Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:58 AM GMT

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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

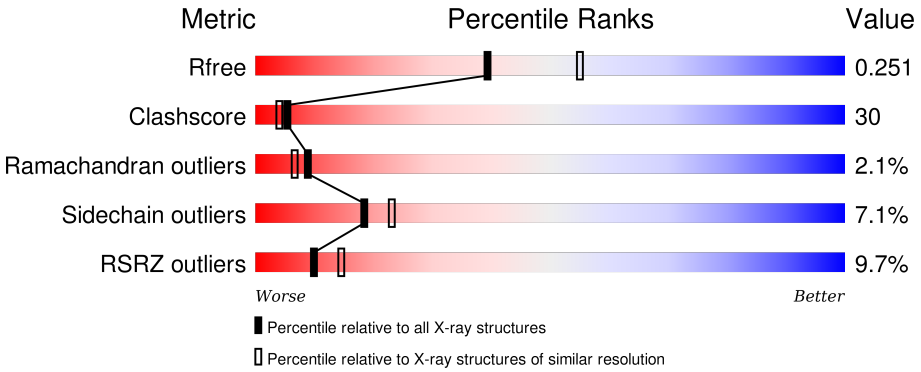
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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% 74% 24%
2	B	483	15% 40% 35% 8% 16%
3	C	100	12% 58% 29% 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

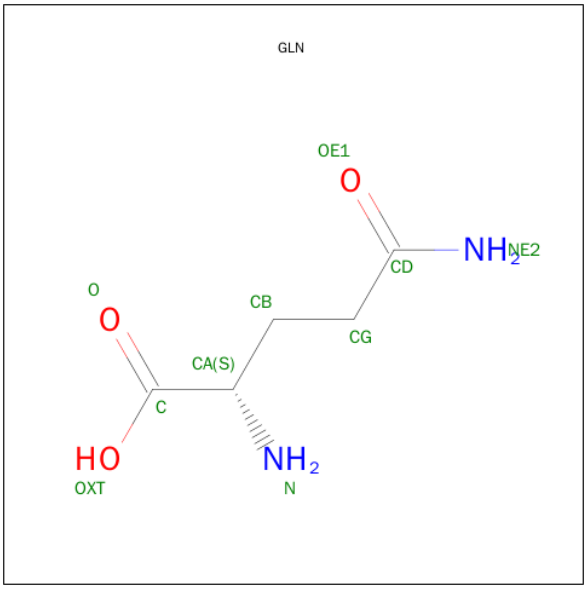
- Molecule 3 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit C.

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

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

- Molecule 5 is GLUTAMINE (three-letter code: GLN) (formula: $C_5H_{10}N_2O_3$).



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

- Molecule 6 is water.

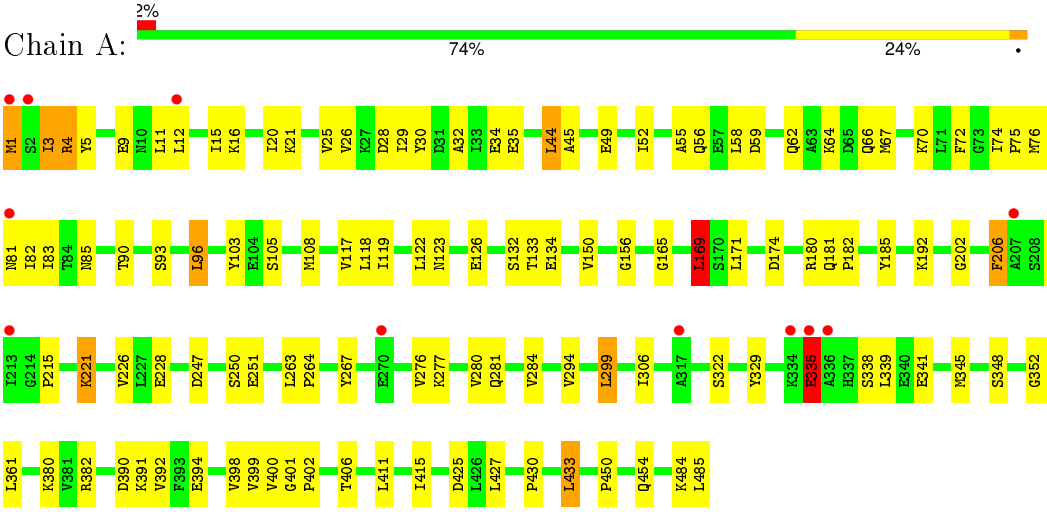
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	239	Total O 239 239	0	0
6	B	117	Total O 117 117	0	0
6	C	37	Total O 37 37	0	0

3 Residue-property plots (i)

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

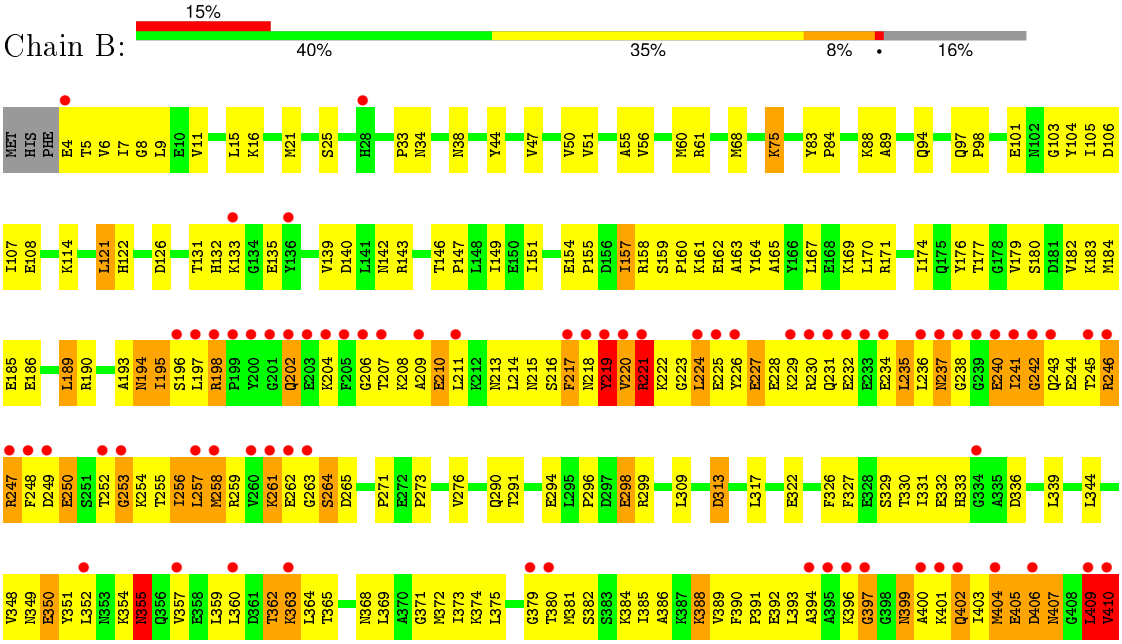
- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

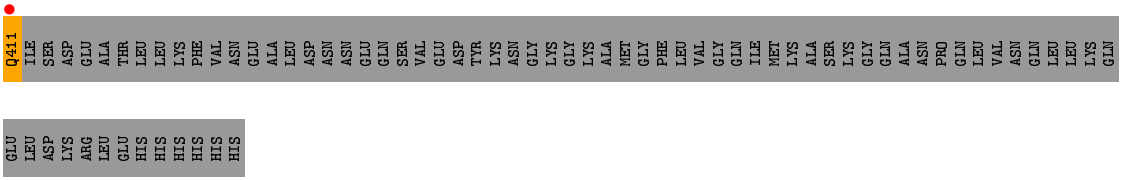
Chain A:



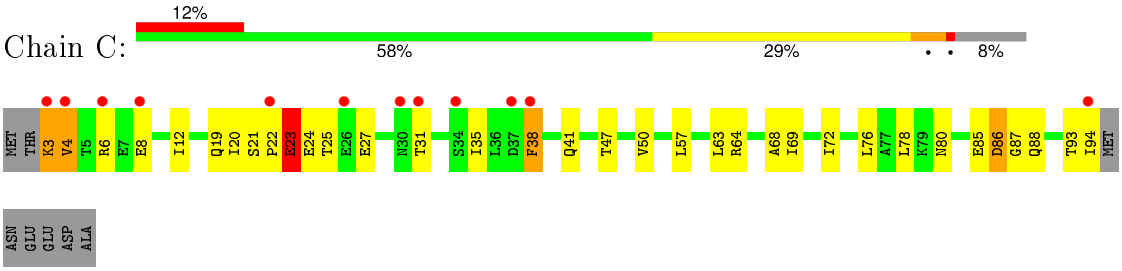
- Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain B:





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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.19Å 88.22Å 183.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 47.92 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.30) 99.6 (47.92-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [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	5525 reflections (9.81%)	DCC
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 , 50.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 64069 reflections	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.36	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(^{o})	Ideal(^{o})
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	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	10	0	7	1	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:NH1	2:B:247:ARG:HB2	1.93	0.82
2:B:360:LEU:HD12	2:B:360:LEU:H	1.42	0.82
1:A:49:GLU:CD	1:A:49:GLU:H	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

Continued on next page...

Continued from previous page...

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:HD12	2:B:257:LEU:N	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:407:ASN:HB3	2:B:409:LEU:CD2	2.15	0.76
2:B:326:PHE:CD2	2:B:359:LEU:HD11	2.20	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: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
2:B:7:ILE:HB	2:B:157:ILE:HG13	1.68	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
2:B:227:GLU:O	2:B:230:ARG:HB3	1.87	0.74
1:A:353:LYS:HG2	1:A:357:ARG:HH12	1.51	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:O	2:B:236:LEU:HD23	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
2:B:375:LEU:HD22	2:B:401:LYS:HD3	1.71	0.71
1:A:382:ARG:HD3	1:A:433:LEU:O	1.90	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:O	2:B:256:ILE:HG13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ILE:HG22	1:A:67:MET:HE2	1.73	0.69
2:B:257:LEU:HD12	2:B:257:LEU:H	1.58	0.69
2:B:220:VAL:HG23	2:B:221:ARG:N	2.06	0.69
1:A:1:MET:HG2	1:A:4:ARG:HE	1.57	0.69
2:B:388:LYS:HZ2	2:B:388:LYS:HA	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:HB2	2:B:232:GLU:HG2	1.79	0.64
2:B:197:LEU:HD23	2:B:232:GLU:HG2	1.80	0.64
2:B:161:LYS:N	2:B:161:LYS:HD2	2.13	0.64
1:A:1:MET:SD	1:A:35:GLU:OE1	2.55	0.64
3:C:86:ASP:HB3	6:C:120:HOH:O	1.97	0.64
2:B:121:LEU:CD2	2:B:151:ILE:HG12	2.28	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
2:B:215:ASN:H	2:B:220:VAL:HG21	1.63	0.63
1:A:3:ILE:CD1	1:A:25:VAL:HG13	2.28	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
2:B:195:ILE:HD11	2:B:197:LEU:CD2	2.30	0.62
1:A:64:LYS:O	1:A:66:GLN:HG3	1.99	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

Continued on next page...

Continued from previous page...

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:N	2:B:246:ARG:HD3	2.15	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:167:LEU:HD21	2:B:221:ARG:HD2	1.80	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
2:B:215:ASN:H	2:B:220:VAL:CG2	2.13	0.61
2:B:198:ARG:NH2	2:B:204:LYS:NZ	2.46	0.61
1:A:29:ILE:HG21	1:A:119:ILE:HG12	1.81	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:HD22	2:B:409:LEU:N	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:H	2:B:364:LEU:HD23	1.67	0.59
2:B:219:TYR:O	2:B:222:LYS:HB3	2.03	0.58
2:B:198:ARG:HD2	2:B:204:LYS:HA	1.83	0.58
2:B:107:ILE:HD12	2:B:108:GLU:H	1.68	0.58
2:B:384:LYS:CA	2:B:384:LYS:HE2	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
3:C:3:LYS:HD3	3:C:4:VAL:H	1.68	0.58
2:B:185:GLU:HG3	2:B:186:GLU:HG3	1.85	0.58
2:B:121:LEU:HD22	2:B:151:ILE:HG12	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:HD21	2:B:149:ILE:HD12	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ILE:HB	2:B:157:ILE:CD1	2.34	0.57
1:A:339:LEU:H	3:C:94:ILE:HG12	1.70	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
2:B:363:LYS:HB3	2:B:394:ALA:O	2.05	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: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
2:B:246:ARG:HA	2:B:258:MET:CG	2.35	0.55
1:A:251:GLU:HB2	6:A:602:HOH:O	2.05	0.55
2:B:401:LYS:HE2	2:B:411:GLN:OE1	2.07	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:326:PHE:HD2	2:B:359:LEU:HD11	1.71	0.55
2:B:365:THR:CG2	2:B:368:ASN:H	2.18	0.55
1:A:180:ARG:HD2	1:A:454:GLN:OE1	2.07	0.55
2:B:246:ARG:CG	2:B:246:ARG:HH11	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
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
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: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
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:181:GLN:HB3	1:A:182:PRO:HD3	1.89	0.53
1:A:62:GLN:HG3	1:A:67:MET:HE1	1.90	0.53

Continued on next page...

Continued from previous page...

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:159:SER:HB2	2:B:161:LYS:HD3	1.89	0.53
2:B:140:ASP:HB2	3:C:88:GLN:NE2	2.24	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
2:B:405:GLU:C	2:B:407:ASN:H	2.12	0.52
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:77:GLY:C	1:A:78:ILE:HD12	2.29	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
2:B:246:ARG:CA	2:B:258:MET:HG2	2.39	0.52
2:B:154:GLU:OE2	2:B:155:PRO:HD2	2.10	0.52
2:B:44:TYR:O	2:B:47:VAL:HG22	2.10	0.52
1:A:329:TYR:HA	3:C:80:ASN:O	2.09	0.52
3:C:63:LEU:N	3:C:63:LEU:HD22	2.25	0.51
2:B:195:ILE:HG23	2:B:209:ALA:HB3	1.91	0.51
1:A:1:MET:N	1:A:28:ASP:HA	2.24	0.51
2:B:348:VAL:O	2:B:352:LEU:HD13	2.10	0.51
2:B:237:ASN:HD22	2:B:237:ASN:C	2.13	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:240:GLU:CD	2:B:241:ILE:H	2.14	0.51
2:B:198:ARG:NH2	2:B:204:LYS:HG2	2.24	0.51
2:B:197:LEU:HB2	2:B:232:GLU:CG	2.40	0.51
2:B:255:THR:O	2:B:255:THR:HG23	2.10	0.51
2:B:170:LEU:O	2:B:174:ILE:HD13	2.10	0.51
2:B:256:ILE:O	2:B:256:ILE:CG1	2.58	0.51
2:B:107:ILE:HG12	2:B:165:ALA:CB	2.38	0.51
1:A:133:THR:HG22	1:A:133:THR:O	2.11	0.51
2:B:7:ILE:CD1	2:B:157:ILE:HD11	2.39	0.51
1:A:185:TYR:O	1:A:450:PRO:HG2	2.11	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:HD12	2:B:196:SER:N	2.27	0.50
1:A:11:LEU:O	1:A:15:ILE:HG13	2.11	0.50
2:B:393:LEU:O	2:B:393:LEU:HD23	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
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
1:A:62:GLN:HE21	1:A:67:MET:HE1	1.77	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:243:GLN:CG	2:B:257:LEU:HD23	2.42	0.49
2:B:132:HIS:NE2	3:C:93:THR:HG21	2.28	0.49
3:C:72:ILE:HD12	3:C:76:LEU:HB3	1.93	0.49
2:B:189:LEU:HD13	2:B:190:ARG:N	2.28	0.49
1:A:21:LYS:HB2	1:A:59:ASP:OD1	2.12	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:259:ARG:HH12	2:B:262:GLU:N	2.11	0.48
2:B:176:TYR:CE1	2:B:296:PRO:HG3	2.48	0.48
2:B:240:GLU:O	2:B:242:GLY:N	2.43	0.48
2:B:227:GLU:HB2	2:B:254:LYS:HE3	1.94	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: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
2:B:220:VAL:O	2:B:222:LYS:N	2.46	0.48
2:B:193:ALA:HB2	2:B:221:ARG:HH21	1.78	0.48
1:A:390:ASP:O	1:A:394:GLU:HG3	2.14	0.48
2:B:246:ARG:HB2	2:B:255:THR:OG1	2.13	0.48
2:B:176:TYR:CZ	2:B:296:PRO:HG3	2.49	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:339:LEU:H	3:C:94:ILE:CD1	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ARG:HG3	1:A:433:LEU:HD12	1.95	0.48
1:A:26:VAL:HG21	1:A:55:ALA:HB2	1.95	0.48
2:B:227:GLU:OE2	2:B:255:THR:HG22	2.14	0.48
1:A:78:ILE:HD12	1:A:78:ILE:N	2.28	0.48
1:A:485:LEU:HB3	6:A:678:HOH:O	2.14	0.48
2:B:202:GLN:C	2:B:204:LYS:H	2.15	0.47
1:A:1:MET:N	1:A:28:ASP:CA	2.77	0.47
2:B:241:ILE:C	2:B:243:GLN:N	2.67	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:98:PRO:HG2	2:B:101:GLU:HG3	1.95	0.47
2:B:88:LYS:O	2:B:89:ALA:HB3	2.14	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
2:B:214:LEU:N	2:B:214:LEU:CD1	2.77	0.47
1:A:484:LYS:O	1:A:485:LEU:HG	2.14	0.47
2:B:6:VAL:O	2:B:6:VAL:HG23	2.15	0.47
1:A:425:ASP:OD2	5:A:501:GLN:N	2.47	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
2:B:372:MET:HE1	2:B:390:PHE:CA	2.45	0.46
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:163:ALA:HB3	2:B:221:ARG:HH12	1.80	0.46
1:A:117:VAL:O	1:A:119:ILE:CD1	2.63	0.46
2:B:211:LEU:HD13	2:B:224:LEU:HG	1.97	0.46
2:B:7:ILE:HD13	2:B:225:GLU:HG2	1.95	0.46
2:B:211:LEU:CD1	2:B:214:LEU:HD11	2.46	0.46
1:A:338:SER:HB3	1:A:341:GLU:CG	2.40	0.46
3:C:94:ILE:HD12	3:C:94:ILE:N	2.31	0.46
2:B:185:GLU:HG3	2:B:186:GLU:N	2.31	0.46
1:A:83:ILE:HD13	1:A:103:TYR:CE1	2.51	0.46
2:B:126:ASP:OD2	2:B:143:ARG:NH1	2.48	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:169:LEU:C	1:A:169:LEU:HD23	2.36	0.46
2:B:250:GLU:O	2:B:253:GLY:CA	2.64	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

Continued on next page...

Continued from previous page...

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
2:B:348:VAL:HG22	2:B:390:PHE:CZ	2.51	0.45
1:A:75:PRO:HB3	1:A:119:ILE:HD11	1.98	0.45
2:B:209:ALA:CB	2:B:246:ARG:NH1	2.64	0.45
2:B:231:GLN:HA	2:B:234:GLU:CG	2.47	0.45
1:A:52:ILE:O	1:A:56:GLN:HG2	2.16	0.45
2:B:143:ARG:O	2:B:146:THR:HG23	2.17	0.45
2:B:220:VAL:CG2	2:B:221:ARG:N	2.78	0.45
1:A:276:VAL:HG21	1:A:406:THR:HA	1.98	0.45
2:B:372:MET:HE3	2:B:393:LEU:HD13	1.98	0.45
2:B:33:PRO:HA	2:B:142:ASN:ND2	2.31	0.45
1:A:391:LYS:HD3	1:A:394:GLU:OE1	2.17	0.45
2:B:365:THR:H	2:B:368:ASN:CG	2.20	0.45
2:B:183:LYS:HB3	2:B:185:GLU:CG	2.47	0.45
3:C:20:ILE:O	3:C:20:ILE:HG23	2.16	0.45
2:B:276:VAL:HG22	6:B:700:HOH:O	2.17	0.45
2:B:359:LEU:C	2:B:359:LEU:HD13	2.37	0.45
2:B:121:LEU:HD23	2:B:151:ILE:HG12	1.99	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
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
2:B:107:ILE:HG13	2:B:108:GLU:N	2.32	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:245:THR:O	2:B:258:MET:HG3	2.18	0.44
2:B:243:GLN:CD	2:B:257:LEU:CD2	2.83	0.44
2:B:411:GLN:HG3	2:B:411:GLN:H	1.36	0.44
1:A:134:GLU:HB2	1:A:415:ILE:HD13	2.00	0.44
2:B:215:ASN:HD22	2:B:215:ASN:N	2.12	0.44
2:B:372:MET:HE1	2:B:390:PHE:HA	2.00	0.44
2:B:331:ILE:C	2:B:333:HIS:H	2.21	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:108:GLU:OE1	2:B:108:GLU:HA	2.17	0.44
2:B:405:GLU:C	2:B:407:ASN:N	2.70	0.44
2:B:400:ALA:C	2:B:402:GLN:H	2.20	0.44
2:B:211:LEU:HD13	2:B:214:LEU:HD11	2.00	0.43
2:B:371:GLY:O	2:B:375:LEU:HG	2.17	0.43
1:A:1:MET:N	1:A:28:ASP:CG	2.72	0.43
2:B:350:GLU:HG2	6:B:657:HOH:O	2.18	0.43
1:A:70:LYS:HE2	1:A:228:GLU:HB2	2.00	0.43
2:B:404:MET:O	2:B:410:VAL:HG23	2.18	0.43
2:B:177:THR:OG1	2:B:179:VAL:HG22	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
2:B:171:ARG:HD2	6:B:659:HOH:O	2.18	0.43
2:B:68:MET:HG2	2:B:103:GLY:HA3	2.00	0.43
2:B:107:ILE:CG1	2:B:165:ALA:HB1	2.41	0.43
1:A:1:MET:HG3	1:A:32:ALA:CA	2.48	0.43
2:B:354:LYS:O	2:B:355:ASN:ND2	2.51	0.43
1:A:78:ILE:HD13	1:A:118:LEU:HD13	1.99	0.43
1:A:74:ILE:HA	1:A:75:PRO:HD3	1.82	0.43
2:B:126:ASP:CG	2:B:143:ARG:NH1	2.72	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:409:LEU:N	2:B:409:LEU:CD2	2.82	0.43
2:B:84:PRO:HB2	2:B:139:VAL:HG21	2.01	0.43
2:B:243:GLN:O	2:B:244:GLU:OE1	2.37	0.43
2:B:107:ILE:CD1	2:B:108:GLU:H	2.31	0.43
2:B:161:LYS:CD	2:B:161:LYS:H	2.30	0.43
1:A:62:GLN:HG3	1:A:67:MET:CE	2.48	0.43
2:B:362:THR:OG1	2:B:364:LEU:HD23	2.18	0.43
2:B:309:LEU:HG	2:B:313:ASP:HB2	2.01	0.43
2:B:6:VAL:HG22	2:B:196:SER:O	2.18	0.42
1:A:15:ILE:HG22	1:A:67:MET:CE	2.45	0.42
1:A:484:LYS:O	1:A:485:LEU:HB2	2.19	0.42
2:B:327:PHE:HB2	2:B:344:LEU:CD1	2.49	0.42
1:A:206:PHE:HB3	1:A:211:ASP:OD1	2.19	0.42
2:B:157:ILE:HD12	2:B:158:ARG:N	2.34	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:VAL:HG23	6:B:609:HOH:O	2.18	0.42
1:A:192:LYS:HE2	6:A:527:HOH:O	2.19	0.42
2:B:198:ARG:NH2	2:B:204:LYS:HZ2	2.17	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
1:A:58:LEU:HD22	1:A:72:PHE:CE2	2.55	0.42
2:B:363:LYS:HG3	2:B:363:LYS:O	2.20	0.42
2:B:380:THR:O	2:B:404:MET:HE1	2.19	0.42
2:B:16:LYS:CG	2:B:180:SER:HA	2.43	0.42
1:A:78:ILE:HG12	1:A:108:MET:SD	2.60	0.42
2:B:21:MET:HE1	2:B:55:ALA:HB3	2.01	0.42
1:A:49:GLU:CD	1:A:49:GLU:N	2.59	0.42
1:A:20:ILE:HG12	1:A:21:LYS:N	2.35	0.42
2:B:107:ILE:CG1	2:B:108:GLU:N	2.83	0.42
1:A:209:SER:OG	1:A:382:ARG:NH2	2.50	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
1:A:44:LEU:HD22	1:A:123:ASN:HA	2.02	0.42
2:B:135:GLU:OE1	2:B:135:GLU:HA	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
2:B:403:ILE:O	2:B:407:ASN:CB	2.63	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:211:LEU:O	2:B:211:LEU:HD12	2.21	0.41
2:B:163:ALA:O	2:B:167:LEU:HG	2.21	0.41
1:A:299:LEU:CD1	1:A:392:VAL:HG21	2.51	0.41
2:B:220:VAL:C	2:B:222:LYS:N	2.72	0.41
2:B:351:TYR:CE2	2:B:394:ALA:HB3	2.56	0.41
3:C:85:GLU:O	3:C:86:ASP:HB2	2.21	0.41
2:B:294:GLU:CG	2:B:298:GLU:OE1	2.68	0.41
3:C:21:SER:HA	3:C:22:PRO:HD3	1.93	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
2:B:221:ARG:HB2	2:B:221:ARG:HE	1.79	0.41
2:B:389:VAL:HG23	2:B:390:PHE:N	2.35	0.41
2:B:34:ASN:ND2	3:C:88:GLN:HA	2.35	0.41
2:B:385:ILE:HD12	2:B:385:ILE:H	1.86	0.41
1:A:90:THR:HA	1:A:96:LEU:HB3	2.02	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:LEU:HD21	2:B:248:PHE:CG	2.57	0.40
3:C:3:LYS:CD	3:C:4:VAL:N	2.80	0.40
2:B:171:ARG:C	2:B:171:ARG:HD3	2.42	0.40
2:B:106:ASP:O	2:B:169:LYS:HE2	2.22	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: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:229:LYS:O	2:B:230:ARG:C	2.59	0.40
1:A:1:MET:HB3	1:A:1:MET:HE3	2.01	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
2:B:237:ASN:ND2	2:B:237:ASN:C	2.74	0.40
2:B:329:SER:O	2:B:332:GLU:HG2	2.21	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
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

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%)	39 48
2	B	406/483 (84%)	345 (85%)	44 (11%)	17 (4%)	3 1
3	C	90/100 (90%)	83 (92%)	5 (6%)	2 (2%)	8 6
All	All	979/1068 (92%)	892 (91%)	66 (7%)	21 (2%)	9 7

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	406/406 (100%)	388 (96%)	18 (4%)	35 46
2	B	354/419 (84%)	318 (90%)	36 (10%)	9 10
3	C	81/88 (92%)	75 (93%)	6 (7%)	17 21
All	All	841/913 (92%)	781 (93%)	60 (7%)	18 23

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Res	Type
1	A	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 carbohydrates 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	$\#\|Z\| > 2$
5	GLN	A	501	1	6,9,9	2.77	1 (16%)	5,11,11	2.77	2 (40%)

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
5	GLN	A	501	1	-	0/5/9/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GLN	OE1-CD	6.68	1.44	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	501	GLN	OE1-CD-NE2	-3.86	111.37	122.46
5	A	501	GLN	CB-CG-CD	4.32	126.21	112.53

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
5	A	501	GLN	1	0

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, 95^{th} 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%)	0.03	12 (2%) 61 70	21, 34, 56, 74	0
2	B	408/483 (84%)	0.77	72 (17%) 2 3	25, 53, 95, 96	0
3	C	92/100 (92%)	0.69	12 (13%) 5 7	34, 56, 83, 88	0
All	All	985/1068 (92%)	0.40	96 (9%) 10 14	21, 41, 95, 96	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	263	GLY	11.2
2	B	224	LEU	10.3
2	B	260	VAL	9.6
2	B	411	GLN	9.3
2	B	240	GLU	9.0
2	B	221	ARG	8.1
2	B	246	ARG	7.8
2	B	241	ILE	7.6
2	B	238	GLY	7.2
2	B	401	LYS	6.5
2	B	205	PHE	6.5
2	B	207	THR	6.4
1	A	1	MET	6.1
3	C	38	PHE	6.0
2	B	239	GLY	5.9
2	B	203	GLU	5.9
2	B	409	LEU	5.6
2	B	236	LEU	5.4
3	C	4	VAL	5.3
2	B	220	VAL	5.3
2	B	201	GLY	5.1
2	B	230	ARG	5.0
2	B	360	LEU	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	242	GLY	5.0
2	B	243	GLN	4.6
3	C	94	ILE	4.5
2	B	198	ARG	4.3
2	B	262	GLU	4.3
2	B	396	LYS	4.3
3	C	26	GLU	4.1
2	B	225	GLU	4.1
2	B	197	LEU	4.0
3	C	22	PRO	3.9
2	B	258	MET	3.8
2	B	232	GLU	3.8
2	B	252	THR	3.8
2	B	400	ALA	3.8
2	B	211	LEU	3.7
2	B	233	GLU	3.4
3	C	34	SER	3.4
2	B	410	VAL	3.2
2	B	204	LYS	3.2
2	B	248	PHE	3.2
2	B	28	HIS	3.2
3	C	3	LYS	3.2
2	B	196	SER	3.1
2	B	218	ASN	3.1
2	B	357	VAL	3.1
2	B	237	ASN	3.0
2	B	200	TYR	3.0
3	C	6	ARG	2.9
2	B	219	TYR	2.9
2	B	363	LYS	2.9
1	A	336	ALA	2.7
2	B	136	TYR	2.7
2	B	402	GLN	2.6
2	B	261	LYS	2.6
2	B	231	GLN	2.6
2	B	202	GLN	2.6
2	B	406	ASP	2.5
2	B	217	PHE	2.5
2	B	257	LEU	2.5
1	A	213	ILE	2.5
1	A	210	LEU	2.5
2	B	4	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	81	ASN	2.4
1	A	334	LYS	2.4
2	B	394	ALA	2.4
3	C	31	THR	2.4
2	B	253	GLY	2.4
2	B	209	ALA	2.4
2	B	397	GLY	2.4
2	B	245	THR	2.4
2	B	334	GLY	2.3
3	C	30	ASN	2.3
2	B	404	MET	2.3
2	B	206	GLY	2.3
1	A	2	SER	2.3
2	B	379	GLY	2.2
3	C	37	ASP	2.2
2	B	199	PRO	2.2
2	B	234	GLU	2.2
2	B	133	LYS	2.2
2	B	352	LEU	2.2
2	B	229	LYS	2.2
1	A	207	ALA	2.1
2	B	395	ALA	2.1
2	B	249	ASP	2.1
2	B	226	TYR	2.1
1	A	270	GLU	2.1
1	A	335	GLU	2.1
1	A	317	ALA	2.1
2	B	247	ARG	2.0
1	A	12	LEU	2.0
2	B	380	THR	2.0
3	C	8	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	GLN	A	501	10/10	0.92	0.20	0.55	21,25,30,31	0
4	MG	B	601	1/1	0.96	0.07	-2.35	52,52,52,52	0

6.5 Other polymers

There are no such residues in this entry.