



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 05:04 PM EST

PDB ID : 2F2A  
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](mailto: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>.

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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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

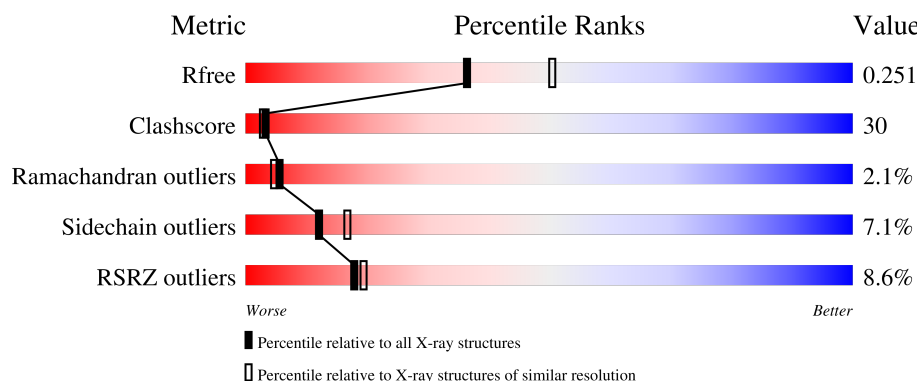
# 1 Overall quality at a glance

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))
$R_{free}$	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

## 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			

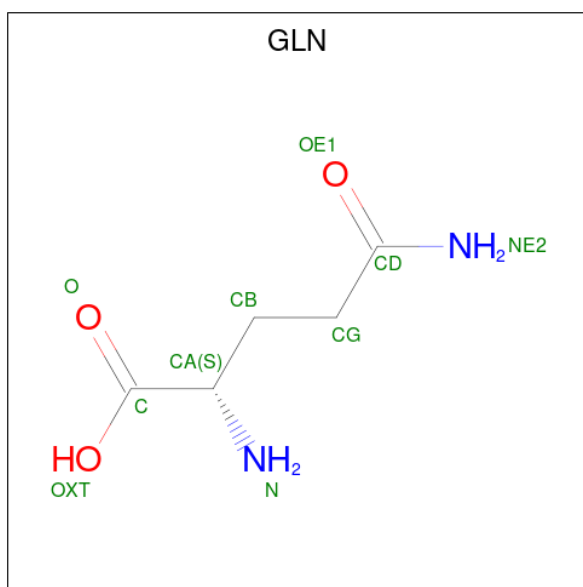
There are 8 discrepancies between the modelled and reference sequences:

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 (three-letter code: GLN) (formula: C<sub>5</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

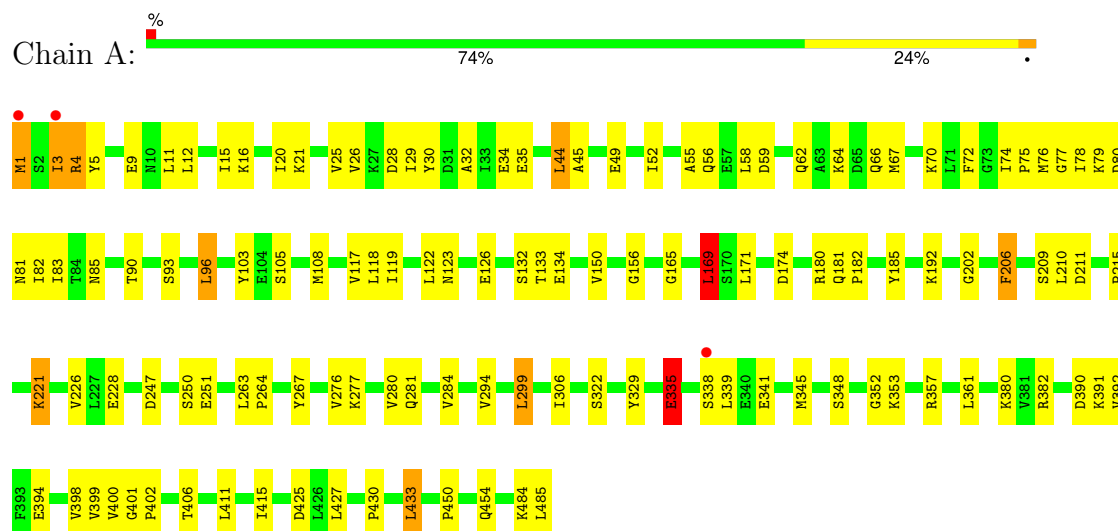
- Molecule 6 is water.

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		

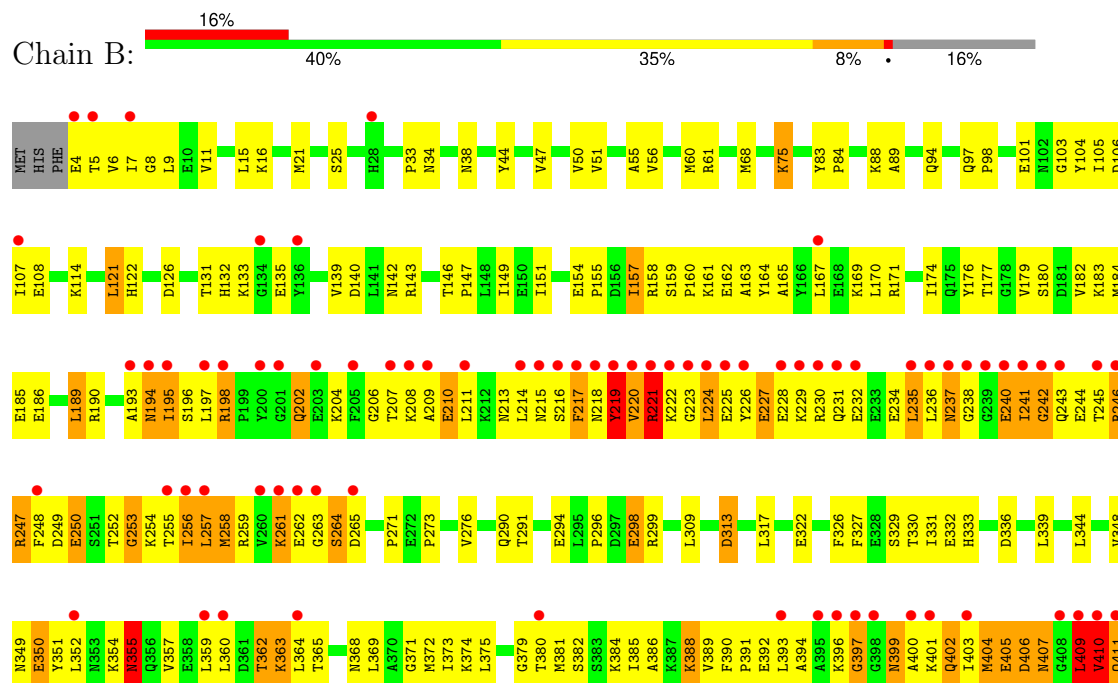
### 3 Residue-property plots

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



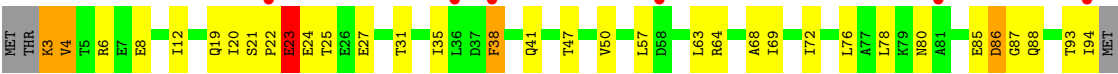
- Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B



ILE  
SER  
ASP  
LYS  
GLU  
ARG  
ALA  
LEU  
THR  
LEU  
LEU  
LYS  
PHE  
VAL  
ASN  
GLU  
ALA  
LEU  
ASP  
ASP  
ASN  
ASN  
GLU  
GLN  
SER  
VAL  
GLU  
ASP  
TYR  
LYS  
ASN  
GLY  
GLY  
LYS  
ALA  
MET  
GLY  
PHE  
LEU  
VAL  
GLY  
GLN  
ILE  
MET  
LYS  
ALA  
SER  
LYS  
GLY  
GLN  
ALA  
ASN  
PRO  
GLN  
LEU  
VAL  
ASN  
GLN  
LEU  
LYS  
GLN  
GLU

LEU  
ASP  
LYS  
ARG  
LEU  
GLU  
HIS  
HIS  
HIS  
HIS  
HIS

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



ASN  
GLU  
GLU  
ASP  
ALA

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	5527 reflections (9.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.3	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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.*

<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, 0.333 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	0.36	0/3784	0.63	1/5116 (0.0%)
2	B	0.35	0/3306	0.67	3/4464 (0.1%)
3	C	0.29	0/734	0.55	0/993
All	All	0.35	0/7824	0.64	4/10573 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	LEU	CA-CB-CG	6.73	130.78	115.30
2	B	410	VAL	N-CA-C	6.13	127.55	111.00
2	B	409	LEU	CA-CB-CG	5.50	127.94	115.30
2	B	258	MET	N-CA-C	5.31	125.34	111.00

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	116	0
2	B	3245	0	3198	322	0
3	C	726	0	717	34	0
4	A	10	0	7	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	458	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 30.

All (458) 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
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:227:GLU:HB2	2:B:254:LYS:HD2	1.56	0.85
2:B:235:LEU:HD12	2:B:240:GLU:HB2	1.57	0.84
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
1:A:49:GLU:H	1:A:49:GLU:CD	1.83	0.82
2:B:401:LYS:HE2	2:B:411:GLN:CD	2.00	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
2:B:240:GLU:C	2:B:242:GLY:H	1.82	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
1:A:402:PRO:HG2	1:A:427:LEU:HD13	1.64	0.79
2:B:214:LEU:HD23	2:B:221:ARG:HB2	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:THR:C	2:B:246:ARG:HD3	2.03	0.79
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
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
3:C:93:THR:C	3:C:94:ILE:HD12	2.07	0.75
2:B:246:ARG:HA	2:B:258:MET:HG2	1.69	0.75
2:B:403:ILE:C	2:B:405:GLU:H	1.87	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:243:GLN:CD	2:B:257:LEU:HD23	2.08	0.73
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: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
1:A:15:ILE:HG22	1:A:67:MET:HE2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HZ2	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
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: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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:LEU:HD21	2:B:221:ARG:NH2	2.14	0.62
2:B:403:ILE:C	2:B:405:GLU:N	2.49	0.62
1:A:402:PRO:HG2	1:A:427:LEU:CD1	2.29	0.62
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
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
1:A:79:LYS:C	1:A:81:ASN:H	2.03	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
3:C:6:ARG:HG3	3:C:25:THR:HG21	1.84	0.60
2:B:241:ILE:C	2:B:243:GLN:H	2.04	0.60
2:B:207:THR:HG23	2:B:208:LYS:N	2.17	0.59
2:B:227:GLU:HB2	2:B:254:LYS:CE	2.32	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
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:240:GLU:C	2:B:242:GLY:N	2.53	0.58
2:B:372:MET:HE1	2:B:389:VAL:HG23	1.84	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: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: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:306:ILE:HG22	3:C:38:PHE:HZ	1.70	0.57
1:A:335:GLU:CD	1:A:335:GLU:H	2.06	0.57
2:B:363:LYS:HB3	2:B:394:ALA:O	2.05	0.57
2:B:7:ILE:HB	2:B:157:ILE:HD11	1.87	0.56
2:B:214:LEU:C	2:B:215:ASN:HD22	2.09	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: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
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:227:GLU:CD	2:B:254:LYS:HD2	2.28	0.53
3:C:47:THR:O	3:C:50:VAL:HG22	2.07	0.53
1:A:62:GLN:HG3	1:A:67:MET:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:GLN:C	2:B:204:LYS:N	2.61	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:1:MET:H2	1:A:28:ASP:CG	2.11	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:405:GLU:C	2:B:407:ASN:H	2.12	0.52
1:A:77:GLY:C	1:A:78:ILE:HD12	2.29	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
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:228:GLU:O	2:B:232:GLU:HB2	2.10	0.52
2:B:161:LYS:HZ3	2:B:226:TYR:HE1	1.57	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
2:B:237:ASN:C	2:B:237:ASN:HD22	2.13	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:240:GLU:CD	2:B:241:ILE:H	2.14	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:62:GLN:HE21	1:A:67:MET:HE1	1.77	0.49
2:B:195:ILE:HD12	2:B:196:SER:H	1.77	0.49
2:B:253:GLY:O	2:B:254:LYS:CD	2.60	0.49
2:B:25:SER:OG	2:B:38:ASN:ND2	2.46	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:399:ASN:ND2	2:B:402:GLN:HB2	2.27	0.49
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:7:ILE:HG22	2:B:8:GLY:N	2.28	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:386:ALA:HA	2:B:389:VAL:HG22	1.95	0.48
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
1:A:390:ASP:O	1:A:394:GLU:HG3	2.14	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:26:VAL:HG21	1:A:55:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:202:GLN:C	2:B:204:LYS:H	2.15	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:CB	2.62	0.47
2:B:88:LYS:O	2:B:89:ALA:HB3	2.14	0.47
2:B:98:PRO:HG2	2:B:101:GLU:HG3	1.95	0.47
2:B:241:ILE:C	2:B:243:GLN:N	2.67	0.47
3:C:68:ALA:C	3:C:69:ILE:HD12	2.34	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: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
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:372:MET:HE1	2:B:390:PHE:CA	2.45	0.46
1:A:117:VAL:O	1:A:119:ILE:CD1	2.63	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
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:169:LEU:C	1:A:169:LEU:HD23	2.36	0.46
1:A:339:LEU:H	3:C:94:ILE:CG1	2.28	0.46
2:B:379:GLY:C	2:B:381:MET:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:225:GLU:CD	2:B:225:GLU:H	2.19	0.45
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: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
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
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
2:B:372:MET:HE3	2:B:393:LEU:HD13	1.98	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
2:B:365:THR:H	2:B:368:ASN:CG	2.20	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:359:LEU:HD13	2:B:359:LEU:C	2.37	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
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: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:243:GLN:CD	2:B:257:LEU:CD2	2.83	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:331:ILE:C	2:B:333:HIS:H	2.21	0.44
2:B:372:MET:HE1	2:B:390:PHE:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:249:ASP:HB3	2:B:252:THR:OG1	2.18	0.44
2:B:400:ALA:C	2:B:402:GLN:H	2.20	0.44
2:B:405:GLU:C	2:B:407:ASN:N	2.70	0.44
2:B:211:LEU:HD13	2:B:214:LEU:HD11	2.00	0.43
1:A:1:MET:N	1:A:28:ASP:CG	2.72	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:240:GLU:CG	2:B:241:ILE:N	2.81	0.43
2:B:265:ASP:HA	6:B:672:HOH:O	2.17	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
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:126:ASP:CG	2:B:143:ARG:NH1	2.72	0.43
2:B:354:LYS:O	2:B:355:ASN:ND2	2.51	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
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
1:A:62:GLN:HG3	1:A:67:MET:CE	2.48	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:15:ILE:HG22	1:A:67:MET:CE	2.45	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:363:LYS:O	2:B:363:LYS:HG3	2.20	0.42
2:B:380:THR:O	2:B:404:MET:HE1	2.19	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
2:B:21:MET:HE1	2:B:55:ALA:HB3	2.01	0.42
1:A:20:ILE:HG12	1:A:21:LYS:N	2.35	0.42
1:A:49:GLU:CD	1:A:49:GLU:N	2.59	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:365:THR:HG22	2:B:368:ASN:CG	2.40	0.42
2:B:368:ASN:OD1	2:B:369:LEU:N	2.53	0.42
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:132:SER:O	1:A:133:THR:HB	2.19	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
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:220:VAL:C	2:B:222:LYS:N	2.72	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:171:ARG:HD3	2:B:171:ARG:C	2.42	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
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
1:A:1:MET:HE3	1:A:1:MET:HB3	2.01	0.40
2:B:229:LYS:O	2:B:230:ARG:C	2.59	0.40
2:B:237:ASN:C	2:B:237:ASN:ND2	2.74	0.40
2:B:329:SER:O	2:B:332:GLU:HG2	2.21	0.40
2:B:372:MET:CE	2:B:390:PHE:HA	2.51	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 [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%)	464 (96%)	17 (4%)	2 (0%)	30	39
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	5

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%)	388 (96%)	18 (4%)	24	35
2	B	354/419 (84%)	318 (90%)	36 (10%)	6	7
3	C	81/88 (92%)	75 (93%)	6 (7%)	11	15
All	All	841/913 (92%)	781 (93%)	60 (7%)	12	17

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	ILE

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Mol	Chain	Res	Type
1	A	4	ARG
1	A	44	LEU
1	A	85	ASN
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	433	LEU
2	B	75	LYS
2	B	121	LEU
2	B	157	ILE
2	B	189	LEU
2	B	194	ASN
2	B	195	ILE
2	B	198	ARG
2	B	202	GLN
2	B	218	ASN
2	B	219	TYR
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	298	GLU
2	B	313	ASP
2	B	317	LEU
2	B	349	ASN
2	B	350	GLU
2	B	355	ASN
2	B	363	LYS
2	B	388	LYS

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Mol	Chain	Res	Type
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	86	ASP

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

Mol	Chain	Res	Type
1	A	56	GLN
1	A	85	ASN
2	B	28	HIS
2	B	194	ASN
2	B	215	ASN
2	B	237	ASN
2	B	290	GLN
2	B	355	ASN
2	B	399	ASN
2	B	402	GLN
3	C	30	ASN
3	C	60	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 [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, 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%)	-0.35	3 (0%) 85 86	21, 34, 56, 74	0
2	B	408/483 (84%)	0.73	76 (18%) 4 5	25, 53, 95, 96	0
3	C	92/100 (92%)	0.58	6 (6%) 26 28	34, 56, 83, 88	0
All	All	985/1068 (92%)	0.18	85 (8%) 18 19	21, 41, 95, 96	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	221	ARG	9.9
2	B	224	LEU	9.5
2	B	411	GLN	7.2
1	A	1	MET	6.6
2	B	246	ARG	6.0
2	B	220	VAL	5.8
2	B	263	GLY	5.1
2	B	241	ILE	5.0
2	B	225	GLU	4.8
2	B	257	LEU	4.6
2	B	260	VAL	4.6
2	B	242	GLY	4.4
2	B	223	GLY	4.3
3	C	94	ILE	4.3
2	B	240	GLU	4.2
2	B	211	LEU	4.1
2	B	205	PHE	4.1
2	B	248	PHE	4.1
3	C	38	PHE	4.0
2	B	232	GLU	3.9
2	B	398	GLY	3.8
2	B	228	GLU	3.7
2	B	217	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	401	LYS	3.5
2	B	203	GLU	3.4
2	B	245	THR	3.4
2	B	229	LYS	3.3
3	C	22	PRO	3.3
2	B	359	LEU	3.1
2	B	214	LEU	3.1
2	B	5	THR	3.1
2	B	256	ILE	3.0
2	B	235	LEU	3.0
2	B	195	ILE	3.0
2	B	226	TYR	3.0
2	B	397	GLY	3.0
2	B	236	LEU	2.9
2	B	207	THR	2.9
2	B	409	LEU	2.9
2	B	219	TYR	2.9
2	B	222	LYS	2.8
2	B	231	GLN	2.7
2	B	216	SER	2.7
2	B	395	ALA	2.7
2	B	243	GLN	2.7
2	B	239	GLY	2.7
2	B	134	GLY	2.6
2	B	28	HIS	2.6
2	B	197	LEU	2.5
2	B	364	LEU	2.5
2	B	201	GLY	2.5
2	B	215	ASN	2.5
2	B	200	TYR	2.4
2	B	107	ILE	2.4
2	B	4	GLU	2.4
2	B	7	ILE	2.4
2	B	193	ALA	2.4
2	B	352	LEU	2.4
2	B	265	ASP	2.4
2	B	136	TYR	2.3
2	B	255	THR	2.3
2	B	360	LEU	2.3
2	B	408	GLY	2.3
2	B	261	LYS	2.3
3	C	36	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	209	ALA	2.2
3	C	58	ASP	2.2
2	B	396	LYS	2.2
2	B	218	ASN	2.2
2	B	380	THR	2.2
2	B	237	ASN	2.2
2	B	230	ARG	2.2
2	B	208	LYS	2.2
1	A	338	SER	2.1
2	B	262	GLU	2.1
2	B	198	ARG	2.1
2	B	400	ALA	2.1
2	B	167	LEU	2.1
3	C	81	ALA	2.1
2	B	403	ILE	2.1
2	B	393	LEU	2.1
2	B	410	VAL	2.0
2	B	238	GLY	2.0
1	A	3	ILE	2.0
2	B	194	ASN	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 monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	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 [i](#)

There are no such residues in this entry.