WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 01:16 AM GMT

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)

This is a full wwPDB validation report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

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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
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance ⓘ

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.

Metric	Percentile Ranks	Value
Rfree		0.239
Clashscore		28
Ramachandran outliers		1.2%
Sidechain outliers		8.7%
RSRZ outliers		7.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
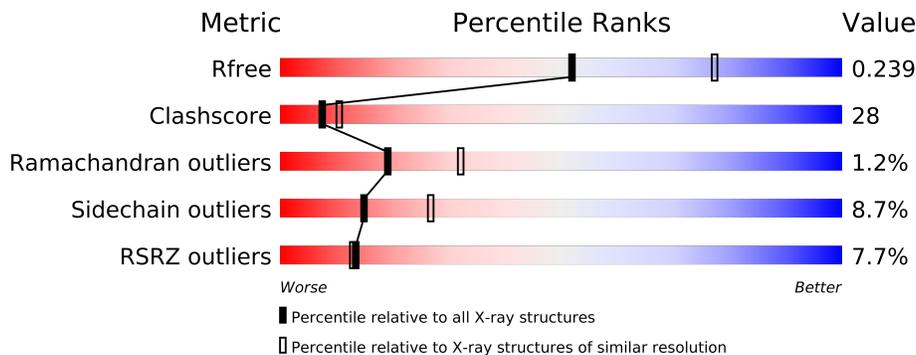
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	485	
2	B	483	
3	C	100	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MG	B	501	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 7806 atoms, of which 0 are hydrogen and 0 are deuterium.

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	A	485	Total	C	N	O	S	0	0	0
			3716	2359	605	739	13			

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

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

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
3	C	99	Total	C	N	O	S	0	0	0
			781	480	130	169	2			

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total 81	O 81	0	0
5	B	47	Total 47	O 47	0	0
5	C	11	Total 11	O 11	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

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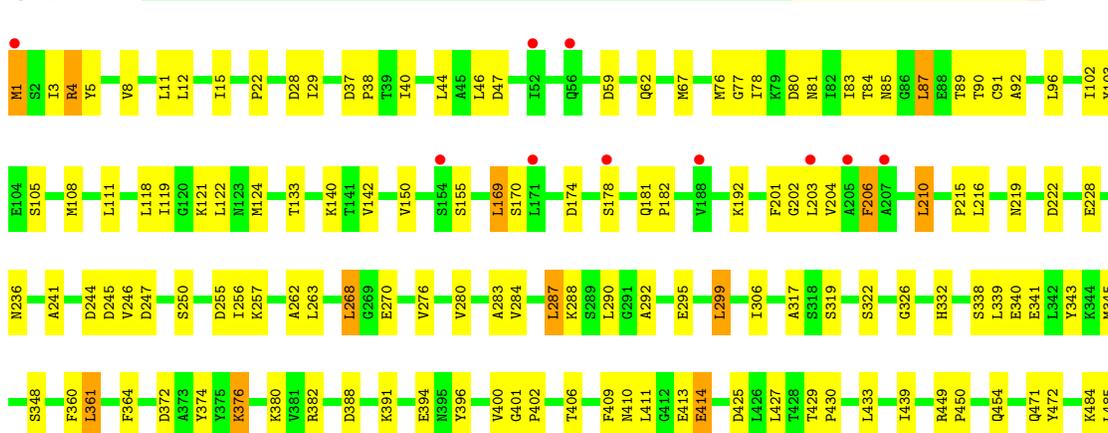
- Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln)amidotransferase subunit B

Chain B:
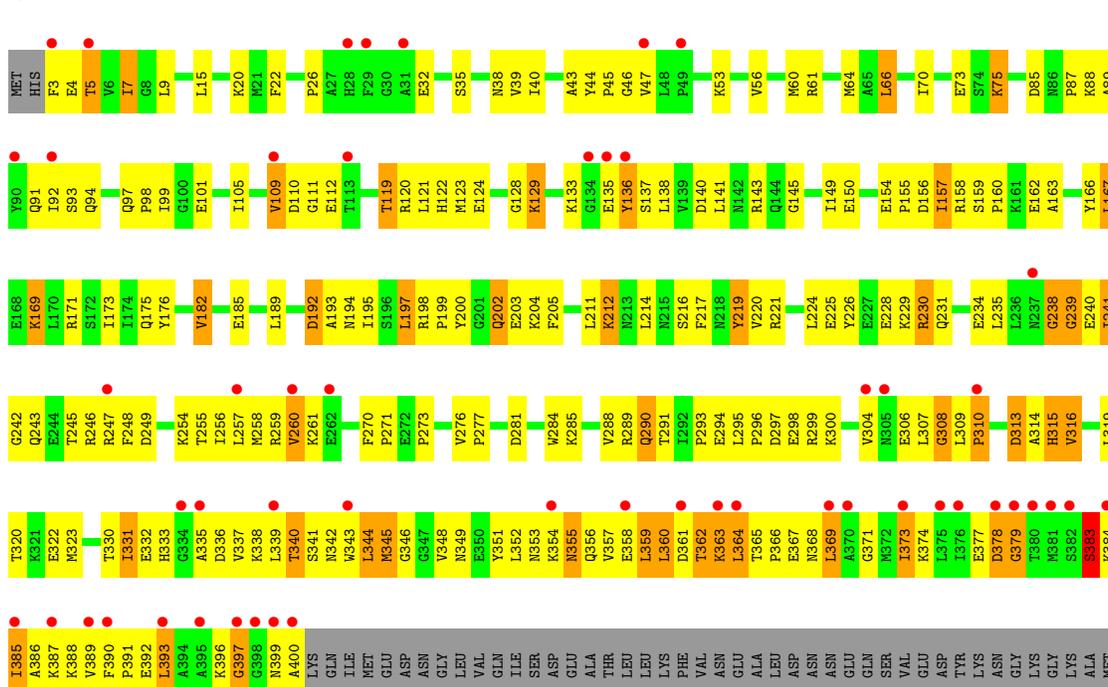
GLY PHE LEU VAL GLY GLN ILE MET LYS ALA SER LYS GLY GLN ALA ASN PRO GLN LEU VAL ASN GLN LEU LEU LYS GLN GLU LEU ASP LYS ARG LEU GLU HIS HIS HIS HIS HIS HIS

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

Chain C:
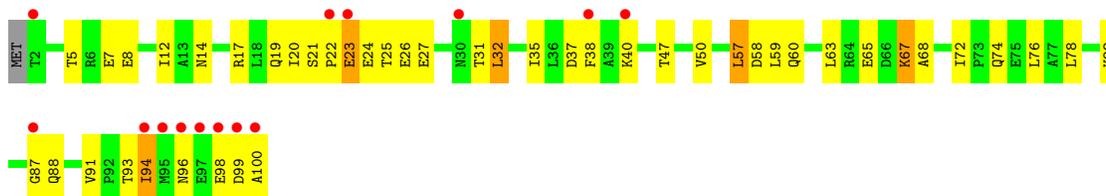
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.92Å 92.04Å 181.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 41.16 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.50) 99.4 (41.16-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$<I/\sigma(I)>$ [1]	6.07 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.275 0.243 , 0.239	Depositor DCC
R_{free} test set	4151 reflections (9.98%)	DCC
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 , 40.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$<\lvert L \rvert> = 0.51, <L^2> = 0.35$	Xtriage
Outliers	1 of 41671 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	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.*

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[1]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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z| > 5$	RMSZ	#$|Z| > 5$
1	A	0.41	0/3784	0.65	0/5116
2	B	0.42	0/3231	0.74	4/4364 (0.1%)
3	C	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	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	383	SER	N-CA-C	7.77	131.99	111.00
2	B	397	GLY	N-CA-C	5.93	127.92	113.10
2	B	5	THR	N-CA-C	-5.36	96.53	111.00
2	B	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	A	472	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3716	0	3709	118	0
2	B	3169	0	3119	278	0
3	C	781	0	760	59	0
4	B	1	0	0	0	0
5	A	81	0	0	3	0
5	B	47	0	0	4	0
5	C	11	0	0	1	0
All	All	7806	0	7588	423	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

All (423) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
2:B:199:PRO:HG2	2:B:202:GLN:NE2	1.85	0.90
1:A:338:SER:HA	3:C:94:ILE:HD11	1.52	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:HG3	2:B:198:ARG:O	1.81	0.80
2:B:364:LEU:CD1	2:B:369:LEU:HB2	2.13	0.79
2:B:295:LEU:HD22	2:B:295:LEU:N	1.98	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

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Atom-1	Atom-2	Distance(Å)	Clash(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
2:B:217:PHE:O	2:B:220:VAL:HG22	1.85	0.77
1:A:247:ASP:OD2	1:A:250:SER:HB3	1.84	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
3:C:98:GLU:CG	3:C:99:ASP:N	2.51	0.73
2:B:348:VAL:HG12	2:B:390:PHE:CZ	2.24	0.73
2:B:5:THR:HG21	2:B:228:GLU:HG3	1.70	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
2:B:386:ALA:HA	2:B:389:VAL:CG2	2.22	0.69
2:B:60:MET:HE3	2:B:70:ILE:HG21	1.74	0.69
1:A:284:VAL:HG12	1:A:288:LYS:HE3	1.74	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:352:LEU:HA	2:B:357:VAL:HG23	1.77	0.67
2:B:256:ILE:N	2:B:256:ILE:HD12	2.09	0.67
1:A:255:ASP:OD1	1:A:257:LYS:HG2	1.94	0.67
2:B:202:GLN:HG2	2:B:203:GLU:N	2.08	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:B:295:LEU:H	2:B:295:LEU:HD22	1.62	0.63
1:A:22:PRO:HD2	1:A:59:ASP:OD1	1.98	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:360:LEU:HG	2:B:360:LEU:O	1.99	0.62
2:B:331:ILE:CG2	2:B:332:GLU:N	2.62	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:249:ASP:HB2	2:B:256:ILE:HD11	1.82	0.62
2:B:133:LYS:HB2	2:B:138:LEU:HD23	1.81	0.62
1:A:83:ILE:HD12	1:A:103:TYR:OH	2.00	0.62
2:B:295:LEU:O	2:B:299:ARG:HB2	2.01	0.61
2:B:256:ILE:HA	5:B:519:HOH:O	2.01	0.61
2:B:344:LEU:HA	2:B:348:VAL:CG2	2.31	0.61
2:B:154:GLU:HG3	2:B:155:PRO:HD2	1.82	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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
2:B:105:ILE:HD11	2:B:166:TYR:CD1	2.37	0.59
2:B:15:LEU:HD11	2:B:149:ILE:HG23	1.84	0.59
2:B:26:PRO:HG3	3:C:68:ALA:HB1	1.84	0.59
1:A:299:LEU:HD12	1:A:388:ASP:HB3	1.85	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
3:C:94:ILE:O	3:C:94:ILE:HG12	2.03	0.58
1:A:361:LEU:HG	3:C:35:ILE:HG21	1.84	0.58
1:A:241:ALA:HB2	3:C:57:LEU:HD11	1.85	0.58
3:C:21:SER:C	3:C:23:GLU:H	2.07	0.57
2:B:98:PRO:HG2	2:B:101:GLU:HG3	1.84	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:362:THR:C	2:B:363:LYS:HD2	2.26	0.56
2:B:60:MET:O	2:B:64:MET:HG3	2.04	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
3:C:98:GLU:CG	3:C:99:ASP:H	2.19	0.55
1:A:276:VAL:HG21	1:A:406:THR:HA	1.88	0.55
3:C:99:ASP:CG	3:C:100:ALA:H	2.09	0.55
2:B:369:LEU:O	2:B:369:LEU:HD22	2.05	0.55
2:B:3:PHE:CG	2:B:3:PHE:O	2.59	0.55
1:A:256:ILE:HD12	1:A:292:ALA:HB2	1.88	0.55
2:B:241:ILE:C	2:B:241:ILE:HD13	2.26	0.55
2:B:295:LEU:CD2	2:B:295:LEU:N	2.70	0.55
1:A:360:PHE:HB3	3:C:32:LEU:HD21	1.87	0.55
2:B:295:LEU:HB3	2:B:296:PRO:CD	2.37	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:61:ARG:HD2	2:B:291:THR:HG23	1.89	0.55
2:B:260:VAL:O	2:B:260:VAL:HG12	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
2:B:193:ALA:CB	2:B:224:LEU:HD11	2.38	0.54
1:A:228:GLU:OE2	1:A:247:ASP:HA	2.08	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
3:C:57:LEU:HD22	3:C:59:LEU:CD1	2.38	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
2:B:355:ASN:HD22	2:B:357:VAL:HG13	1.73	0.53
2:B:288:VAL:CA	2:B:291:THR:HG22	2.39	0.53
2:B:138:LEU:N	2:B:138:LEU:HD22	2.24	0.53
2:B:316:VAL:HG13	2:B:345:MET:CE	2.38	0.52
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:295:LEU:HB3	2:B:296:PRO:HD2	1.90	0.52
2:B:288:VAL:C	2:B:291:THR:HG22	2.30	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: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:91:GLN:NE2	2:B:124:GLU:HB3	2.25	0.52
2:B:355:ASN:ND2	2:B:357:VAL:HG13	2.25	0.52
1:A:340:GLU:OE1	3:C:99:ASP:O	2.28	0.51
1:A:40:ILE:HA	1:A:142:VAL:HG22	1.92	0.51
1:A:364:PHE:HB2	3:C:12:ILE:HD13	1.90	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:306:GLU:O	2:B:307:LEU:HB3	2.09	0.51
2:B:343:TRP:CD1	2:B:373:ILE:HD13	2.45	0.51
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:378:ASP:O	2:B:379:GLY:C	2.50	0.51
1:A:219:ASN:ND2	1:A:222:ASP:OD2	2.42	0.51
2:B:330:THR:HG21	2:B:369:LEU:HD13	1.93	0.50
1:A:361:LEU:HG	3:C:35:ILE:CG2	2.40	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:335:ALA:HB1	2:B:340:THR:HG23	1.92	0.50
2:B:259:ARG:HG3	2:B:260:VAL:N	2.26	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
2:B:7:ILE:HD11	2:B:157:ILE:CD1	2.25	0.50
1:A:206:PHE:C	1:A:206:PHE:CD1	2.85	0.50
2:B:169:LYS:HD3	2:B:169:LYS:O	2.12	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:8:VAL:O	1:A:12:LEU:HB2	2.11	0.50
2:B:331:ILE:HG22	2:B:332:GLU:N	2.27	0.50
1:A:409:PHE:CD1	1:A:414:GLU:HG3	2.46	0.50
1:A:80:ASP:OD1	1:A:89:THR:HA	2.11	0.50
2:B:271:PRO:O	2:B:273:PRO:HD3	2.11	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
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
1:A:133:THR:HG22	1:A:133:THR:O	2.13	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
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
1:A:15:ILE:HG22	1:A:67:MET:HE2	1.94	0.49
3:C:78:LEU:HD11	3:C:87:GLY:HA2	1.95	0.49
2:B:383:SER:O	2:B:386:ALA:HB3	2.13	0.49
2:B:339:LEU:HB3	2:B:373:ILE:CG2	2.43	0.48
1:A:215:PRO:C	1:A:216:LEU:HD12	2.33	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:313:ASP:HA	2:B:345:MET:CE	2.44	0.48
2:B:245:THR:OG1	2:B:261:LYS:HE2	2.13	0.48
2:B:229:LYS:HD2	2:B:229:LYS:N	2.28	0.48
1:A:283:ALA:O	1:A:287:LEU:HD22	2.13	0.48
2:B:7:ILE:HG22	2:B:195:ILE:CG1	2.43	0.48
1:A:484:LYS:O	1:A:485:LEU:CB	2.61	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:429:THR:OG1	1:A:430:PRO:HD3	2.13	0.48
1:A:402:PRO:HG2	1:A:427:LEU:CD1	2.44	0.48
2:B:157:ILE:CD1	2:B:159:SER:H	2.26	0.47
1:A:364:PHE:CD1	1:A:364:PHE:C	2.87	0.47
2:B:378:ASP:O	2:B:379:GLY:O	2.30	0.47
2:B:388:LYS:C	2:B:391:PRO:HD2	2.35	0.47
2:B:300:LYS:NZ	2:B:315:HIS:HB2	2.29	0.47
2:B:362:THR:O	2:B:362:THR:HG23	2.14	0.47
2:B:295:LEU:H	2:B:295:LEU:CD2	2.25	0.47
2:B:167:LEU:CD2	2:B:220:VAL:HG21	2.43	0.47
2:B:240:GLU:OE1	2:B:240:GLU:HA	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:355:ASN:HB2	5:B:547:HOH:O	2.13	0.47
2:B:310:PRO:HB2	2:B:313:ASP:OD1	2.13	0.47
2:B:137:SER:HB2	3:C:91:VAL:HG23	1.96	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
2:B:338:LYS:NZ	2:B:342:ASN:HD21	2.12	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
1:A:374:TYR:OH	3:C:40:LYS:HE3	2.15	0.47
1:A:201:PHE:CD1	1:A:236:ASN:HB3	2.50	0.47
2:B:368:ASN:N	2:B:368:ASN:HD22	2.11	0.47
2:B:216:SER:OG	2:B:219:TYR:HB2	2.14	0.47
2:B:363:LYS:NZ	2:B:363:LYS:HB3	2.30	0.47
2:B:98:PRO:HB3	2:B:120:ARG:NH2	2.29	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:169:LYS:C	2:B:169:LYS:HD3	2.36	0.46
2:B:160:PRO:HG3	2:B:225:GLU:HB3	1.96	0.46
1:A:103:TYR:HB3	2:B:39:VAL:HG11	1.96	0.46
1:A:247:ASP:OD2	1:A:250:SER:CB	2.61	0.46
1:A:78:ILE:HG12	1:A:108:MET:SD	2.56	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:202:GLN:HG2	2:B:204:LYS:N	2.31	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:176:TYR:HE2	2:B:299:ARG:CD	2.29	0.46
2:B:309:LEU:CD1	2:B:338:LYS:CD	2.92	0.46
2:B:290:GLN:CD	2:B:290:GLN:C	2.74	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
2:B:212:LYS:HA	2:B:212:LYS:HD2	1.51	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
1:A:103:TYR:CD1	2:B:39:VAL:HG11	2.51	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:439:ILE:O	1:A:454:GLN:HA	2.16	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:362:THR:HB	5:B:521:HOH:O	2.15	0.45
2:B:257:LEU:C	2:B:257:LEU:HD13	2.37	0.45
2:B:20:LYS:HB3	2:B:145:GLY:O	2.17	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
2:B:157:ILE:CD1	2:B:162:GLU:HB2	2.46	0.45
1:A:410:ASN:HB2	1:A:413:GLU:HB2	1.99	0.45
1:A:284:VAL:CG1	1:A:288:LYS:HE3	2.46	0.45
2:B:368:ASN:N	2:B:368:ASN:ND2	2.65	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:181:GLN:HB3	1:A:182:PRO:HD3	1.99	0.45
2:B:383:SER:O	2:B:386:ALA:N	2.47	0.45
2:B:298:GLU:H	2:B:298:GLU:CD	2.20	0.45
1:A:348:SER:OG	3:C:19:GLN:N	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:7:ILE:CG2	2:B:195:ILE:HG13	2.46	0.44
2:B:135:GLU:OE2	3:C:94:ILE:HG22	2.17	0.44
2:B:61:ARG:HD3	2:B:291:THR:HG23	1.99	0.44
1:A:338:SER:HB2	3:C:100:ALA:OXT	2.18	0.44
1:A:84:THR:CG2	1:A:121:LYS:HE3	2.47	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:CD1	2:B:197:LEU:N	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
2:B:389:VAL:HG23	2:B:390:PHE:N	2.32	0.44
2:B:276:VAL:HG22	2:B:277:PRO:HD2	1.99	0.44
2:B:56:VAL:HG22	2:B:123:MET:CE	2.48	0.44
1:A:210:LEU:HD13	1:A:382:ARG:NH2	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
2:B:247:ARG:CA	2:B:258:MET:HE2	2.48	0.43
2:B:167:LEU:HD23	2:B:220:VAL:HG21	2.00	0.43
2:B:64:MET:HE1	2:B:288:VAL:C	2.38	0.43
1:A:290:LEU:HD13	1:A:471:GLN:HB3	2.00	0.43
1:A:78:ILE:HD12	1:A:78:ILE:N	2.33	0.43
2:B:119:THR:HG22	2:B:154:GLU:HA	1.99	0.43
2:B:38:ASN:OD1	2:B:40:ILE:HB	2.18	0.43
2:B:348:VAL:CG2	2:B:349:ASN:N	2.81	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: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: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
1:A:87:LEU:HD12	1:A:118:LEU:CD2	2.43	0.43
2:B:93:SER:OG	2:B:94:GLN:N	2.51	0.43
1:A:11:LEU:O	1:A:15:ILE:HG13	2.18	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
2:B:270:PHE:HA	2:B:271:PRO:HD3	1.85	0.43
2:B:129:LYS:HE2	2:B:143:ARG:NH2	2.34	0.43
1:A:244:ASP:O	1:A:246:VAL:N	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:20:ILE:HG13	3:C:24:GLU:HB3	1.99	0.43
1:A:256:ILE:CD1	1:A:292:ALA:HB2	2.49	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
2:B:230:ARG:CZ	2:B:246:ARG:HE	2.32	0.42
1:A:425:ASP:HB3	1:A:429:THR:HG23	2.01	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
1:A:90:THR:C	1:A:92:ALA:N	2.71	0.42
2:B:60:MET:HB3	2:B:99:ILE:CD1	2.50	0.42
2:B:137:SER:OG	3:C:93:THR:HB	2.18	0.42
2:B:121:LEU:HA	2:B:150:GLU:O	2.18	0.42
2:B:22:PHE:CE2	2:B:92:ILE:HB	2.55	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
2:B:198:ARG:CG	2:B:198:ARG:O	2.61	0.42
1:A:343:TYR:HB3	3:C:17:ARG:HB3	2.02	0.42
2:B:135:GLU:HA	2:B:135:GLU:OE1	2.19	0.42
1:A:449:ARG:HA	1:A:450:PRO:HD2	1.93	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
2:B:198:ARG:HH11	2:B:198:ARG:HG3	1.84	0.41
2:B:309:LEU:HD11	2:B:338:LYS:CD	2.45	0.41
1:A:47:ASP:HB2	1:A:87:LEU:HD11	2.01	0.41
2:B:214:LEU:HB3	2:B:220:VAL:HG12	2.02	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:309:LEU:HD21	2:B:341:SER:CB	2.51	0.41
1:A:1:MET:O	1:A:4:ARG:HG2	2.21	0.41
2:B:307:LEU:O	2:B:307:LEU:HD23	2.20	0.41
2:B:284:TRP:O	2:B:288:VAL:HG22	2.21	0.41
1:A:108:MET:CE	1:A:111:LEU:HD12	2.50	0.41
2:B:365:THR:HB	2:B:366:PRO:CD	2.50	0.41
1:A:345:MET:HG2	3:C:19:GLN:OE1	2.20	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
2:B:156:ASP:O	2:B:158:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:7:ILE:HG22	2:B:195:ILE:HA	2.03	0.41
1:A:216:LEU:HD12	1:A:216:LEU:N	2.35	0.41
1:A:268:LEU:HA	1:A:268:LEU:HD12	1.93	0.41
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.94	0.41
2:B:64:MET:C	2:B:66:LEU:H	2.24	0.41
1:A:256:ILE:HG23	1:A:471:GLN:CG	2.44	0.41
1:A:37:ASP:N	1:A:38:PRO:CD	2.83	0.41
2:B:105:ILE:HD11	2:B:166:TYR:CE1	2.56	0.41
2:B:43:ALA:HB3	2:B:87:PRO:HB2	2.03	0.41
2:B:316:VAL:HA	2:B:319:LEU:HD13	2.02	0.40
2:B:64:MET:SD	2:B:289:ARG:HD2	2.61	0.40
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
1:A:90:THR:O	1:A:91:CYS:HB2	2.20	0.40
2:B:226:TYR:CD1	2:B:226:TYR:C	2.94	0.40
1:A:317:ALA:C	1:A:319:SER:H	2.24	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
2:B:202:GLN:OE1	2:B:204:LYS:O	2.40	0.40
2:B:5:THR:HG22	2:B:197:LEU:CD1	2.52	0.40
2:B:119:THR:CG2	2:B:154:GLU:HA	2.51	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:358:GLU:HG2	2:B:358:GLU:H	1.68	0.40
2:B:85:ASP:HB2	2:B:128:GLY:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	483/485 (100%)	459 (95%)	23 (5%)	1 (0%)	56	79
2	B	396/483 (82%)	348 (88%)	38 (10%)	10 (2%)	9	12
3	C	97/100 (97%)	85 (88%)	11 (11%)	1 (1%)	22	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	976/1068 (91%)	892 (91%)	72 (7%)	12 (1%)	19 32

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	239	GLY
2	B	308	GLY
2	B	310	PRO
2	B	383	SER
1	A	245	ASP
2	B	337	VAL
2	B	360	LEU
2	B	379	GLY
2	B	293	PRO
2	B	397	GLY
3	C	22	PRO
2	B	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
1	A	406/406 (100%)	387 (95%)	19 (5%)	36 61
2	B	345/419 (82%)	300 (87%)	45 (13%)	6 11
3	C	87/88 (99%)	78 (90%)	9 (10%)	10 19
All	All	838/913 (92%)	765 (91%)	73 (9%)	15 27

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	ARG
1	A	46	LEU
1	A	85	ASN
1	A	87	LEU
1	A	96	LEU

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Mol	Chain	Res	Type
1	A	122	LEU
1	A	169	LEU
1	A	206	PHE
1	A	210	LEU
1	A	263	LEU
1	A	268	LEU
1	A	287	LEU
1	A	299	LEU
1	A	339	LEU
1	A	361	LEU
1	A	376	LYS
1	A	414	GLU
1	A	433	LEU
2	B	4	GLU
2	B	7	ILE
2	B	66	LEU
2	B	73	GLU
2	B	75	LYS
2	B	109	VAL
2	B	119	THR
2	B	129	LYS
2	B	136	TYR
2	B	141	LEU
2	B	157	ILE
2	B	167	LEU
2	B	169	LYS
2	B	182	VAL
2	B	192	ASP
2	B	197	LEU
2	B	202	GLN
2	B	212	LYS
2	B	219	TYR
2	B	230	ARG
2	B	241	ILE
2	B	254	LYS
2	B	260	VAL
2	B	290	GLN
2	B	313	ASP
2	B	315	HIS
2	B	316	VAL
2	B	322	GLU
2	B	331	ILE

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Mol	Chain	Res	Type
2	B	333	HIS
2	B	340	THR
2	B	344	LEU
2	B	345	MET
2	B	353	ASN
2	B	354	LYS
2	B	355	ASN
2	B	359	LEU
2	B	362	THR
2	B	363	LYS
2	B	364	LEU
2	B	369	LEU
2	B	373	ILE
2	B	378	ASP
2	B	385	ILE
2	B	393	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
3	C	58	ASP
3	C	67	LYS
3	C	94	ILE

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

Mol	Chain	Res	Type
1	A	62	GLN
1	A	85	ASN
1	A	281	GLN
1	A	479	HIS
2	B	202	GLN
2	B	290	GLN
2	B	342	ASN
2	B	356	GLN
2	B	368	ASN
3	C	14	ASN
3	C	60	GLN
3	C	74	GLN
3	C	88	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	485/485 (100%)	0.20	10 (2%)	60	63	32, 47, 67, 88	0
2	B	398/483 (82%)	0.67	52 (13%)	4	3	38, 69, 95, 95	0
3	C	99/100 (99%)	0.74	14 (14%)	3	3	45, 69, 95, 95	0
All	All	982/1068 (91%)	0.45	76 (7%)	13	13	32, 55, 95, 95	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	8.4
2	B	381	MET	8.4
2	B	382	SER	8.2
2	B	398	GLY	6.1
3	C	2	THR	5.8
2	B	393	LEU	5.7
2	B	397	GLY	5.7
2	B	237	ASN	5.2
2	B	395	ALA	5.0
3	C	96	ASN	4.8
3	C	94	ILE	4.7
2	B	387	LYS	4.3
3	C	98	GLU	4.0
3	C	97	GLU	3.9
2	B	400	ALA	3.9
2	B	379	GLY	3.9
2	B	369	LEU	3.9
2	B	335	ALA	3.8
2	B	376	ILE	3.7
3	C	22	PRO	3.5
2	B	304	VAL	3.4
2	B	378	ASP	3.4
3	C	99	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	31	ALA	3.3
1	A	203	LEU	3.2
2	B	29	PHE	3.2
2	B	262	GLU	3.1
3	C	100	ALA	3.1
2	B	385	ILE	3.1
2	B	334	GLY	3.0
2	B	109	VAL	2.9
2	B	354	LYS	2.9
3	C	38	PHE	2.9
2	B	135	GLU	2.9
3	C	23	GLU	2.8
3	C	95	MET	2.8
2	B	399	ASN	2.8
3	C	87	GLY	2.7
2	B	389	VAL	2.7
2	B	305	ASN	2.7
1	A	52	ILE	2.7
2	B	28	HIS	2.6
2	B	5	THR	2.6
2	B	310	PRO	2.6
1	A	205	ALA	2.6
2	B	390	PHE	2.5
2	B	113	THR	2.5
2	B	358	GLU	2.5
3	C	30	ASN	2.5
1	A	154	SER	2.4
2	B	363	LYS	2.4
2	B	343	TRP	2.3
1	A	171	LEU	2.3
1	A	207	ALA	2.3
1	A	56	GLN	2.3
2	B	364	LEU	2.2
2	B	260	VAL	2.2
2	B	373	ILE	2.2
2	B	339	LEU	2.2
2	B	247	ARG	2.2
2	B	361	ASP	2.2
2	B	134	GLY	2.2
2	B	3	PHE	2.1
2	B	375	LEU	2.1
2	B	384	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	40	LYS	2.1
1	A	178	SER	2.1
2	B	49	PRO	2.1
2	B	136	TYR	2.0
1	A	188	VAL	2.0
2	B	47	VAL	2.0
2	B	370	ALA	2.0
2	B	380	THR	2.0
2	B	90	TYR	2.0
2	B	257	LEU	2.0
2	B	92	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	MG	B	501	1/1	0.23	2.29	43,43,43,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.