN	2.6
1	B	366	GLN	2.6
1	A	297	TRP	2.5
1	D	234	GLU	2.5
1	C	431	VAL	2.5
1	D	396	LYS	2.5
1	D	214	TYR	2.5
1	A	61	LEU	2.5
1	B	157	HIS	2.5
1	B	312	GLU	2.5
1	C	26	PHE	2.5
1	D	432	ASN	2.5
1	A	424	ALA	2.5
1	D	322	SER	2.5
1	C	427	LEU	2.5
1	D	281	LYS	2.5
1	A	73	GLN	2.5
1	A	401	GLN	2.5
1	D	394	VAL	2.5
1	D	417	VAL	2.5
1	A	445	ARG	2.5
1	D	213	ALA	2.5
1	D	392	GLY	2.4
1	D	362	LYS	2.4
1	B	453	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	438	TYR	2.4
1	C	371	ARG	2.4
1	A	415	VAL	2.4
1	C	297	TRP	2.4
1	B	237	ALA	2.4
1	B	349	ASP	2.4
1	D	280	ILE	2.4
1	C	366	GLN	2.4
1	B	408	PHE	2.4
1	C	395	VAL	2.4
1	A	420	THR	2.4
1	B	86	GLU	2.4
1	D	83	ILE	2.4
1	B	463	LEU	2.4
1	A	408	PHE	2.4
1	C	397	ALA	2.4
1	D	237	ALA	2.4
1	A	214	TYR	2.3
1	A	450	PHE	2.3
1	D	438	TYR	2.3
1	C	72	ASN	2.3
1	A	437	THR	2.3
1	D	290	SER	2.3
1	A	366	GLN	2.3
1	C	401	GLN	2.3
1	D	384	LEU	2.3
1	A	404	PHE	2.3
1	B	362	LYS	2.3
1	D	461	GLU	2.3
1	D	366	GLN	2.3
1	B	468	ILE	2.3
1	D	389	ILE	2.3
1	A	50	GLU	2.3
1	A	394	VAL	2.3
1	B	158	PRO	2.3
1	B	346	THR	2.2
1	B	153	GLY	2.2
1	D	421	GLY	2.2
1	D	312	GLU	2.2
1	A	41	ALA	2.2
1	A	44	LEU	2.2
1	D	235	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	312	GLU	2.2
1	B	239	PHE	2.2
1	B	91	VAL	2.2
1	B	414	VAL	2.2
1	B	316	LYS	2.2
1	C	413	TYR	2.2
1	D	260	THR	2.2
1	A	418	GLY	2.2
1	D	464	ILE	2.2
1	B	339	GLU	2.2
1	B	216	ARG	2.2
1	B	450	PHE	2.2
1	D	158	PRO	2.2
1	A	35	VAL	2.2
1	C	62	VAL	2.2
1	D	395	VAL	2.2
1	B	152	HIS	2.2
1	C	74	GLY	2.2
1	D	132	TYR	2.2
1	D	379	GLY	2.2
1	C	295	ASN	2.1
1	C	392	GLY	2.1
1	C	421	GLY	2.1
1	C	51	ILE	2.1
1	C	211	ARG	2.1
1	A	350	ASP	2.1
1	A	430	LYS	2.1
1	C	2	HIS	2.1
1	D	296	HIS	2.1
1	A	37	TYR	2.1
1	C	234	GLU	2.1
1	C	474	LEU	2.1
1	A	89	ARG	2.1
1	D	89	ARG	2.1
1	C	423	ILE	2.1
1	D	188	SER	2.1
1	D	152	HIS	2.1
1	C	87	PHE	2.1
1	A	64	LEU	2.1
1	D	423	ILE	2.1
1	A	425	LYS	2.1
1	A	426	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	439	TYR	2.1
1	A	328	VAL	2.0
1	A	395	VAL	2.0
1	C	210	VAL	2.0
1	D	305	PHE	2.0
1	D	408	PHE	2.0
1	A	389	ILE	2.0
1	C	361	LYS	2.0
1	A	439	TYR	2.0
1	C	390	ASP	2.0
1	D	92	ASP	2.0
1	C	381	SER	2.0
1	C	291	ALA	2.0
1	A	95	GLU	2.0
1	A	83	ILE	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.