



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:12 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 X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

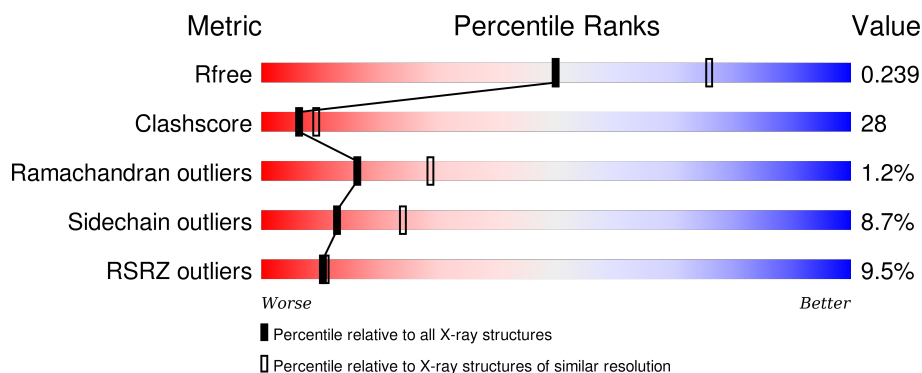
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div>72%</div> <div>26%</div> <div>.</div> </div>
2	B	483	<div> <div>12%</div> <div>36%</div> <div>37%</div> <div>9%</div> <div>18%</div> </div>
3	C	100	<div> <div>17%</div> <div>54%</div> <div>40%</div> <div>5%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	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 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	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

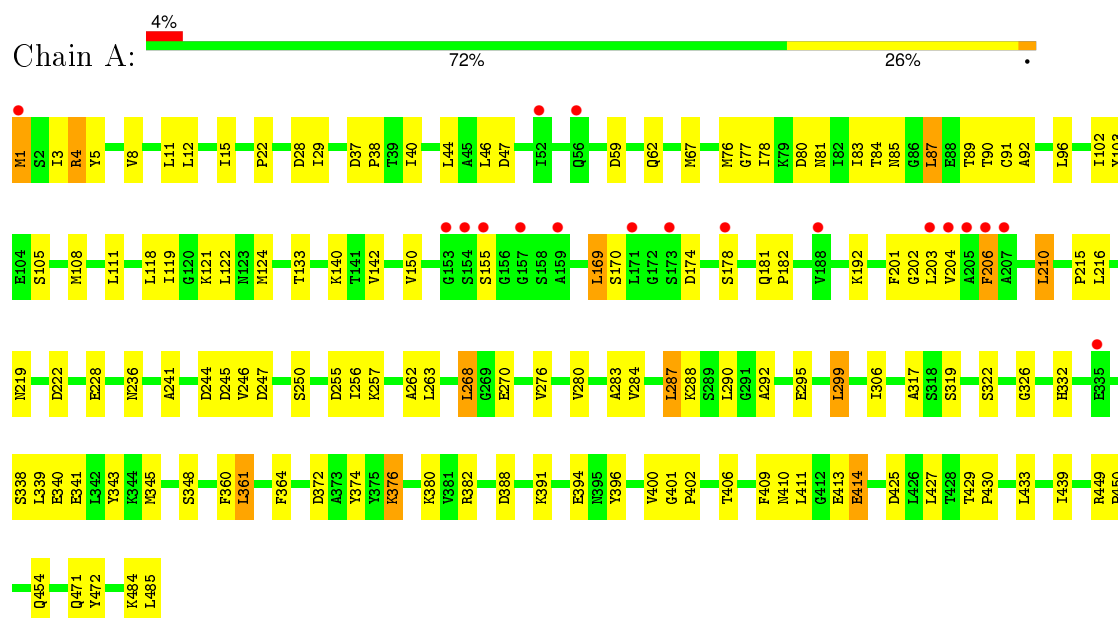
- Molecule 5 is water.

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

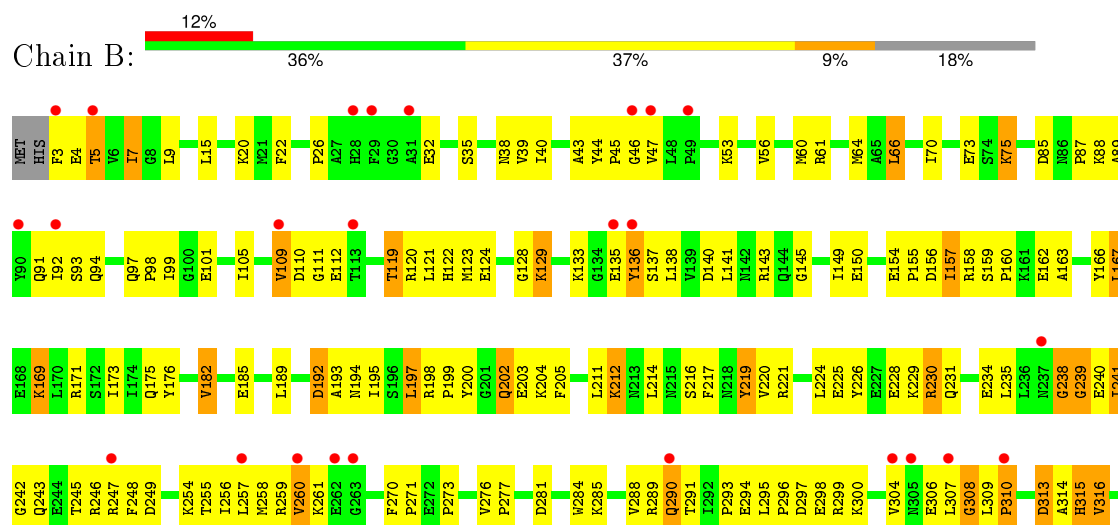
### 3 Residue-property plots

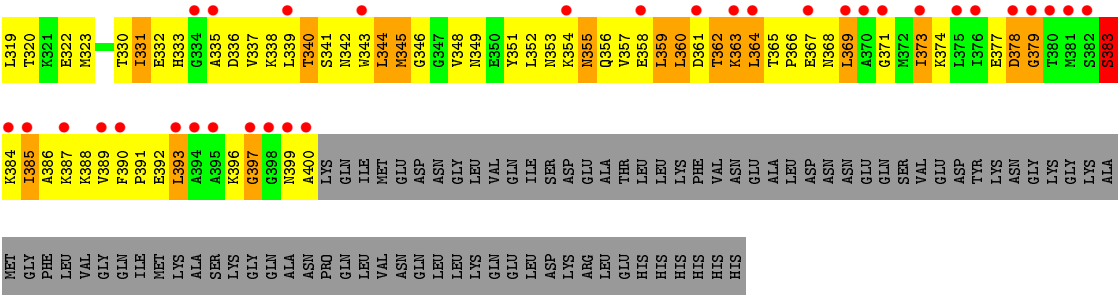
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

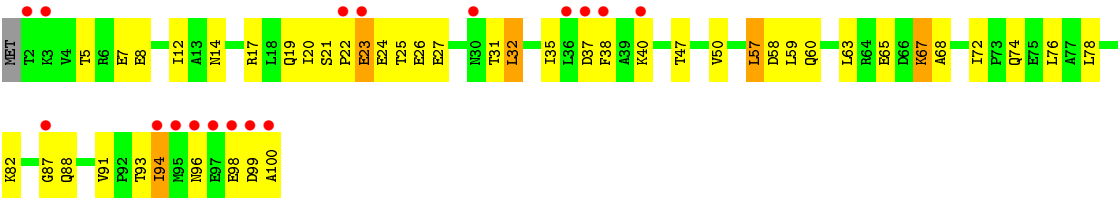


- Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B





● 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	53.1	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 41671 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7806	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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(°)	Ideal(°)
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 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	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

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 distance (Å)	Clash 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
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	Interatomic distance (Å)	Clash 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [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	483/485 (100%)	459 (95%)	23 (5%)	1 (0%)	52	75
2	B	396/483 (82%)	348 (88%)	38 (10%)	10 (2%)	7	10
3	C	97/100 (97%)	85 (88%)	11 (11%)	1 (1%)	19	34
All	All	976/1068 (91%)	892 (91%)	72 (7%)	12 (1%)	16	29

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/406 (100%)	387 (95%)	19 (5%)	32	56
2	B	345/419 (82%)	300 (87%)	45 (13%)	5	9
3	C	87/88 (99%)	78 (90%)	9 (10%)	9	17
All	All	838/913 (92%)	765 (91%)	73 (9%)	13	24

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
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

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Mol	Chain	Res	Type
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
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 molecules 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.

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	485/485 (100%)	0.25	18 (3%) 45 50	32, 47, 67, 88	0
2	B	398/483 (82%)	0.76	58 (14%) 3 3	38, 69, 95, 95	0
3	C	99/100 (99%)	0.83	17 (17%) 2 2	45, 69, 95, 95	0
All	All	982/1068 (91%)	0.52	93 (9%) 10 11	32, 55, 95, 95	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	381	MET	9.7
1	A	1	MET	9.2
2	B	382	SER	8.3
2	B	398	GLY	7.8
2	B	397	GLY	6.3
3	C	2	THR	6.2
2	B	393	LEU	5.8
3	C	96	ASN	5.7
2	B	237	ASN	5.4
2	B	395	ALA	4.8
3	C	94	ILE	4.7
3	C	98	GLU	4.5
2	B	387	LYS	4.5
2	B	379	GLY	4.4
2	B	335	ALA	4.3
3	C	97	GLU	4.2
2	B	400	ALA	4.2
1	A	203	LEU	4.0
2	B	31	ALA	4.0
2	B	376	ILE	3.9
3	C	95	MET	3.9
3	C	99	ASP	3.9
2	B	109	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	378	ASP	3.8
2	B	262	GLU	3.7
2	B	135	GLU	3.7
2	B	369	LEU	3.7
2	B	304	VAL	3.6
3	C	23	GLU	3.6
2	B	305	ASN	3.5
2	B	334	GLY	3.5
3	C	22	PRO	3.3
3	C	100	ALA	3.2
1	A	205	ALA	3.1
2	B	389	VAL	3.1
2	B	29	PHE	3.1
2	B	260	VAL	3.1
2	B	354	LYS	3.1
2	B	113	THR	2.9
2	B	399	ASN	2.9
2	B	343	TRP	2.9
3	C	38	PHE	2.7
2	B	385	ILE	2.7
2	B	358	GLU	2.7
2	B	28	HIS	2.7
2	B	310	PRO	2.7
2	B	384	LYS	2.7
1	A	52	ILE	2.6
2	B	375	LEU	2.6
1	A	154	SER	2.6
1	A	335	GLU	2.6
2	B	47	VAL	2.5
3	C	3	LYS	2.5
2	B	307	LEU	2.5
2	B	136	TYR	2.5
3	C	87	GLY	2.5
1	A	56	GLN	2.4
2	B	390	PHE	2.4
2	B	5	THR	2.4
2	B	290	GLN	2.4
3	C	30	ASN	2.4
1	A	173	SER	2.3
2	B	380	THR	2.3
2	B	364	LEU	2.3
2	B	373	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	367	GLU	2.3
1	A	171	LEU	2.3
2	B	49	PRO	2.3
1	A	188	VAL	2.2
2	B	263	GLY	2.2
3	C	40	LYS	2.2
3	C	37	ASP	2.2
1	A	204	VAL	2.2
2	B	247	ARG	2.2
1	A	178	SER	2.2
1	A	157	GLY	2.2
2	B	92	ILE	2.2
1	A	207	ALA	2.2
2	B	371	GLY	2.1
1	A	206	PHE	2.1
2	B	3	PHE	2.1
2	B	361	ASP	2.1
2	B	370	ALA	2.1
2	B	257	LEU	2.1
1	A	153	GLY	2.1
2	B	339	LEU	2.1
1	A	155	SER	2.1
2	B	394	ALA	2.1
2	B	363	LYS	2.1
2	B	90	TYR	2.0
3	C	36	LEU	2.0
1	A	159	ALA	2.0
2	B	46	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	B	501	1/1	0.78	0.25	2.72	43,43,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.