



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 11:57 AM EDT

PDB ID : 3IP4
Title : The high resolution structure of GatCAB
Authors : Nakamura, A.; Yao, M.; Tanaka, I.
Deposited on : 2009-08-17
Resolution : 1.90 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 : 4.02b-467
Xtriage (Phenix) : 1.13
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

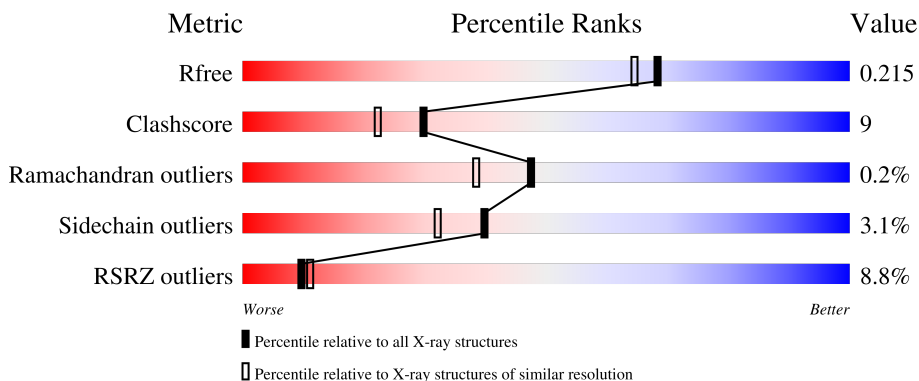
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	485	 88% 12%
2	B	483	 16% 75% 23%
3	C	100	 9% 72% 19% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9101 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
			Total	C	N	O	S			
1	A	485	3730	2366	609	742	13	0	3	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	482	3834	2408	655	755	16	0	3	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	476	LEU	-	expression tag	UNP P64201
B	477	GLU	-	expression tag	UNP P64201
B	478	HIS	-	expression tag	UNP P64201
B	479	HIS	-	expression tag	UNP P64201
B	480	HIS	-	expression tag	UNP P64201
B	481	HIS	-	expression tag	UNP P64201
B	482	HIS	-	expression tag	UNP P64201
B	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
			Total	C	N	O	S			
3	C	92	735	455	122	157	1	0	2	0

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

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

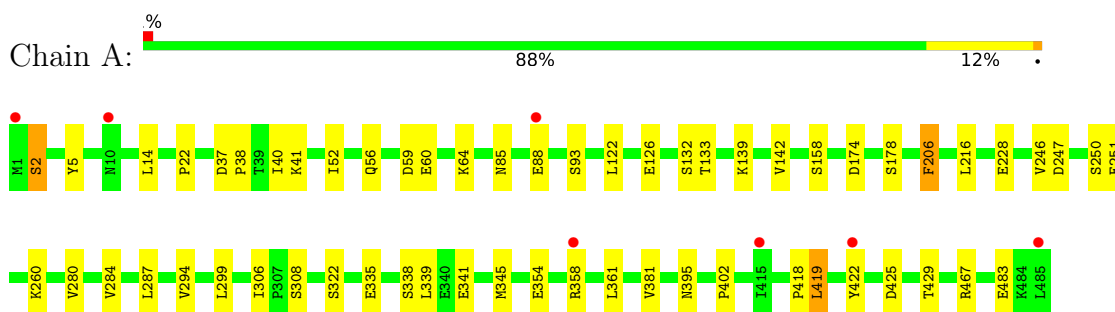
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	410	Total O 410 410	0	0
5	B	300	Total O 300 300	0	0
5	C	91	Total O 91 91	0	0

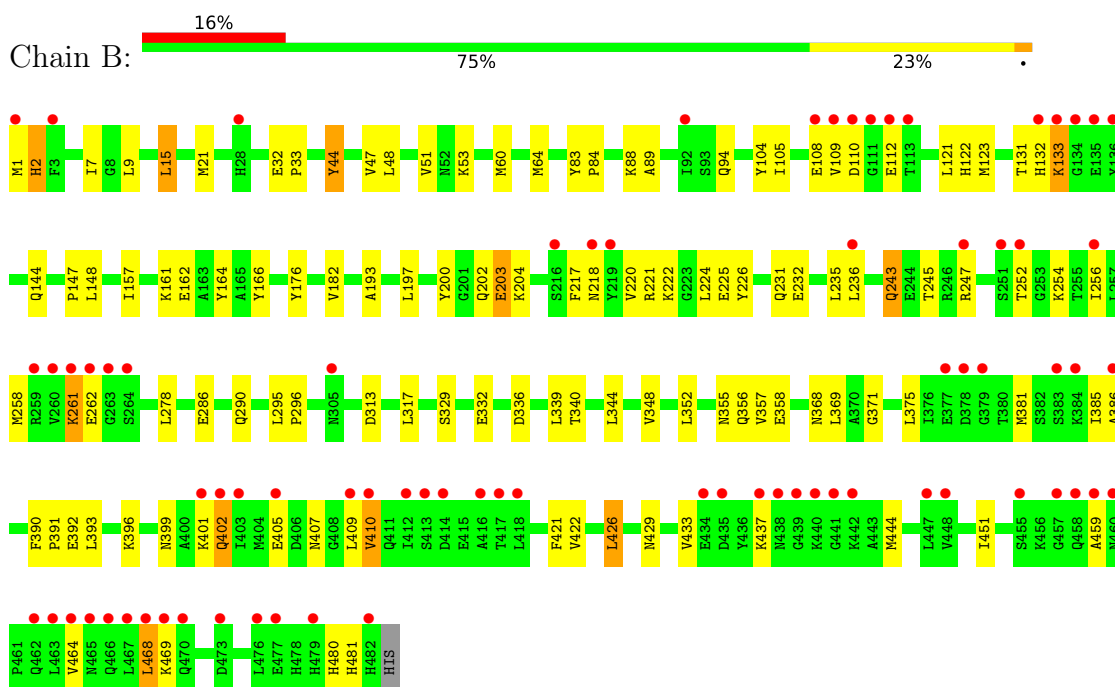
3 Residue-property plots [i](#)

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 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

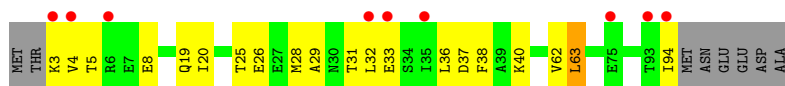


- Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B



- Molecule 3: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit C





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.12Å 92.73Å 180.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 35.67 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-1.90) 99.9 (35.67-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 1.91Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.214 0.197 , 0.215	Depositor DCC
R_{free} test set	4739 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtrriage
Anisotropy	0.417	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9101	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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 [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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.34	0/3812	0.64	2/5153 (0.0%)
2	B	0.29	0/3920	0.57	0/5287
3	C	0.27	0/752	0.56	0/1017
All	All	0.31	0/8484	0.60	2/11457 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	SER	N-CA-C	-11.72	79.37	111.00
1	A	299	LEU	N-CA-C	-5.49	96.19	111.00

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	3730	0	3722	40	0
2	B	3834	0	3774	96	0
3	C	735	0	721	32	0
4	B	1	0	0	0	0
5	A	410	0	0	5	0
5	B	300	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	91	0	0	1	0
All	All	9101	0	8217	156	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 (156) 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)
3:C:3:LYS:HZ2	3:C:33[B]:GLU:HB2	1.43	0.82
2:B:261:LYS:HB2	2:B:261:LYS:NZ	1.95	0.80
1:A:339:LEU:HD22	3:C:94:ILE:HG12	1.67	0.76
3:C:3:LYS:NZ	3:C:33[B]:GLU:HB2	2.02	0.75
1:A:216:LEU:HB3	5:A:797:HOH:O	1.87	0.75
2:B:385:ILE:HD12	5:B:623:HOH:O	1.90	0.71
3:C:33[A]:GLU:HG2	3:C:37:ASP:OD2	1.94	0.68
2:B:399:ASN:OD1	2:B:402[B]:GLN:HB2	1.94	0.68
2:B:243:GLN:HE21	2:B:243:GLN:N	1.91	0.67
2:B:221:ARG:O	2:B:225:GLU:HG3	1.96	0.66
3:C:3:LYS:NZ	3:C:29:ALA:O	2.28	0.66
2:B:329:SER:O	2:B:332:GLU:HG2	1.95	0.66
2:B:108:GLU:HA	2:B:108:GLU:OE1	1.95	0.65
2:B:252:THR:HG22	2:B:254:LYS:HG3	1.77	0.65
2:B:451:ILE:CD1	2:B:468:LEU:HD11	2.28	0.64
2:B:348:VAL:O	2:B:352:LEU:HD13	1.99	0.62
3:C:3:LYS:HE3	3:C:4:VAL:H	1.64	0.61
2:B:261:LYS:HB2	2:B:261:LYS:HZ3	1.65	0.61
1:A:345:MET:HG2	3:C:19:GLN:HE22	1.66	0.61
1:A:260:LYS:HE3	1:A:395:ASN:O	2.01	0.61
2:B:247:ARG:HB3	2:B:258:MET:SD	2.41	0.61
2:B:422:VAL:HG22	2:B:468:LEU:HD12	1.83	0.60
2:B:256:ILE:HD12	2:B:256:ILE:N	2.15	0.60
2:B:426:LEU:HD12	2:B:433:VAL:HG22	1.83	0.60
1:A:122:LEU:HD13	1:A:158:SER:HA	1.84	0.60
1:A:354:GLU:OE2	1:A:422:TYR:OH	2.20	0.60
2:B:336:ASP:OD2	2:B:339:LEU:HD13	2.01	0.60
2:B:222:LYS:HD3	2:B:225:GLU:OE1	2.03	0.59
2:B:437:LYS:O	2:B:437:LYS:HD3	2.03	0.59
2:B:7:ILE:HB	2:B:157:ILE:HB	1.85	0.59
2:B:232:GLU:O	2:B:236:LEU:HD13	2.03	0.58
3:C:5:THR:HG23	3:C:8:GLU:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:LYS:O	2:B:405:GLU:HG2	2.04	0.58
3:C:20:ILE:HD11	3:C:25:THR:HA	1.85	0.58
2:B:451:ILE:HD12	2:B:468:LEU:HD11	1.87	0.57
1:A:306:ILE:HG22	3:C:38:PHE:HZ	1.70	0.57
2:B:340:THR:O	2:B:344:LEU:HD13	2.04	0.57
2:B:429:ASN:O	2:B:433:VAL:HG23	2.04	0.57
1:A:247:ASP:OD2	1:A:250:SER:HB3	2.04	0.57
2:B:371:GLY:O	2:B:375:LEU:HD13	2.04	0.57
1:A:228:GLU:HG2	1:A:246:VAL:O	2.05	0.56
1:A:174:ASP:HA	1:A:178:SER:HB2	1.88	0.54
3:C:63:LEU:HD22	3:C:63:LEU:N	2.22	0.54
2:B:132:HIS:O	2:B:133:LYS:CD	2.55	0.54
2:B:83:TYR:OH	3:C:94:ILE:CG2	2.56	0.54
2:B:444:MET:CE	2:B:468:LEU:HB3	2.39	0.53
2:B:110:ASP:HB2	5:B:660:HOH:O	2.09	0.53
1:A:40:ILE:HA	1:A:142:VAL:HG22	1.91	0.53
1:A:284:VAL:HG13	1:A:294:VAL:HG11	1.90	0.53
1:A:280:VAL:HG21	1:A:402:PRO:HG3	1.90	0.53
2:B:444:MET:HE1	2:B:469:LYS:N	2.23	0.52
3:C:4:VAL:HG21	3:C:32:LEU:HB3	1.90	0.52
1:A:41:LYS:HB3	1:A:139:LYS:HD3	1.91	0.52
2:B:88:LYS:O	2:B:89:ALA:HB3	2.09	0.52
2:B:161:LYS:HZ2	2:B:221:ARG:HD2	1.75	0.52
3:C:3:LYS:HZ2	3:C:33[A]:GLU:HB2	1.74	0.52
3:C:3:LYS:HD3	3:C:33[B]:GLU:HG2	1.92	0.52
3:C:3:LYS:HD3	3:C:33[A]:GLU:OE1	2.10	0.52
1:A:338:SER:OG	1:A:341:GLU:HG3	2.10	0.51
2:B:399:ASN:OD1	2:B:402[A]:GLN:HB3	2.09	0.51
1:A:345:MET:HG2	3:C:19:GLN:NE2	2.25	0.51
3:C:28:MET:HA	3:C:31:THR:HB	1.92	0.51
2:B:109:VAL:HG22	5:B:752:HOH:O	2.10	0.51
2:B:132:HIS:O	2:B:133:LYS:HD2	2.11	0.51
2:B:21:MET:CE	2:B:123:MET:HB3	2.41	0.50
3:C:4:VAL:HG11	3:C:32:LEU:HD23	1.93	0.50
2:B:451:ILE:HD12	2:B:468:LEU:CD1	2.42	0.50
2:B:295:LEU:HB3	2:B:296:PRO:HD2	1.93	0.50
2:B:451:ILE:HD11	2:B:468:LEU:HD11	1.94	0.50
3:C:4:VAL:HG21	3:C:32:LEU:HD23	1.94	0.49
1:A:322:SER:HB3	2:B:89:ALA:CB	2.42	0.49
2:B:444:MET:HE1	2:B:468:LEU:HB3	1.92	0.49
1:A:60:GLU:CG	1:A:64:LYS:NZ	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:VAL:HG23	2:B:110:ASP:N	2.26	0.49
2:B:112:GLU:HA	2:B:112:GLU:OE1	2.11	0.49
2:B:226:TYR:CE2	2:B:254:LYS:HG2	2.47	0.49
2:B:94:GLN:HB2	2:B:122:HIS:HB2	1.94	0.49
3:C:32:LEU:O	3:C:36:LEU:HG	2.12	0.49
1:A:419:LEU:HB2	5:A:748:HOH:O	2.12	0.49
1:A:251:GLU:HB2	5:A:569:HOH:O	2.12	0.49
3:C:3:LYS:HD2	3:C:33[B]:GLU:OE1	2.12	0.49
2:B:105:ILE:HD11	2:B:166:TYR:CD1	2.48	0.48
2:B:109:VAL:HG23	2:B:110:ASP:H	1.79	0.48
1:A:93:SER:HB2	1:A:126:GLU:HG3	1.95	0.47
2:B:84:PRO:HG2	3:C:94:ILE:HD11	1.96	0.47
2:B:1:MET:CE	2:B:236:LEU:HD12	2.45	0.47
2:B:164:TYR:HE2	2:B:218[A]:ASN:HD22	1.61	0.47
2:B:176:TYR:CE1	2:B:296:PRO:HG3	2.50	0.47
1:A:22:PRO:HD2	1:A:59:ASP:OD1	2.15	0.47
2:B:9:LEU:HD12	2:B:166:TYR:CD2	2.50	0.47
2:B:44:TYR:O	2:B:47:VAL:HG22	2.15	0.47
2:B:161:LYS:HZ2	2:B:221:ARG:NH1	2.13	0.47
2:B:2:HIS:HB3	2:B:200:TYR:HD2	1.79	0.46
2:B:197:LEU:HD13	2:B:231:GLN:OE1	2.15	0.46
3:C:62:VAL:C	3:C:63:LEU:HD22	2.35	0.46
2:B:355:ASN:O	2:B:356:GLN:C	2.52	0.46
2:B:421:PHE:HB3	2:B:451:ILE:HG23	1.97	0.46
3:C:36:LEU:O	3:C:40:LYS:HG3	2.15	0.46
2:B:21:MET:HE3	2:B:123:MET:HB3	1.96	0.46
2:B:51:VAL:CG1	3:C:63:LEU:HD13	2.46	0.46
1:A:354:GLU:OE2	1:A:358[B]:ARG:NE	2.49	0.46
2:B:15:LEU:HB2	2:B:147:PRO:HB2	1.97	0.45
2:B:164:TYR:HE2	2:B:218[A]:ASN:ND2	2.15	0.45
2:B:202:GLN:OE1	2:B:204:LYS:HB2	2.17	0.45
2:B:390:PHE:N	2:B:391:PRO:HD2	2.32	0.45
1:A:306:ILE:HG22	3:C:38:PHE:CZ	2.49	0.44
2:B:161:LYS:NZ	2:B:221:ARG:HD2	2.32	0.44
1:A:361:LEU:C	1:A:361:LEU:HD13	2.37	0.44
1:A:467:ARG:NH2	5:A:798:HOH:O	2.35	0.44
2:B:344:LEU:HD11	2:B:369:LEU:HD21	1.99	0.44
2:B:60:MET:O	2:B:64:MET:HG3	2.17	0.44
2:B:121:LEU:C	2:B:121:LEU:HD23	2.38	0.44
1:A:52:ILE:O	1:A:56:GLN:HG3	2.18	0.44
1:A:425:ASP:HB3	1:A:429:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:HIS:O	2:B:133:LYS:HD3	2.17	0.43
2:B:451:ILE:CD1	2:B:468:LEU:CD1	2.95	0.43
2:B:203:GLU:CD	2:B:203:GLU:H	2.20	0.43
2:B:286:GLU:O	2:B:290:GLN:HG2	2.17	0.43
2:B:405:GLU:C	2:B:407:ASN:H	2.21	0.43
2:B:217:PHE:HB2	5:B:721:HOH:O	2.19	0.43
1:A:132:SER:O	1:A:133:THR:HB	2.17	0.43
2:B:243:GLN:HE21	2:B:243:GLN:CA	2.31	0.43
2:B:245:THR:OG1	2:B:261:LYS:NZ	2.52	0.42
2:B:459:ALA:HB1	2:B:464:VAL:HG21	1.99	0.42
1:A:133:THR:HG22	1:A:133:THR:O	2.18	0.42
2:B:295:LEU:HB3	2:B:296:PRO:CD	2.48	0.42
2:B:381:MET:HE3	2:B:386:ALA:HB2	2.01	0.42
1:A:5:TYR:CZ	1:A:483:GLU:HA	2.53	0.42
2:B:109:VAL:HG11	2:B:162:GLU:HG2	2.00	0.42
2:B:392:GLU:OE2	2:B:396:LYS:HD2	2.20	0.42
2:B:407:ASN:CB	2:B:409:LEU:HD13	2.50	0.42
1:A:418:PRO:HA	5:A:767:HOH:O	2.19	0.42
2:B:51:VAL:HG13	3:C:63:LEU:HD13	2.01	0.42
2:B:131:THR:HG22	2:B:132:HIS:O	2.20	0.42
2:B:53:LYS:HD3	5:C:756:HOH:O	2.20	0.41
2:B:480:HIS:ND1	2:B:481:HIS:N	2.68	0.41
2:B:193:ALA:HB1	2:B:224:LEU:HD21	2.01	0.41
3:C:94:ILE:HG22	3:C:94:ILE:O	2.19	0.41
2:B:262:GLU:H	2:B:262:GLU:HG2	1.77	0.41
2:B:410:VAL:O	2:B:410:VAL:CG2	2.67	0.41
3:C:3:LYS:NZ	3:C:33[A]:GLU:HB2	2.35	0.41
1:A:60:GLU:CG	1:A:64:LYS:HZ2	2.33	0.41
2:B:368:ASN:HB2	2:B:393:LEU:HD11	2.01	0.41
1:A:322:SER:CB	2:B:89:ALA:HB3	2.51	0.41
2:B:51:VAL:HG13	3:C:63:LEU:CD1	2.51	0.41
1:A:308:SER:OG	1:A:381:VAL:HG11	2.20	0.41
1:A:37:ASP:N	1:A:38:PRO:CD	2.84	0.41
1:A:60:GLU:OE2	1:A:64:LYS:NZ	2.52	0.41
3:C:4:VAL:CG1	3:C:32:LEU:HD23	2.51	0.40
1:A:358[B]:ARG:NH2	1:A:422:TYR:HE1	2.19	0.40
2:B:2:HIS:HB3	2:B:200:TYR:CD2	2.55	0.40
2:B:104:TYR:CD1	2:B:104:TYR:C	2.94	0.40
1:A:206:PHE:C	1:A:206:PHE:CD1	2.93	0.40
2:B:32:GLU:HA	2:B:33:PRO:HD3	1.97	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	486/485 (100%)	472 (97%)	14 (3%)	0	100	100
2	B	483/483 (100%)	464 (96%)	17 (4%)	2 (0%)	34	24
3	C	92/100 (92%)	90 (98%)	2 (2%)	0	100	100
All	All	1061/1068 (99%)	1026 (97%)	33 (3%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	133	LYS
2	B	182	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	409/406 (101%)	402 (98%)	7 (2%)	60	57
2	B	418/419 (100%)	398 (95%)	20 (5%)	25	16
3	C	83/88 (94%)	81 (98%)	2 (2%)	49	43
All	All	910/913 (100%)	881 (97%)	29 (3%)	40	30

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER

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Mol	Chain	Res	Type
1	A	14	LEU
1	A	85	ASN
1	A	206	PHE
1	A	287	LEU
1	A	335	GLU
1	A	419	LEU
2	B	2	HIS
2	B	15	LEU
2	B	44	TYR
2	B	48	LEU
2	B	144	GLN
2	B	148	LEU
2	B	203	GLU
2	B	235	LEU
2	B	243	GLN
2	B	261	LYS
2	B	278	LEU
2	B	313	ASP
2	B	317	LEU
2	B	357	VAL
2	B	358	GLU
2	B	402[A]	GLN
2	B	402[B]	GLN
2	B	410	VAL
2	B	426	LEU
2	B	468	LEU
3	C	26	GLU
3	C	63	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
2	B	144	GLN
2	B	237	ASN
2	B	243	GLN
2	B	428	ASN
2	B	438	ASN
3	C	19	GLN
3	C	42	ASN

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

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	485/485 (100%)	0.05	7 (1%) 75 77	17, 23, 38, 58	3 (0%)
2	B	482/483 (99%)	0.79	77 (15%) 1 2	19, 39, 64, 79	3 (0%)
3	C	92/100 (92%)	0.54	9 (9%) 7 8	23, 38, 62, 71	2 (2%)
All	All	1059/1068 (99%)	0.43	93 (8%) 10 11	17, 29, 61, 79	8 (0%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	441	GLY	11.7
1	A	1	MET	9.2
3	C	94	ILE	7.3
2	B	440	LYS	6.8
2	B	216[A]	SER	5.9
2	B	263	GLY	5.8
2	B	438	ASN	5.8
2	B	439	GLY	5.7
2	B	413	SER	5.5
2	B	218[A]	ASN	5.4
2	B	1	MET	5.2
1	A	358[A]	ARG	5.2
2	B	262	GLU	5.2
2	B	418	LEU	4.9
2	B	457	GLY	4.4
1	A	10[A]	ASN	4.4
2	B	109	VAL	4.2
2	B	463	LEU	4.2
2	B	112	GLU	4.1
2	B	379	GLY	4.1
2	B	28	HIS	4.1
2	B	409	LEU	4.0
2	B	401	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	136	TYR	3.8
3	C	93	THR	3.7
2	B	260	VAL	3.6
2	B	417	THR	3.6
3	C	4	VAL	3.6
2	B	416	ALA	3.6
2	B	458	GLN	3.5
2	B	470	GLN	3.5
2	B	466	GLN	3.5
2	B	403	ILE	3.5
2	B	476	LEU	3.4
2	B	134	GLY	3.4
2	B	412	ILE	3.4
1	A	88[A]	GLU	3.2
2	B	437	LYS	3.2
2	B	219	TYR	3.2
2	B	434	GLU	3.2
2	B	462	GLN	3.2
2	B	135	GLU	3.1
3	C	6	ARG	3.1
2	B	247	ARG	3.1
2	B	469	LYS	3.1
2	B	132	HIS	3.1
3	C	3	LYS	3.0
2	B	3	PHE	3.0
2	B	460	ASN	3.0
2	B	442	LYS	3.0
2	B	473	ASP	2.9
2	B	482	HIS	2.9
2	B	252	THR	2.8
2	B	465	ASN	2.8
2	B	264	SER	2.8
2	B	402[A]	GLN	2.8
2	B	459	ALA	2.7
2	B	447	LEU	2.7
2	B	477	GLU	2.7
2	B	377	GLU	2.6
2	B	113	THR	2.6
2	B	455	SER	2.5
2	B	410	VAL	2.5
2	B	108	GLU	2.5
3	C	35	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	422	TYR	2.5
2	B	110	ASP	2.4
2	B	111	GLY	2.4
2	B	435	ASP	2.4
1	A	415	ILE	2.4
2	B	259	ARG	2.4
2	B	405	GLU	2.4
3	C	32	LEU	2.3
2	B	92	ILE	2.3
2	B	378	ASP	2.3
2	B	386	ALA	2.3
2	B	467	LEU	2.3
3	C	75[A]	GLU	2.3
2	B	468	LEU	2.2
2	B	448	VAL	2.2
2	B	464	VAL	2.2
2	B	256	ILE	2.2
2	B	133	LYS	2.2
1	A	485	LEU	2.2
2	B	479	HIS	2.2
2	B	305	ASN	2.1
2	B	383	SER	2.1
3	C	33[A]	GLU	2.1
2	B	251	SER	2.1
2	B	384	LYS	2.1
2	B	261	LYS	2.1
2	B	414	ASP	2.0
2	B	236	LEU	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, 95th 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	B-factors(Å ²)	Q<0.9
4	MG	B	802	1/1	0.94	0.22	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.