



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:28 PM EDT

PDB ID : 3IP4 / pdb_00003ip4
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 : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

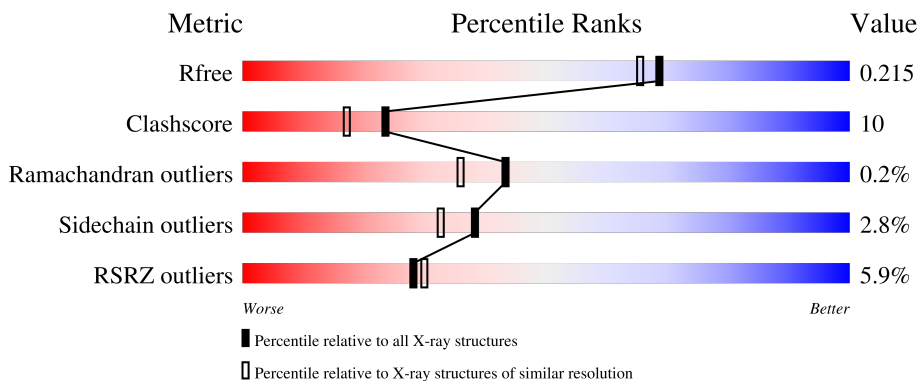
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


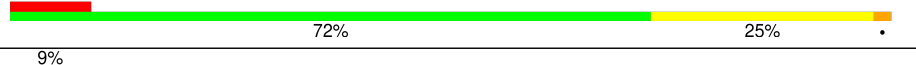
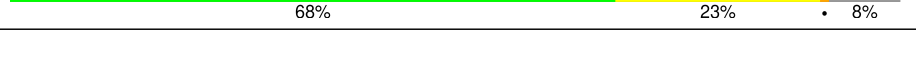
The reported resolution of this entry is 1.90 Å.

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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	 2% 84% 15%
2	B	483	 9% 72% 25%
3	C	100	 9% 68% 23% 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 (CCD ID: MG) (formula: Mg).

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

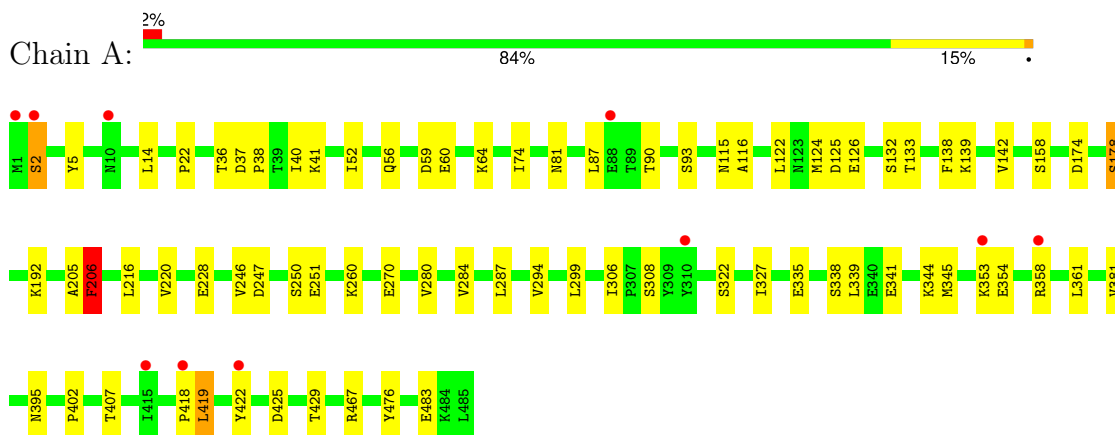
- Molecule 5 is water.

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

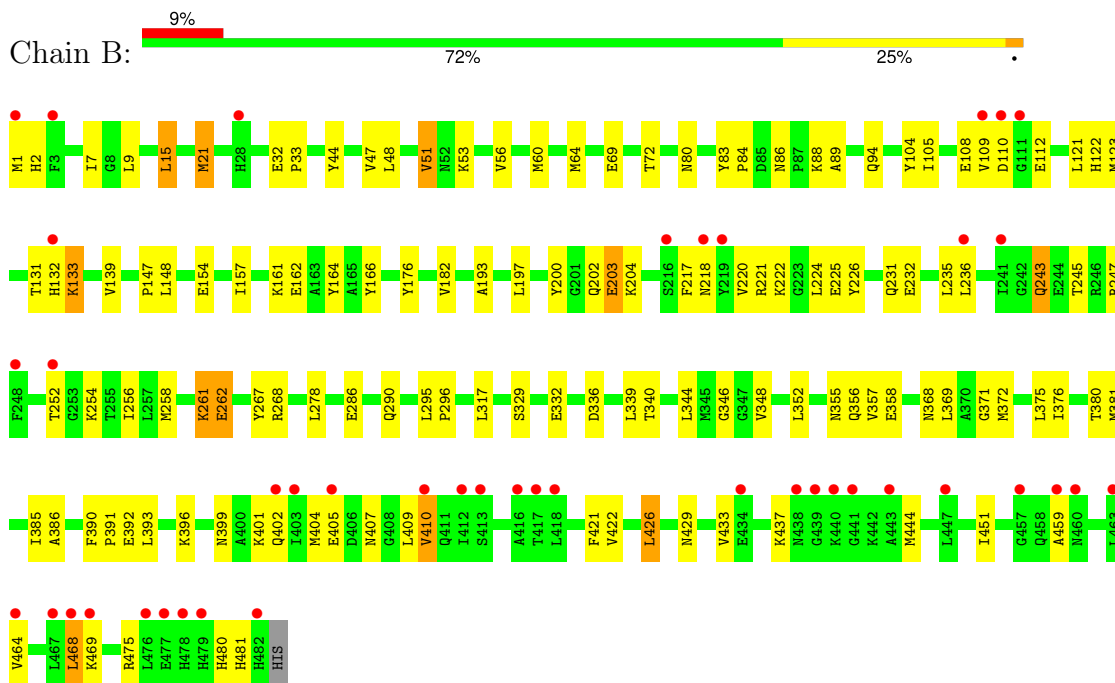
3 Residue-property plots [i](#)

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

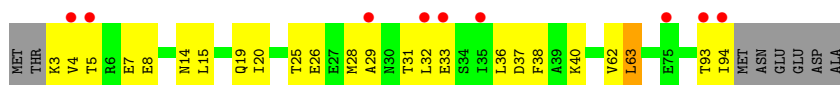


- Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B



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

Chain C:  9% 68% 23% 8%



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 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-1.90) 99.7 (20.00-1.90)	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)	0.35 , 44.7	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	0.96	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	0.42	0/3812	1.00	19/5153 (0.4%)
2	B	0.34	0/3920	0.88	11/5287 (0.2%)
3	C	0.34	0/752	0.81	1/1017 (0.1%)
All	All	0.38	0/8484	0.93	31/11457 (0.3%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	SER	N-CA-C	-19.53	79.37	109.25
2	B	72	THR	N-CA-C	-8.66	102.29	113.12
2	B	475	ARG	N-CA-C	7.86	122.94	112.25
1	A	206	PHE	N-CA-C	-7.41	100.30	111.34
2	B	154	GLU	N-CA-C	-6.76	100.47	110.20
1	A	270	GLU	N-CA-C	6.65	119.38	111.33
1	A	407	THR	N-CA-C	-6.51	102.13	110.53
1	A	205	ALA	N-CA-C	6.38	119.48	110.23
2	B	86	ASN	CA-C-N	6.31	126.51	119.32
2	B	86	ASN	C-N-CA	6.31	126.51	119.32
3	C	93	THR	N-CA-C	6.12	119.35	110.42
1	A	90	THR	N-CA-C	6.09	120.99	113.50
1	A	299	LEU	N-CA-C	-6.01	96.19	108.21
1	A	327	ILE	N-CA-C	5.99	116.63	110.82
2	B	21	MET	N-CA-C	5.96	117.57	111.14
2	B	51	VAL	N-CA-C	5.89	117.32	109.37
2	B	80	ASN	N-CA-C	5.86	118.22	109.25
2	B	346	GLY	N-CA-C	5.83	115.52	110.21
1	A	115	ASN	N-CA-C	5.72	119.56	112.24
1	A	220	VAL	N-CA-C	5.69	115.88	110.42
2	B	69	GLU	N-CA-C	-5.54	100.95	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ILE	N-CA-C	5.43	113.25	107.76
1	A	353	LYS	N-CA-C	5.31	117.07	111.28
2	B	139	VAL	N-CA-C	5.27	115.54	108.17
1	A	344	LYS	N-CA-C	5.25	117.00	111.28
1	A	192	LYS	N-CA-C	-5.18	99.21	109.10
1	A	178	SER	N-CA-C	5.08	118.97	112.87
1	A	116	ALA	N-CA-C	-5.08	103.69	110.55
1	A	125	ASP	N-CA-C	-5.08	103.34	110.50
1	A	138	PHE	N-CA-C	5.04	119.39	112.68
1	A	36	THR	N-CA-C	5.00	119.51	113.41

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	3730	0	3722	42	0
2	B	3834	0	3774	105	0
3	C	735	0	721	33	0
4	B	1	0	0	0	0
5	A	410	0	0	5	0
5	B	300	0	0	4	0
5	C	91	0	0	1	0
All	All	9101	0	8217	168	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 10.

All (168) 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)
2:B:261:LYS:HB2	2:B:261:LYS:NZ	1.95	0.80
3:C:3:LYS:HZ2	3:C:33[B]:GLU:HB2	1.49	0.76
1:A:339:LEU:HD22	3:C:94:ILE:HG12	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:261:LYS:HB2	2:B:261:LYS:HZ2	1.57	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
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:381:MET:HE3	2:B:386:ALA:HB2	1.83	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
2:B:401:LYS:O	2:B:405:GLU:HG2	2.04	0.58
2:B:372:MET:CG	2:B:381:MET:HE1	2.34	0.58
3:C:20:ILE:HD11	3:C:25:THR:HA	1.85	0.58
2:B:381:MET:HE3	2:B:386:ALA:CB	2.34	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:THR:HG22	2:B:404:MET:HE1	1.87	0.56
2:B:372:MET:HG3	2:B:381:MET:HE1	1.87	0.55
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:161:LYS:HZ2	2:B:221:ARG:NH1	2.06	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:468:LEU:HB3	1.89	0.52
3:C:4:VAL:HG21	3:C:32:LEU:HB3	1.90	0.52
2:B:444:MET:HE1	2:B:469:LYS:N	2.23	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
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
3:C:62:VAL:C	3:C:63:LEU:HD22	2.35	0.51
2:B:109:VAL:HG22	5:B:752:HOH:O	2.10	0.51
2:B:355:ASN:O	2:B:356:GLN:C	2.52	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
1:A:60:GLU:CG	1:A:64:LYS:NZ	2.75	0.49
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
1:A:361:LEU:C	1:A:361:LEU:HD13	2.37	0.49
3:C:32:LEU:O	3:C:36:LEU:HG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:203:GLU:CD	2:B:203:GLU:H	2.20	0.48
2:B:405:GLU:C	2:B:407:ASN:H	2.21	0.48
2:B:109:VAL:HG23	2:B:110:ASP:H	1.79	0.48
2:B:121:LEU:C	2:B:121:LEU:HD23	2.38	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:376:ILE:CG1	2:B:381:MET:HE2	2.44	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: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
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: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
3:C:3:LYS:HZ2	3:C:33[A]:GLU:HB2	1.80	0.46
2:B:161:LYS:NZ	2:B:221:ARG:HD2	2.32	0.45
2:B:15:LEU:HB2	2:B:147:PRO:HB2	1.97	0.45
2:B:56:VAL:HG22	2:B:123:MET:HE1	1.98	0.45
2:B:104:TYR:CD1	2:B:104:TYR:C	2.94	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
1:A:206:PHE:C	1:A:206:PHE:CD1	2.93	0.45
1:A:81:ASN:HB3	1:A:124:MET:HE1	1.98	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
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
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
2:B:21:MET:HE1	2:B:123:MET:HB3	2.00	0.44
2:B:132:HIS:O	2:B:133:LYS:HD3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:451:ILE:CD1	2:B:468:LEU:CD1	2.95	0.43
1:A:476:TYR:CD1	1:A:476:TYR:C	2.95	0.43
2:B:376:ILE:HG13	2:B:381:MET:HE2	2.00	0.43
2:B:286:GLU:O	2:B:290:GLN:HG2	2.17	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
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
3:C:7:GLU:CD	3:C:7:GLU:H	2.27	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:O	3:C:94:ILE:HG22	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
2:B:399:ASN:CG	2:B:402[A]:GLN:HB3	2.46	0.41
1:A:308:SER:OG	1:A:381:VAL:HG11	2.20	0.41
2:B:161:LYS:HZ2	2:B:221:ARG:HH11	1.68	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
2:B:267:TYR:O	2:B:268:ARG:C	2.64	0.40
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: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%)	30	22
3	C	92/100 (92%)	90 (98%)	2 (2%)	0	100	100
All	All	1061/1068 (99%)	1026 (97%)	33 (3%)	2 (0%)	43	36

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%)	403 (98%)	6 (2%)	57	56
2	B	418/419 (100%)	403 (96%)	15 (4%)	31	23
3	C	83/88 (94%)	79 (95%)	4 (5%)	23	15
All	All	910/913 (100%)	885 (97%)	25 (3%)	38	34

All (25) 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	206	PHE
1	A	287	LEU
1	A	335	GLU
1	A	419	LEU
2	B	15	LEU
2	B	48	LEU
2	B	148	LEU
2	B	203	GLU
2	B	235	LEU
2	B	243	GLN
2	B	261	LYS
2	B	262	GLU
2	B	278	LEU
2	B	317	LEU
2	B	357	VAL
2	B	358	GLU
2	B	410	VAL
2	B	426	LEU
2	B	468	LEU
3	C	14	ASN
3	C	15	LEU
3	C	26	GLU
3	C	63	LEU

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

Mol	Chain	Res	Type
1	A	50	ASN
1	A	56	GLN
1	A	301	ASN
2	B	144	GLN
2	B	194	ASN
2	B	237	ASN
2	B	243	GLN
2	B	428	ASN
2	B	438	ASN
2	B	462	GLN
3	C	19	GLN
3	C	42	ASN
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 oligosaccharides 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%)	-0.30	10 (2%) 63 67	12, 23, 38, 58	3 (0%)
2	B	482/483 (99%)	0.68	43 (8%) 15 16	19, 39, 64, 79	3 (0%)
3	C	92/100 (92%)	0.71	9 (9%) 13 13	22, 37, 62, 71	2 (2%)
All	All	1059/1068 (99%)	0.23	62 (5%) 28 30	12, 29, 61, 79	8 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	216[A]	SER	8.3
2	B	402[A]	GLN	6.8
2	B	218[A]	ASN	6.7
2	B	441	GLY	5.7
1	A	88[A]	GLU	5.6
1	A	1	MET	5.2
1	A	358[A]	ARG	4.6
1	A	10[A]	ASN	4.6
3	C	75[A]	GLU	4.5
3	C	94	ILE	4.5
3	C	33[A]	GLU	4.2
2	B	439	GLY	4.1
2	B	109	VAL	3.8
2	B	1	MET	3.7
2	B	403	ILE	3.6
2	B	476	LEU	3.6
2	B	28	HIS	3.2
1	A	422	TYR	3.1
2	B	477	GLU	3.1
2	B	3	PHE	3.0
3	C	29	ALA	3.0
2	B	438	ASN	2.9
2	B	412	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	418	LEU	2.8
2	B	457	GLY	2.8
2	B	417	THR	2.8
2	B	241	ILE	2.8
2	B	416	ALA	2.7
2	B	111	GLY	2.7
2	B	219	TYR	2.7
2	B	468	LEU	2.7
2	B	482	HIS	2.7
1	A	310	TYR	2.6
2	B	464	VAL	2.6
1	A	2	SER	2.6
2	B	478	HIS	2.6
1	A	418	PRO	2.5
3	C	93	THR	2.5
2	B	410	VAL	2.5
2	B	479	HIS	2.4
2	B	443	ALA	2.4
2	B	236	LEU	2.3
2	B	463	LEU	2.3
2	B	248	PHE	2.3
3	C	5	THR	2.3
3	C	35	ILE	2.3
3	C	4	VAL	2.3
2	B	405	GLU	2.3
2	B	440	LYS	2.2
2	B	434	GLU	2.2
2	B	447	LEU	2.2
3	C	32	LEU	2.2
2	B	110	ASP	2.2
2	B	460	ASN	2.1
2	B	467	LEU	2.1
2	B	132	HIS	2.1
1	A	415	ILE	2.1
2	B	459	ALA	2.1
1	A	353	LYS	2.1
2	B	413	SER	2.0
2	B	469	LYS	2.0
2	B	252	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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	0.10	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.