



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:48 AM UTC

PDB ID : 2F2A / pdb_00002f2a
Title : Structure of tRNA-Dependent Amidotransferase GatCAB complexed with Gln
Authors : Nakamura, A.; Yao, M.; Tanaka, I.
Deposited on : 2005-11-15
Resolution : 2.30 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
Mogul : 2022.3.0, CSD as543be (2022)
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

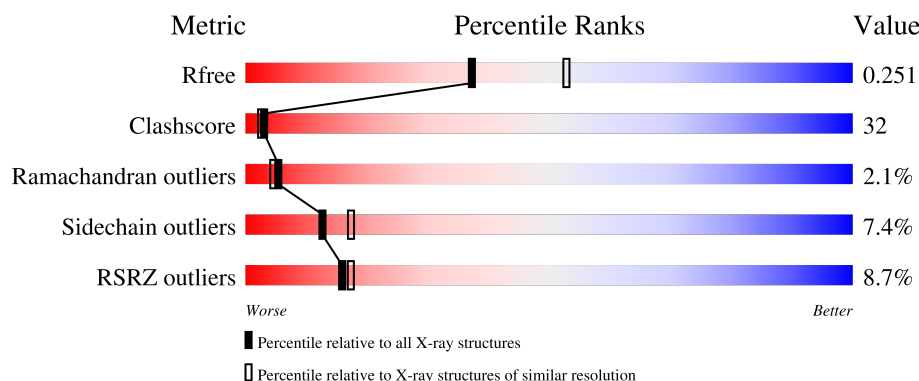
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	71% 25% ..
2	B	483	16% 38% 35% 10% . 16%
3	C	100	7% 55% 32% .. 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8091 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	408	Total	C	N	O	S	0	0	0
			3245	2043	546	643	13			

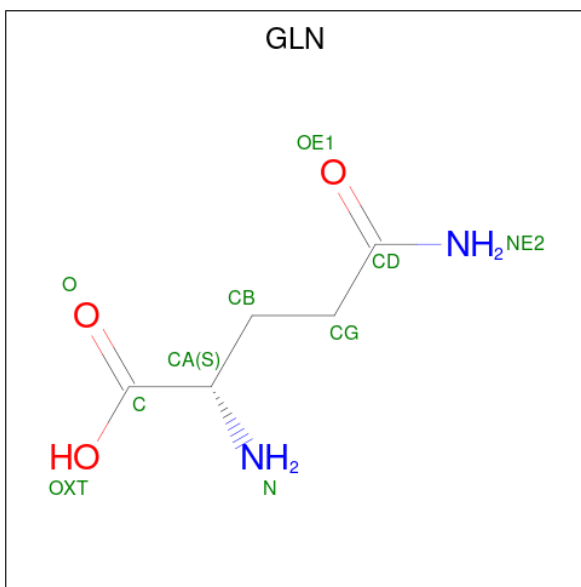
There are 8 discrepancies between the modelled and reference sequences:

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	92	Total	C	N	O	S	0	0	0
			726	450	122	153	1			

- Molecule 4 is GLUTAMINE (CCD ID: GLN) (formula: C₅H₁₀N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

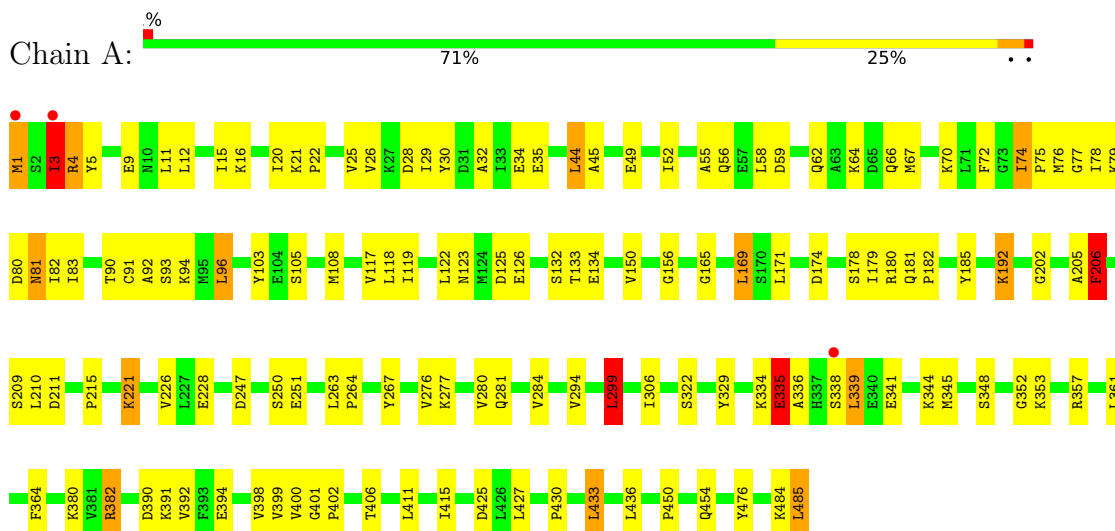
- Molecule 6 is water.

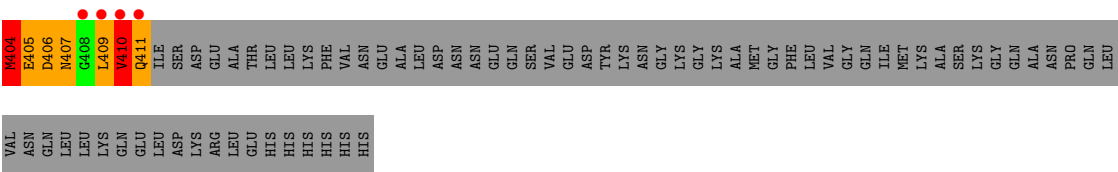
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	239	Total	O	0	0
			239	239		
6	B	117	Total	O	0	0
			117	117		
6	C	37	Total	O	0	0
			37	37		

3 Residue-property plots

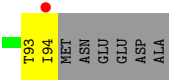
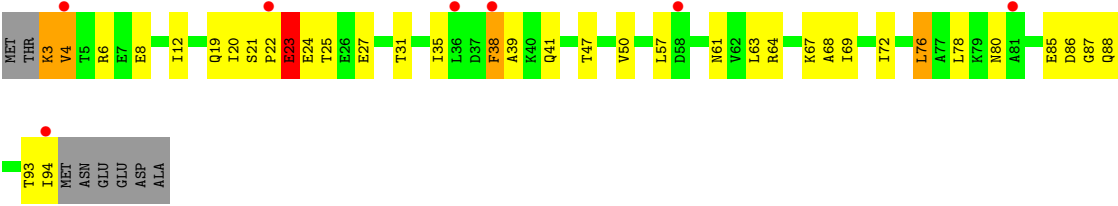
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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





● Molecule 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	77.19Å 88.22Å 183.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.30) 99.8 (20.00-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.252 0.211 , 0.251	Depositor DCC
R_{free} test set	6274 reflections (9.79%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8091	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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	0.43	0/3784	0.98	17/5116 (0.3%)
2	B	0.42	0/3306	1.03	22/4464 (0.5%)
3	C	0.36	0/734	0.80	0/993
All	All	0.42	0/7824	0.98	39/10573 (0.4%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	410	VAL	N-CA-C	12.64	127.55	108.71
2	B	203	GLU	N-CA-C	-12.14	98.44	113.01
1	A	3	ILE	N-CA-C	-11.37	101.99	112.90
2	B	404	MET	N-CA-C	-7.88	102.50	113.37
2	B	229	LYS	N-CA-C	-7.17	103.15	110.97
1	A	179	ILE	N-CA-C	-6.96	105.58	111.56
1	A	299	LEU	CA-C-N	6.86	127.43	119.47
1	A	299	LEU	C-N-CA	6.86	127.43	119.47
2	B	258	MET	N-CA-C	6.83	125.34	110.80
1	A	205	ALA	N-CA-C	6.69	119.99	109.96
2	B	215	ASN	N-CA-C	6.41	122.05	113.72
2	B	252	THR	N-CA-C	-6.36	104.40	111.71
1	A	178	SER	N-CA-C	6.33	120.72	113.19
2	B	72	THR	N-CA-C	-6.25	104.37	112.68
1	A	81	ASN	N-CA-C	-6.23	105.81	113.41
2	B	220	VAL	N-CA-C	6.00	121.82	109.34
2	B	154	GLU	N-CA-C	-5.98	101.43	110.39
2	B	378	ASP	N-CA-C	-5.94	106.58	113.88
2	B	395	ALA	N-CA-C	5.89	117.39	110.97
2	B	96	ASP	N-CA-C	5.77	117.65	111.36
2	B	410	VAL	CA-C-N	5.70	131.97	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	410	VAL	C-N-CA	5.70	131.97	121.70
2	B	120	ARG	N-CA-C	5.62	117.39	108.79
2	B	195	ILE	N-CA-C	5.60	116.55	108.48
2	B	255	THR	N-CA-C	5.59	117.58	108.63
1	A	339	LEU	N-CA-C	-5.51	105.35	111.36
1	A	91	CYS	N-CA-C	-5.37	106.31	112.86
2	B	159	SER	N-CA-C	5.33	112.93	108.13
1	A	344	LYS	N-CA-C	5.27	117.02	111.28
2	B	227	GLU	N-CA-C	5.24	117.79	111.40
1	A	192	LYS	N-CA-C	-5.23	99.10	109.10
2	B	119	THR	N-CA-C	5.12	116.55	111.07
1	A	94	LYS	N-CA-C	-5.11	105.89	111.82
1	A	299	LEU	N-CA-C	-5.11	99.94	108.94
1	A	125	ASP	N-CA-C	-5.09	103.33	110.50
1	A	74	ILE	N-CA-C	5.08	113.00	108.63
1	A	436	LEU	N-CA-C	5.07	117.15	110.36
1	A	206	PHE	N-CA-C	-5.03	100.09	110.80
2	B	51	VAL	N-CA-C	5.02	116.86	109.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3716	0	3708	124	0
2	B	3245	0	3198	338	0
3	C	726	0	717	37	0
4	A	10	0	7	1	0
5	B	1	0	0	0	0
6	A	239	0	0	6	0
6	B	117	0	0	6	0
6	C	37	0	0	1	0
All	All	8091	0	7630	485	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 32.

All (485) 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:209:ALA:HB1	2:B:246:ARG:HH12	1.07	1.10
2:B:246:ARG:HB3	2:B:257:LEU:HA	1.11	1.06
2:B:160:PRO:HB3	2:B:225:GLU:HB2	1.51	0.91
2:B:197:LEU:HD21	2:B:229:LYS:HG2	1.55	0.89
2:B:198:ARG:HH22	2:B:204:LYS:HZ1	1.22	0.87
1:A:49:GLU:H	1:A:49:GLU:CD	1.83	0.87
2:B:193:ALA:HB3	2:B:211:LEU:HD11	1.57	0.87
2:B:220:VAL:HG23	2:B:221:ARG:H	1.39	0.86
2:B:198:ARG:HH22	2:B:204:LYS:NZ	1.72	0.86
2:B:247:ARG:HH11	2:B:247:ARG:HB2	1.40	0.86
2:B:209:ALA:CB	2:B:246:ARG:HH12	1.86	0.86
2:B:401:LYS:HE2	2:B:411:GLN:CD	2.00	0.85
2:B:227:GLU:HB2	2:B:254:LYS:HD2	1.56	0.85
2:B:240:GLU:C	2:B:242:GLY:H	1.82	0.85
2:B:235:LEU:HD12	2:B:240:GLU:HB2	1.57	0.84
2:B:245:THR:C	2:B:246:ARG:HD3	2.03	0.83
1:A:338:SER:HB3	1:A:341:GLU:HG3	1.61	0.83
2:B:107:ILE:HG12	2:B:165:ALA:HB1	1.61	0.83
2:B:247:ARG:HB2	2:B:247:ARG:NH1	1.93	0.82
2:B:360:LEU:H	2:B:360:LEU:HD12	1.42	0.82
2:B:7:ILE:HD12	2:B:157:ILE:HD11	1.62	0.81
2:B:246:ARG:HG2	2:B:246:ARG:HH11	1.45	0.81
2:B:5:THR:CG2	2:B:229:LYS:HD3	2.09	0.81
2:B:246:ARG:HB3	2:B:257:LEU:CA	2.03	0.81
2:B:209:ALA:HB1	2:B:246:ARG:NH1	1.92	0.80
1:A:9:GLU:OE2	1:A:221:LYS:HE2	1.81	0.80
3:C:93:THR:C	3:C:94:ILE:HD12	2.07	0.80
2:B:16:LYS:HG3	2:B:180:SER:HA	1.63	0.80
1:A:1:MET:H2	1:A:28:ASP:CB	1.94	0.80
2:B:372:MET:HE1	2:B:390:PHE:HA	1.64	0.80
1:A:402:PRO:HG2	1:A:427:LEU:HD13	1.64	0.79
2:B:403:ILE:C	2:B:405:GLU:H	1.87	0.79
2:B:372:MET:HE3	2:B:393:LEU:HD13	1.62	0.79
2:B:214:LEU:HD23	2:B:221:ARG:HB2	1.62	0.79
2:B:243:GLN:CD	2:B:257:LEU:HD23	2.08	0.78
2:B:243:GLN:HB3	2:B:246:ARG:HE	1.49	0.78
2:B:257:LEU:N	2:B:257:LEU:HD12	1.97	0.78
2:B:253:GLY:O	2:B:254:LYS:HG2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:LYS:NZ	2:B:388:LYS:HA	2.00	0.77
2:B:249:ASP:O	2:B:253:GLY:HA2	1.84	0.77
2:B:7:ILE:HB	2:B:157:ILE:CG1	2.15	0.76
2:B:326:PHE:CD2	2:B:359:LEU:HD11	2.20	0.76
2:B:407:ASN:HB3	2:B:409:LEU:CD2	2.15	0.76
2:B:371:GLY:O	2:B:374:LYS:HG2	1.86	0.76
2:B:246:ARG:HA	2:B:258:MET:HG2	1.69	0.75
2:B:196:SER:HB2	2:B:206:GLY:O	1.86	0.75
2:B:246:ARG:CB	2:B:257:LEU:HA	2.06	0.75
2:B:7:ILE:HB	2:B:157:ILE:HG13	1.68	0.75
2:B:211:LEU:HD22	2:B:224:LEU:HD12	1.69	0.75
2:B:227:GLU:HB2	2:B:254:LYS:CD	2.17	0.75
1:A:3:ILE:HD11	1:A:25:VAL:HG13	1.67	0.74
2:B:131:THR:HG22	2:B:133:LYS:HG3	1.68	0.74
1:A:353:LYS:HG2	1:A:357:ARG:HH12	1.51	0.74
2:B:227:GLU:O	2:B:230:ARG:HB3	1.87	0.74
2:B:214:LEU:HB3	2:B:221:ARG:HB3	1.68	0.74
2:B:236:LEU:HD23	2:B:236:LEU:O	1.89	0.73
2:B:403:ILE:O	2:B:407:ASN:HB2	1.87	0.73
2:B:384:LYS:HE2	2:B:384:LYS:HA	1.69	0.73
2:B:372:MET:HE2	2:B:389:VAL:HG23	1.70	0.72
2:B:195:ILE:HD11	2:B:197:LEU:HD22	1.72	0.72
2:B:322:GLU:HG2	2:B:360:LEU:HD11	1.72	0.72
2:B:206:GLY:O	2:B:207:THR:HG22	1.90	0.71
1:A:382:ARG:HD3	1:A:433:LEU:O	1.90	0.71
2:B:375:LEU:HD22	2:B:401:LYS:HD3	1.71	0.71
2:B:104:TYR:O	2:B:105:ILE:HD12	1.91	0.71
2:B:184:MET:SD	2:B:216:SER:HA	2.31	0.70
2:B:227:GLU:CB	2:B:254:LYS:HD2	2.20	0.70
2:B:5:THR:HG21	2:B:229:LYS:HD3	1.74	0.70
1:A:30:TYR:O	1:A:34:GLU:HG3	1.91	0.70
2:B:393:LEU:HA	2:B:397:GLY:HA3	1.73	0.70
2:B:256:ILE:HG13	2:B:256:ILE:O	1.92	0.69
2:B:202:GLN:HB3	2:B:204:LYS:H	1.58	0.69
2:B:243:GLN:HB2	2:B:246:ARG:HH21	1.58	0.69
2:B:257:LEU:HD12	2:B:257:LEU:H	1.58	0.69
1:A:1:MET:HG2	1:A:4:ARG:HE	1.57	0.69
2:B:220:VAL:HG23	2:B:221:ARG:N	2.06	0.69
2:B:388:LYS:HA	2:B:388:LYS:HZ3	1.58	0.69
2:B:365:THR:HG22	2:B:368:ASN:ND2	2.08	0.68
2:B:253:GLY:O	2:B:254:LYS:CG	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:ARG:NH1	2:B:261:LYS:HA	2.07	0.68
2:B:157:ILE:HD12	2:B:159:SER:H	1.58	0.68
3:C:31:THR:O	3:C:35:ILE:HD13	1.93	0.67
3:C:3:LYS:CD	3:C:4:VAL:H	2.07	0.67
1:A:284:VAL:HG13	1:A:294:VAL:HG11	1.76	0.67
2:B:227:GLU:HG3	2:B:228:GLU:N	2.09	0.66
2:B:403:ILE:C	2:B:405:GLU:N	2.49	0.66
2:B:4:GLU:HG2	2:B:158:ARG:HD2	1.78	0.66
2:B:350:GLU:O	2:B:354:LYS:HG2	1.95	0.66
2:B:56:VAL:O	2:B:60:MET:HG2	1.96	0.65
1:A:79:LYS:C	1:A:81:ASN:H	2.03	0.65
2:B:161:LYS:H	2:B:161:LYS:HD2	1.61	0.65
2:B:336:ASP:OD2	2:B:339:LEU:HD23	1.97	0.65
1:A:353:LYS:HG2	1:A:357:ARG:NH1	2.10	0.65
2:B:365:THR:HG23	2:B:368:ASN:H	1.61	0.65
2:B:369:LEU:O	2:B:373:ILE:HG12	1.97	0.65
2:B:241:ILE:C	2:B:243:GLN:H	2.04	0.64
2:B:407:ASN:HB3	2:B:409:LEU:HD23	1.79	0.64
2:B:198:ARG:CZ	2:B:204:LYS:HG2	2.27	0.64
2:B:322:GLU:HG3	2:B:360:LEU:HD21	1.80	0.64
2:B:167:LEU:HD13	2:B:217:PHE:CD1	2.32	0.64
2:B:372:MET:HE1	2:B:390:PHE:CA	2.28	0.64
2:B:197:LEU:HD23	2:B:232:GLU:HG2	1.80	0.64
2:B:197:LEU:HB2	2:B:232:GLU:HG2	1.79	0.64
1:A:1:MET:SD	1:A:35:GLU:OE1	2.55	0.64
2:B:121:LEU:CD2	2:B:151:ILE:HG12	2.28	0.64
2:B:161:LYS:HD2	2:B:161:LYS:N	2.13	0.64
3:C:86:ASP:HB3	6:C:120:HOH:O	1.97	0.64
1:A:1:MET:H2	1:A:28:ASP:HB3	1.63	0.63
2:B:182:VAL:HB	2:B:189:LEU:HD23	1.79	0.63
1:A:3:ILE:CD1	1:A:25:VAL:HG13	2.28	0.63
2:B:215:ASN:H	2:B:220:VAL:HG21	1.63	0.63
2:B:227:GLU:CG	2:B:254:LYS:HD2	2.29	0.63
2:B:240:GLU:C	2:B:242:GLY:N	2.53	0.63
2:B:241:ILE:O	2:B:243:GLN:N	2.31	0.63
1:A:64:LYS:O	1:A:66:GLN:HG3	1.99	0.62
2:B:195:ILE:HD11	2:B:197:LEU:CD2	2.30	0.62
2:B:257:LEU:H	2:B:257:LEU:CD1	2.12	0.62
2:B:363:LYS:HA	2:B:363:LYS:HE3	1.81	0.62
2:B:9:LEU:HD21	2:B:221:ARG:NH2	2.14	0.62
1:A:402:PRO:HG2	1:A:427:LEU:CD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:ARG:HD3	2:B:246:ARG:N	2.15	0.62
2:B:167:LEU:HD21	2:B:221:ARG:HD2	1.80	0.62
2:B:216:SER:HB2	2:B:219:TYR:HB2	1.81	0.62
2:B:219:TYR:CD2	2:B:220:VAL:HG13	2.34	0.62
2:B:360:LEU:HD12	2:B:360:LEU:N	2.14	0.61
2:B:399:ASN:HB3	2:B:402:GLN:CB	2.30	0.61
1:A:335:GLU:CD	1:A:335:GLU:H	2.06	0.61
2:B:94:GLN:HB2	2:B:122:HIS:HB2	1.82	0.61
1:A:29:ILE:HG21	1:A:119:ILE:HG12	1.81	0.61
2:B:198:ARG:NH2	2:B:204:LYS:NZ	2.46	0.61
2:B:215:ASN:H	2:B:220:VAL:CG2	2.13	0.61
2:B:163:ALA:CB	2:B:221:ARG:HH12	2.14	0.61
2:B:235:LEU:CD1	2:B:240:GLU:HB2	2.31	0.61
2:B:214:LEU:C	2:B:215:ASN:HD22	2.09	0.61
2:B:409:LEU:N	2:B:409:LEU:HD22	2.16	0.60
2:B:220:VAL:HG12	2:B:248:PHE:HE2	1.66	0.60
1:A:306:ILE:HG22	3:C:38:PHE:CZ	2.36	0.60
1:A:79:LYS:HG2	1:A:81:ASN:HB2	1.82	0.60
1:A:15:ILE:O	1:A:67:MET:HE1	2.02	0.60
3:C:6:ARG:HG3	3:C:25:THR:HG21	1.84	0.60
2:B:227:GLU:HB2	2:B:254:LYS:CE	2.32	0.59
2:B:372:MET:HE3	2:B:393:LEU:CD1	2.32	0.59
2:B:207:THR:HG23	2:B:208:LYS:N	2.17	0.59
2:B:223:GLY:HA2	2:B:226:TYR:CD2	2.37	0.59
2:B:193:ALA:HB3	2:B:211:LEU:CD1	2.30	0.59
2:B:231:GLN:HA	2:B:234:GLU:HG3	1.84	0.59
2:B:364:LEU:HD23	2:B:364:LEU:H	1.67	0.59
1:A:49:GLU:CD	1:A:49:GLU:N	2.59	0.59
2:B:107:ILE:HD12	2:B:108:GLU:H	1.68	0.58
2:B:198:ARG:HD2	2:B:204:LYS:HA	1.83	0.58
2:B:219:TYR:O	2:B:222:LYS:HB3	2.03	0.58
2:B:384:LYS:HE2	2:B:384:LYS:CA	2.33	0.58
2:B:247:ARG:N	2:B:258:MET:HG2	2.18	0.58
2:B:227:GLU:CD	2:B:254:LYS:HD2	2.28	0.58
2:B:185:GLU:HG3	2:B:186:GLU:HG3	1.85	0.58
3:C:3:LYS:HD3	3:C:4:VAL:H	1.68	0.58
1:A:62:GLN:HG3	1:A:67:MET:HE3	1.85	0.58
1:A:247:ASP:OD2	1:A:250:SER:HB3	2.04	0.58
2:B:33:PRO:HA	2:B:142:ASN:HD21	1.69	0.58
2:B:121:LEU:HD22	2:B:151:ILE:HG12	1.85	0.58
2:B:121:LEU:HD21	2:B:149:ILE:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:H2	1:A:28:ASP:CG	2.11	0.57
1:A:339:LEU:H	3:C:94:ILE:HG12	1.70	0.57
2:B:7:ILE:HB	2:B:157:ILE:CD1	2.34	0.57
2:B:83:TYR:CD1	2:B:84:PRO:HD2	2.38	0.57
1:A:345:MET:HG2	6:A:649:HOH:O	2.04	0.57
1:A:77:GLY:C	1:A:78:ILE:HD12	2.29	0.57
2:B:202:GLN:C	2:B:204:LYS:N	2.61	0.57
2:B:405:GLU:C	2:B:407:ASN:H	2.12	0.57
1:A:306:ILE:HG22	3:C:38:PHE:HZ	1.70	0.57
2:B:363:LYS:HB3	2:B:394:ALA:O	2.05	0.57
2:B:372:MET:CG	2:B:381:MET:HE1	2.34	0.56
2:B:7:ILE:HB	2:B:157:ILE:HD11	1.87	0.56
2:B:372:MET:HG3	2:B:381:MET:HE1	1.87	0.56
2:B:237:ASN:C	2:B:237:ASN:HD22	2.13	0.56
2:B:351:TYR:O	2:B:355:ASN:HB2	2.05	0.56
1:A:280:VAL:HG21	1:A:402:PRO:HB3	1.87	0.56
2:B:240:GLU:CD	2:B:241:ILE:H	2.14	0.56
2:B:256:ILE:O	2:B:258:MET:N	2.36	0.56
2:B:257:LEU:N	2:B:257:LEU:CD1	2.65	0.56
1:A:1:MET:H1	1:A:28:ASP:HA	1.71	0.55
1:A:251:GLU:HB2	6:A:602:HOH:O	2.05	0.55
2:B:246:ARG:HA	2:B:258:MET:CG	2.35	0.55
2:B:11:VAL:HG13	2:B:190:ARG:O	2.07	0.55
2:B:194:ASN:HB2	2:B:210:GLU:OE2	2.06	0.55
2:B:401:LYS:HE2	2:B:411:GLN:OE1	2.07	0.55
2:B:326:PHE:HD2	2:B:359:LEU:HD11	1.71	0.55
1:A:180:ARG:HD2	1:A:454:GLN:OE1	2.07	0.55
2:B:365:THR:CG2	2:B:368:ASN:H	2.18	0.55
2:B:246:ARG:HH11	2:B:246:ARG:CG	2.14	0.54
2:B:355:ASN:O	2:B:357:VAL:HG23	2.06	0.54
2:B:216:SER:HB2	2:B:219:TYR:CB	2.38	0.54
2:B:399:ASN:HB3	2:B:402:GLN:HB3	1.87	0.54
2:B:322:GLU:CG	2:B:360:LEU:HD11	2.35	0.54
2:B:242:GLY:O	2:B:243:GLN:HB2	2.08	0.54
1:A:1:MET:HG3	1:A:32:ALA:HA	1.89	0.54
1:A:93:SER:HB2	1:A:126:GLU:HG3	1.89	0.54
2:B:241:ILE:O	2:B:241:ILE:HG22	2.08	0.54
2:B:250:GLU:O	2:B:253:GLY:N	2.40	0.54
2:B:214:LEU:HD12	2:B:214:LEU:N	2.22	0.54
2:B:364:LEU:HA	2:B:368:ASN:HD21	1.73	0.54
2:B:396:LYS:O	2:B:397:GLY:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:GLU:O	3:C:12:ILE:HG12	2.08	0.53
1:A:181:GLN:HB3	1:A:182:PRO:HD3	1.89	0.53
2:B:157:ILE:HD12	2:B:159:SER:N	2.23	0.53
2:B:247:ARG:CB	2:B:258:MET:HE2	2.38	0.53
3:C:47:THR:O	3:C:50:VAL:HG22	2.07	0.53
2:B:249:ASP:O	2:B:253:GLY:CA	2.53	0.53
2:B:140:ASP:HB2	3:C:88:GLN:NE2	2.24	0.53
2:B:159:SER:HB2	2:B:161:LYS:HD3	1.89	0.53
2:B:163:ALA:HB1	2:B:221:ARG:NH1	2.24	0.53
2:B:402:GLN:O	2:B:406:ASP:HB2	2.08	0.53
1:A:380:LYS:HB3	3:C:50:VAL:CG2	2.38	0.53
1:A:398:VAL:HG12	1:A:399:VAL:N	2.23	0.52
2:B:161:LYS:NZ	2:B:226:TYR:HE1	2.06	0.52
1:A:4:ARG:HD3	1:A:165:GLY:O	2.08	0.52
3:C:68:ALA:C	3:C:69:ILE:HD12	2.34	0.52
2:B:241:ILE:C	2:B:243:GLN:N	2.67	0.52
2:B:375:LEU:HD11	2:B:401:LYS:HB2	1.90	0.52
3:C:23:GLU:HG3	3:C:24:GLU:N	2.25	0.52
2:B:154:GLU:HG3	2:B:155:PRO:HD2	1.92	0.52
2:B:202:GLN:C	2:B:204:LYS:H	2.15	0.52
2:B:228:GLU:O	2:B:232:GLU:HB2	2.10	0.52
1:A:329:TYR:HA	3:C:80:ASN:O	2.09	0.52
2:B:44:TYR:O	2:B:47:VAL:HG22	2.10	0.52
2:B:154:GLU:OE2	2:B:155:PRO:HD2	2.10	0.52
2:B:246:ARG:CA	2:B:258:MET:HG2	2.39	0.52
3:C:63:LEU:N	3:C:63:LEU:HD22	2.25	0.51
1:A:1:MET:N	1:A:28:ASP:HA	2.24	0.51
2:B:195:ILE:HG23	2:B:209:ALA:HB3	1.91	0.51
2:B:348:VAL:O	2:B:352:LEU:HD13	2.10	0.51
1:A:150:VAL:HG12	1:A:411:LEU:HD23	1.92	0.51
1:A:78:ILE:HD13	1:A:118:LEU:CD1	2.40	0.51
2:B:198:ARG:NH2	2:B:204:LYS:HG2	2.24	0.51
2:B:170:LEU:O	2:B:174:ILE:HD13	2.10	0.51
2:B:197:LEU:HB2	2:B:232:GLU:CG	2.40	0.51
2:B:255:THR:HG23	2:B:255:THR:O	2.10	0.51
1:A:169:LEU:C	1:A:169:LEU:HD23	2.36	0.51
2:B:379:GLY:C	2:B:381:MET:H	2.19	0.51
1:A:133:THR:O	1:A:133:THR:HG22	2.11	0.51
2:B:107:ILE:HG12	2:B:165:ALA:CB	2.38	0.51
2:B:256:ILE:O	2:B:256:ILE:CG1	2.58	0.51
1:A:185:TYR:O	1:A:450:PRO:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ILE:CD1	2:B:157:ILE:HD11	2.39	0.51
1:A:4:ARG:HD2	1:A:5:TYR:CZ	2.46	0.50
1:A:1:MET:HG2	1:A:4:ARG:NE	2.25	0.50
1:A:11:LEU:O	1:A:15:ILE:HG13	2.11	0.50
2:B:195:ILE:HD12	2:B:196:SER:N	2.27	0.50
2:B:393:LEU:HD23	2:B:393:LEU:O	2.11	0.50
2:B:211:LEU:HA	2:B:246:ARG:O	2.10	0.50
1:A:339:LEU:HB2	3:C:94:ILE:HD13	1.93	0.50
6:A:728:HOH:O	2:B:51:VAL:HG23	2.12	0.50
2:B:330:THR:O	2:B:333:HIS:HB2	2.12	0.50
2:B:220:VAL:CG2	2:B:221:ARG:H	2.20	0.50
2:B:331:ILE:HG13	2:B:332:GLU:N	2.25	0.49
2:B:365:THR:H	2:B:368:ASN:CG	2.20	0.49
1:A:3:ILE:HD13	1:A:11:LEU:HD11	1.93	0.49
2:B:182:VAL:CB	2:B:189:LEU:HD23	2.42	0.49
2:B:405:GLU:C	2:B:407:ASN:N	2.70	0.49
2:B:195:ILE:HD12	2:B:196:SER:H	1.77	0.49
2:B:243:GLN:CD	2:B:257:LEU:CD2	2.83	0.49
2:B:253:GLY:O	2:B:254:LYS:CD	2.60	0.49
2:B:359:LEU:HD13	2:B:359:LEU:C	2.37	0.49
2:B:25:SER:OG	2:B:38:ASN:ND2	2.46	0.49
2:B:225:GLU:CD	2:B:225:GLU:H	2.19	0.49
2:B:271:PRO:O	2:B:273:PRO:HD3	2.12	0.49
2:B:5:THR:HG23	2:B:229:LYS:HD3	1.93	0.49
2:B:132:HIS:NE2	3:C:93:THR:HG21	2.28	0.49
2:B:243:GLN:CG	2:B:257:LEU:HD23	2.42	0.49
3:C:72:ILE:HD12	3:C:76:LEU:HB3	1.93	0.49
1:A:21:LYS:HB2	1:A:59:ASP:OD1	2.12	0.49
2:B:189:LEU:HD13	2:B:190:ARG:N	2.28	0.49
2:B:331:ILE:C	2:B:333:HIS:H	2.21	0.49
2:B:21:MET:HE1	2:B:55:ALA:HB3	1.94	0.49
2:B:399:ASN:ND2	2:B:402:GLN:HB2	2.27	0.49
1:A:62:GLN:CG	1:A:67:MET:HE3	2.42	0.48
2:B:163:ALA:CB	2:B:221:ARG:NH1	2.75	0.48
2:B:176:TYR:CE1	2:B:296:PRO:HG3	2.48	0.48
2:B:259:ARG:HH12	2:B:262:GLU:N	2.11	0.48
2:B:198:ARG:CD	2:B:204:LYS:HA	2.43	0.48
2:B:227:GLU:HB2	2:B:254:LYS:HE3	1.94	0.48
2:B:240:GLU:O	2:B:242:GLY:N	2.43	0.48
2:B:375:LEU:HB2	2:B:381:MET:HE2	1.95	0.48
2:B:386:ALA:HA	2:B:389:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:PHE:CD1	3:C:41:GLN:NE2	2.81	0.48
2:B:360:LEU:H	2:B:360:LEU:CD1	2.21	0.48
2:B:400:ALA:C	2:B:402:GLN:H	2.20	0.48
1:A:390:ASP:O	1:A:394:GLU:HG3	2.14	0.48
2:B:7:ILE:HG22	2:B:8:GLY:N	2.28	0.48
2:B:56:VAL:HG22	2:B:123:MET:HE1	1.95	0.48
2:B:193:ALA:HB2	2:B:221:ARG:HH21	1.78	0.48
2:B:220:VAL:O	2:B:222:LYS:N	2.46	0.48
2:B:176:TYR:CZ	2:B:296:PRO:HG3	2.49	0.48
2:B:246:ARG:HB2	2:B:255:THR:OG1	2.13	0.48
2:B:382:SER:OG	2:B:385:ILE:HD13	2.14	0.48
1:A:117:VAL:O	1:A:119:ILE:HD12	2.14	0.48
1:A:1:MET:N	1:A:28:ASP:CG	2.72	0.48
1:A:26:VAL:HG21	1:A:55:ALA:HB2	1.95	0.48
1:A:339:LEU:H	3:C:94:ILE:CD1	2.27	0.48
1:A:382:ARG:HG3	1:A:433:LEU:HD12	1.95	0.48
2:B:126:ASP:CG	2:B:143:ARG:NH1	2.72	0.48
1:A:78:ILE:HD12	1:A:78:ILE:N	2.28	0.48
2:B:227:GLU:OE2	2:B:255:THR:HG22	2.14	0.48
1:A:485:LEU:HB3	6:A:678:HOH:O	2.14	0.48
1:A:1:MET:N	1:A:28:ASP:CA	2.77	0.47
1:A:484:LYS:O	1:A:485:LEU:CB	2.62	0.47
2:B:98:PRO:HG2	2:B:101:GLU:HG3	1.95	0.47
2:B:213:ASN:ND2	2:B:248:PHE:O	2.46	0.47
2:B:259:ARG:HH12	2:B:261:LYS:HA	1.79	0.47
1:A:398:VAL:CG1	1:A:399:VAL:N	2.77	0.47
1:A:484:LYS:O	1:A:485:LEU:HG	2.14	0.47
2:B:214:LEU:N	2:B:214:LEU:CD1	2.77	0.47
1:A:425:ASP:OD2	4:A:501:GLN:N	2.47	0.47
2:B:6:VAL:HG23	2:B:6:VAL:O	2.15	0.47
2:B:114:LYS:HE2	2:B:162:GLU:OE1	2.15	0.47
1:A:15:ILE:HG22	1:A:67:MET:CE	2.45	0.47
2:B:385:ILE:N	2:B:385:ILE:HD12	2.30	0.47
1:A:430:PRO:HB2	6:A:719:HOH:O	2.14	0.47
1:A:76:MET:H	1:A:119:ILE:HD13	1.79	0.46
2:B:61:ARG:HD2	2:B:291:THR:OG1	2.15	0.46
2:B:365:THR:HG22	2:B:368:ASN:CG	2.40	0.46
1:A:117:VAL:O	1:A:119:ILE:CD1	2.63	0.46
2:B:88:LYS:O	2:B:89:ALA:HB3	2.14	0.46
2:B:163:ALA:HB3	2:B:221:ARG:HH12	1.80	0.46
2:B:7:ILE:HD13	2:B:225:GLU:HG2	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:LEU:HD13	2:B:224:LEU:HG	1.97	0.46
1:A:83:ILE:HD13	1:A:103:TYR:CE1	2.51	0.46
1:A:338:SER:HB3	1:A:341:GLU:CG	2.40	0.46
2:B:126:ASP:OD2	2:B:143:ARG:NH1	2.48	0.46
2:B:185:GLU:HG3	2:B:186:GLU:N	2.31	0.46
2:B:211:LEU:CD1	2:B:214:LEU:HD11	2.46	0.46
3:C:94:ILE:HD12	3:C:94:ILE:N	2.31	0.46
1:A:339:LEU:H	3:C:94:ILE:CG1	2.28	0.46
1:A:12:LEU:HG	1:A:16:LYS:HE3	1.98	0.46
2:B:15:LEU:HB2	2:B:147:PRO:HB2	1.96	0.46
2:B:250:GLU:O	2:B:253:GLY:CA	2.64	0.46
1:A:4:ARG:HD2	1:A:5:TYR:CE2	2.50	0.46
2:B:183:LYS:HB3	2:B:185:GLU:HG2	1.97	0.46
2:B:259:ARG:HG3	2:B:259:ARG:HH11	1.80	0.46
1:A:264:PRO:HG2	1:A:267:TYR:CD2	2.51	0.46
1:A:264:PRO:HG2	1:A:267:TYR:CG	2.51	0.45
2:B:50:VAL:HG23	3:C:64:ARG:HE	1.81	0.45
1:A:75:PRO:HB3	1:A:119:ILE:HD11	1.98	0.45
2:B:348:VAL:HG22	2:B:390:PHE:CZ	2.51	0.45
2:B:209:ALA:CB	2:B:246:ARG:NH1	2.64	0.45
1:A:52:ILE:O	1:A:56:GLN:HG2	2.16	0.45
2:B:171:ARG:HD3	2:B:171:ARG:C	2.42	0.45
2:B:231:GLN:HA	2:B:234:GLU:CG	2.47	0.45
2:B:143:ARG:O	2:B:146:THR:HG23	2.17	0.45
2:B:220:VAL:C	2:B:222:LYS:N	2.72	0.45
1:A:276:VAL:HG21	1:A:406:THR:HA	1.98	0.45
2:B:220:VAL:CG2	2:B:221:ARG:N	2.78	0.45
2:B:229:LYS:O	2:B:230:ARG:C	2.59	0.45
2:B:237:ASN:C	2:B:237:ASN:ND2	2.74	0.45
1:A:391:LYS:HD3	1:A:394:GLU:OE1	2.17	0.45
2:B:33:PRO:HA	2:B:142:ASN:ND2	2.31	0.45
1:A:334:LYS:C	1:A:336:ALA:H	2.25	0.45
2:B:183:LYS:HB3	2:B:185:GLU:CG	2.47	0.45
2:B:276:VAL:HG22	6:B:700:HOH:O	2.17	0.45
3:C:20:ILE:O	3:C:20:ILE:HG23	2.16	0.45
1:A:169:LEU:HG	1:A:226:VAL:HG21	1.98	0.45
2:B:75:LYS:HG3	2:B:97:GLN:OE1	2.16	0.45
2:B:121:LEU:HD23	2:B:151:ILE:HG12	1.99	0.45
2:B:225:GLU:CD	2:B:225:GLU:N	2.75	0.45
1:A:78:ILE:CG2	1:A:82:ILE:HB	2.47	0.44
2:B:294:GLU:O	2:B:299:ARG:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:78:LEU:HD11	3:C:87:GLY:HA2	2.00	0.44
2:B:202:GLN:O	2:B:204:LYS:HG3	2.16	0.44
2:B:290:GLN:HG2	6:B:681:HOH:O	2.17	0.44
1:A:133:THR:OG1	1:A:156:GLY:HA3	2.18	0.44
1:A:322:SER:HB3	2:B:89:ALA:CB	2.47	0.44
2:B:104:TYR:CD1	2:B:104:TYR:C	2.95	0.44
2:B:107:ILE:HG13	2:B:108:GLU:N	2.32	0.44
2:B:245:THR:O	2:B:258:MET:HG3	2.18	0.44
1:A:134:GLU:HB2	1:A:415:ILE:HD13	2.00	0.44
2:B:411:GLN:H	2:B:411:GLN:HG3	1.36	0.44
2:B:215:ASN:HD22	2:B:215:ASN:N	2.12	0.44
2:B:108:GLU:HA	2:B:108:GLU:OE1	2.17	0.44
2:B:163:ALA:HB1	2:B:221:ARG:HH12	1.79	0.44
2:B:247:ARG:HB2	2:B:258:MET:HE2	1.99	0.44
2:B:249:ASP:HB3	2:B:252:THR:OG1	2.18	0.44
2:B:410:VAL:HG22	2:B:411:GLN:CD	2.43	0.44
2:B:196:SER:HB2	2:B:206:GLY:C	2.42	0.43
2:B:211:LEU:HD13	2:B:214:LEU:HD11	2.00	0.43
1:A:70:LYS:HE2	1:A:228:GLU:HB2	2.00	0.43
2:B:177:THR:OG1	2:B:179:VAL:HG22	2.18	0.43
2:B:350:GLU:HG2	6:B:657:HOH:O	2.18	0.43
2:B:371:GLY:O	2:B:375:LEU:HG	2.17	0.43
2:B:404:MET:O	2:B:410:VAL:HG23	2.18	0.43
2:B:68:MET:HG2	2:B:103:GLY:HA3	2.00	0.43
2:B:171:ARG:HD2	6:B:659:HOH:O	2.18	0.43
2:B:265:ASP:HA	6:B:672:HOH:O	2.17	0.43
1:A:1:MET:SD	1:A:35:GLU:CD	3.01	0.43
1:A:1:MET:HG3	1:A:32:ALA:CA	2.48	0.43
2:B:107:ILE:CG1	2:B:165:ALA:HB1	2.41	0.43
2:B:157:ILE:HD12	2:B:157:ILE:C	2.44	0.43
1:A:74:ILE:HA	1:A:75:PRO:HD3	1.82	0.43
1:A:78:ILE:HD13	1:A:118:LEU:HD13	1.99	0.43
2:B:240:GLU:CG	2:B:241:ILE:N	2.81	0.43
2:B:354:LYS:O	2:B:355:ASN:ND2	2.51	0.43
2:B:380:THR:O	2:B:404:MET:HE1	2.18	0.43
2:B:164:TYR:CD2	2:B:222:LYS:HD3	2.53	0.43
2:B:222:LYS:HE2	2:B:226:TYR:OH	2.18	0.43
2:B:247:ARG:H	2:B:258:MET:HG2	1.81	0.43
2:B:84:PRO:HB2	2:B:139:VAL:HG21	2.01	0.43
2:B:409:LEU:CD2	2:B:409:LEU:N	2.82	0.43
1:A:79:LYS:C	1:A:81:ASN:N	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:ILE:CD1	2:B:108:GLU:H	2.31	0.43
2:B:243:GLN:O	2:B:244:GLU:OE1	2.37	0.43
2:B:161:LYS:H	2:B:161:LYS:CD	2.30	0.43
2:B:309:LEU:HG	2:B:313:ASP:HB2	2.01	0.43
2:B:362:THR:OG1	2:B:364:LEU:HD23	2.18	0.43
1:A:206:PHE:HB3	1:A:211:ASP:OD1	2.19	0.42
1:A:484:LYS:O	1:A:485:LEU:HB2	2.19	0.42
2:B:6:VAL:HG22	2:B:196:SER:O	2.18	0.42
2:B:327:PHE:HB2	2:B:344:LEU:CD1	2.49	0.42
1:A:192:LYS:HE2	6:A:527:HOH:O	2.19	0.42
2:B:157:ILE:HD12	2:B:158:ARG:N	2.34	0.42
2:B:276:VAL:HG23	6:B:609:HOH:O	2.18	0.42
2:B:375:LEU:CD2	2:B:401:LYS:HD3	2.43	0.42
3:C:38:PHE:O	3:C:41:GLN:NE2	2.44	0.42
1:A:58:LEU:HD22	1:A:72:PHE:CE2	2.55	0.42
1:A:90:THR:C	1:A:92:ALA:N	2.75	0.42
1:A:126:GLU:OE1	1:A:352:GLY:HA3	2.18	0.42
1:A:174:ASP:HB3	1:A:192:LYS:HG3	2.01	0.42
2:B:198:ARG:NH2	2:B:204:LYS:HZ2	2.17	0.42
2:B:322:GLU:H	2:B:322:GLU:CD	2.28	0.42
3:C:61:ASN:C	3:C:63:LEU:HD22	2.44	0.42
2:B:363:LYS:O	2:B:363:LYS:HG3	2.20	0.42
1:A:62:GLN:HG3	1:A:67:MET:CE	2.48	0.42
2:B:331:ILE:C	2:B:333:HIS:N	2.78	0.42
1:A:78:ILE:HG12	1:A:108:MET:SD	2.60	0.42
2:B:16:LYS:CG	2:B:180:SER:HA	2.43	0.42
1:A:20:ILE:HG12	1:A:21:LYS:N	2.35	0.42
1:A:44:LEU:HD22	1:A:123:ASN:HA	2.02	0.42
1:A:209:SER:OG	1:A:382:ARG:NH2	2.50	0.42
2:B:107:ILE:CG1	2:B:108:GLU:N	2.83	0.42
2:B:368:ASN:OD1	2:B:369:LEU:N	2.53	0.42
1:A:476:TYR:CD1	1:A:476:TYR:C	2.98	0.41
2:B:135:GLU:HA	2:B:135:GLU:OE1	2.19	0.41
1:A:1:MET:H2	1:A:28:ASP:CA	2.32	0.41
1:A:400:VAL:HG22	1:A:401:GLY:N	2.35	0.41
1:A:348:SER:OG	3:C:19:GLN:N	2.53	0.41
2:B:403:ILE:O	2:B:407:ASN:CB	2.63	0.41
2:B:211:LEU:HD12	2:B:211:LEU:O	2.21	0.41
2:B:372:MET:HG2	2:B:381:MET:HE1	2.01	0.41
2:B:400:ALA:C	2:B:402:GLN:N	2.78	0.41
1:A:62:GLN:CB	1:A:67:MET:HE3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LEU:CD1	1:A:392:VAL:HG21	2.51	0.41
2:B:163:ALA:O	2:B:167:LEU:HG	2.21	0.41
2:B:376:ILE:C	2:B:378:ASP:H	2.28	0.41
3:C:67:LYS:HD3	3:C:67:LYS:C	2.45	0.41
1:A:132:SER:O	1:A:133:THR:HB	2.19	0.41
1:A:335:GLU:CD	1:A:335:GLU:N	2.77	0.41
2:B:294:GLU:CG	2:B:298:GLU:OE1	2.68	0.41
2:B:351:TYR:CE2	2:B:394:ALA:HB3	2.56	0.41
3:C:21:SER:HA	3:C:22:PRO:HD3	1.93	0.41
3:C:85:GLU:O	3:C:86:ASP:HB2	2.21	0.41
1:A:44:LEU:HB3	1:A:45:ALA:H	1.76	0.41
2:B:263:GLY:O	2:B:264:SER:HB2	2.21	0.41
1:A:90:THR:HA	1:A:96:LEU:HB3	2.02	0.41
2:B:34:ASN:ND2	3:C:88:GLN:HA	2.35	0.41
2:B:221:ARG:HB2	2:B:221:ARG:HE	1.79	0.41
2:B:385:ILE:HD12	2:B:385:ILE:H	1.86	0.41
2:B:389:VAL:HG23	2:B:390:PHE:N	2.35	0.41
3:C:39:ALA:C	3:C:41:GLN:H	2.28	0.41
1:A:364:PHE:CD1	1:A:364:PHE:C	2.99	0.40
2:B:164:TYR:CD1	2:B:164:TYR:C	2.99	0.40
2:B:167:LEU:HD13	2:B:217:PHE:CE1	2.56	0.40
2:B:211:LEU:CD1	2:B:214:LEU:HD21	2.51	0.40
2:B:224:LEU:HD21	2:B:248:PHE:CG	2.57	0.40
2:B:106:ASP:O	2:B:169:LYS:HE2	2.22	0.40
3:C:3:LYS:CD	3:C:4:VAL:N	2.80	0.40
1:A:1:MET:N	1:A:28:ASP:CB	2.74	0.40
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.85	0.40
1:A:206:PHE:C	1:A:206:PHE:CD1	2.98	0.40
2:B:5:THR:HA	2:B:197:LEU:HD13	2.03	0.40
2:B:246:ARG:N	2:B:246:ARG:CD	2.79	0.40
2:B:329:SER:O	2:B:332:GLU:HG2	2.21	0.40
3:C:3:LYS:O	3:C:4:VAL:HB	2.21	0.40
1:A:76:MET:HG3	1:A:78:ILE:HD11	2.04	0.40
1:A:105:SER:CB	1:A:202:GLY:HA3	2.52	0.40
1:A:277:LYS:O	1:A:281:GLN:HG3	2.22	0.40
2:B:197:LEU:HD23	2:B:232:GLU:CG	2.50	0.40
2:B:390:PHE:HB3	2:B:391:PRO:HD3	2.03	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%)	464 (96%)	17 (4%)	2 (0%)	30	38
2	B	406/483 (84%)	345 (85%)	44 (11%)	17 (4%)	2	1
3	C	90/100 (90%)	83 (92%)	5 (6%)	2 (2%)	5	4
All	All	979/1068 (92%)	892 (91%)	66 (7%)	21 (2%)	5	4

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	217	PHE
2	B	240	GLU
2	B	250	GLU
2	B	257	LEU
2	B	397	GLY
2	B	210	GLU
2	B	219	TYR
2	B	220	VAL
2	B	221	ARG
2	B	241	ILE
2	B	253	GLY
2	B	261	LYS
2	B	264	SER
2	B	355	ASN
1	A	335	GLU
1	A	80	ASP
3	C	23	GLU
2	B	238	GLY
2	B	362	THR
3	C	4	VAL
2	B	242	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%)	386 (95%)	20 (5%)	22	34
2	B	354/419 (84%)	318 (90%)	36 (10%)	7	8
3	C	81/88 (92%)	75 (93%)	6 (7%)	13	17
All	All	841/913 (92%)	779 (93%)	62 (7%)	13	17

All (62) 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	22	PRO
1	A	44	LEU
1	A	96	LEU
1	A	122	LEU
1	A	169	LEU
1	A	171	LEU
1	A	206	PHE
1	A	210	LEU
1	A	215	PRO
1	A	221	LYS
1	A	263	LEU
1	A	299	LEU
1	A	335	GLU
1	A	361	LEU
1	A	382	ARG
1	A	433	LEU
1	A	485	LEU
2	B	105	ILE
2	B	121	LEU
2	B	157	ILE
2	B	189	LEU
2	B	194	ASN
2	B	195	ILE

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Mol	Chain	Res	Type
2	B	198	ARG
2	B	202	GLN
2	B	218	ASN
2	B	221	ARG
2	B	224	LEU
2	B	227	GLU
2	B	235	LEU
2	B	237	ASN
2	B	246	ARG
2	B	247	ARG
2	B	256	ILE
2	B	258	MET
2	B	298	GLU
2	B	317	LEU
2	B	350	GLU
2	B	355	ASN
2	B	359	LEU
2	B	363	LYS
2	B	387	LYS
2	B	388	LYS
2	B	392	GLU
2	B	399	ASN
2	B	402	GLN
2	B	404	MET
2	B	405	GLU
2	B	406	ASP
2	B	407	ASN
2	B	409	LEU
2	B	410	VAL
2	B	411	GLN
3	C	3	LYS
3	C	23	GLU
3	C	27	GLU
3	C	38	PHE
3	C	57	LEU
3	C	76	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	85	ASN

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Mol	Chain	Res	Type
1	A	301	ASN
1	A	471	GLN
2	B	28	HIS
2	B	194	ASN
2	B	215	ASN
2	B	237	ASN
2	B	290	GLN
2	B	315	HIS
2	B	355	ASN
2	B	402	GLN
3	C	11	HIS
3	C	14	ASN
3	C	30	ASN
3	C	55	HIS
3	C	60	GLN
3	C	80	ASN
3	C	88	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GLN	A	501	-	8,9,9	3.39	2 (25%)	8,11,11	2.26	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLN	A	501	-	-	0/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	GLN	OE1-CD	6.78	1.44	1.23
4	A	501	GLN	OXT-C	6.51	1.51	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	GLN	OE1-CD-NE2	-4.18	111.37	122.53
4	A	501	GLN	CB-CG-CD	4.02	126.21	112.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	GLN	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	485/485 (100%)	-0.25	3 (0%) 85 86	21, 34, 56, 74	0
2	B	408/483 (84%)	0.82	76 (18%) 3 4	25, 53, 95, 96	0
3	C	92/100 (92%)	0.68	7 (7%) 20 21	34, 56, 83, 88	0
All	All	985/1068 (92%)	0.28	86 (8%) 16 17	21, 41, 95, 96	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	221	ARG	9.8
2	B	224	LEU	9.6
2	B	411	GLN	7.2
1	A	1	MET	6.7
2	B	246	ARG	6.0
2	B	220	VAL	6.0
2	B	263	GLY	5.2
2	B	241	ILE	5.1
2	B	225	GLU	4.8
2	B	257	LEU	4.7
2	B	260	VAL	4.7
2	B	242	GLY	4.5
2	B	223	GLY	4.5
3	C	94	ILE	4.4
2	B	211	LEU	4.2
2	B	205	PHE	4.2
2	B	248	PHE	4.2
2	B	240	GLU	4.1
3	C	38	PHE	4.1
2	B	398	GLY	3.9
2	B	232	GLU	3.9
2	B	217	PHE	3.7
2	B	228	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	401	LYS	3.5
2	B	245	THR	3.5
3	C	22	PRO	3.4
2	B	203	GLU	3.4
2	B	229	LYS	3.3
2	B	359	LEU	3.2
2	B	214	LEU	3.2
2	B	5	THR	3.2
2	B	235	LEU	3.1
2	B	256	ILE	3.1
2	B	226	TYR	3.1
2	B	195	ILE	3.1
2	B	397	GLY	3.1
2	B	236	LEU	3.1
2	B	219	TYR	3.0
2	B	207	THR	3.0
2	B	409	LEU	3.0
2	B	395	ALA	2.8
2	B	216	SER	2.8
2	B	239	GLY	2.8
2	B	231	GLN	2.8
2	B	222	LYS	2.8
2	B	134	GLY	2.8
2	B	243	GLN	2.7
2	B	28	HIS	2.7
2	B	197	LEU	2.7
2	B	364	LEU	2.6
2	B	200	TYR	2.6
2	B	201	GLY	2.6
2	B	107	ILE	2.6
2	B	215	ASN	2.5
2	B	7	ILE	2.5
2	B	193	ALA	2.5
2	B	352	LEU	2.5
2	B	136	TYR	2.5
2	B	4	GLU	2.4
2	B	265	ASP	2.4
2	B	255	THR	2.4
2	B	360	LEU	2.4
2	B	408	GLY	2.4
2	B	209	ALA	2.4
3	C	36	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	380	THR	2.3
2	B	218	ASN	2.3
2	B	261	LYS	2.3
3	C	58	ASP	2.3
2	B	237	ASN	2.3
2	B	396	LYS	2.3
2	B	400	ALA	2.2
1	A	338	SER	2.2
2	B	230	ARG	2.2
3	C	81	ALA	2.2
2	B	167	LEU	2.2
2	B	262	GLU	2.2
2	B	208	LYS	2.2
2	B	198	ARG	2.2
2	B	393	LEU	2.2
2	B	403	ILE	2.2
2	B	410	VAL	2.2
2	B	238	GLY	2.1
1	A	3	ILE	2.1
2	B	194	ASN	2.1
3	C	4	VAL	2.1

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 oligosaccharides 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. 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	GLN	A	501	10/10	0.93	0.08	21,25,30,31	0
5	MG	B	601	1/1	0.98	0.03	52,52,52,52	0

6.5 Other polymers ⓘ

There are no such residues in this entry.