



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 06:56 PM EDT

PDB ID : 2DQN
Title : Structure of tRNA-Dependent Amidotransferase GatCAB complexed with Asn
Authors : Nakamura, A.; Yao, M.; Tanaka, I.
Deposited on : 2006-05-29
Resolution : 2.55 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

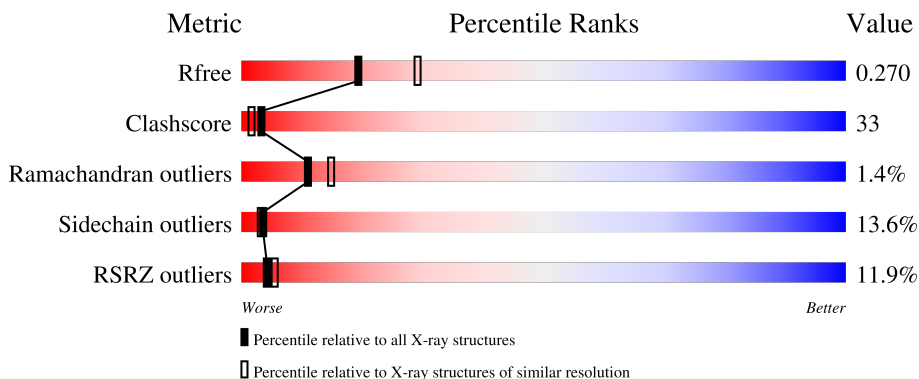
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	
2	B	483	
3	C	100	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7925 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
			Total	C	N	O	S			
1	A	485	3716	2359	605	739	13	0	0	0

- Molecule 2 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	405	3228	2034	542	639	13	0	0	0

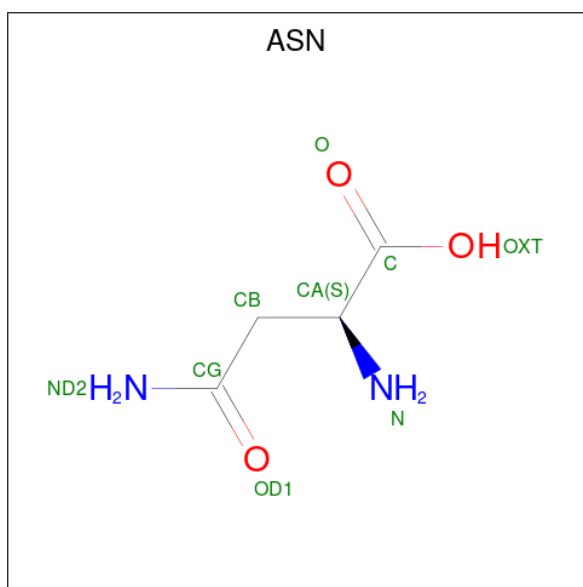
There are 8 discrepancies between the modelled and reference sequences:

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
			Total	C	N	O	S			
3	C	98	774	476	129	167	2	0	0	0

- Molecule 4 is ASPARAGINE (three-letter code: ASN) (formula: C₄H₈N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	4	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		

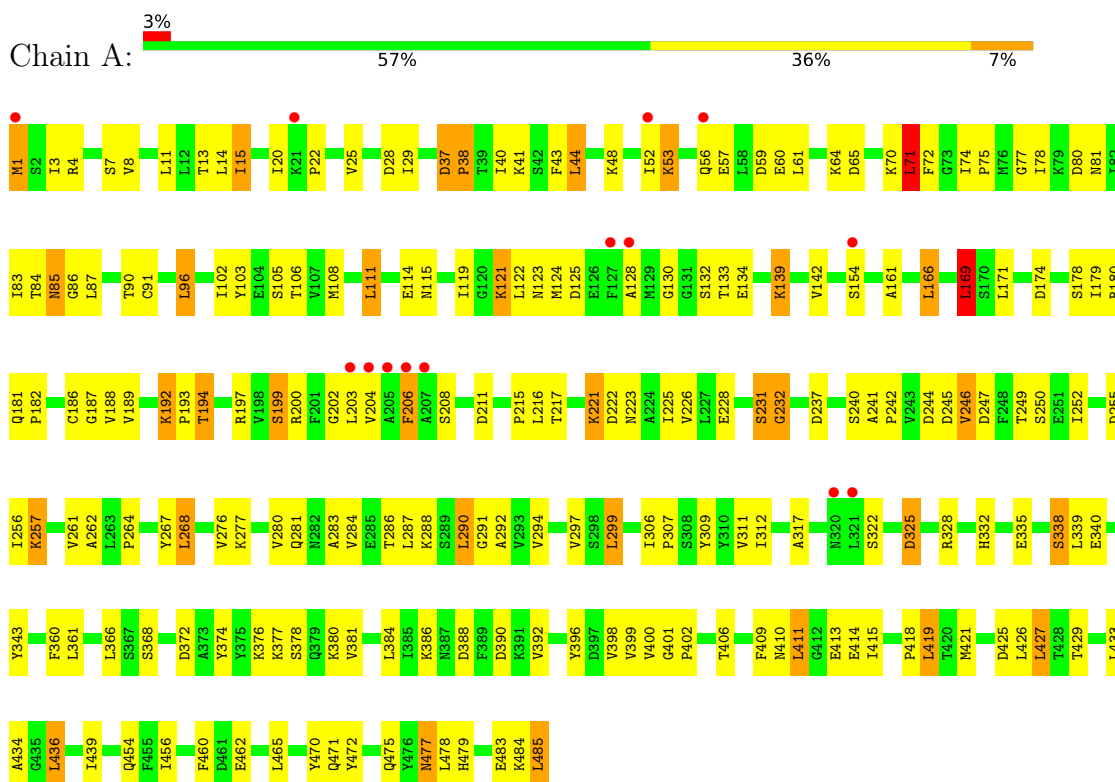
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	121	Total	O	0	0
			121	121		
6	B	61	Total	O	0	0
			61	61		
6	C	15	Total	O	0	0
			15	15		

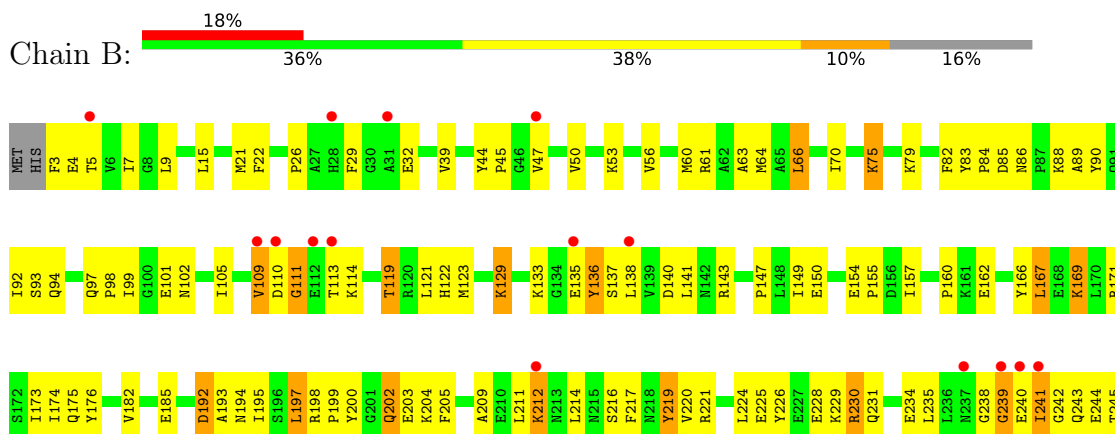
3 Residue-property plots i

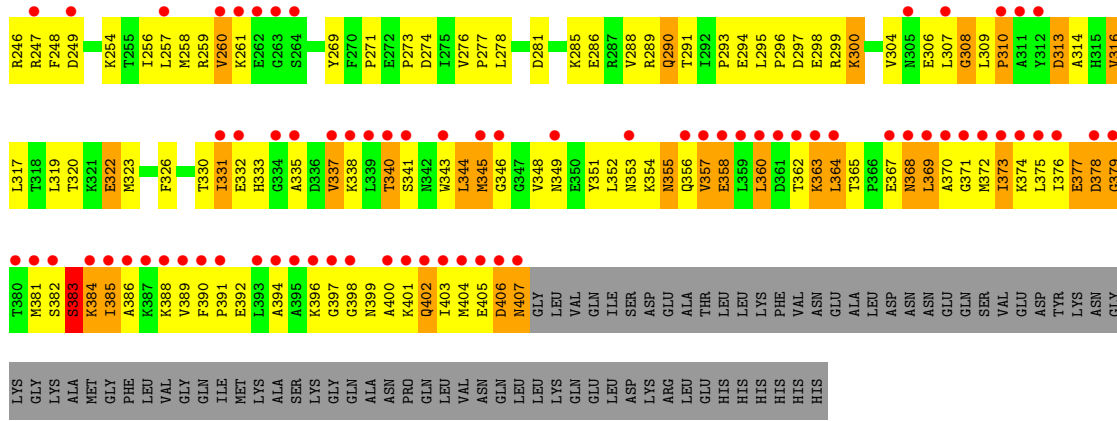
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

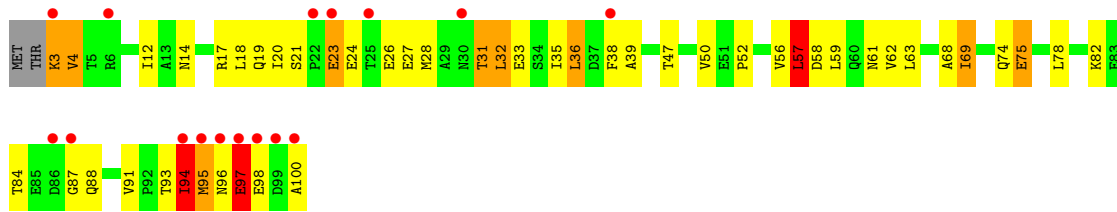


- Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.81Å 92.36Å 182.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.55 41.19 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-2.55) 98.8 (41.19-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 2.54Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.271 0.233 , 0.270	Depositor DCC
R_{free} test set	3915 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtrriage
Anisotropy	0.566	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7925	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.48	0/3784	0.75	3/5116 (0.1%)
2	B	0.45	0/3290	0.79	4/4442 (0.1%)
3	C	0.41	0/782	0.82	3/1056 (0.3%)
All	All	0.46	0/7856	0.78	10/10614 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	111	GLY	N-CA-C	-11.22	85.04	113.10
3	C	97	GLU	N-CA-C	9.27	136.02	111.00
2	B	383	SER	N-CA-C	7.53	131.33	111.00
3	C	57	LEU	CA-CB-CG	-6.62	100.08	115.30
1	A	231	SER	N-CA-C	6.27	127.92	111.00
1	A	71	LEU	N-CA-C	-6.08	94.60	111.00
1	A	169	LEU	CA-CB-CG	5.78	128.60	115.30
2	B	397	GLY	N-CA-C	5.27	126.28	113.10
3	C	94	ILE	N-CA-C	-5.27	96.78	111.00
2	B	382	SER	N-CA-C	5.18	124.99	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	472	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3716	0	3709	183	0
2	B	3228	0	3176	293	0
3	C	774	0	753	69	0
4	A	9	0	5	3	0
5	B	1	0	0	0	0
6	A	121	0	0	5	0
6	B	61	0	0	6	0
6	C	15	0	0	1	0
All	All	7925	0	7643	505	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 33.

All (505) 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:199:PRO:HG2	2:B:202:GLN:HE22	1.12	1.12
2:B:357:VAL:HG11	2:B:363:LYS:HE2	1.32	1.09
2:B:192:ASP:OD2	2:B:212:LYS:HD3	1.63	0.98
3:C:23:GLU:OE1	3:C:24:GLU:HG3	1.63	0.96
1:A:194:THR:HG22	1:A:462:GLU:OE2	1.68	0.92
2:B:355:ASN:HB3	2:B:357:VAL:HG22	1.53	0.90
2:B:344:LEU:HD12	2:B:348:VAL:HG21	1.52	0.89
2:B:368:ASN:HD22	2:B:369:LEU:N	1.71	0.88
2:B:357:VAL:HG11	2:B:363:LYS:CE	2.05	0.87
1:A:286:THR:O	1:A:290:LEU:HD12	1.74	0.86
2:B:371:GLY:O	2:B:374:LYS:HG2	1.76	0.85
3:C:47:THR:O	3:C:50:VAL:HG12	1.77	0.85
2:B:331:ILE:HD11	2:B:337:VAL:HG13	1.58	0.85
2:B:309:LEU:HD11	2:B:338:LYS:HD2	1.57	0.84
1:A:255:ASP:OD1	1:A:257:LYS:HE2	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:PRO:HG2	2:B:202:GLN:NE2	1.92	0.84
2:B:383:SER:O	2:B:384:LYS:C	2.14	0.83
2:B:26:PRO:HG3	3:C:68:ALA:HB1	1.60	0.83
2:B:368:ASN:HD22	2:B:368:ASN:C	1.82	0.83
1:A:180:ARG:HD2	1:A:192:LYS:HB3	1.60	0.83
2:B:343:TRP:O	2:B:348:VAL:HG13	1.78	0.83
1:A:1:MET:HG2	1:A:4:ARG:HD2	1.60	0.82
1:A:372:ASP:HA	1:A:376:LYS:HB2	1.59	0.82
2:B:368:ASN:ND2	2:B:369:LEU:N	2.28	0.82
2:B:304:VAL:O	2:B:308:GLY:HA2	1.81	0.81
2:B:309:LEU:CD1	2:B:338:LYS:HD2	2.10	0.81
2:B:364:LEU:HD12	2:B:365:THR:H	1.45	0.81
1:A:194:THR:HG21	1:A:460:PHE:HA	1.63	0.81
1:A:247:ASP:OD2	1:A:250:SER:HB3	1.80	0.81
1:A:84:THR:OG1	1:A:121:LYS:HE3	1.81	0.81
2:B:364:LEU:HD12	2:B:365:THR:N	1.96	0.80
1:A:477:ASN:C	1:A:477:ASN:HD22	1.83	0.80
2:B:403:ILE:O	2:B:407:ASN:HB2	1.81	0.79
2:B:390:PHE:HB3	2:B:391:PRO:HD3	1.64	0.79
2:B:388:LYS:O	2:B:388:LYS:HD3	1.82	0.79
2:B:140:ASP:HB2	3:C:88:GLN:NE2	1.97	0.79
2:B:348:VAL:HG12	2:B:390:PHE:CZ	2.18	0.78
2:B:356:GLN:HA	2:B:356:GLN:NE2	1.99	0.77
2:B:82:PHE:HB2	3:C:17:ARG:HE	1.48	0.77
1:A:306:ILE:HG22	3:C:38:PHE:HZ	1.50	0.76
2:B:400:ALA:O	2:B:404:MET:HG3	1.85	0.76
2:B:198:ARG:O	2:B:198:ARG:HG3	1.86	0.75
2:B:217:PHE:O	2:B:220:VAL:HG22	1.87	0.74
1:A:204:VAL:HG22	2:B:45:PRO:HB2	1.70	0.74
2:B:375:LEU:HD21	2:B:404:MET:SD	2.26	0.74
2:B:313:ASP:HA	2:B:345:MET:SD	2.28	0.74
3:C:75:GLU:OE1	3:C:75:GLU:HA	1.88	0.74
3:C:94:ILE:HG12	3:C:94:ILE:O	1.87	0.74
1:A:340:GLU:HB2	3:C:100:ALA:O	1.88	0.73
2:B:221:ARG:O	2:B:225:GLU:HG2	1.89	0.73
2:B:399:ASN:HD21	2:B:401:LYS:HB3	1.53	0.73
2:B:281:ASP:O	2:B:285:LYS:HG3	1.87	0.73
2:B:288:VAL:O	2:B:291:THR:HG22	1.88	0.72
3:C:35:ILE:O	3:C:38:PHE:HB3	1.88	0.72
2:B:352:LEU:HA	2:B:357:VAL:HG23	1.72	0.72
1:A:249:THR:HA	1:A:252:ILE:HD12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:386:ALA:HA	2:B:389:VAL:HG22	1.69	0.72
2:B:94:GLN:HB2	2:B:122:HIS:HB2	1.71	0.71
1:A:221:LYS:O	1:A:225:ILE:HD12	1.89	0.71
2:B:388:LYS:HE2	2:B:392:GLU:CG	2.20	0.71
2:B:5:THR:HG21	2:B:228:GLU:HG3	1.72	0.71
2:B:75:LYS:HG3	2:B:97:GLN:OE1	1.90	0.71
3:C:27:GLU:O	3:C:31:THR:HG22	1.90	0.71
2:B:348:VAL:O	2:B:352:LEU:HD13	1.90	0.71
1:A:264:PRO:HB3	1:A:299:LEU:HD22	1.73	0.70
2:B:243:GLN:HG3	2:B:261:LYS:HG3	1.74	0.70
2:B:364:LEU:HD13	2:B:368:ASN:HD21	1.56	0.70
2:B:375:LEU:CD2	2:B:404:MET:SD	2.80	0.70
2:B:202:GLN:HG2	2:B:203:GLU:N	2.05	0.70
2:B:364:LEU:HD11	2:B:369:LEU:HB2	1.74	0.69
1:A:178:SER:OG	4:A:511:ASN:ND2	2.25	0.69
2:B:256:ILE:HD12	2:B:256:ILE:N	2.07	0.69
3:C:93:THR:C	3:C:95:MET:H	1.96	0.69
2:B:404:MET:HB2	6:B:547:HOH:O	1.91	0.68
2:B:300:LYS:HG3	6:B:553:HOH:O	1.92	0.68
1:A:306:ILE:HG22	3:C:38:PHE:CZ	2.29	0.67
2:B:307:LEU:HD23	2:B:307:LEU:O	1.95	0.67
2:B:61:ARG:CD	2:B:291:THR:HG23	2.24	0.67
1:A:192:LYS:O	1:A:192:LYS:HG3	1.94	0.66
3:C:96:ASN:OD1	3:C:97:GLU:N	2.29	0.66
2:B:386:ALA:HA	2:B:389:VAL:CG2	2.25	0.66
1:A:57:GLU:O	1:A:61:LEU:HD23	1.96	0.66
2:B:160:PRO:HB3	2:B:224:LEU:HB3	1.78	0.65
1:A:78:ILE:HD12	1:A:108:MET:HE1	1.78	0.65
1:A:280:VAL:HG21	1:A:402:PRO:HB3	1.77	0.65
2:B:388:LYS:HE2	2:B:392:GLU:HG3	1.78	0.65
1:A:72:PHE:H	1:A:74:ILE:HG12	1.62	0.65
1:A:434:ALA:HB3	1:A:436:LEU:HD22	1.78	0.64
2:B:171:ARG:NH1	2:B:175:GLN:HG3	2.13	0.64
1:A:139:LYS:NZ	1:A:139:LYS:HB3	2.13	0.64
2:B:259:ARG:HG3	2:B:259:ARG:HH11	1.62	0.64
1:A:194:THR:HG21	1:A:460:PHE:CA	2.28	0.63
3:C:97:GLU:OE2	3:C:97:GLU:HA	1.98	0.63
2:B:7:ILE:HG22	2:B:195:ILE:HG13	1.81	0.63
3:C:57:LEU:HD23	3:C:58:ASP:H	1.62	0.63
1:A:277:LYS:O	1:A:281:GLN:HG3	1.99	0.63
2:B:247:ARG:HB3	2:B:258:MET:HE2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:28:MET:HA	3:C:31:THR:HG23	1.80	0.63
3:C:59:LEU:HD23	3:C:59:LEU:N	2.13	0.62
2:B:56:VAL:HA	2:B:123:MET:HE3	1.79	0.62
2:B:320:THR:OG1	2:B:323:MET:HB3	2.00	0.62
1:A:132:SER:O	1:A:133:THR:HB	2.00	0.62
2:B:288:VAL:HA	2:B:291:THR:HG22	1.81	0.62
2:B:82:PHE:CD1	3:C:17:ARG:HG3	2.34	0.62
1:A:1:MET:H2	1:A:28:ASP:CG	2.02	0.62
2:B:344:LEU:HA	2:B:348:VAL:HG22	1.81	0.62
2:B:3:PHE:HE1	2:B:197:LEU:HD23	1.65	0.62
1:A:377:LYS:O	1:A:381:VAL:HG23	1.99	0.62
1:A:284:VAL:HG12	1:A:288:LYS:HE3	1.82	0.61
3:C:3:LYS:HA	6:C:109:HOH:O	2.00	0.61
1:A:409:PHE:CD1	1:A:414:GLU:HG3	2.35	0.61
2:B:309:LEU:HG	2:B:310:PRO:HD2	1.82	0.61
2:B:388:LYS:HE2	2:B:392:GLU:HG2	1.82	0.61
1:A:29:ILE:HG21	1:A:119:ILE:HG12	1.82	0.61
2:B:133:LYS:HB2	2:B:138:LEU:HD23	1.81	0.61
2:B:5:THR:HG22	2:B:197:LEU:HG	1.82	0.61
2:B:88:LYS:O	2:B:89:ALA:HB3	1.99	0.61
2:B:364:LEU:CD1	2:B:369:LEU:HB2	2.30	0.61
2:B:368:ASN:HB2	2:B:398:GLY:O	2.00	0.61
2:B:197:LEU:HD13	2:B:231:GLN:OE1	2.01	0.61
2:B:105:ILE:HD11	2:B:166:TYR:CD1	2.36	0.61
2:B:140:ASP:HB2	3:C:88:GLN:HE21	1.64	0.60
1:A:252:ILE:HG23	1:A:470:TYR:CG	2.37	0.60
2:B:300:LYS:HG2	2:B:314:ALA:HB1	1.82	0.60
2:B:378:ASP:OD1	2:B:379:GLY:N	2.35	0.60
1:A:374:TYR:HE2	3:C:36:LEU:HG	1.66	0.60
2:B:44:TYR:O	2:B:47:VAL:HG22	2.01	0.60
1:A:477:ASN:C	1:A:477:ASN:ND2	2.55	0.60
2:B:333:HIS:CE1	2:B:367:GLU:HA	2.37	0.59
2:B:61:ARG:HD3	2:B:291:THR:HG23	1.84	0.59
2:B:241:ILE:HD13	2:B:241:ILE:C	2.23	0.59
2:B:247:ARG:HB3	2:B:258:MET:CE	2.32	0.59
2:B:331:ILE:CG2	2:B:332:GLU:N	2.65	0.59
1:A:84:THR:HG23	1:A:121:LYS:HE2	1.85	0.59
1:A:256:ILE:HG23	1:A:471:GLN:HG3	1.84	0.59
1:A:332:HIS:HB3	3:C:82:LYS:HD2	1.84	0.59
1:A:139:LYS:HB3	1:A:139:LYS:HZ3	1.68	0.58
1:A:276:VAL:HG21	1:A:406:THR:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:LEU:CD2	2:B:337:VAL:HG11	2.34	0.58
2:B:333:HIS:HE1	2:B:367:GLU:HA	1.67	0.58
1:A:244:ASP:O	1:A:246:VAL:HG22	2.04	0.58
2:B:61:ARG:HD2	2:B:291:THR:HG23	1.85	0.58
2:B:202:GLN:HG2	2:B:204:LYS:H	1.68	0.58
1:A:197:ARG:O	1:A:231:SER:O	2.22	0.58
2:B:249:ASP:HB2	2:B:256:ILE:HD11	1.86	0.58
3:C:20:ILE:HD11	3:C:24:GLU:HB3	1.86	0.58
1:A:194:THR:HG21	1:A:460:PHE:H	1.69	0.57
1:A:484:LYS:C	1:A:485:LEU:HD23	2.25	0.57
1:A:84:THR:CG2	1:A:121:LYS:HE2	2.34	0.57
2:B:383:SER:O	2:B:386:ALA:N	2.35	0.57
2:B:295:LEU:O	2:B:299:ARG:HB2	2.05	0.57
1:A:284:VAL:HG13	1:A:294:VAL:HG11	1.87	0.57
2:B:109:VAL:O	2:B:111:GLY:N	2.38	0.57
2:B:226:TYR:HB2	6:B:522:HOH:O	2.03	0.57
1:A:221:LYS:HZ2	1:A:252:ILE:HG21	1.70	0.57
1:A:290:LEU:HD11	1:A:475:GLN:HG3	1.87	0.57
1:A:41:LYS:HB3	1:A:139:LYS:HD3	1.85	0.57
1:A:264:PRO:HA	1:A:297:VAL:O	2.05	0.57
3:C:93:THR:C	3:C:95:MET:N	2.57	0.57
1:A:60:GLU:O	1:A:64:LYS:HG3	2.05	0.56
1:A:71:LEU:O	1:A:114:GLU:O	2.22	0.56
2:B:219:TYR:CD1	2:B:248:PHE:HE2	2.23	0.56
2:B:230:ARG:NH1	2:B:246:ARG:HE	2.04	0.56
1:A:70:LYS:HZ3	1:A:70:LYS:HB3	1.70	0.56
2:B:176:TYR:CE1	2:B:296:PRO:HG3	2.40	0.56
2:B:383:SER:O	2:B:385:ILE:N	2.37	0.56
2:B:344:LEU:HA	2:B:348:VAL:CG2	2.36	0.56
1:A:188:VAL:CG1	1:A:217:THR:O	2.54	0.56
2:B:193:ALA:CB	2:B:224:LEU:HD11	2.36	0.56
3:C:97:GLU:OE2	3:C:97:GLU:CA	2.53	0.56
2:B:211:LEU:HD12	2:B:224:LEU:HD12	1.88	0.56
2:B:133:LYS:HB2	2:B:138:LEU:CD2	2.36	0.56
2:B:295:LEU:HD22	2:B:295:LEU:N	2.21	0.56
2:B:340:THR:O	2:B:344:LEU:HD22	2.05	0.56
1:A:299:LEU:HD12	1:A:388:ASP:HB3	1.88	0.55
1:A:411:LEU:HB2	6:A:624:HOH:O	2.06	0.55
2:B:276:VAL:CG2	3:C:59:LEU:O	2.55	0.55
2:B:352:LEU:HD21	2:B:360:LEU:CD1	2.37	0.55
2:B:22:PHE:CE2	2:B:92:ILE:HB	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:LEU:HD23	1:A:485:LEU:N	2.22	0.55
2:B:316:VAL:HG13	2:B:345:MET:CE	2.36	0.55
1:A:242:PRO:HD2	3:C:59:LEU:HD11	1.87	0.55
1:A:134:GLU:HB2	1:A:415:ILE:HD13	1.88	0.55
1:A:206:PHE:CE1	1:A:317:ALA:HB2	2.42	0.54
2:B:276:VAL:HG21	3:C:59:LEU:O	2.06	0.54
2:B:294:GLU:HB2	2:B:299:ARG:HH11	1.72	0.54
3:C:78:LEU:HD22	3:C:84:THR:HG21	1.88	0.54
2:B:26:PRO:HD3	3:C:69:ILE:O	2.08	0.54
1:A:228:GLU:HG2	1:A:246:VAL:O	2.08	0.54
2:B:343:TRP:O	2:B:346:GLY:O	2.26	0.54
2:B:364:LEU:CD1	2:B:368:ASN:HD21	2.20	0.54
2:B:369:LEU:HD22	2:B:369:LEU:O	2.06	0.54
2:B:199:PRO:HD3	2:B:235:LEU:HD21	1.90	0.54
2:B:330:THR:HG21	2:B:369:LEU:HD13	1.88	0.54
1:A:325:ASP:HB3	1:A:343:TYR:CE1	2.43	0.54
2:B:278:LEU:HD21	3:C:63:LEU:HD11	1.89	0.54
2:B:247:ARG:CB	2:B:258:MET:HE2	2.38	0.54
2:B:352:LEU:HD21	2:B:360:LEU:HD12	1.89	0.54
2:B:15:LEU:HD11	2:B:149:ILE:HG23	1.90	0.53
1:A:328:ARG:HG3	1:A:328:ARG:HH11	1.74	0.53
1:A:306:ILE:CG2	3:C:38:PHE:HZ	2.21	0.53
1:A:84:THR:OG1	1:A:87:LEU:HB3	2.09	0.53
1:A:188:VAL:HG12	1:A:189:VAL:N	2.24	0.53
1:A:194:THR:HG21	1:A:460:PHE:N	2.23	0.53
2:B:276:VAL:HG11	3:C:62:VAL:HG23	1.91	0.53
2:B:375:LEU:HD23	2:B:404:MET:SD	2.49	0.52
3:C:69:ILE:O	3:C:69:ILE:HG22	2.08	0.52
1:A:361:LEU:HD13	3:C:35:ILE:CG2	2.39	0.52
2:B:271:PRO:O	2:B:273:PRO:HD3	2.09	0.52
2:B:79:LYS:HE2	2:B:269:TYR:OH	2.09	0.52
2:B:307:LEU:HD21	2:B:337:VAL:CG1	2.39	0.52
2:B:60:MET:HB3	2:B:99:ILE:HD11	1.91	0.52
2:B:121:LEU:C	2:B:121:LEU:HD23	2.30	0.52
2:B:241:ILE:HD13	2:B:242:GLY:N	2.25	0.52
1:A:380:LYS:HG2	3:C:50:VAL:HG13	1.91	0.52
1:A:8:VAL:HB	1:A:222:ASP:OD1	2.10	0.52
1:A:264:PRO:CB	1:A:299:LEU:HD22	2.40	0.52
2:B:175:GLN:NE2	2:B:322:GLU:OE2	2.42	0.52
2:B:307:LEU:HG	2:B:337:VAL:HG11	1.92	0.52
2:B:372:MET:O	2:B:376:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:ARG:N	2:B:258:MET:HE2	2.25	0.51
2:B:365:THR:HG22	6:B:552:HOH:O	2.10	0.51
1:A:262:ALA:HB2	1:A:396:TYR:CG	2.46	0.51
2:B:154:GLU:HG3	2:B:155:PRO:HD2	1.91	0.51
3:C:32:LEU:HD12	3:C:36:LEU:HD22	1.92	0.51
2:B:136:TYR:N	2:B:136:TYR:CD1	2.79	0.51
2:B:344:LEU:HD13	2:B:348:VAL:HG11	1.92	0.51
2:B:307:LEU:O	2:B:307:LEU:CD2	2.59	0.51
1:A:188:VAL:HG13	1:A:217:THR:O	2.11	0.51
2:B:238:GLY:O	2:B:239:GLY:O	2.29	0.51
2:B:288:VAL:C	2:B:291:THR:HG22	2.31	0.51
2:B:351:TYR:CE1	2:B:357:VAL:HG21	2.46	0.51
2:B:9:LEU:HD12	2:B:166:TYR:CD2	2.45	0.51
2:B:61:ARG:HD3	2:B:291:THR:CG2	2.41	0.51
2:B:83:TYR:HD2	2:B:85:ASP:CG	2.14	0.51
1:A:161:ALA:O	1:A:166:LEU:HB2	2.11	0.50
1:A:257:LYS:HD2	1:A:257:LYS:O	2.11	0.50
1:A:309:TYR:OH	4:A:511:ASN:HB2	2.11	0.50
2:B:63:ALA:HB2	2:B:121:LEU:HD13	1.93	0.50
1:A:322:SER:HB3	2:B:89:ALA:CB	2.40	0.50
2:B:98:PRO:HG2	2:B:101:GLU:HG3	1.92	0.50
2:B:338:LYS:O	2:B:341:SER:HB3	2.11	0.50
1:A:130:GLY:N	4:A:511:ASN:O	2.44	0.50
1:A:139:LYS:NZ	1:A:139:LYS:CB	2.73	0.50
2:B:309:LEU:CG	2:B:310:PRO:HD2	2.42	0.50
2:B:3:PHE:N	2:B:200:TYR:CD2	2.79	0.50
2:B:3:PHE:O	2:B:3:PHE:CG	2.61	0.50
1:A:14:LEU:O	1:A:20:ILE:HG22	2.12	0.50
1:A:90:THR:HA	1:A:96:LEU:HB3	1.93	0.50
2:B:288:VAL:CA	2:B:291:THR:HG22	2.42	0.50
2:B:392:GLU:OE2	2:B:396:LYS:HG3	2.11	0.50
1:A:15:ILE:HG13	1:A:20:ILE:HG23	1.94	0.50
1:A:72:PHE:O	1:A:115:ASN:O	2.29	0.50
1:A:261:VAL:HB	1:A:294:VAL:HG22	1.94	0.50
1:A:338:SER:HB2	3:C:100:ALA:OXT	2.12	0.50
1:A:105:SER:CB	1:A:202:GLY:HA3	2.42	0.49
1:A:237:ASP:O	1:A:240:SER:OG	2.28	0.49
1:A:339:LEU:CD2	3:C:95:MET:HE3	2.42	0.49
2:B:306:GLU:O	2:B:307:LEU:HB3	2.10	0.49
2:B:276:VAL:HG21	3:C:59:LEU:C	2.33	0.49
1:A:1:MET:H1	1:A:28:ASP:HA	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:TYR:CZ	2:B:296:PRO:HG3	2.46	0.49
2:B:229:LYS:N	2:B:229:LYS:HD2	2.27	0.49
2:B:331:ILE:HG22	2:B:332:GLU:N	2.28	0.49
2:B:348:VAL:CG2	2:B:349:ASN:N	2.75	0.49
1:A:368:SER:HA	6:A:531:HOH:O	2.12	0.49
2:B:259:ARG:HG3	2:B:259:ARG:NH1	2.26	0.49
2:B:399:ASN:ND2	2:B:401:LYS:HB3	2.25	0.49
1:A:77:GLY:O	1:A:78:ILE:HD13	2.13	0.49
2:B:169:LYS:O	2:B:169:LYS:HD3	2.13	0.49
2:B:331:ILE:HG22	2:B:332:GLU:H	1.78	0.49
2:B:340:THR:HG23	2:B:373:ILE:HD12	1.94	0.49
3:C:74:GLN:NE2	3:C:87:GLY:HA2	2.27	0.49
2:B:202:GLN:HG2	2:B:204:LYS:N	2.28	0.49
1:A:1:MET:O	1:A:4:ARG:HG2	2.13	0.49
1:A:174:ASP:HB2	1:A:179:ILE:HB	1.95	0.49
1:A:299:LEU:CD1	1:A:392:VAL:HG21	2.42	0.49
2:B:356:GLN:O	2:B:358:GLU:HG2	2.13	0.49
1:A:374:TYR:CE2	3:C:36:LEU:HG	2.47	0.48
2:B:93:SER:OG	2:B:94:GLN:N	2.46	0.48
2:B:363:LYS:CB	2:B:363:LYS:NZ	2.76	0.48
3:C:75:GLU:OE1	3:C:75:GLU:CA	2.58	0.48
1:A:206:PHE:CD1	1:A:206:PHE:C	2.84	0.48
2:B:288:VAL:HA	2:B:291:THR:CG2	2.42	0.48
2:B:343:TRP:CD1	2:B:373:ILE:HD13	2.48	0.48
2:B:356:GLN:HA	2:B:356:GLN:HE21	1.76	0.48
2:B:368:ASN:C	2:B:368:ASN:ND2	2.51	0.48
2:B:402:GLN:O	2:B:406:ASP:HB2	2.13	0.48
1:A:37:ASP:N	1:A:38:PRO:CD	2.77	0.48
1:A:192:LYS:NZ	1:A:193:PRO:O	2.36	0.48
2:B:7:ILE:HA	2:B:194:ASN:O	2.14	0.48
1:A:78:ILE:CD1	1:A:108:MET:HE1	2.43	0.48
2:B:309:LEU:HD12	2:B:310:PRO:HD3	1.95	0.48
1:A:241:ALA:HA	3:C:59:LEU:HD11	1.95	0.48
2:B:7:ILE:HG22	2:B:195:ILE:CG1	2.44	0.48
1:A:22:PRO:HD2	1:A:59:ASP:OD1	2.14	0.48
2:B:405:GLU:C	2:B:407:ASN:H	2.16	0.48
2:B:86:ASN:HD21	2:B:90:TYR:N	2.12	0.48
2:B:234:GLU:O	2:B:239:GLY:HA3	2.14	0.48
2:B:260:VAL:HG12	2:B:260:VAL:O	2.14	0.48
2:B:276:VAL:HG22	2:B:277:PRO:HD2	1.95	0.48
2:B:278:LEU:HA	3:C:61:ASN:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:309:LEU:HD12	2:B:310:PRO:CD	2.44	0.48
2:B:137:SER:N	3:C:91:VAL:O	2.47	0.47
1:A:90:THR:O	1:A:91:CYS:HB2	2.14	0.47
2:B:247:ARG:CA	2:B:258:MET:HE2	2.43	0.47
2:B:357:VAL:CG1	2:B:363:LYS:HE2	2.24	0.47
3:C:47:THR:HB	3:C:50:VAL:CG1	2.44	0.47
3:C:58:ASP:O	3:C:59:LEU:C	2.52	0.47
2:B:88:LYS:O	2:B:89:ALA:CB	2.63	0.47
2:B:352:LEU:O	2:B:356:GLN:N	2.47	0.47
2:B:307:LEU:HD21	2:B:337:VAL:HG11	1.96	0.47
2:B:176:TYR:HE2	2:B:299:ARG:CD	2.27	0.47
2:B:209:ALA:HA	2:B:244:GLU:O	2.15	0.47
1:A:169:LEU:C	1:A:169:LEU:HD22	2.35	0.47
1:A:325:ASP:HB3	1:A:343:TYR:HE1	1.79	0.47
2:B:259:ARG:HG3	2:B:260:VAL:N	2.29	0.47
2:B:377:GLU:HG3	2:B:378:ASP:N	2.28	0.47
2:B:169:LYS:HE2	2:B:173:ILE:HD11	1.97	0.47
2:B:7:ILE:HG22	2:B:195:ILE:CB	2.45	0.46
2:B:245:THR:OG1	2:B:261:LYS:HE2	2.15	0.46
1:A:280:VAL:O	1:A:283:ALA:HB3	2.14	0.46
2:B:64:MET:HE2	2:B:70:ILE:HG13	1.98	0.46
2:B:290:GLN:C	2:B:290:GLN:CD	2.74	0.46
2:B:295:LEU:HB3	2:B:296:PRO:HD2	1.96	0.46
1:A:242:PRO:CD	3:C:59:LEU:HD11	2.45	0.46
2:B:129:LYS:HE2	2:B:143:ARG:NH2	2.31	0.46
1:A:261:VAL:HG22	1:A:398:VAL:CG2	2.45	0.46
1:A:361:LEU:HD13	3:C:35:ILE:HG22	1.96	0.46
1:A:439:ILE:O	1:A:454:GLN:HA	2.16	0.46
2:B:83:TYR:CD2	2:B:85:ASP:CG	2.89	0.46
2:B:307:LEU:O	2:B:309:LEU:N	2.49	0.46
1:A:15:ILE:HG21	1:A:72:PHE:HD2	1.81	0.46
3:C:26:GLU:HA	3:C:26:GLU:OE1	2.15	0.46
3:C:27:GLU:O	3:C:31:THR:CG2	2.60	0.46
1:A:61:LEU:N	1:A:61:LEU:HD22	2.31	0.46
2:B:220:VAL:HG23	2:B:221:ARG:N	2.31	0.46
2:B:401:LYS:HG2	2:B:401:LYS:O	2.16	0.46
1:A:11:LEU:O	1:A:15:ILE:HD12	2.15	0.46
2:B:317:LEU:HG	2:B:345:MET:CE	2.45	0.46
3:C:93:THR:HG23	3:C:93:THR:O	2.15	0.46
2:B:129:LYS:CE	2:B:143:ARG:HH21	2.28	0.46
2:B:169:LYS:HD3	2:B:169:LYS:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:GLU:O	2:B:299:ARG:HD2	2.16	0.45
3:C:47:THR:HB	3:C:50:VAL:HG12	1.98	0.45
1:A:268:LEU:O	1:A:277:LYS:HE2	2.16	0.45
2:B:214:LEU:HB3	2:B:220:VAL:HG12	1.98	0.45
2:B:371:GLY:HA2	2:B:374:LYS:HE2	1.99	0.45
1:A:111:LEU:HD12	1:A:111:LEU:HA	1.79	0.45
1:A:311:VAL:HG11	1:A:374:TYR:O	2.16	0.45
2:B:167:LEU:CD2	2:B:220:VAL:HG21	2.46	0.45
2:B:389:VAL:HG23	2:B:390:PHE:N	2.31	0.45
1:A:426:LEU:HG	1:A:427:LEU:HD13	1.98	0.45
2:B:138:LEU:N	2:B:138:LEU:HD22	2.31	0.45
2:B:198:ARG:HG3	2:B:198:ARG:HH11	1.81	0.45
1:A:61:LEU:CD2	1:A:61:LEU:H	2.30	0.45
2:B:313:ASP:HA	2:B:345:MET:HE1	1.97	0.45
2:B:330:THR:CG2	2:B:340:THR:HG21	2.46	0.45
3:C:4:VAL:HG12	3:C:4:VAL:O	2.16	0.45
2:B:121:LEU:HA	2:B:150:GLU:O	2.16	0.45
2:B:300:LYS:O	2:B:304:VAL:HG23	2.16	0.45
1:A:84:THR:CG2	1:A:121:LYS:CE	2.95	0.45
2:B:5:THR:HG22	2:B:197:LEU:CD1	2.47	0.45
2:B:202:GLN:HE21	2:B:202:GLN:HB3	1.49	0.45
2:B:56:VAL:HG22	2:B:123:MET:CE	2.47	0.45
1:A:206:PHE:CD1	1:A:317:ALA:HB2	2.52	0.45
1:A:376:LYS:HE2	3:C:52:PRO:HG2	1.99	0.45
1:A:84:THR:HB	6:A:547:HOH:O	2.15	0.44
2:B:138:LEU:CD2	2:B:138:LEU:N	2.80	0.44
2:B:185:GLU:CD	2:B:185:GLU:H	2.19	0.44
2:B:298:GLU:CD	2:B:298:GLU:H	2.20	0.44
2:B:53:LYS:HB2	3:C:63:LEU:HB3	2.00	0.44
3:C:78:LEU:HD22	3:C:84:THR:CG2	2.48	0.44
1:A:103:TYR:CD1	2:B:39:VAL:HG11	2.52	0.44
2:B:363:LYS:NZ	2:B:363:LYS:HB3	2.32	0.44
2:B:364:LEU:CD1	2:B:368:ASN:ND2	2.81	0.44
2:B:64:MET:C	2:B:66:LEU:N	2.71	0.44
2:B:300:LYS:C	2:B:300:LYS:HD2	2.38	0.44
2:B:344:LEU:CD1	2:B:348:VAL:HG11	2.47	0.44
3:C:28:MET:O	3:C:32:LEU:HB2	2.16	0.44
1:A:125:ASP:CG	1:A:133:THR:HA	2.38	0.44
1:A:215:PRO:HG2	1:A:223:ASN:OD1	2.18	0.44
1:A:257:LYS:HA	1:A:291:GLY:HA3	1.98	0.44
2:B:373:ILE:O	2:B:377:GLU:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ILE:HA	1:A:142:VAL:HG22	2.00	0.44
1:A:400:VAL:HG22	1:A:401:GLY:N	2.32	0.44
3:C:74:GLN:HE21	3:C:87:GLY:HA2	1.83	0.43
2:B:198:ARG:HB3	2:B:205:PHE:CD2	2.53	0.43
2:B:351:TYR:HE1	2:B:357:VAL:HG21	1.81	0.43
2:B:174:ILE:HG21	2:B:182:VAL:HG11	2.00	0.43
2:B:240:GLU:HA	2:B:240:GLU:OE1	2.18	0.43
1:A:7:SER:HB2	1:A:222:ASP:OD2	2.17	0.43
2:B:333:HIS:ND1	2:B:370:ALA:HB2	2.33	0.43
2:B:21:MET:N	2:B:147:PRO:HD3	2.33	0.43
1:A:208:SER:HB3	2:B:274:ASP:OD1	2.19	0.43
1:A:257:LYS:O	1:A:257:LYS:CD	2.67	0.43
1:A:264:PRO:HG2	1:A:267:TYR:CD2	2.54	0.43
2:B:64:MET:SD	2:B:289:ARG:HD2	2.58	0.43
2:B:309:LEU:HD12	2:B:309:LEU:HA	1.62	0.43
2:B:216:SER:OG	2:B:219:TYR:HB2	2.17	0.43
2:B:286:GLU:O	2:B:289:ARG:N	2.51	0.43
1:A:186:CYS:O	1:A:188:VAL:HG23	2.18	0.43
2:B:7:ILE:CG2	2:B:195:ILE:HG13	2.48	0.43
1:A:48:LYS:HG2	1:A:52:ILE:HD12	2.00	0.43
1:A:418:PRO:HA	1:A:421:MET:HB3	2.01	0.43
1:A:1:MET:CG	1:A:4:ARG:HD2	2.42	0.42
1:A:44:LEU:HD22	1:A:123:ASN:HA	2.00	0.42
1:A:81:ASN:HB3	1:A:124:MET:HE1	2.01	0.42
1:A:221:LYS:HZ2	1:A:252:ILE:CG2	2.30	0.42
1:A:181:GLN:HB3	1:A:182:PRO:HD3	2.01	0.42
2:B:114:LYS:HE2	2:B:162:GLU:OE1	2.19	0.42
2:B:330:THR:HG22	2:B:340:THR:HG21	2.01	0.42
3:C:20:ILE:CD1	3:C:24:GLU:HB3	2.48	0.42
1:A:128:ALA:HA	1:A:154:SER:CB	2.49	0.42
1:A:221:LYS:NZ	1:A:252:ILE:HB	2.34	0.42
2:B:388:LYS:C	2:B:391:PRO:HD2	2.39	0.42
3:C:21:SER:O	3:C:24:GLU:N	2.50	0.42
1:A:78:ILE:O	1:A:121:LYS:HA	2.20	0.42
1:A:386:LYS:HE3	1:A:390:ASP:OD2	2.19	0.42
1:A:484:LYS:O	1:A:485:LEU:CB	2.67	0.42
1:A:256:ILE:HD12	1:A:292:ALA:HB2	2.01	0.42
2:B:343:TRP:CE3	2:B:343:TRP:HA	2.54	0.42
1:A:203:LEU:HD21	1:A:211:ASP:HB3	2.01	0.42
1:A:339:LEU:HB2	3:C:95:MET:HE1	2.01	0.42
3:C:50:VAL:HG13	3:C:50:VAL:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:SER:HB2	1:A:202:GLY:HA3	2.00	0.42
1:A:187:GLY:HA2	6:A:549:HOH:O	2.19	0.42
2:B:197:LEU:CD1	2:B:197:LEU:N	2.83	0.42
2:B:313:ASP:HA	2:B:345:MET:CE	2.49	0.42
1:A:419:LEU:HD13	1:A:419:LEU:HA	1.76	0.42
2:B:344:LEU:O	2:B:348:VAL:HG22	2.19	0.42
2:B:405:GLU:C	2:B:407:ASN:N	2.73	0.42
1:A:188:VAL:HG12	1:A:217:THR:O	2.19	0.42
1:A:299:LEU:HD13	1:A:392:VAL:HG21	2.00	0.42
1:A:410:ASN:HB2	1:A:413:GLU:HB2	2.02	0.42
2:B:119:THR:HG22	2:B:154:GLU:CA	2.50	0.42
2:B:212:LYS:HD2	2:B:212:LYS:HA	1.60	0.42
2:B:257:LEU:C	2:B:257:LEU:HD13	2.40	0.42
1:A:85:ASN:HD22	1:A:86:GLY:N	2.18	0.42
1:A:425:ASP:HB3	1:A:429:THR:HG23	2.02	0.42
2:B:7:ILE:HD11	2:B:157:ILE:CG2	2.50	0.42
2:B:119:THR:HG22	2:B:154:GLU:HA	2.01	0.42
2:B:297:ASP:HB2	2:B:298:GLU:OE2	2.19	0.42
1:A:231:SER:O	1:A:232:GLY:O	2.38	0.41
1:A:339:LEU:HD21	2:B:84:PRO:HD3	2.02	0.41
2:B:378:ASP:CG	2:B:379:GLY:N	2.73	0.41
3:C:28:MET:HA	3:C:31:THR:CG2	2.46	0.41
1:A:91:CYS:SG	1:A:204:VAL:HG11	2.60	0.41
1:A:169:LEU:HG	1:A:226:VAL:HG21	2.03	0.41
2:B:316:VAL:HA	2:B:319:LEU:HD13	2.01	0.41
3:C:12:ILE:N	3:C:12:ILE:HD13	2.35	0.41
2:B:113:THR:HG22	2:B:114:LYS:N	2.35	0.41
2:B:176:TYR:HE2	2:B:299:ARG:HD3	1.85	0.41
2:B:295:LEU:HB3	2:B:296:PRO:CD	2.50	0.41
2:B:3:PHE:HB2	6:B:524:HOH:O	2.20	0.41
2:B:60:MET:HB3	2:B:99:ILE:CD1	2.50	0.41
2:B:363:LYS:HB2	2:B:394:ALA:O	2.21	0.41
1:A:75:PRO:HB3	1:A:119:ILE:CD1	2.50	0.41
1:A:247:ASP:OD2	1:A:250:SER:CB	2.62	0.41
2:B:56:VAL:HG22	2:B:123:MET:HE1	2.02	0.41
2:B:230:ARG:CZ	2:B:246:ARG:HE	2.33	0.41
2:B:276:VAL:HG22	2:B:277:PRO:CD	2.51	0.41
2:B:335:ALA:HB1	2:B:340:THR:HG23	2.03	0.41
2:B:60:MET:O	2:B:64:MET:HG3	2.19	0.41
1:A:1:MET:HG2	1:A:4:ARG:CD	2.39	0.41
1:A:306:ILE:N	1:A:307:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:ASP:HB2	2:B:256:ILE:CD1	2.49	0.41
1:A:43:PHE:O	1:A:139:LYS:HE3	2.21	0.41
1:A:57:GLU:O	1:A:60:GLU:HB2	2.21	0.41
2:B:174:ILE:CG2	2:B:182:VAL:HG11	2.51	0.41
2:B:338:LYS:HZ2	2:B:338:LYS:HB3	1.85	0.41
1:A:53:LYS:HE2	1:A:57:GLU:OE2	2.21	0.41
1:A:70:LYS:HZ1	1:A:228:GLU:HB2	1.86	0.41
1:A:200:ARG:NH2	2:B:274:ASP:OD1	2.39	0.41
1:A:322:SER:CB	2:B:89:ALA:HB3	2.50	0.41
1:A:477:ASN:ND2	1:A:479:HIS:H	2.18	0.41
2:B:29:PHE:CD1	2:B:29:PHE:N	2.89	0.41
2:B:64:MET:C	2:B:66:LEU:H	2.23	0.41
2:B:105:ILE:HD11	2:B:166:TYR:CE1	2.56	0.41
2:B:135:GLU:OE1	2:B:135:GLU:HA	2.20	0.41
2:B:202:GLN:CG	2:B:203:GLU:N	2.82	0.41
2:B:202:GLN:CG	2:B:204:LYS:H	2.33	0.41
2:B:363:LYS:HB3	2:B:363:LYS:HZ3	1.86	0.41
1:A:15:ILE:HD11	1:A:25:VAL:HG21	2.03	0.41
1:A:132:SER:O	1:A:133:THR:CB	2.66	0.41
1:A:192:LYS:O	1:A:192:LYS:CG	2.67	0.41
1:A:312:ILE:HG13	1:A:378:SER:HB3	2.03	0.41
2:B:212:LYS:HB2	2:B:258:MET:HE3	2.03	0.41
2:B:285:LYS:O	2:B:289:ARG:HB2	2.21	0.41
2:B:307:LEU:CG	2:B:337:VAL:HG11	2.49	0.41
2:B:192:ASP:OD2	2:B:212:LYS:CD	2.52	0.40
2:B:295:LEU:HD22	2:B:295:LEU:H	1.84	0.40
1:A:166:LEU:HA	1:A:166:LEU:HD12	1.86	0.40
1:A:483:GLU:HB2	6:A:564:HOH:O	2.20	0.40
2:B:160:PRO:HG3	2:B:225:GLU:HB3	2.03	0.40
3:C:36:LEU:O	3:C:39:ALA:HB3	2.21	0.40
1:A:44:LEU:HD23	1:A:80:ASP:OD2	2.21	0.40
1:A:106:THR:HB	1:A:199:SER:OG	2.22	0.40
1:A:376:LYS:CE	3:C:52:PRO:HG2	2.52	0.40
1:A:15:ILE:HG13	1:A:20:ILE:CG2	2.51	0.40
1:A:399:VAL:HB	1:A:456:ILE:HB	2.03	0.40
2:B:32:GLU:HB3	6:B:515:HOH:O	2.21	0.40
2:B:226:TYR:CD1	2:B:226:TYR:C	2.95	0.40
1:A:103:TYR:HB3	2:B:39:VAL:HG11	2.02	0.40
2:B:326:PHE:CZ	2:B:364:LEU:HG	2.57	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%)	462 (96%)	20 (4%)	1 (0%)	47	60
2	B	403/483 (83%)	364 (90%)	28 (7%)	11 (3%)	5	4
3	C	96/100 (96%)	89 (93%)	5 (5%)	2 (2%)	7	7
All	All	982/1068 (92%)	915 (93%)	53 (5%)	14 (1%)	11	15

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	GLY
2	B	239	GLY
2	B	308	GLY
2	B	381	MET
2	B	383	SER
2	B	110	ASP
2	B	379	GLY
2	B	102	ASN
2	B	310	PRO
2	B	337	VAL
2	B	384	LYS
3	C	95	MET
2	B	293	PRO
3	C	94	ILE

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%)	356 (88%)	50 (12%)	4	4
2	B	352/419 (84%)	305 (87%)	47 (13%)	4	3
3	C	86/88 (98%)	69 (80%)	17 (20%)	1	1
All	All	844/913 (92%)	730 (86%)	114 (14%)	3	3

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	ILE
1	A	13	THR
1	A	15	ILE
1	A	37	ASP
1	A	38	PRO
1	A	44	LEU
1	A	53	LYS
1	A	56	GLN
1	A	65	ASP
1	A	71	LEU
1	A	83	ILE
1	A	85	ASN
1	A	96	LEU
1	A	102	ILE
1	A	111	LEU
1	A	121	LYS
1	A	122	LEU
1	A	139	LYS
1	A	166	LEU
1	A	169	LEU
1	A	171	LEU
1	A	192	LYS
1	A	194	THR
1	A	199	SER
1	A	206	PHE
1	A	216	LEU
1	A	221	LYS
1	A	245	ASP
1	A	246	VAL
1	A	257	LYS
1	A	268	LEU
1	A	287	LEU
1	A	290	LEU

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Mol	Chain	Res	Type
1	A	299	LEU
1	A	325	ASP
1	A	335	GLU
1	A	338	SER
1	A	360	PHE
1	A	366	LEU
1	A	384	LEU
1	A	411	LEU
1	A	419	LEU
1	A	427	LEU
1	A	433	LEU
1	A	436	LEU
1	A	465	LEU
1	A	477	ASN
1	A	478	LEU
1	A	485	LEU
2	B	4	GLU
2	B	50	VAL
2	B	66	LEU
2	B	75	LYS
2	B	109	VAL
2	B	119	THR
2	B	129	LYS
2	B	136	TYR
2	B	141	LEU
2	B	167	LEU
2	B	169	LYS
2	B	192	ASP
2	B	197	LEU
2	B	202	GLN
2	B	212	LYS
2	B	219	TYR
2	B	230	ARG
2	B	241	ILE
2	B	254	LYS
2	B	260	VAL
2	B	290	GLN
2	B	300	LYS
2	B	313	ASP
2	B	316	VAL
2	B	322	GLU
2	B	331	ILE

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Mol	Chain	Res	Type
2	B	340	THR
2	B	344	LEU
2	B	345	MET
2	B	353	ASN
2	B	354	LYS
2	B	355	ASN
2	B	357	VAL
2	B	358	GLU
2	B	360	LEU
2	B	362	THR
2	B	363	LYS
2	B	364	LEU
2	B	368	ASN
2	B	369	LEU
2	B	373	ILE
2	B	377	GLU
2	B	378	ASP
2	B	385	ILE
2	B	402	GLN
2	B	406	ASP
2	B	407	ASN
3	C	3	LYS
3	C	4	VAL
3	C	14	ASN
3	C	18	LEU
3	C	19	GLN
3	C	23	GLU
3	C	31	THR
3	C	32	LEU
3	C	33	GLU
3	C	36	LEU
3	C	56	VAL
3	C	57	LEU
3	C	69	ILE
3	C	75	GLU
3	C	94	ILE
3	C	97	GLU
3	C	98	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	85	ASN
1	A	387	ASN
1	A	477	ASN
2	B	86	ASN
2	B	194	ASN
2	B	202	GLN
2	B	290	GLN
2	B	315	HIS
2	B	356	GLN
2	B	368	ASN
2	B	399	ASN
2	B	402	GLN
3	C	60	GLN
3	C	74	GLN
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 monosaccharides 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	ASN	A	511	-	6,8,8	0.74	0	8,10,10	3.46	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	ASN	A	511	-	-	2/8/8/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	511	ASN	CA-CB-CG	9.03	130.19	112.24
4	A	511	ASN	O-C-CA	2.62	131.39	122.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	511	ASN	CA-CB-CG-OD1
4	A	511	ASN	CA-CB-CG-ND2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	511	ASN	3	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%)	0.27	14 (2%) 51 59	24, 38, 58, 80	0
2	B	405/483 (83%)	1.10	88 (21%) 0 0	30, 67, 95, 95	0
3	C	98/100 (98%)	0.94	16 (16%) 1 1	42, 62, 95, 95	0
All	All	988/1068 (92%)	0.67	118 (11%) 4 5	24, 49, 95, 95	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	382	SER	10.5
2	B	381	MET	9.6
2	B	403	ILE	9.6
1	A	1	MET	9.1
2	B	400	ALA	8.9
3	C	96	ASN	8.4
2	B	260	VAL	7.4
3	C	95	MET	7.2
3	C	94	ILE	6.3
3	C	99	ASP	6.1
2	B	375	LEU	5.9
2	B	398	GLY	5.9
2	B	404	MET	5.6
2	B	376	ILE	5.6
2	B	405	GLU	5.5
3	C	97	GLU	5.4
3	C	98	GLU	5.3
2	B	401	LYS	5.2
3	C	100	ALA	5.0
2	B	363	LYS	4.7
2	B	361	ASP	4.7
2	B	358	GLU	4.6
2	B	390	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	109	VAL	4.5
2	B	362	THR	4.4
2	B	262	GLU	4.3
2	B	397	GLY	4.3
2	B	387	LYS	4.0
2	B	378	ASP	3.9
2	B	337	VAL	3.8
3	C	23	GLU	3.8
2	B	395	ALA	3.8
2	B	380	THR	3.8
2	B	263	GLY	3.7
2	B	364	LEU	3.6
2	B	384	LYS	3.6
2	B	360	LEU	3.5
2	B	388	LYS	3.5
2	B	307	LEU	3.5
2	B	393	LEU	3.5
2	B	112	GLU	3.4
2	B	379	GLY	3.4
1	A	52	ILE	3.4
2	B	135	GLU	3.4
2	B	237	ASN	3.3
2	B	339	LEU	3.3
2	B	370	ALA	3.3
2	B	372	MET	3.3
2	B	31	ALA	3.3
2	B	261	LYS	3.3
2	B	335	ALA	3.3
2	B	331	ILE	3.3
2	B	28	HIS	3.2
2	B	305	ASN	3.2
3	C	86	ASP	3.1
3	C	38	PHE	3.0
2	B	239	GLY	3.0
1	A	206	PHE	3.0
1	A	203	LEU	3.0
2	B	264	SER	3.0
2	B	311	ALA	2.9
2	B	402	GLN	2.9
2	B	391	PRO	2.9
2	B	340	THR	2.9
2	B	373	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	359	LEU	2.8
2	B	353	ASN	2.8
2	B	338	LYS	2.7
1	A	127	PHE	2.7
2	B	385	ILE	2.7
1	A	56	GLN	2.7
2	B	312	TYR	2.7
2	B	396	LYS	2.7
3	C	22	PRO	2.7
2	B	110	ASP	2.7
1	A	154	SER	2.6
3	C	30	ASN	2.6
2	B	371	GLY	2.6
2	B	257	LEU	2.6
2	B	407	ASN	2.6
2	B	406	ASP	2.6
2	B	310	PRO	2.6
2	B	357	VAL	2.5
2	B	212	LYS	2.5
2	B	346	GLY	2.4
2	B	5	THR	2.4
2	B	394	ALA	2.4
2	B	389	VAL	2.4
2	B	113	THR	2.4
2	B	386	ALA	2.4
2	B	367	GLU	2.4
2	B	345	MET	2.3
2	B	334	GLY	2.3
2	B	247	ARG	2.3
2	B	341	SER	2.3
2	B	249	ASP	2.3
3	C	6	ARG	2.3
2	B	343	TRP	2.3
1	A	128	ALA	2.3
1	A	207	ALA	2.3
3	C	25	THR	2.3
2	B	368	ASN	2.3
1	A	205	ALA	2.2
2	B	369	LEU	2.2
1	A	321	LEU	2.2
3	C	3	LYS	2.2
1	A	204	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	138	LEU	2.2
1	A	21	LYS	2.1
2	B	356	GLN	2.1
1	A	320	ASN	2.1
2	B	374	LYS	2.1
2	B	349	ASN	2.1
2	B	332	GLU	2.0
2	B	240	GLU	2.0
2	B	47	VAL	2.0
3	C	87	GLY	2.0
2	B	241	ILE	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, 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(Å ²)	Q<0.9
5	MG	B	501	1/1	0.86	0.23	33,33,33,33	0
4	ASN	A	511	9/9	0.96	0.24	32,36,39,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.