



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:55 PM UTC

PDB ID : 1BXB / pdb_00001bxb
Title : XYLOSE ISOMERASE FROM THERMUS THERMOPHILUS
Authors : Chang, C.; Park, B.C.; Lee, D.-S.; Suh, S.W.
Deposited on : 1998-10-02
Resolution : 2.20 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

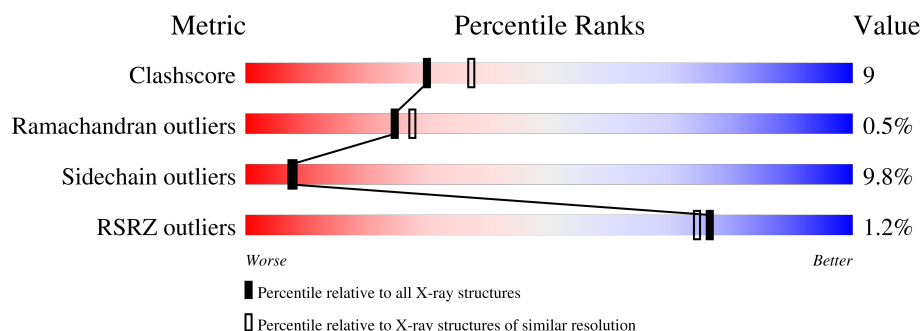
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	387	2% 78% 18% .
1	B	387	% 78% 18% .
1	C	387	% 77% 19% .
1	D	387	% 77% 19% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13488 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 XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			3101	1980	544	568	9			
1	B	387	Total	C	N	O	S	0	0	0
			3101	1980	544	568	9			
1	C	387	Total	C	N	O	S	0	0	0
			3101	1980	544	568	9			
1	D	387	Total	C	N	O	S	0	0	0
			3101	1980	544	568	9			

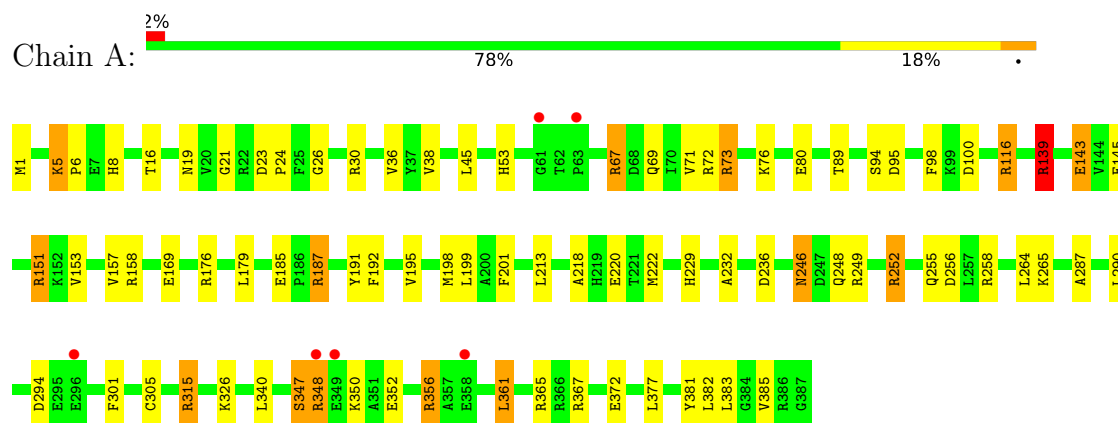
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	277	Total	O	0	0
			277	277		
2	B	267	Total	O	0	0
			267	267		
2	C	273	Total	O	0	0
			273	273		
2	D	267	Total	O	0	0
			267	267		

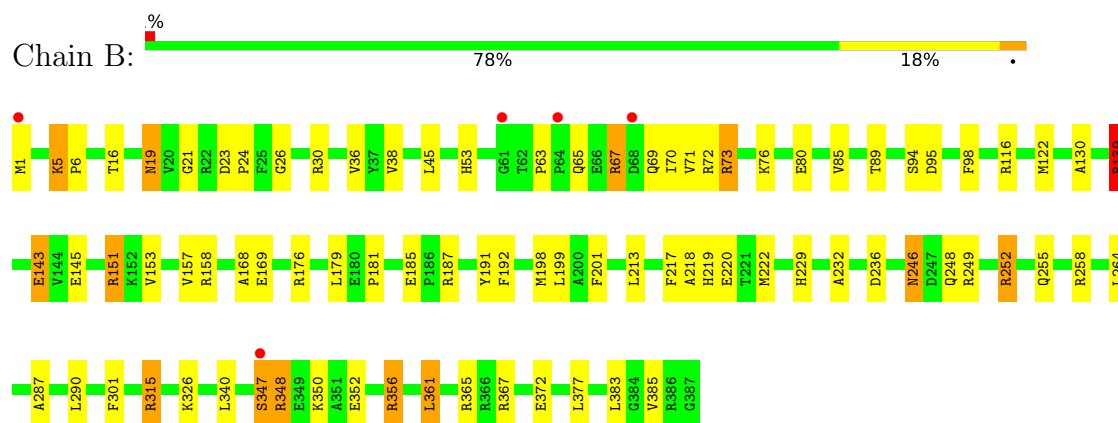
3 Residue-property plots

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.

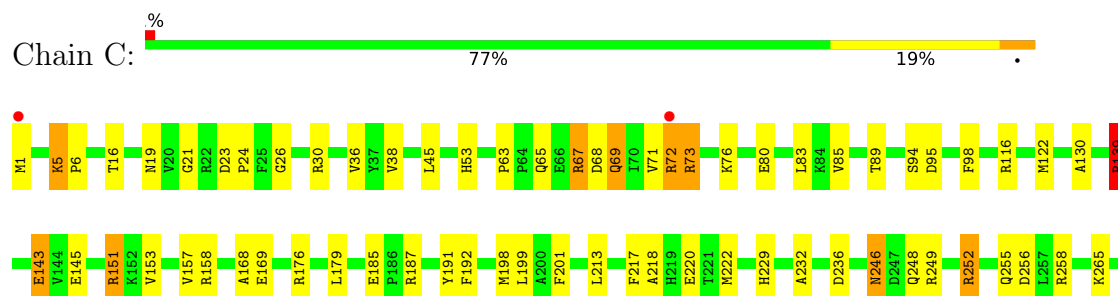
• Molecule 1: XYLOSE ISOMERASE

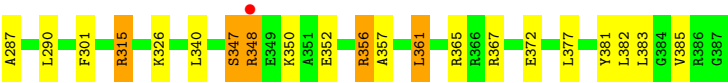


• Molecule 1: XYLOSE ISOMERASE

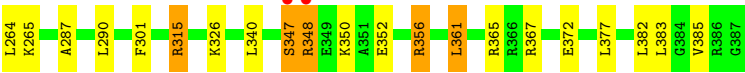
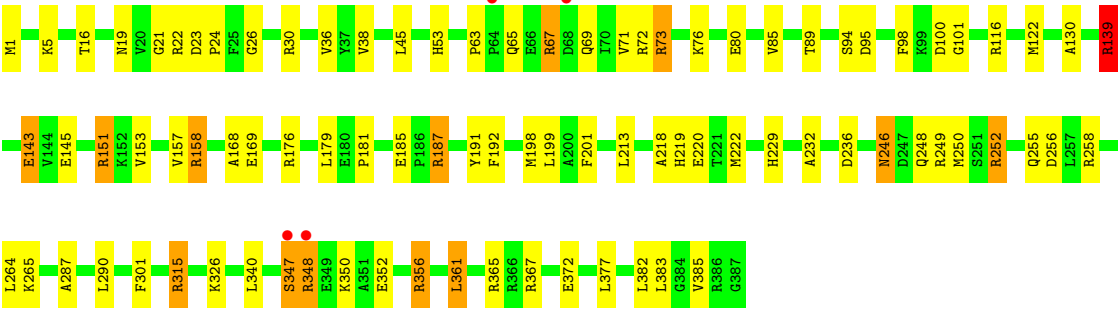
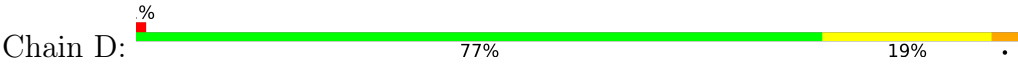


• Molecule 1: XYLOSE ISOMERASE





● Molecule 1: XYLOSE ISOMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.34Å 144.05Å 155.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20 8.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	70.7 (8.00-2.20) 69.1 (8.00-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.99Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.180 , 0.230 0.174 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13488	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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	0.62	0/3181	0.79	0/4307
1	B	0.62	0/3181	0.80	0/4307
1	C	0.60	0/3181	0.80	0/4307
1	D	0.60	0/3181	0.79	0/4307
All	All	0.61	0/12724	0.79	0/17228

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	6
1	B	0	5
1	C	0	6
1	D	0	6
All	All	0	23

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	ARG	Sidechain
1	A	187	ARG	Sidechain
1	A	258	ARG	Sidechain
1	A	30	ARG	Sidechain
1	A	356	ARG	Sidechain
1	A	381	TYR	Sidechain
1	B	139	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	187	ARG	Sidechain
1	B	258	ARG	Sidechain
1	B	30	ARG	Sidechain
1	B	356	ARG	Sidechain
1	C	139	ARG	Sidechain
1	C	187	ARG	Sidechain
1	C	258	ARG	Sidechain
1	C	30	ARG	Sidechain
1	C	356	ARG	Sidechain
1	C	381	TYR	Sidechain
1	D	139	ARG	Sidechain
1	D	158	ARG	Sidechain
1	D	187	ARG	Sidechain
1	D	258	ARG	Sidechain
1	D	30	ARG	Sidechain
1	D	356	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	3101	0	3016	57	4
1	B	3101	0	3016	59	1
1	C	3101	0	3016	62	2
1	D	3101	0	3016	66	2
2	A	277	0	0	5	0
2	B	267	0	0	6	2
2	C	273	0	0	4	2
2	D	267	0	0	6	5
All	All	13488	0	12064	209	9

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 9.

All (209) 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:B:248:GLN:HE22	1:B:255:GLN:H	1.10	0.97
1:D:248:GLN:HE22	1:D:255:GLN:H	1.15	0.93
1:C:248:GLN:HE22	1:C:255:GLN:H	1.10	0.91
1:A:248:GLN:HE22	1:A:255:GLN:H	1.11	0.91
1:C:24:PRO:HG3	1:D:24:PRO:HG3	1.56	0.88
1:A:24:PRO:HG3	1:B:24:PRO:HG3	1.59	0.84
1:D:347:SER:HB2	1:D:350:LYS:HB2	1.58	0.84
1:B:347:SER:HB2	1:B:350:LYS:HB2	1.61	0.82
1:B:347:SER:O	1:B:348:ARG:HB3	1.81	0.80
1:C:347:SER:HB2	1:C:350:LYS:HB2	1.61	0.80
1:A:347:SER:HB2	1:A:350:LYS:HB2	1.63	0.80
1:A:347:SER:O	1:A:348:ARG:HB3	1.82	0.78
1:D:347:SER:O	1:D:348:ARG:HB3	1.83	0.78
1:C:347:SER:O	1:C:348:ARG:HB3	1.83	0.77
1:D:347:SER:HB3	1:D:350:LYS:H	1.51	0.75
1:A:347:SER:HB3	1:A:350:LYS:H	1.52	0.75
1:C:347:SER:HB3	1:C:350:LYS:H	1.51	0.74
1:D:218:ALA:O	1:D:222:MET:HG3	1.88	0.72
1:D:153:VAL:O	1:D:157:VAL:HG12	1.90	0.71
1:C:153:VAL:O	1:C:157:VAL:HG12	1.91	0.71
1:B:347:SER:HB3	1:B:350:LYS:H	1.54	0.70
1:A:19:ASN:ND2	1:A:21:GLY:H	1.90	0.70
1:C:19:ASN:ND2	1:C:21:GLY:H	1.91	0.69
1:B:153:VAL:O	1:B:157:VAL:HG12	1.93	0.68
1:B:19:ASN:ND2	1:B:21:GLY:H	1.90	0.68
1:D:249:ARG:O	1:D:252:ARG:HD3	1.94	0.68
1:C:248:GLN:NE2	1:C:255:GLN:H	1.88	0.67
1:D:248:GLN:NE2	1:D:255:GLN:H	1.92	0.67
1:A:153:VAL:O	1:A:157:VAL:HG12	1.95	0.66
1:A:199:LEU:HG	1:A:213:LEU:HD11	1.78	0.66
1:B:218:ALA:H	1:B:246:ASN:HD21	1.45	0.65
1:A:249:ARG:O	1:A:252:ARG:HD3	1.97	0.65
1:D:199:LEU:HG	1:D:213:LEU:HD11	1.77	0.64
1:A:248:GLN:NE2	1:A:255:GLN:H	1.89	0.64
1:D:19:ASN:ND2	1:D:21:GLY:H	1.96	0.64
1:C:199:LEU:HG	1:C:213:LEU:HD11	1.80	0.64
1:C:249:ARG:O	1:C:252:ARG:HD3	1.98	0.63
1:B:199:LEU:HG	1:B:213:LEU:HD11	1.80	0.62
1:B:249:ARG:O	1:B:252:ARG:HD3	1.99	0.61
1:A:383:LEU:O	1:D:315:ARG:NH2	2.34	0.60
1:A:246:ASN:HD22	1:A:246:ASN:C	2.07	0.60
1:C:356:ARG:HD3	2:C:434:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:VAL:HG13	1:A:201:PHE:CZ	2.36	0.60
1:D:246:ASN:C	1:D:246:ASN:HD22	2.10	0.60
1:D:218:ALA:H	1:D:246:ASN:HD21	1.50	0.59
2:B:571:HOH:O	1:D:229:HIS:HD2	1.84	0.59
1:B:23:ASP:HB2	1:B:24:PRO:CD	2.32	0.59
1:D:23:ASP:HB2	1:D:24:PRO:CD	2.32	0.59
1:B:248:GLN:NE2	1:B:255:GLN:H	1.91	0.58
1:B:232:ALA:O	1:D:151:ARG:NH2	2.36	0.58
1:C:157:VAL:HG13	1:C:201:PHE:CZ	2.38	0.58
1:B:383:LEU:O	1:C:315:ARG:NH2	2.38	0.57
1:B:151:ARG:NH2	1:D:232:ALA:O	2.37	0.57
1:B:246:ASN:C	1:B:246:ASN:HD22	2.12	0.57
1:C:248:GLN:HE22	1:C:255:GLN:N	1.93	0.57
1:C:23:ASP:HB2	1:C:24:PRO:CD	2.34	0.57
1:B:19:ASN:HD22	1:B:21:GLY:H	1.50	0.56
1:A:19:ASN:HD22	1:A:21:GLY:H	1.52	0.56
1:A:315:ARG:NH2	1:D:383:LEU:O	2.39	0.56
1:C:218:ALA:O	1:C:222:MET:HG3	2.05	0.56
1:A:218:ALA:O	1:A:222:MET:HG3	2.05	0.56
1:A:232:ALA:O	1:C:151:ARG:NH2	2.38	0.56
1:A:23:ASP:HB2	1:A:24:PRO:CD	2.35	0.55
2:A:634:HOH:O	1:C:229:HIS:HD2	1.89	0.55
1:A:151:ARG:NH2	1:C:232:ALA:O	2.38	0.55
1:B:157:VAL:HG13	1:B:201:PHE:CZ	2.42	0.55
1:A:372:GLU:HG2	1:D:301:PHE:HB2	1.87	0.55
1:A:248:GLN:HE22	1:A:255:GLN:N	1.94	0.55
1:A:95:ASP:OD1	1:C:365:ARG:HD3	2.07	0.54
1:A:236:ASP:HB2	1:C:151:ARG:HH22	1.73	0.54
1:C:16:THR:HB	1:C:287:ALA:O	2.07	0.54
1:B:236:ASP:HB2	1:D:151:ARG:HH22	1.71	0.54
1:D:157:VAL:HG13	1:D:201:PHE:CZ	2.43	0.54
1:C:143:GLU:HG3	1:D:290:LEU:HD22	1.90	0.54
1:B:151:ARG:HH22	1:D:236:ASP:HB2	1.73	0.54
1:B:372:GLU:HG2	1:C:301:PHE:HB2	1.90	0.54
1:D:151:ARG:NH1	2:D:524:HOH:O	2.35	0.54
1:A:151:ARG:HH22	1:C:236:ASP:HB2	1.73	0.53
1:C:94:SER:HA	1:D:26:GLY:HA2	1.90	0.53
1:B:315:ARG:NH2	1:C:383:LEU:O	2.42	0.53
1:A:98:PHE:O	1:A:139:ARG:HG2	2.09	0.53
1:C:218:ALA:H	1:C:246:ASN:HD21	1.55	0.53
1:A:229:HIS:HD2	2:C:460:HOH:O	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ASP:HB2	1:B:24:PRO:HD3	1.91	0.53
1:C:19:ASN:HD22	1:C:21:GLY:H	1.57	0.53
1:A:53:HIS:HA	1:A:89:THR:O	2.09	0.52
1:C:23:ASP:HB2	1:C:24:PRO:HD3	1.91	0.52
1:B:218:ALA:O	1:B:222:MET:HG3	2.09	0.52
1:D:23:ASP:HB2	1:D:24:PRO:HD3	1.92	0.52
1:A:157:VAL:HG13	1:A:201:PHE:HZ	1.75	0.52
1:B:53:HIS:HA	1:B:89:THR:O	2.09	0.52
1:C:53:HIS:HA	1:C:89:THR:O	2.11	0.51
1:D:53:HIS:HA	1:D:89:THR:O	2.10	0.51
1:C:67:ARG:O	1:C:71:VAL:HG23	2.10	0.51
1:A:23:ASP:HB2	1:A:24:PRO:HD3	1.91	0.51
1:C:246:ASN:C	1:C:246:ASN:HD22	2.19	0.51
1:D:16:THR:HB	1:D:287:ALA:O	2.10	0.51
1:D:122:MET:CE	1:D:168:ALA:HB2	2.42	0.50
1:B:176:ARG:HH11	1:B:176:ARG:HG3	1.75	0.50
1:C:98:PHE:O	1:C:139:ARG:HG2	2.12	0.50
1:D:176:ARG:HH11	1:D:176:ARG:HG3	1.76	0.49
1:A:176:ARG:HG3	1:A:176:ARG:HH11	1.76	0.49
1:A:67:ARG:O	1:A:71:VAL:HG23	2.12	0.49
1:A:365:ARG:HD3	1:C:95:ASP:OD1	2.12	0.49
1:D:361:LEU:O	1:D:365:ARG:HG3	2.12	0.49
1:A:361:LEU:O	1:A:365:ARG:HG3	2.13	0.49
1:D:248:GLN:HE22	1:D:255:GLN:N	1.98	0.49
1:C:151:ARG:NH1	2:C:650:HOH:O	2.39	0.48
1:B:67:ARG:O	1:B:71:VAL:HG23	2.14	0.48
1:C:176:ARG:HH11	1:C:176:ARG:HG3	1.78	0.48
1:C:347:SER:O	1:C:348:ARG:CB	2.59	0.48
1:C:361:LEU:O	1:C:365:ARG:HG3	2.12	0.48
1:A:356:ARG:HD3	2:A:608:HOH:O	2.14	0.48
1:A:218:ALA:H	1:A:246:ASN:HD21	1.60	0.48
1:D:67:ARG:O	1:D:71:VAL:HG23	2.14	0.48
1:A:26:GLY:HA2	1:B:94:SER:HA	1.96	0.48
1:B:151:ARG:NH1	2:B:423:HOH:O	2.40	0.48
1:B:301:PHE:HB2	1:C:372:GLU:HG2	1.95	0.48
1:A:151:ARG:NH1	2:A:552:HOH:O	2.41	0.47
1:C:157:VAL:HG13	1:C:201:PHE:HZ	1.76	0.47
1:A:16:THR:HB	1:A:287:ALA:O	2.15	0.47
1:C:26:GLY:HA2	1:D:94:SER:HA	1.95	0.47
1:D:98:PHE:O	1:D:139:ARG:HG2	2.14	0.47
1:D:157:VAL:HG11	1:D:192:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:LEU:HD22	1:D:143:GLU:HG3	1.95	0.47
1:B:361:LEU:O	1:B:365:ARG:HG3	2.15	0.47
1:D:122:MET:HE1	1:D:168:ALA:HB2	1.97	0.47
1:B:347:SER:CB	1:B:350:LYS:H	2.23	0.46
1:B:157:VAL:HG13	1:B:201:PHE:HZ	1.80	0.46
1:B:16:THR:HB	1:B:287:ALA:O	2.15	0.46
1:B:249:ARG:NH2	2:B:420:HOH:O	2.49	0.46
1:B:347:SER:O	1:B:348:ARG:CB	2.59	0.46
1:B:95:ASP:OD1	1:D:365:ARG:HD3	2.15	0.46
1:C:290:LEU:HD22	1:D:143:GLU:CG	2.46	0.46
1:C:69:GLN:O	1:C:72:ARG:HG3	2.16	0.46
1:B:365:ARG:HD3	1:D:95:ASP:OD1	2.17	0.45
1:B:181:PRO:O	1:B:219:HIS:HD2	2.00	0.45
1:C:347:SER:CB	1:C:350:LYS:H	2.26	0.45
1:D:347:SER:CB	1:D:350:LYS:H	2.26	0.45
1:B:218:ALA:N	1:B:246:ASN:HD21	2.14	0.45
1:C:153:VAL:HG11	1:C:191:TYR:CE2	2.52	0.45
1:B:229:HIS:HD2	2:D:404:HOH:O	1.99	0.45
1:D:19:ASN:HD22	1:D:21:GLY:H	1.64	0.45
1:D:356:ARG:HD3	2:D:478:HOH:O	2.16	0.45
1:A:94:SER:HA	1:B:26:GLY:HA2	1.99	0.44
1:A:290:LEU:HD22	1:B:143:GLU:HG3	1.99	0.44
1:A:100:ASP:HA	1:A:187:ARG:NH2	2.32	0.44
1:D:85:VAL:O	1:D:130:ALA:HA	2.18	0.44
1:D:63:PRO:C	1:D:65:GLN:H	2.26	0.43
1:A:153:VAL:HG11	1:A:191:TYR:CE2	2.53	0.43
1:A:301:PHE:HB2	1:D:372:GLU:HG2	1.99	0.43
1:B:122:MET:CE	1:B:168:ALA:HB2	2.49	0.43
1:C:122:MET:HE1	1:C:168:ALA:HB2	2.01	0.43
1:C:143:GLU:CG	1:D:290:LEU:HD22	2.48	0.43
1:A:143:GLU:CG	1:B:290:LEU:HD22	2.48	0.43
1:B:157:VAL:HG11	1:B:192:PHE:CZ	2.53	0.43
1:D:157:VAL:HG13	1:D:201:PHE:HZ	1.83	0.43
1:A:157:VAL:HG11	1:A:192:PHE:CZ	2.53	0.43
1:B:198:MET:HB2	1:B:213:LEU:HD21	2.01	0.43
1:A:143:GLU:HG3	1:B:290:LEU:HD22	2.00	0.43
1:D:249:ARG:NH2	2:D:521:HOH:O	2.51	0.43
1:D:22:ARG:NH2	2:D:553:HOH:O	2.51	0.42
1:B:98:PHE:O	1:B:139:ARG:HG2	2.19	0.42
1:B:85:VAL:O	1:B:130:ALA:HA	2.18	0.42
1:D:250:MET:O	1:D:252:ARG:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:HA	1:A:382:LEU:HD11	2.02	0.42
1:A:347:SER:O	1:A:348:ARG:CB	2.60	0.42
1:C:217:PHE:HB3	1:C:246:ASN:ND2	2.33	0.42
1:A:116:ARG:NH2	1:C:357:ALA:O	2.51	0.42
1:C:5:LYS:HB3	1:C:6:PRO:HD2	2.01	0.42
1:C:122:MET:CE	1:C:168:ALA:HB2	2.49	0.42
1:C:36:VAL:HG21	1:C:73:ARG:HD2	2.00	0.42
1:C:157:VAL:HG11	1:C:192:PHE:CZ	2.54	0.42
1:D:100:ASP:HA	1:D:187:ARG:NH2	2.34	0.42
1:A:198:MET:HB2	1:A:213:LEU:HD21	2.02	0.42
1:C:218:ALA:N	1:C:246:ASN:HD21	2.17	0.42
1:D:181:PRO:O	1:D:219:HIS:HD2	2.02	0.42
1:D:181:PRO:O	1:D:219:HIS:CD2	2.73	0.42
1:C:249:ARG:NH2	2:C:647:HOH:O	2.53	0.41
1:D:198:MET:HB2	1:D:213:LEU:HD21	2.03	0.41
1:B:264:LEU:HG	2:B:442:HOH:O	2.20	0.41
1:B:356:ARG:HD3	2:B:646:HOH:O	2.19	0.41
1:A:5:LYS:HB3	1:A:6:PRO:HD2	2.01	0.41
1:B:217:PHE:HB3	1:B:246:ASN:ND2	2.35	0.41
1:D:256:ASP:HB3	1:D:287:ALA:HA	2.01	0.41
1:A:290:LEU:HD22	1:B:143:GLU:CG	2.51	0.41
1:B:63:PRO:C	1:B:65:GLN:H	2.26	0.41
1:C:198:MET:HB2	1:C:213:LEU:HD21	2.03	0.41
1:D:264:LEU:HD23	1:D:264:LEU:HA	1.94	0.41
1:D:36:VAL:HG21	1:D:73:ARG:HD2	2.02	0.41
1:D:246:ASN:C	1:D:246:ASN:ND2	2.77	0.41
1:C:85:VAL:O	1:C:130:ALA:HA	2.20	0.41
1:D:153:VAL:HG11	1:D:191:TYR:CE2	2.55	0.41
1:D:347:SER:O	1:D:348:ARG:CB	2.60	0.41
1:B:36:VAL:HG21	1:B:73:ARG:HD2	2.02	0.41
1:B:264:LEU:HA	1:B:264:LEU:HD23	1.89	0.41
1:C:265:LYS:HA	1:C:382:LEU:HD11	2.02	0.41
1:A:249:ARG:NH2	2:A:549:HOH:O	2.54	0.41
1:A:264:LEU:HG	2:A:571:HOH:O	2.20	0.41
1:B:153:VAL:HG11	1:B:191:TYR:CE2	2.56	0.41
1:C:63:PRO:C	1:C:65:GLN:H	2.29	0.40
1:D:264:LEU:HG	2:D:543:HOH:O	2.22	0.40
1:A:256:ASP:HB3	1:A:287:ALA:HA	2.03	0.40
1:D:265:LYS:HA	1:D:382:LEU:HD11	2.04	0.40
1:A:36:VAL:HG21	1:A:73:ARG:HD2	2.03	0.40
1:A:195:VAL:HG13	1:A:213:LEU:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:LYS:HB3	1:B:6:PRO:HD2	2.03	0.40
1:C:256:ASP:HB3	1:C:287:ALA:HA	2.04	0.40
2:B:571:HOH:O	1:D:229:HIS:CD2	2.68	0.40

All (9) 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:C:68:ASP:N	2:D:456:HOH:O[2_435]	2.08	0.12
1:A:301:PHE:O	2:D:594:HOH:O[4_436]	2.09	0.11
1:C:356:ARG:NE	2:B:597:HOH:O[4_526]	2.12	0.08
1:D:248:GLN:OE1	2:B:545:HOH:O[3_456]	2.13	0.07
1:B:70:ILE:O	2:C:547:HOH:O[4_426]	2.14	0.06
1:A:305:CYS:N	2:D:594:HOH:O[4_436]	2.15	0.05
1:A:8:HIS:O	2:C:556:HOH:O[2_534]	2.16	0.04
1:A:294:ASP:O	2:D:645:HOH:O[4_436]	2.17	0.03
1:D:101:GLY:O	2:D:413:HOH:O[2_435]	2.17	0.03

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	385/387 (100%)	371 (96%)	12 (3%)	2 (0%)	24	27
1	B	385/387 (100%)	371 (96%)	12 (3%)	2 (0%)	24	27
1	C	385/387 (100%)	371 (96%)	12 (3%)	2 (0%)	24	27
1	D	385/387 (100%)	371 (96%)	12 (3%)	2 (0%)	24	27
All	All	1540/1548 (100%)	1484 (96%)	48 (3%)	8 (0%)	24	27

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	348	ARG
1	C	348	ARG
1	D	348	ARG
1	B	348	ARG
1	A	185	GLU
1	B	185	GLU
1	C	185	GLU
1	D	185	GLU

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	310/311 (100%)	280 (90%)	30 (10%)	8	8
1	B	310/311 (100%)	279 (90%)	31 (10%)	7	7
1	C	310/311 (100%)	279 (90%)	31 (10%)	7	7
1	D	310/311 (100%)	280 (90%)	30 (10%)	8	8
All	All	1240/1244 (100%)	1118 (90%)	122 (10%)	7	8

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LYS
1	A	38	VAL
1	A	45	LEU
1	A	67	ARG
1	A	69	GLN
1	A	72	ARG
1	A	73	ARG
1	A	76	LYS
1	A	80	GLU
1	A	116	ARG
1	A	139	ARG
1	A	143	GLU
1	A	145	GLU

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Mol	Chain	Res	Type
1	A	151	ARG
1	A	158	ARG
1	A	169	GLU
1	A	179	LEU
1	A	220	GLU
1	A	246	ASN
1	A	252	ARG
1	A	315	ARG
1	A	326	LYS
1	A	340	LEU
1	A	347	SER
1	A	352	GLU
1	A	361	LEU
1	A	367	ARG
1	A	377	LEU
1	A	385	VAL
1	B	1	MET
1	B	5	LYS
1	B	19	ASN
1	B	38	VAL
1	B	45	LEU
1	B	67	ARG
1	B	69	GLN
1	B	72	ARG
1	B	73	ARG
1	B	76	LYS
1	B	80	GLU
1	B	116	ARG
1	B	139	ARG
1	B	143	GLU
1	B	145	GLU
1	B	151	ARG
1	B	158	ARG
1	B	169	GLU
1	B	179	LEU
1	B	220	GLU
1	B	246	ASN
1	B	252	ARG
1	B	315	ARG
1	B	326	LYS
1	B	340	LEU
1	B	347	SER

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Mol	Chain	Res	Type
1	B	352	GLU
1	B	361	LEU
1	B	367	ARG
1	B	377	LEU
1	B	385	VAL
1	C	1	MET
1	C	5	LYS
1	C	38	VAL
1	C	45	LEU
1	C	67	ARG
1	C	69	GLN
1	C	72	ARG
1	C	73	ARG
1	C	76	LYS
1	C	80	GLU
1	C	83	LEU
1	C	116	ARG
1	C	139	ARG
1	C	143	GLU
1	C	145	GLU
1	C	151	ARG
1	C	158	ARG
1	C	169	GLU
1	C	179	LEU
1	C	220	GLU
1	C	246	ASN
1	C	252	ARG
1	C	315	ARG
1	C	326	LYS
1	C	340	LEU
1	C	347	SER
1	C	352	GLU
1	C	361	LEU
1	C	367	ARG
1	C	377	LEU
1	C	385	VAL
1	D	1	MET
1	D	5	LYS
1	D	38	VAL
1	D	45	LEU
1	D	67	ARG
1	D	69	GLN

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Mol	Chain	Res	Type
1	D	72	ARG
1	D	73	ARG
1	D	76	LYS
1	D	80	GLU
1	D	116	ARG
1	D	139	ARG
1	D	143	GLU
1	D	145	GLU
1	D	151	ARG
1	D	158	ARG
1	D	169	GLU
1	D	179	LEU
1	D	220	GLU
1	D	246	ASN
1	D	252	ARG
1	D	315	ARG
1	D	326	LYS
1	D	340	LEU
1	D	347	SER
1	D	352	GLU
1	D	361	LEU
1	D	367	ARG
1	D	377	LEU
1	D	385	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	51	ASN
1	A	219	HIS
1	A	229	HIS
1	A	233	GLN
1	A	246	ASN
1	A	248	GLN
1	B	19	ASN
1	B	219	HIS
1	B	229	HIS
1	B	233	GLN
1	B	246	ASN
1	B	248	GLN
1	C	19	ASN

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Mol	Chain	Res	Type
1	C	51	ASN
1	C	219	HIS
1	C	229	HIS
1	C	233	GLN
1	C	246	ASN
1	C	248	GLN
1	D	19	ASN
1	D	51	ASN
1	D	219	HIS
1	D	229	HIS
1	D	233	GLN
1	D	246	ASN
1	D	248	GLN

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 [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	387/387 (100%)	-0.55	6 (1%) 70 67	2, 10, 41, 59	0
1	B	387/387 (100%)	-0.58	5 (1%) 75 73	2, 10, 39, 61	0
1	C	387/387 (100%)	-0.57	3 (0%) 82 80	2, 12, 40, 63	0
1	D	387/387 (100%)	-0.54	4 (1%) 79 77	2, 12, 40, 62	0
All	All	1548/1548 (100%)	-0.56	18 (1%) 76 74	2, 11, 40, 63	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	64	PRO	3.9
1	B	1	MET	3.8
1	C	1	MET	3.8
1	D	68	ASP	3.3
1	B	64	PRO	2.9
1	A	63	PRO	2.7
1	B	61	GLY	2.5
1	A	358	GLU	2.5
1	D	347	SER	2.5
1	A	348	ARG	2.4
1	C	348	ARG	2.3
1	D	348	ARG	2.2
1	A	349	GLU	2.2
1	A	296	GLU	2.2
1	A	61	GLY	2.1
1	B	68	ASP	2.0
1	B	347	SER	2.0
1	C	72	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.