



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:36 AM UTC

PDB ID : 2G5H / pdb_00002g5h
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

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
Xtriage (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

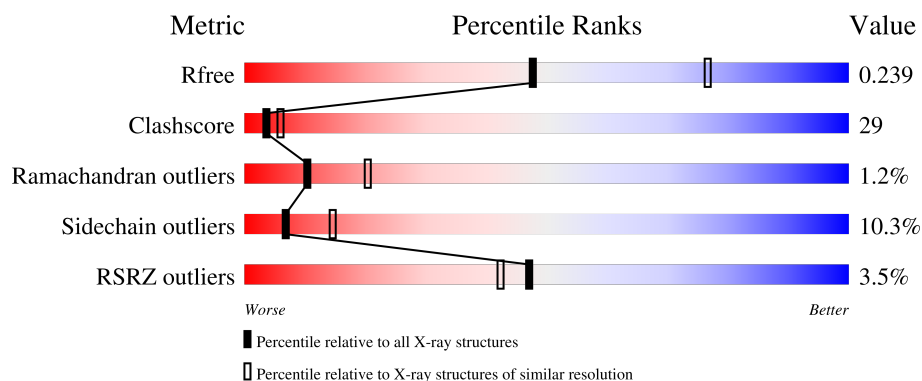
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	6% 69% 27% ..
2	B	483	6% 31% 38% 13% • 18%
3	C	100	4% 55% 34% 10% •

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 (CCD ID: MG) (formula: Mg).

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

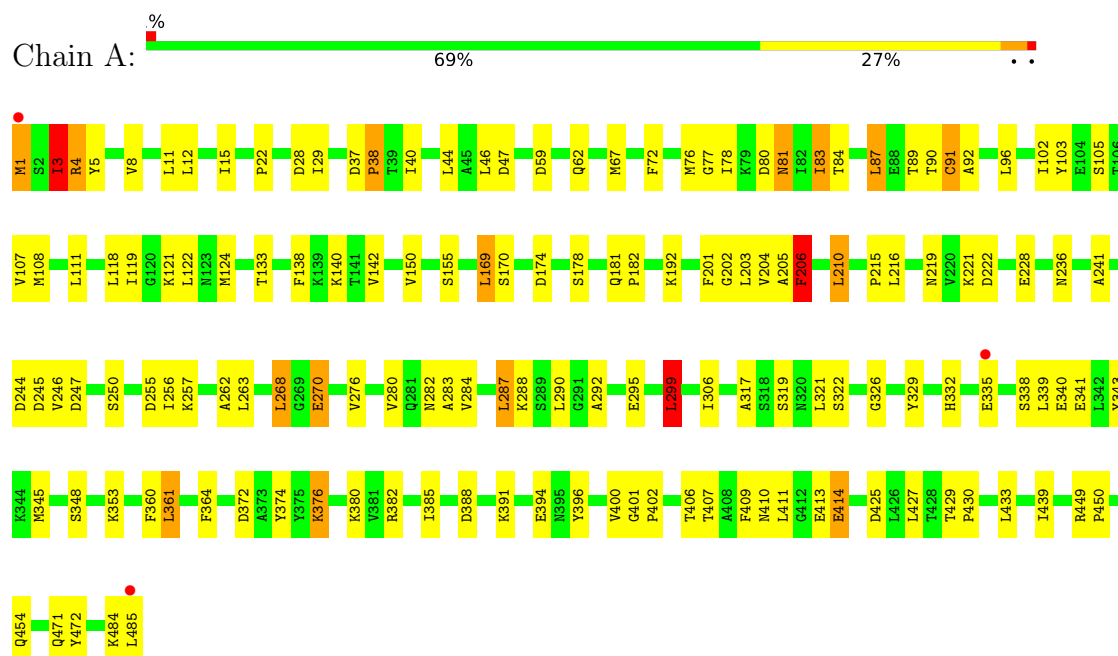
- Molecule 5 is water.

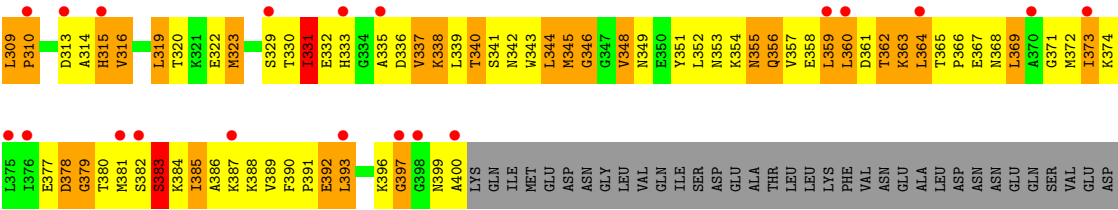
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total 81	O 81	0	0
5	B	47	Total 47	O 47	0	0
5	C	11	Total 11	O 11	0	0

3 Residue-property plots [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.

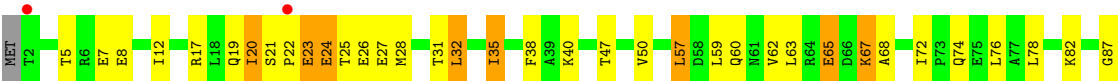
- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A





TYR	LYS	ASN	GLY	LYS	GLY	LYS	ALA	MET	PHE	LEU	VAL	GLY	GLN	ILE	MET	LYS	ALA	SER	LYS	GLY	GLN	ALA	ASN	PRO	GLN	LEU	ILE	VAL	ASN	GLU	ASP	ASN	GLY	LEU	LEU	LYS	GLN	VAL	GLU	ILE	SER	ASP	LYS	ARG	LEU	GLU	THR	LEU	LEU	LYS	VAL	PHE	ASN	GLU	ALA	LEU	ASP	ASN	GLN	SER	VAL	GLU	ASP
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● Molecule 3: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.92Å 92.04Å 181.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.50) 99.2 (20.00-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ 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	4160 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7806	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

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

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

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	0.49	0/3784	1.02	14/5116 (0.3%)
2	B	0.50	1/3231 (0.0%)	1.11	39/4364 (0.9%)
3	C	0.50	0/789	1.01	1/1066 (0.1%)
All	All	0.49	1/7804 (0.0%)	1.06	54/10546 (0.5%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	381	MET	SD-CE	8.56	2.00	1.79

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	383	SER	N-CA-C	9.95	131.99	110.80
2	B	382	SER	N-CA-C	8.59	122.84	109.52
2	B	154	GLU	N-CA-C	-8.21	98.07	110.39
2	B	307	LEU	N-CA-C	-7.57	100.92	111.52
1	A	205	ALA	N-CA-C	7.56	121.36	110.10
2	B	380	THR	N-CA-C	-7.55	98.02	109.79
2	B	237	ASN	N-CA-C	7.47	119.43	111.28
2	B	158	ARG	N-CA-C	7.10	121.64	112.41
2	B	51	VAL	N-CA-C	7.08	118.49	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	86	ASN	CA-C-N	7.05	127.36	119.32
2	B	86	ASN	C-N-CA	7.05	127.36	119.32
2	B	5	THR	N-CA-C	-6.82	96.53	108.20
2	B	232	GLU	N-CA-C	-6.66	104.10	111.36
2	B	244	GLU	N-CA-C	6.40	118.91	109.24
2	B	53	LYS	N-CA-C	6.28	118.13	111.28
2	B	72	THR	N-CA-C	-6.24	105.32	113.12
2	B	397	GLY	N-CA-C	6.22	127.92	113.18
2	B	381	MET	N-CA-C	6.05	123.68	110.80
2	B	96	ASP	N-CA-C	-6.04	101.57	110.52
1	A	138	PHE	N-CA-C	5.97	120.58	113.12
1	A	407	THR	N-CA-C	-5.92	103.12	110.41
2	B	80	ASN	N-CA-C	5.92	118.31	109.25
1	A	91	CYS	N-CA-C	-5.90	105.66	112.86
2	B	236	LEU	N-CA-C	5.89	117.50	111.14
1	A	270	GLU	N-CA-C	5.88	118.48	111.71
1	A	206	PHE	N-CA-C	-5.87	102.09	111.02
1	A	3	ILE	N-CA-C	-5.87	107.02	112.83
1	A	83	ILE	N-CA-C	5.81	116.91	109.30
2	B	309	LEU	CA-C-N	5.70	126.96	119.84
2	B	309	LEU	C-N-CA	5.70	126.96	119.84
2	B	111	GLY	N-CA-C	-5.66	99.77	113.18
1	A	299	LEU	N-CA-C	-5.62	99.06	108.94
2	B	289	ARG	N-CA-C	-5.60	104.86	110.97
2	B	346	GLY	N-CA-C	-5.57	103.01	111.14
1	A	353	LYS	N-CA-C	5.57	117.79	111.11
1	A	299	LEU	CA-C-N	5.54	126.77	119.84
1	A	299	LEU	C-N-CA	5.54	126.77	119.84
2	B	21	MET	N-CA-C	5.53	116.99	111.07
2	B	119	THR	N-CA-C	5.50	118.20	111.82
2	B	294	GLU	N-CA-C	-5.47	99.81	108.73
3	C	98	GLU	N-CA-C	-5.45	99.19	110.80
2	B	299	ARG	N-CA-C	-5.45	104.99	111.69
1	A	282	ASN	N-CA-C	-5.36	105.60	111.82
2	B	331	ILE	N-CA-C	5.22	115.33	110.42
1	A	81	ASN	N-CA-C	-5.22	106.15	112.88
2	B	270	PHE	CA-C-N	5.21	126.36	119.84
2	B	270	PHE	C-N-CA	5.21	126.36	119.84
2	B	329	SER	N-CA-C	-5.14	105.76	111.36
2	B	120	ARG	N-CA-C	5.13	116.64	108.79
2	B	215	ASN	N-CA-C	5.12	119.62	113.17
2	B	61	ARG	N-CA-C	-5.11	105.35	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	97	GLN	CA-C-N	-5.09	114.70	119.85
2	B	97	GLN	C-N-CA	-5.09	114.70	119.85
2	B	306	GLU	N-CA-C	-5.06	101.06	109.46

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	126	0
2	B	3169	0	3119	293	0
3	C	781	0	760	62	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	447	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 29.

All (447) 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
2:B:247:ARG:HB3	2:B:258:MET:HE2	1.49	0.92
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:SER:HA	3:C:94:ILE:HD11	1.52	0.90
2:B:199:PRO:HG2	2:B:202:GLN:NE2	1.85	0.90
2:B:344:LEU:HD12	2:B:348:VAL:HG21	1.55	0.89
2:B:56:VAL:HG22	2:B:123:MET:HE1	1.54	0.89
2:B:343:TRP:O	2:B:348:VAL:HG13	1.74	0.87
1:A:1:MET:H2	1:A:28:ASP:CB	1.89	0.85
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
2:B:304:VAL:O	2:B:308:GLY:HA2	1.79	0.82
2:B:351:TYR:CE1	2:B:357:VAL:HG21	2.15	0.81
2:B:388:LYS:O	2:B:388:LYS:HD3	1.81	0.81
2:B:198:ARG:O	2:B:198:ARG:HG3	1.81	0.80
2:B:295:LEU:HD22	2:B:295:LEU:N	1.98	0.79
2:B:364:LEU:CD1	2:B:369:LEU:HB2	2.13	0.79
1:A:84:THR:OG1	1:A:121:LYS:HE3	1.84	0.78
2:B:309:LEU:HD11	2:B:338:LYS:HD2	1.66	0.77
2:B:348:VAL:O	2:B:352:LEU:HD13	1.83	0.77
1:A:87:LEU:HD12	1:A:118:LEU:HD21	1.67	0.77
2:B:364:LEU:HD11	2:B:369:LEU:HB2	1.64	0.77
1:A:247:ASP:OD2	1:A:250:SER:HB3	1.84	0.77
2:B:217:PHE:O	2:B:220:VAL:HG22	1.85	0.77
2:B:320:THR:OG1	2:B:323:MET:HB3	1.85	0.76
1:A:364:PHE:HD2	3:C:12:ILE:HD11	1.49	0.76
1:A:4:ARG:HD2	1:A:5:TYR:CE2	2.20	0.76
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
1:A:77:GLY:C	1:A:78:ILE:HD12	2.12	0.74
2:B:5:THR:HG21	2:B:228:GLU:HG3	1.70	0.73
2:B:348:VAL:HG12	2:B:390:PHE:CZ	2.24	0.73
3:C:98:GLU:CG	3:C:99:ASP:N	2.51	0.73
1:A:1:MET:CG	1:A:4:ARG:HE	2.00	0.73
2:B:313:ASP:HA	2:B:345:MET:SD	2.28	0.73
2:B:316:VAL:HG13	2:B:345:MET:HE2	1.71	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:247:ARG:CB	2:B:258:MET:HE2	2.21	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ILE:HG23	1:A:471:GLN:HG3	1.72	0.70
3:C:72:ILE:HD12	3:C:76:LEU:HB3	1.74	0.70
2:B:182:VAL:HG12	2:B:189:LEU:HD23	1.72	0.70
1:A:284:VAL:HG12	1:A:288:LYS:HE3	1.74	0.69
2:B:386:ALA:HA	2:B:389:VAL:CG2	2.22	0.69
2:B:221:ARG:O	2:B:225:GLU:HG2	1.93	0.69
2:B:309:LEU:CD1	2:B:338:LYS:HD2	2.23	0.69
2:B:390:PHE:HB3	2:B:391:PRO:HD3	1.74	0.68
3:C:99:ASP:OD1	3:C:100:ALA:N	2.21	0.68
2:B:309:LEU:HD12	2:B:310:PRO:HD3	1.74	0.68
3:C:57:LEU:HD22	3:C:59:LEU:HD13	1.76	0.68
2:B:338:LYS:HZ2	2:B:338:LYS:HB3	1.57	0.68
2:B:344:LEU:HA	2:B:348:VAL:HG22	1.74	0.68
1:A:1:MET:H2	1:A:28:ASP:CA	2.07	0.68
3:C:96:ASN:O	3:C:99:ASP:OD1	2.12	0.67
2:B:256:ILE:HD12	2:B:256:ILE:N	2.09	0.67
2:B:352:LEU:HA	2:B:357:VAL:HG23	1.77	0.67
1:A:255:ASP:OD1	1:A:257:LYS:HG2	1.94	0.67
1:A:169:LEU:C	1:A:169:LEU:HD22	2.19	0.67
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:359:LEU:C	2:B:361:ASP:H	2.02	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: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
1:A:360:PHE:CD2	3:C:28:MET:HE3	2.33	0.63
2:B:7:ILE:HG22	2:B:195:ILE:HG13	1.80	0.63
1:A:22:PRO:HD2	1:A:59:ASP:OD1	1.98	0.63
2:B:295:LEU:HD22	2:B:295:LEU:H	1.62	0.63
2:B:32:GLU:O	2:B:35:SER:OG	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:SER:C	3:C:23:GLU:H	2.07	0.62
2:B:157:ILE:HD12	2:B:159:SER:H	1.62	0.62
1:A:169:LEU:HD22	1:A:170:SER:N	2.13	0.62
2:B:331:ILE:CG2	2:B:332:GLU:N	2.62	0.62
2:B:360:LEU:HG	2:B:360:LEU:O	1.99	0.62
2:B:5:THR:HG22	2:B:197:LEU:HG	1.81	0.62
2:B:94:GLN:HB2	2:B:122:HIS:HB2	1.80	0.62
2:B:340:THR:HG23	2:B:373:ILE:HD12	1.81	0.62
2:B:399:ASN:O	2:B:400:ALA:C	2.41	0.62
2:B:133:LYS:HB2	2:B:138:LEU:HD23	1.81	0.62
2:B:249:ASP:HB2	2:B:256:ILE:HD11	1.82	0.62
1:A:83:ILE:HD12	1:A:103:TYR:OH	2.00	0.62
2:B:256:ILE:HA	5:B:519:HOH:O	2.01	0.61
2:B:295:LEU:O	2:B:299:ARG:HB2	2.01	0.61
2:B:154:GLU:HG3	2:B:155:PRO:HD2	1.82	0.61
2:B:344:LEU:HA	2:B:348:VAL:CG2	2.31	0.61
1:A:140:LYS:HD3	5:A:512:HOH:O	2.00	0.61
2:B:88:LYS:O	2:B:89:ALA:HB3	2.00	0.61
2:B:362:THR:C	2:B:363:LYS:HD2	2.26	0.61
2:B:309:LEU:HG	2:B:310:PRO:HD2	1.83	0.61
1:A:1:MET:H2	1:A:28:ASP:CG	2.08	0.60
2:B:230:ARG:NH1	2:B:246:ARG:HE	2.00	0.60
3:C:99:ASP:CG	3:C:100:ALA:H	2.09	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:241:ILE:HD13	2:B:241:ILE:C	2.26	0.60
2:B:3:PHE:N	2:B:200:TYR:CD2	2.69	0.60
2:B:15:LEU:HD11	2:B:149:ILE:HG23	1.84	0.59
2:B:105:ILE:HD11	2:B:166:TYR:CD1	2.37	0.59
2:B:199:PRO:HD3	2:B:235:LEU:HD21	1.84	0.59
2:B:388:LYS:HE2	2:B:392:GLU:HG2	1.84	0.59
1:A:299:LEU:HD12	1:A:388:ASP:HB3	1.85	0.59
2:B:26:PRO:HG3	3:C:68:ALA:HB1	1.84	0.59
2:B:352:LEU:HA	2:B:357:VAL:CG2	2.33	0.58
3:C:27:GLU:O	3:C:31:THR:HG23	2.03	0.58
1:A:361:LEU:HG	3:C:35:ILE:HG21	1.84	0.58
3:C:94:ILE:HG12	3:C:94:ILE:O	2.03	0.58
1:A:241:ALA:HB2	3:C:57:LEU:HD11	1.85	0.58
2:B:98:PRO:HG2	2:B:101:GLU:HG3	1.84	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:219:TYR:CD1	2:B:248:PHE:HE2	2.22	0.57
2:B:288:VAL:C	2:B:291:THR:HG22	2.30	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:359:LEU:C	2:B:361:ASP:N	2.62	0.56
2:B:336:ASP:OD2	2:B:339:LEU:HD23	2.06	0.56
2:B:60:MET:O	2:B:64:MET:HG3	2.04	0.56
2:B:176:TYR:CE1	2:B:296:PRO:HG3	2.41	0.56
1:A:276:VAL:HG21	1:A:406:THR:HA	1.88	0.55
3:C:21:SER:C	3:C:23:GLU:N	2.64	0.55
3:C:98:GLU:CG	3:C:99:ASP:H	2.19	0.55
1:A:256:ILE:HD12	1:A:292:ALA:HB2	1.88	0.55
2:B:3:PHE:O	2:B:3:PHE:CG	2.59	0.55
2:B:290:GLN:C	2:B:290:GLN:CD	2.74	0.55
2:B:369:LEU:HD22	2:B:369:LEU:O	2.05	0.55
2:B:378:ASP:O	2:B:379:GLY:C	2.50	0.55
1:A:360:PHE:HB3	3:C:32:LEU:HD21	1.87	0.55
2:B:295:LEU:N	2:B:295:LEU:CD2	2.70	0.55
2:B:295:LEU:HB3	2:B:296:PRO:CD	2.37	0.55
2:B:61:ARG:HD2	2:B:291:THR:HG23	1.89	0.55
2:B:260:VAL:HG12	2:B:260:VAL:O	2.06	0.55
1:A:338:SER:OG	1:A:341:GLU:HG3	2.07	0.55
2:B:351:TYR:HD1	2:B:352:LEU:HD12	1.71	0.54
1:A:102:ILE:HG12	2:B:44:TYR:CE2	2.43	0.54
2:B:309:LEU:HD12	2:B:310:PRO:CD	2.36	0.54
2:B:384:LYS:HE3	2:B:387:LYS:NZ	2.23	0.54
1:A:228:GLU:OE2	1:A:247:ASP:HA	2.08	0.54
2:B:193:ALA:CB	2:B:224:LEU:HD11	2.38	0.54
2:B:171:ARG:NH1	2:B:175:GLN:HG3	2.23	0.54
2:B:53:LYS:HB2	3:C:63:LEU:HB3	1.88	0.53
1:A:15:ILE:HG22	1:A:67:MET:HE1	1.90	0.53
1:A:215:PRO:C	1:A:216:LEU:HD12	2.33	0.53
2:B:176:TYR:HE2	2:B:299:ARG:HD3	1.73	0.53
2:B:392:GLU:O	2:B:396:LYS:HB2	2.08	0.53
1:A:204:VAL:HG22	2:B:45:PRO:HB2	1.90	0.53
2:B:109:VAL:O	2:B:110:ASP:C	2.52	0.53
2:B:234:GLU:O	2:B:239:GLY:HA3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:LEU:HD22	3:C:59:LEU:CD1	2.38	0.53
2:B:355:ASN:HD22	2:B:357:VAL:HG13	1.73	0.53
2:B:138:LEU:N	2:B:138:LEU:HD22	2.24	0.53
2:B:288:VAL:CA	2:B:291:THR:HG22	2.39	0.53
1:A:206:PHE:CD1	1:A:206:PHE:C	2.85	0.52
1:A:364:PHE:CD1	1:A:364:PHE:C	2.87	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:316:VAL:HG13	2:B:345:MET:CE	2.38	0.52
2:B:295:LEU:HB3	2:B:296:PRO:HD2	1.90	0.52
2:B:388:LYS:C	2:B:391:PRO:HD2	2.35	0.52
2:B:91:GLN:NE2	2:B:124:GLU:HB3	2.25	0.52
2:B:202:GLN:HG2	2:B:204:LYS:H	1.75	0.52
3:C:21:SER:O	3:C:23:GLU:N	2.43	0.52
1:A:81:ASN:HB3	1:A:124:MET:HE1	1.92	0.52
2:B:355:ASN:ND2	2:B:357:VAL:HG13	2.25	0.52
1:A:40:ILE:HA	1:A:142:VAL:HG22	1.92	0.51
1:A:340:GLU:OE1	3:C:99:ASP:O	2.28	0.51
1:A:364:PHE:HB2	3:C:12:ILE:HD13	1.90	0.51
2:B:306:GLU:O	2:B:307:LEU:HB3	2.09	0.51
2:B:331:ILE:HG22	2:B:332:GLU:H	1.75	0.51
3:C:35:ILE:O	3:C:38:PHE:HB3	2.10	0.51
2:B:276:VAL:HG21	3:C:59:LEU:C	2.35	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:169:LYS:HD3	2:B:169:LYS:C	2.36	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
1:A:219:ASN:ND2	1:A:222:ASP:OD2	2.42	0.51
1:A:67:MET:HE2	1:A:72:PHE:CE1	2.45	0.51
1:A:361:LEU:HG	3:C:35:ILE:CG2	2.40	0.50
2:B:60:MET:HE2	2:B:288:VAL:HG21	1.92	0.50
2:B:316:VAL:CG1	2:B:345:MET:HE2	2.40	0.50
2:B:330:THR:HG21	2:B:369:LEU:HD13	1.93	0.50
2:B:176:TYR:CZ	2:B:296:PRO:HG3	2.46	0.50
3:C:63:LEU:N	3:C:63:LEU:HD22	2.27	0.50
2:B:259:ARG:HG3	2:B:260:VAL:N	2.26	0.50
2:B:335:ALA:HB1	2:B:340:THR:HG23	1.92	0.50
2:B:355:ASN:HB3	2:B:357:VAL:HG22	1.93	0.50
3:C:26:GLU:HB2	5:C:110:HOH:O	2.11	0.50
2:B:185:GLU:CD	2:B:185:GLU:H	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ILE:HD11	2:B:157:ILE:CD1	2.25	0.50
2:B:169:LYS:HD3	2:B:169:LYS:O	2.12	0.50
2:B:257:LEU:C	2:B:257:LEU:HD13	2.37	0.50
1:A:8:VAL:O	1:A:12:LEU:HB2	2.11	0.50
2:B:136:TYR:N	2:B:136:TYR:CD1	2.80	0.50
3:C:74:GLN:NE2	3:C:87:GLY:HA3	2.27	0.50
1:A:80:ASP:OD1	1:A:89:THR:HA	2.11	0.50
1:A:409:PHE:CD1	1:A:414:GLU:HG3	2.46	0.50
2:B:271:PRO:O	2:B:273:PRO:HD3	2.11	0.50
2:B:331:ILE:HG22	2:B:332:GLU:N	2.27	0.50
2:B:7:ILE:CG1	2:B:157:ILE:HG13	2.42	0.49
2:B:60:MET:HB3	2:B:99:ILE:HD11	1.94	0.49
2:B:298:GLU:CD	2:B:298:GLU:H	2.20	0.49
3:C:21:SER:OG	3:C:23:GLU:HG3	2.11	0.49
1:A:1:MET:H2	1:A:28:ASP:HB3	1.75	0.49
1:A:133:THR:O	1:A:133:THR:HG22	2.13	0.49
2:B:7:ILE:HG22	2:B:195:ILE:CB	2.43	0.49
3:C:59:LEU:O	3:C:60:GLN:HG3	2.10	0.49
3:C:65:GLU:HB3	3:C:67:LYS:HD2	1.93	0.49
1:A:380:LYS:HB3	3:C:50:VAL:CG1	2.43	0.49
2:B:238:GLY:O	2:B:239:GLY:O	2.30	0.49
1:A:1:MET:N	1:A:28:ASP:CG	2.71	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
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
2:B:9:LEU:HD12	2:B:166:TYR:CD2	2.48	0.48
2:B:363:LYS:HD2	2:B:363:LYS:N	2.27	0.48
2:B:393:LEU:HD22	2:B:393:LEU:O	2.14	0.48
1:A:283:ALA:O	1:A:287:LEU:HD22	2.13	0.48
2:B:229:LYS:N	2:B:229:LYS:HD2	2.28	0.48
2:B:245:THR:OG1	2:B:261:LYS:HE2	2.13	0.48
2:B:313:ASP:HA	2:B:345:MET:CE	2.44	0.48
1:A:484:LYS:O	1:A:485:LEU:CB	2.61	0.48
2:B:7:ILE:HG22	2:B:195:ILE:CG1	2.43	0.48
1:A:429:THR:OG1	1:A:430:PRO:HD3	2.13	0.48
2:B:7:ILE:HA	2:B:194:ASN:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:VAL:HG21	3:C:59:LEU:CB	2.44	0.48
1:A:402:PRO:HG2	1:A:427:LEU:CD1	2.44	0.48
2:B:169:LYS:HZ3	2:B:297:ASP:CG	2.22	0.48
2:B:338:LYS:NZ	2:B:342:ASN:HD21	2.12	0.48
1:A:62:GLN:CB	1:A:67:MET:HE3	2.44	0.47
2:B:157:ILE:CD1	2:B:159:SER:H	2.26	0.47
2:B:300:LYS:NZ	2:B:315:HIS:HB2	2.29	0.47
2:B:338:LYS:HZ2	2:B:338:LYS:CB	2.25	0.47
2:B:378:ASP:O	2:B:379:GLY:O	2.30	0.47
2:B:167:LEU:CD2	2:B:220:VAL:HG21	2.43	0.47
2:B:240:GLU:HA	2:B:240:GLU:OE1	2.14	0.47
2:B:295:LEU:H	2:B:295:LEU:CD2	2.25	0.47
2:B:362:THR:O	2:B:362:THR:HG23	2.14	0.47
2:B:336:ASP:CG	2:B:339:LEU:HD23	2.39	0.47
3:C:47:THR:HB	3:C:50:VAL:HG12	1.96	0.47
2:B:137:SER:HB2	3:C:91:VAL:HG23	1.96	0.47
2:B:310:PRO:HB2	2:B:313:ASP:OD1	2.13	0.47
2:B:355:ASN:HB2	5:B:547:HOH:O	2.13	0.47
1:A:90:THR:C	1:A:92:ALA:N	2.71	0.47
2:B:294:GLU:O	2:B:299:ARG:HD2	2.15	0.47
2:B:378:ASP:OD1	2:B:379:GLY:N	2.48	0.47
1:A:201:PHE:CD1	1:A:236:ASN:HB3	2.50	0.47
1:A:374:TYR:OH	3:C:40:LYS:HE3	2.15	0.47
2:B:64:MET:C	2:B:66:LEU:N	2.71	0.47
2:B:88:LYS:O	2:B:89:ALA:CB	2.63	0.47
2:B:98:PRO:HB3	2:B:120:ARG:HH21	1.78	0.47
2:B:169:LYS:HE2	2:B:173:ILE:HD11	1.96	0.47
2:B:300:LYS:HZ3	2:B:315:HIS:HB2	1.79	0.47
2:B:368:ASN:HD22	2:B:368:ASN:N	2.11	0.47
2:B:60:MET:HE3	2:B:70:ILE:HG21	1.97	0.47
2:B:216:SER:OG	2:B:219:TYR:HB2	2.14	0.47
2:B:98:PRO:HB3	2:B:120:ARG:NH2	2.29	0.47
2:B:363:LYS:NZ	2:B:363:LYS:HB3	2.30	0.47
2:B:356:GLN:HA	2:B:356:GLN:NE2	2.31	0.46
1:A:107:VAL:HG23	1:A:108:MET:HE2	1.98	0.46
1:A:103:TYR:HB3	2:B:39:VAL:HG11	1.96	0.46
2:B:160:PRO:HG3	2:B:225:GLU:HB3	1.96	0.46
1:A:78:ILE:HG12	1:A:108:MET:SD	2.56	0.46
1:A:247:ASP:OD2	1:A:250:SER:CB	2.61	0.46
1:A:360:PHE:CE2	3:C:28:MET:HE3	2.50	0.46
2:B:309:LEU:CG	2:B:310:PRO:HD2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:309:LEU:HD21	2:B:341:SER:HB2	1.98	0.46
2:B:176:TYR:HE2	2:B:299:ARG:CD	2.29	0.46
2:B:202:GLN:HG2	2:B:204:LYS:N	2.31	0.46
2:B:309:LEU:CD1	2:B:338:LYS:CD	2.92	0.46
2:B:340:THR:O	2:B:344:LEU:HD22	2.15	0.46
2:B:385:ILE:O	2:B:389:VAL:HG13	2.15	0.46
2:B:64:MET:C	2:B:66:LEU:H	2.24	0.46
2:B:159:SER:OG	2:B:162:GLU:HG3	2.15	0.46
2:B:363:LYS:O	2:B:364:LEU:C	2.59	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:212:LYS:HA	2:B:212:LYS:HD2	1.51	0.46
1:A:1:MET:N	1:A:28:ASP:CA	2.72	0.45
1:A:103:TYR:CD1	2:B:39:VAL:HG11	2.51	0.45
1:A:317:ALA:C	1:A:319:SER:H	2.24	0.45
1:A:439:ILE:O	1:A:454:GLN:HA	2.16	0.45
2:B:220:VAL:HG23	2:B:221:ARG:N	2.32	0.45
2:B:259:ARG:HG3	2:B:259:ARG:NH1	2.30	0.45
2:B:313:ASP:HA	2:B:345:MET:HE1	1.98	0.45
1:A:76:MET:HB3	1:A:169:LEU:HD11	1.97	0.45
2:B:241:ILE:HD13	2:B:242:GLY:N	2.31	0.45
1:A:338:SER:CB	3:C:99:ASP:HB2	2.46	0.45
2:B:20:LYS:HB3	2:B:145:GLY:O	2.17	0.45
2:B:226:TYR:CD1	2:B:226:TYR:C	2.94	0.45
2:B:362:THR:HB	5:B:521:HOH:O	2.15	0.45
1:A:4:ARG:HD2	1:A:5:TYR:CD2	2.52	0.45
1:A:410:ASN:HB2	1:A:413:GLU:HB2	1.99	0.45
2:B:157:ILE:CD1	2:B:162:GLU:HB2	2.46	0.45
2:B:197:LEU:HD13	2:B:231:GLN:CD	2.42	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
1:A:181:GLN:HB3	1:A:182:PRO:HD3	1.99	0.45
3:C:62:VAL:C	3:C:63:LEU:HD22	2.42	0.45
1:A:348:SER:OG	3:C:19:GLN:N	2.50	0.45
2:B:383:SER:O	2:B:386:ALA:N	2.47	0.45
2:B:7:ILE:CG2	2:B:195:ILE:HG13	2.46	0.44
2:B:61:ARG:HD3	2:B:291:THR:HG23	1.99	0.44
2:B:135:GLU:OE2	3:C:94:ILE:HG22	2.17	0.44
2:B:336:ASP:O	2:B:337:VAL:C	2.60	0.44
1:A:84:THR:CG2	1:A:121:LYS:HE3	2.47	0.44
1:A:338:SER:HB2	3:C:100:ALA:OXT	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:ARG:NH1	2:B:255:THR:O	2.50	0.44
2:B:64:MET:HE1	2:B:288:VAL:HG23	1.99	0.44
2:B:197:LEU:N	2:B:197:LEU:CD1	2.80	0.44
2:B:383:SER:O	2:B:384:LYS:C	2.60	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:169:LYS:NZ	2:B:297:ASP:OD2	2.50	0.44
1:A:210:LEU:HD13	1:A:382:ARG:NH2	2.32	0.44
2:B:276:VAL:HG22	2:B:277:PRO:HD2	1.99	0.44
2:B:389:VAL:HG23	2:B:390:PHE:N	2.32	0.44
2:B:198:ARG:HB3	2:B:205:PHE:CD2	2.53	0.44
1:A:62:GLN:HB2	1:A:67:MET:HE3	1.99	0.43
2:B:144:GLN:CD	2:B:145:GLY:N	2.76	0.43
2:B:336:ASP:CB	2:B:339:LEU:HD23	2.48	0.43
2:B:344:LEU:O	2:B:348:VAL:HG22	2.18	0.43
1:A:290:LEU:HD13	1:A:471:GLN:HB3	2.00	0.43
2:B:167:LEU:HD23	2:B:220:VAL:HG21	2.00	0.43
2:B:247:ARG:CA	2:B:258:MET:HE2	2.48	0.43
1:A:15:ILE:HG22	1:A:67:MET:CE	2.47	0.43
1:A:78:ILE:HD12	1:A:78:ILE:N	2.33	0.43
2:B:38:ASN:OD1	2:B:40:ILE:HB	2.18	0.43
2:B:119:THR:HG22	2:B:154:GLU:HA	1.99	0.43
2:B:286:GLU:O	2:B:287:ARG:C	2.61	0.43
2:B:372:MET:HE1	2:B:390:PHE:CD1	2.53	0.43
2:B:348:VAL:CG2	2:B:349:ASN:N	2.81	0.43
2:B:371:GLY:O	2:B:372:MET:C	2.62	0.43
1:A:105:SER:HB2	1:A:202:GLY:HA3	2.00	0.43
1:A:262:ALA:HB2	1:A:396:TYR:CG	2.54	0.43
2:B:202:GLN:HE21	2:B:202:GLN:HB3	1.51	0.43
2:B:249:ASP:HB2	2:B:256:ILE:CD1	2.47	0.43
1:A:11:LEU:O	1:A:15:ILE:HG13	2.18	0.43
1:A:87:LEU:HD12	1:A:118:LEU:CD2	2.43	0.43
2:B:93:SER:OG	2:B:94:GLN:N	2.51	0.43
2:B:157:ILE:HD13	2:B:163:ALA:N	2.34	0.43
3:C:99:ASP:O	3:C:100:ALA:HB3	2.19	0.43
2:B:129:LYS:HE2	2:B:143:ARG:NH2	2.34	0.43
2:B:164:TYR:CD1	2:B:164:TYR:C	2.96	0.43
2:B:247:ARG:HB3	2:B:258:MET:CE	2.35	0.43
2:B:270:PHE:HA	2:B:271:PRO:HD3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:330:THR:CG2	2:B:340:THR:HG21	2.49	0.43
2:B:386:ALA:CA	2:B:389:VAL:HG22	2.43	0.43
1:A:244:ASP:O	1:A:246:VAL:N	2.52	0.43
2:B:137:SER:C	2:B:138:LEU:HD22	2.44	0.43
3:C:20:ILE:HG13	3:C:24:GLU:HB3	1.99	0.43
1:A:105:SER:CB	1:A:202:GLY:HA3	2.49	0.43
1:A:203:LEU:O	2:B:46:GLY:HA2	2.19	0.43
1:A:256:ILE:CD1	1:A:292:ALA:HB2	2.49	0.43
1:A:425:ASP:HB3	1:A:429:THR:HG23	2.01	0.42
2:B:181:ASP:O	2:B:182:VAL:C	2.61	0.42
2:B:230:ARG:CZ	2:B:246:ARG:HE	2.32	0.42
1:A:1:MET:H1	1:A:28:ASP:HA	1.84	0.42
2:B:157:ILE:HD13	2:B:162:GLU:HB2	2.01	0.42
2:B:389:VAL:O	2:B:393:LEU:HB3	2.19	0.42
2:B:22:PHE:CE2	2:B:92:ILE:HB	2.55	0.42
2:B:60:MET:HB3	2:B:99:ILE:CD1	2.50	0.42
2:B:121:LEU:HA	2:B:150:GLU:O	2.18	0.42
2:B:137:SER:OG	3:C:93:THR:HB	2.18	0.42
2:B:372:MET:HE1	2:B:390:PHE:HD1	1.84	0.42
1:A:391:LYS:O	1:A:394:GLU:HB2	2.20	0.42
2:B:121:LEU:C	2:B:121:LEU:HD23	2.44	0.42
2:B:297:ASP:HB2	2:B:298:GLU:OE2	2.19	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:64:MET:HE1	2:B:288:VAL:C	2.45	0.42
1:A:343:TYR:HB3	3:C:17:ARG:HB3	2.02	0.42
2:B:198:ARG:O	2:B:198:ARG:CG	2.61	0.42
1:A:449:ARG:HA	1:A:450:PRO:HD2	1.93	0.42
2:B:135:GLU:OE1	2:B:135:GLU:HA	2.19	0.42
1:A:338:SER:HB3	3:C:99:ASP:HB2	2.02	0.42
2:B:60:MET:O	2:B:64:MET:HE2	2.18	0.42
3:C:5:THR:HB	3:C:7:GLU:OE1	2.20	0.42
2:B:112:GLU:N	5:B:517:HOH:O	2.52	0.41
1:A:3:ILE:HG13	1:A:28:ASP:OD2	2.20	0.41
1:A:47:ASP:HB2	1:A:87:LEU:HD11	2.01	0.41
1:A:155:SER:HB2	1:A:178:SER:O	2.19	0.41
2:B:140:ASP:HB2	3:C:88:GLN:HE21	1.84	0.41
2:B:198:ARG:HG3	2:B:198:ARG:HH11	1.84	0.41
2:B:214:LEU:HB3	2:B:220:VAL:HG12	2.02	0.41
2:B:309:LEU:HD11	2:B:338:LYS:CD	2.45	0.41
2:B:309:LEU:HD21	2:B:341:SER:CB	2.51	0.41

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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:HD23	2:B:307:LEU:O	2.20	0.41
2:B:355:ASN:C	2:B:357:VAL:N	2.78	0.41
1:A:108:MET:CE	1:A:111:LEU:HD12	2.50	0.41
1:A:345:MET:HG2	3:C:19:GLN:OE1	2.20	0.41
2:B:284:TRP:O	2:B:288:VAL:HG22	2.21	0.41
2:B:365:THR:HB	2:B:366:PRO:CD	2.50	0.41
2:B:216:SER:O	2:B:217:PHE:C	2.64	0.41
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.94	0.41
1:A:216:LEU:HD12	1:A:216:LEU:N	2.35	0.41
1:A:268:LEU:HD12	1:A:268:LEU:HA	1.93	0.41
2:B:7:ILE:HG22	2:B:195:ILE:HA	2.03	0.41
2:B:156:ASP:O	2:B:158:ARG:HG2	2.21	0.41
1:A:37:ASP:N	1:A:38:PRO:CD	2.83	0.41
1:A:256:ILE:HG23	1:A:471:GLN:CG	2.44	0.41
1:A:329:TYR:C	1:A:329:TYR:CD1	2.99	0.41
2:B:43:ALA:HB3	2:B:87:PRO:HB2	2.03	0.41
2:B:105:ILE:HD11	2:B:166:TYR:CE1	2.56	0.41
1:A:332:HIS:HB3	3:C:82:LYS:CD	2.51	0.40
2:B:64:MET:SD	2:B:289:ARG:HD2	2.61	0.40
2:B:316:VAL:HA	2:B:319:LEU:HD13	2.02	0.40
1:A:62:GLN:HG3	1:A:67:MET:HE3	2.04	0.40
1:A:90:THR:O	1:A:91:CYS:HB2	2.20	0.40
2:B:385:ILE:HG23	2:B:389:VAL:HG11	2.03	0.40
1:A:322:SER:HB3	2:B:89:ALA:CB	2.52	0.40
1:A:326:GLY:O	1:A:332:HIS:ND1	2.51	0.40
2:B:5:THR:HG22	2:B:197:LEU:CD1	2.52	0.40
2:B:85:ASP:HB2	2:B:128:GLY:O	2.21	0.40
2:B:119:THR:CG2	2:B:154:GLU:HA	2.51	0.40
2:B:202:GLN:OE1	2:B:204:LYS:O	2.40	0.40
2:B:358:GLU:H	2:B:358:GLU:HG2	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

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%)	43	63
2	B	396/483 (82%)	348 (88%)	38 (10%)	10 (2%)	4	7
3	C	97/100 (97%)	85 (88%)	11 (11%)	1 (1%)	12	24
All	All	976/1068 (91%)	892 (91%)	72 (7%)	12 (1%)	10	20

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 ⓘ

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%)	382 (94%)	24 (6%)	18	37
2	B	345/419 (82%)	293 (85%)	52 (15%)	3	5
3	C	87/88 (99%)	77 (88%)	10 (12%)	5	11
All	All	838/913 (92%)	752 (90%)	86 (10%)	7	14

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	ILE
1	A	4	ARG
1	A	38	PRO
1	A	46	LEU
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	221	LYS
1	A	263	LEU
1	A	268	LEU
1	A	287	LEU
1	A	299	LEU
1	A	321	LEU
1	A	335	GLU
1	A	339	LEU
1	A	361	LEU
1	A	376	LYS
1	A	385	ILE
1	A	414	GLU
1	A	433	LEU
2	B	4	GLU
2	B	7	ILE
2	B	50	VAL
2	B	66	LEU
2	B	73	GLU
2	B	108	GLU
2	B	109	VAL
2	B	114	LYS
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	185	GLU
2	B	197	LEU
2	B	202	GLN

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Mol	Chain	Res	Type
2	B	212	LYS
2	B	236	LEU
2	B	241	ILE
2	B	254	LYS
2	B	256	ILE
2	B	260	VAL
2	B	290	GLN
2	B	315	HIS
2	B	316	VAL
2	B	319	LEU
2	B	322	GLU
2	B	323	MET
2	B	331	ILE
2	B	333	HIS
2	B	338	LYS
2	B	340	THR
2	B	344	LEU
2	B	345	MET
2	B	348	VAL
2	B	353	ASN
2	B	354	LYS
2	B	355	ASN
2	B	356	GLN
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	392	GLU
2	B	393	LEU
3	C	8	GLU
3	C	20	ILE
3	C	23	GLU
3	C	24	GLU
3	C	32	LEU
3	C	35	ILE
3	C	57	LEU
3	C	65	GLU
3	C	67	LYS

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Mol	Chain	Res	Type
3	C	94	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	281	GLN
1	A	379	GLN
1	A	479	HIS
2	B	202	GLN
2	B	290	GLN
2	B	342	ASN
2	B	355	ASN
2	B	356	GLN
3	C	14	ASN
3	C	42	ASN
3	C	60	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

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(Å ²)	Q<0.9
1	A	485/485 (100%)	-0.20	3 (0%) 85 83	32, 47, 67, 88	0
2	B	398/483 (82%)	0.63	27 (6%) 23 20	38, 69, 95, 95	0
3	C	99/100 (99%)	0.50	4 (4%) 42 38	45, 69, 95, 95	0
All	All	982/1068 (91%)	0.21	34 (3%) 47 42	32, 55, 95, 95	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	7.4
2	B	335	ALA	5.5
2	B	382	SER	3.8
2	B	398	GLY	3.8
2	B	393	LEU	3.8
2	B	381	MET	3.8
2	B	400	ALA	3.5
2	B	397	GLY	3.4
2	B	237	ASN	3.3
1	A	485	LEU	3.2
2	B	359	LEU	3.1
2	B	360	LEU	3.0
2	B	315	HIS	2.8
3	C	99	ASP	2.8
2	B	364	LEU	2.7
3	C	96	ASN	2.6
2	B	376	ILE	2.5
1	A	335	GLU	2.5
3	C	2	THR	2.5
2	B	290	GLN	2.4
2	B	28	HIS	2.4
3	C	22	PRO	2.4
2	B	109	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	310	PRO	2.3
2	B	5	THR	2.2
2	B	333	HIS	2.2
2	B	313	ASP	2.2
2	B	3	PHE	2.2
2	B	303	TYR	2.1
2	B	387	LYS	2.1
2	B	370	ALA	2.1
2	B	329	SER	2.1
2	B	375	LEU	2.1
2	B	373	ILE	2.1

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($\text{\AA}^2$)	Q<0.9
4	MG	B	501	1/1	0.78	0.10	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.