



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:14 PM UTC

PDB ID : 3L2D / pdb_00003l2d
Title : Glycocyamine kinase, beta-beta homodimer from marine worm *Namalycastis* sp.
Authors : Lim, K.; Pullalarevu, S.; Herzberg, O.
Deposited on : 2009-12-15
Resolution : 2.40 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

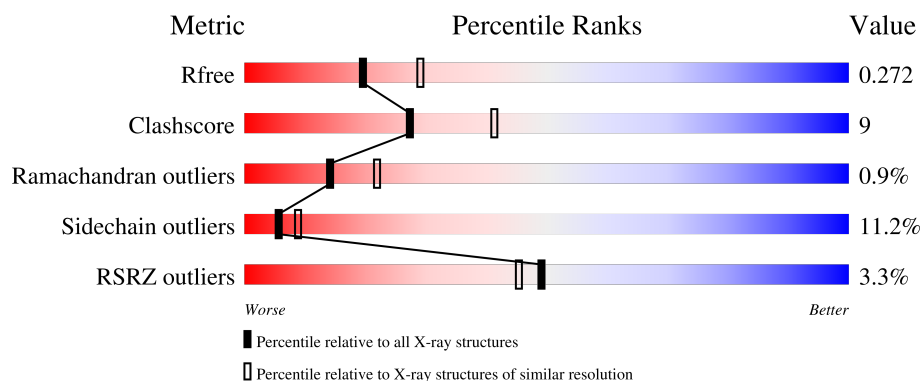
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	390	3% 72% 18% 6%
1	B	390	4% 72% 21% 6%
1	C	390	2% 73% 17% 6%
1	D	390	3% 75% 17% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12453 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 Glycocyamine kinase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	B	379	Total	C	N	O	S	0	0	0
			3005	1892	533	559	21			
1	C	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	D	379	Total	C	N	O	S	0	0	0
			3005	1892	533	559	21			

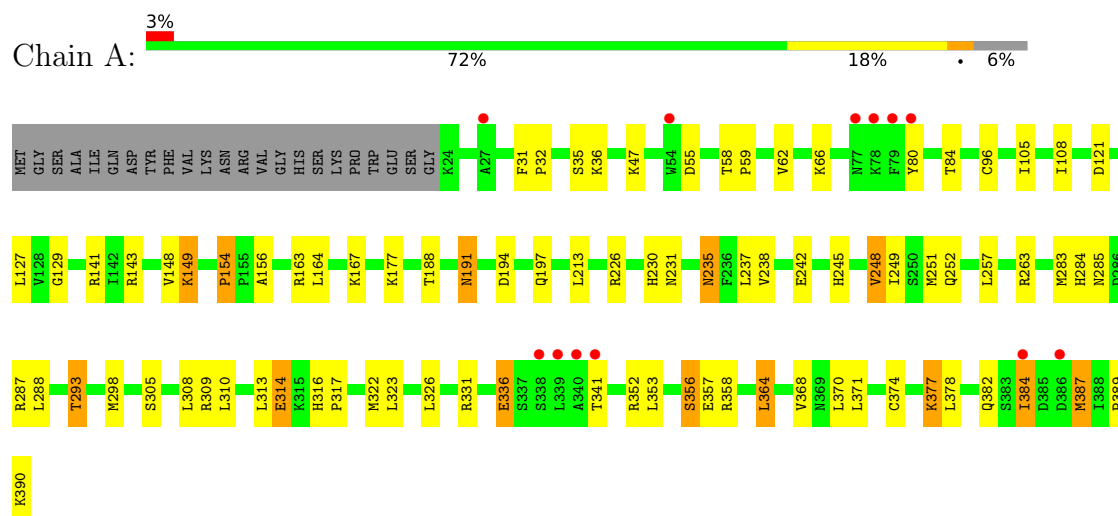
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	149	Total	O	0	0
			149	149		
2	B	140	Total	O	0	0
			140	140		
2	C	181	Total	O	0	0
			181	181		
2	D	153	Total	O	0	0
			153	153		

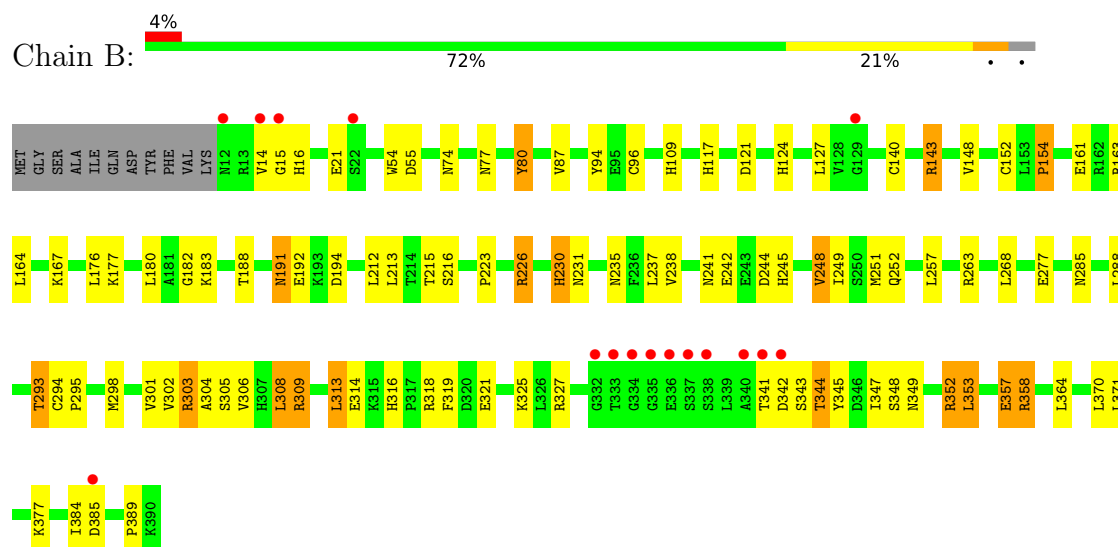
3 Residue-property plots

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: Glycocyamine kinase beta chain

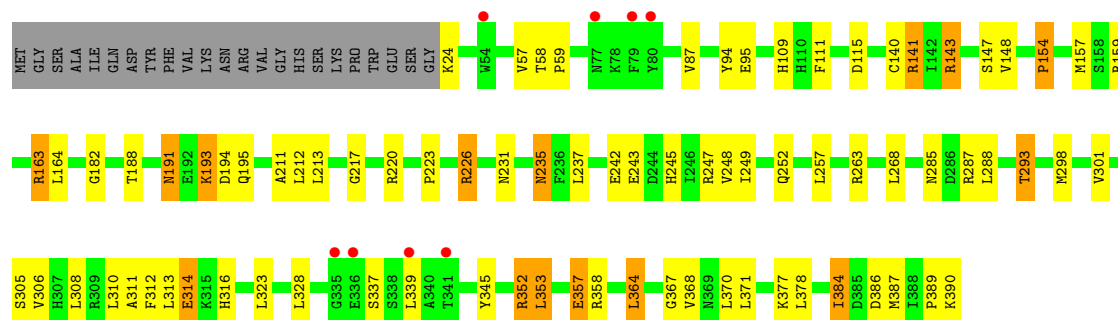


• Molecule 1: Glycocyamine kinase beta chain

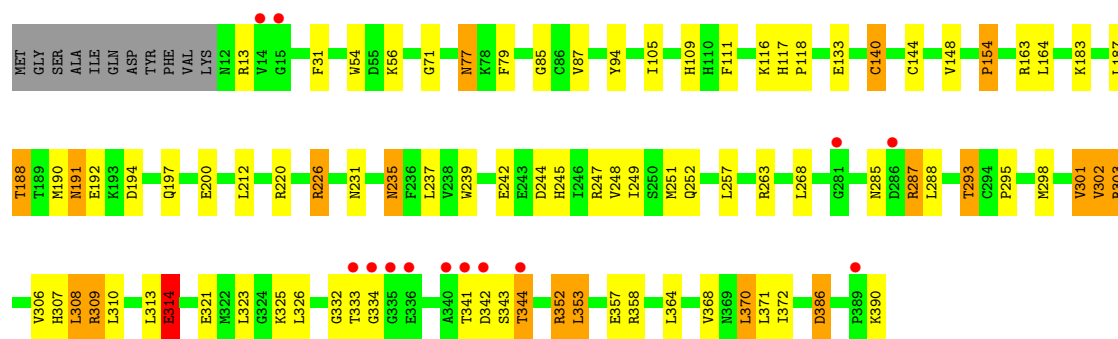
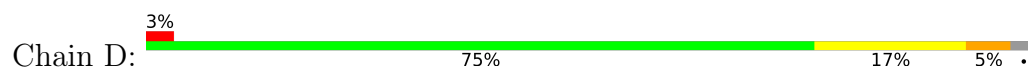


• Molecule 1: Glycocyamine kinase beta chain





● Molecule 1: Glycocyamine kinase beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.62Å 99.72Å 93.30Å 90.00° 92.38° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.40) 99.6 (50.00-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.39Å)	Xtriage
Refinement program	CNS, REFMAC 5.0	Depositor
R, R_{free}	0.197 , 0.267 0.214 , 0.272	Depositor DCC
R_{free} test set	3048 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12453	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 9.21% 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	0.82	0/2972	1.00	2/3997 (0.1%)
1	B	0.85	0/3071	1.05	10/4131 (0.2%)
1	C	0.90	0/2972	1.04	5/3997 (0.1%)
1	D	0.88	2/3071 (0.1%)	1.06	6/4131 (0.1%)
All	All	0.86	2/12086 (0.0%)	1.04	23/16256 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	302	VAL	CA-CB	5.49	1.60	1.54
1	D	154	PRO	CA-C	5.47	1.57	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	353	LEU	N-CA-C	7.79	123.48	111.56
1	C	154	PRO	N-CA-C	7.67	120.06	110.70
1	D	154	PRO	N-CA-C	7.08	119.34	110.70
1	A	154	PRO	N-CA-C	6.84	119.04	110.70
1	B	154	PRO	N-CA-C	6.71	118.89	110.70
1	C	337	SER	N-CA-C	6.57	118.16	110.41
1	D	54	TRP	CA-C-N	6.14	129.13	120.28
1	D	54	TRP	C-N-CA	6.14	129.13	120.28
1	B	55	ASP	N-CA-C	5.72	119.52	112.54
1	B	294	CYS	CA-C-N	5.42	125.08	119.56
1	B	294	CYS	C-N-CA	5.42	125.08	119.56
1	D	353	LEU	N-CA-C	5.38	119.79	111.56
1	C	357	GLU	N-CA-C	-5.37	105.33	111.07
1	D	54	TRP	CA-CB-CG	5.36	123.78	113.60
1	A	80	TYR	N-CA-C	5.34	117.31	108.13
1	D	303	ARG	CB-CA-C	-5.31	102.28	110.78
1	B	54	TRP	CA-C-N	5.26	129.50	120.72
1	B	54	TRP	C-N-CA	5.26	129.50	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	ASP	CB-CA-C	-5.11	99.63	110.31
1	B	96	CYS	N-CA-C	5.10	117.50	111.33
1	C	211	ALA	N-CA-C	5.05	116.47	111.07
1	B	303	ARG	CB-CA-C	-5.02	102.59	111.22
1	B	353	LEU	N-CA-C	5.01	119.23	111.56

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	2910	0	2879	46	0
1	B	3005	0	2966	62	0
1	C	2910	0	2879	56	0
1	D	3005	0	2966	57	0
2	A	149	0	0	3	0
2	B	140	0	0	5	0
2	C	181	0	0	3	0
2	D	153	0	0	3	0
All	All	12453	0	11690	215	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 9.

All (215) 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:D:298:MET:HE3	1:D:353:LEU:HD11	1.46	0.98
1:A:231:ASN:HD21	1:A:235:ASN:ND2	1.70	0.88
1:C:298:MET:HE1	1:C:353:LEU:HD11	1.57	0.86
1:B:298:MET:CE	1:B:353:LEU:HD11	2.06	0.85
1:C:298:MET:CE	1:C:353:LEU:HD11	2.09	0.82
1:B:191:ASN:ND2	1:B:194:ASP:H	1.77	0.82
1:A:298:MET:CE	1:A:353:LEU:HD11	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:HIS:CE1	1:A:384:ILE:HD11	2.16	0.81
1:C:285:ASN:HD22	1:C:288:LEU:H	1.28	0.80
1:B:252:GLN:NE2	1:B:263:ARG:HH22	1.79	0.80
1:D:298:MET:CE	1:D:353:LEU:HD11	2.12	0.79
1:B:252:GLN:HE21	1:B:263:ARG:HH22	1.30	0.78
1:C:148:VAL:H	1:C:245:HIS:HD2	1.30	0.77
1:C:252:GLN:HE21	1:C:263:ARG:HH22	1.31	0.76
1:A:231:ASN:HD21	1:A:235:ASN:HD21	1.33	0.76
1:A:252:GLN:HE21	1:A:263:ARG:HH22	1.32	0.76
1:B:148:VAL:H	1:B:245:HIS:HD2	1.33	0.75
1:D:77:ASN:HD22	1:D:79:PHE:H	1.32	0.75
1:A:249:ILE:HD11	2:A:1039:HOH:O	1.86	0.75
1:C:94:TYR:OH	1:C:287:ARG:NH1	2.20	0.74
1:D:154:PRO:HD2	1:D:293:THR:HG22	1.68	0.74
1:A:121:ASP:HB3	1:A:356:SER:OG	1.86	0.73
1:C:316:HIS:CE1	1:C:384:ILE:HD11	2.24	0.73
1:D:191:ASN:C	1:D:191:ASN:HD22	1.96	0.73
1:C:220:ARG:O	1:C:226:ARG:NH2	2.21	0.72
1:A:148:VAL:H	1:A:245:HIS:HD2	1.33	0.72
1:D:341:THR:HB	2:D:1260:HOH:O	1.91	0.71
1:D:231:ASN:HD21	1:D:235:ASN:HD21	1.40	0.70
1:A:298:MET:HE2	1:A:353:LEU:HD11	1.73	0.69
1:A:378:LEU:HD21	1:A:384:ILE:HD12	1.73	0.69
1:C:231:ASN:HD21	1:C:235:ASN:HD21	1.39	0.69
1:D:247:ARG:NH1	1:D:249:ILE:HD11	2.08	0.69
1:B:285:ASN:HD22	1:B:288:LEU:H	1.42	0.68
1:D:231:ASN:HD21	1:D:235:ASN:ND2	1.92	0.68
1:D:285:ASN:HD22	1:D:288:LEU:H	1.42	0.68
1:B:321:GLU:OE1	1:B:325:LYS:NZ	2.27	0.67
1:C:148:VAL:H	1:C:245:HIS:CD2	2.12	0.67
1:C:247:ARG:NH1	1:C:249:ILE:HD11	2.10	0.66
1:B:140:CYS:HB3	1:B:306:VAL:HG12	1.77	0.66
1:B:309:ARG:HG2	1:B:344:THR:HG22	1.76	0.65
1:B:385:ASP:HB2	2:B:1623:HOH:O	1.97	0.65
1:A:384:ILE:HA	1:A:387:MET:HG3	1.80	0.64
1:A:287:ARG:NH1	1:A:288:LEU:HD21	2.14	0.62
1:D:191:ASN:HD21	1:D:194:ASP:H	1.45	0.62
1:D:252:GLN:HE21	1:D:263:ARG:HH22	1.48	0.61
1:B:191:ASN:HD21	1:B:194:ASP:H	1.48	0.61
1:C:154:PRO:HD2	1:C:293:THR:HG22	1.82	0.60
1:D:332:GLY:O	1:D:333:THR:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:VAL:O	1:B:16:HIS:N	2.33	0.60
1:D:94:TYR:OH	1:D:287:ARG:NH1	2.35	0.60
1:D:148:VAL:H	1:D:245:HIS:HD2	1.48	0.59
1:B:349:ASN:O	1:B:352:ARG:NH2	2.35	0.59
1:C:247:ARG:HH12	1:C:249:ILE:HD11	1.65	0.59
1:C:231:ASN:HD21	1:C:235:ASN:ND2	2.00	0.59
1:C:191:ASN:ND2	1:C:194:ASP:H	2.00	0.59
1:A:298:MET:HE3	1:A:353:LEU:HD11	1.85	0.59
1:A:55:ASP:OD2	1:A:55:ASP:N	2.34	0.58
1:A:285:ASN:HD22	1:A:288:LEU:H	1.51	0.58
1:D:188:THR:HG23	2:D:1379:HOH:O	2.04	0.58
1:B:191:ASN:C	1:B:191:ASN:HD22	2.12	0.58
1:C:287:ARG:NH1	1:C:288:LEU:HD21	2.19	0.58
1:B:148:VAL:H	1:B:245:HIS:CD2	2.18	0.58
1:B:252:GLN:HE21	1:B:263:ARG:NH2	2.00	0.58
1:A:384:ILE:HD13	1:A:384:ILE:H	1.69	0.57
1:A:377:LYS:HE3	1:A:382:GLN:NE2	2.20	0.57
1:D:140:CYS:HB3	1:D:306:VAL:HG12	1.86	0.57
1:B:223:PRO:O	1:B:226:ARG:HB2	2.05	0.57
1:A:310:LEU:O	1:A:314:GLU:HB2	2.04	0.56
1:A:149:LYS:HE3	1:A:283:MET:HA	1.86	0.56
1:B:176:LEU:HB3	1:B:180:LEU:O	2.05	0.56
1:C:252:GLN:NE2	1:C:263:ARG:HH22	2.00	0.56
1:A:141:ARG:HD2	1:A:305:SER:OG	2.05	0.56
1:D:307:HIS:CE1	1:D:333:THR:HG21	2.41	0.55
1:C:191:ASN:HD22	1:C:191:ASN:C	2.13	0.55
1:B:14:VAL:C	1:B:16:HIS:H	2.15	0.55
1:A:238:VAL:HG22	1:A:248:VAL:HB	1.89	0.55
1:A:287:ARG:HH12	1:A:288:LEU:HD21	1.71	0.55
1:B:77:ASN:ND2	1:C:378:LEU:O	2.40	0.55
1:B:298:MET:HE3	1:B:353:LEU:HD11	1.88	0.54
1:B:230:HIS:C	1:B:230:HIS:CD2	2.85	0.54
1:C:148:VAL:N	1:C:245:HIS:HD2	2.03	0.54
1:C:352:ARG:HD3	2:C:1158:HOH:O	2.07	0.54
1:D:105:ILE:HG23	1:D:298:MET:HE1	1.89	0.54
1:D:191:ASN:C	1:D:191:ASN:ND2	2.65	0.53
1:D:342:ASP:HB3	1:D:344:THR:HG22	1.90	0.53
1:D:342:ASP:HB3	1:D:344:THR:CG2	2.38	0.52
1:D:191:ASN:ND2	1:D:194:ASP:H	2.07	0.52
1:C:182:GLY:HA3	1:C:231:ASN:HA	1.91	0.52
1:B:226:ARG:HD2	1:B:241:ASN:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:HIS:ND1	1:B:353:LEU:O	2.35	0.52
1:B:80:TYR:HB2	1:C:312:PHE:CE2	2.45	0.51
1:B:109:HIS:HD2	2:B:1101:HOH:O	1.93	0.51
1:D:321:GLU:O	1:D:325:LYS:HG3	2.10	0.51
1:D:71:GLY:HA3	1:D:85:GLY:O	2.11	0.51
1:C:377:LYS:HG2	1:C:384:ILE:HG22	1.91	0.50
1:D:326:LEU:HD21	1:D:370:LEU:HD12	1.93	0.50
1:C:316:HIS:CE1	1:C:384:ILE:CD1	2.94	0.50
1:B:121:ASP:OD2	1:B:358:ARG:NH1	2.45	0.50
1:B:327:ARG:HD2	2:B:1005:HOH:O	2.12	0.50
1:D:117:HIS:ND1	1:D:118:PRO:HD2	2.26	0.49
1:C:140:CYS:HB3	1:C:306:VAL:HG12	1.93	0.49
1:A:129:GLY:O	2:A:1358:HOH:O	2.20	0.49
1:D:77:ASN:ND2	1:D:79:PHE:H	2.06	0.49
1:D:386:ASP:OD1	1:D:386:ASP:N	2.45	0.49
1:B:230:HIS:HD2	1:B:230:HIS:O	1.96	0.49
1:B:124:HIS:HB2	2:B:1294:HOH:O	2.11	0.49
1:D:144:CYS:SG	1:D:248:VAL:CG1	3.01	0.49
1:A:322:MET:O	1:A:326:LEU:HG	2.13	0.49
1:B:314:GLU:CD	1:B:343:SER:HB3	2.37	0.49
1:D:133:GLU:HG2	2:D:1292:HOH:O	2.12	0.49
1:A:364:LEU:O	1:A:368:VAL:HG23	2.13	0.48
1:A:143:ARG:HB3	1:A:249:ILE:HG23	1.94	0.48
1:A:191:ASN:ND2	1:A:194:ASP:H	2.11	0.48
1:B:182:GLY:HA3	1:B:231:ASN:HA	1.96	0.48
1:C:328:LEU:HD11	1:C:367:GLY:HA3	1.96	0.48
1:C:310:LEU:O	1:C:314:GLU:HB2	2.14	0.48
1:C:301:VAL:HG12	1:C:301:VAL:O	2.14	0.47
1:D:325:LYS:NZ	1:D:390:LYS:O	2.36	0.47
1:A:141:ARG:CD	1:A:305:SER:OG	2.62	0.47
1:C:223:PRO:O	1:C:226:ARG:HG2	2.14	0.47
1:D:303:ARG:HG2	1:D:352:ARG:NH1	2.29	0.47
1:B:308:LEU:O	1:B:344:THR:HA	2.14	0.47
1:D:187:LEU:HD12	1:D:226:ARG:HB2	1.95	0.47
1:C:95:GLU:HB2	2:C:1558:HOH:O	2.14	0.47
1:D:109:HIS:HE1	1:D:295:PRO:O	1.98	0.47
1:B:80:TYR:CE2	1:C:311:ALA:HB1	2.50	0.47
1:B:352:ARG:HD3	2:B:1290:HOH:O	2.14	0.47
1:C:364:LEU:HD22	1:C:368:VAL:HG23	1.97	0.47
1:B:238:VAL:HG22	1:B:248:VAL:HB	1.97	0.47
1:A:154:PRO:HD2	1:A:293:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:ASP:OD1	1:D:293:THR:HG23	2.16	0.46
1:B:154:PRO:HD2	1:B:293:THR:HG22	1.96	0.46
1:B:191:ASN:HD21	1:B:194:ASP:CG	2.24	0.46
1:D:190:MET:HG3	1:D:191:ASN:O	2.14	0.46
1:B:303:ARG:HG2	1:B:352:ARG:NH1	2.30	0.46
1:B:342:ASP:HB2	1:B:344:THR:CG2	2.45	0.46
1:A:58:THR:OG1	1:A:62:VAL:HB	2.16	0.46
1:A:316:HIS:CG	1:A:317:PRO:HD2	2.50	0.46
1:C:141:ARG:HD2	1:C:305:SER:OG	2.16	0.46
1:C:217:GLY:O	1:C:220:ARG:HD3	2.16	0.46
1:A:149:LYS:HE3	1:A:284:HIS:H	1.80	0.46
1:B:316:HIS:CD2	1:B:318:ARG:H	2.34	0.46
1:D:111:PHE:CG	1:D:353:LEU:HD13	2.51	0.46
1:D:144:CYS:HA	1:D:301:VAL:O	2.15	0.46
1:D:148:VAL:N	1:D:245:HIS:HD2	2.14	0.46
1:C:109:HIS:CE1	1:C:298:MET:HE2	2.51	0.46
1:C:163:ARG:NH2	1:D:31:PHE:O	2.44	0.45
1:D:285:ASN:HD22	1:D:288:LEU:N	2.09	0.45
1:B:313:LEU:HD13	1:B:319:PHE:CD1	2.51	0.45
1:D:287:ARG:HH11	1:D:287:ARG:HG2	1.80	0.45
1:A:36:LYS:NZ	2:A:1271:HOH:O	2.49	0.45
1:C:243:GLU:O	1:C:293:THR:CG2	2.65	0.45
1:D:308:LEU:HD13	1:D:310:LEU:HD11	1.99	0.45
1:A:191:ASN:HD22	1:A:194:ASP:H	1.64	0.45
1:C:191:ASN:HD21	1:C:194:ASP:H	1.64	0.45
1:D:164:LEU:C	1:D:164:LEU:HD23	2.42	0.45
1:C:193:LYS:HB3	2:C:1057:HOH:O	2.16	0.44
1:C:143:ARG:HB3	1:C:249:ILE:HG23	1.99	0.44
1:C:298:MET:HE3	1:C:353:LEU:HD21	1.98	0.44
1:A:31:PHE:CD1	1:A:32:PRO:HD2	2.52	0.44
1:C:235:ASN:C	1:C:235:ASN:HD22	2.24	0.44
1:D:239:TRP:CE3	1:D:247:ARG:NH1	2.85	0.44
1:D:301:VAL:HA	1:D:352:ARG:HG2	1.99	0.44
1:D:308:LEU:O	1:D:344:THR:HA	2.18	0.44
1:A:374:CYS:SG	1:A:387:MET:HE2	2.57	0.44
1:C:191:ASN:CG	1:C:193:LYS:HG3	2.43	0.44
1:C:147:SER:HA	1:C:245:HIS:HB2	2.00	0.44
1:B:305:SER:HA	1:B:347:ILE:O	2.16	0.44
1:C:154:PRO:HA	1:C:157:MET:HG2	1.99	0.43
1:A:58:THR:HB	1:A:59:PRO:HD2	2.00	0.43
1:B:74:ASN:HD21	1:B:215:THR:HG21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:GLU:HG2	1:B:345:TYR:OH	2.17	0.43
1:C:243:GLU:O	1:C:293:THR:HG21	2.17	0.43
1:C:364:LEU:HD22	1:C:368:VAL:CG2	2.49	0.43
1:A:230:HIS:HD2	1:A:231:ASN:O	2.01	0.43
1:B:244:ASP:OD1	1:B:293:THR:HG23	2.19	0.43
1:A:66:LYS:NZ	1:B:16:HIS:HE1	2.17	0.43
1:B:109:HIS:HE1	1:B:295:PRO:O	2.01	0.43
1:B:143:ARG:HA	1:B:248:VAL:O	2.18	0.43
1:B:226:ARG:CD	1:B:241:ASN:O	2.67	0.43
1:A:148:VAL:H	1:A:245:HIS:CD2	2.24	0.43
1:A:84:THR:HG23	1:A:108:ILE:HD11	2.00	0.42
1:A:105:ILE:HG23	1:A:298:MET:HE1	2.01	0.42
1:B:191:ASN:HD22	1:B:194:ASP:H	1.60	0.42
1:D:220:ARG:O	1:D:226:ARG:NH2	2.41	0.42
1:B:182:GLY:HA3	1:B:230:HIS:O	2.19	0.42
1:B:309:ARG:HG2	1:B:344:THR:CG2	2.46	0.42
1:C:159:ARG:O	1:C:163:ARG:HD3	2.20	0.42
1:C:314:GLU:HG2	1:C:345:TYR:OH	2.19	0.42
1:D:368:VAL:HG12	1:D:372:ILE:HD12	2.01	0.42
1:D:77:ASN:HD21	1:D:79:PHE:HB2	1.83	0.42
1:D:309:ARG:HG2	1:D:344:THR:HG22	2.00	0.42
1:B:302:VAL:HG21	1:B:357:GLU:HB3	2.02	0.42
1:C:212:LEU:HD22	1:C:213:LEU:HD12	2.01	0.42
1:D:105:ILE:HG12	1:D:298:MET:HE1	2.01	0.42
1:B:342:ASP:HB2	1:B:344:THR:HG23	2.02	0.42
1:A:252:GLN:HE21	1:A:263:ARG:NH2	2.10	0.42
1:A:105:ILE:HG12	1:A:298:MET:HE1	2.02	0.41
1:A:156:ALA:HB1	1:B:16:HIS:HA	2.02	0.41
1:D:191:ASN:ND2	1:D:194:ASP:HB2	2.36	0.41
1:B:249:ILE:N	1:B:249:ILE:HD12	2.35	0.41
1:C:58:THR:O	1:C:59:PRO:C	2.63	0.41
1:B:304:ALA:O	1:B:348:SER:HA	2.19	0.41
1:C:111:PHE:CE1	1:C:115:ASP:HB3	2.55	0.41
1:B:94:TYR:CZ	1:B:288:LEU:HD11	2.55	0.41
1:C:364:LEU:O	1:C:368:VAL:HG23	2.21	0.41
1:B:152:CYS:HB2	1:B:161:GLU:OE1	2.20	0.41
1:D:235:ASN:HB2	1:D:263:ARG:NH2	2.36	0.41
1:D:334:GLY:HA3	1:D:341:THR:CG2	2.51	0.41
1:B:377:LYS:HG2	1:B:384:ILE:HG22	2.03	0.40
1:C:298:MET:HE3	1:C:298:MET:HB2	1.81	0.40
1:C:378:LEU:HD21	1:C:384:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:GLU:OE1	1:D:343:SER:OG	2.38	0.40
1:A:384:ILE:HD13	1:A:384:ILE:N	2.34	0.40
1:B:94:TYR:CE2	1:B:288:LEU:HD11	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	365/390 (94%)	345 (94%)	16 (4%)	4 (1%)	11	18
1	B	377/390 (97%)	356 (94%)	18 (5%)	3 (1%)	16	25
1	C	365/390 (94%)	348 (95%)	14 (4%)	3 (1%)	16	25
1	D	377/390 (97%)	359 (95%)	15 (4%)	3 (1%)	16	25
All	All	1484/1560 (95%)	1408 (95%)	63 (4%)	13 (1%)	14	22

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	GLU
1	B	15	GLY
1	B	242	GLU
1	B	389	PRO
1	C	389	PRO
1	D	242	GLU
1	C	242	GLU
1	C	314	GLU
1	D	13	ARG
1	D	314	GLU
1	A	314	GLU
1	A	336	GLU

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Mol	Chain	Res	Type
1	A	389	PRO

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	316/335 (94%)	278 (88%)	38 (12%)	5	7
1	B	326/335 (97%)	288 (88%)	38 (12%)	5	7
1	C	316/335 (94%)	284 (90%)	32 (10%)	7	11
1	D	326/335 (97%)	290 (89%)	36 (11%)	6	9
All	All	1284/1340 (96%)	1140 (89%)	144 (11%)	6	9

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	47	LYS
1	A	96	CYS
1	A	127	LEU
1	A	149	LYS
1	A	163	ARG
1	A	164	LEU
1	A	167	LYS
1	A	177	LYS
1	A	188	THR
1	A	191	ASN
1	A	197	GLN
1	A	213	LEU
1	A	226	ARG
1	A	235	ASN
1	A	237	LEU
1	A	248	VAL
1	A	251	MET
1	A	257	LEU
1	A	293	THR

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Mol	Chain	Res	Type
1	A	308	LEU
1	A	309	ARG
1	A	313	LEU
1	A	323	LEU
1	A	331	ARG
1	A	336	GLU
1	A	341	THR
1	A	352	ARG
1	A	356	SER
1	A	357	GLU
1	A	358	ARG
1	A	364	LEU
1	A	370	LEU
1	A	371	LEU
1	A	377	LYS
1	A	384	ILE
1	A	387	MET
1	A	390	LYS
1	B	21	GLU
1	B	80	TYR
1	B	87	VAL
1	B	127	LEU
1	B	143	ARG
1	B	163	ARG
1	B	164	LEU
1	B	167	LYS
1	B	177	LYS
1	B	183	LYS
1	B	188	THR
1	B	191	ASN
1	B	192	GLU
1	B	212	LEU
1	B	213	LEU
1	B	216	SER
1	B	226	ARG
1	B	230	HIS
1	B	235	ASN
1	B	237	LEU
1	B	248	VAL
1	B	251	MET
1	B	257	LEU
1	B	268	LEU

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Mol	Chain	Res	Type
1	B	277	GLU
1	B	293	THR
1	B	301	VAL
1	B	308	LEU
1	B	309	ARG
1	B	313	LEU
1	B	341	THR
1	B	344	THR
1	B	352	ARG
1	B	357	GLU
1	B	358	ARG
1	B	364	LEU
1	B	370	LEU
1	B	371	LEU
1	C	24	LYS
1	C	57	VAL
1	C	87	VAL
1	C	141	ARG
1	C	143	ARG
1	C	163	ARG
1	C	164	LEU
1	C	188	THR
1	C	191	ASN
1	C	193	LYS
1	C	195	GLN
1	C	226	ARG
1	C	235	ASN
1	C	237	LEU
1	C	248	VAL
1	C	257	LEU
1	C	268	LEU
1	C	293	THR
1	C	308	LEU
1	C	313	LEU
1	C	323	LEU
1	C	339	LEU
1	C	352	ARG
1	C	357	GLU
1	C	358	ARG
1	C	364	LEU
1	C	370	LEU
1	C	371	LEU

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Mol	Chain	Res	Type
1	C	384	ILE
1	C	386	ASP
1	C	387	MET
1	C	390	LYS
1	D	56	LYS
1	D	77	ASN
1	D	87	VAL
1	D	116	LYS
1	D	140	CYS
1	D	163	ARG
1	D	183	LYS
1	D	188	THR
1	D	191	ASN
1	D	192	GLU
1	D	197	GLN
1	D	200	GLU
1	D	212	LEU
1	D	226	ARG
1	D	235	ASN
1	D	237	LEU
1	D	251	MET
1	D	257	LEU
1	D	268	LEU
1	D	287	ARG
1	D	293	THR
1	D	301	VAL
1	D	302	VAL
1	D	308	LEU
1	D	309	ARG
1	D	313	LEU
1	D	314	GLU
1	D	323	LEU
1	D	344	THR
1	D	352	ARG
1	D	357	GLU
1	D	358	ARG
1	D	364	LEU
1	D	370	LEU
1	D	371	LEU
1	D	386	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	109	HIS
1	A	191	ASN
1	A	195	GLN
1	A	230	HIS
1	A	235	ASN
1	A	245	HIS
1	A	252	GLN
1	A	280	HIS
1	A	285	ASN
1	A	307	HIS
1	A	316	HIS
1	A	382	GLN
1	B	16	HIS
1	B	38	ASN
1	B	109	HIS
1	B	191	ASN
1	B	197	GLN
1	B	235	ASN
1	B	245	HIS
1	B	252	GLN
1	B	285	ASN
1	B	307	HIS
1	B	316	HIS
1	C	30	ASN
1	C	109	HIS
1	C	124	HIS
1	C	191	ASN
1	C	197	GLN
1	C	235	ASN
1	C	245	HIS
1	C	252	GLN
1	C	285	ASN
1	C	316	HIS
1	C	382	GLN
1	D	16	HIS
1	D	38	ASN
1	D	77	ASN
1	D	109	HIS
1	D	124	HIS
1	D	191	ASN
1	D	195	GLN
1	D	230	HIS

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Mol	Chain	Res	Type
1	D	235	ASN
1	D	245	HIS
1	D	252	GLN
1	D	285	ASN
1	D	316	HIS

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	367/390 (94%)	0.36	12 (3%) 49 45	36, 43, 62, 73	0
1	B	379/390 (97%)	0.40	16 (4%) 40 36	31, 42, 68, 76	0
1	C	367/390 (94%)	0.17	8 (2%) 62 58	31, 39, 56, 71	0
1	D	379/390 (97%)	0.28	13 (3%) 48 44	32, 41, 59, 72	0
All	All	1492/1560 (95%)	0.30	49 (3%) 49 45	31, 42, 62, 76	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	GLY	4.5
1	B	334	GLY	4.0
1	D	15	GLY	4.0
1	D	334	GLY	3.8
1	D	342	ASP	3.8
1	B	333	THR	3.7
1	B	337	SER	3.7
1	D	333	THR	3.7
1	D	335	GLY	3.6
1	B	12	ASN	3.5
1	C	79	PHE	3.5
1	A	339	LEU	3.4
1	C	80	TYR	3.4
1	A	80	TYR	3.4
1	C	339	LEU	3.3
1	B	341	THR	3.3
1	B	332	GLY	3.3
1	B	14	VAL	3.3
1	D	14	VAL	3.3
1	A	78	LYS	3.3
1	B	336	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	386	ASP	3.0
1	B	338	SER	3.0
1	D	281	GLY	2.9
1	A	77	ASN	2.8
1	A	341	THR	2.8
1	A	54	TRP	2.8
1	C	336	GLU	2.7
1	D	341	THR	2.7
1	C	77	ASN	2.7
1	C	54	TRP	2.6
1	A	27	ALA	2.6
1	B	15	GLY	2.5
1	B	340	ALA	2.5
1	A	338	SER	2.5
1	B	129	GLY	2.4
1	A	79	PHE	2.4
1	D	340	ALA	2.4
1	B	342	ASP	2.3
1	A	340	ALA	2.3
1	B	385	ASP	2.3
1	D	389	PRO	2.3
1	C	341	THR	2.3
1	D	344	THR	2.2
1	C	335	GLY	2.2
1	A	384	ILE	2.2
1	D	336	GLU	2.2
1	B	22	SER	2.1
1	D	286	ASP	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.