



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:01 pm BST

PDB ID : 3L2D
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

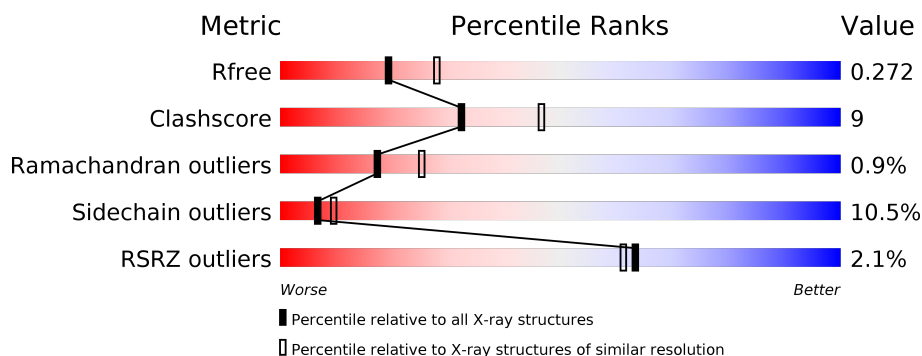
1 Overall quality at a glance

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 on 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	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>• 6%</div> </div> </div>
1	B	390	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>• • •</div> </div> </div>
1	C	390	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>• 6%</div> </div> </div>
1	D	390	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• •</div> </div> </div>

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			

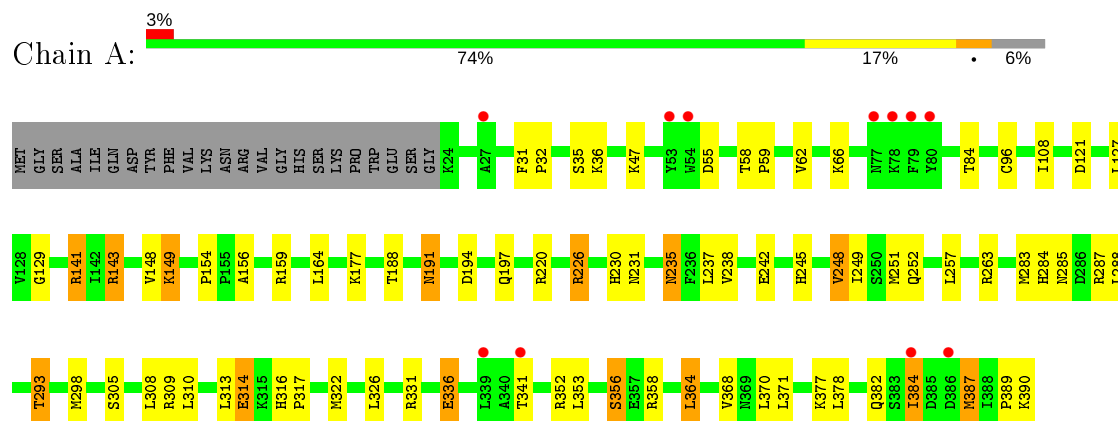
- Molecule 2 is water.

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		

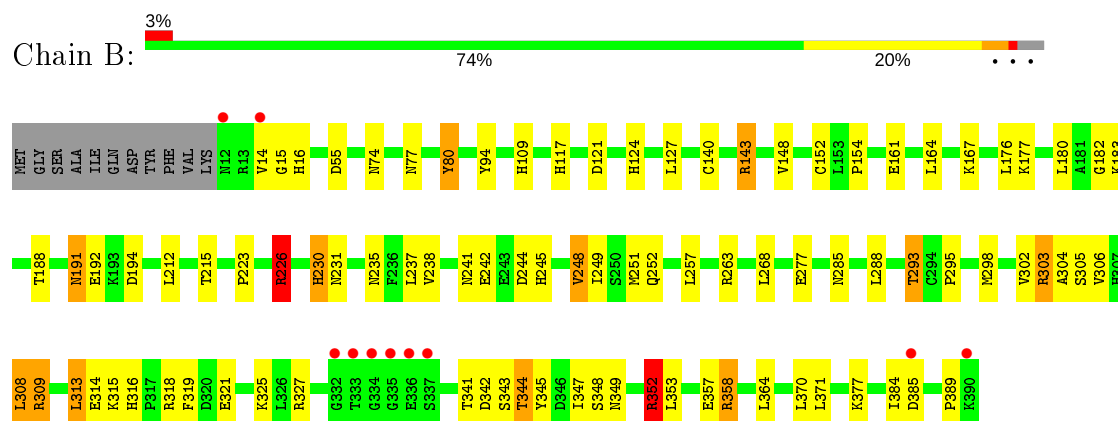
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

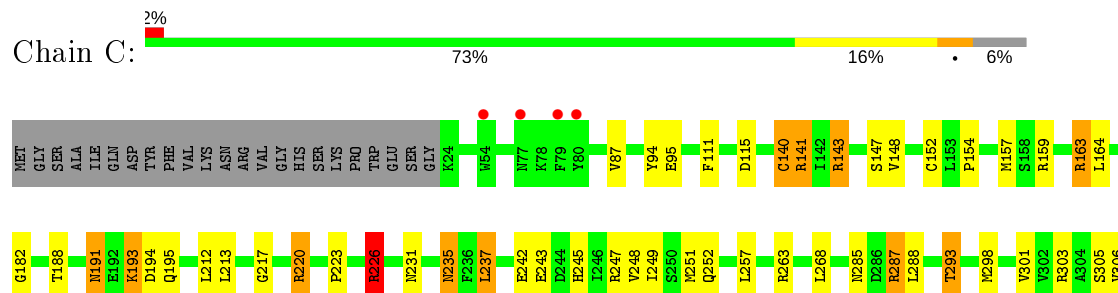
• Molecule 1: Glycocyamine kinase beta chain

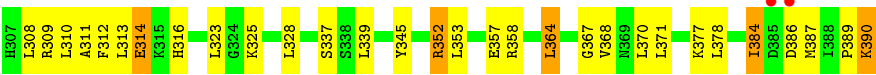


• Molecule 1: Glycocyamine kinase beta chain

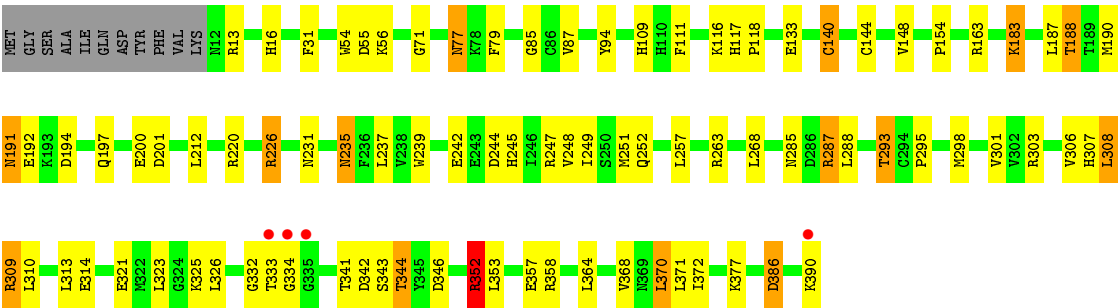


• Molecule 1: Glycocyamine kinase beta chain





● 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 43.97 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.40) 99.6 (43.97-2.40)	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 0.213 , 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)	0.35 , 42.9	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	0.68	0/2972	0.83	7/3997 (0.2%)
1	B	0.69	0/3071	0.82	4/4131 (0.1%)
1	C	0.73	1/2972 (0.0%)	0.86	6/3997 (0.2%)
1	D	0.71	0/3071	0.84	7/4131 (0.2%)
All	All	0.70	1/12086 (0.0%)	0.84	24/16256 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	152	CYS	CB-SG	-5.50	1.72	1.81

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	226	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	D	226	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	B	352	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	B	352	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	A	226	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	A	226	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	C	220	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	C	220	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	C	226	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	226	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	220	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	D	352	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	220	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	D	163	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	D	346	ASP	CB-CG-OD1	5.43	123.19	118.30
1	B	55	ASP	CB-CA-C	-5.38	99.63	110.40
1	A	159	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	226	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	D	54	TRP	CA-CB-CG	5.30	123.78	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	237	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	159	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	287	ARG	NE-CZ-NH2	5.11	122.85	120.30
1	D	226	ARG	CD-NE-CZ	5.02	130.63	123.60

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	2910	0	2879	43	0
1	B	3005	0	2966	63	0
1	C	2910	0	2879	54	0
1	D	3005	0	2966	55	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	4	0
All	All	12453	0	11690	208	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 (208) 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:298:MET:HE2	1:A:353:LEU:HD11	1.49	0.93
1:A:231:ASN:HD21	1:A:235:ASN:ND2	1.70	0.88
1:C:298:MET:HE1	1:C:353:LEU:HD11	1.56	0.87
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

Continued on next page...

Continued from previous page...

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: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: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:191:ASN:C	1:D:191:ASN:HD22	1.96	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:D:298:MET:HE2	1:D:353:LEU:HD11	1.76	0.67
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:D:298:MET:HE3	1:D:353:LEU:HD11	1.77	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:GLY:O	1:D:333:THR:HG23	2.02	0.60
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:55:ASP:N	1:A:55:ASP:OD2	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: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:H	1:A:384:ILE:HD13	1.69	0.57
1:A:377:LYS:HE3	1:A:382:GLN:NE2	2.20	0.57
1:D:325:LYS:NZ	1:D:390:LYS:O	2.36	0.57
1:C:298:MET:HE3	1:C:353:LEU:HD21	1.86	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:B:298:MET:HE3	1:B:353:LEU:HD11	1.89	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: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:B:191:ASN:C	1:B:191:ASN:HD22	2.12	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:191:ASN:HD22	1:C:191:ASN:C	2.13	0.50
1:B:14:VAL:C	1:B:16:HIS:H	2.15	0.50
1:B:315:LYS:HZ2	1:C:337:SER:CB	2.23	0.50
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:D:191:ASN:ND2	1:D:191:ASN:C	2.65	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:B:230:HIS:CD2	1:B:230:HIS:C	2.85	0.49
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:386:ASP:OD1	1:D:386:ASP:N	2.45	0.49
1:D:77:ASN:ND2	1:D:79:PHE:H	2.06	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: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:O	1:C:301:VAL:HG12	2.14	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:183:LYS:NZ	2:D:1309:HOH:O	2.47	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:352:ARG:HD3	2:B:1290:HOH:O	2.14	0.47
1:B:80:TYR:CE2	1:C:311:ALA:HB1	2.50	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PRO:HD2	1:A:293:THR:HG22	1.97	0.46
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:D:190:MET:HG3	1:D:191:ASN:O	2.14	0.46
1:B:342:ASP:HB2	1:B:344:THR:CG2	2.45	0.46
1:B:303:ARG:HG2	1:B:352:ARG:NH1	2.30	0.46
1:A:316:HIS:CG	1:A:317:PRO:HD2	2.50	0.46
1:A:58:THR:OG1	1:A:62:VAL:HB	2.16	0.46
1:C:217:GLY:O	1:C:220:ARG:HD3	2.16	0.46
1:C:141:ARG:HD2	1:C:305:SER:OG	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:148:VAL:N	1:D:245:HIS:HD2	2.14	0.46
1:D:144:CYS:HA	1:D:301:VAL:O	2.15	0.46
1:D:285:ASN:HD22	1:D:288:LEU:N	2.09	0.45
1:C:163:ARG:NH2	1:D:31:PHE:O	2.44	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:C:325:LYS:HZ3	1:C:390:LYS:HB3	1.82	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:A:31:PHE:CD1	1:A:32:PRO:HD2	2.52	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:B:314:GLU:CD	1:B:343:SER:HB3	2.37	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:109:HIS:HE1	1:B:295:PRO:O	2.01	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: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:309:ARG:HG2	1:D:344:THR:HG22	2.00	0.42
1:D:77:ASN:HD21	1:D:79:PHE:HB2	1.83	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: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: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:191:ASN:HD21	1:B:194:ASP:CG	2.24	0.41
1:B:249:ILE:N	1:B:249:ILE:HD12	2.35	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:A:387:MET:HE3	1:A:387:MET:HB3	1.74	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:152:CYS:HB2	1:B:161:GLU:OE1	2.20	0.41
1:C:235:ASN:C	1:C:235:ASN:HD22	2.24	0.41
1:B:377:LYS:HG2	1:B:384:ILE:HG22	2.03	0.40
1:C:378:LEU:HD21	1:C:384:ILE:HD12	2.03	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%)	14	20
1	B	377/390 (97%)	356 (94%)	18 (5%)	3 (1%)	19	29
1	C	365/390 (94%)	348 (95%)	14 (4%)	3 (1%)	19	29
1	D	377/390 (97%)	359 (95%)	15 (4%)	3 (1%)	19	29
All	All	1484/1560 (95%)	1408 (95%)	63 (4%)	13 (1%)	17	25

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
1	A	389	PRO

5.3.2 Protein sidechains [i](#)

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%)	283 (90%)	33 (10%)	7	10
1	B	326/335 (97%)	294 (90%)	32 (10%)	8	11
1	C	316/335 (94%)	282 (89%)	34 (11%)	6	9
1	D	326/335 (97%)	290 (89%)	36 (11%)	6	8
All	All	1284/1340 (96%)	1149 (90%)	135 (10%)	7	9

All (135) 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	141	ARG
1	A	149	LYS
1	A	164	LEU
1	A	177	LYS
1	A	188	THR
1	A	191	ASN
1	A	197	GLN
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
1	A	308	LEU
1	A	309	ARG
1	A	313	LEU
1	A	331	ARG
1	A	336	GLU
1	A	341	THR
1	A	352	ARG
1	A	356	SER
1	A	358	ARG
1	A	364	LEU
1	A	370	LEU
1	A	371	LEU
1	A	384	ILE
1	A	387	MET
1	A	390	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	80	TYR
1	B	127	LEU
1	B	143	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	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
1	B	277	GLU
1	B	293	THR
1	B	303	ARG
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	358	ARG
1	B	364	LEU
1	B	370	LEU
1	B	371	LEU
1	C	87	VAL
1	C	140	CYS
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	226	ARG
1	C	235	ASN
1	C	237	LEU
1	C	248	VAL
1	C	251	MET
1	C	257	LEU
1	C	268	LEU
1	C	293	THR
1	C	303	ARG
1	C	308	LEU
1	C	309	ARG
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
1	C	384	ILE
1	C	386	ASP
1	C	387	MET
1	C	390	LYS
1	D	16	HIS
1	D	55	ASP
1	D	56	LYS
1	D	77	ASN
1	D	87	VAL
1	D	116	LYS
1	D	140	CYS
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	201	ASP
1	D	212	LEU
1	D	235	ASN
1	D	237	LEU
1	D	251	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	257	LEU
1	D	268	LEU
1	D	287	ARG
1	D	293	THR
1	D	308	LEU
1	D	309	ARG
1	D	313	LEU
1	D	323	LEU
1	D	343	SER
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	377	LYS
1	D	386	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	191	ASN
1	A	230	HIS
1	A	235	ASN
1	A	245	HIS
1	A	252	GLN
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	77	ASN
1	B	109	HIS
1	B	191	ASN
1	B	235	ASN
1	B	245	HIS
1	B	252	GLN
1	B	285	ASN
1	B	307	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	316	HIS
1	C	109	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	D	16	HIS
1	D	38	ASN
1	D	77	ASN
1	D	124	HIS
1	D	191	ASN
1	D	195	GLN
1	D	230	HIS
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 carbohydrates 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	367/390 (94%)	0.05	11 (2%) 50 49	36, 43, 62, 73	0
1	B	379/390 (97%)	0.06	10 (2%) 56 54	31, 42, 68, 76	0
1	C	367/390 (94%)	-0.04	6 (1%) 72 70	31, 39, 56, 71	0
1	D	379/390 (97%)	-0.02	4 (1%) 80 79	32, 41, 59, 72	0
All	All	1492/1560 (95%)	0.01	31 (2%) 63 61	31, 42, 62, 76	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	GLY	8.2
1	B	333	THR	6.3
1	A	79	PHE	5.9
1	A	80	TYR	5.3
1	D	334	GLY	5.1
1	C	79	PHE	4.7
1	C	80	TYR	4.3
1	A	78	LYS	3.8
1	A	54	TRP	3.6
1	A	386	ASP	3.4
1	C	54	TRP	3.3
1	B	12	ASN	3.2
1	B	337	SER	3.1
1	D	333	THR	3.0
1	A	77	ASN	2.8
1	B	390	LYS	2.6
1	D	335	GLY	2.6
1	B	332	GLY	2.5
1	C	386	ASP	2.5
1	A	384	ILE	2.5
1	B	336	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	27	ALA	2.5
1	B	14	VAL	2.4
1	B	335	GLY	2.4
1	C	77	ASN	2.3
1	A	339	LEU	2.3
1	C	385	ASP	2.2
1	B	385	ASP	2.1
1	A	53	TYR	2.1
1	A	341	THR	2.1
1	D	390	LYS	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 carbohydrates 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.