

# Full wwPDB X-ray Structure Validation Report (i)

#### Mar 5, 2024 – 10:54 AM EST

PDB ID	:	2G5H
Title	:	Structure of tRNA-Dependent Amidotransferase GatCAB
Authors	:	Nakamura, A.; Yao, M.; Tanaka, I.
Deposited on	:	2006-02-23
Resolution	:	2.50  Å(reported)
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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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
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)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Motric	Whole archive	Similar resolution
Wiethic	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	А	485	3% 72	2%	2	.6% •	
2	В	483	36%	37%	9%	18%	
3	С	100	16%		40%	5%•	



#### 2G5H

# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7806 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 Glutamyl-tRNA(Gln) amidotransferase subunit A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	485	Total 3716	C 2359	N 605	O 739	S 13	0	0	0

 • Molecule 2 is a protein called Aspartyl/glutamyl-tRNA (Asn/Gln) amidotransferase subunit B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	В	398	Total 3169	C 1999	N 532	O 626	S 12	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	476	LEU	-	expression tag	UNP P64201
В	477	GLU	-	expression tag	UNP P64201
В	478	HIS	-	expression tag	UNP P64201
В	479	HIS	-	expression tag	UNP P64201
В	480	HIS	-	expression tag	UNP P64201
В	481	HIS	-	expression tag	UNP P64201
В	482	HIS	-	expression tag	UNP P64201
В	483	HIS	-	expression tag	UNP P64201

• Molecule 3 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit C.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	С	99	Total 781	C 480	N 130	O 169	${ m S} { m 2}$	0	0	0

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total Mg 1 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	81	Total         O           81         81	0	0
5	В	47	$\begin{array}{cc} \text{Total} & \text{O} \\ 47 & 47 \end{array}$	0	0
5	С	11	Total         O           11         11	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.









## 

• Molecule 3: Aspartyl/glutamyl-tRNA<br/>(Asn/Gln) amidotransferase subunit C





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	70.92Å 92.04Å 181.45Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(A)	20.00 - 2.50	Depositor
Resolution (A)	41.16 - 2.50	EDS
% Data completeness	99.4 (20.00-2.50)	Depositor
(in resolution range)	99.4 (41.16 - 2.50)	EDS
$R_{merge}$	0.04	Depositor
R <sub>sym</sub>	0.04	Depositor
$< I/\sigma(I) > 1$	$6.07 (at 2.51 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
P. P.	0.238 , $0.275$	Depositor
$n, n_{free}$	0.243 , $0.239$	DCC
$R_{free}$ test set	4160 reflections $(9.98\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	53.1	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , $40.8$	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.51, < L^2>=0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7806	wwPDB-VP
Average B, all atoms $(Å^2)$	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

# 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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).

Mal	Mol Chain		lengths	Bond angles		
1VIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.41	0/3784	0.65	0/5116	
2	В	0.42	0/3231	0.74	4/4364~(0.1%)	
3	С	0.42	0/789	0.70	0/1066	
All	All	0.42	0/7804	0.70	4/10546~(0.0%)	

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	А	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	383	SER	N-CA-C	7.77	131.99	111.00
2	В	397	GLY	N-CA-C	5.93	127.92	113.10
2	В	5	THR	N-CA-C	-5.36	96.53	111.00
2	В	111	GLY	N-CA-C	-5.33	99.77	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	472	TYR	Sidechain



## 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	А	3716	0	3709	118	0
2	В	3169	0	3119	278	0
3	С	781	0	760	59	0
4	В	1	0	0	0	0
5	А	81	0	0	3	0
5	В	47	0	0	4	0
5	С	11	0	0	1	0
All	All	7806	0	7588	423	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 28.

All (423) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:192:ASP:OD2	2:B:212:LYS:HD3	1.53	1.08
2:B:199:PRO:HG2	2:B:202:GLN:HE22	1.08	1.07
2:B:7:ILE:HD11	2:B:157:ILE:HD11	1.36	1.04
3:C:98:GLU:HG3	3:C:99:ASP:N	1.85	0.91
2:B:371:GLY:O	2:B:374:LYS:HG2	1.72	0.90
1:A:338:SER:HA	3:C:94:ILE:HD11	1.52	0.90
2:B:199:PRO:HG2	2:B:202:GLN:NE2	1.85	0.90
2:B:344:LEU:HD12	2:B:348:VAL:HG21	1.55	0.89
2:B:343:TRP:O	2:B:348:VAL:HG13	1.74	0.87
3:C:94:ILE:HD13	3:C:94:ILE:H	1.41	0.85
3:C:20:ILE:HD11	3:C:25:THR:HA	1.60	0.84
1:A:1:MET:H2	1:A:28:ASP:CB	1.91	0.83
2:B:304:VAL:O	2:B:308:GLY:HA2	1.79	0.82
2:B:351:TYR:CE1	2:B:357:VAL:HG21	2.15	0.81
2:B:388:LYS:O	2:B:388:LYS:HD3	1.81	0.81
2:B:198:ARG:O	2:B:198:ARG:HG3	1.81	0.80
2:B:295:LEU:HD22	2:B:295:LEU:N	1.98	0.79
2:B:364:LEU:CD1	2:B:369:LEU:HB2	2.13	0.79
1:A:84:THR:OG1	1:A:121:LYS:HE3	1.84	0.78
2:B:309:LEU:HD11	2:B:338:LYS:HD2	1.66	0.77



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:348:VAL:O	2:B:352:LEU:HD13	1.83	0.77
1:A:87:LEU:HD12	1:A:118:LEU:HD21	1.67	0.77
2:B:364:LEU:HD11	2:B:369:LEU:HB2	1.64	0.77
1:A:247:ASP:OD2	1:A:250:SER:HB3	1.84	0.77
2:B:217:PHE:O	2:B:220:VAL:HG22	1.85	0.77
2:B:320:THR:OG1	2:B:323:MET:HB3	1.85	0.76
1:A:364:PHE:HD2	3:C:12:ILE:HD11	1.49	0.76
1:A:4:ARG:HD2	1:A:5:TYR:CE2	2.20	0.76
1:A:1:MET:H2	1:A:28:ASP:CA	1.99	0.75
3:C:47:THR:O	3:C:50:VAL:HG12	1.87	0.75
2:B:386:ALA:HA	2:B:389:VAL:HG22	1.68	0.75
2:B:388:LYS:HE2	2:B:392:GLU:CG	2.17	0.74
2:B:5:THR:HG21	2:B:228:GLU:HG3	1.70	0.73
2:B:348:VAL:HG12	2:B:390:PHE:CZ	2.24	0.73
3:C:98:GLU:CG	3:C:99:ASP:N	2.51	0.73
1:A:1:MET:CG	1:A:4:ARG:HE	2.00	0.73
2:B:313:ASP:HA	2:B:345:MET:SD	2.28	0.73
2:B:388:LYS:HE2	2:B:392:GLU:HG3	1.71	0.73
2:B:160:PRO:HB3	2:B:224:LEU:HB3	1.72	0.72
2:B:288:VAL:O	2:B:291:THR:HG22	1.89	0.72
2:B:243:GLN:HG3	2:B:261:LYS:HG3	1.72	0.72
2:B:197:LEU:HD13	2:B:231:GLN:OE1	1.91	0.70
1:A:484:LYS:O	1:A:485:LEU:HB2	1.88	0.70
1:A:256:ILE:HG23	1:A:471:GLN:HG3	1.72	0.70
1:A:77:GLY:C	1:A:78:ILE:HD12	2.12	0.70
3:C:72:ILE:HD12	3:C:76:LEU:HB3	1.74	0.70
2:B:182:VAL:HG12	2:B:189:LEU:HD23	1.72	0.70
1:A:284:VAL:HG12	1:A:288:LYS:HE3	1.74	0.69
2:B:60:MET:HE3	2:B:70:ILE:HG21	1.74	0.69
2:B:386:ALA:HA	2:B:389:VAL:CG2	2.22	0.69
2:B:221:ARG:O	2:B:225:GLU:HG2	1.93	0.69
2:B:309:LEU:CD1	2:B:338:LYS:HD2	2.23	0.69
2:B:390:PHE:HB3	2:B:391:PRO:HD3	1.74	0.68
3:C:99:ASP:OD1	3:C:100:ALA:N	2.21	0.68
2:B:309:LEU:HD12	2:B:310:PRO:HD3	1.74	0.68
3:C:57:LEU:HD22	3:C:59:LEU:HD13	1.76	0.68
2:B:344:LEU:HA	2:B:348:VAL:HG22	1.74	0.68
3:C:96:ASN:O	3:C:99:ASP:OD1	2.12	0.67
2:B:256:ILE:HD12	2:B:256:ILE:N	2.09	0.67
2:B:352:LEU:HA	2:B:357:VAL:HG23	1.77	0.67
1:A:255:ASP:OD1	1:A:257:LYS:HG2	1.94	$0.\overline{67}$



	A h C	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
2:B:202:GLN:HG2	2:B:203:GLU:N	2.08	0.67	
3:C:20:ILE:HD11	3:C:25:THR:CA	2.24	0.66	
2:B:281:ASP:O	2:B:285:LYS:HG3	1.94	0.66	
2:B:3:PHE:HE1	2:B:197:LEU:HD23	1.61	0.66	
1:A:1:MET:HG2	1:A:4:ARG:HE	1.60	0.66	
2:B:288:VAL:HA	2:B:291:THR:HG22	1.77	0.66	
3:C:94:ILE:HD13	3:C:94:ILE:N	2.11	0.66	
2:B:7:ILE:HG12	2:B:157:ILE:HG13	1.79	0.65	
2:B:359:LEU:O	2:B:361:ASP:N	2.30	0.65	
3:C:94:ILE:H	3:C:94:ILE:CD1	2.10	0.65	
1:A:402:PRO:HG2	1:A:427:LEU:HD13	1.79	0.65	
1:A:150:VAL:HG12	1:A:411:LEU:HD23	1.79	0.64	
2:B:44:TYR:O	2:B:47:VAL:HG22	1.96	0.64	
2:B:247:ARG:HB3	2:B:258:MET:HE2	1.79	0.64	
2:B:351:TYR:HE1	2:B:357:VAL:HG21	1.62	0.64	
1:A:1:MET:N	1:A:28:ASP:HA	2.13	0.64	
1:A:174:ASP:HB3	1:A:192:LYS:HG3	1.78	0.64	
2:B:7:ILE:HG22	2:B:195:ILE:HG13	1.80	0.63	
1:A:22:PRO:HD2	1:A:59:ASP:OD1	1.98	0.63	
2:B:295:LEU:HD22	2:B:295:LEU:H	1.62	0.63	
2:B:338:LYS:HZ2	2:B:338:LYS:HB3	1.62	0.63	
2:B:32:GLU:O	2:B:35:SER:OG	2.16	0.62	
2:B:157:ILE:HD12	2:B:159:SER:H	1.62	0.62	
1:A:169:LEU:C	1:A:169:LEU:HD22	2.19	0.62	
1:A:169:LEU:HD22	1:A:170:SER:N	2.13	0.62	
2:B:331:ILE:CG2	2:B:332:GLU:N	2.62	0.62	
2:B:360:LEU:HG	2:B:360:LEU:O	1.99	0.62	
2:B:5:THR:HG22	2:B:197:LEU:HG	1.81	0.62	
2:B:94:GLN:HB2	2:B:122:HIS:HB2	1.80	0.62	
2:B:340:THR:HG23	2:B:373:ILE:HD12	1.81	0.62	
2:B:133:LYS:HB2	2:B:138:LEU:HD23	1.81	0.62	
2:B:249:ASP:HB2	2:B:256:ILE:HD11	1.82	0.62	
1:A:83:ILE:HD12	1:A:103:TYR:OH	2.00	0.62	
2:B:256:ILE:HA	5:B:519:HOH:O	2.01	0.61	
2:B:295:LEU:O	2:B:299:ARG:HB2	2.01	0.61	
2:B:154:GLU:HG3	2:B:155:PRO:HD2	1.82	0.61	
2:B:344:LEU:HA	2:B:348:VAL:CG2	2.31	0.61	
1:A:140:LYS:HD3	5:A:512:HOH:O	2.00	0.61	
2:B:88:LYS:O	2:B:89:ALA:HB3	2.00	0.61	
2:B:309:LEU:HG	2:B:310:PRO:HD2	1.83	0.61	
2:B:359:LEU:C	2:B:361:ASP:H	2.02	0.60	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:B:230:ARG:NH1	2:B:246:ARG:HE	2.00	0.60	
2:B:300:LYS:HG3	2:B:314:ALA:HB1	1.84	0.60	
1:A:29:ILE:HG21	1:A:119:ILE:HG12	1.82	0.60	
2:B:3:PHE:N	2:B:200:TYR:CD2	2.69	0.60	
2:B:15:LEU:HD11	2:B:149:ILE:HG23	1.84	0.59	
2:B:105:ILE:HD11	2:B:166:TYR:CD1	2.37	0.59	
2:B:199:PRO:HD3	2:B:235:LEU:HD21	1.84	0.59	
2:B:388:LYS:HE2	2:B:392:GLU:HG2	1.84	0.59	
1:A:299:LEU:HD12	1:A:388:ASP:HB3	1.85	0.59	
2:B:26:PRO:HG3	3:C:68:ALA:HB1	1.84	0.59	
2:B:352:LEU:HA	2:B:357:VAL:CG2	2.33	0.58	
1:A:1:MET:H2	1:A:28:ASP:HA	1.66	0.58	
3:C:27:GLU:O	3:C:31:THR:HG23	2.03	0.58	
1:A:361:LEU:HG	3:C:35:ILE:HG21	1.84	0.58	
3:C:94:ILE:HG12	3:C:94:ILE:O	2.03	0.58	
1:A:241:ALA:HB2	3:C:57:LEU:HD11	1.85	0.58	
2:B:98:PRO:HG2	2:B:101:GLU:HG3	1.84	0.57	
3:C:21:SER:C	3:C:23:GLU:H	2.07	0.57	
2:B:75:LYS:HG3	2:B:97:GLN:OE1	2.04	0.57	
2:B:133:LYS:HB2	2:B:138:LEU:CD2	2.34	0.57	
2:B:259:ARG:HG3	2:B:259:ARG:HH11	1.69	0.57	
1:A:306:ILE:HG22	3:C:38:PHE:HZ	1.70	0.57	
2:B:399:ASN:O	2:B:400:ALA:C	2.41	0.57	
2:B:219:TYR:CD1	2:B:248:PHE:HE2	2.22	0.57	
1:A:1:MET:HG3	1:A:4:ARG:HE	1.70	0.57	
2:B:61:ARG:CD	2:B:291:THR:HG23	2.34	0.57	
2:B:336:ASP:HB3	2:B:339:LEU:HD23	1.86	0.57	
2:B:348:VAL:HG12	2:B:390:PHE:CE1	2.40	0.57	
2:B:336:ASP:OD2	2:B:339:LEU:HD23	2.06	0.56	
2:B:247:ARG:HB3	2:B:258:MET:CE	2.35	0.56	
2:B:60:MET:O	2:B:64:MET:HG3	2.04	0.56	
2:B:362:THR:C	2:B:363:LYS:HD2	2.26	0.56	
2:B:338:LYS:HZ2	2:B:342:ASN:HD21	1.54	0.56	
2:B:176:TYR:CE1	2:B:296:PRO:HG3	2.41	0.56	
1:A:276:VAL:HG21	1:A:406:THR:HA	1.88	0.55	
3:C:98:GLU:CG	3:C:99:ASP:H	2.19	0.55	
1:A:256:ILE:HD12	1:A:292:ALA:HB2	1.88	0.55	
2:B:3:PHE:O	2:B:3:PHE:CG	2.59	0.55	
2:B:369:LEU:HD22	2:B:369:LEU:O	2.05	0.55	
3:C:99:ASP:CG	3:C:100:ALA:H	2.09	0.55	
2:B:241:ILE:HD13	2:B:241:ILE:C	2.26	0.55	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:360:PHE:HB3	3:C:32:LEU:HD21	1.87	0.55	
2:B:295:LEU:N	2:B:295:LEU:CD2	2.70	0.55	
2:B:295:LEU:HB3	2:B:296:PRO:CD	2.37	0.55	
2:B:61:ARG:HD2	2:B:291:THR:HG23	1.89	0.55	
2:B:260:VAL:HG12	2:B:260:VAL:O	2.06	0.55	
1:A:338:SER:OG	1:A:341:GLU:HG3	2.07	0.55	
2:B:351:TYR:HD1	2:B:352:LEU:HD12	1.71	0.54	
1:A:102:ILE:HG12	2:B:44:TYR:CE2	2.43	0.54	
2:B:309:LEU:HD12	2:B:310:PRO:CD	2.36	0.54	
2:B:384:LYS:HE3	2:B:387:LYS:NZ	2.23	0.54	
1:A:228:GLU:OE2	1:A:247:ASP:HA	2.08	0.54	
2:B:193:ALA:CB	2:B:224:LEU:HD11	2.38	0.54	
2:B:171:ARG:NH1	2:B:175:GLN:HG3	2.23	0.54	
2:B:300:LYS:HZ3	2:B:315:HIS:HB2	1.72	0.53	
2:B:53:LYS:HB2	3:C:63:LEU:HB3	1.88	0.53	
2:B:176:TYR:HE2	2:B:299:ARG:HD3	1.73	0.53	
2:B:392:GLU:O	2:B:396:LYS:HB2	2.08	0.53	
1:A:204:VAL:HG22	2:B:45:PRO:HB2	1.90	0.53	
2:B:234:GLU:O	2:B:239:GLY:HA3	2.08	0.53	
3:C:57:LEU:HD22	3:C:59:LEU:CD1	2.38	0.53	
2:B:355:ASN:HD22	2:B:357:VAL:HG13	1.73	0.53	
2:B:138:LEU:N	2:B:138:LEU:HD22	2.24	0.53	
2:B:288:VAL:CA	2:B:291:THR:HG22	2.39	0.53	
2:B:211:LEU:HD12	2:B:224:LEU:HD12	1.92	0.52	
2:B:288:VAL:HA	2:B:291:THR:CG2	2.38	0.52	
2:B:316:VAL:HG13	2:B:345:MET:CE	2.38	0.52	
2:B:288:VAL:C	2:B:291:THR:HG22	2.30	0.52	
2:B:295:LEU:HB3	2:B:296:PRO:HD2	1.90	0.52	
2:B:313:ASP:HA	2:B:345:MET:HE1	1.90	0.52	
2:B:359:LEU:C	2:B:361:ASP:N	2.62	0.52	
2:B:91:GLN:NE2	2:B:124:GLU:HB3	2.25	0.52	
2:B:202:GLN:HG2	2:B:204:LYS:H	1.75	0.52	
3:C:21:SER:O	3:C:23:GLU:N	2.43	0.52	
2:B:355:ASN:ND2	2:B:357:VAL:HG13	2.25	0.52	
1:A:40:ILE:HA	1:A:142:VAL:HG22	1.92	0.51	
1:A:340:GLU:OE1	3:C:99:ASP:O	2.28	0.51	
1:A:364:PHE:HB2	3:C:12:ILE:HD13	1.90	0.51	
2:B:306:GLU:O	2:B:307:LEU:HB3	2.09	0.51	
2:B:331:ILE:HG22	2:B:332:GLU:H	1.75	0.51	
3:C:35:ILE:O	3:C:38:PHE:HB3	2.10	0.51	
2:B:343:TRP:CD1	2:B:373:ILE:HD13	2.45	0.51	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:C:47:THR:HB	3:C:50:VAL:CG1	2.40	0.51
2:B:374:LYS:HA	2:B:377:GLU:HB3	1.92	0.51
2:B:138:LEU:CD2	2:B:138:LEU:N	2.74	0.51
3:C:21:SER:C	3:C:23:GLU:N	2.64	0.51
1:A:219:ASN:ND2	1:A:222:ASP:OD2	2.42	0.51
2:B:378:ASP:O	2:B:379:GLY:C	2.50	0.51
1:A:361:LEU:HG	3:C:35:ILE:CG2	2.40	0.50
2:B:330:THR:HG21	2:B:369:LEU:HD13	1.93	0.50
2:B:176:TYR:CZ	2:B:296:PRO:HG3	2.46	0.50
3:C:63:LEU:N	3:C:63:LEU:HD22	2.27	0.50
2:B:259:ARG:HG3	2:B:260:VAL:N	2.26	0.50
2:B:335:ALA:HB1	2:B:340:THR:HG23	1.92	0.50
2:B:355:ASN:HB3	2:B:357:VAL:HG22	1.93	0.50
3:C:26:GLU:HB2	5:C:110:HOH:O	2.11	0.50
1:A:206:PHE:CD1	1:A:206:PHE:C	2.85	0.50
2:B:7:ILE:HD11	2:B:157:ILE:CD1	2.25	0.50
2:B:169:LYS:O	2:B:169:LYS:HD3	2.12	0.50
1:A:8:VAL:O	1:A:12:LEU:HB2	2.11	0.50
2:B:136:TYR:N	2:B:136:TYR:CD1	2.80	0.50
3:C:74:GLN:NE2	3:C:87:GLY:HA3	2.27	0.50
1:A:80:ASP:OD1	1:A:89:THR:HA	2.11	0.50
1:A:409:PHE:CD1	1:A:414:GLU:HG3	2.46	0.50
2:B:271:PRO:O	2:B:273:PRO:HD3	2.11	0.50
2:B:331:ILE:HG22	2:B:332:GLU:N	2.27	0.50
2:B:7:ILE:CG1	2:B:157:ILE:HG13	2.42	0.49
2:B:60:MET:HB3	2:B:99:ILE:HD11	1.94	0.49
3:C:21:SER:OG	3:C:23:GLU:HG3	2.11	0.49
1:A:133:THR:O	1:A:133:THR:HG22	2.13	0.49
2:B:7:ILE:HG22	2:B:195:ILE:CB	2.43	0.49
3:C:59:LEU:O	3:C:60:GLN:HG3	2.10	0.49
3:C:65:GLU:HB3	3:C:67:LYS:HD2	1.93	0.49
1:A:380:LYS:HB3	3:C:50:VAL:CG1	2.43	0.49
2:B:238:GLY:O	2:B:239:GLY:O	2.30	0.49
2:B:247:ARG:CB	2:B:258:MET:HE2	2.41	0.49
2:B:340:THR:CG2	2:B:373:ILE:HD12	2.42	0.49
2:B:343:TRP:O	2:B:346:GLY:O	2.31	0.49
2:B:366:PRO:HD2	2:B:367:GLU:OE2	2.13	0.49
1:A:15:ILE:HG22	1:A:67:MET:HE2	1.94	0.49
2:B:157:ILE:HD12	2:B:158:ARG:N	2.26	0.49
2:B:388:LYS:HA	2:B:391:PRO:HD2	1.94	0.49
3:C:78:LEU:HD11	3:C:87:GLY:HA2	1.95	0.49



	to as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:383:SER:O	2:B:386:ALA:HB3	2.13	0.49
1:A:215:PRO:C	1:A:216:LEU:HD12	2.33	0.48
2:B:339:LEU:HB3	2:B:373:ILE:CG2	2.43	0.48
2:B:9:LEU:HD12	2:B:166:TYR:CD2	2.48	0.48
2:B:109:VAL:O	2:B:110:ASP:C	2.52	0.48
2:B:363:LYS:HD2	2:B:363:LYS:N	2.27	0.48
2:B:393:LEU:HD22	2:B:393:LEU:O	2.14	0.48
1:A:283:ALA:O	1:A:287:LEU:HD22	2.13	0.48
2:B:229:LYS:N	2:B:229:LYS:HD2	2.28	0.48
2:B:245:THR:OG1	2:B:261:LYS:HE2	2.13	0.48
2:B:313:ASP:HA	2:B:345:MET:CE	2.44	0.48
1:A:484:LYS:O	1:A:485:LEU:CB	2.61	0.48
2:B:7:ILE:HG22	2:B:195:ILE:CG1	2.43	0.48
1:A:429:THR:OG1	1:A:430:PRO:HD3	2.13	0.48
2:B:7:ILE:HA	2:B:194:ASN:O	2.13	0.48
2:B:276:VAL:HG21	3:C:59:LEU:CB	2.44	0.48
1:A:402:PRO:HG2	1:A:427:LEU:CD1	2.44	0.48
1:A:364:PHE:CD1	1:A:364:PHE:C	2.87	0.47
2:B:157:ILE:CD1	2:B:159:SER:H	2.26	0.47
2:B:378:ASP:O	2:B:379:GLY:O	2.30	0.47
2:B:300:LYS:NZ	2:B:315:HIS:HB2	2.29	0.47
2:B:388:LYS:C	2:B:391:PRO:HD2	2.35	0.47
2:B:167:LEU:CD2	2:B:220:VAL:HG21	2.43	0.47
2:B:240:GLU:HA	2:B:240:GLU:OE1	2.14	0.47
2:B:295:LEU:H	2:B:295:LEU:CD2	2.25	0.47
2:B:362:THR:O	2:B:362:THR:HG23	2.14	0.47
1:A:1:MET:H2	1:A:28:ASP:HB3	1.78	0.47
3:C:47:THR:HB	3:C:50:VAL:HG12	1.96	0.47
2:B:137:SER:HB2	3:C:91:VAL:HG23	1.96	0.47
2:B:310:PRO:HB2	2:B:313:ASP:OD1	2.13	0.47
2:B:355:ASN:HB2	5:B:547:HOH:O	2.13	0.47
2:B:247:ARG:N	2:B:258:MET:HE2	2.30	0.47
2:B:294:GLU:O	2:B:299:ARG:HD2	2.15	0.47
2:B:378:ASP:OD1	2:B:379:GLY:N	2.48	0.47
1:A:201:PHE:CD1	1:A:236:ASN:HB3	2.50	0.47
1:A:374:TYR:OH	3:C:40:LYS:HE3	2.15	0.47
2:B:88:LYS:O	2:B:89:ALA:CB	2.63	0.47
2:B:98:PRO:HB3	2:B:120:ARG:HH21	1.78	0.47
2:B:169:LYS:HE2	2:B:173:ILE:HD11	1.96	0.47
2:B:338:LYS:NZ	2:B:342:ASN:HD21	2.12	0.47
2:B:368:ASN:HD22	2:B:368:ASN:N	2.11	0.47



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:B:216:SER:OG	2:B:219:TYR:HB2	2.14	0.47	
2:B:98:PRO:HB3	2:B:120:ARG:NH2	2.29	0.47	
2:B:363:LYS:NZ	2:B:363:LYS:HB3	2.30	0.47	
2:B:276:VAL:HG21	3:C:59:LEU:C	2.35	0.47	
2:B:212:LYS:HB2	2:B:258:MET:HE3	1.97	0.46	
2:B:356:GLN:HA	2:B:356:GLN:NE2	2.31	0.46	
2:B:169:LYS:HD3	2:B:169:LYS:C	2.36	0.46	
1:A:103:TYR:HB3	2:B:39:VAL:HG11	1.96	0.46	
2:B:160:PRO:HG3	2:B:225:GLU:HB3	1.96	0.46	
1:A:78:ILE:HG12	1:A:108:MET:SD	2.56	0.46	
1:A:247:ASP:OD2	1:A:250:SER:CB	2.61	0.46	
1:A:1:MET:H2	1:A:28:ASP:CG	2.18	0.46	
2:B:309:LEU:CG	2:B:310:PRO:HD2	2.45	0.46	
2:B:309:LEU:HD21	2:B:341:SER:HB2	1.98	0.46	
2:B:176:TYR:HE2	2:B:299:ARG:CD	2.29	0.46	
2:B:202:GLN:HG2	2:B:204:LYS:N	2.31	0.46	
2:B:290:GLN:C	2:B:290:GLN:CD	2.74	0.46	
2:B:309:LEU:CD1	2:B:338:LYS:CD	2.92	0.46	
2:B:340:THR:O	2:B:344:LEU:HD22	2.15	0.46	
2:B:385:ILE:O	2:B:389:VAL:HG13	2.15	0.46	
2:B:159:SER:OG	2:B:162:GLU:HG3	2.15	0.46	
1:A:81:ASN:HB3	1:A:124:MET:HE1	1.97	0.46	
1:A:280:VAL:HG21	1:A:402:PRO:HB3	1.97	0.46	
2:B:119:THR:HG22	2:B:154:GLU:CA	2.46	0.46	
2:B:185:GLU:CD	2:B:185:GLU:H	2.18	0.46	
2:B:212:LYS:HA	2:B:212:LYS:HD2	1.51	0.46	
1:A:103:TYR:CD1	2:B:39:VAL:HG11	2.51	0.45	
1:A:439:ILE:O	1:A:454:GLN:HA	2.16	0.45	
2:B:220:VAL:HG23	2:B:221:ARG:N	2.32	0.45	
2:B:259:ARG:HG3	2:B:259:ARG:NH1	2.30	0.45	
1:A:76:MET:HB3	1:A:169:LEU:HD11	1.97	0.45	
2:B:241:ILE:HD13	2:B:242:GLY:N	2.31	0.45	
1:A:338:SER:CB	3:C:99:ASP:HB2	2.46	0.45	
2:B:20:LYS:HB3	2:B:145:GLY:O	2.17	0.45	
2:B:257:LEU:C	2:B:257:LEU:HD13	2.37	0.45	
2:B:362:THR:HB	5:B:521:HOH:O	2.15	0.45	
1:A:4:ARG:HD2	1:A:5:TYR:CD2	2.52	0.45	
1:A:15:ILE:HG22	1:A:67:MET:CE	2.47	0.45	
1:A:410:ASN:HB2	1:A:413:GLU:HB2	1.99	0.45	
2:B:157:ILE:CD1	2:B:162:GLU:HB2	2.46	0.45	
1:A:284:VAL:CG1	1:A:288:LYS:HE3	2.46	0.45	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:368:ASN:N	2:B:368:ASN:ND2	2.65	0.45
1:A:181:GLN:HB3	1:A:182:PRO:HD3	1.99	0.45
2:B:64:MET:C	2:B:66:LEU:N	2.71	0.45
2:B:169:LYS:NZ	2:B:297:ASP:OD2	2.50	0.45
1:A:348:SER:OG	3:C:19:GLN:N	2.50	0.45
2:B:298:GLU:CD	2:B:298:GLU:H	2.20	0.45
2:B:383:SER:O	2:B:386:ALA:N	2.47	0.45
2:B:7:ILE:CG2	2:B:195:ILE:HG13	2.46	0.44
2:B:61:ARG:HD3	2:B:291:THR:HG23	1.99	0.44
2:B:135:GLU:OE2	3:C:94:ILE:HG22	2.17	0.44
1:A:84:THR:CG2	1:A:121:LYS:HE3	2.47	0.44
1:A:338:SER:HB2	3:C:100:ALA:OXT	2.18	0.44
2:B:246:ARG:NH1	2:B:255:THR:O	2.50	0.44
1:A:1:MET:N	1:A:28:ASP:CG	2.71	0.44
2:B:197:LEU:N	2:B:197:LEU:CD1	2.80	0.44
1:A:295:GLU:HB3	5:A:558:HOH:O	2.17	0.44
1:A:62:GLN:HG3	1:A:67:MET:CE	2.48	0.44
1:A:270:GLU:HB3	5:A:503:HOH:O	2.17	0.44
1:A:372:ASP:HA	1:A:376:LYS:HB3	2.00	0.44
1:A:210:LEU:HD13	1:A:382:ARG:NH2	2.32	0.44
2:B:56:VAL:HG22	2:B:123:MET:CE	2.48	0.44
2:B:276:VAL:HG22	2:B:277:PRO:HD2	1.99	0.44
2:B:389:VAL:HG23	2:B:390:PHE:N	2.32	0.44
2:B:198:ARG:HB3	2:B:205:PHE:CD2	2.53	0.44
2:B:384:LYS:HE3	2:B:387:LYS:HZ1	1.82	0.44
2:B:336:ASP:CB	2:B:339:LEU:HD23	2.48	0.43
2:B:344:LEU:O	2:B:348:VAL:HG22	2.18	0.43
1:A:290:LEU:HD13	1:A:471:GLN:HB3	2.00	0.43
2:B:64:MET:HE1	2:B:288:VAL:C	2.38	0.43
2:B:167:LEU:HD23	2:B:220:VAL:HG21	2.00	0.43
2:B:247:ARG:CA	2:B:258:MET:HE2	2.48	0.43
1:A:78:ILE:HD12	1:A:78:ILE:N	2.33	0.43
2:B:38:ASN:OD1	2:B:40:ILE:HB	2.18	0.43
2:B:119:THR:HG22	2:B:154:GLU:HA	1.99	0.43
2:B:348:VAL:CG2	2:B:349:ASN:N	2.81	0.43
1:A:105:SER:HB2	1:A:202:GLY:HA3	2.00	0.43
1:A:262:ALA:HB2	1:A:396:TYR:CG	2.54	0.43
2:B:202:GLN:HE21	2:B:202:GLN:HB3	1.51	0.43
2:B:249:ASP:HB2	2:B:256:ILE:CD1	2.47	0.43
1:A:11:LEU:O	1:A:15:ILE:HG13	2.18	0.43
1:A:87:LEU:HD12	1:A:118:LEU:CD2	2.43	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap $(\text{\AA})$
2:B:93:SER:OG	2:B:94:GLN:N	2.51	0.43
2:B:157:ILE:HD13	2:B:163:ALA:N	2.34	0.43
3:C:99:ASP:O	3:C:100:ALA:HB3	2.19	0.43
2:B:129:LYS:HE2	2:B:143:ARG:NH2	2.34	0.43
2:B:270:PHE:HA	2:B:271:PRO:HD3	1.85	0.43
2:B:330:THR:CG2	2:B:340:THR:HG21	2.49	0.43
2:B:386:ALA:CA	2:B:389:VAL:HG22	2.43	0.43
1:A:244:ASP:O	1:A:246:VAL:N	2.52	0.43
3:C:20:ILE:HG13	3:C:24:GLU:HB3	1.99	0.43
1:A:105:SER:CB	1:A:202:GLY:HA3	2.49	0.43
1:A:203:LEU:O	2:B:46:GLY:HA2	2.19	0.43
1:A:256:ILE:CD1	1:A:292:ALA:HB2	2.49	0.43
1:A:425:ASP:HB3	1:A:429:THR:HG23	2.01	0.42
2:B:230:ARG:CZ	2:B:246:ARG:HE	2.32	0.42
1:A:90:THR:C	1:A:92:ALA:N	2.71	0.42
2:B:157:ILE:HD13	2:B:162:GLU:HB2	2.01	0.42
2:B:389:VAL:O	2:B:393:LEU:HB3	2.19	0.42
2:B:22:PHE:CE2	2:B:92:ILE:HB	2.55	0.42
2:B:60:MET:HB3	2:B:99:ILE:CD1	2.50	0.42
2:B:121:LEU:HA	2:B:150:GLU:O	2.18	0.42
2:B:137:SER:OG	3:C:93:THR:HB	2.18	0.42
1:A:391:LYS:O	1:A:394:GLU:HB2	2.20	0.42
2:B:297:ASP:HB2	2:B:298:GLU:OE2	2.19	0.42
2:B:316:VAL:HG13	2:B:345:MET:HE2	2.01	0.42
1:A:284:VAL:O	1:A:288:LYS:HG3	2.19	0.42
1:A:400:VAL:HG22	1:A:401:GLY:N	2.34	0.42
1:A:343:TYR:HB3	3:C:17:ARG:HB3	2.02	0.42
2:B:198:ARG:O	2:B:198:ARG:CG	2.61	0.42
1:A:449:ARG:HA	1:A:450:PRO:HD2	1.93	0.42
2:B:135:GLU:OE1	2:B:135:GLU:HA	2.19	0.42
1:A:338:SER:HB3	3:C:99:ASP:HB2	2.02	0.42
3:C:5:THR:HB	3:C:7:GLU:OE1	2.20	0.42
2:B:112:GLU:N	5:B:517:HOH:O	2.52	0.41
1:A:3:ILE:HG13	1:A:28:ASP:OD2	2.20	0.41
1:A:47:ASP:HB2	1:A:87:LEU:HD11	2.01	0.41
1:A:155:SER:HB2	1:A:178:SER:O	2.19	0.41
2:B:140:ASP:HB2	3:C:88:GLN:HE21	1.84	0.41
2:B:198:ARG:HG3	2:B:198:ARG:HH11	1.84	0.41
2:B:214:LEU:HB3	2:B:220:VAL:HG12	2.02	0.41
2:B:309:LEU:HD11	2:B:338:LYS:CD	2.45	0.41
2:B:309:LEU:HD21	2:B:341:SER:CB	2.51	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance (\text{\AA})$	overlap (Å)
1:A:1:MET:O	1:A:4:ARG:HG2	2.21	0.41
2:B:307:LEU:HD23	2:B:307:LEU:O	2.20	0.41
1:A:108:MET:CE	1:A:111:LEU:HD12	2.50	0.41
1:A:345:MET:HG2	3:C:19:GLN:OE1	2.20	0.41
2:B:284:TRP:O	2:B:288:VAL:HG22	2.21	0.41
2:B:365:THR:HB	2:B:366:PRO:CD	2.50	0.41
2:B:336:ASP:CG	2:B:339:LEU:HD23	2.39	0.41
2:B:363:LYS:O	2:B:364:LEU:C	2.59	0.41
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.94	0.41
1:A:216:LEU:HD12	1:A:216:LEU:N	2.35	0.41
1:A:268:LEU:HD12	1:A:268:LEU:HA	1.93	0.41
2:B:7:ILE:HG22	2:B:195:ILE:HA	2.03	0.41
2:B:156:ASP:O	2:B:158:ARG:HG2	2.21	0.41
1:A:37:ASP:N	1:A:38:PRO:CD	2.83	0.41
1:A:256:ILE:HG23	1:A:471:GLN:CG	2.44	0.41
2:B:64:MET:C	2:B:66:LEU:H	2.24	0.41
2:B:43:ALA:HB3	2:B:87:PRO:HB2	2.03	0.41
2:B:105:ILE:HD11	2:B:166:TYR:CE1	2.56	0.41
1:A:62:GLN:HG3	1:A:67:MET:HE1	2.02	0.40
1:A:332:HIS:HB3	3:C:82:LYS:CD	2.51	0.40
2:B:64:MET:SD	2:B:289:ARG:HD2	2.61	0.40
2:B:316:VAL:HA	2:B:319:LEU:HD13	2.02	0.40
1:A:90:THR:O	1:A:91:CYS:HB2	2.20	0.40
1:A:317:ALA:C	1:A:319:SER:H	2.24	0.40
2:B:226:TYR:CD1	2:B:226:TYR:C	2.94	0.40
2:B:385:ILE:HG23	2:B:389:VAL:HG11	2.03	0.40
2:B:197:LEU:HD13	2:B:231:GLN:CD	2.42	0.40
1:A:322:SER:HB3	2:B:89:ALA:CB	2.52	0.40
1:A:326:GLY:O	1:A:332:HIS:ND1	2.51	0.40
2:B:5:THR:HG22	2:B:197:LEU:CD1	2.52	0.40
2:B:85:ASP:HB2	2:B:128:GLY:O	2.21	0.40
2:B:119:THR:CG2	2:B:154:GLU:HA	2.51	0.40
2:B:202:GLN:OE1	2:B:204:LYS:O	2.40	0.40
2:B:358:GLU:H	2:B:358:GLU:HG2	1.68	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	Perce	entiles
1	А	483/485 (100%)	459 (95%)	23~(5%)	1 (0%)	47	68
2	В	396/483~(82%)	348 (88%)	38 (10%)	10 (2%)	5	8
3	С	97/100~(97%)	85 (88%)	11 (11%)	1 (1%)	15	28
All	All	976/1068 (91%)	892 (91%)	72 (7%)	12 (1%)	13	24

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	239	GLY
2	В	308	GLY
2	В	310	PRO
2	В	383	SER
1	А	245	ASP
2	В	337	VAL
2	В	360	LEU
2	В	379	GLY
2	В	293	PRO
2	В	397	GLY
3	С	22	PRO
2	В	238	GLY

#### 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
Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	406/406 (100%)	387~(95%)	19 (5%)	26 49
2	В	345/419~(82%)	300 (87%)	45 (13%)	4 7
3	С	87/88~(99%)	78~(90%)	9 (10%)	7 14
All	All	838/913~(92%)	765~(91%)	73 (9%)	10 20

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	1	MET
1	А	4	ARG
1	А	46	LEU
1	А	85	ASN
1	А	87	LEU
1	А	96	LEU
1	А	122	LEU
1	А	169	LEU
1	А	206	PHE
1	А	210	LEU
1	А	263	LEU
1	А	268	LEU
1	А	287	LEU
1	А	299	LEU
1	А	339	LEU
1	А	361	LEU
1	А	376	LYS
1	А	414	GLU
1	А	433	LEU
2	В	4	GLU
2	В	7	ILE
2	В	66	LEU
2	В	73	GLU
2	В	75	LYS
2	В	109	VAL
2	В	119	THR
2	В	129	LYS
2	В	136	TYR
2	В	141	LEU
2	В	157	ILE
2	В	167	LEU



Mol	Chain	Res	Tvpe
2	B	169	LYS
2	B	182	VAL
2	B	192	ASP
2	B	192	LEU
2	B	202	GLN
2	B	202	LYS
2	B	212	TYB
2	B	230	ARG
2	B	230 241	ILE
2	B	254	LYS
$\frac{2}{2}$	B	261	VAL
$\frac{2}{2}$	B	200	GLN
2	R	313	ASP
2	B	315	HIS
$\frac{2}{2}$	B	316	VAL
2 9	R	300	CLU
$\frac{2}{2}$	B	322	ILE
2	R	333	HIS
2	B	3/10	THR
$\frac{2}{2}$	B	340	LEU
2	B	3/5	MET
$\frac{2}{2}$	B	340	ASN
2	B	354	LVS
$\frac{2}{2}$	B	355	ASN
2	B	350	LEU
2	B	362	THB
$\frac{2}{2}$	B	363	LVS
2	B	364	LEU
2	R	360	LEU
2	B	373	
$\frac{2}{2}$	R	378	ASP
2	B	385	ILE
$\frac{2}{2}$	B	303	LEU
3	C	8	GLU
3	C	14	ASN
3	C	23	GLU
3	C	32	LEU
3	C	37	ASP
3	C	57	LEU
् <u>र</u>		58	
े २	C	67	LVS
ວ 		01	
3	U	94	

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

Mol	Chain	Res	Type
1	А	62	GLN
1	А	85	ASN
1	А	281	GLN
1	А	479	HIS
2	В	202	GLN
2	В	290	GLN
2	В	342	ASN
2	В	356	GLN
2	В	368	ASN
3	С	14	ASN
3	С	60	GLN
3	С	74	GLN
3	C	88	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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



# 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 (i)

# 6.1 Protein, DNA and RNA chains (i)

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,  $95^{th}$  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	А	485/485~(100%)	0.19	14 (2%) 51 55	32, 47, 67, 88	0
2	В	398/483~(82%)	0.68	52 (13%) 3 3	38, 69, 95, 95	0
3	С	99/100~(99%)	0.75	16 (16%) 1 1	45, 69, 95, 95	0
All	All	982/1068~(91%)	0.45	82 (8%) 11 11	32, 55, 95, 95	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	381	MET	9.1
1	А	1	MET	8.8
2	В	382	SER	7.9
2	В	398	GLY	7.3
2	В	397	GLY	6.1
3	С	2	THR	6.0
2	В	393	LEU	5.6
3	С	96	ASN	5.4
2	В	237	ASN	5.2
2	В	395	ALA	4.6
3	С	94	ILE	4.5
3	С	98	GLU	4.4
2	В	387	LYS	4.3
3	С	97	GLU	4.1
2	В	379	GLY	4.1
2	В	335	ALA	4.1
2	В	400	ALA	4.0
1	А	203	LEU	3.8
2	В	109	VAL	3.8
3	С	95	MET	3.8
2	В	31	ALA	3.7
2	В	376	ILE	3.7
3	С	99	ASP	3.6



Mol	Chain	Res	Type	RSRZ
2	В	262	GLU	3.6
2	В	369	LEU	3.5
2	В	378	ASP	3.5
2	В	135	GLU	3.5
3	С	23	GLU	3.5
2	В	305	ASN	3.4
2	В	304	VAL	3.4
2	В	334	GLY	3.3
3	С	22	PRO	3.1
3	С	100	ALA	3.1
1	А	205	ALA	3.0
2	В	354	LYS	3.0
2	В	260	VAL	2.9
2	В	389	VAL	2.9
2	В	29	PHE	2.9
2	В	399	ASN	2.8
2	В	113	THR	2.7
2	В	343	TRP	2.7
2	В	358	GLU	2.6
3	С	38	PHE	2.6
2	В	375	LEU	2.5
2	В	385	ILE	2.5
2	В	28	HIS	2.5
2	В	310	PRO	2.5
1	А	52	ILE	2.5
2	В	384	LYS	2.5
1	А	154	SER	2.5
1	А	335	GLU	2.5
3	С	3	LYS	2.4
3	С	87	GLY	2.4
2	В	307	LEU	2.4
2	B	136	TYR	2.4
2	В	47	VAL	2.3
3	C	30	ASN	2.3
2	В	290	GLN	2.3
2	B	5	THR	2.3
2	В	390	PHE	2.2
1	A	56	GLN	2.2
1	A	173	SER	2.2
2	В	373	ILE	2.2
2	В	367	GLU	2.2
2	В	364	LEU	2.2



Mol	Chain	Res Type		RSRZ	
2	В	380	THR	2.2	
1	А	171	LEU	2.2	
2	В	49	PRO	2.1	
3	С	40	LYS	2.1	
2	В	247	ARG	2.1	
1	А	178	SER	2.1	
1	А	188	VAL	2.1	
2	В	92	ILE	2.1	
2	В	263	GLY	2.1	
2	В	361	ASP	2.0	
3	С	37	ASP	2.0	
1	А	204	VAL	2.0	
1	A	206	PHE	2.0	
2	В	370	ALA	2.0	
2	В	394	ALA	2.0	
1	А	157	GLY	2.0	
2	В	3	PHE	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 monosaccharides in this entry.

### 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
4	MG	В	501	1/1	0.78	0.25	43,43,43,43	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

