



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:03 pm BST

PDB ID : 3L2E  
Title : Glycocyamine kinase, alpha-beta heterodimer from marine worm *Namalycastis* sp.  
Authors : Lim, K.; Pullalarevu, S.; Herzberg, O.  
Deposited on : 2009-12-15  
Resolution : 2.60 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](mailto: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.

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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

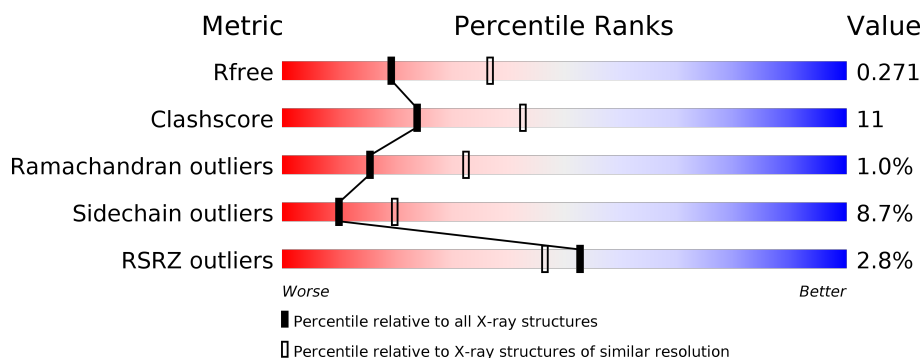
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	374	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>•</div> </div> </div>
1	C	374	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>5%</div> </div> </div>
2	B	390	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>• • •</div> </div> </div>
2	D	390	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>5%</div> <div>• • •</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12299 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 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2976	1878	522	555	21			
1	C	373	Total	C	N	O	S	0	0	0
			2976	1878	522	555	21			

- Molecule 2 is a protein called Glycocyamine kinase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	383	Total	C	N	O	S	0	0	0
			3048	1925	539	563	21			
2	D	380	Total	C	N	O	S	0	0	0
			3031	1914	536	560	21			

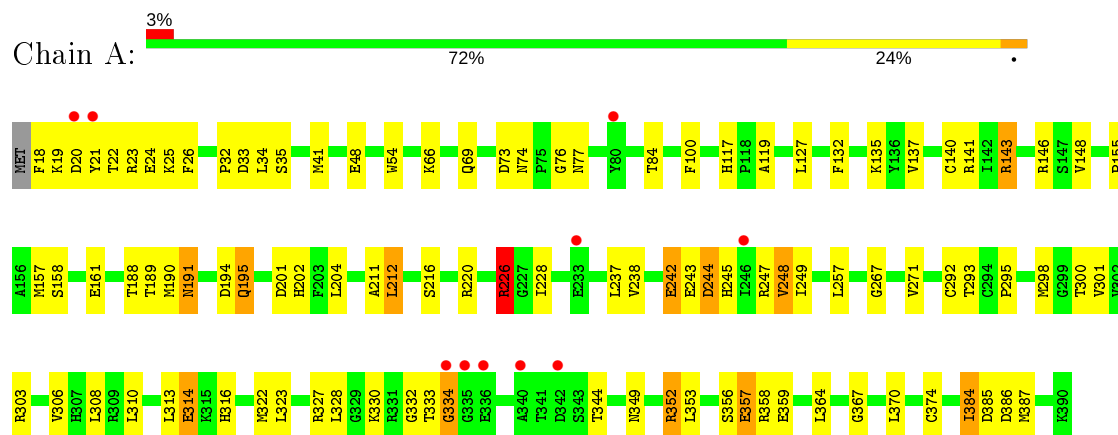
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		
3	B	74	Total	O	0	0
			74	74		
3	C	54	Total	O	0	0
			54	54		
3	D	79	Total	O	0	0
			79	79		

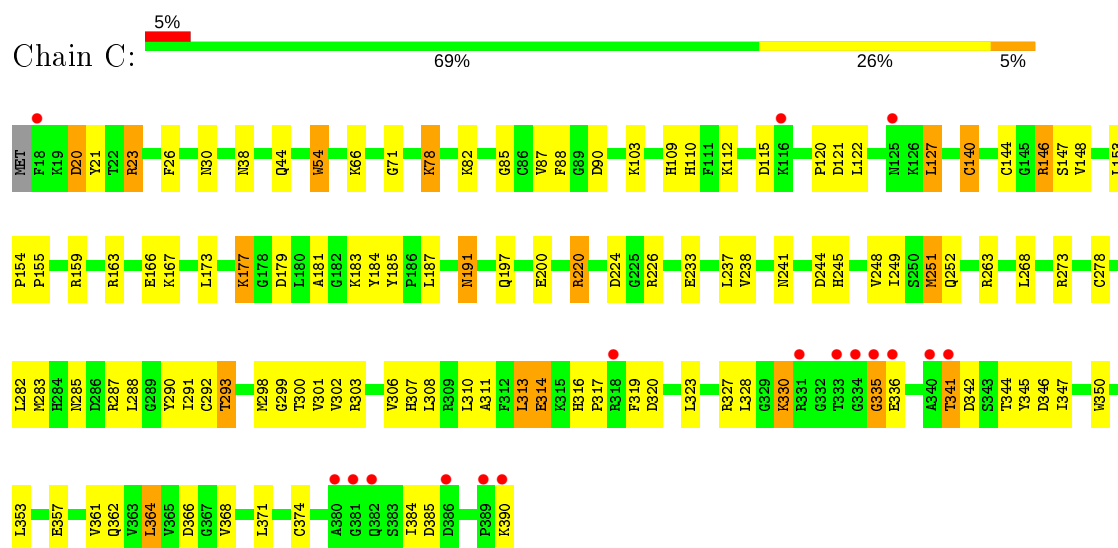
### 3 Residue-property plots [i](#)

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.

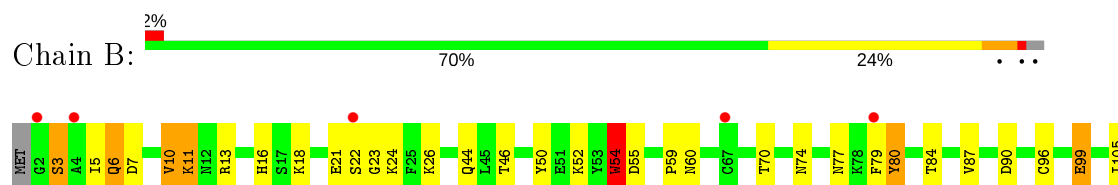
#### • Molecule 1: Glycocyamine kinase alpha chain

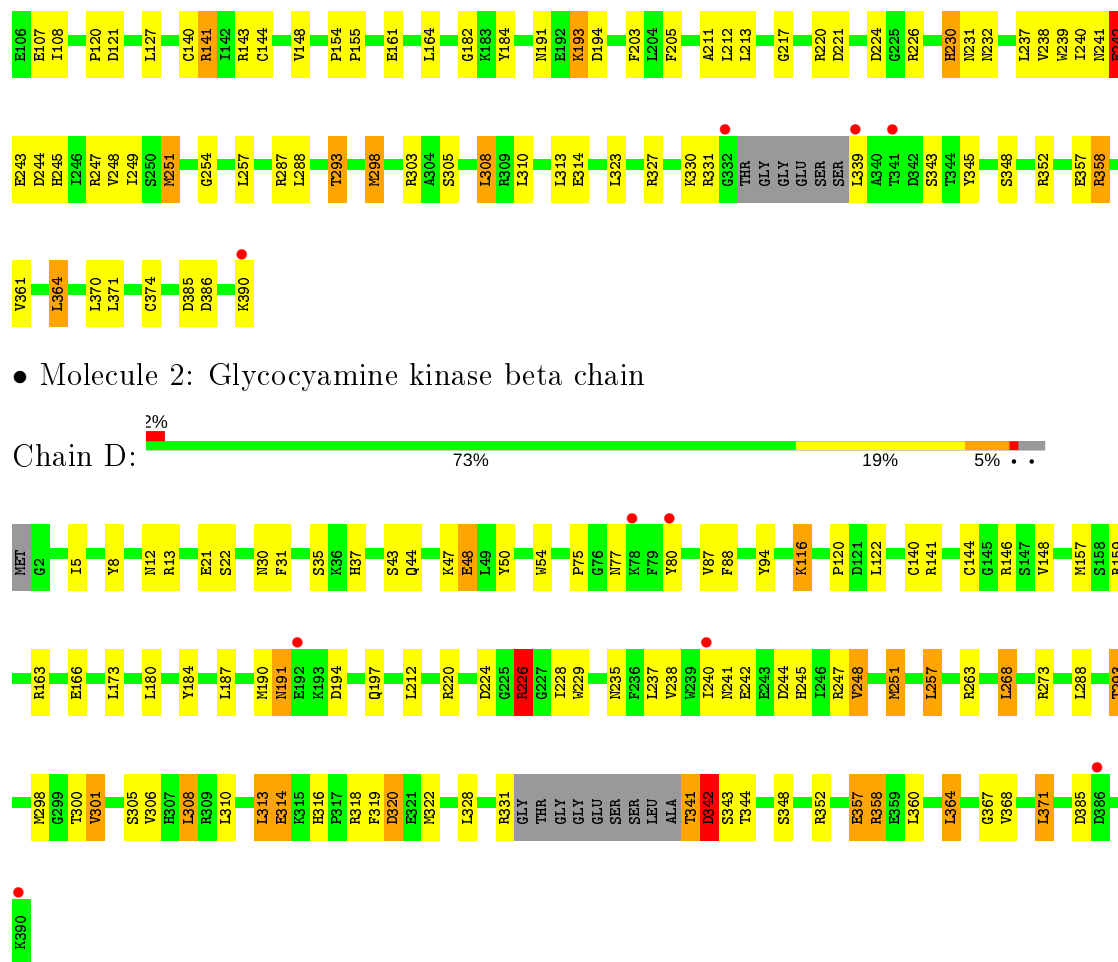


#### • Molecule 1: Glycocyamine kinase alpha chain



#### • Molecule 2: Glycocyamine kinase beta chain





• Molecule 2: Glycocyamine kinase beta chain

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.09Å 98.20Å 93.12Å 90.00° 91.29° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 19.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.60) 90.7 (19.99-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.11 (at 2.59Å)	Xtriage
Refinement program	CNS, REFMAC 5.0	Depositor
R, $R_{free}$	0.192 , 0.266 0.210 , 0.271	Depositor DCC
$R_{free}$ test set	2118 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.4	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12299	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.75	0/3041	0.81	4/4090 (0.1%)
1	C	0.67	0/3041	0.75	4/4090 (0.1%)
2	B	0.79	3/3115 (0.1%)	0.80	1/4189 (0.0%)
2	D	0.73	0/3098	0.81	2/4166 (0.0%)
All	All	0.74	3/12295 (0.0%)	0.79	11/16535 (0.1%)

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	C	0	2
2	D	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	96	CYS	CB-SG	-6.80	1.70	1.82
2	B	140	CYS	CB-SG	-5.42	1.73	1.81
2	B	374	CYS	CB-SG	-5.11	1.73	1.81

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	A	226	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	A	146	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	33	ASP	CB-CG-OD1	5.34	123.11	118.30
2	D	226	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	327	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	B	54	TRP	CA-CB-CG	5.13	123.44	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	343	SER	N-CA-C	-5.08	97.27	111.00
1	C	146	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	220	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	146	ARG	NE-CZ-NH2	-5.05	117.77	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	335	GLY	Peptide
1	C	341	THR	Peptide
2	D	342	ASP	Peptide

## 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	2976	0	2933	59	0
1	C	2976	0	2933	75	0
2	B	3048	0	3012	73	0
2	D	3031	0	2993	68	0
3	A	61	0	0	3	0
3	B	74	0	0	4	0
3	C	54	0	0	0	0
3	D	79	0	0	4	0
All	All	12299	0	11871	266	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 11.

All (266) 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:191:ASN:C	1:A:191:ASN:HD22	1.74	0.88
2:B:148:VAL:H	2:B:245:HIS:HD2	1.25	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:ASN:HD21	2:B:211:ALA:HB1	1.40	0.84
1:C:341:THR:HG22	1:C:344:THR:HB	1.59	0.83
2:D:140:CYS:HB3	2:D:306:VAL:HG12	1.63	0.78
2:D:358:ARG:HH11	2:D:358:ARG:HG2	1.53	0.73
1:C:78:LYS:CE	1:C:78:LYS:H	2.02	0.72
2:B:84:THR:HG23	2:B:108:ILE:HD11	1.71	0.71
2:D:30:ASN:ND2	2:D:50:TYR:OH	2.25	0.70
2:D:364:LEU:O	2:D:368:VAL:HG23	1.93	0.69
1:C:298:MET:HE2	1:C:353:LEU:HD11	1.76	0.68
1:A:332:GLY:O	1:A:334:GLY:N	2.25	0.68
1:A:191:ASN:HD21	1:A:194:ASP:H	1.42	0.68
2:D:148:VAL:H	2:D:245:HIS:HD2	1.42	0.68
2:B:357:GLU:O	2:B:361:VAL:HG23	1.93	0.67
1:A:191:ASN:ND2	1:A:194:ASP:H	1.93	0.67
1:C:287:ARG:NH1	1:C:288:LEU:HD21	2.10	0.66
1:C:78:LYS:HE2	1:C:78:LYS:H	1.61	0.66
1:A:191:ASN:C	1:A:191:ASN:ND2	2.48	0.66
2:B:244:ASP:OD1	2:B:293:THR:HG23	1.98	0.63
1:C:146:ARG:NH2	1:C:300:THR:O	2.32	0.63
2:B:87:VAL:HG11	2:B:155:PRO:HG2	1.80	0.62
2:B:74:ASN:ND2	2:B:211:ALA:HB1	2.13	0.62
2:B:87:VAL:HG11	2:B:155:PRO:CG	2.29	0.62
1:C:357:GLU:O	1:C:361:VAL:HG23	1.98	0.62
1:A:310:LEU:O	1:A:314:GLU:HB3	2.00	0.61
2:B:257:LEU:O	2:B:257:LEU:HD23	2.00	0.61
1:A:316:HIS:CE1	1:A:384:ILE:HD11	2.36	0.61
2:B:191:ASN:ND2	2:B:193:LYS:HG2	2.16	0.61
2:B:257:LEU:HD11	2:B:364:LEU:HD13	1.84	0.60
2:D:77:ASN:ND2	2:D:80:TYR:CE1	2.69	0.60
1:C:120:PRO:HA	1:C:357:GLU:OE2	2.02	0.60
2:D:341:THR:O	2:D:342:ASP:C	2.40	0.60
1:C:87:VAL:HG11	1:C:155:PRO:HG2	1.83	0.60
2:D:191:ASN:ND2	2:D:194:ASP:H	2.00	0.60
1:C:140:CYS:HB3	1:C:306:VAL:HG12	1.83	0.60
1:C:110:HIS:HD1	1:C:350:TRP:HH2	1.50	0.59
2:B:288:LEU:HD22	2:B:298:MET:HE1	1.85	0.59
1:C:226:ARG:HD2	1:C:241:ASN:O	2.03	0.59
2:B:26:LYS:HA	3:B:1029:HOH:O	2.03	0.58
1:C:299:GLY:HA3	1:C:353:LEU:HD23	1.85	0.58
2:D:220:ARG:O	2:D:226:ARG:NH2	2.35	0.58
2:D:163:ARG:HD2	2:D:224:ASP:OD1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:VAL:CG1	2:B:155:PRO:HG2	2.34	0.58
2:B:191:ASN:ND2	2:B:194:ASP:H	2.02	0.58
1:C:173:LEU:HD11	1:C:238:VAL:HG11	1.85	0.58
1:A:244:ASP:OD2	1:A:292:CYS:HB3	2.05	0.56
1:C:307:HIS:HA	1:C:345:TYR:O	2.06	0.56
2:B:323:LEU:HD21	2:B:330:LYS:HB3	1.87	0.55
1:C:310:LEU:HD13	1:C:313:LEU:HD13	1.88	0.55
1:C:87:VAL:HG11	1:C:155:PRO:CG	2.37	0.55
2:D:251:MET:N	2:D:251:MET:SD	2.80	0.55
2:B:226:ARG:HD2	2:B:241:ASN:O	2.06	0.55
1:A:48:GLU:OE1	1:A:48:GLU:N	2.38	0.55
2:D:342:ASP:HB3	2:D:344:THR:OG1	2.07	0.54
2:B:10:VAL:HG22	2:B:59:PRO:O	2.06	0.54
1:C:90:ASP:HA	1:C:153:LEU:HG	1.89	0.54
1:C:330:LYS:O	1:C:330:LYS:HG3	2.07	0.54
1:A:247:ARG:CZ	1:A:249:ILE:HD11	2.37	0.54
2:B:44:GLN:NE2	2:B:107:GLU:OE1	2.40	0.54
1:A:298:MET:HE2	1:A:353:LEU:HD11	1.90	0.54
1:A:316:HIS:NE2	1:A:384:ILE:HD11	2.23	0.54
1:C:220:ARG:O	1:C:226:ARG:NH2	2.40	0.54
1:C:313:LEU:HD22	1:C:319:PHE:HD1	1.73	0.53
1:A:23:ARG:HB3	3:A:1131:HOH:O	2.09	0.53
2:B:148:VAL:H	2:B:245:HIS:CD2	2.14	0.53
1:A:19:LYS:HE3	2:B:164:LEU:HD12	1.90	0.53
1:C:163:ARG:O	1:C:167:LYS:HG3	2.08	0.53
2:B:6:GLN:O	2:B:10:VAL:HG23	2.08	0.53
1:A:140:CYS:HB3	1:A:306:VAL:HG12	1.91	0.53
1:C:179:ASP:HB2	1:C:233:GLU:OE2	2.09	0.53
2:B:24:LYS:HZ3	2:B:26:LYS:HE2	1.74	0.52
1:C:311:ALA:O	1:C:314:GLU:HG2	2.09	0.52
1:C:44:GLN:OE1	1:C:103:LYS:HB3	2.09	0.52
2:B:121:ASP:O	2:B:357:GLU:HG2	2.10	0.52
1:A:148:VAL:H	1:A:245:HIS:HD2	1.57	0.52
2:B:191:ASN:HD22	2:B:193:LYS:HG2	1.75	0.52
1:C:285:ASN:HB2	1:C:291:ILE:HD11	1.92	0.52
1:C:313:LEU:HD22	1:C:319:PHE:CD1	2.45	0.51
1:C:30:ASN:O	2:D:159:ARG:HD2	2.10	0.51
2:B:105:ILE:HG12	2:B:298:MET:HE1	1.92	0.51
2:D:173:LEU:HD13	2:D:229:TRP:CG	2.45	0.51
2:B:182:GLY:HA3	2:B:231:ASN:HA	1.92	0.51
2:B:120:PRO:HA	2:B:357:GLU:OE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:VAL:CG1	1:C:155:PRO:HG2	2.41	0.51
2:D:358:ARG:HH11	2:D:358:ARG:CG	2.22	0.51
1:A:20:ASP:HB2	3:A:1174:HOH:O	2.10	0.51
2:D:146:ARG:NH2	2:D:300:THR:O	2.43	0.51
2:B:305:SER:HB3	2:B:348:SER:HB3	1.92	0.51
2:B:141:ARG:HB2	2:B:251:MET:HB3	1.92	0.51
2:B:205:PHE:CD1	2:B:242:GLU:HG2	2.46	0.51
1:A:66:LYS:HE2	2:B:16:HIS:NE2	2.26	0.51
2:B:217:GLY:O	2:B:220:ARG:NH1	2.44	0.50
2:B:314:GLU:HG2	2:B:345:TYR:OH	2.11	0.50
2:B:77:ASN:HB2	2:B:80:TYR:HB2	1.94	0.50
1:C:78:LYS:HE3	1:C:78:LYS:H	1.73	0.50
2:B:308:LEU:HD13	2:B:310:LEU:HD11	1.93	0.50
1:C:159:ARG:HD2	2:D:30:ASN:O	2.10	0.50
1:A:143:ARG:HB2	1:A:249:ILE:HD13	1.92	0.50
1:A:308:LEU:O	1:A:344:THR:HA	2.12	0.50
1:A:188:THR:HG23	1:A:189:THR:HG23	1.93	0.50
1:A:298:MET:CE	1:A:353:LEU:HD11	2.41	0.50
2:D:238:VAL:HG22	2:D:248:VAL:HB	1.94	0.50
2:B:74:ASN:HD21	2:B:211:ALA:CB	2.18	0.50
2:B:182:GLY:HA2	2:B:232:ASN:OD1	2.12	0.49
2:D:228:ILE:N	2:D:228:ILE:HD12	2.27	0.49
2:D:247:ARG:HD3	3:D:1206:HOH:O	2.12	0.49
2:B:154:PRO:HD2	2:B:293:THR:HG22	1.94	0.49
1:C:187:LEU:HD12	1:C:226:ARG:HB2	1.94	0.49
1:C:121:ASP:O	1:C:357:GLU:HG2	2.12	0.49
2:B:55:ASP:N	2:B:55:ASP:OD2	2.40	0.49
2:B:323:LEU:CD2	2:B:330:LYS:HB3	2.44	0.48
2:B:184:TYR:HE1	2:B:240:ILE:HD12	1.78	0.48
2:B:21:GLU:O	2:B:23:GLY:N	2.45	0.48
1:C:112:LYS:N	1:C:115:ASP:OD2	2.47	0.48
2:B:221:ASP:O	2:B:224:ASP:HB3	2.14	0.48
2:D:37:HIS:CD2	2:D:75:PRO:HA	2.49	0.48
1:A:158:SER:OG	1:A:161:GLU:HG3	2.13	0.48
1:C:302:VAL:HG21	1:C:357:GLU:HB3	1.94	0.48
1:C:308:LEU:HD12	1:C:347:ILE:HD12	1.96	0.48
2:D:310:LEU:O	2:D:314:GLU:HB3	2.13	0.47
1:C:122:LEU:HD21	1:C:357:GLU:HG3	1.96	0.47
2:B:213:LEU:H	2:B:213:LEU:HD22	1.80	0.47
1:A:370:LEU:CD2	1:A:374:CYS:SG	3.02	0.47
1:C:163:ARG:HD2	1:C:224:ASP:OD1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:122:LEU:CD2	2:D:357:GLU:HG3	2.45	0.47
1:A:119:ALA:HA	3:A:1082:HOH:O	2.14	0.47
2:B:239:TRP:CE3	2:B:242:GLU:HG3	2.50	0.47
2:D:244:ASP:OD1	2:D:293:THR:HG23	2.14	0.47
2:D:140:CYS:CB	2:D:306:VAL:HG12	2.40	0.47
2:D:48:GLU:N	2:D:48:GLU:OE2	2.48	0.47
1:A:22:THR:HB	1:A:25:LYS:H	1.79	0.47
1:A:247:ARG:NE	1:A:249:ILE:HD11	2.29	0.47
2:B:52:LYS:HE2	2:B:99:GLU:OE2	2.15	0.47
1:A:357:GLU:HG2	1:A:357:GLU:H	1.53	0.46
1:C:249:ILE:HG22	1:C:251:MET:HE3	1.97	0.46
1:C:374:CYS:HB3	1:C:384:ILE:HD13	1.98	0.46
2:B:220:ARG:O	2:B:226:ARG:NH2	2.48	0.46
2:D:235:ASN:OD1	2:D:263:ARG:HD2	2.16	0.46
1:A:303:ARG:HG2	1:A:352:ARG:NH1	2.31	0.46
2:B:13:ARG:NH1	2:B:161:GLU:OE1	2.47	0.46
2:D:313:LEU:HD21	2:D:322:MET:HE1	1.97	0.46
1:A:370:LEU:HD23	1:A:374:CYS:SG	2.55	0.46
2:B:121:ASP:OD1	2:B:358:ARG:HG2	2.16	0.46
2:D:31:PHE:CD2	2:D:47:LYS:HD3	2.50	0.46
1:A:22:THR:HG22	1:A:24:GLU:HG2	1.97	0.46
1:C:335:GLY:O	1:C:336:GLU:HG2	2.15	0.46
1:A:132:PHE:CB	1:A:137:VAL:HG21	2.46	0.46
2:D:226:ARG:HD2	2:D:241:ASN:O	2.15	0.46
2:B:24:LYS:HE2	2:B:26:LYS:HG3	1.98	0.46
1:C:183:LYS:HG3	1:C:185:TYR:CE1	2.51	0.46
1:C:20:ASP:N	1:C:20:ASP:OD1	2.49	0.46
2:B:3:SER:O	2:B:7:ASP:OD1	2.33	0.46
1:C:244:ASP:OD1	1:C:292:CYS:HB3	2.15	0.46
1:A:238:VAL:HG22	1:A:248:VAL:HB	1.98	0.45
1:A:356:SER:OG	1:A:359:GLU:HG3	2.16	0.45
2:B:287:ARG:NH1	2:B:288:LEU:HD21	2.31	0.45
1:C:87:VAL:HG12	1:C:88:PHE:N	2.29	0.45
2:D:191:ASN:C	2:D:191:ASN:HD22	2.19	0.45
2:D:240:ILE:N	2:D:240:ILE:HD12	2.31	0.45
2:D:273:ARG:HG2	2:D:273:ARG:HH11	1.81	0.45
1:A:155:PRO:HD3	1:A:293:THR:HG22	1.97	0.45
2:D:35:SER:C	3:D:1261:HOH:O	2.55	0.45
2:B:11:LYS:HG2	2:B:18:LYS:NZ	2.31	0.45
2:B:184:TYR:CE1	2:B:240:ILE:HD12	2.52	0.45
1:C:154:PRO:HD2	1:C:293:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:157:MET:O	2:D:220:ARG:NH2	2.47	0.45
1:A:328:LEU:HD11	1:A:367:GLY:HA3	1.98	0.45
1:C:109:HIS:CB	1:C:353:LEU:HD12	2.47	0.45
1:A:204:LEU:HA	1:A:228:ILE:CD1	2.46	0.45
2:B:254:GLY:HA3	3:B:1125:HOH:O	2.17	0.45
1:C:191:ASN:HD22	1:C:191:ASN:N	2.14	0.45
1:C:252:GLN:HE21	1:C:263:ARG:HH22	1.64	0.44
2:B:287:ARG:HH12	2:B:288:LEU:HD21	1.82	0.44
1:A:220:ARG:O	1:A:226:ARG:NH2	2.34	0.44
2:D:94:TYR:CZ	2:D:288:LEU:HD11	2.52	0.44
2:B:226:ARG:N	2:B:226:ARG:HD3	2.31	0.44
2:D:320:ASP:N	2:D:320:ASP:OD2	2.36	0.44
1:A:21:TYR:HB2	2:B:5:ILE:HD12	1.99	0.44
1:C:71:GLY:HA3	1:C:85:GLY:O	2.17	0.44
2:D:313:LEU:HD13	2:D:319:PHE:CE1	2.52	0.44
2:B:46:THR:HB	3:B:1106:HOH:O	2.17	0.44
1:A:157:MET:O	1:A:220:ARG:NH2	2.50	0.44
1:A:26:PHE:HB2	2:B:5:ILE:CD1	2.48	0.44
2:B:50:TYR:O	2:B:54:TRP:HB3	2.18	0.43
1:C:328:LEU:HD22	1:C:364:LEU:HD23	2.00	0.43
1:C:299:GLY:CA	1:C:353:LEU:HD23	2.47	0.43
2:D:180:LEU:HD21	2:D:263:ARG:HG3	2.00	0.43
1:C:148:VAL:H	1:C:245:HIS:HD2	1.66	0.43
2:D:120:PRO:HA	2:D:357:GLU:OE2	2.18	0.43
1:C:191:ASN:HD22	1:C:191:ASN:H	1.64	0.43
2:D:305:SER:HB3	2:D:348:SER:HB3	1.99	0.43
2:D:257:LEU:HD11	2:D:364:LEU:HD13	2.00	0.43
1:A:148:VAL:H	1:A:245:HIS:CD2	2.35	0.43
1:C:147:SER:O	1:C:283:MET:N	2.51	0.43
1:C:87:VAL:CG1	1:C:88:PHE:N	2.81	0.43
2:D:116:LYS:HB3	3:D:1009:HOH:O	2.18	0.43
2:D:358:ARG:NH1	2:D:358:ARG:HG2	2.29	0.43
1:A:242:GLU:HG2	1:A:243:GLU:N	2.34	0.43
1:A:267:GLY:O	1:A:271:VAL:HG23	2.19	0.43
1:A:349:ASN:O	1:A:352:ARG:NH2	2.52	0.43
2:D:328:LEU:HD11	2:D:367:GLY:HA3	2.00	0.43
1:A:32:PRO:HB2	1:A:34:LEU:HD21	2.00	0.43
1:C:320:ASP:OD1	1:C:330:LYS:HD3	2.19	0.43
2:D:144:CYS:HA	2:D:301:VAL:O	2.18	0.43
2:D:87:VAL:HG12	2:D:88:PHE:N	2.34	0.43
1:A:155:PRO:HD3	1:A:293:THR:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:CYS:CB	1:A:306:VAL:HG12	2.48	0.42
1:C:273:ARG:HG2	1:C:273:ARG:HH11	1.84	0.42
1:C:146:ARG:HD2	1:C:282:LEU:HD13	2.01	0.42
2:D:12:ASN:O	2:D:13:ARG:C	2.58	0.42
2:D:313:LEU:HD13	2:D:319:PHE:CD1	2.54	0.42
1:A:212:LEU:O	1:A:216:SER:HB3	2.19	0.42
1:C:364:LEU:O	1:C:368:VAL:HG23	2.19	0.42
1:C:127:LEU:HD22	1:C:362:GLN:OE1	2.19	0.42
2:D:8:TYR:CE2	2:D:12:ASN:ND2	2.86	0.42
1:A:117:HIS:HE1	1:A:300:THR:HG23	1.85	0.42
1:C:38:ASN:ND2	1:C:82:LYS:HG3	2.34	0.42
2:D:144:CYS:SG	2:D:268:LEU:HD11	2.59	0.42
2:D:187:LEU:HD23	2:D:190:MET:HE3	2.01	0.42
2:B:288:LEU:HD22	2:B:298:MET:CE	2.49	0.42
2:D:308:LEU:HD13	2:D:310:LEU:HD21	2.01	0.42
2:D:43:SER:HB2	2:D:44:GLN:HE21	1.84	0.42
1:C:316:HIS:CG	1:C:317:PRO:HD2	2.55	0.42
2:D:341:THR:O	2:D:342:ASP:O	2.37	0.42
1:A:66:LYS:HE2	2:B:16:HIS:CD2	2.55	0.41
1:C:146:ARG:CZ	1:C:290:TYR:CD2	3.02	0.41
2:B:143:ARG:HB2	2:B:249:ILE:HG12	2.02	0.41
2:B:144:CYS:SG	2:B:248:VAL:HG12	2.60	0.41
2:D:166:GLU:OE2	2:D:184:TYR:OH	2.31	0.41
2:B:203:PHE:HE2	2:B:230:HIS:ND1	2.19	0.41
2:B:24:LYS:HE3	3:B:1029:HOH:O	2.20	0.41
2:B:60:ASN:HD22	2:B:90:ASP:CB	2.33	0.41
1:C:298:MET:CE	1:C:353:LEU:HD11	2.49	0.41
2:D:298:MET:HE3	2:D:298:MET:HB2	1.91	0.41
1:C:148:VAL:H	1:C:245:HIS:CD2	2.39	0.41
2:D:300:THR:HG21	2:D:360:LEU:HD12	2.03	0.41
1:C:21:TYR:HB2	2:D:5:ILE:HD12	2.02	0.41
1:A:84:THR:HG21	1:A:295:PRO:HD2	2.03	0.41
1:A:298:MET:HE2	1:A:298:MET:HB3	1.86	0.41
1:C:177:LYS:HA	1:C:181:ALA:HB2	2.02	0.41
1:C:306:VAL:O	1:C:346:ASP:HA	2.21	0.41
2:D:358:ARG:NH1	2:D:358:ARG:CG	2.81	0.41
2:D:371:LEU:HD12	2:D:371:LEU:HA	1.92	0.41
1:A:322:MET:SD	1:A:370:LEU:HD22	2.60	0.41
1:A:41:MET:HG2	1:A:100:PHE:HZ	1.85	0.41
1:A:69:GLN:HE21	1:A:73:ASP:CG	2.23	0.41
1:C:54:TRP:C	1:C:54:TRP:CD1	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:LEU:C	2:B:257:LEU:HD23	2.40	0.41
1:C:122:LEU:CD2	1:C:357:GLU:HG3	2.51	0.41
2:D:116:LYS:NZ	3:D:1268:HOH:O	2.51	0.41
2:D:122:LEU:HD21	2:D:357:GLU:HG3	2.02	0.41
1:C:23:ARG:HB3	1:C:54:TRP:CZ3	2.56	0.41
1:A:74:ASN:OD1	1:A:211:ALA:HB1	2.20	0.40
2:D:148:VAL:H	2:D:245:HIS:CD2	2.29	0.40
2:D:364:LEU:HD22	2:D:368:VAL:CG2	2.51	0.40
1:A:201:ASP:O	1:A:202:HIS:HB2	2.21	0.40
2:B:154:PRO:HG2	2:B:243:GLU:O	2.21	0.40
1:C:88:PHE:O	1:C:153:LEU:HD12	2.21	0.40
1:C:26:PHE:HB2	2:D:5:ILE:CD1	2.50	0.40
2:B:238:VAL:HG22	2:B:248:VAL:HG23	2.04	0.40
2:D:21:GLU:HG2	2:D:22:SER:N	2.36	0.40
2:D:316:HIS:CD2	2:D:318:ARG:H	2.40	0.40
1:A:190:MET:HG2	1:A:195:GLN:HE21	1.87	0.40
2:B:314:GLU:OE2	2:B:343:SER:HA	2.21	0.40
1:C:166:GLU:HG3	1:C:184:TYR:OH	2.22	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	371/374 (99%)	348 (94%)	17 (5%)	6 (2%)	9	19
1	C	371/374 (99%)	345 (93%)	24 (6%)	2 (0%)	29	52
2	B	379/390 (97%)	356 (94%)	19 (5%)	4 (1%)	14	30
2	D	376/390 (96%)	360 (96%)	13 (4%)	3 (1%)	19	39
All	All	1497/1528 (98%)	1409 (94%)	73 (5%)	15 (1%)	15	32

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	22	SER
2	B	80	TYR
1	A	242	GLU
1	C	314	GLU
2	D	242	GLU
1	A	76	GLY
1	A	334	GLY
1	A	135	LYS
1	A	333	THR
2	B	242	GLU
2	D	342	ASP
2	B	10	VAL
1	C	301	VAL
1	A	301	VAL
2	D	301	VAL

### 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	323/324 (100%)	295 (91%)	28 (9%)	10	20
1	C	323/324 (100%)	295 (91%)	28 (9%)	10	20
2	B	330/335 (98%)	298 (90%)	32 (10%)	8	15
2	D	329/335 (98%)	303 (92%)	26 (8%)	12	24
All	All	1305/1318 (99%)	1191 (91%)	114 (9%)	10	20

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	PHE
1	A	35	SER
1	A	54	TRP
1	A	77	ASN
1	A	127	LEU
1	A	141	ARG
1	A	143	ARG

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Mol	Chain	Res	Type
1	A	191	ASN
1	A	195	GLN
1	A	212	LEU
1	A	226	ARG
1	A	237	LEU
1	A	244	ASP
1	A	248	VAL
1	A	257	LEU
1	A	313	LEU
1	A	314	GLU
1	A	323	LEU
1	A	327	ARG
1	A	330	LYS
1	A	352	ARG
1	A	357	GLU
1	A	358	ARG
1	A	364	LEU
1	A	384	ILE
1	A	385	ASP
1	A	386	ASP
1	A	387	MET
2	B	3	SER
2	B	6	GLN
2	B	11	LYS
2	B	54	TRP
2	B	70	THR
2	B	79	PHE
2	B	99	GLU
2	B	127	LEU
2	B	141	ARG
2	B	193	LYS
2	B	212	LEU
2	B	230	HIS
2	B	237	LEU
2	B	242	GLU
2	B	247	ARG
2	B	251	MET
2	B	293	THR
2	B	298	MET
2	B	303	ARG
2	B	308	LEU
2	B	313	LEU

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Mol	Chain	Res	Type
2	B	327	ARG
2	B	331	ARG
2	B	339	LEU
2	B	352	ARG
2	B	358	ARG
2	B	364	LEU
2	B	370	LEU
2	B	371	LEU
2	B	385	ASP
2	B	386	ASP
2	B	390	LYS
1	C	20	ASP
1	C	23	ARG
1	C	54	TRP
1	C	66	LYS
1	C	78	LYS
1	C	127	LEU
1	C	140	CYS
1	C	144	CYS
1	C	177	LYS
1	C	191	ASN
1	C	197	GLN
1	C	200	GLU
1	C	237	LEU
1	C	248	VAL
1	C	251	MET
1	C	268	LEU
1	C	278	CYS
1	C	293	THR
1	C	303	ARG
1	C	313	LEU
1	C	323	LEU
1	C	330	LYS
1	C	342	ASP
1	C	364	LEU
1	C	366	ASP
1	C	371	LEU
1	C	385	ASP
1	C	390	LYS
2	D	48	GLU
2	D	54	TRP
2	D	116	LYS

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Mol	Chain	Res	Type
2	D	141	ARG
2	D	191	ASN
2	D	197	GLN
2	D	212	LEU
2	D	226	ARG
2	D	237	LEU
2	D	248	VAL
2	D	251	MET
2	D	257	LEU
2	D	268	LEU
2	D	293	THR
2	D	308	LEU
2	D	313	LEU
2	D	314	GLU
2	D	320	ASP
2	D	331	ARG
2	D	341	THR
2	D	352	ARG
2	D	357	GLU
2	D	358	ARG
2	D	364	LEU
2	D	371	LEU
2	D	385	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	109	HIS
1	A	191	ASN
1	A	195	GLN
1	A	230	HIS
1	A	245	HIS
1	A	307	HIS
1	A	382	GLN
2	B	38	ASN
2	B	60	ASN
2	B	74	ASN
2	B	109	HIS
2	B	191	ASN
2	B	202	HIS
2	B	245	HIS

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Mol	Chain	Res	Type
2	B	316	HIS
2	B	382	GLN
1	C	38	ASN
1	C	69	GLN
1	C	195	GLN
1	C	245	HIS
1	C	252	GLN
2	D	30	ASN
2	D	109	HIS
2	D	124	HIS
2	D	191	ASN
2	D	245	HIS
2	D	252	GLN
2	D	316	HIS
2	D	382	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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	373/374 (99%)	0.09	10 (2%) 54 48	43, 51, 62, 74	0
1	C	373/374 (99%)	0.09	17 (4%) 32 26	43, 51, 64, 73	0
2	B	383/390 (98%)	-0.04	9 (2%) 60 54	43, 51, 61, 74	0
2	D	380/390 (97%)	-0.12	6 (1%) 72 68	43, 51, 62, 69	0
All	All	1509/1528 (98%)	0.01	42 (2%) 53 46	43, 51, 62, 74	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	GLY	5.1
1	C	390	LYS	5.1
1	C	380	ALA	4.9
1	A	336	GLU	4.5
1	A	334	GLY	4.4
1	C	381	GLY	3.9
1	C	336	GLU	3.9
2	B	341	THR	3.8
2	B	79	PHE	3.8
1	C	335	GLY	3.7
1	A	340	ALA	3.6
2	B	339	LEU	3.4
2	B	4	ALA	3.3
1	C	333	THR	3.2
1	C	331	ARG	3.1
2	B	332	GLY	3.1
1	C	340	ALA	2.9
1	C	341	THR	2.9
2	D	80	TYR	2.7
2	D	192	GLU	2.6
1	A	80	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	389	PRO	2.6
1	A	342	ASP	2.5
2	D	390	LYS	2.5
1	C	18	PHE	2.5
1	A	20	ASP	2.5
2	D	386	ASP	2.5
2	B	22	SER	2.4
1	A	246	ILE	2.4
2	D	240	ILE	2.4
2	B	2	GLY	2.4
1	C	318	ARG	2.3
1	C	334	GLY	2.3
2	B	390	LYS	2.2
2	B	67	CYS	2.2
1	C	116	LYS	2.1
1	C	125	ASN	2.1
1	A	21	TYR	2.1
1	C	382	GLN	2.1
1	C	386	ASP	2.1
2	D	78	LYS	2.1
1	A	233	GLU	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.