



Full wwPDB EM Validation Report ⓘ

Feb 11, 2024 – 09:55 PM EST

PDB ID : 3DCO
EMDB ID : EMD-5038
Title : Drosophila NOD (3DC4) and Bovine Tubulin (1JFF) Docked into the 11-Angstrom Cryo-EM Map of Nucleotide-Free NOD Complexed to the Microtubule
Authors : Sindelar, C.V.; Cochran, J.C.; Kull, F.J.
Deposited on : 2008-06-04
Resolution : 11.00 Å (reported)
Based on initial models : 1JFF, 3DC4

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

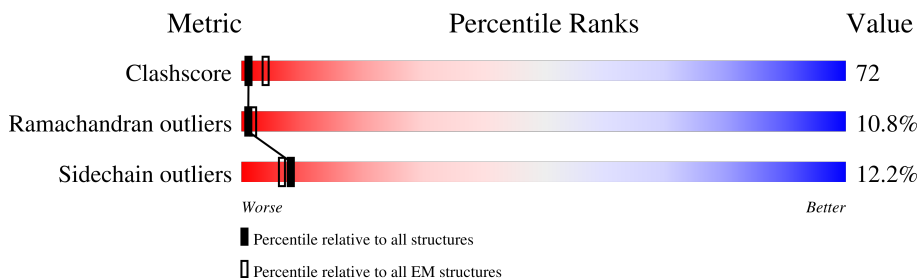
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.00 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	N	344	84% 55% 26% 15% 16% 57% 17% 9%
2	A	451	51% 20% 56% 18%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8977 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Kinesin-like protein Nod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	N	291	2247	1420	397	416	14	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	-14	MET	-	expression tag	UNP P18105
N	-13	ALA	-	expression tag	UNP P18105
N	-12	SER	-	expression tag	UNP P18105
N	-11	ASP	-	expression tag	UNP P18105
N	-10	TYR	-	expression tag	UNP P18105
N	-9	LYS	-	expression tag	UNP P18105
N	-8	ASP	-	expression tag	UNP P18105
N	-7	ASP	-	expression tag	UNP P18105
N	-6	ASP	-	expression tag	UNP P18105
N	-5	ASP	-	expression tag	UNP P18105
N	-4	LYS	-	expression tag	UNP P18105
N	-3	ARG	-	expression tag	UNP P18105
N	-2	ARG	-	expression tag	UNP P18105
N	-1	ARG	-	expression tag	UNP P18105
N	0	GLY	-	expression tag	UNP P18105
N	319	ALA	-	expression tag	UNP P18105
N	320	ALA	-	expression tag	UNP P18105
N	321	ALA	-	expression tag	UNP P18105
N	322	LEU	-	expression tag	UNP P18105
N	323	GLU	-	expression tag	UNP P18105
N	324	HIS	-	expression tag	UNP P18105
N	325	HIS	-	expression tag	UNP P18105
N	326	HIS	-	expression tag	UNP P18105
N	327	HIS	-	expression tag	UNP P18105
N	328	HIS	-	expression tag	UNP P18105
N	329	HIS	-	expression tag	UNP P18105

- Molecule 2 is a protein called Bovine Alpha Tubulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	412	3227	2043	551	613	20	0	0

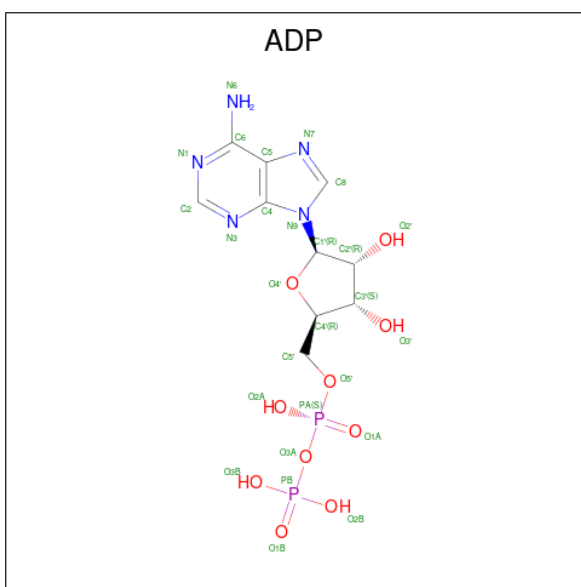
- Molecule 3 is a protein called Bovine Beta Tubulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	426	3351	2105	575	646	25	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	N	1	Total	Mg	0
			1	1	
4	A	1	Total	Mg	0
			1	1	

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

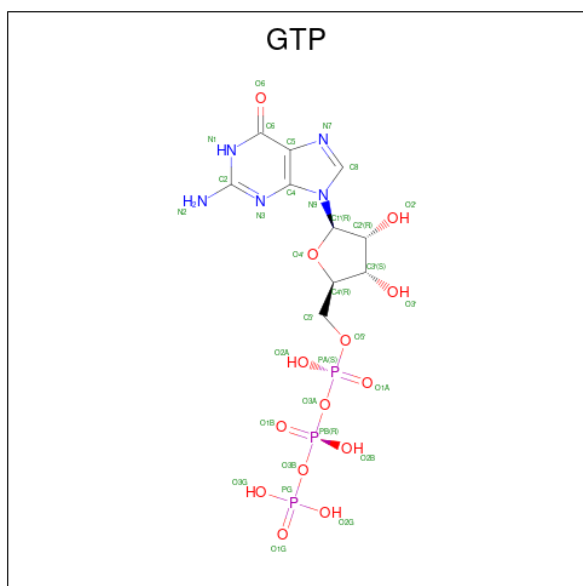


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	N	1	27	10	5	10	2	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

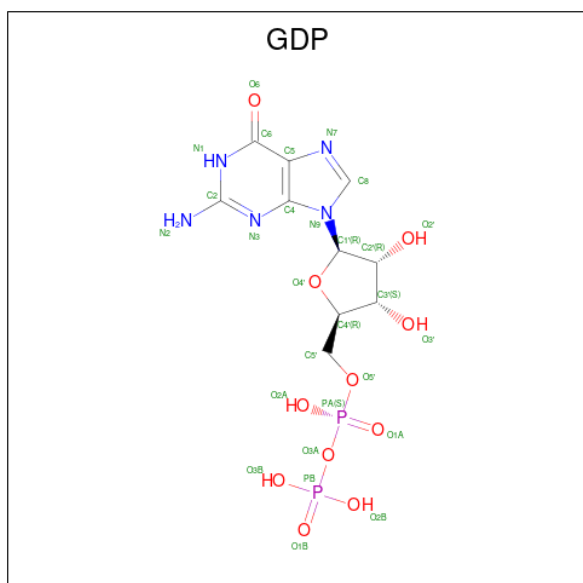
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Zn	0
			1	1	

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



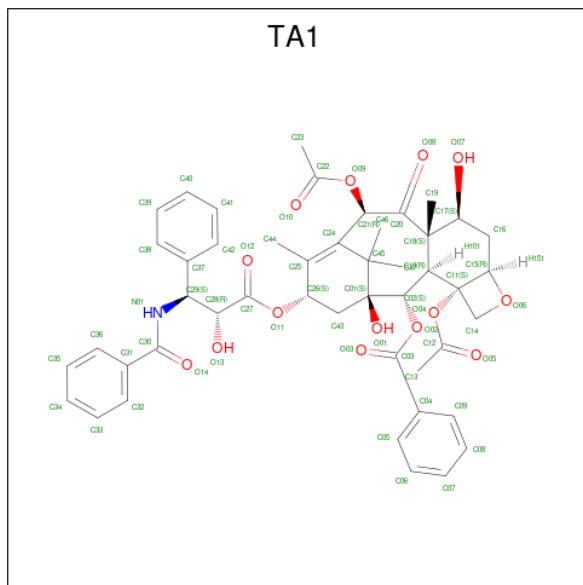
Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
8	B	1	28	10	5	11	2	0

- Molecule 9 is TAXOL (three-letter code: TA1) (formula: $C_{47}H_{51}NO_{14}$).

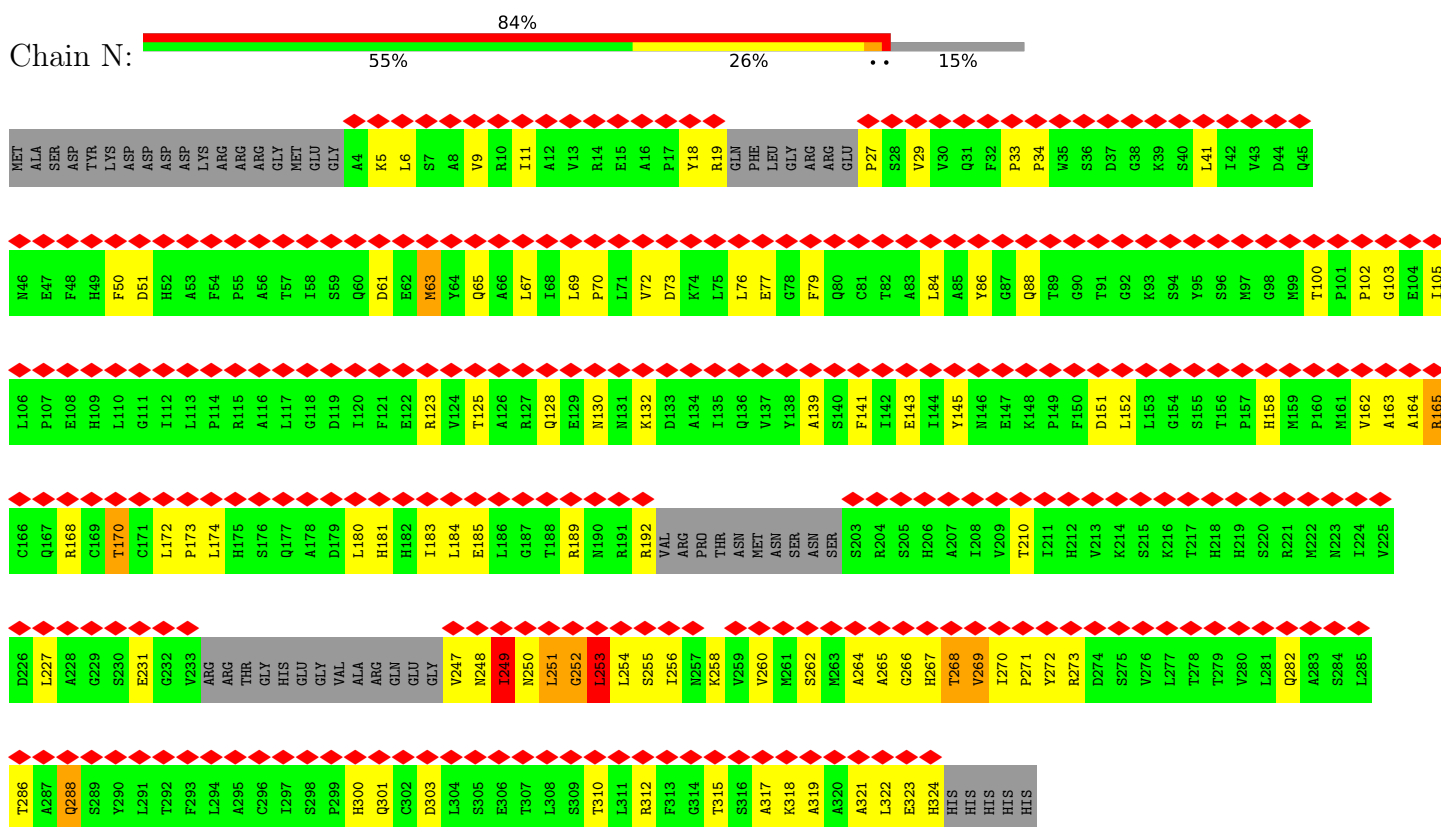


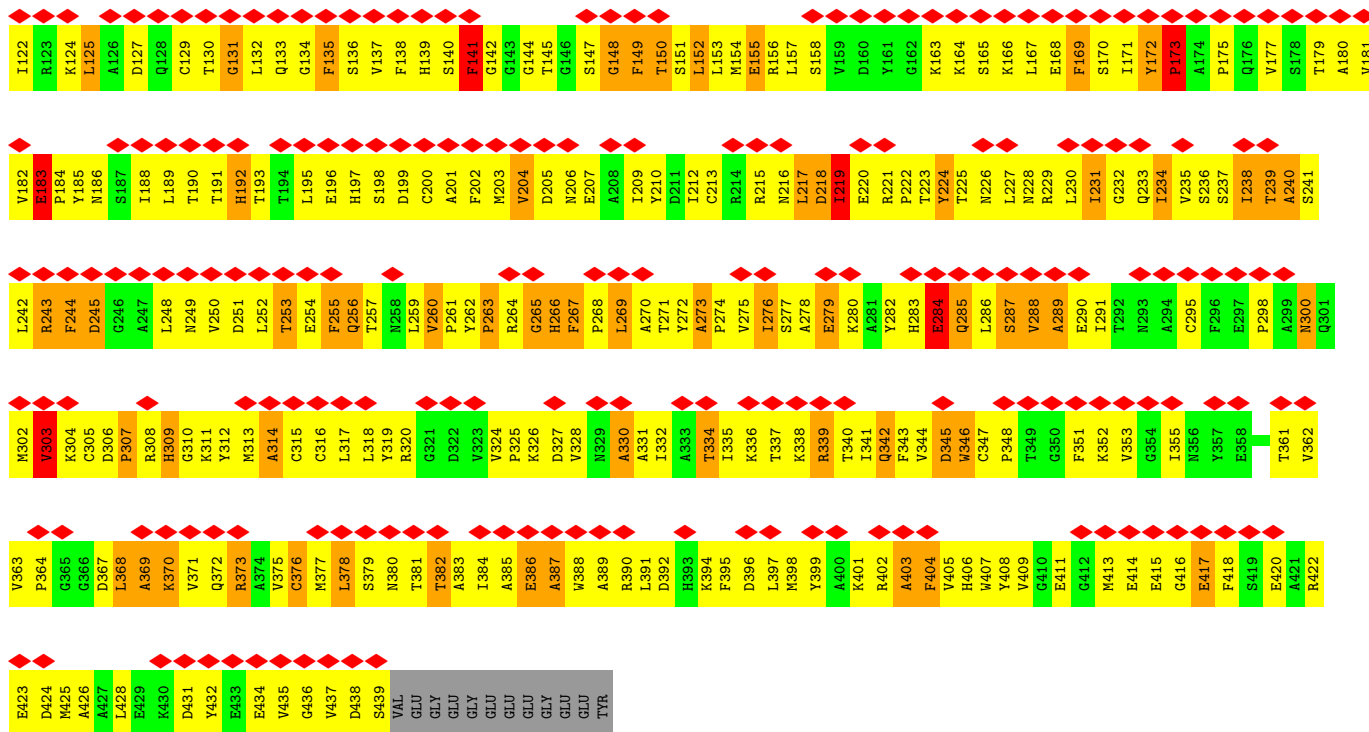
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	B	1	62	47	1	14	0

3 Residue-property plots

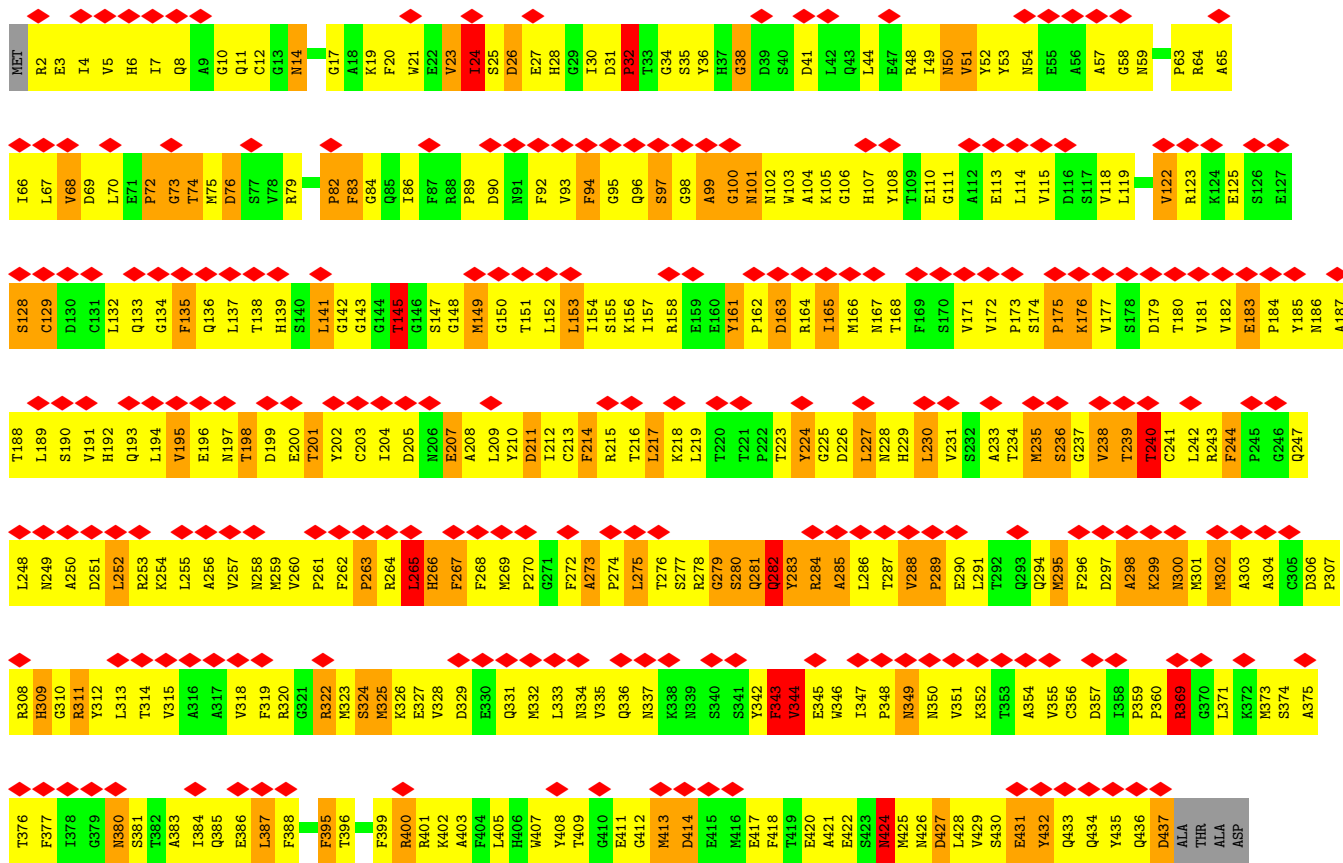
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Kinesin-like protein Nod





● Molecule 3: Bovine Beta Tubulin



GLU
GLN
GLY
GLU
PHE
GLU
GLU
GLY
GLU
GLU
ASP
GLU
ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	JEOL 4000EX	Depositor
Voltage (kV)	400	Depositor
Electron dose ($e^-/\text{Å}^2$)	16	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	60000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.100	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	360, 360, 360	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2, 2, 2	Depositor

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: ADP, ZN, GTP, TA1, MG, GDP

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	N	0.31	0/2293	0.60	3/3110 (0.1%)
2	A	0.50	0/3300	0.73	0/4482
3	B	0.51	0/3426	0.76	2/4642 (0.0%)
All	All	0.46	0/9019	0.71	5/12234 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	268	THR	CB-CA-C	-9.04	87.20	111.60
1	N	288	GLN	CB-CA-C	-6.56	97.29	110.40
3	B	235	MET	CG-SD-CE	6.09	109.95	100.20
1	N	130	ASN	N-CA-C	-5.55	96.02	111.00
3	B	217	LEU	N-CA-C	-5.37	96.51	111.00

There are no chirality outliers.

There are no planarity outliers.

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	N	2247	0	2247	212	0
2	A	3227	0	3143	580	0
3	B	3351	0	3227	619	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	N	1	0	0	0	0
5	N	27	0	12	0	0
6	A	1	0	0	0	0
7	B	32	0	12	4	0
8	B	28	0	12	1	0
9	B	62	0	51	6	0
All	All	8977	0	8704	1270	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 72.

All (1270) 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)
1:N:254:LEU:CD2	2:A:409:VAL:CG1	1.78	1.58
1:N:271:PRO:HB3	3:B:263:PRO:CG	1.22	1.57
1:N:271:PRO:CB	3:B:263:PRO:CG	1.92	1.47
1:N:254:LEU:HD22	2:A:409:VAL:CG1	1.01	1.46
1:N:271:PRO:CB	3:B:263:PRO:HG2	1.48	1.36
1:N:266:GLY:O	3:B:434:GLN:CB	1.72	1.34
1:N:268:THR:HG23	3:B:430:SER:O	1.26	1.28
1:N:248:ASN:O	1:N:249:ILE:CG2	1.81	1.27
1:N:248:ASN:O	1:N:249:ILE:HG23	1.29	1.24
1:N:227:LEU:CD1	1:N:253:LEU:HD21	1.67	1.23
1:N:254:LEU:CD1	2:A:409:VAL:HG12	1.70	1.21
1:N:268:THR:HG23	3:B:430:SER:C	1.40	1.17
3:B:234:THR:HG21	3:B:270:PRO:HB2	1.23	1.16
1:N:266:GLY:C	3:B:434:GLN:CB	2.14	1.16
2:A:243:ARG:NH2	2:A:252:LEU:H	1.45	1.13
1:N:266:GLY:O	3:B:434:GLN:HB2	1.36	1.13
1:N:254:LEU:HD13	2:A:409:VAL:HG12	1.20	1.12
1:N:271:PRO:HB3	3:B:263:PRO:CB	1.79	1.12
1:N:312:ARG:HH22	2:A:417:GLU:HA	1.05	1.11
1:N:266:GLY:C	3:B:434:GLN:HB3	1.69	1.11
1:N:312:ARG:NH2	2:A:417:GLU:CA	2.15	1.10
1:N:227:LEU:HD12	1:N:253:LEU:HD21	1.18	1.09
1:N:268:THR:HG22	1:N:268:THR:O	1.50	1.09
3:B:93:VAL:HG11	3:B:118:VAL:HG22	1.30	1.09
1:N:312:ARG:NH2	2:A:417:GLU:HA	1.68	1.07
1:N:254:LEU:CD2	2:A:409:VAL:HG13	1.58	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:268:THR:OG1	3:B:433:GLN:N	1.89	1.05
2:A:109:THR:HG22	2:A:110:ILE:N	1.70	1.04
1:N:271:PRO:CB	3:B:263:PRO:HG3	1.87	1.03
2:A:243:ARG:HH21	2:A:252:LEU:N	1.57	1.03
1:N:254:LEU:HD21	2:A:409:VAL:HG13	1.40	1.02
3:B:172:VAL:HG11	3:B:387:LEU:HD21	1.37	1.02
1:N:268:THR:OG1	3:B:434:GLN:N	1.91	1.01
2:A:11:GLN:HG3	2:A:74:VAL:HG11	1.43	1.01
1:N:254:LEU:CD2	2:A:409:VAL:HG11	1.62	1.01
1:N:268:THR:O	3:B:432:TYR:N	1.72	1.01
3:B:236:SER:O	3:B:240:THR:HG23	1.61	1.01
1:N:273:ARG:HH11	3:B:196:GLU:CB	1.73	1.00
1:N:266:GLY:CA	3:B:434:GLN:HB3	1.89	1.00
1:N:268:THR:CG2	3:B:430:SER:C	2.28	1.00
1:N:268:THR:HB	3:B:431:GLU:OE1	1.60	1.00
3:B:299:LYS:H	3:B:299:LYS:HD3	1.24	1.00
1:N:254:LEU:HD22	2:A:409:VAL:HG13	1.19	0.97
2:A:98:ASP:HB2	2:A:105:ARG:HH21	1.31	0.96
1:N:266:GLY:O	3:B:434:GLN:C	2.03	0.95
1:N:266:GLY:C	3:B:434:GLN:HB2	1.80	0.95
1:N:265:ALA:HB2	2:A:401:LYS:HG2	1.49	0.94
2:A:259:LEU:HD11	2:A:378:LEU:HD13	1.47	0.94
3:B:273:ALA:HB3	3:B:274:PRO:HD3	1.48	0.94
3:B:281:GLN:O	3:B:283:TYR:N	2.00	0.94
2:A:251:ASP:N	2:A:254:GLU:HG3	1.82	0.94
1:N:268:THR:OG1	3:B:432:TYR:C	2.04	0.94
2:A:237:SER:HB2	2:A:376:CYS:SG	2.08	0.94
3:B:132:LEU:HD23	3:B:164:ARG:HG3	1.50	0.93
2:A:31:GLN:HB3	2:A:32:PRO:HD2	1.51	0.93
2:A:316:CYS:HB3	2:A:378:LEU:HD11	1.48	0.93
1:N:312:ARG:NH2	2:A:417:GLU:HG2	1.83	0.92
3:B:264:ARG:O	3:B:265:LEU:HB3	1.69	0.92
2:A:251:ASP:H	2:A:254:GLU:HG3	1.33	0.92
1:N:265:ALA:HB1	2:A:401:LYS:HD3	1.50	0.92
1:N:271:PRO:CG	3:B:263:PRO:HG2	2.00	0.92
1:N:271:PRO:CG	3:B:263:PRO:CG	2.47	0.92
1:N:268:THR:H	3:B:434:GLN:HG3	1.35	0.91
1:N:248:ASN:C	1:N:249:ILE:HG22	1.88	0.91
3:B:70:LEU:H	3:B:145:THR:HG21	1.33	0.91
2:A:151:SER:HB3	2:A:193:THR:HG21	1.51	0.90
1:N:248:ASN:O	1:N:249:ILE:HG22	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:147:SER:O	3:B:151:THR:HB	1.71	0.89
3:B:8:GLN:OE1	3:B:67:LEU:HD22	1.72	0.89
3:B:93:VAL:HG11	3:B:118:VAL:CG2	2.03	0.89
3:B:102:ASN:HD21	3:B:408:TYR:HA	1.38	0.88
2:A:343:PHE:CZ	2:A:351:PHE:CE1	2.61	0.88
3:B:101:ASN:HD21	3:B:143:GLY:HA2	1.38	0.88
1:N:227:LEU:CD1	1:N:253:LEU:CD2	2.51	0.88
2:A:119:LEU:HD23	2:A:122:ILE:HD11	1.53	0.88
1:N:268:THR:HA	3:B:434:GLN:CG	2.03	0.88
3:B:264:ARG:HB2	3:B:266:HIS:CD2	2.08	0.88
3:B:311:ARG:HD3	3:B:342:TYR:HA	1.56	0.88
1:N:268:THR:CG2	3:B:430:SER:O	2.18	0.88
2:A:147:SER:HB2	2:A:190:THR:OG1	1.73	0.88
2:A:109:THR:HG22	2:A:110:ILE:H	1.33	0.88
1:N:312:ARG:NH2	2:A:417:GLU:CG	2.36	0.87
3:B:276:THR:HB	3:B:281:GLN:HG3	1.56	0.87
2:A:407:TRP:HE1	3:B:260:VAL:HG23	1.38	0.87
2:A:110:ILE:HG23	2:A:111:GLY:H	1.38	0.87
2:A:122:ILE:HD12	2:A:157:LEU:HD21	1.54	0.87
3:B:6:HIS:CE1	3:B:8:GLN:HG2	2.10	0.86
3:B:153:LEU:O	3:B:157:ILE:HG12	1.75	0.86
1:N:312:ARG:NH2	2:A:417:GLU:N	2.23	0.86
1:N:248:ASN:C	1:N:249:ILE:CG2	2.36	0.86
1:N:268:THR:CG2	3:B:433:GLN:H	1.85	0.86
1:N:254:LEU:CG	2:A:409:VAL:CG1	2.53	0.86
3:B:195:VAL:HG13	3:B:196:GLU:HG2	1.57	0.86
3:B:360:PRO:HG2	3:B:371:LEU:HB3	1.56	0.86
3:B:10:GLY:HA2	3:B:145:THR:HB	1.55	0.86
2:A:264:ARG:O	2:A:266:HIS:N	2.09	0.85
1:N:266:GLY:O	3:B:434:GLN:HB3	1.63	0.85
3:B:242:LEU:HD22	3:B:250:ALA:H	1.41	0.85
2:A:234:ILE:HG13	2:A:270:ALA:HB1	1.59	0.84
3:B:234:THR:HG21	3:B:270:PRO:CB	2.06	0.84
1:N:84:LEU:HD21	1:N:253:LEU:CD2	2.06	0.84
1:N:312:ARG:HH22	2:A:417:GLU:CA	1.81	0.84
2:A:204:VAL:HG11	2:A:231:ILE:HD12	1.59	0.84
3:B:4:ILE:HD13	3:B:136:GLN:HE21	1.42	0.84
3:B:20:PHE:CD2	3:B:235:MET:SD	2.71	0.84
3:B:19:LYS:HG3	3:B:228:ASN:HB3	1.57	0.84
3:B:324:SER:HB3	3:B:327:GLU:HG2	1.60	0.84
1:N:273:ARG:HH11	3:B:196:GLU:HB3	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:264:ARG:HB2	2:A:266:HIS:CD2	2.13	0.83
2:A:316:CYS:HB3	2:A:378:LEU:CD1	2.08	0.83
3:B:3:GLU:O	3:B:133:GLN:HB3	1.78	0.83
3:B:101:ASN:ND2	3:B:143:GLY:HA2	1.94	0.83
3:B:209:LEU:HB3	3:B:227:LEU:HD22	1.59	0.83
3:B:148:GLY:O	3:B:151:THR:HG22	1.79	0.83
3:B:156:LYS:HE2	3:B:156:LYS:HA	1.61	0.83
1:N:254:LEU:CG	2:A:409:VAL:HG12	2.08	0.82
2:A:184:PRO:HG2	2:A:398:MET:HE1	1.60	0.82
1:N:227:LEU:HD11	1:N:253:LEU:HD21	1.62	0.82
1:N:268:THR:CA	3:B:434:GLN:CG	2.58	0.82
2:A:106:GLY:O	2:A:111:GLY:HA3	1.78	0.82
2:A:23:LEU:HD23	2:A:236:SER:HB2	1.61	0.82
1:N:268:THR:H	3:B:434:GLN:CG	1.92	0.81
3:B:147:SER:HB2	3:B:190:SER:HB3	1.60	0.81
3:B:287:THR:O	3:B:288:VAL:HG23	1.78	0.81
1:N:103:GLY:H	1:N:181:HIS:HD2	1.29	0.81
2:A:151:SER:CB	2:A:193:THR:HG21	2.09	0.81
3:B:110:GLU:O	3:B:113:GLU:HG2	1.79	0.81
1:N:267:HIS:C	3:B:431:GLU:HG2	1.83	0.81
3:B:150:GLY:HA2	3:B:153:LEU:HD22	1.59	0.81
2:A:248:LEU:HD23	2:A:353:VAL:O	1.80	0.81
3:B:264:ARG:HB2	3:B:266:HIS:HD2	1.45	0.81
1:N:268:THR:N	3:B:434:GLN:HB2	1.96	0.81
2:A:267:PHE:N	2:A:267:PHE:CD1	2.49	0.81
3:B:54:ASN:HD21	3:B:64:ARG:HD3	1.46	0.81
3:B:20:PHE:CZ	3:B:24:ILE:HD12	2.15	0.80
3:B:236:SER:O	3:B:240:THR:CG2	2.29	0.80
1:N:268:THR:N	3:B:434:GLN:HG3	1.95	0.80
2:A:234:ILE:HD13	2:A:234:ILE:O	1.81	0.80
3:B:191:VAL:HG11	3:B:425:MET:HG3	1.60	0.80
2:A:220:GLU:C	2:A:222:PRO:HD3	2.02	0.80
2:A:6:SER:HB3	2:A:136:SER:OG	1.81	0.80
1:N:273:ARG:NH1	3:B:196:GLU:CB	2.45	0.80
1:N:312:ARG:HH21	2:A:417:GLU:HG2	1.44	0.80
3:B:68:VAL:HG12	3:B:149:MET:SD	2.22	0.80
1:N:268:THR:N	3:B:434:GLN:CG	2.45	0.80
2:A:313:MET:HB3	2:A:344:VAL:HG21	1.63	0.79
2:A:7:ILE:HG22	2:A:66:VAL:HG22	1.63	0.79
2:A:132:LEU:HD23	2:A:132:LEU:H	1.46	0.79
3:B:265:LEU:HD12	3:B:265:LEU:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:271:PRO:CG	3:B:263:PRO:HG3	2.10	0.79
3:B:413:MET:HG3	3:B:414:ASP:H	1.47	0.79
2:A:241:SER:O	2:A:244:PHE:HB3	1.82	0.79
2:A:204:VAL:HG13	2:A:209:ILE:HD11	1.65	0.79
3:B:259:MET:HA	3:B:314:THR:HG21	1.65	0.79
2:A:11:GLN:HG3	2:A:74:VAL:CG1	2.13	0.78
2:A:69:ASP:HA	2:A:145:THR:HG21	1.66	0.78
1:N:253:LEU:O	1:N:256:ILE:HB	1.83	0.78
2:A:199:ASP:HB3	2:A:256:GLN:NE2	1.98	0.78
2:A:109:THR:CG2	2:A:110:ILE:N	2.44	0.78
2:A:172:TYR:C	2:A:172:TYR:HD1	1.87	0.78
1:N:265:ALA:HB2	2:A:401:LYS:CG	2.13	0.78
1:N:273:ARG:HH11	3:B:196:GLU:HB2	1.46	0.78
2:A:155:GLU:HA	2:A:197:HIS:ND1	1.99	0.78
3:B:234:THR:CG2	3:B:270:PRO:HB2	2.11	0.78
2:A:243:ARG:HH21	2:A:252:LEU:H	0.79	0.77
3:B:396:THR:HG23	3:B:422:GLU:OE2	1.83	0.77
3:B:205:ASP:OD1	3:B:304:ALA:HB2	1.84	0.77
3:B:192:HIS:ND1	3:B:424:ASN:OD1	2.18	0.77
2:A:223:THR:HB	2:A:225:THR:HG22	1.67	0.77
2:A:425:MET:HE2	2:A:428:LEU:HD23	1.64	0.77
3:B:259:MET:HG2	3:B:314:THR:HG21	1.67	0.77
1:N:268:THR:CG2	3:B:433:GLN:N	2.45	0.77
1:N:268:THR:HA	3:B:434:GLN:HG3	1.64	0.77
2:A:110:ILE:HG23	2:A:111:GLY:N	1.99	0.77
1:N:266:GLY:O	3:B:434:GLN:CA	2.33	0.76
2:A:231:ILE:HA	2:A:234:ILE:HG22	1.66	0.76
3:B:35:SER:HB3	3:B:59:ASN:HA	1.65	0.76
1:N:271:PRO:HB3	3:B:263:PRO:HG2	0.77	0.76
1:N:253:LEU:HA	1:N:256:ILE:HD12	1.65	0.76
2:A:221:ARG:O	2:A:221:ARG:HD3	1.85	0.76
3:B:176:LYS:HE3	3:B:207:GLU:HG3	1.68	0.76
3:B:250:ALA:HA	3:B:254:LYS:HE2	1.68	0.76
2:A:7:ILE:HD12	2:A:153:LEU:HD21	1.68	0.76
1:N:273:ARG:NH1	3:B:196:GLU:HB2	2.01	0.75
3:B:198:THR:O	3:B:265:LEU:HD22	1.85	0.75
2:A:167:LEU:HG	2:A:200:CYS:HB3	1.69	0.75
2:A:225:THR:O	2:A:229:ARG:HG3	1.85	0.75
2:A:101:ASN:ND2	3:B:254:LYS:HD2	2.02	0.75
2:A:344:VAL:HG11	2:A:346:TRP:CE2	2.21	0.75
1:N:19:ARG:H	1:N:300:HIS:HE1	1.32	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:268:THR:HA	3:B:434:GLN:HG2	1.67	0.75
2:A:163:LYS:O	2:A:164:LYS:HG2	1.86	0.75
2:A:205:ASP:CB	2:A:303:VAL:HA	2.17	0.75
3:B:19:LYS:HG3	3:B:228:ASN:CB	2.17	0.75
3:B:209:LEU:HG	3:B:230:LEU:HD22	1.69	0.75
1:N:271:PRO:CB	3:B:263:PRO:CB	2.53	0.75
2:A:4:CYS:SG	2:A:252:LEU:HD11	2.27	0.75
3:B:103:TRP:CZ3	3:B:108:TYR:HE1	2.05	0.74
1:N:269:VAL:C	3:B:264:ARG:HD3	2.08	0.74
2:A:331:ALA:O	2:A:335:ILE:HG12	1.86	0.74
2:A:172:TYR:OH	2:A:387:ALA:HB1	1.87	0.74
1:N:164:ALA:HB1	1:N:168:ARG:HB3	1.69	0.74
1:N:266:GLY:HA3	3:B:434:GLN:HB3	1.69	0.74
2:A:362:VAL:HG13	2:A:368:LEU:HD12	1.68	0.74
2:A:276:ILE:HG23	2:A:369:ALA:CB	2.16	0.74
2:A:264:ARG:C	2:A:266:HIS:H	1.91	0.74
3:B:242:LEU:HD13	3:B:250:ALA:C	2.08	0.74
2:A:317:LEU:HB3	2:A:319:TYR:HE1	1.52	0.74
3:B:168:THR:HB	3:B:201:THR:HG23	1.68	0.74
2:A:63:PRO:O	2:A:64:ARG:HG2	1.88	0.73
2:A:104:ALA:HB2	2:A:413:MET:HG3	1.71	0.73
3:B:8:GLN:CD	3:B:67:LEU:HD22	2.08	0.73
2:A:104:ALA:CB	2:A:413:MET:HG3	2.18	0.73
2:A:112:LYS:O	2:A:115:ILE:HG22	1.89	0.73
3:B:76:ASP:HA	3:B:79:ARG:HG2	1.71	0.73
3:B:217:LEU:O	3:B:219:LEU:N	2.22	0.73
2:A:7:ILE:HD11	2:A:137:VAL:HG22	1.71	0.73
3:B:217:LEU:C	3:B:219:LEU:H	1.91	0.73
3:B:191:VAL:CG1	3:B:425:MET:HG3	2.19	0.73
2:A:31:GLN:HB3	2:A:32:PRO:CD	2.18	0.72
2:A:105:ARG:O	2:A:110:ILE:HG22	1.89	0.72
3:B:274:PRO:HG2	3:B:371:LEU:HD21	1.70	0.72
2:A:25:CYS:HB2	2:A:30:ILE:O	1.89	0.72
1:N:270:ILE:N	3:B:264:ARG:HD3	2.04	0.72
1:N:227:LEU:HD11	1:N:253:LEU:CD2	2.18	0.72
1:N:265:ALA:HB1	2:A:401:LYS:CD	2.20	0.72
1:N:271:PRO:HG3	3:B:263:PRO:HG3	1.70	0.72
2:A:103:TYR:CD2	2:A:189:LEU:HD13	2.24	0.72
3:B:356:CYS:SG	3:B:357:ASP:N	2.62	0.72
2:A:242:LEU:HG	2:A:250:VAL:O	1.88	0.72
1:N:268:THR:CA	3:B:434:GLN:HG2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:7:ILE:CG1	2:A:137:VAL:HG22	2.20	0.72
1:N:265:ALA:CB	2:A:401:LYS:HG2	2.20	0.72
2:A:306:ASP:O	2:A:308:ARG:N	2.20	0.72
3:B:6:HIS:HE1	3:B:8:GLN:HG2	1.52	0.72
2:A:172:TYR:C	2:A:172:TYR:CD1	2.61	0.72
3:B:70:LEU:HG	3:B:145:THR:CG2	2.20	0.72
3:B:48:ARG:HG2	3:B:243:ARG:O	1.90	0.71
3:B:237:GLY:O	3:B:241:CYS:HB3	1.90	0.71
1:N:268:THR:O	1:N:269:VAL:HG23	1.88	0.71
3:B:201:THR:OG1	3:B:265:LEU:HD11	1.90	0.71
3:B:243:ARG:NH2	3:B:252:LEU:HG	2.05	0.71
3:B:111:GLY:O	3:B:115:VAL:HG23	1.89	0.71
3:B:431:GLU:OE1	3:B:432:TYR:HA	1.91	0.71
3:B:255:LEU:O	3:B:259:MET:HG3	1.91	0.71
2:A:12:ALA:HB3	2:A:140:SER:OG	1.91	0.71
2:A:317:LEU:HD12	2:A:351:PHE:HD2	1.56	0.71
2:A:166:LYS:HE3	2:A:199:ASP:OD1	1.90	0.70
3:B:10:GLY:O	3:B:14:ASN:HB2	1.90	0.70
3:B:299:LYS:HD3	3:B:299:LYS:N	2.04	0.70
1:N:268:THR:HG21	3:B:433:GLN:N	1.99	0.70
3:B:8:GLN:NE2	3:B:17:GLY:HA3	2.06	0.70
2:A:259:LEU:HD11	2:A:378:LEU:CD1	2.20	0.70
3:B:70:LEU:HG	3:B:145:THR:HG23	1.74	0.70
3:B:175:PRO:HD2	3:B:207:GLU:OE2	1.91	0.70
2:A:148:GLY:O	2:A:151:SER:HB2	1.91	0.70
2:A:312:TYR:O	2:A:344:VAL:HG23	1.90	0.70
3:B:291:LEU:O	3:B:295:MET:HG3	1.91	0.70
1:N:254:LEU:HD22	2:A:409:VAL:HG11	0.70	0.70
1:N:271:PRO:HG3	3:B:263:PRO:CG	2.21	0.70
2:A:5:ILE:HG22	2:A:6:SER:N	2.07	0.70
1:N:268:THR:CA	3:B:434:GLN:HG3	2.20	0.70
2:A:88:HIS:C	2:A:90:GLU:H	1.95	0.70
2:A:343:PHE:CZ	2:A:351:PHE:HE1	2.08	0.70
2:A:205:ASP:HB3	2:A:303:VAL:HA	1.73	0.69
2:A:242:LEU:HD21	2:A:250:VAL:HB	1.71	0.69
3:B:24:ILE:HD11	3:B:52:TYR:CE1	2.28	0.69
2:A:234:ILE:HG21	2:A:302:MET:HE3	1.72	0.69
2:A:237:SER:CB	2:A:376:CYS:SG	2.80	0.69
3:B:234:THR:O	3:B:238:VAL:HG23	1.92	0.69
2:A:63:PRO:C	2:A:64:ARG:HG2	2.12	0.69
3:B:180:THR:HG22	3:B:181:VAL:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:244:PHE:HD2	2:A:245:ASP:N	1.89	0.69
2:A:381:THR:C	2:A:383:ALA:H	1.95	0.69
3:B:209:LEU:HD23	3:B:227:LEU:HB3	1.75	0.69
1:N:312:ARG:NH2	2:A:417:GLU:CB	2.56	0.69
2:A:394:LYS:HG2	3:B:348:PRO:HG3	1.75	0.69
2:A:222:PRO:HD2	3:B:326:LYS:HB3	1.74	0.69
3:B:359:PRO:HB2	3:B:360:PRO:HD2	1.74	0.69
2:A:133:GLN:HG2	2:A:243:ARG:HH22	1.57	0.68
1:N:88:GLN:HE22	1:N:303:ASP:HB3	1.58	0.68
1:N:268:THR:O	1:N:269:VAL:CG2	2.41	0.68
2:A:141:PHE:O	2:A:147:SER:HB3	1.94	0.68
1:N:271:PRO:HB3	3:B:263:PRO:HB2	1.73	0.68
2:A:199:ASP:HB3	2:A:256:GLN:HE21	1.57	0.68
2:A:407:TRP:HE1	3:B:260:VAL:CG2	2.07	0.68
1:N:268:THR:H	3:B:434:GLN:CB	2.06	0.68
2:A:71:GLU:HG3	3:B:2:ARG:HH21	1.58	0.68
2:A:217:LEU:HD12	2:A:277:SER:HB3	1.75	0.68
2:A:371:VAL:HG12	2:A:372:GLN:H	1.57	0.68
2:A:221:ARG:N	2:A:222:PRO:HD3	2.09	0.68
3:B:204:ILE:HD13	3:B:231:VAL:HG22	1.76	0.68
2:A:95:GLY:O	2:A:97:GLU:N	2.27	0.68
2:A:7:ILE:HD12	2:A:153:LEU:CD2	2.24	0.68
2:A:115:ILE:CD1	2:A:119:LEU:HG	2.23	0.68
2:A:152:LEU:HA	2:A:155:GLU:HB2	1.76	0.68
2:A:298:PRO:HB3	2:A:307:PRO:HD2	1.74	0.67
3:B:251:ASP:O	3:B:253:ARG:N	2.26	0.67
3:B:257:VAL:O	3:B:257:VAL:HG12	1.93	0.67
3:B:325:MET:CE	3:B:355:VAL:HG21	2.24	0.67
3:B:328:VAL:O	3:B:332:MET:HG2	1.94	0.67
2:A:343:PHE:HZ	2:A:351:PHE:CE1	2.10	0.67
3:B:107:HIS:CD2	3:B:151:THR:CG2	2.78	0.67
3:B:242:LEU:CD2	3:B:250:ALA:H	2.06	0.67
2:A:102:ASN:HB2	2:A:408:TYR:CE2	2.29	0.67
1:N:271:PRO:HB2	3:B:263:PRO:CG	2.20	0.67
3:B:230:LEU:HD23	3:B:231:VAL:N	2.10	0.67
3:B:250:ALA:HB1	3:B:254:LYS:HB2	1.75	0.67
3:B:256:ALA:O	3:B:260:VAL:HG22	1.94	0.67
3:B:276:THR:HB	3:B:281:GLN:CG	2.25	0.67
3:B:310:GLY:HA3	3:B:436:GLN:HE21	1.59	0.67
2:A:251:ASP:O	2:A:254:GLU:HB2	1.94	0.67
1:N:162:VAL:HA	1:N:165:ARG:NH1	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:265:ALA:CB	2:A:401:LYS:CG	2.72	0.67
1:N:315:THR:HG21	2:A:420:GLU:OE2	1.94	0.67
2:A:175:PRO:HG3	2:A:304:LYS:HG2	1.76	0.67
3:B:66:ILE:C	3:B:67:LEU:HD23	2.15	0.67
3:B:172:VAL:HG11	3:B:387:LEU:CD2	2.22	0.67
3:B:182:VAL:HG23	3:B:186:ASN:HD21	1.60	0.67
1:N:185:GLU:HG2	1:N:189:ARG:NH1	2.10	0.66
2:A:276:ILE:O	2:A:369:ALA:HB2	1.95	0.66
3:B:108:TYR:CD1	3:B:413:MET:HE1	2.30	0.66
3:B:44:LEU:HD12	3:B:49:ILE:HD13	1.76	0.66
1:N:50:PHE:HA	1:N:318:LYS:HE3	1.76	0.66
3:B:243:ARG:HH22	3:B:252:LEU:HG	1.59	0.66
2:A:172:TYR:HD1	2:A:173:PRO:N	1.93	0.66
3:B:325:MET:HE2	3:B:355:VAL:HG21	1.78	0.66
1:N:268:THR:N	3:B:434:GLN:CB	2.58	0.66
2:A:100:ALA:CB	2:A:105:ARG:HD3	2.26	0.66
3:B:4:ILE:HG21	3:B:136:GLN:HG2	1.76	0.66
2:A:68:VAL:HG11	2:A:149:PHE:CZ	2.30	0.66
1:N:266:GLY:O	3:B:434:GLN:O	2.13	0.66
3:B:281:GLN:O	3:B:283:TYR:HB2	1.96	0.66
2:A:206:ASN:OD1	2:A:227:LEU:HD13	1.96	0.65
3:B:265:LEU:HD12	3:B:265:LEU:C	2.16	0.65
1:N:151:ASP:OD2	1:N:170:THR:HG22	1.96	0.65
2:A:243:ARG:NH2	2:A:252:LEU:N	2.28	0.65
2:A:341:ILE:HG12	2:A:341:ILE:O	1.95	0.65
2:A:217:LEU:HD11	2:A:367:ASP:O	1.96	0.65
3:B:325:MET:HE3	3:B:325:MET:HA	1.77	0.65
1:N:312:ARG:HH21	2:A:417:GLU:CB	2.09	0.65
3:B:158:ARG:NE	3:B:197:ASN:O	2.30	0.65
3:B:66:ILE:CD1	3:B:122:VAL:HG12	2.26	0.65
3:B:267:PHE:N	3:B:267:PHE:CD1	2.62	0.65
1:N:139:ALA:HB2	1:N:174:LEU:HD11	1.78	0.65
1:N:312:ARG:HB3	2:A:416:GLY:HA3	1.78	0.65
3:B:103:TRP:HZ3	3:B:108:TYR:HE1	1.42	0.65
3:B:242:LEU:CD1	3:B:255:LEU:HD11	2.25	0.65
2:A:344:VAL:HG12	2:A:345:ASP:N	2.12	0.65
3:B:66:ILE:HD13	3:B:122:VAL:HG12	1.79	0.65
2:A:271:THR:HG23	2:A:300:ASN:O	1.97	0.65
2:A:313:MET:HB3	2:A:344:VAL:CG2	2.26	0.65
3:B:422:GLU:O	3:B:426:ASN:HB2	1.97	0.65
3:B:431:GLU:O	3:B:434:GLN:HG2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:305:CYS:SG	2:A:384:ILE:HD13	2.37	0.65
2:A:372:GLN:O	2:A:373:ARG:HB3	1.96	0.65
3:B:413:MET:HG2	3:B:418:PHE:HE1	1.61	0.65
2:A:115:ILE:HG23	2:A:116:ASP:N	2.12	0.64
2:A:315:CYS:HB3	2:A:377:MET:HE2	1.78	0.64
2:A:402:ARG:O	2:A:403:ALA:C	2.36	0.64
2:A:224:TYR:CD1	3:B:325:MET:HG2	2.33	0.64
3:B:35:SER:HB3	3:B:59:ASN:CA	2.26	0.64
3:B:241:CYS:O	3:B:244:PHE:HB2	1.97	0.64
3:B:242:LEU:HD12	3:B:255:LEU:HD11	1.78	0.64
3:B:105:LYS:O	3:B:110:GLU:HB2	1.98	0.64
3:B:192:HIS:O	3:B:195:VAL:HG12	1.98	0.64
3:B:284:ARG:O	3:B:286:LEU:N	2.31	0.64
3:B:332:MET:HE3	3:B:351:VAL:HG11	1.78	0.64
3:B:427:ASP:O	3:B:430:SER:HB3	1.97	0.64
2:A:209:ILE:HG23	2:A:230:LEU:HD23	1.79	0.64
2:A:317:LEU:HD12	2:A:351:PHE:CD2	2.32	0.64
3:B:243:ARG:HH21	3:B:252:LEU:H	1.45	0.64
2:A:151:SER:O	2:A:155:GLU:HB2	1.98	0.64
1:N:312:ARG:HH21	2:A:417:GLU:CG	2.02	0.63
2:A:276:ILE:HG23	2:A:369:ALA:HB2	1.80	0.63
3:B:133:GLN:HG3	3:B:165:ILE:HD11	1.80	0.63
3:B:172:VAL:CG1	3:B:387:LEU:HD21	2.24	0.63
2:A:175:PRO:HG2	2:A:207:GLU:OE1	1.98	0.63
3:B:180:THR:CG2	3:B:181:VAL:N	2.61	0.63
1:N:271:PRO:CB	3:B:263:PRO:HB2	2.26	0.63
2:A:273:ALA:HB3	2:A:274:PRO:HD3	1.81	0.63
2:A:386:GLU:O	2:A:389:ALA:N	2.31	0.63
9:B:601:TA1:H463	9:B:601:TA1:H261	1.80	0.63
1:N:11:ILE:HB	1:N:318:LYS:NZ	2.13	0.63
2:A:7:ILE:HG22	2:A:66:VAL:CG2	2.28	0.63
3:B:114:LEU:O	3:B:118:VAL:HG23	1.97	0.63
3:B:205:ASP:OD1	3:B:304:ALA:N	2.32	0.63
3:B:282:GLN:O	3:B:282:GLN:HG2	1.97	0.63
1:N:6:LEU:H	1:N:324:HIS:HD2	1.46	0.63
1:N:268:THR:HG21	3:B:433:GLN:H	1.54	0.63
2:A:269:LEU:O	2:A:378:LEU:HA	1.99	0.63
3:B:315:VAL:HG13	3:B:377:PHE:CE1	2.34	0.63
3:B:318:VAL:HA	3:B:354:ALA:HB3	1.81	0.63
2:A:234:ILE:HD13	2:A:234:ILE:C	2.18	0.63
3:B:4:ILE:HA	3:B:134:GLY:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:107:HIS:HD2	3:B:151:THR:CG2	2.12	0.63
2:A:315:CYS:HB3	2:A:377:MET:CE	2.29	0.62
3:B:137:LEU:HD22	3:B:154:ILE:CG2	2.28	0.62
3:B:299:LYS:O	3:B:300:ASN:HB2	1.97	0.62
1:N:6:LEU:H	1:N:324:HIS:CD2	2.17	0.62
1:N:84:LEU:HD21	1:N:253:LEU:HD21	1.80	0.62
2:A:7:ILE:CD1	2:A:137:VAL:HG22	2.29	0.62
2:A:288:VAL:O	2:A:290:GLU:N	2.33	0.62
2:A:317:LEU:HD11	2:A:351:PHE:HE2	1.63	0.62
2:A:236:SER:O	2:A:240:ALA:HB3	1.99	0.62
3:B:115:VAL:HG21	3:B:152:LEU:CD2	2.30	0.62
2:A:278:ALA:HA	2:A:282:TYR:OH	2.00	0.62
1:N:269:VAL:HG22	3:B:428:LEU:HD12	1.81	0.62
2:A:317:LEU:HB3	2:A:319:TYR:CE1	2.33	0.62
3:B:253:ARG:O	3:B:256:ALA:N	2.33	0.62
2:A:152:LEU:HD12	2:A:153:LEU:N	2.14	0.62
2:A:205:ASP:HB2	2:A:303:VAL:HA	1.82	0.62
2:A:267:PHE:HD1	2:A:267:PHE:H	1.47	0.62
3:B:63:PRO:HD2	3:B:86:ILE:HG12	1.80	0.62
2:A:179:THR:HG22	3:B:352:LYS:NZ	2.15	0.61
3:B:4:ILE:HG23	3:B:134:GLY:O	2.00	0.61
3:B:230:LEU:O	3:B:233:ALA:HB3	2.00	0.61
2:A:166:LYS:H	2:A:199:ASP:CG	2.03	0.61
2:A:177:VAL:HG11	3:B:329:ASP:HB3	1.82	0.61
3:B:70:LEU:CG	3:B:145:THR:HG23	2.30	0.61
2:A:102:ASN:OD1	2:A:105:ARG:HB3	1.99	0.61
2:A:118:VAL:HG11	2:A:149:PHE:HZ	1.65	0.61
3:B:54:ASN:ND2	3:B:64:ARG:HD3	2.15	0.61
3:B:273:ALA:HB3	3:B:274:PRO:CD	2.29	0.61
2:A:23:LEU:HD22	2:A:232:GLY:O	1.99	0.61
3:B:114:LEU:HD23	3:B:149:MET:CE	2.30	0.61
2:A:88:HIS:O	2:A:90:GLU:N	2.33	0.61
2:A:179:THR:HG21	3:B:248:LEU:HD21	1.81	0.61
2:A:115:ILE:HG13	2:A:152:LEU:HD13	1.81	0.61
2:A:169:PHE:CE1	2:A:235:VAL:HG22	2.36	0.61
2:A:179:THR:HG21	3:B:248:LEU:CD2	2.30	0.61
2:A:362:VAL:HG13	2:A:368:LEU:HB2	1.83	0.61
2:A:168:GLU:OE1	2:A:198:SER:HB2	2.01	0.60
2:A:181:VAL:HG21	3:B:258:ASN:O	2.01	0.60
3:B:204:ILE:CD1	3:B:231:VAL:HG13	2.30	0.60
3:B:211:ASP:OD1	3:B:212:ILE:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:268:THR:CB	3:B:433:GLN:N	2.59	0.60
2:A:167:LEU:HA	2:A:200:CYS:O	2.01	0.60
2:A:311:LYS:HE3	2:A:342:GLN:CD	2.22	0.60
2:A:407:TRP:NE1	3:B:260:VAL:HG23	2.14	0.60
2:A:435:VAL:HG12	2:A:435:VAL:O	2.02	0.60
3:B:19:LYS:CG	3:B:228:ASN:HB3	2.31	0.60
3:B:70:LEU:H	3:B:145:THR:CG2	2.10	0.60
3:B:204:ILE:HG21	3:B:231:VAL:HG22	1.84	0.60
3:B:205:ASP:OD1	3:B:304:ALA:CB	2.50	0.60
1:N:158:HIS:HA	1:N:192:ARG:NH2	2.16	0.60
2:A:11:GLN:HE21	2:A:74:VAL:HG22	1.66	0.60
2:A:177:VAL:CG1	3:B:329:ASP:HB3	2.31	0.60
2:A:345:ASP:C	2:A:347:CYS:H	2.04	0.60
3:B:285:ALA:HB1	3:B:290:GLU:HG2	1.82	0.60
1:N:250:ASN:O	1:N:251:LEU:CB	2.49	0.60
3:B:324:SER:C	3:B:326:LYS:H	2.03	0.60
3:B:324:SER:CB	3:B:327:GLU:HG2	2.30	0.60
3:B:279:GLY:O	3:B:282:GLN:HB3	2.01	0.60
2:A:191:THR:HG21	2:A:425:MET:SD	2.41	0.60
3:B:70:LEU:N	3:B:145:THR:HG21	2.11	0.60
3:B:324:SER:O	3:B:328:VAL:HG23	2.01	0.60
1:N:18:TYR:HH	1:N:27:PRO:N	1.99	0.60
2:A:229:ARG:NH1	2:A:363:VAL:HG21	2.16	0.60
3:B:49:ILE:O	3:B:51:VAL:N	2.35	0.60
2:A:119:LEU:O	2:A:122:ILE:HG12	2.02	0.59
1:N:273:ARG:CZ	3:B:196:GLU:HG3	2.32	0.59
2:A:344:VAL:HG11	2:A:346:TRP:NE1	2.16	0.59
3:B:102:ASN:ND2	3:B:407:TRP:O	2.35	0.59
1:N:163:ALA:H	1:N:165:ARG:NH2	1.99	0.59
3:B:68:VAL:CG1	3:B:149:MET:SD	2.90	0.59
2:A:115:ILE:HD13	2:A:115:ILE:O	2.02	0.59
2:A:278:ALA:HB2	2:A:369:ALA:HA	1.85	0.59
3:B:30:ILE:HD13	3:B:53:TYR:CE2	2.38	0.59
3:B:161:TYR:C	3:B:163:ASP:H	2.05	0.59
2:A:371:VAL:HG12	2:A:372:GLN:N	2.17	0.59
3:B:93:VAL:CG1	3:B:118:VAL:HG22	2.19	0.59
3:B:89:PRO:HA	3:B:92:PHE:CD1	2.38	0.59
3:B:115:VAL:HG21	3:B:152:LEU:HD23	1.84	0.59
2:A:119:LEU:CD2	2:A:122:ILE:HD11	2.28	0.59
2:A:284:GLU:O	2:A:286:LEU:N	2.35	0.59
3:B:128:SER:OG	3:B:129:CYS:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:141:LEU:CD1	3:B:141:LEU:N	2.65	0.59
3:B:332:MET:CE	3:B:351:VAL:HG11	2.32	0.59
2:A:6:SER:HA	2:A:136:SER:O	2.02	0.58
3:B:408:TYR:CG	3:B:418:PHE:HZ	2.20	0.58
2:A:369:ALA:O	2:A:370:LYS:HB3	2.03	0.58
2:A:110:ILE:CG2	2:A:111:GLY:H	2.15	0.58
2:A:248:LEU:CD2	2:A:353:VAL:O	2.49	0.58
2:A:413:MET:O	2:A:414:GLU:HG3	2.03	0.58
2:A:88:HIS:C	2:A:90:GLU:N	2.57	0.58
2:A:317:LEU:HD11	2:A:351:PHE:CE2	2.38	0.58
3:B:307:PRO:HB3	3:B:312:TYR:OH	2.04	0.58
2:A:2:ARG:N	2:A:131:GLY:O	2.36	0.58
2:A:166:LYS:HD2	2:A:197:HIS:O	2.04	0.58
2:A:268:PRO:HA	2:A:379:SER:O	2.04	0.58
2:A:381:THR:C	2:A:383:ALA:N	2.56	0.58
3:B:198:THR:HG22	3:B:265:LEU:HD22	1.86	0.58
1:N:253:LEU:O	1:N:256:ILE:N	2.36	0.58
2:A:218:ASP:O	2:A:219:ILE:HG23	2.04	0.58
3:B:180:THR:CG2	3:B:181:VAL:H	2.17	0.58
3:B:299:LYS:O	3:B:300:ASN:CB	2.51	0.58
3:B:320:ARG:O	3:B:359:PRO:HA	2.04	0.58
2:A:407:TRP:O	2:A:411:GLU:HG2	2.02	0.58
3:B:183:GLU:HB3	3:B:184:PRO:CD	2.33	0.58
3:B:70:LEU:C	3:B:99:ALA:HB2	2.24	0.57
2:A:362:VAL:HG11	2:A:368:LEU:O	2.04	0.57
1:N:252:GLY:O	1:N:255:SER:N	2.37	0.57
2:A:345:ASP:O	2:A:347:CYS:N	2.38	0.57
3:B:283:TYR:C	3:B:284:ARG:HG2	2.25	0.57
3:B:319:PHE:CD2	3:B:375:ALA:HB2	2.40	0.57
3:B:5:VAL:CG2	3:B:135:PHE:HD2	2.18	0.57
3:B:253:ARG:O	3:B:254:LYS:C	2.42	0.57
3:B:270:PRO:HA	3:B:377:PHE:O	2.04	0.57
3:B:349:ASN:C	3:B:349:ASN:HD22	2.06	0.57
1:N:63:MET:HE2	1:N:67:LEU:HB3	1.85	0.57
2:A:152:LEU:HA	2:A:155:GLU:CB	2.35	0.57
1:N:264:ALA:HB2	1:N:324:HIS:CE1	2.40	0.57
2:A:202:PHE:CE2	2:A:378:LEU:HD22	2.38	0.57
2:A:362:VAL:CG1	2:A:368:LEU:HB2	2.35	0.57
3:B:149:MET:O	3:B:153:LEU:HD13	2.05	0.57
3:B:151:THR:OG1	3:B:193:GLN:HB3	2.03	0.57
3:B:217:LEU:C	3:B:219:LEU:N	2.55	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:63:PRO:HD3	2:A:86:LEU:O	2.04	0.57
2:A:139:HIS:CE1	2:A:170:SER:HB3	2.40	0.57
2:A:165:SER:HA	2:A:199:ASP:OD2	2.04	0.57
2:A:175:PRO:HG3	2:A:304:LYS:CG	2.35	0.57
2:A:117:LEU:HD11	2:A:121:ARG:HH22	1.69	0.57
3:B:30:ILE:HA	3:B:35:SER:O	2.04	0.57
3:B:273:ALA:CB	3:B:274:PRO:HD3	2.30	0.57
2:A:286:LEU:HD12	2:A:290:GLU:HG2	1.87	0.57
3:B:6:HIS:HB3	3:B:65:ALA:HB2	1.87	0.57
3:B:14:ASN:OD1	3:B:75:MET:HG2	2.05	0.57
3:B:132:LEU:CD2	3:B:164:ARG:HG3	2.32	0.57
3:B:259:MET:CA	3:B:314:THR:HG21	2.35	0.57
1:N:63:MET:CE	1:N:67:LEU:HB3	2.35	0.56
2:A:210:TYR:CE2	2:A:227:LEU:HD11	2.40	0.56
2:A:394:LYS:HG2	3:B:348:PRO:CG	2.35	0.56
3:B:301:MET:CE	3:B:377:PHE:HE2	2.18	0.56
2:A:19:ALA:CB	2:A:228:ASN:HB3	2.35	0.56
2:A:209:ILE:CG2	2:A:227:LEU:HD22	2.35	0.56
2:A:338:LYS:O	2:A:340:THR:N	2.34	0.56
3:B:216:THR:O	3:B:217:LEU:HD12	2.05	0.56
2:A:11:GLN:HE22	3:B:249:ASN:ND2	2.03	0.56
2:A:71:GLU:HG3	3:B:2:ARG:NH2	2.19	0.56
2:A:409:VAL:C	2:A:411:GLU:H	2.09	0.56
2:A:436:GLY:C	2:A:438:ASP:H	2.08	0.56
3:B:31:ASP:O	3:B:32:PRO:C	2.44	0.56
3:B:50:ASN:O	3:B:64:ARG:NH2	2.38	0.56
3:B:319:PHE:HA	3:B:375:ALA:HA	1.86	0.56
2:A:216:ASN:O	2:A:217:LEU:HB2	2.05	0.56
2:A:264:ARG:HB2	2:A:266:HIS:HD2	1.67	0.56
2:A:331:ALA:O	2:A:334:THR:HG22	2.05	0.56
3:B:274:PRO:CG	3:B:371:LEU:HD21	2.34	0.56
1:N:268:THR:H	3:B:434:GLN:HB2	1.63	0.56
2:A:209:ILE:HG22	2:A:227:LEU:HD22	1.88	0.56
3:B:312:TYR:O	3:B:344:VAL:HB	2.05	0.56
3:B:70:LEU:CD1	3:B:145:THR:HG23	2.35	0.56
1:N:312:ARG:HH21	2:A:417:GLU:CA	2.11	0.56
3:B:4:ILE:HD13	3:B:136:GLN:NE2	2.18	0.56
3:B:139:HIS:HE1	3:B:168:THR:HG23	1.71	0.56
3:B:204:ILE:HG21	3:B:231:VAL:CG2	2.36	0.56
3:B:422:GLU:O	3:B:426:ASN:N	2.37	0.56
1:N:253:LEU:HA	1:N:256:ILE:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:242:LEU:C	2:A:244:PHE:H	2.09	0.56
3:B:324:SER:C	3:B:326:LYS:N	2.59	0.56
2:A:313:MET:O	2:A:314:ALA:HB2	2.04	0.56
3:B:151:THR:OG1	3:B:193:GLN:CB	2.54	0.56
3:B:182:VAL:HG23	3:B:186:ASN:ND2	2.20	0.56
3:B:272:PHE:HB3	3:B:275:LEU:HD22	1.88	0.56
3:B:191:VAL:HA	3:B:194:LEU:HD12	1.87	0.55
3:B:311:ARG:HD2	3:B:344:VAL:H	1.71	0.55
1:N:163:ALA:H	1:N:165:ARG:CZ	2.20	0.55
2:A:388:TRP:CE3	2:A:388:TRP:HA	2.41	0.55
3:B:165:ILE:HD13	3:B:165:ILE:H	1.71	0.55
2:A:16:ILE:HD12	2:A:171:ILE:HD11	1.87	0.55
3:B:250:ALA:CA	3:B:254:LYS:HE2	2.35	0.55
1:N:158:HIS:HA	1:N:192:ARG:HH21	1.71	0.55
3:B:19:LYS:O	3:B:23:VAL:HG23	2.06	0.55
3:B:190:SER:O	3:B:194:LEU:HG	2.06	0.55
3:B:311:ARG:HG2	3:B:311:ARG:HH11	1.71	0.55
2:A:253:THR:O	2:A:256:GLN:HG2	2.06	0.55
3:B:223:THR:HG22	3:B:224:TYR:N	2.21	0.55
1:N:253:LEU:HA	1:N:256:ILE:CD1	2.36	0.55
2:A:382:THR:O	2:A:382:THR:HG22	2.05	0.55
3:B:119:LEU:O	3:B:123:ARG:HG3	2.06	0.55
3:B:147:SER:O	3:B:151:THR:CB	2.52	0.55
2:A:381:THR:OG1	2:A:383:ALA:HB3	2.07	0.55
1:N:29:VAL:HG11	1:N:301:GLN:HA	1.88	0.55
2:A:6:SER:O	2:A:65:ALA:HB1	2.07	0.55
2:A:231:ILE:HA	2:A:234:ILE:CG2	2.36	0.55
3:B:166:MET:HB3	3:B:198:THR:OG1	2.06	0.55
3:B:5:VAL:HG22	3:B:135:PHE:CD2	2.42	0.55
3:B:253:ARG:O	3:B:257:VAL:N	2.33	0.55
3:B:310:GLY:CA	3:B:436:GLN:HE21	2.19	0.55
2:A:408:TYR:CD1	2:A:418:PHE:HZ	2.24	0.54
3:B:210:TYR:HD2	3:B:227:LEU:HD21	1.71	0.54
2:A:101:ASN:CG	3:B:254:LYS:HD2	2.28	0.54
3:B:20:PHE:CE2	3:B:24:ILE:HD12	2.43	0.54
2:A:118:VAL:HG21	2:A:149:PHE:CZ	2.42	0.54
3:B:239:THR:O	3:B:241:CYS:N	2.41	0.54
2:A:9:VAL:CG1	2:A:139:HIS:HB3	2.38	0.54
2:A:98:ASP:CB	2:A:105:ARG:HH21	2.14	0.54
3:B:44:LEU:O	3:B:49:ILE:HG12	2.07	0.54
2:A:150:THR:O	2:A:153:LEU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:194:LEU:C	3:B:196:GLU:H	2.11	0.54
2:A:17:GLY:O	2:A:21:TRP:HB2	2.08	0.54
2:A:115:ILE:HD13	2:A:115:ILE:C	2.28	0.54
3:B:297:ASP:OD1	3:B:298:ALA:N	2.39	0.54
3:B:325:MET:CE	3:B:355:VAL:HG11	2.38	0.54
3:B:325:MET:O	3:B:329:ASP:HB2	2.07	0.54
3:B:331:GLN:O	3:B:335:VAL:HG23	2.08	0.54
1:N:84:LEU:HD21	1:N:253:LEU:HD23	1.88	0.54
2:A:5:ILE:CG2	2:A:6:SER:N	2.70	0.54
3:B:27:GLU:O	3:B:27:GLU:HG2	2.08	0.54
3:B:204:ILE:HD13	3:B:231:VAL:HG13	1.89	0.54
3:B:239:THR:HG22	3:B:240:THR:N	2.22	0.54
2:A:173:PRO:HB2	2:A:391:LEU:CD1	2.38	0.54
3:B:322:ARG:HG3	3:B:322:ARG:HH11	1.73	0.54
3:B:31:ASP:HB3	3:B:32:PRO:HD2	1.89	0.54
3:B:323:MET:HG3	3:B:328:VAL:HG21	1.90	0.54
1:N:264:ALA:HB2	1:N:324:HIS:HE1	1.73	0.53
3:B:424:ASN:ND2	3:B:424:ASN:C	2.62	0.53
2:A:5:ILE:O	2:A:135:PHE:HA	2.09	0.53
2:A:150:THR:O	2:A:151:SER:C	2.47	0.53
2:A:163:LYS:O	2:A:163:LYS:HG2	2.08	0.53
2:A:339:ARG:C	2:A:341:ILE:H	2.11	0.53
3:B:67:LEU:HD23	3:B:67:LEU:N	2.22	0.53
3:B:259:MET:HG2	3:B:314:THR:CG2	2.38	0.53
3:B:259:MET:CG	3:B:314:THR:HG21	2.36	0.53
3:B:427:ASP:OD1	3:B:428:LEU:N	2.41	0.53
3:B:431:GLU:O	3:B:434:GLN:CG	2.56	0.53
2:A:215:ARG:C	2:A:216:ASN:HD22	2.12	0.53
3:B:21:TRP:CZ2	3:B:65:ALA:HB2	2.44	0.53
3:B:36:TYR:CZ	3:B:38:GLY:HA3	2.43	0.53
3:B:424:ASN:C	3:B:424:ASN:HD22	2.09	0.53
3:B:68:VAL:HG12	3:B:149:MET:CE	2.38	0.53
3:B:229:HIS:ND1	3:B:229:HIS:C	2.62	0.53
3:B:343:PHE:O	3:B:344:VAL:O	2.26	0.53
2:A:110:ILE:O	2:A:112:LYS:N	2.41	0.53
3:B:4:ILE:CG2	3:B:136:GLN:HG2	2.38	0.53
3:B:242:LEU:HD22	3:B:250:ALA:N	2.19	0.53
1:N:251:LEU:O	1:N:255:SER:OG	2.26	0.53
2:A:98:ASP:O	2:A:110:ILE:HD13	2.08	0.53
2:A:248:LEU:HB3	2:A:355:ILE:H	1.73	0.53
1:N:79:PHE:HD2	1:N:288:GLN:O	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:182:VAL:O	2:A:184:PRO:N	2.41	0.53
2:A:243:ARG:CZ	2:A:252:LEU:HG	2.39	0.53
3:B:133:GLN:HE21	3:B:252:LEU:HB2	1.73	0.53
3:B:213:CYS:SG	3:B:219:LEU:HD23	2.48	0.53
2:A:121:ARG:O	2:A:125:LEU:HB2	2.08	0.53
3:B:179:ASP:HB2	8:B:600:GDP:H3'	1.90	0.53
3:B:226:ASP:O	3:B:227:LEU:C	2.46	0.53
2:A:324:VAL:O	2:A:327:ASP:HB2	2.08	0.53
3:B:141:LEU:HA	3:B:147:SER:HB3	1.91	0.53
3:B:345:GLU:C	3:B:347:ILE:H	2.12	0.53
2:A:196:GLU:C	2:A:197:HIS:CD2	2.82	0.53
2:A:275:VAL:HG21	2:A:300:ASN:OD1	2.09	0.53
3:B:212:ILE:O	3:B:216:THR:HB	2.09	0.53
3:B:210:TYR:CD2	3:B:227:LEU:HD21	2.44	0.52
1:N:265:ALA:HB2	2:A:401:LYS:CB	2.39	0.52
2:A:101:ASN:ND2	7:B:500:GTP:O3G	2.42	0.52
2:A:264:ARG:C	2:A:266:HIS:N	2.60	0.52
1:N:319:ALA:CB	2:A:402:ARG:HH22	2.22	0.52
2:A:173:PRO:HB2	2:A:391:LEU:HD11	1.91	0.52
3:B:198:THR:HG22	3:B:265:LEU:CD2	2.39	0.52
3:B:431:GLU:OE1	3:B:432:TYR:CA	2.57	0.52
2:A:344:VAL:HG12	2:A:345:ASP:H	1.74	0.52
2:A:408:TYR:O	2:A:411:GLU:N	2.39	0.52
3:B:5:VAL:HG23	3:B:5:VAL:O	2.09	0.52
2:A:206:ASN:OD1	2:A:227:LEU:CD1	2.58	0.52
3:B:70:LEU:HD12	3:B:145:THR:HG23	1.91	0.52
3:B:107:HIS:HD2	3:B:151:THR:HG22	1.72	0.52
3:B:226:ASP:O	3:B:229:HIS:N	2.42	0.52
2:A:251:ASP:OD1	2:A:252:LEU:N	2.43	0.52
2:A:362:VAL:HG13	2:A:368:LEU:CD1	2.38	0.52
3:B:188:THR:HA	3:B:425:MET:CE	2.40	0.52
3:B:200:GLU:N	3:B:265:LEU:HD13	2.25	0.52
3:B:264:ARG:HE	3:B:264:ARG:HA	1.75	0.52
3:B:360:PRO:HB2	9:B:601:TA1:H281	1.91	0.52
2:A:231:ILE:CA	2:A:234:ILE:HG22	2.38	0.52
3:B:107:HIS:CD2	3:B:151:THR:HG22	2.45	0.52
3:B:295:MET:SD	3:B:375:ALA:O	2.68	0.52
3:B:314:THR:CG2	3:B:315:VAL:N	2.73	0.52
3:B:8:GLN:OE1	3:B:14:ASN:ND2	2.42	0.52
3:B:149:MET:O	3:B:149:MET:HG2	2.10	0.52
3:B:149:MET:O	3:B:153:LEU:HD22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:23:LEU:HD23	2:A:236:SER:CB	2.37	0.52
3:B:425:MET:O	3:B:428:LEU:HB3	2.09	0.52
1:N:262:SER:HG	3:B:262:PHE:HD2	1.57	0.51
2:A:119:LEU:HD11	2:A:156:ARG:CD	2.40	0.51
2:A:243:ARG:NH2	2:A:251:ASP:OD1	2.44	0.51
2:A:345:ASP:OD2	2:A:439:SER:HB3	2.10	0.51
3:B:251:ASP:O	3:B:252:LEU:C	2.49	0.51
1:N:84:LEU:CD2	1:N:253:LEU:CD2	2.83	0.51
2:A:8:HIS:HB3	2:A:13:GLY:O	2.09	0.51
2:A:201:ALA:O	2:A:267:PHE:HA	2.10	0.51
2:A:234:ILE:HB	2:A:302:MET:HE1	1.91	0.51
1:N:143:GLU:HB3	1:N:152:LEU:HD11	1.92	0.51
2:A:4:CYS:HA	2:A:134:GLY:O	2.10	0.51
2:A:9:VAL:HG21	2:A:149:PHE:CD1	2.46	0.51
2:A:171:ILE:O	2:A:171:ILE:HG22	2.10	0.51
2:A:191:THR:HG23	2:A:192:HIS:N	2.25	0.51
2:A:231:ILE:HD13	2:A:231:ILE:N	2.25	0.51
2:A:283:HIS:O	2:A:284:GLU:C	2.47	0.51
3:B:49:ILE:O	3:B:50:ASN:C	2.48	0.51
3:B:103:TRP:CE2	3:B:189:LEU:HB3	2.45	0.51
3:B:320:ARG:HA	3:B:356:CYS:HB3	1.92	0.51
1:N:252:GLY:O	1:N:256:ILE:N	2.42	0.51
2:A:239:THR:O	2:A:240:ALA:C	2.48	0.51
2:A:172:TYR:OH	2:A:387:ALA:O	2.24	0.51
3:B:240:THR:HG23	3:B:241:CYS:H	1.76	0.51
3:B:260:VAL:HG23	3:B:260:VAL:O	2.10	0.51
2:A:244:PHE:C	2:A:244:PHE:CD2	2.83	0.51
2:A:244:PHE:CD2	2:A:245:ASP:N	2.76	0.51
1:N:86:TYR:CE2	1:N:310:THR:HG23	2.46	0.51
2:A:24:TYR:CE2	2:A:240:ALA:HB2	2.45	0.51
3:B:21:TRP:HZ2	3:B:65:ALA:HB2	1.76	0.51
3:B:277:SER:OG	3:B:281:GLN:HB2	2.10	0.51
2:A:133:GLN:HB3	2:A:243:ARG:HH12	1.76	0.51
1:N:247:VAL:O	1:N:248:ASN:HB2	2.10	0.51
2:A:67:PHE:HE1	2:A:87:PHE:CE2	2.29	0.51
3:B:113:GLU:HG3	3:B:114:LEU:N	2.26	0.51
2:A:417:GLU:HA	2:A:417:GLU:OE1	2.10	0.50
3:B:5:VAL:CG2	3:B:135:PHE:CD2	2.94	0.50
2:A:12:ALA:CB	2:A:140:SER:OG	2.59	0.50
2:A:119:LEU:HA	2:A:122:ILE:HG12	1.93	0.50
2:A:261:PRO:HB2	2:A:262:TYR:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:413:MET:HG3	3:B:414:ASP:N	2.22	0.50
2:A:310:GLY:HA3	2:A:383:ALA:N	2.26	0.50
3:B:168:THR:O	3:B:201:THR:HA	2.12	0.50
3:B:323:MET:HG3	3:B:328:VAL:CG2	2.41	0.50
3:B:3:GLU:HA	3:B:51:VAL:HA	1.93	0.50
3:B:265:LEU:O	3:B:266:HIS:O	2.29	0.50
3:B:296:PHE:CZ	3:B:315:VAL:HG11	2.46	0.50
2:A:16:ILE:HG23	2:A:17:GLY:N	2.26	0.50
2:A:196:GLU:O	2:A:197:HIS:CD2	2.65	0.50
3:B:156:LYS:HA	3:B:156:LYS:CE	2.38	0.50
2:A:132:LEU:CD2	2:A:164:LYS:HE3	2.42	0.50
2:A:140:SER:O	2:A:142:GLY:N	2.44	0.50
2:A:402:ARG:O	2:A:403:ALA:O	2.29	0.50
3:B:49:ILE:HG13	3:B:50:ASN:H	1.76	0.50
3:B:298:ALA:O	3:B:299:LYS:C	2.50	0.50
1:N:253:LEU:O	1:N:256:ILE:CB	2.59	0.50
2:A:5:ILE:O	2:A:136:SER:N	2.40	0.50
2:A:147:SER:CB	2:A:190:THR:OG1	2.52	0.50
3:B:176:LYS:CE	3:B:207:GLU:HG3	2.39	0.50
1:N:72:VAL:O	1:N:76:LEU:HD13	2.12	0.49
1:N:272:TYR:CG	1:N:282:GLN:HG3	2.47	0.49
2:A:11:GLN:O	2:A:14:VAL:HB	2.12	0.49
2:A:115:ILE:CG2	2:A:116:ASP:N	2.75	0.49
2:A:115:ILE:HD11	2:A:119:LEU:HG	1.92	0.49
2:A:238:ILE:O	2:A:242:LEU:HB2	2.11	0.49
3:B:333:LEU:O	3:B:336:GLN:N	2.45	0.49
3:B:369:ARG:C	3:B:369:ARG:HD2	2.32	0.49
1:N:9:VAL:HB	1:N:321:ALA:HB1	1.94	0.49
2:A:227:LEU:O	2:A:231:ILE:HG12	2.12	0.49
3:B:24:ILE:HG22	3:B:25:SER:N	2.27	0.49
3:B:262:PHE:O	3:B:264:ARG:N	2.45	0.49
3:B:336:GLN:HE22	3:B:349:ASN:ND2	2.10	0.49
2:A:305:CYS:O	2:A:306:ASP:C	2.49	0.49
3:B:8:GLN:HB3	3:B:14:ASN:HA	1.94	0.49
3:B:387:LEU:HD23	3:B:388:PHE:CD2	2.47	0.49
1:N:84:LEU:CD2	1:N:253:LEU:HD23	2.42	0.49
3:B:69:ASP:HA	3:B:145:THR:HG21	1.95	0.49
3:B:265:LEU:HD12	3:B:266:HIS:O	2.12	0.49
2:A:133:GLN:CB	2:A:243:ARG:HH12	2.24	0.49
3:B:4:ILE:HG22	3:B:5:VAL:N	2.27	0.49
3:B:209:LEU:O	3:B:210:TYR:C	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:5:LYS:HD2	1:N:264:ALA:HA	1.93	0.49
1:N:19:ARG:HA	1:N:19:ARG:NE	2.27	0.49
2:A:414:GLU:OE1	2:A:414:GLU:N	2.46	0.49
3:B:102:ASN:HB3	3:B:105:LYS:HB2	1.95	0.49
3:B:199:ASP:O	3:B:200:GLU:HG3	2.13	0.49
3:B:345:GLU:O	3:B:347:ILE:N	2.45	0.49
3:B:383:ALA:C	3:B:385:GLN:H	2.15	0.49
1:N:319:ALA:HB3	2:A:402:ARG:HH22	1.78	0.49
2:A:149:PHE:HE1	2:A:153:LEU:HD22	1.77	0.49
2:A:234:ILE:CG1	2:A:270:ALA:HB1	2.38	0.49
3:B:4:ILE:HD12	3:B:239:THR:CG2	2.42	0.49
2:A:118:VAL:HG21	2:A:149:PHE:CE2	2.48	0.49
2:A:158:SER:OG	2:A:197:HIS:HB3	2.13	0.49
2:A:163:LYS:C	2:A:164:LYS:HG2	2.33	0.49
2:A:192:HIS:CD2	2:A:424:ASP:OD2	2.66	0.49
2:A:392:ASP:O	2:A:395:PHE:HB3	2.13	0.49
3:B:142:GLY:HA3	3:B:183:GLU:OE2	2.13	0.49
2:A:115:ILE:O	2:A:116:ASP:C	2.51	0.49
2:A:122:ILE:CD1	2:A:157:LEU:HD21	2.35	0.49
2:A:191:THR:CG2	2:A:192:HIS:N	2.76	0.49
2:A:274:PRO:CB	2:A:371:VAL:HG21	2.43	0.49
3:B:280:SER:O	3:B:282:GLN:N	2.45	0.49
3:B:296:PHE:HZ	3:B:315:VAL:HG11	1.78	0.49
1:N:271:PRO:HB2	3:B:263:PRO:HG3	1.88	0.49
3:B:173:PRO:HB3	3:B:183:GLU:HG2	1.93	0.49
1:N:63:MET:HE3	1:N:67:LEU:HD23	1.94	0.48
3:B:175:PRO:CD	3:B:207:GLU:OE1	2.61	0.48
2:A:9:VAL:HG11	2:A:150:THR:OG1	2.13	0.48
2:A:99:ALA:O	2:A:100:ALA:HB3	2.14	0.48
2:A:155:GLU:OE1	2:A:197:HIS:HE1	1.96	0.48
3:B:2:ARG:NH1	3:B:251:ASP:OD2	2.46	0.48
3:B:133:GLN:NE2	3:B:252:LEU:HB2	2.27	0.48
3:B:211:ASP:OD1	3:B:212:ILE:HG13	2.13	0.48
3:B:431:GLU:OE1	3:B:432:TYR:N	2.46	0.48
2:A:188:ILE:O	2:A:191:THR:HG22	2.13	0.48
2:A:283:HIS:O	2:A:285:GLN:N	2.45	0.48
2:A:151:SER:OG	2:A:193:THR:HG21	2.13	0.48
3:B:49:ILE:HG13	3:B:50:ASN:N	2.28	0.48
3:B:173:PRO:HB3	3:B:183:GLU:CG	2.42	0.48
1:N:231:GLU:O	1:N:249:ILE:CD1	2.61	0.48
1:N:251:LEU:O	1:N:255:SER:N	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:104:ALA:CB	2:A:408:TYR:HD2	2.26	0.48
2:A:231:ILE:O	2:A:235:VAL:HG23	2.12	0.48
3:B:20:PHE:CG	3:B:235:MET:SD	3.07	0.48
3:B:399:PHE:O	3:B:400:ARG:C	2.52	0.48
2:A:105:ARG:HH11	2:A:105:ARG:HG3	1.78	0.48
2:A:242:LEU:C	2:A:244:PHE:N	2.66	0.48
2:A:369:ALA:O	2:A:370:LYS:CB	2.62	0.48
3:B:103:TRP:HZ3	3:B:108:TYR:CE1	2.27	0.48
3:B:209:LEU:CD2	3:B:227:LEU:HD13	2.44	0.48
3:B:307:PRO:HB3	3:B:312:TYR:CZ	2.49	0.48
2:A:253:THR:O	2:A:254:GLU:C	2.52	0.48
1:N:265:ALA:CB	2:A:401:LYS:CD	2.91	0.48
2:A:5:ILE:HG22	2:A:6:SER:H	1.78	0.48
2:A:97:GLU:HB2	2:A:110:ILE:HD11	1.96	0.48
2:A:151:SER:HB3	2:A:193:THR:CG2	2.34	0.48
2:A:204:VAL:CG1	2:A:209:ILE:HD11	2.42	0.48
3:B:154:ILE:HG22	3:B:166:MET:CE	2.44	0.48
3:B:176:LYS:HG3	3:B:177:VAL:H	1.78	0.48
3:B:237:GLY:O	3:B:241:CYS:CB	2.61	0.48
3:B:269:MET:HB3	3:B:303:ALA:HB2	1.94	0.48
3:B:137:LEU:HD22	3:B:154:ILE:HG21	1.95	0.48
3:B:175:PRO:O	3:B:176:LYS:C	2.52	0.48
3:B:209:LEU:O	3:B:213:CYS:N	2.47	0.48
3:B:308:ARG:HG3	3:B:342:TYR:OH	2.13	0.48
1:N:251:LEU:O	1:N:255:SER:CB	2.61	0.48
2:A:132:LEU:HD21	2:A:164:LYS:HE3	1.96	0.48
2:A:203:MET:SD	2:A:267:PHE:HB3	2.53	0.48
2:A:339:ARG:C	2:A:341:ILE:N	2.68	0.48
2:A:107:HIS:CE1	2:A:152:LEU:HB3	2.49	0.47
2:A:110:ILE:CG2	2:A:111:GLY:N	2.71	0.47
3:B:191:VAL:HG13	3:B:192:HIS:N	2.28	0.47
3:B:297:ASP:OD2	3:B:299:LYS:HE2	2.14	0.47
1:N:102:PRO:HD3	1:N:184:LEU:HD12	1.96	0.47
1:N:231:GLU:O	1:N:249:ILE:HD13	2.14	0.47
2:A:34:GLY:C	2:A:61:HIS:N	2.68	0.47
2:A:286:LEU:CD1	2:A:290:GLU:HG2	2.44	0.47
2:A:317:LEU:CD1	2:A:351:PHE:CD2	2.97	0.47
2:A:335:ILE:O	2:A:337:THR:N	2.47	0.47
3:B:198:THR:HG23	3:B:200:GLU:H	1.79	0.47
1:N:11:ILE:HB	1:N:318:LYS:HZ1	1.77	0.47
2:A:210:TYR:CE2	2:A:227:LEU:HD21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:76:LEU:HD21	1:N:123:ARG:HB2	1.96	0.47
1:N:254:LEU:HD21	2:A:409:VAL:CG1	2.03	0.47
1:N:267:HIS:O	3:B:435:TYR:CD1	2.46	0.47
2:A:19:ALA:HB2	2:A:228:ASN:HB3	1.96	0.47
2:A:148:GLY:O	2:A:151:SER:CB	2.61	0.47
2:A:155:GLU:HG2	2:A:197:HIS:CE1	2.49	0.47
2:A:175:PRO:HD2	2:A:207:GLU:HB3	1.97	0.47
2:A:345:ASP:C	2:A:347:CYS:N	2.68	0.47
2:A:386:GLU:O	2:A:388:TRP:N	2.47	0.47
3:B:243:ARG:N	3:B:243:ARG:HD3	2.26	0.47
3:B:384:ILE:HG23	3:B:384:ILE:O	2.14	0.47
2:A:6:SER:OG	2:A:65:ALA:HB2	2.14	0.47
2:A:115:ILE:HG23	2:A:116:ASP:H	1.79	0.47
2:A:154:MET:HA	2:A:157:LEU:HD12	1.96	0.47
3:B:185:TYR:HD2	3:B:395:PHE:CE1	2.33	0.47
2:A:217:LEU:CD1	2:A:277:SER:HA	2.44	0.47
2:A:230:LEU:O	2:A:233:GLN:N	2.35	0.47
2:A:396:ASP:O	2:A:397:LEU:C	2.53	0.47
3:B:24:ILE:CD1	3:B:52:TYR:CE1	2.97	0.47
3:B:168:THR:CB	3:B:201:THR:HG23	2.38	0.47
3:B:242:LEU:CD1	3:B:250:ALA:HB3	2.45	0.47
1:N:252:GLY:O	1:N:253:LEU:C	2.52	0.47
1:N:267:HIS:C	3:B:431:GLU:CG	2.62	0.47
2:A:25:CYS:SG	2:A:83:TYR:HE2	2.38	0.47
2:A:96:LYS:O	2:A:97:GLU:O	2.31	0.47
2:A:226:ASN:O	2:A:229:ARG:N	2.48	0.47
2:A:256:GLN:HA	2:A:260:VAL:HG13	1.97	0.47
2:A:384:ILE:HG22	2:A:388:TRP:CD1	2.49	0.47
3:B:101:ASN:ND2	3:B:101:ASN:O	2.47	0.47
3:B:115:VAL:CG2	3:B:152:LEU:HD23	2.44	0.47
3:B:134:GLY:HA3	3:B:165:ILE:HG12	1.97	0.47
1:N:165:ARG:H	1:N:165:ARG:HD2	1.79	0.47
2:A:120:ASP:O	2:A:124:LYS:HB2	2.15	0.47
2:A:191:THR:O	2:A:195:LEU:HB2	2.15	0.47
3:B:264:ARG:HA	3:B:264:ARG:NE	2.29	0.47
3:B:287:THR:N	3:B:290:GLU:OE1	2.48	0.47
2:A:278:ALA:O	2:A:279:GLU:HG2	2.15	0.47
2:A:4:CYS:SG	2:A:252:LEU:CD1	3.02	0.47
2:A:147:SER:O	2:A:190:THR:HG23	2.14	0.47
2:A:384:ILE:HG22	2:A:384:ILE:O	2.15	0.47
3:B:387:LEU:O	3:B:387:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:185:TYR:OH	2:A:399:TYR:HA	2.15	0.46
3:B:242:LEU:HD11	3:B:250:ALA:HB3	1.97	0.46
2:A:22:GLU:O	2:A:23:LEU:C	2.54	0.46
2:A:114:ILE:O	2:A:118:VAL:HG23	2.16	0.46
2:A:392:ASP:OD2	2:A:422:ARG:NE	2.48	0.46
3:B:70:LEU:O	3:B:99:ALA:HB2	2.15	0.46
3:B:133:GLN:O	3:B:165:ILE:CD1	2.64	0.46
3:B:226:ASP:O	3:B:229:HIS:HB3	2.14	0.46
3:B:237:GLY:HA3	3:B:376:THR:OG1	2.15	0.46
3:B:263:PRO:O	3:B:264:ARG:C	2.52	0.46
3:B:272:PHE:CE1	9:B:601:TA1:H391	2.50	0.46
1:N:271:PRO:CD	3:B:263:PRO:HG2	2.44	0.46
2:A:11:GLN:O	2:A:15:GLN:HG3	2.15	0.46
2:A:210:TYR:CZ	2:A:227:LEU:HD11	2.51	0.46
2:A:407:TRP:O	2:A:411:GLU:CG	2.63	0.46
3:B:20:PHE:O	3:B:24:ILE:HB	2.14	0.46
3:B:175:PRO:HD2	3:B:207:GLU:CD	2.35	0.46
1:N:253:LEU:HA	1:N:256:ILE:CG1	2.45	0.46
2:A:117:LEU:HD12	2:A:121:ARG:HH12	1.80	0.46
2:A:243:ARG:NH2	2:A:252:LEU:CB	2.78	0.46
3:B:307:PRO:C	3:B:309:HIS:H	2.18	0.46
2:A:224:TYR:HD1	3:B:247:GLN:HB3	1.80	0.46
2:A:224:TYR:CG	3:B:325:MET:HG2	2.50	0.46
2:A:196:GLU:C	2:A:197:HIS:HD2	2.19	0.46
2:A:241:SER:HB3	2:A:320:ARG:NH2	2.29	0.46
2:A:260:VAL:O	2:A:260:VAL:CG2	2.63	0.46
2:A:278:ALA:HB2	2:A:369:ALA:CA	2.45	0.46
3:B:243:ARG:HH21	3:B:252:LEU:N	2.12	0.46
3:B:324:SER:OG	3:B:326:LYS:HB3	2.16	0.46
9:B:601:TA1:H463	9:B:601:TA1:C26	2.46	0.46
2:A:23:LEU:CD2	2:A:232:GLY:O	2.64	0.46
2:A:145:THR:O	2:A:149:PHE:HB3	2.15	0.46
2:A:179:THR:HG22	3:B:352:LYS:HZ2	1.80	0.46
2:A:241:SER:C	2:A:244:PHE:HB3	2.36	0.46
2:A:286:LEU:O	2:A:287:SER:O	2.34	0.46
2:A:324:VAL:HG12	2:A:326:LYS:H	1.81	0.46
3:B:208:ALA:O	3:B:212:ILE:HG13	2.16	0.46
1:N:273:ARG:HD3	3:B:196:GLU:HB3	1.59	0.46
2:A:155:GLU:HA	2:A:197:HIS:CE1	2.49	0.46
2:A:203:MET:SD	2:A:267:PHE:CB	3.04	0.46
2:A:265:GLY:O	2:A:266:HIS:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:328:VAL:C	2:A:330:ALA:H	2.16	0.46
2:A:381:THR:O	2:A:383:ALA:N	2.49	0.46
2:A:436:GLY:O	2:A:438:ASP:N	2.48	0.46
3:B:102:ASN:ND2	3:B:104:ALA:HB3	2.31	0.46
3:B:360:PRO:O	3:B:369:ARG:C	2.54	0.46
3:B:408:TYR:O	3:B:411:GLU:HB2	2.16	0.46
1:N:51:ASP:OD1	1:N:318:LYS:NZ	2.49	0.46
2:A:11:GLN:CG	2:A:74:VAL:HG11	2.28	0.46
2:A:95:GLY:C	2:A:97:GLU:N	2.69	0.46
2:A:317:LEU:CD1	2:A:351:PHE:CE2	2.99	0.46
3:B:103:TRP:CE3	3:B:189:LEU:HD13	2.50	0.46
3:B:196:GLU:O	3:B:197:ASN:OD1	2.34	0.46
3:B:274:PRO:HG2	3:B:371:LEU:CD2	2.43	0.46
1:N:65:GLN:NE2	1:N:69:LEU:HD22	2.31	0.46
2:A:9:VAL:HG21	2:A:149:PHE:HD1	1.80	0.46
2:A:10:GLY:O	2:A:11:GLN:C	2.53	0.46
2:A:204:VAL:HG21	2:A:231:ILE:HG23	1.97	0.46
2:A:286:LEU:HG	2:A:290:GLU:HB2	1.97	0.46
2:A:316:CYS:HB3	2:A:378:LEU:HD12	1.95	0.46
2:A:423:GLU:O	2:A:426:ALA:HB3	2.16	0.46
2:A:99:ALA:H	3:B:2:ARG:HH22	1.63	0.45
2:A:308:ARG:O	2:A:309:HIS:HB3	2.16	0.45
3:B:154:ILE:HD12	3:B:155:SER:N	2.31	0.45
3:B:194:LEU:O	3:B:265:LEU:HD23	2.16	0.45
3:B:209:LEU:HD23	3:B:227:LEU:HD13	1.98	0.45
3:B:288:VAL:N	3:B:289:PRO:CD	2.80	0.45
3:B:323:MET:CE	3:B:328:VAL:HG22	2.46	0.45
3:B:325:MET:HE2	3:B:355:VAL:CG2	2.46	0.45
2:A:5:ILE:CG2	2:A:6:SER:H	2.29	0.45
2:A:119:LEU:HD11	2:A:156:ARG:HD2	1.97	0.45
2:A:255:PHE:O	2:A:256:GLN:C	2.53	0.45
2:A:288:VAL:HA	2:A:291:ILE:HG12	1.97	0.45
2:A:7:ILE:HG13	2:A:137:VAL:HG22	1.98	0.45
2:A:117:LEU:HD11	2:A:121:ARG:NH2	2.30	0.45
2:A:180:ALA:HA	3:B:352:LYS:NZ	2.31	0.45
2:A:243:ARG:NH2	2:A:252:LEU:HB2	2.31	0.45
2:A:346:TRP:HZ2	2:A:435:VAL:HG12	1.81	0.45
3:B:11:GLN:O	3:B:14:ASN:HB3	2.16	0.45
3:B:113:GLU:CG	3:B:114:LEU:N	2.79	0.45
3:B:137:LEU:HD22	3:B:154:ILE:HG23	1.98	0.45
3:B:242:LEU:C	3:B:244:PHE:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:313:LEU:O	3:B:347:ILE:HD12	2.16	0.45
1:N:269:VAL:HG13	3:B:264:ARG:CZ	2.45	0.45
2:A:256:GLN:O	2:A:260:VAL:HG13	2.15	0.45
2:A:344:VAL:CG1	2:A:345:ASP:N	2.78	0.45
3:B:115:VAL:HG21	3:B:152:LEU:HD21	1.98	0.45
3:B:188:THR:HA	3:B:425:MET:HE3	1.97	0.45
3:B:210:TYR:CE2	3:B:227:LEU:HD11	2.52	0.45
2:A:7:ILE:HD11	2:A:137:VAL:CG2	2.44	0.45
2:A:104:ALA:HB1	2:A:413:MET:HG3	1.96	0.45
2:A:204:VAL:HG12	2:A:204:VAL:O	2.17	0.45
2:A:212:ILE:HD11	2:A:302:MET:H	1.82	0.45
2:A:404:PHE:CD1	2:A:404:PHE:N	2.83	0.45
2:A:434:GLU:C	2:A:436:GLY:H	2.18	0.45
3:B:6:HIS:HB3	3:B:21:TRP:HZ2	1.81	0.45
2:A:166:LYS:CE	2:A:199:ASP:OD1	2.62	0.45
3:B:250:ALA:HB1	3:B:254:LYS:CB	2.44	0.45
3:B:273:ALA:CB	3:B:274:PRO:CD	2.93	0.45
1:N:100:THR:HG21	1:N:105:ILE:HD11	1.98	0.45
2:A:271:THR:O	2:A:376:CYS:HA	2.17	0.45
2:A:303:VAL:O	2:A:303:VAL:CG1	2.65	0.45
3:B:324:SER:O	3:B:326:LYS:N	2.50	0.45
2:A:392:ASP:OD2	2:A:422:ARG:CZ	2.65	0.45
2:A:408:TYR:CG	2:A:418:PHE:HZ	2.34	0.45
3:B:167:ASN:HA	3:B:200:GLU:O	2.17	0.45
3:B:194:LEU:C	3:B:196:GLU:N	2.70	0.45
2:A:11:GLN:HE21	2:A:74:VAL:CG2	2.29	0.45
2:A:11:GLN:NE2	2:A:74:VAL:HG22	2.30	0.45
2:A:103:TYR:CD1	2:A:148:GLY:HA2	2.52	0.45
2:A:132:LEU:H	2:A:132:LEU:CD2	2.23	0.45
2:A:148:GLY:O	2:A:149:PHE:C	2.54	0.45
2:A:182:VAL:O	2:A:184:PRO:CD	2.65	0.45
2:A:291:ILE:HD12	2:A:375:VAL:HG23	1.99	0.45
3:B:23:VAL:O	3:B:25:SER:N	2.50	0.45
3:B:72:PRO:O	3:B:74:THR:N	2.50	0.45
2:A:210:TYR:CD2	2:A:227:LEU:HD21	2.51	0.45
3:B:82:PRO:C	3:B:84:GLY:H	2.20	0.45
3:B:135:PHE:CD1	3:B:135:PHE:N	2.84	0.45
3:B:224:TYR:O	3:B:225:GLY:C	2.53	0.45
3:B:307:PRO:C	3:B:309:HIS:N	2.71	0.45
3:B:360:PRO:HG2	3:B:371:LEU:CB	2.38	0.45
1:N:256:ILE:O	1:N:260:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:172:TYR:CD1	2:A:173:PRO:N	2.80	0.44
2:A:229:ARG:NH1	2:A:229:ARG:HG2	2.31	0.44
2:A:286:LEU:O	2:A:287:SER:C	2.55	0.44
2:A:288:VAL:C	2:A:290:GLU:N	2.71	0.44
3:B:67:LEU:HD12	3:B:92:PHE:CD2	2.51	0.44
1:N:69:LEU:HB3	1:N:70:PRO:HD3	1.99	0.44
2:A:152:LEU:HD12	2:A:152:LEU:C	2.38	0.44
2:A:180:ALA:HA	3:B:352:LYS:HZ3	1.82	0.44
2:A:274:PRO:HB2	2:A:371:VAL:HG21	1.98	0.44
2:A:276:ILE:HG12	2:A:277:SER:N	2.32	0.44
3:B:24:ILE:CG2	3:B:25:SER:N	2.80	0.44
3:B:67:LEU:HD12	3:B:92:PHE:CE2	2.52	0.44
3:B:106:GLY:O	3:B:149:MET:HB2	2.16	0.44
3:B:141:LEU:N	3:B:141:LEU:HD12	2.33	0.44
1:N:269:VAL:CG2	3:B:428:LEU:HD12	2.47	0.44
2:A:209:ILE:CD1	2:A:231:ILE:HD11	2.47	0.44
2:A:334:THR:CG2	2:A:335:ILE:N	2.79	0.44
2:A:343:PHE:CE1	2:A:351:PHE:HE1	2.36	0.44
3:B:4:ILE:HD12	3:B:239:THR:HG21	1.98	0.44
3:B:94:PHE:N	3:B:94:PHE:CD2	2.84	0.44
3:B:102:ASN:OD1	3:B:408:TYR:CZ	2.70	0.44
3:B:230:LEU:HD21	3:B:302:MET:HE2	1.98	0.44
3:B:288:VAL:N	3:B:289:PRO:HD2	2.32	0.44
3:B:312:TYR:HA	3:B:381:SER:HA	1.99	0.44
2:A:12:ALA:HB2	7:B:500:GTP:C8	2.52	0.44
3:B:189:LEU:HD23	3:B:421:ALA:CB	2.48	0.44
2:A:72:PRO:HG2	2:A:73:THR:H	1.83	0.44
2:A:153:LEU:O	2:A:157:LEU:HG	2.18	0.44
2:A:295:CYS:HB3	2:A:377:MET:HG2	1.99	0.44
2:A:362:VAL:HG13	2:A:368:LEU:CG	2.48	0.44
3:B:239:THR:O	3:B:240:THR:C	2.56	0.44
1:N:249:ILE:CG1	1:N:250:ASN:N	2.80	0.44
2:A:144:GLY:H	7:B:500:GTP:PG	2.41	0.44
2:A:413:MET:C	2:A:414:GLU:HG3	2.36	0.44
3:B:8:GLN:CG	3:B:67:LEU:HD22	2.47	0.44
3:B:175:PRO:HG2	3:B:207:GLU:OE1	2.16	0.44
3:B:287:THR:O	3:B:288:VAL:CG2	2.58	0.44
3:B:409:THR:HA	3:B:413:MET:HB3	1.99	0.44
1:N:251:LEU:CA	1:N:254:LEU:HB2	2.48	0.44
2:A:121:ARG:HG2	2:A:121:ARG:HH11	1.83	0.44
2:A:272:TYR:CE2	2:A:274:PRO:HD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:278:ALA:CA	2:A:282:TYR:OH	2.65	0.44
3:B:12:CYS:C	3:B:14:ASN:N	2.71	0.44
3:B:114:LEU:HD23	3:B:149:MET:HE3	2.00	0.44
3:B:295:MET:SD	3:B:375:ALA:HB3	2.57	0.44
2:A:218:ASP:C	2:A:219:ILE:HG12	2.37	0.44
2:A:377:MET:O	2:A:377:MET:HG3	2.18	0.44
2:A:388:TRP:HA	2:A:388:TRP:HE3	1.79	0.44
3:B:7:ILE:N	3:B:136:GLN:O	2.51	0.44
3:B:14:ASN:O	3:B:17:GLY:N	2.50	0.44
3:B:168:THR:CG2	3:B:201:THR:HG23	2.48	0.44
3:B:182:VAL:O	3:B:183:GLU:C	2.56	0.44
3:B:242:LEU:HD22	3:B:250:ALA:O	2.17	0.44
1:N:312:ARG:HH21	2:A:417:GLU:N	2.10	0.44
2:A:23:LEU:O	2:A:26:LEU:HB3	2.17	0.44
2:A:115:ILE:CG1	2:A:152:LEU:HD13	2.46	0.44
2:A:121:ARG:HG2	2:A:121:ARG:NH1	2.33	0.44
2:A:132:LEU:HD23	2:A:132:LEU:N	2.26	0.44
2:A:231:ILE:HD13	2:A:231:ILE:H	1.82	0.44
3:B:52:TYR:HE1	3:B:240:THR:HB	1.82	0.44
3:B:72:PRO:HG2	3:B:73:GLY:H	1.83	0.44
3:B:161:TYR:CD1	3:B:161:TYR:N	2.86	0.44
3:B:161:TYR:O	3:B:163:ASP:N	2.51	0.44
2:A:63:PRO:HG2	2:A:91:GLN:OE1	2.17	0.43
2:A:224:TYR:HD2	2:A:224:TYR:HA	1.73	0.43
2:A:268:PRO:CA	2:A:379:SER:O	2.65	0.43
2:A:283:HIS:O	2:A:283:HIS:ND1	2.49	0.43
2:A:287:SER:N	2:A:290:GLU:OE1	2.51	0.43
3:B:26:ASP:C	3:B:28:HIS:H	2.21	0.43
1:N:125:THR:O	1:N:128:GLN:HG2	2.17	0.43
2:A:262:TYR:HB3	2:A:263:PRO:HD2	2.00	0.43
3:B:167:ASN:HD21	3:B:252:LEU:HD22	1.82	0.43
1:N:139:ALA:HA	1:N:210:THR:O	2.18	0.43
1:N:250:ASN:O	1:N:251:LEU:HB2	2.19	0.43
1:N:258:LYS:HD2	2:A:406:HIS:HA	1.74	0.43
1:N:322:LEU:O	1:N:323:GLU:HB2	2.19	0.43
2:A:175:PRO:CG	2:A:304:LYS:HG2	2.47	0.43
2:A:252:LEU:O	2:A:253:THR:C	2.56	0.43
2:A:363:VAL:CG1	2:A:364:PRO:HD2	2.48	0.43
3:B:409:THR:C	3:B:411:GLU:H	2.22	0.43
2:A:184:PRO:HG2	2:A:398:MET:CE	2.41	0.43
3:B:161:TYR:C	3:B:163:ASP:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:103:TYR:O	2:A:104:ALA:C	2.57	0.43
2:A:172:TYR:HA	2:A:173:PRO:HD3	1.92	0.43
2:A:179:THR:HG22	3:B:352:LYS:HZ1	1.80	0.43
2:A:310:GLY:HA3	2:A:383:ALA:CA	2.49	0.43
3:B:212:ILE:O	3:B:212:ILE:HG22	2.18	0.43
3:B:229:HIS:HE2	9:B:601:TA1:H361	1.83	0.43
2:A:21:TRP:HE1	2:A:63:PRO:HB3	1.83	0.43
2:A:63:PRO:C	2:A:64:ARG:CG	2.83	0.43
3:B:68:VAL:HG11	3:B:153:LEU:HD21	2.00	0.43
2:A:13:GLY:C	2:A:16:ILE:HG22	2.38	0.43
2:A:207:GLU:O	2:A:210:TYR:N	2.51	0.43
3:B:301:MET:O	3:B:303:ALA:N	2.51	0.43
3:B:435:TYR:C	3:B:437:ASP:N	2.72	0.43
3:B:168:THR:N	3:B:200:GLU:O	2.43	0.43
3:B:359:PRO:CB	3:B:360:PRO:HD2	2.45	0.43
3:B:383:ALA:C	3:B:385:GLN:N	2.72	0.43
3:B:105:LYS:HG2	3:B:110:GLU:CG	2.48	0.43
3:B:108:TYR:CE1	3:B:413:MET:HE1	2.53	0.43
3:B:118:VAL:O	3:B:122:VAL:HG13	2.19	0.43
1:N:172:LEU:HA	1:N:173:PRO:HD3	1.92	0.43
2:A:147:SER:HB2	2:A:186:ASN:O	2.19	0.43
2:A:154:MET:CE	2:A:166:LYS:HB3	2.48	0.43
2:A:209:ILE:CD1	2:A:231:ILE:CD1	2.97	0.43
2:A:238:ILE:O	2:A:242:LEU:CB	2.67	0.43
2:A:238:ILE:HD11	2:A:378:LEU:HD23	2.01	0.43
2:A:343:PHE:HZ	2:A:351:PHE:CZ	2.36	0.42
3:B:72:PRO:O	3:B:73:GLY:C	2.58	0.42
3:B:103:TRP:HB2	3:B:186:ASN:HA	2.01	0.42
3:B:210:TYR:O	3:B:214:PHE:N	2.52	0.42
2:A:8:HIS:HA	2:A:138:PHE:HB2	2.00	0.42
2:A:409:VAL:C	2:A:411:GLU:N	2.71	0.42
3:B:70:LEU:HB2	3:B:99:ALA:CB	2.48	0.42
3:B:192:HIS:NE2	3:B:420:GLU:HG2	2.34	0.42
3:B:240:THR:HG23	3:B:241:CYS:N	2.33	0.42
1:N:73:ASP:O	1:N:77:GLU:HG3	2.19	0.42
2:A:16:ILE:CG2	2:A:17:GLY:N	2.82	0.42
2:A:436:GLY:C	2:A:438:ASP:N	2.72	0.42
3:B:288:VAL:C	3:B:290:GLU:N	2.70	0.42
3:B:399:PHE:O	3:B:402:LYS:N	2.29	0.42
1:N:33:PRO:HA	1:N:34:PRO:HD3	1.91	0.42
1:N:103:GLY:H	1:N:181:HIS:CD2	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:268:THR:HG23	3:B:433:GLN:H	1.75	0.42
2:A:76:ASP:O	2:A:79:ARG:N	2.52	0.42
2:A:231:ILE:C	2:A:233:GLN:N	2.73	0.42
3:B:48:ARG:HG2	3:B:243:ARG:HB3	2.01	0.42
3:B:204:ILE:HD13	3:B:231:VAL:CG2	2.45	0.42
2:A:8:HIS:CD2	2:A:138:PHE:CD1	3.07	0.42
2:A:304:LYS:O	2:A:304:LYS:HG3	2.19	0.42
2:A:363:VAL:HG13	2:A:364:PRO:HD2	2.02	0.42
3:B:243:ARG:HD3	3:B:243:ARG:HA	1.62	0.42
3:B:333:LEU:O	3:B:334:ASN:C	2.58	0.42
2:A:105:ARG:O	2:A:110:ILE:CG2	2.64	0.42
2:A:210:TYR:OH	3:B:325:MET:HB3	2.20	0.42
2:A:378:LEU:HD12	2:A:378:LEU:O	2.19	0.42
2:A:390:ARG:HG3	2:A:390:ARG:HH11	1.83	0.42
3:B:153:LEU:HD13	3:B:153:LEU:N	2.34	0.42
3:B:242:LEU:HB3	3:B:250:ALA:O	2.20	0.42
3:B:299:LYS:H	3:B:299:LYS:CD	2.07	0.42
3:B:343:PHE:CD2	3:B:350:ASN:ND2	2.88	0.42
2:A:13:GLY:HA2	2:A:16:ILE:CG2	2.50	0.42
2:A:15:GLN:NE2	7:B:500:GTP:N7	2.67	0.42
2:A:25:CYS:SG	2:A:26:LEU:N	2.92	0.42
2:A:101:ASN:ND2	3:B:254:LYS:CD	2.75	0.42
2:A:213:CYS:O	2:A:219:ILE:HG13	2.20	0.42
3:B:250:ALA:CB	3:B:254:LYS:HE2	2.50	0.42
1:N:321:ALA:O	1:N:324:HIS:HB2	2.19	0.42
2:A:95:GLY:C	2:A:97:GLU:H	2.23	0.42
2:A:119:LEU:HD11	2:A:156:ARG:HD3	2.01	0.42
3:B:2:ARG:NH1	3:B:251:ASP:CG	2.73	0.42
3:B:106:GLY:O	3:B:149:MET:CA	2.68	0.42
2:A:149:PHE:O	2:A:150:THR:C	2.56	0.42
2:A:175:PRO:HG3	2:A:304:LYS:CB	2.50	0.42
2:A:328:VAL:C	2:A:330:ALA:N	2.73	0.42
3:B:6:HIS:HB3	3:B:65:ALA:CB	2.48	0.42
3:B:25:SER:O	3:B:28:HIS:N	2.53	0.42
3:B:138:THR:O	3:B:139:HIS:HB3	2.19	0.42
3:B:171:VAL:HG12	3:B:171:VAL:O	2.20	0.42
1:N:6:LEU:HD23	1:N:286:THR:O	2.20	0.42
2:A:242:LEU:HD11	2:A:250:VAL:HG23	2.02	0.42
2:A:305:CYS:SG	2:A:383:ALA:HB1	2.60	0.42
2:A:402:ARG:O	2:A:405:VAL:N	2.49	0.42
3:B:35:SER:CB	3:B:59:ASN:HA	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:187:ALA:O	3:B:188:THR:C	2.57	0.42
3:B:422:GLU:O	3:B:426:ASN:CB	2.67	0.42
1:N:269:VAL:HG13	3:B:264:ARG:NH1	2.35	0.41
2:A:104:ALA:HB3	2:A:408:TYR:HD2	1.84	0.41
2:A:255:PHE:O	2:A:257:THR:N	2.53	0.41
3:B:82:PRO:HB2	3:B:83:PHE:H	1.56	0.41
3:B:199:ASP:C	3:B:265:LEU:HD13	2.40	0.41
3:B:202:TYR:CE2	3:B:268:PHE:HD1	2.38	0.41
3:B:210:TYR:O	3:B:211:ASP:C	2.57	0.41
3:B:301:MET:HE1	3:B:377:PHE:HE2	1.84	0.41
2:A:67:PHE:HB2	2:A:92:LEU:HD23	2.02	0.41
2:A:76:ASP:O	2:A:80:THR:N	2.53	0.41
2:A:115:ILE:CD1	2:A:115:ILE:C	2.87	0.41
3:B:276:THR:O	9:B:601:TA1:H192	2.20	0.41
1:N:61:ASP:O	1:N:65:GLN:HG2	2.20	0.41
3:B:175:PRO:O	3:B:177:VAL:N	2.53	0.41
3:B:273:ALA:HB1	3:B:291:LEU:HG	2.01	0.41
3:B:274:PRO:HD3	3:B:374:SER:HA	2.03	0.41
3:B:310:GLY:HA3	3:B:436:GLN:NE2	2.29	0.41
3:B:399:PHE:O	3:B:401:ARG:N	2.53	0.41
1:N:180:LEU:O	1:N:183:ILE:HG13	2.20	0.41
2:A:23:LEU:HD11	2:A:361:THR:O	2.21	0.41
2:A:152:LEU:C	2:A:152:LEU:CD1	2.89	0.41
3:B:261:PRO:HB2	3:B:262:PHE:CD1	2.54	0.41
3:B:333:LEU:HD11	3:B:337:ASN:HD21	1.85	0.41
1:N:103:GLY:N	1:N:181:HIS:HD2	2.08	0.41
1:N:268:THR:CG2	3:B:429:VAL:O	2.68	0.41
3:B:119:LEU:O	3:B:122:VAL:HG22	2.21	0.41
3:B:135:PHE:CD1	3:B:166:MET:SD	3.14	0.41
3:B:239:THR:CG2	3:B:240:THR:N	2.80	0.41
3:B:269:MET:HE1	3:B:381:SER:OG	2.20	0.41
3:B:380:ASN:C	3:B:380:ASN:HD22	2.24	0.41
3:B:427:ASP:OD1	3:B:427:ASP:C	2.58	0.41
2:A:67:PHE:CE1	2:A:87:PHE:CE2	3.08	0.41
2:A:115:ILE:CG2	2:A:116:ASP:H	2.32	0.41
2:A:243:ARG:NH2	2:A:252:LEU:HG	2.35	0.41
2:A:255:PHE:O	2:A:259:LEU:N	2.50	0.41
3:B:168:THR:HB	3:B:198:THR:HG21	2.03	0.41
1:N:165:ARG:HD2	1:N:165:ARG:N	2.36	0.41
2:A:166:LYS:HB2	2:A:199:ASP:OD1	2.20	0.41
2:A:282:TYR:HD2	2:A:284:GLU:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:182:VAL:O	3:B:184:PRO:N	2.54	0.41
3:B:409:THR:C	3:B:411:GLU:N	2.73	0.41
1:N:249:ILE:HG12	1:N:250:ASN:N	2.36	0.41
2:A:101:ASN:HD21	3:B:254:LYS:NZ	2.18	0.41
2:A:149:PHE:CD1	2:A:150:THR:N	2.89	0.41
2:A:414:GLU:C	2:A:416:GLY:N	2.74	0.41
3:B:132:LEU:O	3:B:164:ARG:HD2	2.21	0.41
3:B:259:MET:HE3	3:B:268:PHE:CE1	2.56	0.41
3:B:417:GLU:O	3:B:420:GLU:HB3	2.21	0.41
1:N:11:ILE:HD11	1:N:317:ALA:HB3	2.03	0.41
1:N:145:TYR:CD2	1:N:192:ARG:HD2	2.56	0.41
2:A:100:ALA:O	2:A:102:ASN:N	2.49	0.41
2:A:226:ASN:O	2:A:227:LEU:C	2.59	0.41
2:A:272:TYR:O	2:A:300:ASN:ND2	2.54	0.41
2:A:288:VAL:O	2:A:289:ALA:C	2.59	0.41
2:A:384:ILE:O	2:A:385:ALA:C	2.59	0.41
3:B:98:GLY:C	3:B:100:GLY:H	2.25	0.41
3:B:102:ASN:ND2	3:B:408:TYR:HA	2.20	0.41
3:B:147:SER:CB	3:B:190:SER:HB3	2.42	0.41
1:N:265:ALA:CB	2:A:401:LYS:HB3	2.51	0.41
2:A:251:ASP:CA	2:A:254:GLU:HG3	2.49	0.41
2:A:263:PRO:O	2:A:264:ARG:C	2.56	0.41
2:A:332:ILE:CD1	2:A:353:VAL:HG22	2.51	0.41
2:A:401:LYS:O	2:A:402:ARG:HB2	2.21	0.41
2:A:413:MET:C	2:A:414:GLU:CG	2.90	0.41
3:B:242:LEU:HD23	3:B:242:LEU:HA	1.76	0.41
3:B:307:PRO:O	3:B:309:HIS:N	2.53	0.41
3:B:311:ARG:HG2	3:B:311:ARG:NH1	2.34	0.41
1:N:29:VAL:CG1	1:N:301:GLN:HA	2.50	0.40
2:A:384:ILE:C	2:A:386:GLU:N	2.72	0.40
3:B:11:GLN:HA	3:B:74:THR:HG21	2.04	0.40
3:B:23:VAL:O	3:B:24:ILE:C	2.60	0.40
3:B:125:GLU:O	3:B:128:SER:HB3	2.22	0.40
3:B:187:ALA:O	3:B:190:SER:N	2.54	0.40
3:B:409:THR:O	3:B:412:GLY:N	2.48	0.40
1:N:84:LEU:C	1:N:84:LEU:HD23	2.41	0.40
2:A:199:ASP:CB	2:A:256:GLN:NE2	2.77	0.40
3:B:291:LEU:HD21	3:B:373:MET:HG2	2.03	0.40
2:A:14:VAL:HG11	2:A:75:ILE:HD13	2.04	0.40
2:A:273:ALA:O	2:A:275:VAL:N	2.54	0.40
2:A:289:ALA:HB3	2:A:290:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:20:PHE:CD2	3:B:235:MET:CG	3.04	0.40
3:B:98:GLY:O	3:B:100:GLY:N	2.49	0.40
3:B:405:LEU:HD23	3:B:405:LEU:O	2.21	0.40
1:N:249:ILE:HG23	1:N:250:ASN:H	1.87	0.40
1:N:265:ALA:CB	2:A:401:LYS:CB	3.00	0.40
2:A:182:VAL:O	2:A:183:GLU:C	2.60	0.40
2:A:209:ILE:HD13	2:A:231:ILE:HD11	2.04	0.40
2:A:335:ILE:C	2:A:337:THR:N	2.73	0.40
3:B:70:LEU:HB2	3:B:99:ALA:HB2	2.03	0.40
3:B:133:GLN:CG	3:B:165:ILE:HD11	2.49	0.40
3:B:315:VAL:CG1	3:B:377:PHE:CE1	3.05	0.40
2:A:318:LEU:HB2	2:A:376:CYS:SG	2.61	0.40
3:B:35:SER:HB3	3:B:59:ASN:OD1	2.22	0.40
3:B:95:GLY:C	3:B:97:SER:H	2.25	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 PDB entries followed by that with respect to all EM entries.

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	N	283/344 (82%)	265 (94%)	13 (5%)	5 (2%)	8	40
2	A	408/451 (90%)	266 (65%)	83 (20%)	59 (14%)	0	4
3	B	424/445 (95%)	274 (65%)	94 (22%)	56 (13%)	0	5
All	All	1115/1240 (90%)	805 (72%)	190 (17%)	120 (11%)	1	8

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	96	LYS
2	A	97	GLU
2	A	108	TYR

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Mol	Chain	Res	Type
2	A	109	THR
2	A	141	PHE
2	A	183	GLU
2	A	217	LEU
2	A	240	ALA
2	A	249	ASN
2	A	255	PHE
2	A	266	HIS
2	A	280	LYS
2	A	284	GLU
2	A	285	GLN
2	A	289	ALA
2	A	309	HIS
2	A	346	TRP
2	A	370	LYS
2	A	387	ALA
2	A	403	ALA
2	A	437	VAL
3	B	23	VAL
3	B	24	ILE
3	B	32	PRO
3	B	50	ASN
3	B	82	PRO
3	B	97	SER
3	B	128	SER
3	B	176	LYS
3	B	183	GLU
3	B	218	LYS
3	B	238	VAL
3	B	239	THR
3	B	240	THR
3	B	252	LEU
3	B	263	PRO
3	B	266	HIS
3	B	273	ALA
3	B	278	ARG
3	B	280	SER
3	B	281	GLN
3	B	282	GLN
3	B	288	VAL
3	B	294	GLN
3	B	295	MET

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Mol	Chain	Res	Type
3	B	343	PHE
3	B	344	VAL
3	B	346	TRP
3	B	369	ARG
3	B	403	ALA
1	N	251	LEU
1	N	252	GLY
2	A	24	TYR
2	A	63	PRO
2	A	103	TYR
2	A	111	GLY
2	A	131	GLY
2	A	218	ASP
2	A	219	ILE
2	A	238	ILE
2	A	265	GLY
2	A	287	SER
2	A	314	ALA
2	A	339	ARG
2	A	342	GLN
2	A	373	ARG
2	A	386	GLU
3	B	38	GLY
3	B	73	GLY
3	B	175	PRO
3	B	265	LEU
3	B	279	GLY
3	B	298	ALA
3	B	300	ASN
3	B	311	ARG
2	A	104	ALA
2	A	148	GLY
2	A	149	PHE
2	A	173	PRO
2	A	239	THR
2	A	245	ASP
2	A	263	PRO
2	A	279	GLU
2	A	288	VAL
2	A	330	ALA
2	A	336	LYS
2	A	369	ALA

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Mol	Chain	Res	Type
3	B	34	GLY
3	B	83	PHE
3	B	99	ALA
3	B	100	GLY
3	B	302	MET
3	B	386	GLU
2	A	89	PRO
2	A	129	CYS
2	A	300	ASN
2	A	348	PRO
3	B	96	GLN
3	B	395	PHE
2	A	256	GLN
2	A	303	VAL
2	A	307	PRO
2	A	382	THR
3	B	57	ALA
3	B	74	THR
3	B	285	ALA
1	N	253	LEU
2	A	31	GLN
2	A	273	ALA
3	B	51	VAL
3	B	58	GLY
3	B	145	THR
3	B	162	PRO
3	B	400	ARG
3	B	424	ASN
3	B	195	VAL
1	N	269	VAL
2	A	115	ILE
3	B	72	PRO
1	N	249	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 PDB entries followed by that with respect to all EM entries.

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	N	248/293 (85%)	240 (97%)	8 (3%)	39	61
2	A	347/377 (92%)	298 (86%)	49 (14%)	3	16
3	B	367/381 (96%)	307 (84%)	60 (16%)	2	13
All	All	962/1051 (92%)	845 (88%)	117 (12%)	8	20

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	41	LEU
1	N	63	MET
1	N	132	LYS
1	N	141	PHE
1	N	165	ARG
1	N	170	THR
1	N	249	ILE
1	N	253	LEU
2	A	6	SER
2	A	20	CYS
2	A	21	TRP
2	A	32	PRO
2	A	76	ASP
2	A	82	THR
2	A	98	ASP
2	A	115	ILE
2	A	120	ASP
2	A	125	LEU
2	A	127	ASP
2	A	130	THR
2	A	135	PHE
2	A	141	PHE
2	A	150	THR
2	A	152	LEU
2	A	155	GLU
2	A	169	PHE
2	A	172	TYR
2	A	173	PRO
2	A	183	GLU
2	A	192	HIS
2	A	204	VAL
2	A	219	ILE
2	A	224	TYR
2	A	231	ILE

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Mol	Chain	Res	Type
2	A	234	ILE
2	A	243	ARG
2	A	244	PHE
2	A	253	THR
2	A	260	VAL
2	A	267	PHE
2	A	269	LEU
2	A	276	ILE
2	A	284	GLU
2	A	303	VAL
2	A	325	PRO
2	A	334	THR
2	A	345	ASP
2	A	352	LYS
2	A	368	LEU
2	A	376	CYS
2	A	378	LEU
2	A	380	ASN
2	A	404	PHE
2	A	415	GLU
2	A	417	GLU
2	A	431	ASP
2	A	432	TYR
3	B	14	ASN
3	B	24	ILE
3	B	26	ASP
3	B	32	PRO
3	B	41	ASP
3	B	68	VAL
3	B	76	ASP
3	B	90	ASP
3	B	94	PHE
3	B	101	ASN
3	B	122	VAL
3	B	129	CYS
3	B	135	PHE
3	B	141	LEU
3	B	145	THR
3	B	149	MET
3	B	153	LEU
3	B	161	TYR
3	B	163	ASP

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Mol	Chain	Res	Type
3	B	165	ILE
3	B	174	SER
3	B	198	THR
3	B	201	THR
3	B	203	CYS
3	B	207	GLU
3	B	211	ASP
3	B	214	PHE
3	B	215	ARG
3	B	224	TYR
3	B	227	LEU
3	B	230	LEU
3	B	236	SER
3	B	240	THR
3	B	244	PHE
3	B	265	LEU
3	B	267	PHE
3	B	275	LEU
3	B	282	GLN
3	B	283	TYR
3	B	284	ARG
3	B	289	PRO
3	B	299	LYS
3	B	306	ASP
3	B	309	HIS
3	B	322	ARG
3	B	324	SER
3	B	325	MET
3	B	343	PHE
3	B	344	VAL
3	B	349	ASN
3	B	369	ARG
3	B	380	ASN
3	B	387	LEU
3	B	413	MET
3	B	414	ASP
3	B	424	ASN
3	B	427	ASP
3	B	431	GLU
3	B	432	TYR
3	B	437	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34)

such sidechains are listed below:

Mol	Chain	Res	Type
1	N	49	HIS
1	N	65	GLN
1	N	88	GLN
1	N	181	HIS
1	N	300	HIS
1	N	324	HIS
2	A	11	GLN
2	A	15	GLN
2	A	28	HIS
2	A	128	GLN
2	A	133	GLN
2	A	139	HIS
2	A	197	HIS
2	A	216	ASN
2	A	226	ASN
2	A	256	GLN
2	A	309	HIS
2	A	380	ASN
3	B	14	ASN
3	B	91	ASN
3	B	101	ASN
3	B	102	ASN
3	B	107	HIS
3	B	136	GLN
3	B	139	HIS
3	B	197	ASN
3	B	282	GLN
3	B	331	GLN
3	B	334	ASN
3	B	337	ASN
3	B	349	ASN
3	B	380	ASN
3	B	406	HIS
3	B	436	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	ADP	N	401	4	24,29,29	1.28	3 (12%)	29,45,45	1.85	7 (24%)
7	GTP	B	500	4	26,34,34	1.29	4 (15%)	32,54,54	1.11	3 (9%)
9	TA1	B	601	-	68,68,68	2.00	19 (27%)	105,105,105	1.39	11 (10%)
8	GDP	B	600	-	24,30,30	2.60	9 (37%)	30,47,47	2.93	8 (26%)

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	ADP	N	401	4	-	3/12/32/32	0/3/3/3
7	GTP	B	500	4	-	3/18/38/38	0/3/3/3
9	TA1	B	601	-	-	9/41/127/127	0/7/7/7
8	GDP	B	600	-	-	4/12/32/32	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	600	GDP	O4'-C1'	6.28	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	600	GDP	O6-C6	5.68	1.34	1.23
9	B	601	TA1	C06-C05	5.27	1.50	1.38
9	B	601	TA1	C18-C10	5.13	1.69	1.57
8	B	600	GDP	C2-N1	4.67	1.49	1.37
9	B	601	TA1	C08-C07	-4.58	1.25	1.38
9	B	601	TA1	C05-C04	4.31	1.46	1.39
9	B	601	TA1	C45-C24	3.96	1.61	1.54
8	B	600	GDP	PB-O2B	-3.79	1.40	1.54
7	B	500	GTP	C5-C6	-3.71	1.39	1.47
9	B	601	TA1	O02-C03	3.59	1.41	1.34
5	N	401	ADP	PB-O3B	3.53	1.68	1.54
8	B	600	GDP	C8-N7	3.53	1.41	1.35
9	B	601	TA1	C36-C31	3.37	1.45	1.39
9	B	601	TA1	C25-C24	3.24	1.39	1.34
9	B	601	TA1	C46-C45	3.14	1.60	1.53
9	B	601	TA1	C43-C01	3.08	1.60	1.54
9	B	601	TA1	C11-C10	3.05	1.61	1.54
8	B	600	GDP	C5-C6	-2.88	1.41	1.47
9	B	601	TA1	C43-C26	2.79	1.58	1.52
7	B	500	GTP	C6-N1	2.59	1.41	1.37
9	B	601	TA1	C26-C25	2.48	1.56	1.51
9	B	601	TA1	C18-C20	2.43	1.62	1.55
8	B	600	GDP	C2-N3	-2.39	1.27	1.33
7	B	500	GTP	C8-N7	-2.38	1.31	1.35
9	B	601	TA1	C01-C45	2.37	1.66	1.56
8	B	600	GDP	PB-O3B	2.36	1.63	1.54
9	B	601	TA1	C04-C03	-2.33	1.44	1.50
9	B	601	TA1	C16-C15	2.24	1.56	1.52
9	B	601	TA1	C37-C29	2.17	1.54	1.52
7	B	500	GTP	O4'-C1'	2.13	1.44	1.41
5	N	401	ADP	O4'-C1'	2.09	1.44	1.41
8	B	600	GDP	O3'-C3'	2.09	1.47	1.43
9	B	601	TA1	C10-C02	2.09	1.62	1.57
5	N	401	ADP	C2'-C3'	2.04	1.58	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	600	GDP	C8-N7-C5	9.30	120.69	102.99
8	B	600	GDP	N2-C2-N3	6.25	131.90	119.74
8	B	600	GDP	C5-C6-N1	6.10	124.73	113.95
5	N	401	ADP	PA-O3A-PB	-5.36	114.43	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	601	TA1	C06-C05-C04	-4.85	114.60	120.34
9	B	601	TA1	C07-C08-C09	4.70	127.36	120.19
5	N	401	ADP	N3-C2-N1	-4.39	121.82	128.68
8	B	600	GDP	O6-C6-C5	-4.25	116.07	124.37
8	B	600	GDP	N2-C2-N1	-4.17	107.83	116.71
9	B	601	TA1	C05-C04-C03	-3.96	111.46	120.40
8	B	600	GDP	C2-N1-C6	-3.74	118.20	125.10
9	B	601	TA1	C09-C04-C03	3.52	128.36	120.40
8	B	600	GDP	C2'-C3'-C4'	3.39	109.22	102.64
9	B	601	TA1	C17-C18-C20	3.13	109.83	102.59
5	N	401	ADP	O3'-C3'-C2'	-3.08	101.86	111.82
5	N	401	ADP	O4'-C1'-C2'	-3.02	102.52	106.93
9	B	601	TA1	C45-C01-C02	3.00	115.19	111.91
9	B	601	TA1	O04-C11-C14	-2.89	101.77	108.09
7	B	500	GTP	O2G-PG-O3B	2.66	113.57	104.64
9	B	601	TA1	O01-C01-C43	2.55	113.42	107.03
5	N	401	ADP	C2'-C3'-C4'	-2.32	98.13	102.64
8	B	600	GDP	O2'-C2'-C3'	2.26	119.13	111.82
5	N	401	ADP	O2B-PB-O3A	2.24	112.16	104.64
9	B	601	TA1	C14-C11-C15	-2.16	83.10	85.40
9	B	601	TA1	C10-C18-C17	-2.15	102.35	106.54
9	B	601	TA1	O06-C15-C11	2.15	93.00	90.58
7	B	500	GTP	O5'-C5'-C4'	2.07	116.11	108.99
5	N	401	ADP	PA-O5'-C5'	-2.03	109.79	121.68
7	B	500	GTP	O3G-PG-O3B	2.02	111.41	104.64

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	N	401	ADP	PA-O3A-PB-O2B
8	B	600	GDP	PA-O3A-PB-O2B
8	B	600	GDP	C5'-O5'-PA-O3A
8	B	600	GDP	C5'-O5'-PA-O1A
9	B	601	TA1	O02-C03-C04-C05
9	B	601	TA1	O02-C03-C04-C09
9	B	601	TA1	O03-C03-C04-C09
9	B	601	TA1	O03-C03-C04-C05
9	B	601	TA1	N01-C30-C31-C36
9	B	601	TA1	O14-C30-C31-C36
9	B	601	TA1	N01-C30-C31-C32
9	B	601	TA1	O14-C30-C31-C32

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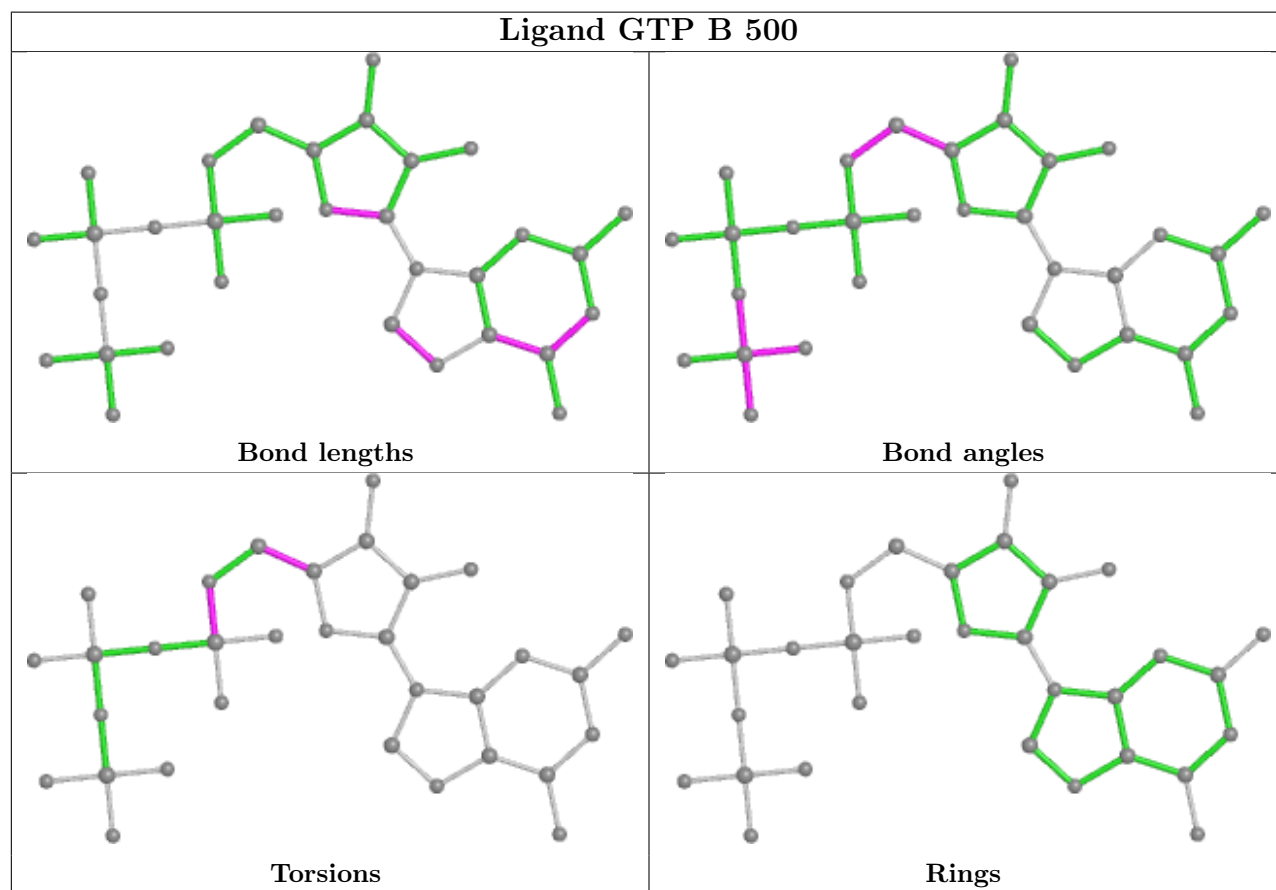
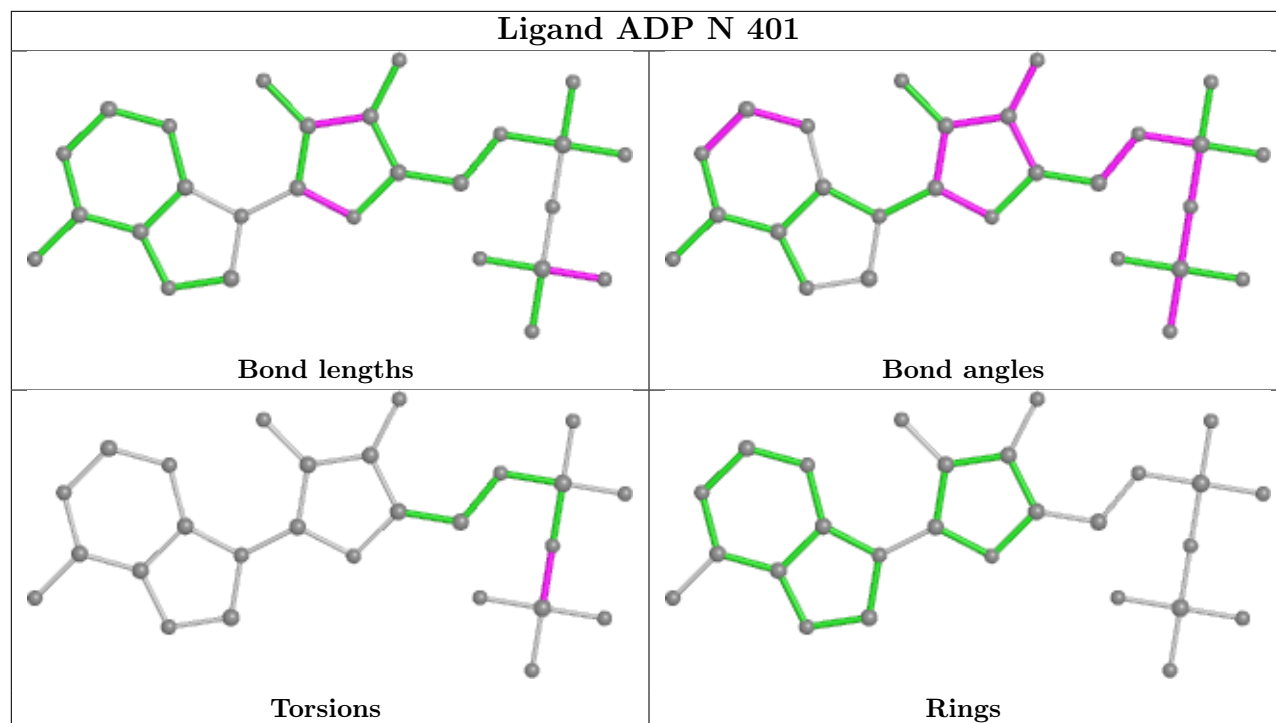
Mol	Chain	Res	Type	Atoms
7	B	500	GTP	C3'-C4'-C5'-O5'
7	B	500	GTP	O4'-C4'-C5'-O5'
5	N	401	ADP	PA-O3A-PB-O1B
5	N	401	ADP	PA-O3A-PB-O3B
8	B	600	GDP	PA-O3A-PB-O3B
9	B	601	TA1	C15-C11-O04-C12
7	B	500	GTP	C5'-O5'-PA-O1A

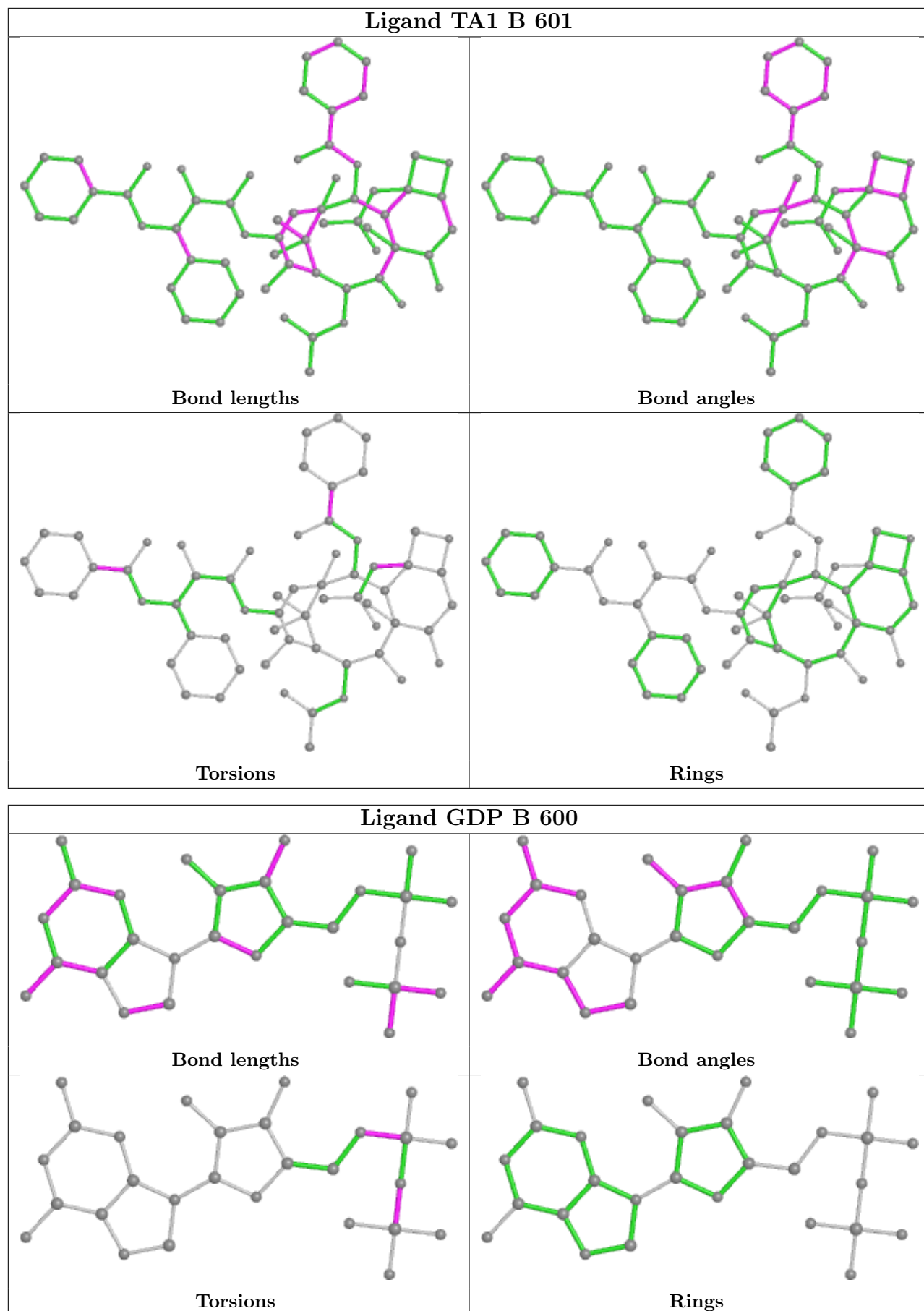
There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	500	GTP	4	0
9	B	601	TA1	6	0
8	B	600	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

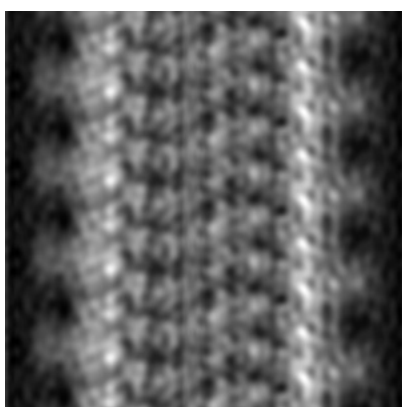
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5038. These allow visual inspection of the internal detail of the map and identification of artifacts.

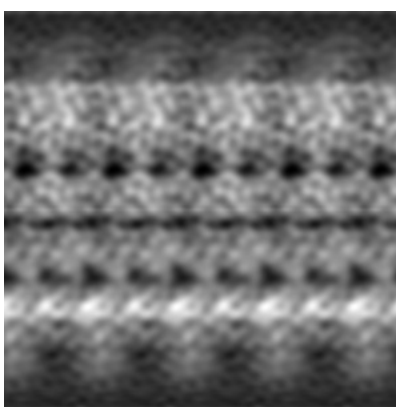
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

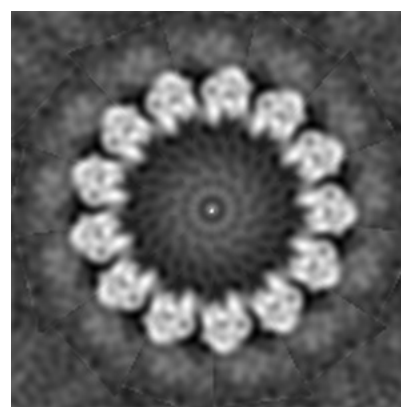
6.1.1 Primary map



X



Y

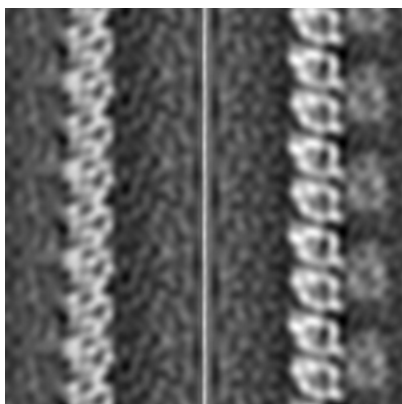


Z

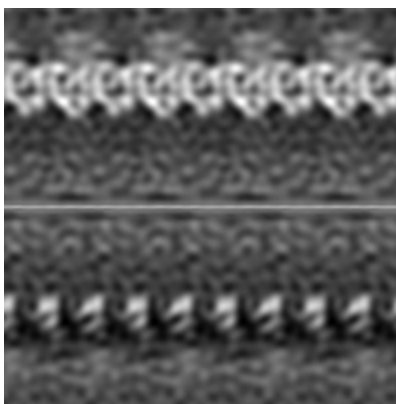
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

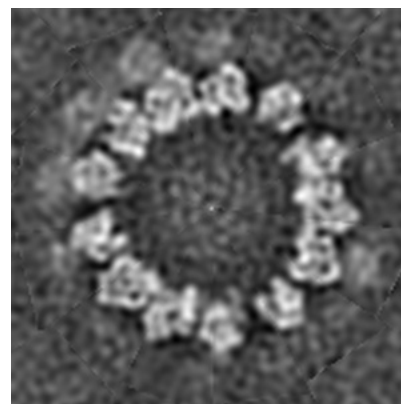
6.2.1 Primary map



X Index: 90



Y Index: 90

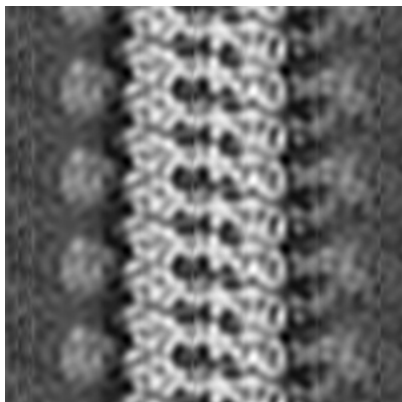


Z Index: 90

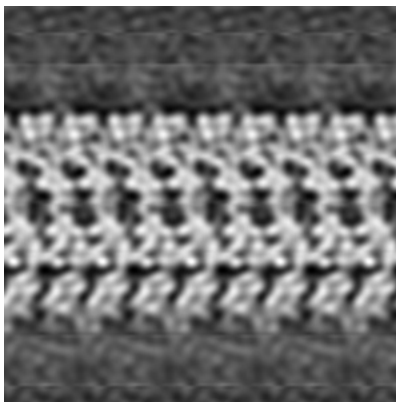
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

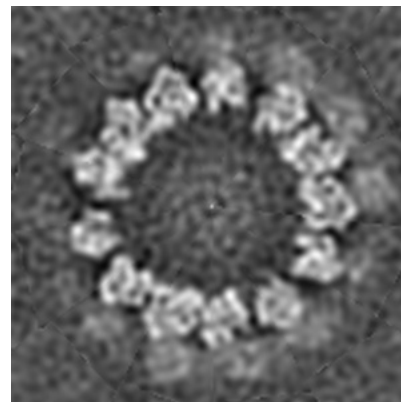
6.3.1 Primary map



X Index: 133



Y Index: 47

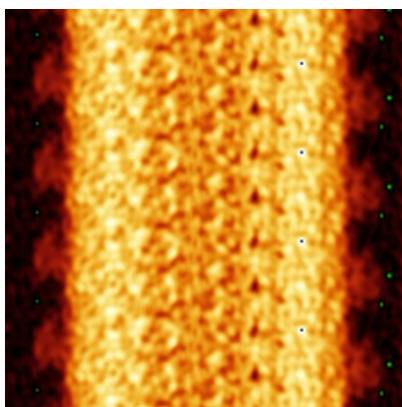


Z Index: 27

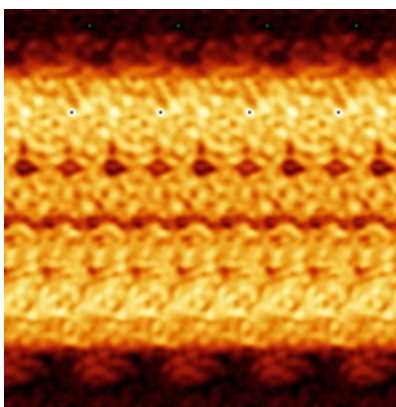
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

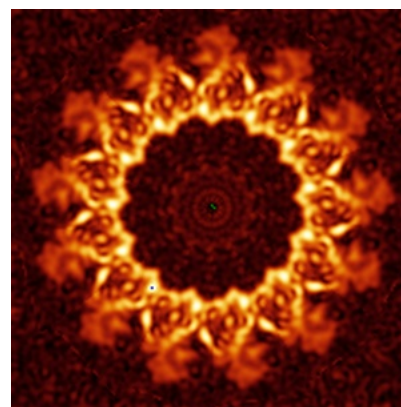
6.4.1 Primary map



X



Y

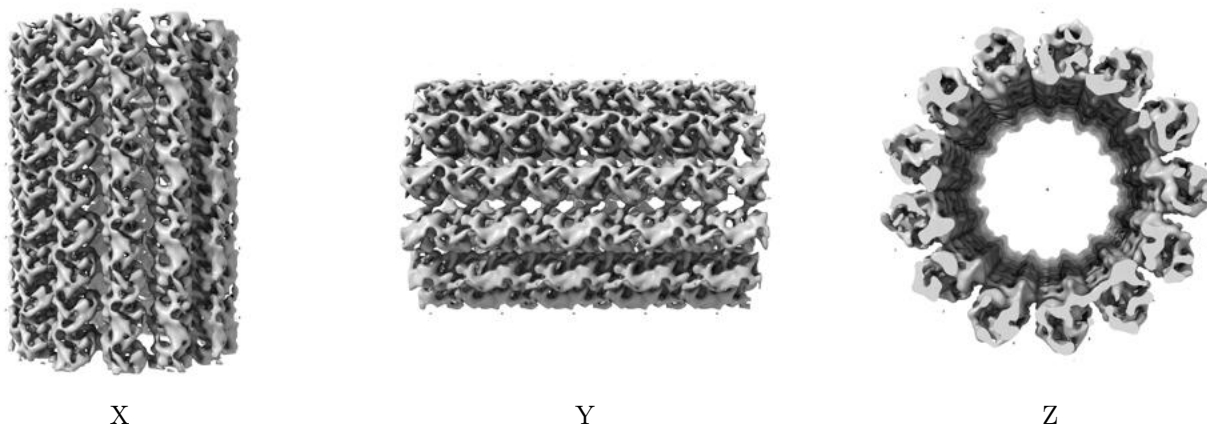


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

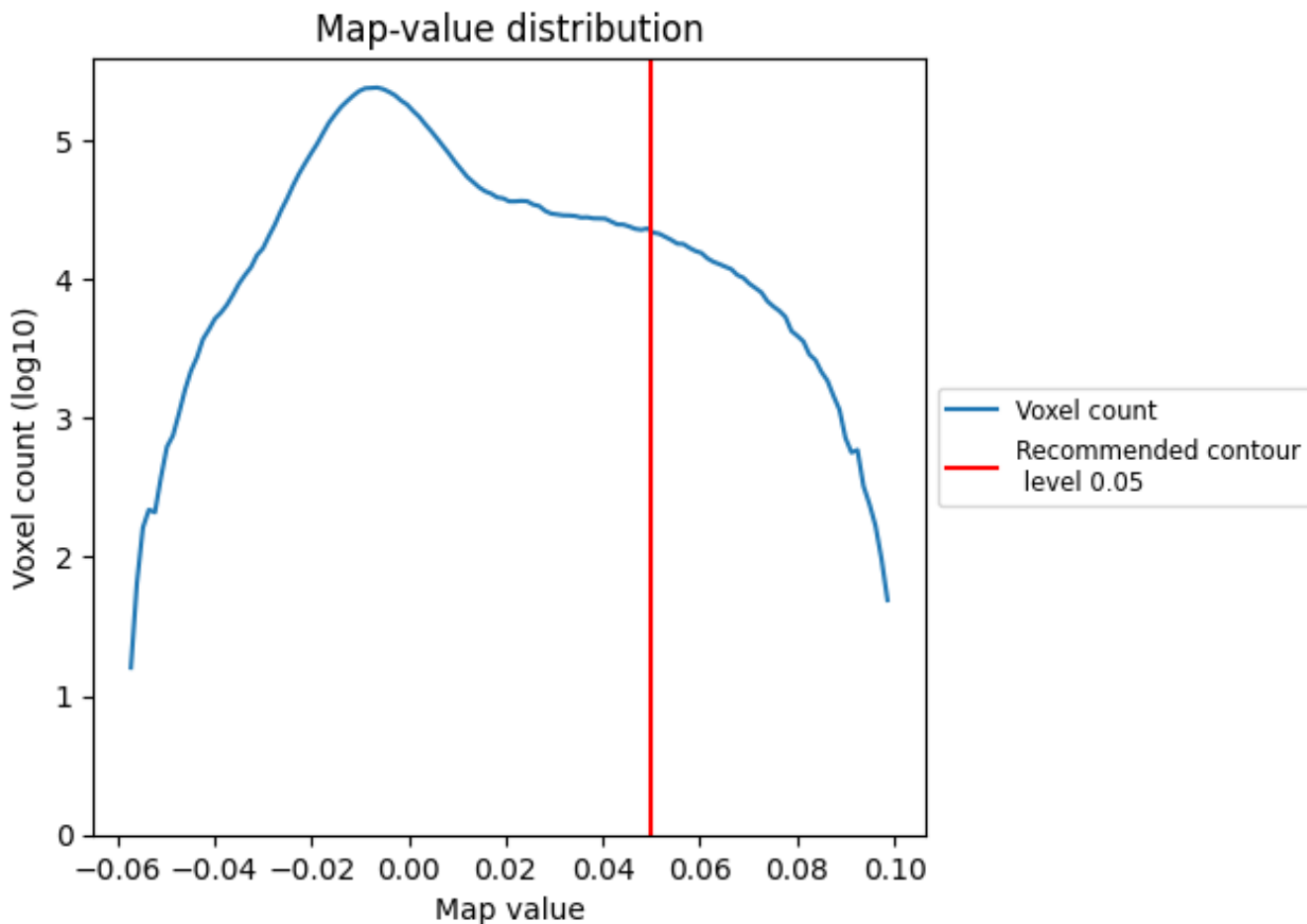
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

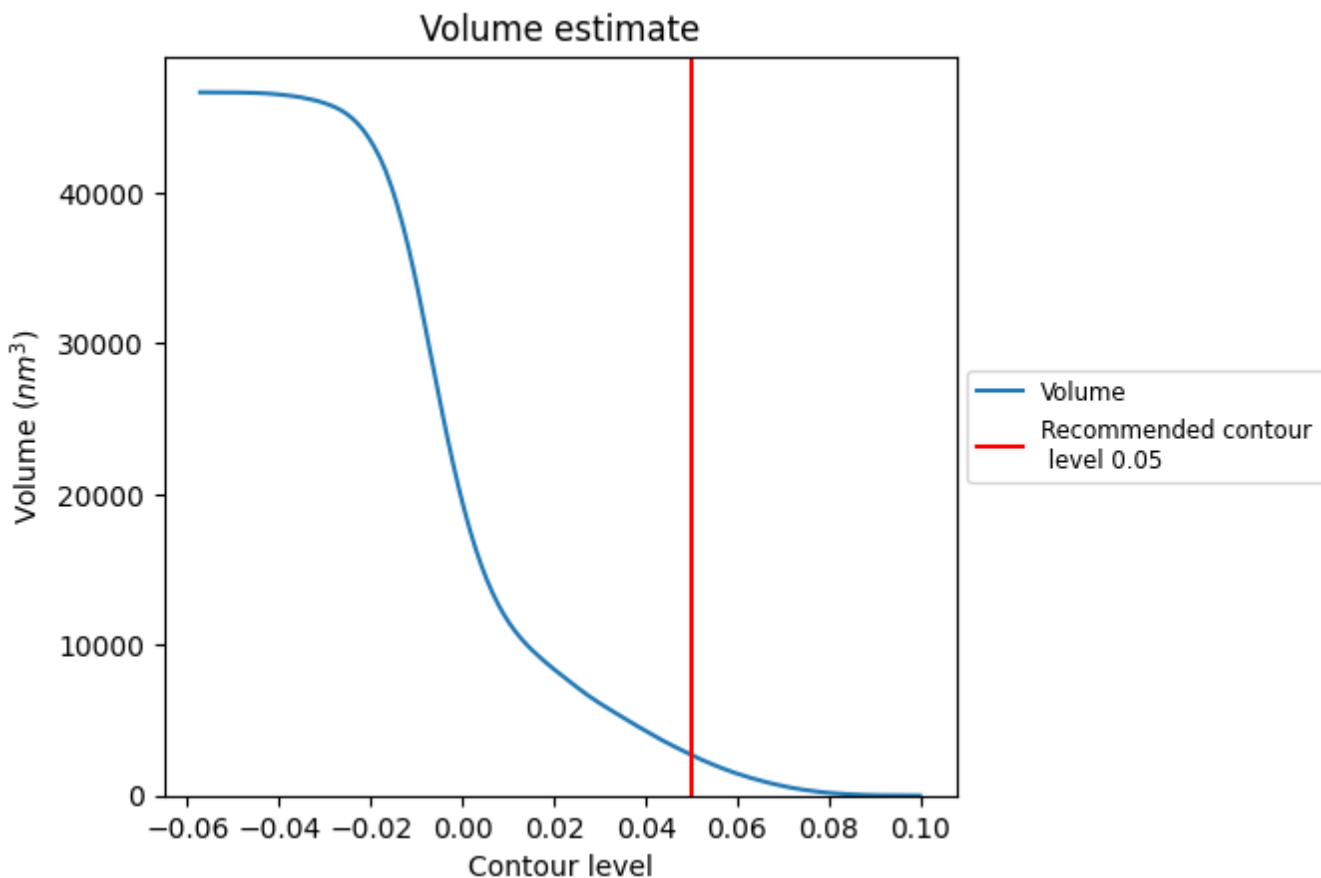
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

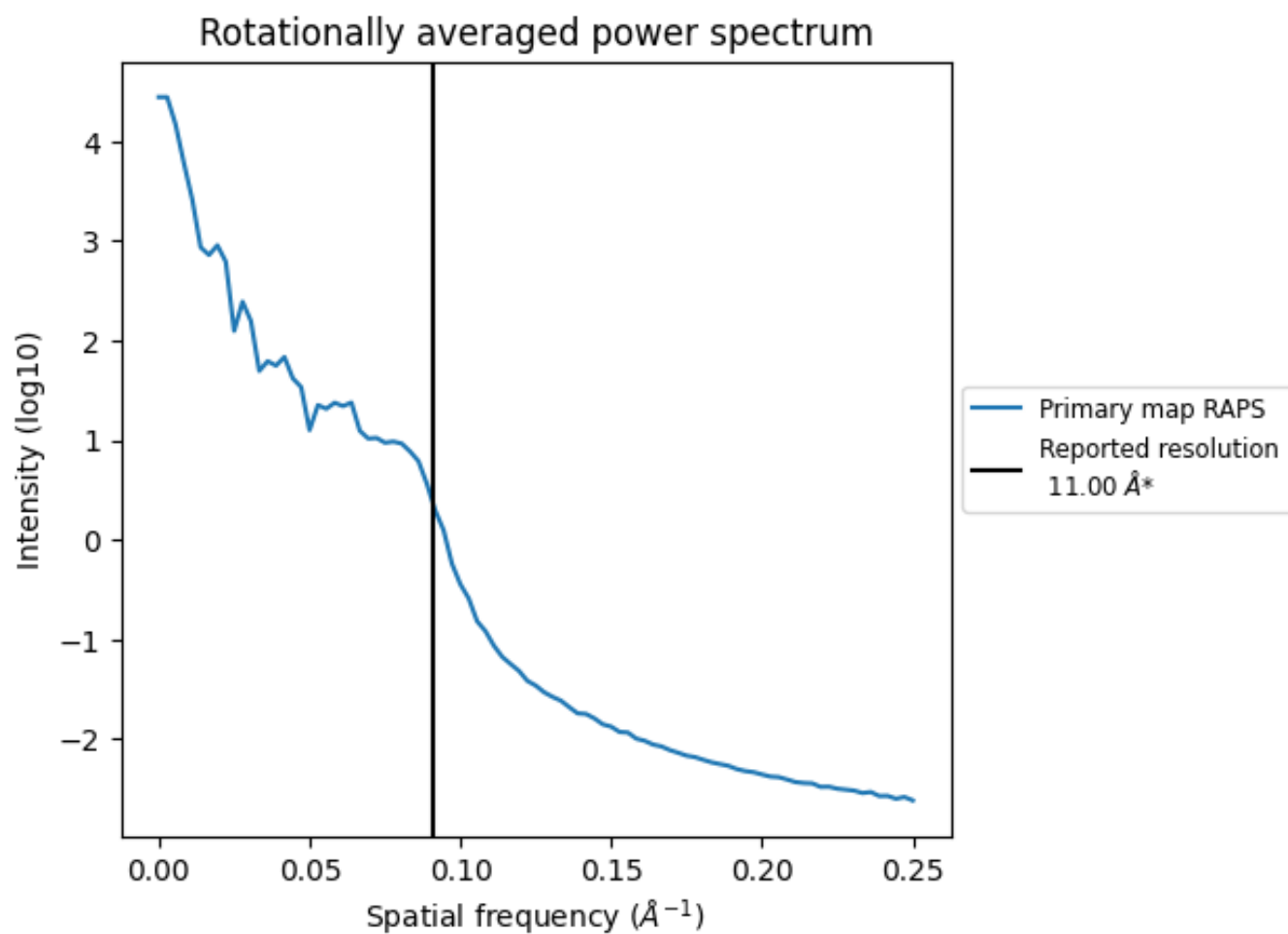
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2696 nm^3 ; this corresponds to an approximate mass of 2436 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.091\AA^{-1}

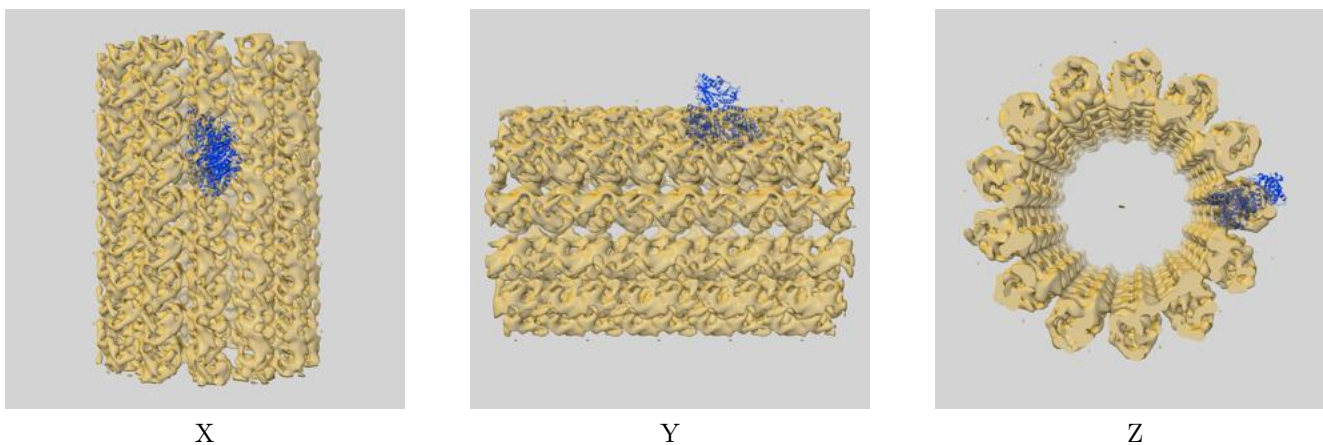
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

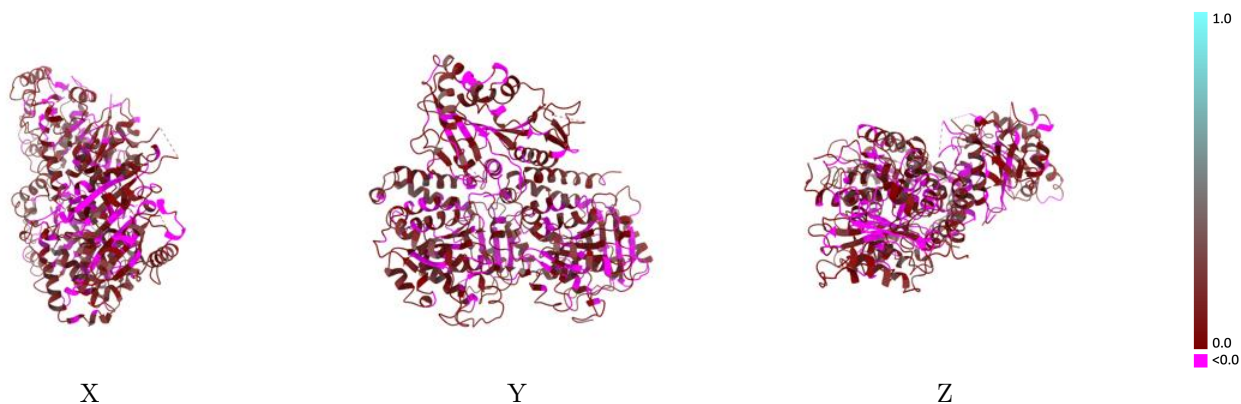
This section contains information regarding the fit between EMDB map EMD-5038 and PDB model 3DCO. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



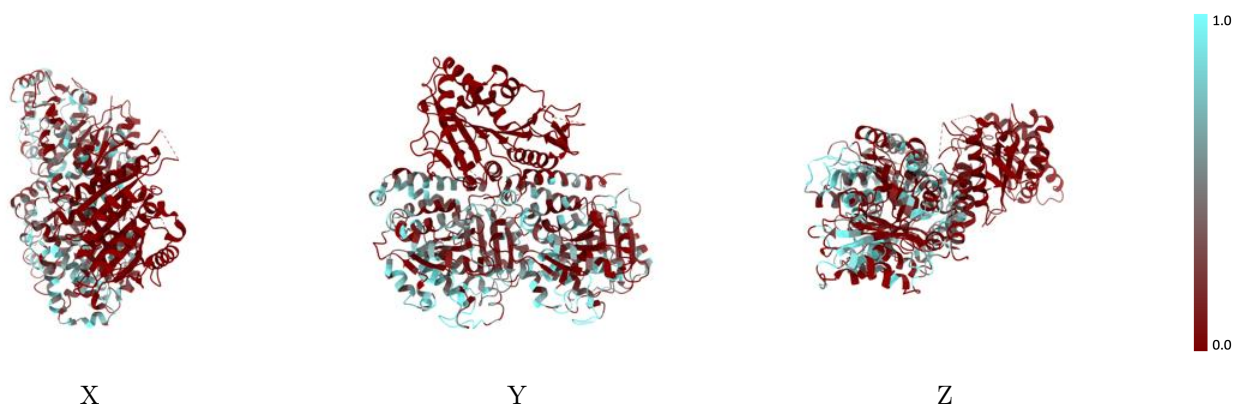
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



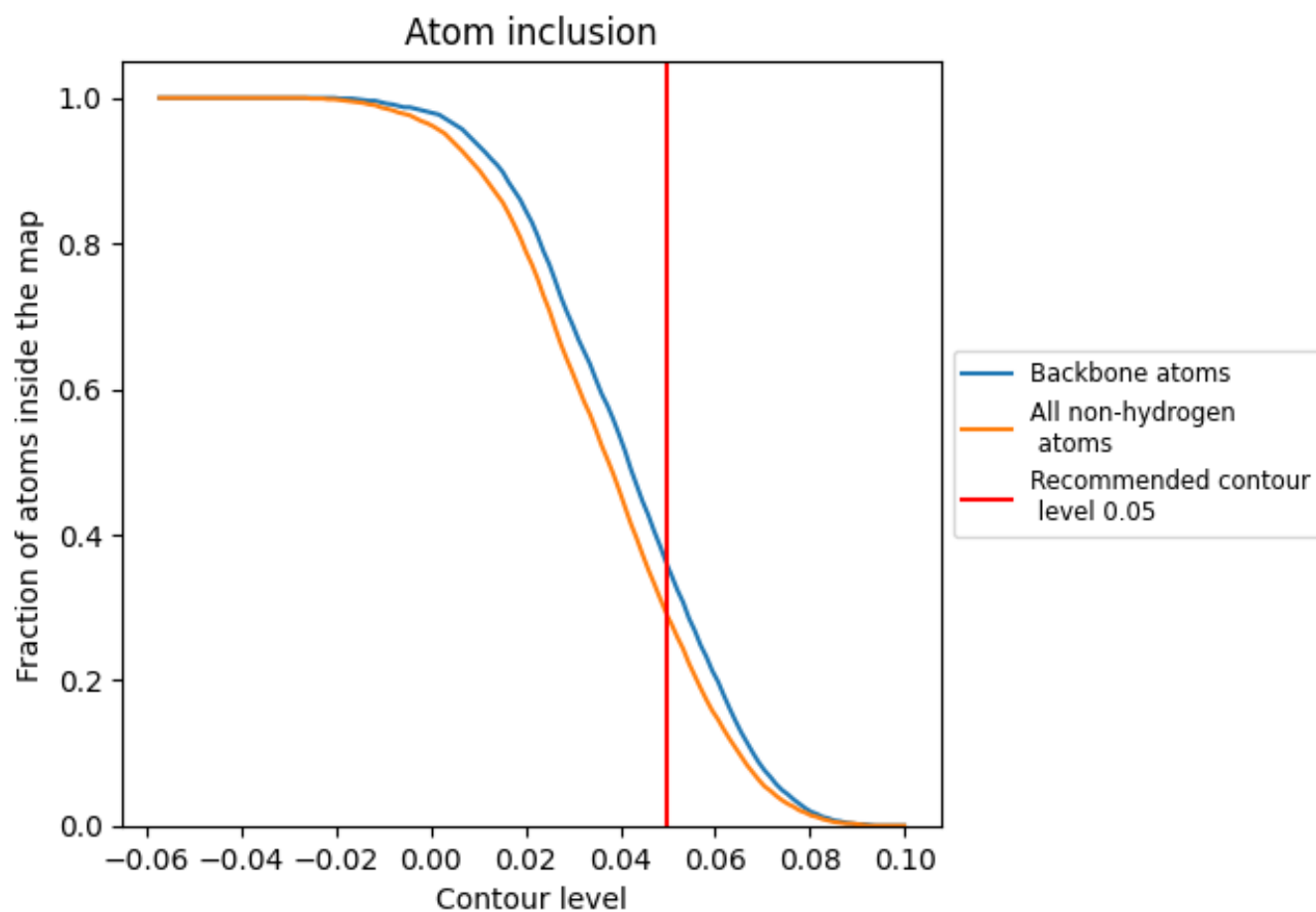
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).









9.4 Atom inclusion [i](#)



At the recommended contour level, 36% of all backbone atoms, 29% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2870	 0.0740
A	 0.3520	 0.0780
B	 0.4140	 0.0840
N	 0.0020	 0.0530

