



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:35 PM UTC

PDB ID : 8XL7 / pdb_00008xl7
EMDB ID : EMD-38440
Title : Structure of human 3-methylcrotonyl-CoA carboxylase in complex with acetyl-CoA (MCC-ACO)
Authors : Zhou, F.Y.; Zhang, Y.Y.; Zhou, Q.; Hu, Q.
Deposited on : 2023-12-25
Resolution : 2.85 Å(reported)

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:

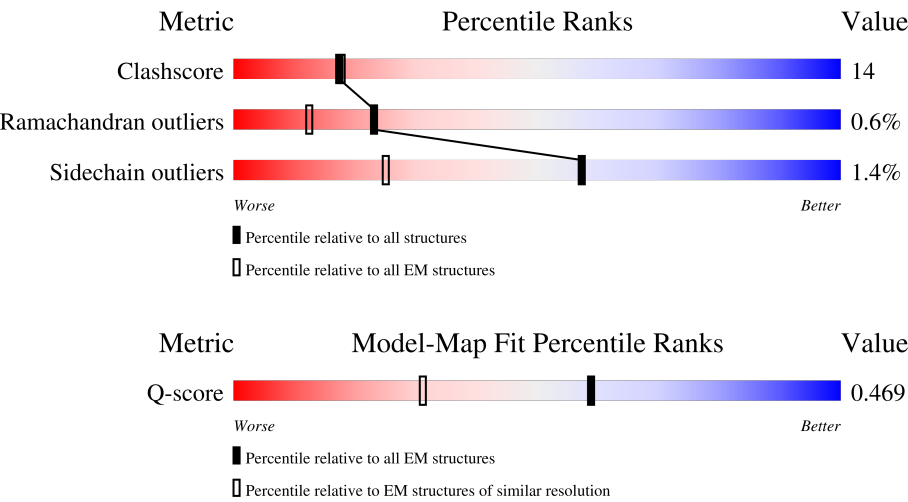
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.85 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11965 (2.35 - 3.35)

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	A	725	9% 24% 71%
1	C	725	8% 24% 71%
1	E	725	12% 24% 71%
1	G	725	36% 74% 6% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	725	
1	K	725	
2	B	563	
2	D	563	
2	F	563	
2	H	563	
2	J	563	
2	L	563	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BTN	A	801	-	-	X	-
3	BTN	G	801	-	-	X	-
3	BTN	I	801	-	-	X	-
3	BTN	K	801	-	-	X	-
4	ACO	J	601	-	-	X	-
4	ACO	J	602	-	-	X	-
4	ACO	L	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 44314 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.

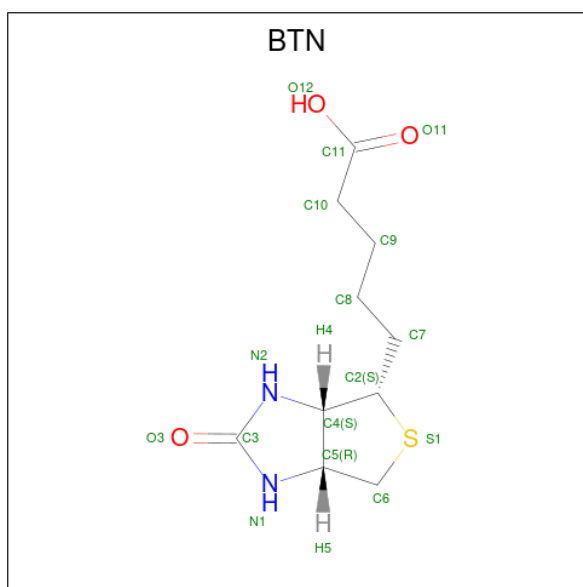
- Molecule 1 is a protein called Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	210	Total	C	N	O	S	0	0
			1615	1022	272	310	11		
1	C	210	Total	C	N	O	S	0	0
			1615	1022	272	310	11		
1	E	210	Total	C	N	O	S	0	0
			1615	1022	272	310	11		
1	G	584	Total	C	N	O	S	0	0
			4517	2847	789	852	29		
1	I	660	Total	C	N	O	S	0	0
			5121	3220	902	966	33		
1	K	584	Total	C	N	O	S	0	0
			4517	2847	789	852	29		

- Molecule 2 is a protein called Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial.

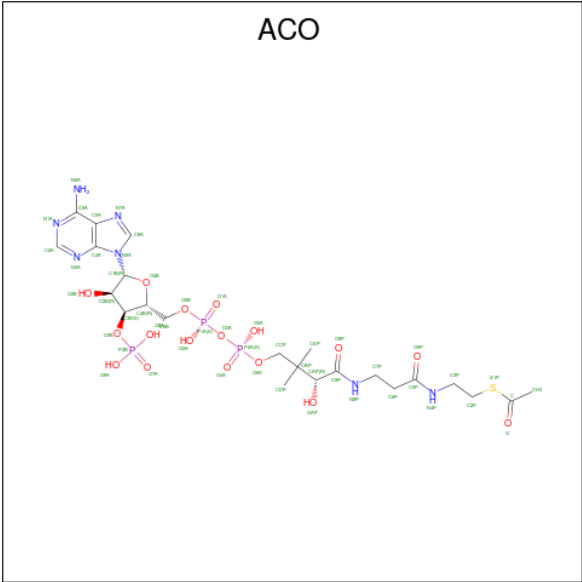
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	541	Total	C	N	O	S	0	0
			4153	2633	726	775	19		
2	D	541	Total	C	N	O	S	0	0
			4153	2633	726	775	19		
2	F	541	Total	C	N	O	S	0	0
			4153	2633	726	775	19		
2	H	541	Total	C	N	O	S	0	0
			4153	2633	726	775	19		
2	J	541	Total	C	N	O	S	0	0
			4153	2633	726	775	19		
2	L	541	Total	C	N	O	S	0	0
			4153	2633	726	775	19		

- Molecule 3 is BIOTIN (CCD ID: BTN) (formula: $C_{10}H_{16}N_2O_3S$) (labeled as "Ligand of Interest" by depositor).

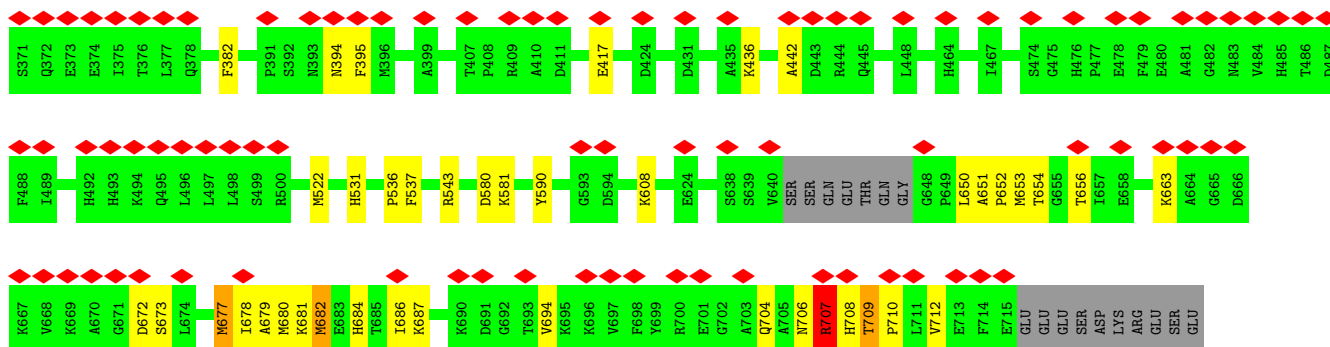


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	C	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	E	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	G	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	I	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	K	1	Total	C	N	O	S	0
			15	10	2	2	1	

- Molecule 4 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).

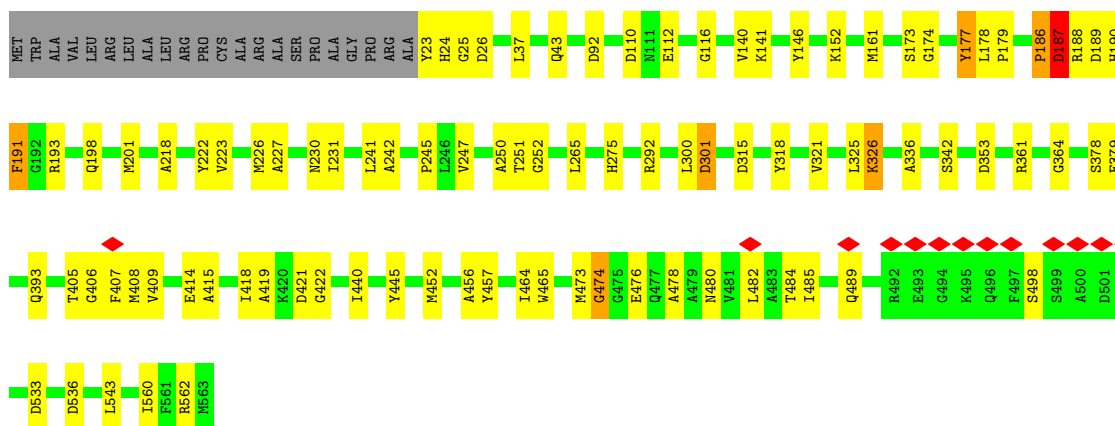


Mol	Chain	Residues	Atoms						AltConf
4	B	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
4	B	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
4	F	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
4	J	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
4	J	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
4	L	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	



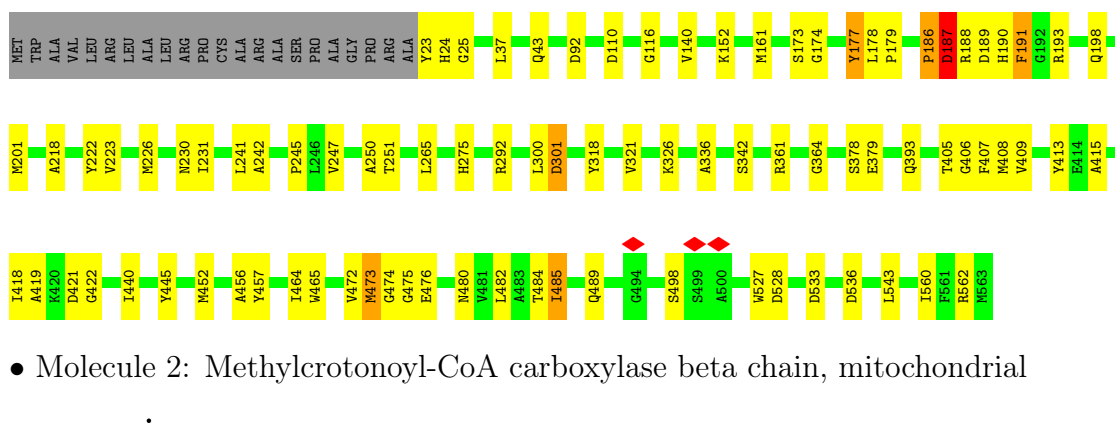
- Molecule 2: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

Chain B: 79% 16% ..



- Molecule 2: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

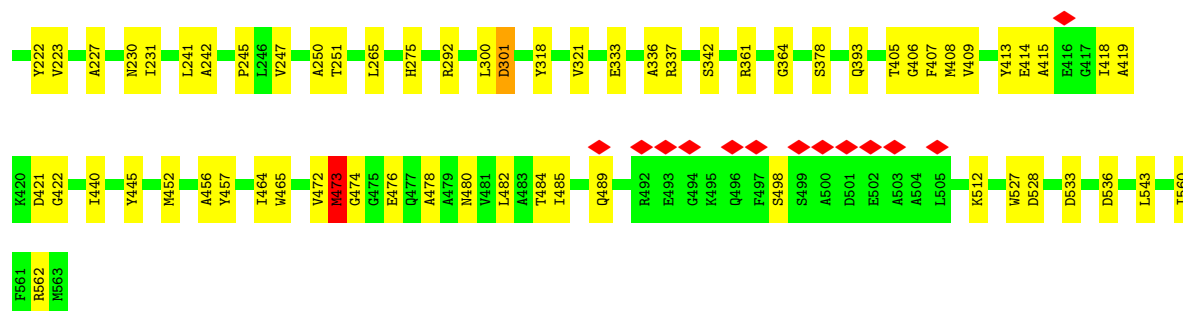
Chain D: 80% 14% ..



- Molecule 2: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

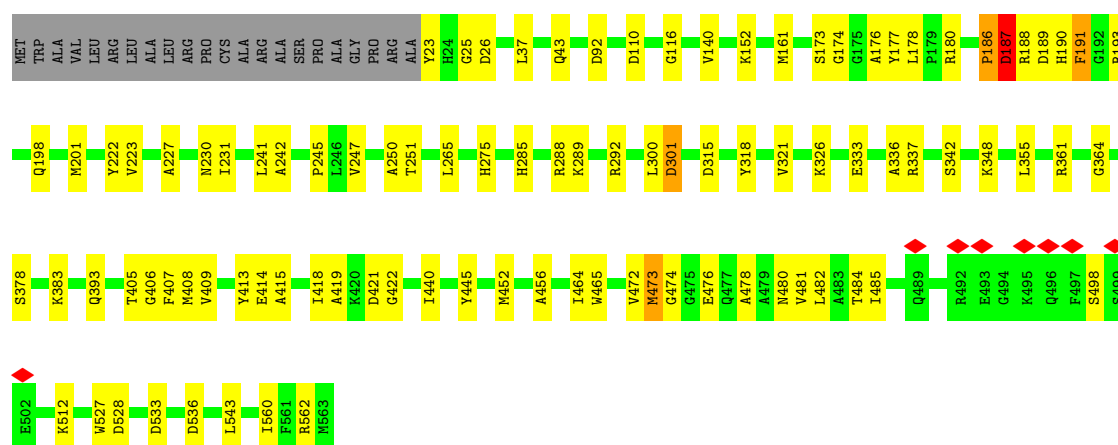
Chain F: 80% 15% ..





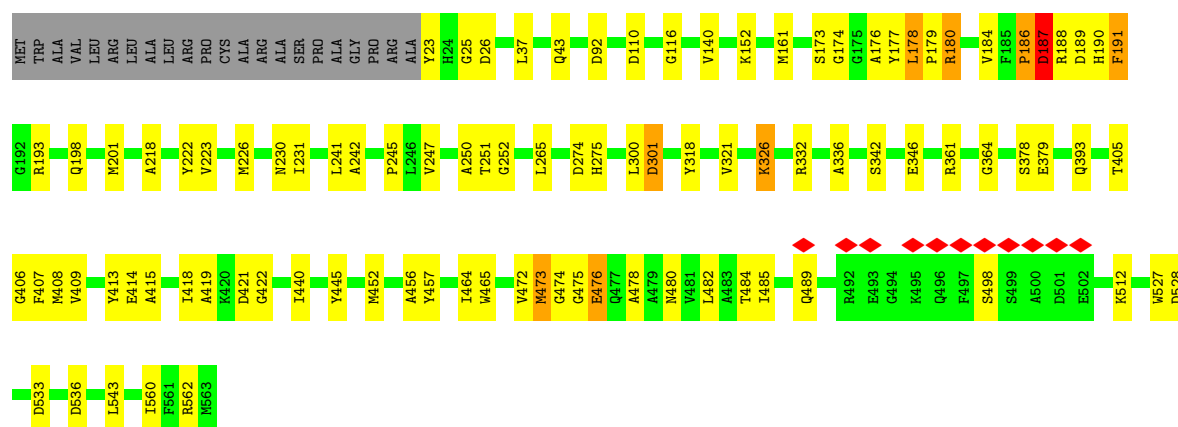
- Molecule 2: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

Chain H: 79% 16%



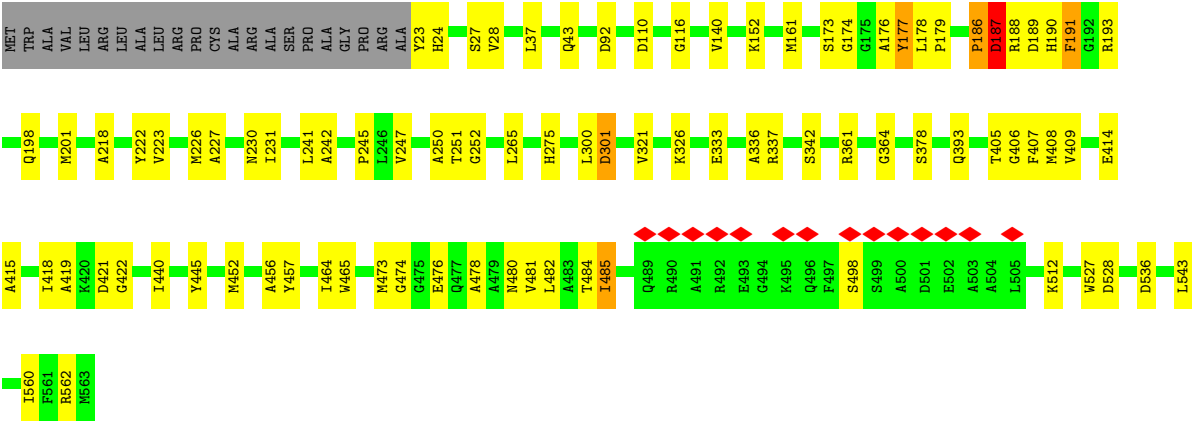
- Molecule 2: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

Chain J: 79% 16%



- Molecule 2: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

Chain L: 80% 15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117900	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.641	Depositor
Minimum map value	-2.441	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	517.104, 517.104, 517.104	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0773, 1.0773, 1.0773	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: ACO, BTN

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	0.47	0/1640	0.66	2/2205 (0.1%)
1	C	0.47	0/1640	0.66	2/2205 (0.1%)
1	E	0.47	0/1640	0.66	2/2205 (0.1%)
1	G	0.51	0/4602	0.67	7/6216 (0.1%)
1	I	0.52	0/5216	0.67	7/7036 (0.1%)
1	K	0.51	0/4602	0.67	7/6216 (0.1%)
2	B	0.63	0/4238	0.73	4/5731 (0.1%)
2	D	0.63	0/4238	0.72	4/5731 (0.1%)
2	F	0.63	0/4238	0.73	4/5731 (0.1%)
2	H	0.64	0/4238	0.73	3/5731 (0.1%)
2	J	0.64	0/4238	0.74	4/5731 (0.1%)
2	L	0.63	0/4238	0.73	4/5731 (0.1%)
All	All	0.58	0/44768	0.70	50/60469 (0.1%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	395	PHE	N-CA-C	8.89	123.96	111.52
1	I	395	PHE	N-CA-C	8.86	123.92	111.52
1	G	395	PHE	N-CA-C	8.83	123.88	111.52
1	I	394	ASN	CA-C-N	6.30	131.10	122.34
1	I	394	ASN	C-N-CA	6.30	131.10	122.34
1	G	394	ASN	CA-C-N	6.30	131.09	122.34
1	G	394	ASN	C-N-CA	6.30	131.09	122.34
1	K	394	ASN	CA-C-N	6.28	131.07	122.34
1	K	394	ASN	C-N-CA	6.28	131.07	122.34
2	D	191	PHE	N-CA-C	5.93	123.43	110.80
2	L	191	PHE	N-CA-C	5.92	123.42	110.80
2	F	191	PHE	N-CA-C	5.92	123.41	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	191	PHE	N-CA-C	5.92	123.40	110.80
2	B	191	PHE	N-CA-C	5.91	123.39	110.80
2	J	191	PHE	N-CA-C	5.91	123.39	110.80
2	H	177	TYR	N-CA-C	-5.70	99.60	108.90
2	F	457	TYR	CA-C-N	5.47	128.74	122.83
2	F	457	TYR	C-N-CA	5.47	128.74	122.83
2	J	457	TYR	CA-C-N	5.47	128.74	122.83
2	J	457	TYR	C-N-CA	5.47	128.74	122.83
2	L	457	TYR	CA-C-N	5.46	128.72	122.83
2	L	457	TYR	C-N-CA	5.46	128.72	122.83
2	B	457	TYR	CA-C-N	5.45	128.72	122.83
2	B	457	TYR	C-N-CA	5.45	128.72	122.83
2	D	457	TYR	CA-C-N	5.44	128.71	122.83
2	D	457	TYR	C-N-CA	5.44	128.71	122.83
1	G	394	ASN	O-C-N	5.40	129.06	122.58
1	K	394	ASN	O-C-N	5.39	129.05	122.58
1	I	394	ASN	O-C-N	5.38	129.03	122.58
1	C	536	PRO	CA-C-N	5.33	131.72	121.54
1	C	536	PRO	C-N-CA	5.33	131.72	121.54
1	G	536	PRO	CA-C-N	5.33	131.72	121.54
1	G	536	PRO	C-N-CA	5.33	131.72	121.54
1	A	536	PRO	CA-C-N	5.33	131.72	121.54
1	A	536	PRO	C-N-CA	5.33	131.72	121.54
1	I	536	PRO	CA-C-N	5.32	131.71	121.54
1	I	536	PRO	C-N-CA	5.32	131.71	121.54
1	K	536	PRO	CA-C-N	5.32	131.70	121.54
1	K	536	PRO	C-N-CA	5.32	131.70	121.54
1	E	536	PRO	CA-C-N	5.31	131.69	121.54
1	E	536	PRO	C-N-CA	5.31	131.69	121.54
2	H	498	SER	N-CA-C	5.24	117.41	111.02
1	I	69	LYS	N-CA-C	-5.22	105.67	111.36
2	J	498	SER	N-CA-C	5.22	117.39	111.02
2	L	498	SER	N-CA-C	5.22	117.39	111.02
2	B	498	SER	N-CA-C	5.21	117.38	111.02
2	D	498	SER	N-CA-C	5.21	117.38	111.02
1	G	69	LYS	N-CA-C	-5.20	105.69	111.36
2	F	498	SER	N-CA-C	5.19	117.35	111.02
1	K	69	LYS	N-CA-C	-5.17	105.73	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1615	0	1645	81	0
1	C	1615	0	1645	78	0
1	E	1615	0	1645	80	0
1	G	4517	0	4533	88	0
1	I	5121	0	5133	94	0
1	K	4517	0	4533	101	0
2	B	4153	0	4130	207	0
2	D	4153	0	4130	198	0
2	F	4153	0	4130	204	0
2	H	4153	0	4130	212	0
2	J	4153	0	4130	210	0
2	L	4153	0	4130	220	0
3	A	15	0	15	8	0
3	C	15	0	15	6	0
3	E	15	0	15	5	0
3	G	15	0	15	8	0
3	I	15	0	15	9	0
3	K	15	0	15	7	0
4	B	102	0	68	27	0
4	F	51	0	34	17	0
4	J	102	0	68	55	0
4	L	51	0	34	24	0
All	All	44314	0	44208	1206	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 14.

All (1206) 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:C:680:MET:CE	2:F:406:GLY:HA3	1.42	1.49
1:A:680:MET:CE	2:D:406:GLY:HA3	1.41	1.46
2:J:406:GLY:HA3	1:K:680:MET:CE	1.48	1.43
2:D:407:PHE:CE2	2:J:241:LEU:HD13	1.54	1.42
1:G:680:MET:CE	2:L:406:GLY:HA3	1.49	1.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:GLY:HA3	1:E:680:MET:CE	1.48	1.40
2:B:241:LEU:HD13	2:H:407:PHE:CE2	1.57	1.38
2:H:406:GLY:HA3	1:I:680:MET:CE	1.52	1.38
2:H:408:MET:CE	1:I:653:MET:HG3	1.52	1.37
2:D:485:ILE:CD1	4:J:602:ACO:H71	1.54	1.36
1:A:653:MET:HG3	2:D:408:MET:CE	1.54	1.35
2:F:241:LEU:HD13	2:L:407:PHE:CE2	1.61	1.35
1:C:653:MET:HG3	2:F:408:MET:CE	1.57	1.35
2:D:241:LEU:HD13	2:J:407:PHE:CE2	1.60	1.34
2:H:408:MET:HE1	1:I:653:MET:CG	1.57	1.33
2:J:408:MET:CE	1:K:653:MET:HG3	1.60	1.31
2:B:407:PHE:CE2	2:H:241:LEU:HD13	1.63	1.31
1:A:653:MET:CG	2:D:408:MET:HE1	1.63	1.28
2:F:407:PHE:CE2	2:L:241:LEU:HD13	1.67	1.28
1:I:652:PRO:O	1:I:707:ARG:HG2	1.33	1.28
2:F:485:ILE:HD11	4:L:601:ACO:O9P	1.33	1.27
1:K:652:PRO:O	1:K:707:ARG:HG2	1.33	1.27
1:C:652:PRO:O	1:C:707:ARG:HG2	1.33	1.26
1:C:653:MET:CG	2:F:408:MET:HE1	1.66	1.25
1:G:707:ARG:HD3	1:G:708:HIS:N	1.52	1.25
2:B:408:MET:CE	1:E:653:MET:HG3	1.64	1.25
2:J:408:MET:HE1	1:K:653:MET:CG	1.67	1.24
1:E:707:ARG:HD3	1:E:708:HIS:N	1.52	1.24
1:A:707:ARG:HD3	1:A:708:HIS:N	1.52	1.24
1:G:653:MET:HG3	2:L:408:MET:CE	1.68	1.24
1:E:652:PRO:O	1:E:707:ARG:HG2	1.33	1.23
1:G:652:PRO:O	1:G:707:ARG:HG2	1.33	1.23
1:K:707:ARG:HD3	1:K:708:HIS:N	1.52	1.22
1:C:707:ARG:HD3	1:C:708:HIS:N	1.52	1.22
1:I:707:ARG:HD3	1:I:708:HIS:N	1.52	1.22
1:A:652:PRO:O	1:A:707:ARG:HG2	1.33	1.22
2:D:251:THR:HG23	2:J:409:VAL:CG2	1.72	1.19
4:B:601:ACO:H71	2:H:485:ILE:HD12	1.24	1.19
1:G:680:MET:HE1	2:L:406:GLY:HA3	1.19	1.18
2:F:241:LEU:CG	2:L:419:ALA:HB2	1.73	1.18
2:H:481:VAL:O	2:H:485:ILE:HG22	1.40	1.18
2:B:408:MET:HE1	1:E:653:MET:CG	1.73	1.17
2:B:409:VAL:CG2	2:H:251:THR:HG23	1.76	1.16
1:E:590:TYR:OH	1:E:608:LYS:HD3	1.46	1.16
2:D:407:PHE:HE2	2:J:241:LEU:CD1	1.59	1.16
2:F:251:THR:HG23	2:L:409:VAL:CG2	1.74	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:251:THR:CG2	2:J:409:VAL:CG2	2.24	1.15
1:G:653:MET:CG	2:L:408:MET:HE1	1.76	1.15
1:I:590:TYR:OH	1:I:608:LYS:HD3	1.46	1.15
1:A:590:TYR:OH	1:A:608:LYS:HD3	1.46	1.14
2:D:409:VAL:CG2	2:J:251:THR:HG23	1.76	1.14
2:D:485:ILE:HD12	4:J:602:ACO:C7P	1.77	1.14
1:G:590:TYR:OH	1:G:608:LYS:HD3	1.46	1.14
1:C:680:MET:HE3	2:F:406:GLY:HA3	1.29	1.14
2:B:419:ALA:HB2	2:H:241:LEU:CG	1.78	1.13
2:H:408:MET:SD	1:I:653:MET:SD	2.47	1.13
1:C:590:TYR:OH	1:C:608:LYS:HD3	1.46	1.13
1:K:590:TYR:OH	1:K:608:LYS:HD3	1.46	1.12
2:D:241:LEU:CG	2:J:419:ALA:HB2	1.78	1.12
2:B:251:THR:HG23	2:H:409:VAL:CG2	1.78	1.12
2:F:419:ALA:HB2	2:L:241:LEU:CG	1.78	1.12
1:A:707:ARG:HD3	1:A:708:HIS:H	0.96	1.12
1:G:680:MET:HE3	2:L:406:GLY:HA3	1.30	1.12
1:K:707:ARG:HD3	1:K:708:HIS:H	0.96	1.11
2:D:485:ILE:CD1	4:J:602:ACO:C7P	2.28	1.11
2:J:406:GLY:HA3	1:K:680:MET:HE1	1.13	1.11
1:A:653:MET:SD	2:D:408:MET:SD	2.49	1.11
1:C:653:MET:SD	2:F:408:MET:SD	2.49	1.10
2:B:178:LEU:CD2	2:H:478:ALA:HB1	1.80	1.10
2:D:409:VAL:CG2	2:J:251:THR:CG2	2.30	1.10
2:B:409:VAL:CG2	2:H:251:THR:CG2	2.29	1.10
2:F:409:VAL:CG2	2:L:251:THR:HG23	1.79	1.10
1:I:707:ARG:HD3	1:I:708:HIS:H	0.96	1.10
2:B:241:LEU:CG	2:H:419:ALA:HB2	1.81	1.09
2:B:241:LEU:CD1	2:H:407:PHE:HE2	1.64	1.09
1:G:707:ARG:HD3	1:G:708:HIS:H	0.96	1.09
2:B:406:GLY:HA3	1:E:680:MET:HE1	1.14	1.09
2:D:251:THR:CG2	2:J:409:VAL:HG23	1.82	1.09
2:D:485:ILE:HD12	4:J:602:ACO:H71	1.11	1.09
2:H:406:GLY:HA3	1:I:680:MET:HE1	1.19	1.09
2:D:419:ALA:HB2	2:J:241:LEU:CG	1.83	1.08
1:E:707:ARG:HD3	1:E:708:HIS:H	0.96	1.08
2:F:485:ILE:CD1	4:L:601:ACO:H71	1.82	1.08
1:G:653:MET:HG3	2:L:408:MET:HE1	1.21	1.08
1:A:680:MET:HE3	2:D:406:GLY:HA3	1.30	1.08
1:C:653:MET:HG3	2:F:408:MET:HE1	1.09	1.08
2:H:474:GLY:H	1:I:681:LYS:NZ	1.52	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:408:MET:HE1	1:E:653:MET:HG3	1.15	1.08
2:J:408:MET:HE1	1:K:653:MET:HG3	1.08	1.08
2:D:241:LEU:CD1	2:J:407:PHE:HE2	1.65	1.08
2:F:251:THR:CG2	2:L:409:VAL:CG2	2.31	1.08
2:F:178:LEU:CD2	2:L:478:ALA:HB1	1.83	1.07
2:F:251:THR:CG2	2:L:409:VAL:HG23	1.84	1.07
4:F:601:ACO:HH32	2:L:473:MET:HE1	1.29	1.07
2:B:251:THR:CG2	2:H:409:VAL:CG2	2.33	1.06
2:B:409:VAL:HG23	2:H:251:THR:CG2	1.85	1.06
2:F:409:VAL:CG2	2:L:251:THR:CG2	2.32	1.06
1:K:257:GLU:HG2	1:K:322:GLU:HG3	1.36	1.06
1:A:680:MET:HE1	2:D:406:GLY:HA3	1.07	1.06
2:B:406:GLY:HA3	1:E:680:MET:HE3	1.32	1.06
1:C:707:ARG:HD3	1:C:708:HIS:H	0.96	1.06
2:B:407:PHE:HE2	2:H:241:LEU:CD1	1.68	1.06
2:F:241:LEU:CD1	2:L:407:PHE:HE2	1.67	1.05
2:F:409:VAL:HG23	2:L:251:THR:CG2	1.85	1.05
2:J:408:MET:SD	1:K:653:MET:SD	2.54	1.05
2:B:408:MET:SD	1:E:653:MET:SD	2.55	1.05
1:G:653:MET:SD	2:L:408:MET:SD	2.54	1.05
2:J:406:GLY:HA3	1:K:680:MET:HE3	1.35	1.04
2:H:406:GLY:HA3	1:I:680:MET:HE3	1.37	1.04
1:I:257:GLU:HG2	1:I:322:GLU:HG3	1.37	1.04
1:A:680:MET:CE	2:D:406:GLY:CA	2.35	1.04
2:B:178:LEU:HD21	2:H:478:ALA:CB	1.87	1.04
2:J:474:GLY:H	1:K:681:LYS:NZ	1.53	1.04
2:B:419:ALA:HB2	2:H:241:LEU:HG	1.39	1.04
2:D:485:ILE:HD13	4:J:602:ACO:H61	1.40	1.04
1:G:257:GLU:HG2	1:G:322:GLU:HG3	1.37	1.03
2:D:419:ALA:HB2	2:J:241:LEU:HG	1.40	1.03
1:A:653:MET:HG3	2:D:408:MET:HE1	1.06	1.03
1:C:680:MET:HE1	2:F:406:GLY:HA3	1.10	1.03
4:F:601:ACO:HH32	2:L:473:MET:CE	1.88	1.03
2:D:241:LEU:HG	2:J:419:ALA:HB2	1.36	1.02
2:F:178:LEU:HD21	2:L:478:ALA:CB	1.88	1.02
2:F:241:LEU:HG	2:L:419:ALA:HB2	1.36	1.02
1:A:680:MET:HE1	2:D:406:GLY:CA	1.88	1.02
2:B:241:LEU:HG	2:H:419:ALA:HB2	1.41	1.02
1:C:680:MET:CE	2:F:406:GLY:CA	2.37	1.02
2:F:485:ILE:HD12	4:L:601:ACO:H71	1.03	1.02
2:D:407:PHE:CE2	2:J:241:LEU:CD1	2.39	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:THR:CG2	2:H:409:VAL:HG23	1.91	1.01
2:D:178:LEU:CD2	2:J:478:ALA:HB1	1.90	1.01
1:C:680:MET:HE1	2:F:406:GLY:CA	1.90	1.01
2:D:178:LEU:HD21	2:J:478:ALA:HB1	1.05	1.00
2:D:409:VAL:HG23	2:J:251:THR:CG2	1.89	1.00
2:F:241:LEU:HD21	2:L:419:ALA:CB	1.90	1.00
2:F:407:PHE:HE2	2:L:241:LEU:CD1	1.73	1.00
2:F:478:ALA:HB1	2:L:178:LEU:HD21	1.01	1.00
4:F:601:ACO:HH31	2:L:473:MET:HE2	1.40	1.00
2:F:478:ALA:HB1	2:L:178:LEU:CD2	1.89	1.00
2:F:419:ALA:HB2	2:L:241:LEU:HG	1.42	1.00
2:H:408:MET:HE1	1:I:653:MET:HG3	1.03	0.99
2:F:241:LEU:CD2	2:L:419:ALA:HB2	1.90	0.99
2:D:407:PHE:CD2	2:J:241:LEU:HD13	1.97	0.99
4:B:601:ACO:C7P	2:H:485:ILE:HD12	1.92	0.99
2:D:251:THR:HG21	2:J:409:VAL:HG23	1.44	0.99
4:F:601:ACO:CH3	2:L:473:MET:CE	2.39	0.99
2:F:419:ALA:CB	2:L:241:LEU:HD21	1.94	0.98
2:J:177:TYR:HD2	2:J:180:ARG:HG3	1.27	0.98
2:B:245:PRO:HB3	2:H:484:THR:HG21	1.45	0.98
2:B:406:GLY:CA	1:E:680:MET:CE	2.41	0.98
4:J:601:ACO:H21	4:J:601:ACO:H61A	1.29	0.98
2:D:485:ILE:HD11	4:J:602:ACO:H71	1.46	0.98
2:F:478:ALA:CB	2:L:178:LEU:HD21	1.94	0.98
2:B:406:GLY:CA	1:E:680:MET:HE1	1.94	0.97
3:G:801:BTN:O3	2:L:407:PHE:HB2	1.65	0.97
1:A:682:MET:CG	2:D:405:THR:HG21	1.95	0.97
1:G:361:ARG:HH22	1:K:442:ALA:HB3	1.30	0.97
2:J:406:GLY:CA	1:K:680:MET:HE1	1.94	0.96
1:C:682:MET:CG	2:F:405:THR:HG21	1.95	0.96
2:D:409:VAL:HG12	2:J:242:ALA:HB2	1.46	0.96
2:F:407:PHE:HE2	2:L:241:LEU:HD13	1.05	0.96
2:J:406:GLY:CA	1:K:680:MET:CE	2.42	0.96
2:B:241:LEU:HD13	2:H:407:PHE:CD2	2.00	0.96
2:J:177:TYR:CD2	2:J:180:ARG:HG3	1.99	0.96
2:B:241:LEU:CD1	2:H:407:PHE:CE2	2.43	0.96
1:G:680:MET:CE	2:L:406:GLY:CA	2.43	0.96
1:I:442:ALA:HB3	1:K:361:ARG:HH22	1.28	0.96
2:F:419:ALA:HB2	2:L:241:LEU:CD2	1.95	0.96
4:B:601:ACO:H71	2:H:485:ILE:CD1	1.95	0.95
4:B:602:ACO:HH33	2:H:178:LEU:HD11	1.48	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:ALA:HB1	1:I:680:MET:HG3	1.46	0.95
1:A:707:ARG:HD2	1:A:708:HIS:ND1	1.82	0.95
2:F:485:ILE:HD12	4:L:601:ACO:C7P	1.96	0.95
4:B:602:ACO:HH33	2:H:178:LEU:CD1	1.96	0.95
2:B:178:LEU:HD21	2:H:478:ALA:HB1	0.96	0.95
1:C:707:ARG:HD2	1:C:708:HIS:ND1	1.82	0.95
1:G:707:ARG:HD2	1:G:708:HIS:ND1	1.82	0.95
1:G:680:MET:HE1	2:L:406:GLY:CA	1.97	0.94
4:B:602:ACO:CH3	2:H:178:LEU:CD1	2.45	0.94
1:E:707:ARG:HD2	1:E:708:HIS:ND1	1.82	0.94
2:D:241:LEU:CD1	2:J:407:PHE:CE2	2.45	0.94
2:H:405:THR:HG21	1:I:682:MET:HG2	1.48	0.94
2:D:484:THR:HG21	2:J:245:PRO:HB3	1.46	0.94
2:B:242:ALA:HB2	2:H:409:VAL:HG12	1.44	0.94
1:K:707:ARG:HD2	1:K:708:HIS:ND1	1.82	0.94
2:B:419:ALA:CB	2:H:241:LEU:HD21	1.97	0.94
1:C:682:MET:HG2	2:F:405:THR:HG21	1.47	0.93
2:B:407:PHE:HE2	2:H:241:LEU:HD13	1.00	0.93
1:I:707:ARG:HD2	1:I:708:HIS:ND1	1.82	0.93
2:J:405:THR:HG21	1:K:682:MET:CG	1.99	0.93
2:B:484:THR:HG21	2:H:245:PRO:HB3	1.48	0.93
1:A:682:MET:HG2	2:D:405:THR:HG21	1.47	0.93
2:F:178:LEU:HD21	2:L:478:ALA:HB1	0.94	0.93
2:F:484:THR:HG21	2:L:245:PRO:HB3	1.51	0.93
2:B:409:VAL:HG23	2:H:251:THR:HG21	1.50	0.93
2:B:241:LEU:HD21	2:H:419:ALA:CB	1.99	0.92
2:B:241:LEU:CD2	2:H:419:ALA:HB2	2.00	0.92
2:B:419:ALA:HB2	2:H:241:LEU:CD2	1.98	0.92
2:D:178:LEU:HD21	2:J:478:ALA:CB	1.97	0.92
4:F:601:ACO:CH3	2:L:473:MET:HE2	1.96	0.92
2:F:409:VAL:HG23	2:L:251:THR:HG21	1.50	0.92
2:J:485:ILE:HD11	4:J:601:ACO:H143	1.49	0.92
2:F:242:ALA:HB2	2:L:409:VAL:HG12	1.50	0.92
2:D:409:VAL:HG23	2:J:251:THR:HG21	1.51	0.92
2:D:485:ILE:CD1	4:J:602:ACO:C6P	2.47	0.92
2:F:445:TYR:CD1	2:F:473:MET:O	2.23	0.92
2:D:241:LEU:HD13	2:J:407:PHE:CD2	2.04	0.91
2:J:405:THR:HG21	1:K:682:MET:HG2	1.50	0.91
2:H:406:GLY:CA	1:I:680:MET:CE	2.47	0.91
1:C:681:LYS:HB3	2:F:405:THR:HB	1.52	0.91
2:B:485:ILE:HD12	4:B:602:ACO:H62	1.50	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:681:LYS:HB3	2:L:405:THR:HB	1.53	0.91
2:B:407:PHE:CD2	2:H:241:LEU:HD13	2.06	0.91
1:I:442:ALA:HB3	1:K:361:ARG:NH2	1.86	0.91
4:B:602:ACO:CH3	2:H:178:LEU:HD11	2.01	0.90
1:A:681:LYS:HB3	2:D:405:THR:HB	1.53	0.90
2:B:409:VAL:HG12	2:H:242:ALA:HB2	1.51	0.90
2:D:187:ASP:HB2	2:D:190:HIS:CE1	2.07	0.90
2:D:489:GLN:NE2	4:J:602:ACO:H51A	1.86	0.90
2:B:407:PHE:HB2	3:E:801:BTN:O3	1.71	0.90
2:B:405:THR:HB	1:E:681:LYS:HB3	1.54	0.90
2:H:406:GLY:CA	1:I:680:MET:HE1	2.01	0.90
2:L:187:ASP:HB2	2:L:190:HIS:CE1	2.07	0.90
2:D:245:PRO:HB3	2:J:484:THR:HG21	1.51	0.89
2:H:187:ASP:HB2	2:H:190:HIS:CE1	2.07	0.89
2:D:251:THR:HG23	2:J:409:VAL:HG21	1.52	0.89
2:B:187:ASP:HB2	2:B:190:HIS:CE1	2.07	0.89
2:D:241:LEU:HD21	2:J:419:ALA:CB	2.01	0.89
2:D:241:LEU:CD2	2:J:419:ALA:HB2	2.02	0.89
2:J:187:ASP:HB2	2:J:190:HIS:CE1	2.07	0.89
2:H:405:THR:HG21	1:I:682:MET:CG	2.02	0.89
2:D:484:THR:CG2	2:J:245:PRO:HB3	2.02	0.89
2:F:187:ASP:HB2	2:F:190:HIS:CE1	2.07	0.89
2:F:409:VAL:HG12	2:L:242:ALA:HB2	1.54	0.89
2:F:241:LEU:HD13	2:L:407:PHE:CD2	2.07	0.89
2:F:407:PHE:CD2	2:L:241:LEU:HD13	2.08	0.88
2:D:419:ALA:CB	2:J:241:LEU:HD21	2.04	0.88
1:C:653:MET:CG	2:F:408:MET:CE	2.37	0.88
2:B:405:THR:HG21	1:E:682:MET:CG	2.03	0.88
4:F:601:ACO:CH3	2:L:473:MET:HE1	2.04	0.88
1:A:653:MET:CG	2:D:408:MET:CE	2.36	0.88
2:B:245:PRO:HB3	2:H:484:THR:CG2	2.03	0.88
2:D:242:ALA:HB2	2:J:409:VAL:HG12	1.54	0.88
2:D:241:LEU:HD13	2:J:407:PHE:HE2	0.98	0.88
1:G:361:ARG:NH2	1:K:442:ALA:HB3	1.89	0.87
2:B:407:PHE:CE2	2:H:241:LEU:CD1	2.48	0.87
2:D:409:VAL:HG21	2:J:251:THR:HG23	1.56	0.87
2:D:419:ALA:HB2	2:J:241:LEU:CD2	2.04	0.87
2:D:245:PRO:HB3	2:J:484:THR:CG2	2.04	0.87
2:F:251:THR:HG21	2:L:409:VAL:HG23	1.53	0.87
2:F:241:LEU:HD13	2:L:407:PHE:HE2	0.97	0.87
2:B:484:THR:CG2	2:H:245:PRO:HB3	2.04	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:590:TYR:HH	1:C:608:LYS:HD3	1.38	0.86
2:F:489:GLN:NE2	4:L:601:ACO:H52A	1.90	0.86
1:I:590:TYR:HH	1:I:608:LYS:HD3	1.38	0.86
2:B:179:PRO:HA	2:H:512:LYS:HE2	1.55	0.86
2:F:230:ASN:ND2	2:L:562:ARG:HH12	1.72	0.86
1:G:707:ARG:HD2	1:G:708:HIS:CE1	2.11	0.86
1:G:707:ARG:HD2	1:G:708:HIS:CG	2.11	0.86
2:J:405:THR:HB	1:K:681:LYS:HB3	1.58	0.86
1:A:707:ARG:HD2	1:A:708:HIS:CE1	2.11	0.85
2:B:251:THR:HG21	2:H:409:VAL:HG23	1.55	0.85
1:E:707:ARG:HD2	1:E:708:HIS:CG	2.11	0.85
2:H:408:MET:CE	1:I:653:MET:CG	2.32	0.85
1:I:707:ARG:HD2	1:I:708:HIS:CE1	2.11	0.85
2:B:405:THR:HG21	1:E:682:MET:HG2	1.57	0.85
1:E:590:TYR:OH	1:E:608:LYS:CD	2.25	0.85
1:G:682:MET:CG	2:L:405:THR:HG21	2.06	0.85
1:C:707:ARG:HD2	1:C:708:HIS:CE1	2.11	0.85
2:H:481:VAL:O	2:H:485:ILE:CG2	2.24	0.85
1:E:707:ARG:HD2	1:E:708:HIS:CE1	2.11	0.85
1:I:707:ARG:HD2	1:I:708:HIS:CG	2.11	0.85
2:F:484:THR:CG2	2:L:245:PRO:HB3	2.06	0.85
1:I:590:TYR:OH	1:I:608:LYS:CD	2.25	0.85
2:J:408:MET:CE	1:K:653:MET:CG	2.40	0.85
2:B:409:VAL:HG21	2:H:251:THR:HG23	1.58	0.85
2:F:245:PRO:HB3	2:L:484:THR:HG21	1.57	0.85
1:A:707:ARG:HD2	1:A:708:HIS:CG	2.11	0.84
1:G:442:ALA:HB3	1:I:361:ARG:HH22	1.42	0.84
2:J:473:MET:HE1	4:J:601:ACO:CH3	2.07	0.84
1:C:707:ARG:HD2	1:C:708:HIS:CG	2.11	0.84
1:K:707:ARG:HD2	1:K:708:HIS:CE1	2.11	0.84
1:A:590:TYR:OH	1:A:608:LYS:CD	2.25	0.84
3:C:801:BTN:O3	2:F:407:PHE:HB2	1.77	0.84
2:D:409:VAL:HG12	2:J:242:ALA:CB	2.07	0.84
2:D:489:GLN:HE21	4:J:602:ACO:H51A	1.37	0.84
1:K:590:TYR:OH	1:K:608:LYS:CD	2.24	0.84
1:G:590:TYR:HH	1:G:608:LYS:HD3	1.40	0.84
1:A:590:TYR:HH	1:A:608:LYS:HD3	1.39	0.84
2:F:241:LEU:HD11	2:L:419:ALA:CA	2.08	0.84
1:C:590:TYR:OH	1:C:608:LYS:CD	2.25	0.84
2:D:409:VAL:HB	2:J:247:VAL:HG12	1.60	0.84
2:H:405:THR:HB	1:I:681:LYS:HB3	1.60	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:407:PHE:HB2	3:K:801:BTN:O3	1.76	0.83
2:B:242:ALA:CB	2:H:409:VAL:HG12	2.07	0.83
1:E:590:TYR:HH	1:E:608:LYS:HD3	1.38	0.83
1:K:707:ARG:HD2	1:K:708:HIS:CG	2.11	0.83
1:G:590:TYR:OH	1:G:608:LYS:CD	2.25	0.83
1:A:680:MET:HG3	2:J:250:ALA:HB1	1.60	0.83
2:F:409:VAL:HG21	2:L:251:THR:HG23	1.60	0.83
2:J:474:GLY:N	1:K:681:LYS:NZ	2.26	0.83
2:B:251:THR:HG23	2:H:409:VAL:HG21	1.61	0.83
3:G:801:BTN:O3	2:L:407:PHE:CB	2.26	0.83
2:F:485:ILE:CD1	4:L:601:ACO:O9P	2.24	0.82
2:F:251:THR:HG23	2:L:409:VAL:HG21	1.60	0.82
2:F:241:LEU:HD21	2:L:419:ALA:HB1	1.60	0.82
2:H:408:MET:HE2	1:I:653:MET:HG3	1.61	0.82
2:D:485:ILE:CD1	4:J:602:ACO:H61	2.09	0.82
4:F:601:ACO:O1A	4:F:601:ACO:H122	1.78	0.82
1:G:682:MET:HG2	2:L:405:THR:HG21	1.59	0.82
2:H:407:PHE:HB2	3:I:801:BTN:O3	1.79	0.82
2:L:174:GLY:HA2	4:L:601:ACO:CEP	2.10	0.81
2:F:251:THR:HG23	2:L:409:VAL:HG23	1.49	0.81
2:B:247:VAL:HG12	2:H:409:VAL:HB	1.62	0.81
2:B:408:MET:CE	1:E:653:MET:CG	2.44	0.81
3:A:801:BTN:O3	2:D:407:PHE:HB2	1.80	0.81
2:J:473:MET:HE1	4:J:601:ACO:HH31	1.63	0.80
2:D:179:PRO:HA	2:J:512:LYS:HE2	1.63	0.80
2:D:241:LEU:HD11	2:J:419:ALA:CA	2.11	0.80
2:F:241:LEU:CD2	2:L:419:ALA:CB	2.56	0.80
2:B:419:ALA:CA	2:H:241:LEU:HD11	2.10	0.80
2:D:250:ALA:HB1	1:K:680:MET:HG3	1.63	0.80
2:F:241:LEU:CD1	2:L:407:PHE:CE2	2.48	0.80
2:F:419:ALA:CA	2:L:241:LEU:HD11	2.11	0.80
2:B:485:ILE:CD1	4:B:602:ACO:H62	2.11	0.79
2:F:419:ALA:HB1	2:L:241:LEU:HD21	1.64	0.79
2:D:562:ARG:HH12	2:J:230:ASN:ND2	1.80	0.79
2:B:419:ALA:HB1	2:H:241:LEU:HD21	1.65	0.78
2:D:247:VAL:HG12	2:J:409:VAL:HB	1.65	0.78
2:B:473:MET:HE3	4:B:602:ACO:O	1.84	0.78
1:G:653:MET:HE3	2:L:408:MET:CE	2.13	0.78
2:F:241:LEU:HD11	2:L:419:ALA:HA	1.65	0.78
2:D:230:ASN:ND2	2:J:562:ARG:HH12	1.83	0.77
2:D:241:LEU:HD11	2:J:419:ALA:HA	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:407:PHE:CE2	2:L:241:LEU:CD1	2.53	0.77
2:D:489:GLN:NE2	4:J:602:ACO:C5B	2.47	0.77
2:B:241:LEU:HD11	2:H:419:ALA:CA	2.15	0.77
2:D:485:ILE:HD13	4:J:602:ACO:C6P	2.10	0.77
2:F:242:ALA:CB	2:L:409:VAL:HG12	2.14	0.77
2:F:245:PRO:HB3	2:L:484:THR:CG2	2.14	0.77
2:B:409:VAL:HG12	2:H:242:ALA:CB	2.14	0.77
2:B:409:VAL:HB	2:H:247:VAL:HG12	1.67	0.77
2:F:562:ARG:HH12	2:L:230:ASN:ND2	1.83	0.77
2:J:473:MET:CE	4:J:601:ACO:HH32	2.15	0.77
2:B:407:PHE:CB	3:E:801:BTN:O3	2.33	0.77
1:C:707:ARG:CD	1:C:708:HIS:N	2.44	0.77
2:D:241:LEU:HD21	2:J:419:ALA:HB1	1.66	0.76
4:J:601:ACO:H4B	4:J:601:ACO:O7A	1.85	0.76
1:K:590:TYR:HH	1:K:608:LYS:HD3	1.47	0.76
1:A:707:ARG:CD	1:A:708:HIS:N	2.44	0.76
2:B:241:LEU:HD21	2:H:419:ALA:HB2	1.65	0.76
2:B:265:LEU:HD21	2:H:415:ALA:HA	1.67	0.76
1:I:682:MET:HE2	1:I:684:HIS:NE2	2.01	0.76
1:A:682:MET:HE2	1:A:684:HIS:NE2	2.01	0.76
2:B:419:ALA:HA	2:H:241:LEU:HD11	1.68	0.76
1:G:682:MET:HE2	1:G:684:HIS:NE2	2.01	0.75
2:F:419:ALA:HB2	2:L:241:LEU:HD21	1.60	0.75
2:H:482:LEU:HA	2:H:485:ILE:CG2	2.16	0.75
2:J:473:MET:CE	4:J:601:ACO:CH3	2.65	0.75
2:B:230:ASN:ND2	2:H:562:ARG:HH12	1.84	0.75
2:D:415:ALA:HA	2:J:265:LEU:HD21	1.66	0.75
2:D:419:ALA:CA	2:J:241:LEU:HD11	2.17	0.75
2:D:242:ALA:CB	2:J:409:VAL:HG12	2.16	0.75
1:E:682:MET:HE2	1:E:684:HIS:NE2	2.01	0.75
1:E:680:MET:HG3	2:H:250:ALA:HB1	1.68	0.75
1:I:707:ARG:CD	1:I:708:HIS:N	2.44	0.75
1:K:682:MET:HE2	1:K:684:HIS:NE2	2.01	0.75
1:C:682:MET:HE2	1:C:684:HIS:NE2	2.01	0.74
1:E:707:ARG:CD	1:E:708:HIS:N	2.44	0.74
2:B:419:ALA:HB2	2:H:241:LEU:HD21	1.64	0.74
1:G:707:ARG:CD	1:G:708:HIS:N	2.44	0.74
2:J:485:ILE:CD1	4:J:601:ACO:N8P	2.50	0.74
2:D:407:PHE:HE2	2:J:241:LEU:HD13	0.95	0.74
2:F:247:VAL:HG12	2:L:409:VAL:HB	1.67	0.74
2:H:407:PHE:CB	3:I:801:BTN:O3	2.35	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:LEU:HD21	2:H:419:ALA:HB1	1.69	0.74
2:F:179:PRO:HA	2:L:512:LYS:HE2	1.69	0.74
2:H:408:MET:CE	1:I:653:MET:HE3	2.17	0.74
1:C:653:MET:HG3	2:F:408:MET:HE2	1.68	0.74
2:F:482:LEU:HD12	2:L:178:LEU:CD2	2.18	0.74
1:G:442:ALA:HB3	1:I:361:ARG:NH2	2.02	0.74
2:F:187:ASP:HB2	2:F:190:HIS:ND1	2.03	0.74
2:F:489:GLN:NE2	4:L:601:ACO:O9A	2.21	0.73
2:B:187:ASP:HB2	2:B:190:HIS:ND1	2.03	0.73
2:F:222:TYR:OH	2:L:407:PHE:CZ	2.40	0.73
2:F:512:LYS:HE2	2:L:179:PRO:HA	1.68	0.73
2:J:407:PHE:CB	3:K:801:BTN:O3	2.36	0.73
1:K:707:ARG:CD	1:K:708:HIS:N	2.44	0.73
2:L:187:ASP:HB2	2:L:190:HIS:ND1	2.03	0.73
2:F:250:ALA:HB1	1:G:680:MET:HG3	1.70	0.73
2:H:187:ASP:HB2	2:H:190:HIS:ND1	2.03	0.73
2:B:241:LEU:HD11	2:H:419:ALA:HA	1.70	0.73
2:B:408:MET:CE	1:E:653:MET:HE3	2.18	0.73
4:B:602:ACO:CH3	2:H:178:LEU:HD12	2.18	0.73
2:D:472:VAL:HG13	2:D:473:MET:HG3	1.70	0.73
1:A:653:MET:HG3	2:D:408:MET:HE2	1.67	0.73
2:B:562:ARG:HH12	2:H:230:ASN:ND2	1.86	0.73
2:D:187:ASP:HB2	2:D:190:HIS:ND1	2.03	0.73
2:D:485:ILE:HD12	4:J:602:ACO:C6P	2.16	0.72
2:L:174:GLY:HA2	4:L:601:ACO:H141	1.70	0.72
2:F:265:LEU:HD21	2:L:415:ALA:HA	1.68	0.72
2:B:419:ALA:CB	2:H:241:LEU:CD2	2.63	0.72
2:J:187:ASP:HB2	2:J:190:HIS:ND1	2.03	0.72
2:H:408:MET:HE1	1:I:653:MET:SD	2.28	0.72
2:B:485:ILE:CD1	4:B:602:ACO:C6P	2.67	0.72
2:B:222:TYR:OH	2:H:407:PHE:CZ	2.43	0.72
3:C:801:BTN:O3	2:F:407:PHE:CB	2.37	0.72
2:D:419:ALA:HB1	2:J:241:LEU:HD21	1.72	0.72
2:J:485:ILE:CD1	4:J:601:ACO:H143	2.20	0.72
2:D:419:ALA:HA	2:J:241:LEU:HD11	1.70	0.71
2:B:482:LEU:CD1	2:H:178:LEU:HD22	2.20	0.71
2:B:489:GLN:NE2	4:B:602:ACO:O9A	2.24	0.71
2:F:407:PHE:CZ	2:L:222:TYR:OH	2.43	0.71
2:F:409:VAL:HG12	2:L:242:ALA:CB	2.20	0.71
1:C:653:MET:HE3	2:F:408:MET:CE	2.19	0.71
2:D:482:LEU:O	2:D:485:ILE:HG22	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:472:VAL:HG13	2:F:473:MET:HG2	1.72	0.71
2:L:482:LEU:O	2:L:485:ILE:HG22	1.91	0.70
2:H:482:LEU:O	2:H:485:ILE:HG23	1.91	0.70
1:A:531:HIS:CD2	2:B:300:LEU:HB2	2.26	0.70
1:C:531:HIS:CD2	2:D:300:LEU:HB2	2.26	0.70
1:I:531:HIS:CD2	2:J:300:LEU:HB2	2.26	0.70
1:G:653:MET:CG	2:L:408:MET:CE	2.46	0.70
2:F:419:ALA:HA	2:L:241:LEU:HD11	1.71	0.70
4:F:601:ACO:H72	2:L:485:ILE:CD1	2.22	0.70
2:F:230:ASN:ND2	2:L:562:ARG:NH1	2.39	0.70
1:G:681:LYS:NZ	2:L:474:GLY:H	1.89	0.69
2:J:408:MET:CE	1:K:653:MET:HE3	2.22	0.69
2:B:241:LEU:HD13	2:H:407:PHE:HE2	0.97	0.69
1:K:531:HIS:CD2	2:L:300:LEU:HB2	2.26	0.69
2:B:250:ALA:O	1:I:680:MET:HA	1.92	0.69
1:E:531:HIS:CD2	2:F:300:LEU:HB2	2.27	0.69
1:G:707:ARG:CD	1:G:708:HIS:CG	2.75	0.69
1:I:707:ARG:CD	1:I:708:HIS:CG	2.75	0.69
1:K:707:ARG:CD	1:K:708:HIS:CG	2.76	0.69
2:B:241:LEU:O	3:I:801:BTN:H5	1.92	0.69
2:B:407:PHE:CZ	2:H:222:TYR:OH	2.46	0.69
2:F:419:ALA:CB	2:L:241:LEU:CD2	2.61	0.69
1:G:531:HIS:CD2	2:H:300:LEU:HB2	2.26	0.69
1:G:650:LEU:HA	1:G:709:THR:O	1.93	0.69
1:A:650:LEU:HA	1:A:709:THR:O	1.93	0.69
1:E:650:LEU:HA	1:E:709:THR:O	1.93	0.69
2:H:408:MET:CE	1:I:653:MET:SD	2.80	0.68
2:J:173:SER:OG	2:J:174:GLY:N	2.23	0.68
3:A:801:BTN:O3	2:D:407:PHE:CB	2.41	0.68
2:F:409:VAL:HB	2:L:247:VAL:HG12	1.75	0.68
1:A:653:MET:HE3	2:D:408:MET:CE	2.23	0.68
1:A:707:ARG:CD	1:A:708:HIS:CG	2.75	0.68
1:C:680:MET:HG3	2:L:250:ALA:HB1	1.75	0.68
2:D:445:TYR:CD1	2:D:473:MET:O	2.47	0.68
4:J:601:ACO:H141	4:J:601:ACO:N7A	2.08	0.68
1:E:707:ARG:CD	1:E:708:HIS:CG	2.75	0.68
1:I:650:LEU:HA	1:I:709:THR:O	1.93	0.68
2:B:415:ALA:HA	2:H:265:LEU:HD21	1.75	0.68
1:C:707:ARG:CD	1:C:708:HIS:CG	2.75	0.68
2:F:489:GLN:HE21	4:L:601:ACO:H52A	1.59	0.68
1:K:650:LEU:HA	1:K:709:THR:O	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:474:GLY:N	1:I:681:LYS:NZ	2.36	0.67
2:D:407:PHE:CZ	2:J:222:TYR:OH	2.47	0.67
4:B:601:ACO:O9A	4:B:601:ACO:H4B	1.92	0.67
1:C:650:LEU:HA	1:C:709:THR:O	1.93	0.67
2:F:485:ILE:HD11	4:L:601:ACO:C9P	2.21	0.67
2:F:415:ALA:HA	2:L:265:LEU:HD21	1.74	0.67
2:B:406:GLY:CA	1:E:680:MET:HE3	2.18	0.67
2:D:409:VAL:HG22	2:J:251:THR:CG2	2.24	0.67
4:B:601:ACO:HH33	2:H:473:MET:HE3	1.76	0.67
2:D:409:VAL:CG2	2:J:251:THR:HG21	2.17	0.67
2:D:241:LEU:CD2	2:J:419:ALA:CB	2.66	0.66
1:C:680:MET:HE3	2:F:406:GLY:CA	2.15	0.66
2:D:265:LEU:HD21	2:J:415:ALA:HA	1.77	0.66
1:G:543:ARG:NH2	2:H:536:ASP:OD1	2.29	0.66
1:K:543:ARG:NH2	2:L:536:ASP:OD1	2.29	0.66
2:B:485:ILE:HD12	4:B:602:ACO:C6P	2.22	0.65
2:F:482:LEU:HD12	2:L:178:LEU:HD22	1.77	0.65
1:A:543:ARG:NH2	2:B:536:ASP:OD1	2.29	0.65
1:I:543:ARG:NH2	2:J:536:ASP:OD1	2.29	0.65
2:B:409:VAL:HG22	2:H:251:THR:CG2	2.27	0.65
2:J:474:GLY:HA3	1:K:681:LYS:HE2	1.79	0.65
2:D:222:TYR:OH	2:J:407:PHE:CZ	2.50	0.65
2:B:478:ALA:HB1	2:H:178:LEU:HD21	1.78	0.65
1:E:543:ARG:NH2	2:F:536:ASP:OD1	2.29	0.65
2:F:178:LEU:CD2	2:L:482:LEU:HD12	2.26	0.65
1:I:442:ALA:CB	1:K:361:ARG:NH2	2.58	0.65
2:B:251:THR:CG2	2:H:409:VAL:HG22	2.27	0.65
1:C:543:ARG:NH2	2:D:536:ASP:OD1	2.29	0.65
2:B:478:ALA:HB1	2:H:178:LEU:CD2	2.27	0.65
2:D:409:VAL:HG23	2:J:251:THR:HG23	1.59	0.64
1:K:537:PHE:CZ	2:L:543:LEU:HD22	2.32	0.64
1:E:537:PHE:CZ	2:F:543:LEU:HD22	2.32	0.64
1:G:680:MET:HE3	2:L:406:GLY:CA	2.17	0.64
2:J:326:LYS:HD2	1:K:682:MET:HA	1.78	0.64
2:J:408:MET:HE2	1:K:653:MET:HG3	1.71	0.64
2:D:178:LEU:CD2	2:J:482:LEU:HD12	2.27	0.64
2:B:242:ALA:CB	2:H:409:VAL:CG1	2.75	0.64
1:C:537:PHE:CZ	2:D:543:LEU:HD22	2.32	0.64
2:F:409:VAL:HG23	2:L:251:THR:HG23	1.54	0.64
2:J:489:GLN:NE2	4:J:601:ACO:O9A	2.30	0.64
2:D:562:ARG:NH1	2:J:230:ASN:ND2	2.45	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:537:PHE:CZ	2:H:543:LEU:HD22	2.32	0.64
1:I:537:PHE:CZ	2:J:543:LEU:HD22	2.32	0.64
4:L:601:ACO:H4B	4:L:601:ACO:O7A	1.95	0.64
2:B:489:GLN:HE21	4:B:602:ACO:H3B	1.63	0.64
2:F:419:ALA:HB2	2:L:241:LEU:CD1	2.28	0.63
2:B:241:LEU:CD2	2:H:419:ALA:CB	2.65	0.63
1:A:537:PHE:CZ	2:B:543:LEU:HD22	2.32	0.63
2:D:409:VAL:CG1	2:J:242:ALA:CB	2.76	0.63
2:J:474:GLY:H	1:K:681:LYS:HZ3	1.39	0.63
2:D:251:THR:CG2	2:J:409:VAL:HG22	2.22	0.63
2:D:241:LEU:CD1	2:J:419:ALA:HB2	2.28	0.63
2:F:485:ILE:CD1	4:L:601:ACO:C7P	2.67	0.63
1:I:652:PRO:HD2	1:I:677:MET:SD	2.40	0.62
2:B:408:MET:HE2	1:E:653:MET:HG3	1.73	0.62
2:J:408:MET:HE1	1:K:653:MET:SD	2.40	0.62
1:C:652:PRO:HD2	1:C:677:MET:SD	2.40	0.62
1:G:652:PRO:HD2	1:G:677:MET:SD	2.40	0.62
2:B:419:ALA:HB2	2:H:241:LEU:CD1	2.29	0.62
1:K:652:PRO:HD2	1:K:677:MET:SD	2.40	0.62
1:E:531:HIS:CD2	2:F:300:LEU:H	2.18	0.62
1:E:652:PRO:HD2	1:E:677:MET:SD	2.40	0.62
4:J:601:ACO:H141	4:J:601:ACO:HN8	1.63	0.62
1:A:680:MET:HE3	2:D:406:GLY:CA	2.15	0.62
1:I:531:HIS:CD2	2:J:300:LEU:H	2.18	0.62
1:I:682:MET:CE	1:I:684:HIS:NE2	2.63	0.62
1:K:531:HIS:CD2	2:L:300:LEU:H	2.18	0.62
1:C:682:MET:CE	1:C:684:HIS:NE2	2.63	0.62
2:D:241:LEU:O	3:K:801:BTN:H5	2.00	0.61
1:E:682:MET:CE	1:E:684:HIS:NE2	2.63	0.61
1:G:653:MET:HE3	2:L:408:MET:HE1	1.81	0.61
1:K:682:MET:CE	1:K:684:HIS:NE2	2.63	0.61
1:C:531:HIS:CD2	2:D:300:LEU:H	2.18	0.61
1:G:653:MET:CE	2:L:408:MET:HE1	2.30	0.61
1:G:682:MET:CE	1:G:684:HIS:NE2	2.63	0.61
4:J:601:ACO:HN8	4:J:601:ACO:CEP	2.13	0.61
1:A:531:HIS:CD2	2:B:300:LEU:H	2.18	0.61
1:A:652:PRO:HD2	1:A:677:MET:SD	2.40	0.61
1:G:531:HIS:CD2	2:H:300:LEU:H	2.18	0.61
2:D:301:ASP:OD1	2:D:301:ASP:N	2.34	0.61
1:C:681:LYS:HE2	2:F:474:GLY:HA3	1.82	0.61
2:L:176:ALA:O	4:L:601:ACO:HH33	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:ASN:ND2	2:H:562:ARG:NH1	2.49	0.61
2:F:251:THR:CG2	2:L:409:VAL:HG22	2.28	0.61
2:F:301:ASP:OD1	2:F:301:ASP:N	2.34	0.61
2:F:562:ARG:NH1	2:L:230:ASN:ND2	2.49	0.61
2:B:178:LEU:CD2	2:H:482:LEU:HD12	2.31	0.60
2:D:419:ALA:CB	2:J:241:LEU:CD2	2.69	0.60
1:A:682:MET:CE	1:A:684:HIS:NE2	2.63	0.60
3:A:801:BTN:O11	2:D:445:TYR:CB	2.49	0.60
2:D:178:LEU:HD22	2:J:482:LEU:HD12	1.82	0.60
1:G:361:ARG:NH2	1:K:442:ALA:CB	2.63	0.60
2:H:408:MET:HE1	1:I:653:MET:CE	2.31	0.60
2:F:241:LEU:CD1	2:L:419:ALA:HB2	2.31	0.60
2:H:301:ASP:OD1	2:H:301:ASP:N	2.34	0.60
2:H:482:LEU:HA	2:H:485:ILE:HG21	1.82	0.60
1:A:653:MET:CG	2:D:408:MET:SD	2.88	0.60
2:B:141:LYS:HE2	2:B:146:TYR:OH	2.02	0.60
1:C:653:MET:SD	2:F:408:MET:HE1	2.41	0.60
2:F:418:ILE:HG23	2:L:241:LEU:HD12	1.84	0.60
2:D:251:THR:HG21	2:J:409:VAL:CG2	2.13	0.59
2:F:241:LEU:HD12	2:L:418:ILE:HG23	1.83	0.59
1:A:653:MET:SD	2:D:408:MET:HE1	2.41	0.59
2:B:482:LEU:HD12	2:H:178:LEU:CD2	2.32	0.59
1:C:707:ARG:CZ	1:C:708:HIS:NE2	2.66	0.59
2:F:482:LEU:HD12	2:L:178:LEU:HD23	1.83	0.59
1:A:653:MET:HG3	2:D:408:MET:SD	2.40	0.59
2:B:301:ASP:OD1	2:B:301:ASP:N	2.34	0.59
2:H:406:GLY:CA	1:I:680:MET:HE3	2.25	0.59
2:L:176:ALA:HB3	4:L:601:ACO:HH32	1.84	0.59
1:G:653:MET:HG3	2:L:408:MET:HE2	1.73	0.59
1:I:707:ARG:CZ	1:I:708:HIS:NE2	2.66	0.59
2:L:301:ASP:OD1	2:L:301:ASP:N	2.34	0.59
1:C:653:MET:HG3	2:F:408:MET:SD	2.43	0.59
1:E:707:ARG:CZ	1:E:708:HIS:NE2	2.66	0.59
1:K:707:ARG:CZ	1:K:708:HIS:NE2	2.66	0.59
3:A:801:BTN:H5	2:J:241:LEU:O	2.01	0.59
1:G:653:MET:SD	2:L:408:MET:HE1	2.42	0.59
2:B:178:LEU:HD22	2:H:482:LEU:HD12	1.85	0.58
2:D:230:ASN:ND2	2:J:562:ARG:NH1	2.49	0.58
1:G:707:ARG:CZ	1:G:708:HIS:NE2	2.66	0.58
2:J:485:ILE:HD13	4:J:601:ACO:N8P	2.18	0.58
3:C:801:BTN:O11	2:F:445:TYR:CB	2.51	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:472:VAL:O	2:H:473:MET:HB3	2.03	0.58
1:A:653:MET:SD	2:D:408:MET:CE	2.90	0.58
1:A:680:MET:HA	2:J:250:ALA:O	2.04	0.58
1:A:707:ARG:CZ	1:A:708:HIS:NE2	2.66	0.58
4:F:601:ACO:HH31	2:L:473:MET:CE	2.12	0.58
2:J:408:MET:CE	1:K:653:MET:SD	2.91	0.58
2:B:251:THR:HB	1:I:654:THR:O	2.02	0.58
4:F:601:ACO:H72	2:L:485:ILE:HD13	1.86	0.58
2:B:408:MET:HE1	1:E:653:MET:SD	2.43	0.58
2:L:173:SER:OG	2:L:174:GLY:N	2.37	0.58
2:D:250:ALA:O	1:K:680:MET:HA	2.04	0.58
2:H:472:VAL:O	2:H:472:VAL:HG22	2.04	0.58
1:A:682:MET:HG3	2:D:405:THR:HG21	1.85	0.57
1:G:653:MET:CE	2:L:408:MET:SD	2.92	0.57
2:H:173:SER:OG	2:H:174:GLY:N	2.37	0.57
2:B:173:SER:OG	2:B:174:GLY:N	2.37	0.57
2:H:408:MET:CE	1:I:653:MET:CE	2.82	0.57
2:J:407:PHE:HZ	2:J:422:GLY:HA3	1.69	0.57
2:L:176:ALA:H	4:L:601:ACO:HH32	1.69	0.57
2:B:562:ARG:NH1	2:H:230:ASN:ND2	2.53	0.57
1:C:651:ALA:HB3	1:C:709:THR:HG22	1.87	0.57
1:G:651:ALA:HB3	1:G:709:THR:HG22	1.87	0.57
1:A:651:ALA:HB3	1:A:709:THR:HG22	1.87	0.57
2:D:489:GLN:NE2	4:J:602:ACO:O9A	2.38	0.57
2:F:173:SER:OG	2:F:174:GLY:N	2.37	0.57
2:H:407:PHE:HZ	2:H:422:GLY:HA3	1.69	0.57
2:B:407:PHE:HZ	2:B:422:GLY:HA3	1.69	0.57
2:F:407:PHE:HZ	2:F:422:GLY:HA3	1.69	0.57
1:C:653:MET:SD	2:F:408:MET:CE	2.90	0.57
2:J:301:ASP:OD1	2:J:301:ASP:N	2.34	0.57
2:L:174:GLY:CA	4:L:601:ACO:CEP	2.81	0.57
2:D:189:ASP:OD2	2:J:188:ARG:NH2	2.38	0.57
1:G:653:MET:SD	2:L:408:MET:CE	2.93	0.57
4:J:601:ACO:H61A	4:J:601:ACO:C2P	2.11	0.57
1:I:651:ALA:HB3	1:I:709:THR:HG22	1.87	0.56
2:B:408:MET:CE	1:E:653:MET:SD	2.93	0.56
2:B:408:MET:HE1	1:E:653:MET:CE	2.35	0.56
1:C:653:MET:CG	2:F:408:MET:SD	2.90	0.56
1:E:651:ALA:HB3	1:E:709:THR:HG22	1.87	0.56
2:H:361:ARG:NH1	2:H:364:GLY:O	2.38	0.56
2:B:409:VAL:CG1	2:H:242:ALA:CB	2.82	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:173:SER:OG	2:D:174:GLY:N	2.37	0.56
2:D:407:PHE:HZ	2:D:422:GLY:HA3	1.69	0.56
2:J:361:ARG:NH1	2:J:364:GLY:O	2.38	0.56
1:K:651:ALA:HB3	1:K:709:THR:HG22	1.87	0.56
2:B:241:LEU:CD1	2:H:419:ALA:HB2	2.35	0.56
4:J:602:ACO:O1A	4:J:602:ACO:OAP	2.23	0.56
2:B:408:MET:HE1	1:E:653:MET:HE3	1.87	0.56
2:D:361:ARG:NH1	2:D:364:GLY:O	2.38	0.56
2:H:482:LEU:O	2:H:485:ILE:CG2	2.53	0.56
2:J:485:ILE:CD1	4:J:601:ACO:C7P	2.84	0.56
2:B:361:ARG:NH1	2:B:364:GLY:O	2.38	0.56
1:C:653:MET:CE	2:F:408:MET:HE1	2.37	0.55
2:D:188:ARG:NH2	2:J:189:ASP:OD2	2.39	0.55
2:F:361:ARG:NH1	2:F:364:GLY:O	2.38	0.55
4:L:601:ACO:O5P	4:L:601:ACO:N8P	2.31	0.55
2:B:445:TYR:CB	3:E:801:BTN:O11	2.54	0.55
2:D:527:TRP:CZ3	2:J:186:PRO:HG2	2.41	0.55
3:E:801:BTN:H5	2:H:241:LEU:O	2.07	0.55
2:F:178:LEU:HD22	2:L:482:LEU:HD12	1.87	0.55
2:J:180:ARG:O	2:J:184:VAL:HG23	2.07	0.55
2:L:528:ASP:OD1	2:L:528:ASP:N	2.38	0.55
1:A:679:ALA:O	1:A:680:MET:CB	2.55	0.55
2:D:251:THR:HG23	2:J:409:VAL:HG23	1.53	0.55
2:L:407:PHE:HZ	2:L:422:GLY:HA3	1.69	0.55
2:J:177:TYR:O	2:J:178:LEU:HB2	2.05	0.55
2:L:361:ARG:NH1	2:L:364:GLY:O	2.38	0.55
1:G:679:ALA:O	1:G:680:MET:CB	2.55	0.55
2:J:406:GLY:CA	1:K:680:MET:HE3	2.21	0.55
1:A:654:THR:O	2:J:251:THR:HB	2.05	0.55
2:D:528:ASP:OD1	2:D:528:ASP:N	2.38	0.55
2:F:241:LEU:HD11	2:L:419:ALA:N	2.21	0.55
2:B:218:ALA:HB1	3:I:801:BTN:C6	2.37	0.55
2:B:418:ILE:HG23	2:H:241:LEU:HD12	1.88	0.55
2:D:230:ASN:HD22	2:J:562:ARG:HH12	1.54	0.55
2:D:242:ALA:CB	2:J:409:VAL:CG1	2.85	0.55
2:B:482:LEU:CD1	2:H:178:LEU:CD2	2.85	0.54
2:F:178:LEU:HD23	2:L:482:LEU:HD12	1.89	0.54
2:F:230:ASN:HD22	2:L:562:ARG:HH12	1.50	0.54
1:I:679:ALA:O	1:I:680:MET:CB	2.55	0.54
2:B:393:GLN:OE1	2:L:560:ILE:HD11	2.07	0.54
1:C:653:MET:CE	2:F:408:MET:SD	2.95	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:679:ALA:O	1:E:680:MET:CB	2.55	0.54
2:J:445:TYR:CB	3:K:801:BTN:O11	2.55	0.54
2:F:242:ALA:CB	2:L:409:VAL:CG1	2.83	0.54
2:D:393:GLN:OE1	2:H:560:ILE:HD11	2.08	0.54
2:F:528:ASP:OD1	2:F:528:ASP:N	2.38	0.54
2:H:528:ASP:N	2:H:528:ASP:OD1	2.38	0.54
2:J:408:MET:HE1	1:K:653:MET:CE	2.38	0.54
4:J:602:ACO:O5P	4:J:602:ACO:H21	2.07	0.54
4:L:601:ACO:O6A	4:L:601:ACO:OAP	2.23	0.54
2:B:560:ILE:HD11	2:L:393:GLN:OE1	2.08	0.54
1:C:679:ALA:O	1:C:680:MET:CB	2.55	0.54
2:H:408:MET:SD	1:I:653:MET:CG	2.93	0.54
2:B:528:ASP:OD1	2:B:528:ASP:N	2.38	0.54
2:F:241:LEU:O	3:G:801:BTN:H5	2.08	0.54
2:F:409:VAL:HG22	2:L:251:THR:CG2	2.32	0.54
1:G:653:MET:CE	2:L:408:MET:CE	2.83	0.54
2:J:528:ASP:N	2:J:528:ASP:OD1	2.38	0.54
2:D:562:ARG:HH12	2:J:230:ASN:HD22	1.52	0.54
2:L:174:GLY:HA2	4:L:601:ACO:H142	1.88	0.54
2:B:482:LEU:HD12	2:H:178:LEU:HD22	1.90	0.54
1:C:654:THR:O	2:L:251:THR:HB	2.08	0.54
2:D:419:ALA:HB2	2:J:241:LEU:CD1	2.37	0.54
4:F:601:ACO:OAP	2:L:485:ILE:HD11	2.08	0.54
2:J:473:MET:CE	4:J:601:ACO:HH31	2.32	0.54
4:J:601:ACO:H21	4:J:601:ACO:N6A	2.12	0.53
4:J:601:ACO:CEP	4:J:601:ACO:C8A	2.85	0.53
4:J:601:ACO:H141	4:J:601:ACO:C8A	2.38	0.53
2:H:474:GLY:H	1:I:681:LYS:HZ3	1.53	0.53
2:H:23:TYR:OH	1:I:522:MET:HE3	2.08	0.53
2:J:472:VAL:O	2:J:473:MET:HB3	2.07	0.53
1:K:679:ALA:O	1:K:680:MET:CB	2.55	0.53
4:F:601:ACO:O5P	2:L:481:VAL:CG1	2.57	0.53
2:J:474:GLY:H	3:K:801:BTN:C11	2.20	0.53
2:B:408:MET:CE	1:E:653:MET:CE	2.87	0.53
1:A:653:MET:CE	2:D:408:MET:SD	2.96	0.53
3:C:801:BTN:H5	2:L:241:LEU:O	2.09	0.53
2:D:489:GLN:HE21	4:J:602:ACO:C5B	2.12	0.53
2:B:218:ALA:HB1	3:I:801:BTN:H5	1.90	0.53
2:B:251:THR:HG23	2:H:409:VAL:HG23	1.58	0.53
2:J:408:MET:SD	1:K:653:MET:HG3	2.48	0.53
1:C:707:ARG:NE	1:C:708:HIS:CD2	2.77	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:680:MET:HA	2:H:250:ALA:O	2.09	0.52
2:H:482:LEU:CA	2:H:485:ILE:CG2	2.84	0.52
1:I:707:ARG:NE	1:I:708:HIS:CD2	2.77	0.52
2:B:408:MET:SD	1:E:653:MET:CE	2.97	0.52
1:C:707:ARG:CD	1:C:708:HIS:CD2	2.93	0.52
3:G:801:BTN:O11	2:L:445:TYR:CB	2.57	0.52
1:K:707:ARG:NE	1:K:708:HIS:CD2	2.77	0.52
2:D:186:PRO:HG2	2:J:527:TRP:CZ3	2.45	0.52
2:B:186:PRO:HG2	2:H:527:TRP:CZ3	2.45	0.52
1:C:653:MET:CE	2:F:408:MET:CE	2.86	0.52
1:E:679:ALA:O	1:E:680:MET:HB3	2.10	0.52
1:G:673:SER:HA	1:G:687:LYS:HG2	1.92	0.52
2:J:177:TYR:CE2	2:J:180:ARG:HG3	2.44	0.52
1:K:707:ARG:CD	1:K:708:HIS:CD2	2.93	0.52
1:A:673:SER:HA	1:A:687:LYS:HG2	1.92	0.52
1:A:680:MET:HE1	2:D:406:GLY:C	2.35	0.52
2:D:489:GLN:HE22	4:J:602:ACO:C5B	2.23	0.52
1:G:417:GLU:OE1	1:G:436:LYS:NZ	2.43	0.52
1:G:707:ARG:CD	1:G:708:HIS:CD2	2.93	0.52
2:H:92:ASP:OD2	2:L:23:TYR:HB2	2.09	0.52
1:K:679:ALA:O	1:K:680:MET:HB3	2.10	0.52
1:A:707:ARG:NE	1:A:708:HIS:CD2	2.77	0.52
2:B:241:LEU:HD12	2:H:418:ILE:HG23	1.91	0.52
2:B:409:VAL:CG2	2:H:251:THR:HG21	2.20	0.52
2:F:227:ALA:O	2:L:562:ARG:NH2	2.43	0.52
2:F:482:LEU:CD1	2:L:178:LEU:CD2	2.87	0.52
1:I:679:ALA:O	1:I:680:MET:HB3	2.10	0.52
1:A:707:ARG:CD	1:A:708:HIS:CD2	2.93	0.52
1:E:707:ARG:CD	1:E:708:HIS:CD2	2.93	0.52
2:F:250:ALA:O	1:G:680:MET:HA	2.10	0.52
1:A:679:ALA:O	1:A:680:MET:HB3	2.10	0.52
1:I:417:GLU:OE1	1:I:436:LYS:NZ	2.43	0.52
1:I:673:SER:HA	1:I:687:LYS:HG2	1.92	0.52
1:I:707:ARG:CD	1:I:708:HIS:CD2	2.93	0.51
1:C:673:SER:HA	1:C:687:LYS:HG2	1.92	0.51
1:G:653:MET:HE3	2:L:408:MET:SD	2.50	0.51
1:G:707:ARG:NE	1:G:708:HIS:CD2	2.77	0.51
2:B:189:ASP:OD2	2:H:188:ARG:NH2	2.43	0.51
1:C:653:MET:HE3	2:F:408:MET:HE1	1.92	0.51
1:A:653:MET:CE	2:D:408:MET:CE	2.89	0.51
2:J:408:MET:HE1	1:K:653:MET:HE3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:485:ILE:HD12	4:J:601:ACO:C7P	2.40	0.51
1:A:707:ARG:HB2	2:D:413:TYR:OH	2.11	0.51
2:B:188:ARG:NH2	2:H:189:ASP:OD2	2.43	0.51
2:H:408:MET:SD	1:I:653:MET:CE	2.98	0.51
4:B:601:ACO:H143	4:B:601:ACO:O9P	2.10	0.51
1:C:680:MET:HE1	2:F:406:GLY:C	2.35	0.51
2:F:409:VAL:CG1	2:L:242:ALA:CB	2.87	0.51
2:B:408:MET:SD	1:E:653:MET:CG	2.97	0.51
2:D:161:MET:HE2	2:D:201:MET:HG3	1.93	0.51
2:J:378:SER:OG	2:J:421:ASP:OD2	2.29	0.51
1:A:653:MET:CE	2:D:408:MET:HE1	2.40	0.51
2:B:218:ALA:HB1	3:I:801:BTN:H61	1.93	0.51
1:G:653:MET:CG	2:L:408:MET:SD	2.98	0.51
1:G:679:ALA:O	1:G:680:MET:HB3	2.10	0.51
2:H:25:GLY:HA3	1:I:522:MET:SD	2.50	0.51
4:J:601:ACO:HH33	4:J:601:ACO:HN4	1.76	0.51
2:B:161:MET:HE2	2:B:201:MET:HG3	1.93	0.51
4:B:602:ACO:HH31	2:H:178:LEU:HD11	1.87	0.51
1:G:653:MET:HG3	2:L:408:MET:SD	2.51	0.51
2:D:116:GLY:O	2:D:152:LYS:NZ	2.42	0.51
1:E:673:SER:HA	1:E:687:LYS:HG2	1.92	0.51
2:J:161:MET:HE2	2:J:201:MET:HG3	1.93	0.51
1:K:417:GLU:OE1	1:K:436:LYS:NZ	2.43	0.51
1:K:673:SER:HA	1:K:687:LYS:HG2	1.92	0.51
2:B:141:LYS:HD2	4:B:601:ACO:O7A	2.11	0.50
1:E:707:ARG:NE	1:E:708:HIS:CD2	2.77	0.50
2:F:161:MET:HE2	2:F:201:MET:HG3	1.93	0.50
2:F:378:SER:OG	2:F:421:ASP:OD2	2.29	0.50
2:H:378:SER:OG	2:H:421:ASP:OD2	2.29	0.50
1:C:679:ALA:O	1:C:680:MET:HB3	2.10	0.50
2:D:407:PHE:HE2	2:J:241:LEU:HD11	1.66	0.50
2:D:489:GLN:NE2	4:J:602:ACO:H52A	2.25	0.50
1:G:656:THR:HG22	1:G:704:GLN:HG3	1.94	0.50
1:A:656:THR:HG22	1:A:704:GLN:HG3	1.94	0.50
2:D:251:THR:HB	1:K:654:THR:O	2.12	0.50
2:F:177:TYR:CE2	2:F:179:PRO:HD2	2.46	0.50
2:F:456:ALA:O	2:L:193:ARG:NH1	2.45	0.50
2:J:408:MET:SD	1:K:653:MET:CG	2.96	0.50
1:C:656:THR:HG22	1:C:704:GLN:HG3	1.93	0.50
1:C:682:MET:HG3	2:F:405:THR:HG21	1.86	0.50
1:E:654:THR:O	2:H:251:THR:HB	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:656:THR:HG22	1:E:704:GLN:HG3	1.94	0.50
2:L:116:GLY:O	2:L:152:LYS:NZ	2.42	0.50
2:L:176:ALA:HB3	4:L:601:ACO:CH3	2.41	0.50
2:B:230:ASN:HD22	2:H:562:ARG:HH12	1.58	0.50
2:B:408:MET:SD	1:E:653:MET:HG3	2.49	0.50
2:H:116:GLY:O	2:H:152:LYS:NZ	2.42	0.50
2:J:177:TYR:CD2	2:J:180:ARG:CG	2.86	0.50
4:J:601:ACO:N8P	4:J:601:ACO:CEP	2.73	0.50
2:B:177:TYR:CE2	2:B:179:PRO:HD2	2.46	0.50
2:D:245:PRO:HB3	2:J:484:THR:HG23	1.90	0.50
2:H:161:MET:HE2	2:H:201:MET:HG3	1.93	0.50
2:B:116:GLY:O	2:B:152:LYS:NZ	2.42	0.49
2:B:562:ARG:HH12	2:H:230:ASN:HD22	1.60	0.49
2:D:177:TYR:CE2	2:D:179:PRO:HD2	2.46	0.49
2:D:241:LEU:HD12	2:J:418:ILE:HG23	1.93	0.49
2:F:414:GLU:OE2	2:L:241:LEU:HB2	2.12	0.49
2:J:177:TYR:CE2	2:J:180:ARG:CG	2.96	0.49
2:B:23:TYR:OH	1:E:522:MET:HE3	2.12	0.49
1:K:656:THR:HG22	1:K:704:GLN:HG3	1.94	0.49
1:I:656:THR:HG22	1:I:704:GLN:HG3	1.94	0.49
2:J:408:MET:SD	1:K:653:MET:CE	3.00	0.49
2:D:321:VAL:HG21	2:D:465:TRP:HZ3	1.78	0.49
2:L:177:TYR:CE2	2:L:179:PRO:HD2	2.46	0.49
2:J:321:VAL:HG21	2:J:465:TRP:HZ3	1.78	0.49
2:J:408:MET:CE	1:K:653:MET:CE	2.89	0.49
2:B:419:ALA:N	2:H:241:LEU:HD11	2.28	0.49
2:H:26:ASP:OD1	2:H:26:ASP:N	2.45	0.49
2:H:408:MET:HE1	1:I:653:MET:HE3	1.89	0.49
1:I:259:GLN:OE1	1:I:274:ARG:NH1	2.46	0.49
2:L:161:MET:HE2	2:L:201:MET:HG3	1.93	0.49
2:F:419:ALA:N	2:L:241:LEU:HD11	2.26	0.49
2:F:562:ARG:HH12	2:L:230:ASN:HD22	1.59	0.49
2:J:474:GLY:HA3	1:K:681:LYS:CE	2.43	0.49
3:A:801:BTN:H5	2:J:218:ALA:HB1	1.94	0.49
4:B:601:ACO:O9P	4:B:601:ACO:H122	2.12	0.49
2:F:241:LEU:HB2	2:L:414:GLU:OE2	2.13	0.49
2:F:560:ILE:HD11	2:J:393:GLN:OE1	2.13	0.49
2:H:292:ARG:HG3	2:L:24:HIS:CE1	2.48	0.49
2:D:489:GLN:HE22	4:J:602:ACO:H52A	1.78	0.49
2:L:174:GLY:CA	4:L:601:ACO:H142	2.43	0.49
2:F:188:ARG:NH2	2:L:189:ASP:OD2	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:321:VAL:HG21	2:H:465:TRP:HZ3	1.78	0.48
2:B:405:THR:HG21	1:E:682:MET:HG3	1.90	0.48
2:J:472:VAL:O	2:J:472:VAL:HG22	2.12	0.48
2:B:378:SER:OG	2:B:421:ASP:OD2	2.29	0.48
2:B:527:TRP:CZ3	2:H:186:PRO:HG2	2.47	0.48
2:F:189:ASP:OD2	2:L:188:ARG:NH2	2.46	0.48
2:F:241:LEU:HD12	2:L:418:ILE:HG13	1.96	0.48
2:F:251:THR:HB	1:G:654:THR:O	2.13	0.48
1:G:442:ALA:CB	1:I:361:ARG:NH2	2.74	0.48
2:J:23:TYR:OH	1:K:522:MET:HE3	2.13	0.48
2:L:110:ASP:OD1	2:L:110:ASP:N	2.45	0.48
2:B:321:VAL:HG21	2:B:465:TRP:HZ3	1.78	0.48
1:C:654:THR:HG22	1:C:706:ASN:HD22	1.79	0.48
2:D:378:SER:OG	2:D:421:ASP:OD2	2.29	0.48
4:J:601:ACO:H8A	4:J:601:ACO:H142	1.96	0.48
1:K:259:GLN:OE1	1:K:274:ARG:NH1	2.46	0.48
1:A:707:ARG:NH1	1:A:708:HIS:CE1	2.82	0.48
2:B:250:ALA:O	1:I:680:MET:CA	2.61	0.48
4:B:601:ACO:H72	2:H:485:ILE:HD12	1.91	0.48
2:D:110:ASP:N	2:D:110:ASP:OD1	2.45	0.48
1:E:707:ARG:NH1	1:E:708:HIS:CE1	2.82	0.48
2:F:419:ALA:CB	2:L:241:LEU:HD11	2.43	0.48
2:F:440:ILE:HB	2:F:464:ILE:HG22	1.96	0.48
1:I:654:THR:HG22	1:I:706:ASN:HD22	1.79	0.48
2:J:475:GLY:O	2:J:478:ALA:N	2.47	0.48
2:L:378:SER:OG	2:L:421:ASP:OD2	2.29	0.48
2:D:475:GLY:O	2:D:476:GLU:C	2.54	0.48
2:F:250:ALA:HB3	2:L:409:VAL:HG21	1.96	0.48
2:F:482:LEU:HD11	2:L:178:LEU:HB3	1.95	0.48
1:K:654:THR:HG22	1:K:706:ASN:HD22	1.79	0.48
2:L:321:VAL:HG21	2:L:465:TRP:HZ3	1.78	0.48
4:B:602:ACO:HH31	2:H:178:LEU:CD1	2.42	0.48
4:F:601:ACO:N6A	4:F:601:ACO:H21	2.28	0.48
2:L:440:ILE:HB	2:L:464:ILE:HG22	1.96	0.48
1:A:522:MET:HE3	2:D:23:TYR:OH	2.14	0.48
2:B:23:TYR:OH	1:E:522:MET:CE	2.62	0.48
2:F:321:VAL:HG21	2:F:465:TRP:HZ3	1.78	0.48
1:G:654:THR:HG22	1:G:706:ASN:HD22	1.79	0.48
1:G:707:ARG:NH1	1:G:708:HIS:CE1	2.82	0.48
2:B:408:MET:SD	1:E:653:MET:HE3	2.54	0.48
2:B:440:ILE:HB	2:B:464:ILE:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:193:ARG:NH1	2:L:456:ALA:O	2.47	0.48
2:J:485:ILE:CD1	4:J:601:ACO:HN8	2.27	0.48
1:G:259:GLN:OE1	1:G:274:ARG:NH1	2.46	0.47
2:B:218:ALA:HB1	3:I:801:BTN:C5	2.44	0.47
1:C:531:HIS:NE2	2:D:300:LEU:HB2	2.29	0.47
2:H:285:HIS:HE1	2:L:27:SER:O	1.96	0.47
1:K:707:ARG:NH1	1:K:708:HIS:CE1	2.82	0.47
2:B:110:ASP:OD1	2:B:110:ASP:N	2.45	0.47
1:E:531:HIS:NE2	2:F:300:LEU:HB2	2.30	0.47
2:D:440:ILE:HB	2:D:464:ILE:HG22	1.96	0.47
1:G:531:HIS:NE2	2:H:300:LEU:HB2	2.30	0.47
2:J:336:ALA:O	2:J:342:SER:OG	2.31	0.47
2:B:409:VAL:HG23	2:H:251:THR:HG23	1.53	0.47
2:B:419:ALA:CB	2:H:241:LEU:HD11	2.43	0.47
1:C:707:ARG:NH1	1:C:708:HIS:CE1	2.82	0.47
2:D:418:ILE:HG23	2:J:241:LEU:HD12	1.97	0.47
1:A:654:THR:HG22	1:A:706:ASN:HD22	1.79	0.47
2:D:241:LEU:HD11	2:J:419:ALA:CB	2.43	0.47
2:F:393:GLN:OE1	2:J:560:ILE:HD11	2.14	0.47
2:H:23:TYR:OH	1:I:522:MET:CE	2.62	0.47
1:I:707:ARG:NH1	1:I:708:HIS:CE1	2.82	0.47
2:J:110:ASP:OD1	2:J:110:ASP:N	2.45	0.47
2:J:440:ILE:HB	2:J:464:ILE:HG22	1.96	0.47
2:J:485:ILE:HD13	4:J:601:ACO:HN8	1.76	0.47
1:K:707:ARG:HD3	1:K:707:ARG:C	2.30	0.47
2:L:482:LEU:C	2:L:485:ILE:HG22	2.40	0.47
2:B:241:LEU:HD11	2:H:419:ALA:N	2.30	0.47
1:G:681:LYS:NZ	2:L:474:GLY:N	2.61	0.47
1:K:531:HIS:NE2	2:L:300:LEU:HB2	2.29	0.47
2:B:26:ASP:OD1	2:B:26:ASP:N	2.45	0.47
2:D:178:LEU:HD23	2:J:482:LEU:HD12	1.95	0.47
2:F:562:ARG:NH2	2:L:227:ALA:O	2.47	0.47
2:H:440:ILE:HB	2:H:464:ILE:HG22	1.96	0.47
1:E:654:THR:HG22	1:E:706:ASN:HD22	1.79	0.47
2:F:419:ALA:HB2	2:L:241:LEU:HD11	1.97	0.47
1:C:707:ARG:HB2	2:F:413:TYR:OH	2.15	0.46
2:F:110:ASP:N	2:F:110:ASP:OD1	2.45	0.46
2:F:336:ALA:O	2:F:342:SER:OG	2.31	0.46
1:G:682:MET:HG3	2:L:405:THR:HG21	1.92	0.46
2:H:110:ASP:OD1	2:H:110:ASP:N	2.45	0.46
2:J:178:LEU:HD21	4:J:602:ACO:HH31	1.95	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:653:MET:HE3	2:F:408:MET:SD	2.54	0.46
1:C:707:ARG:HD2	1:C:708:HIS:CD2	2.50	0.46
1:G:680:MET:HE1	2:L:406:GLY:C	2.41	0.46
4:J:602:ACO:O5P	4:J:602:ACO:N8P	2.47	0.46
2:B:452:MET:HE3	2:B:452:MET:HB3	1.80	0.46
2:D:482:LEU:C	2:D:485:ILE:HG22	2.40	0.46
4:B:602:ACO:O5P	4:B:602:ACO:H21	2.16	0.46
1:I:531:HIS:NE2	2:J:300:LEU:HB2	2.30	0.46
2:B:187:ASP:CG	2:H:527:TRP:CD1	2.94	0.46
2:F:527:TRP:CZ3	2:L:186:PRO:HG2	2.50	0.46
1:K:707:ARG:HD2	1:K:708:HIS:CD2	2.50	0.46
2:B:250:ALA:O	1:I:680:MET:N	2.49	0.46
2:H:336:ALA:O	2:H:342:SER:OG	2.31	0.46
2:J:405:THR:OG1	1:K:682:MET:SD	2.70	0.46
4:J:601:ACO:HH33	4:J:601:ACO:N4P	2.31	0.46
2:B:241:LEU:HD12	2:H:418:ILE:HG13	1.98	0.46
2:H:413:TYR:OH	1:I:707:ARG:HB2	2.15	0.46
2:H:445:TYR:CB	3:I:801:BTN:O11	2.63	0.46
3:A:801:BTN:O11	2:D:445:TYR:HB2	2.16	0.46
2:D:527:TRP:CD1	2:J:187:ASP:CG	2.94	0.46
1:G:707:ARG:HD2	1:G:708:HIS:CD2	2.50	0.46
2:H:482:LEU:C	2:H:485:ILE:HG22	2.41	0.46
2:J:116:GLY:O	2:J:152:LYS:NZ	2.42	0.46
2:B:178:LEU:HD23	2:H:482:LEU:HD12	1.98	0.46
2:J:485:ILE:HD11	4:J:601:ACO:CEP	2.34	0.46
2:J:485:ILE:HD13	4:J:601:ACO:C7P	2.46	0.46
2:D:318:TYR:OH	2:D:533:ASP:OD1	2.32	0.45
2:D:484:THR:HG23	2:J:245:PRO:HB3	1.93	0.45
1:E:652:PRO:HD3	1:E:686:ILE:HD11	1.98	0.45
4:F:601:ACO:HH32	4:F:601:ACO:H22	1.73	0.45
1:I:707:ARG:HD2	1:I:708:HIS:CD2	2.50	0.45
1:A:531:HIS:NE2	2:B:300:LEU:HB2	2.30	0.45
1:A:704:GLN:HG2	2:J:252:GLY:O	2.17	0.45
2:B:527:TRP:CD1	2:H:187:ASP:CG	2.95	0.45
4:B:602:ACO:O9P	4:B:602:ACO:H141	2.16	0.45
3:C:801:BTN:H5	2:L:218:ALA:HB1	1.99	0.45
2:D:336:ALA:O	2:D:342:SER:OG	2.31	0.45
1:C:652:PRO:HD3	1:C:686:ILE:HD11	1.98	0.45
2:H:482:LEU:C	2:H:485:ILE:CG2	2.89	0.45
1:A:653:MET:HE3	2:D:408:MET:HE1	1.95	0.45
1:G:709:THR:HA	1:G:710:PRO:HD3	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:418:ILE:HG13	2:J:241:LEU:HD12	1.99	0.45
2:F:241:LEU:HD11	2:L:419:ALA:CB	2.46	0.45
3:G:801:BTN:C3	2:L:407:PHE:CB	2.94	0.45
2:B:193:ARG:NH1	2:H:456:ALA:O	2.50	0.45
2:H:482:LEU:CA	2:H:485:ILE:HG22	2.47	0.45
1:A:707:ARG:HD2	1:A:708:HIS:CD2	2.50	0.45
2:D:292:ARG:HG3	2:F:24:HIS:CE1	2.52	0.45
2:F:116:GLY:O	2:F:152:LYS:NZ	2.42	0.45
1:G:652:PRO:HD3	1:G:686:ILE:HD11	1.98	0.45
1:K:652:PRO:HD3	1:K:686:ILE:HD11	1.98	0.45
1:K:653:MET:CG	1:K:654:THR:N	2.80	0.45
1:A:653:MET:CG	1:A:654:THR:N	2.80	0.45
1:C:694:VAL:HG13	1:C:712:VAL:HG13	1.99	0.45
2:F:26:ASP:OD1	2:F:26:ASP:N	2.45	0.45
1:I:652:PRO:HD3	1:I:686:ILE:HD11	1.98	0.45
2:J:37:LEU:O	2:J:43:GLN:NE2	2.50	0.45
2:B:227:ALA:O	2:H:562:ARG:NH2	2.50	0.44
2:B:414:GLU:OE2	2:H:241:LEU:HB2	2.17	0.44
2:F:473:MET:HE2	2:F:473:MET:HB3	1.65	0.44
2:F:482:LEU:CD1	2:L:178:LEU:HD23	2.46	0.44
1:I:694:VAL:HG13	1:I:712:VAL:HG13	1.99	0.44
1:A:652:PRO:HD3	1:A:686:ILE:HD11	1.98	0.44
2:B:252:GLY:O	1:I:704:GLN:HG2	2.18	0.44
2:B:473:MET:CE	4:B:602:ACO:O	2.59	0.44
1:C:522:MET:HE3	2:F:23:TYR:OH	2.18	0.44
1:A:522:MET:CE	2:D:23:TYR:OH	2.66	0.44
3:A:801:BTN:C6	2:J:218:ALA:HB1	2.47	0.44
2:B:379:GLU:H	2:B:379:GLU:HG2	1.60	0.44
1:G:707:ARG:CD	1:G:708:HIS:CE1	2.94	0.44
2:L:37:LEU:O	2:L:43:GLN:NE2	2.50	0.44
1:C:653:MET:CG	1:C:654:THR:N	2.80	0.44
2:D:187:ASP:CG	2:J:527:TRP:CD1	2.96	0.44
2:D:241:LEU:HD11	2:J:419:ALA:N	2.31	0.44
2:F:37:LEU:O	2:F:43:GLN:NE2	2.50	0.44
2:F:527:TRP:CD1	2:L:187:ASP:CG	2.95	0.44
1:G:653:MET:CG	1:G:654:THR:N	2.80	0.44
1:G:694:VAL:HG13	1:G:712:VAL:HG13	1.99	0.44
2:J:406:GLY:C	1:K:680:MET:HE1	2.41	0.44
1:A:694:VAL:HG13	1:A:712:VAL:HG13	1.99	0.44
2:B:24:HIS:CE1	2:F:292:ARG:HG3	2.53	0.44
2:F:241:LEU:N	2:L:414:GLU:OE2	2.39	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:484:THR:HG23	2:L:245:PRO:HB3	1.92	0.44
2:L:176:ALA:N	4:L:601:ACO:HH32	2.32	0.44
2:L:326:LYS:HB2	2:L:326:LYS:HE2	1.79	0.44
3:A:801:BTN:H61	2:J:218:ALA:HB1	2.00	0.44
2:B:292:ARG:HG3	2:D:24:HIS:CE1	2.53	0.44
2:B:353:ASP:OD1	2:B:353:ASP:N	2.46	0.44
2:J:318:TYR:OH	2:J:533:ASP:OD1	2.32	0.44
1:A:653:MET:HE3	2:D:408:MET:SD	2.56	0.44
2:B:37:LEU:O	2:B:43:GLN:NE2	2.50	0.44
1:G:285:ILE:HG23	1:G:286:ILE:N	2.33	0.44
2:L:300:LEU:HD23	2:L:300:LEU:HA	1.86	0.44
1:E:608:LYS:HB2	1:E:608:LYS:HE3	1.74	0.44
2:H:326:LYS:HE2	2:H:326:LYS:HB2	1.79	0.44
2:B:318:TYR:OH	2:B:533:ASP:OD1	2.32	0.43
2:F:482:LEU:CD1	2:L:178:LEU:HD22	2.45	0.43
1:G:608:LYS:HB2	1:G:608:LYS:HE3	1.74	0.43
2:H:318:TYR:OH	2:H:533:ASP:OD1	2.32	0.43
1:I:707:ARG:CD	1:I:708:HIS:CE1	2.94	0.43
2:J:413:TYR:OH	1:K:707:ARG:HB2	2.18	0.43
2:J:452:MET:HE3	2:J:452:MET:HB3	1.80	0.43
4:J:601:ACO:N8P	4:J:601:ACO:H141	2.25	0.43
1:K:608:LYS:HB2	1:K:608:LYS:HE3	1.74	0.43
2:B:406:GLY:C	1:E:680:MET:HE1	2.41	0.43
2:D:379:GLU:H	2:D:379:GLU:HG2	1.59	0.43
1:E:653:MET:CG	1:E:654:THR:N	2.80	0.43
4:F:601:ACO:C7P	2:L:485:ILE:CD1	2.93	0.43
2:B:562:ARG:NH2	2:H:227:ALA:O	2.51	0.43
2:D:37:LEU:O	2:D:43:GLN:NE2	2.50	0.43
1:E:580:ASP:OD1	1:E:581:LYS:N	2.52	0.43
2:F:178:LEU:CD2	2:L:482:LEU:CD1	2.95	0.43
2:F:527:TRP:NE1	2:L:187:ASP:OD2	2.51	0.43
1:A:653:MET:HG2	2:D:408:MET:HE1	1.82	0.43
1:E:707:ARG:HD3	1:E:707:ARG:C	2.30	0.43
1:E:707:ARG:HD2	1:E:708:HIS:CD2	2.50	0.43
2:H:37:LEU:O	2:H:43:GLN:NE2	2.50	0.43
2:H:289:LYS:HE2	2:L:28:VAL:CG1	2.48	0.43
2:J:23:TYR:HB2	2:L:92:ASP:OD2	2.18	0.43
2:J:25:GLY:HA3	1:K:522:MET:SD	2.57	0.43
1:K:285:ILE:HG23	1:K:286:ILE:N	2.33	0.43
1:A:580:ASP:OD1	1:A:581:LYS:N	2.52	0.43
1:C:707:ARG:CD	1:C:708:HIS:CE1	2.94	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:801:BTN:O11	2:F:445:TYR:HB2	2.17	0.43
1:E:682:MET:HE2	1:E:684:HIS:CD2	2.54	0.43
2:J:489:GLN:HE21	4:J:601:ACO:H3B	1.83	0.43
2:L:333:GLU:O	2:L:337:ARG:NH1	2.49	0.43
1:E:694:VAL:HG13	1:E:712:VAL:HG13	1.99	0.43
2:F:318:TYR:OH	2:F:533:ASP:OD1	2.32	0.43
3:G:801:BTN:O3	2:L:407:PHE:CG	2.71	0.43
1:I:580:ASP:OD1	1:I:581:LYS:N	2.52	0.43
1:I:653:MET:CG	1:I:654:THR:N	2.80	0.43
2:J:23:TYR:OH	1:K:522:MET:CE	2.66	0.43
2:J:231:ILE:HG13	2:J:275:HIS:HB2	2.01	0.43
1:K:580:ASP:OD1	1:K:581:LYS:N	2.52	0.43
1:K:694:VAL:HG13	1:K:712:VAL:HG13	1.99	0.43
2:L:198:GLN:HE22	2:L:223:VAL:HG13	1.84	0.43
2:L:482:LEU:HA	2:L:485:ILE:HG22	2.01	0.43
2:B:92:ASP:OD2	2:D:23:TYR:HB2	2.19	0.43
2:B:315:ASP:OD1	2:B:315:ASP:N	2.48	0.43
2:B:336:ALA:O	2:B:342:SER:OG	2.31	0.43
2:F:452:MET:HE3	2:F:452:MET:HB3	1.80	0.43
2:H:315:ASP:OD1	2:H:315:ASP:N	2.47	0.43
2:J:198:GLN:HE22	2:J:223:VAL:HG13	1.84	0.43
2:B:419:ALA:HB2	2:H:241:LEU:HD11	1.99	0.43
2:B:456:ALA:O	2:H:193:ARG:NH1	2.50	0.43
1:C:580:ASP:OD1	1:C:581:LYS:N	2.52	0.43
2:D:452:MET:HE3	2:D:452:MET:HB3	1.80	0.43
2:D:485:ILE:HD11	4:J:602:ACO:C7P	2.26	0.43
1:I:682:MET:HE2	1:I:684:HIS:CD2	2.54	0.43
2:B:198:GLN:HE22	2:B:223:VAL:HG13	1.84	0.43
2:B:231:ILE:HG13	2:B:275:HIS:HB2	2.01	0.43
2:D:231:ILE:HG13	2:D:275:HIS:HB2	2.01	0.43
1:E:709:THR:HA	1:E:710:PRO:HD3	1.81	0.43
2:F:231:ILE:HG13	2:F:275:HIS:HB2	2.01	0.43
4:F:601:ACO:O9P	4:F:601:ACO:H131	2.19	0.43
2:B:25:GLY:HA3	1:E:522:MET:SD	2.59	0.42
1:C:681:LYS:CE	2:F:474:GLY:HA3	2.49	0.42
2:D:482:LEU:HA	2:D:485:ILE:HG22	2.00	0.42
2:H:333:GLU:O	2:H:337:ARG:NH1	2.49	0.42
1:I:285:ILE:HG23	1:I:286:ILE:N	2.33	0.42
2:J:405:THR:HG21	1:K:682:MET:HG3	1.90	0.42
2:L:176:ALA:O	4:L:601:ACO:CH3	2.67	0.42
2:B:484:THR:HG23	2:H:245:PRO:HB3	1.93	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:178:LEU:CD2	2:J:482:LEU:CD1	2.95	0.42
2:D:198:GLN:HE22	2:D:223:VAL:HG13	1.84	0.42
1:I:681:LYS:HE3	3:I:801:BTN:H102	1.86	0.42
1:A:681:LYS:HE2	2:D:474:GLY:HA3	2.01	0.42
2:B:562:ARG:HE	2:B:562:ARG:HB2	1.68	0.42
2:F:186:PRO:HG2	2:L:527:TRP:CZ3	2.54	0.42
1:G:580:ASP:OD1	1:G:581:LYS:N	2.52	0.42
2:H:198:GLN:HE22	2:H:223:VAL:HG13	1.84	0.42
2:B:482:LEU:HD12	2:H:178:LEU:HD23	2.00	0.42
2:J:408:MET:SD	1:K:653:MET:HE3	2.60	0.42
2:J:474:GLY:CA	1:K:681:LYS:NZ	2.82	0.42
1:K:709:THR:HA	1:K:710:PRO:HD3	1.81	0.42
2:B:241:LEU:HD11	2:H:419:ALA:CB	2.50	0.42
1:C:704:GLN:HG2	2:L:252:GLY:O	2.20	0.42
2:F:198:GLN:HE22	2:F:223:VAL:HG13	1.84	0.42
3:G:801:BTN:O11	2:L:445:TYR:HB2	2.20	0.42
2:L:226:MET:HE3	2:L:226:MET:HB3	1.89	0.42
1:A:706:ASN:O	1:A:709:THR:HB	2.20	0.42
1:A:709:THR:HA	1:A:710:PRO:HD3	1.81	0.42
1:E:707:ARG:CD	1:E:708:HIS:CE1	2.94	0.42
1:K:706:ASN:O	1:K:709:THR:HB	2.20	0.42
1:A:682:MET:HE2	1:A:684:HIS:CD2	2.54	0.42
2:B:112:GLU:OE1	2:B:146:TYR:OH	2.29	0.42
2:D:226:MET:HE3	2:D:226:MET:HB3	1.89	0.42
2:F:251:THR:HG21	2:L:409:VAL:CG2	2.24	0.42
2:B:245:PRO:HB3	2:H:484:THR:HG23	1.96	0.42
1:C:680:MET:HA	2:L:250:ALA:O	2.19	0.42
1:C:682:MET:HE2	1:C:684:HIS:CD2	2.54	0.42
2:D:419:ALA:N	2:J:241:LEU:HD11	2.35	0.42
2:D:560:ILE:HD11	2:H:393:GLN:OE1	2.19	0.42
1:K:682:MET:HE2	1:K:684:HIS:CD2	2.54	0.42
1:A:522:MET:SD	2:D:25:GLY:HA3	2.60	0.42
2:B:527:TRP:NE1	2:H:187:ASP:OD2	2.53	0.42
2:D:92:ASP:OD2	2:F:23:TYR:HB2	2.20	0.42
2:H:355:LEU:O	2:H:383:LYS:NZ	2.41	0.42
1:I:706:ASN:O	1:I:709:THR:HB	2.20	0.42
2:J:332:ARG:NH2	2:J:346:GLU:OE2	2.46	0.42
1:K:590:TYR:OH	1:K:608:LYS:CE	2.68	0.42
2:L:231:ILE:HG13	2:L:275:HIS:HB2	2.01	0.42
2:L:336:ALA:O	2:L:342:SER:OG	2.31	0.42
1:G:706:ASN:O	1:G:709:THR:HB	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:801:BTN:C3	2:L:407:PHE:HB3	2.50	0.41
2:J:26:ASP:OD1	2:J:26:ASP:N	2.45	0.41
1:K:263:ASP:C	1:K:263:ASP:OD1	2.63	0.41
2:F:474:GLY:O	2:F:476:GLU:OE1	2.38	0.41
2:H:231:ILE:HG13	2:H:275:HIS:HB2	2.01	0.41
2:J:300:LEU:HD23	2:J:300:LEU:HA	1.86	0.41
2:B:226:MET:HE3	2:B:226:MET:HB3	1.89	0.41
1:C:706:ASN:O	1:C:709:THR:HB	2.20	0.41
2:D:187:ASP:CB	2:D:190:HIS:ND1	2.80	0.41
2:D:241:LEU:HB2	2:J:414:GLU:OE2	2.20	0.41
2:D:326:LYS:HB2	2:D:326:LYS:HE2	1.79	0.41
2:F:174:GLY:HA2	4:F:601:ACO:H142	2.01	0.41
2:J:379:GLU:H	2:J:379:GLU:HG2	1.60	0.41
1:A:682:MET:SD	2:D:405:THR:OG1	2.67	0.41
2:H:406:GLY:C	1:I:680:MET:HE1	2.44	0.41
2:B:187:ASP:OD2	2:H:527:TRP:NE1	2.53	0.41
2:B:326:LYS:HA	2:B:326:LYS:HD2	1.90	0.41
2:B:476:GLU:O	2:B:480:ASN:ND2	2.53	0.41
1:C:522:MET:CE	2:F:23:TYR:OH	2.68	0.41
1:C:590:TYR:OH	1:C:608:LYS:CE	2.68	0.41
1:C:707:ARG:NE	1:C:708:HIS:NE2	2.69	0.41
2:D:476:GLU:O	2:D:480:ASN:ND2	2.53	0.41
2:F:178:LEU:HB3	2:L:482:LEU:HD11	2.02	0.41
2:H:178:LEU:C	2:H:180:ARG:H	2.28	0.41
1:K:707:ARG:CD	1:K:708:HIS:CE1	2.94	0.41
1:A:651:ALA:O	1:A:707:ARG:HA	2.21	0.41
1:A:675:MET:O	1:A:686:ILE:N	2.50	0.41
2:B:300:LEU:HD23	2:B:300:LEU:HA	1.86	0.41
2:B:418:ILE:HG13	2:H:241:LEU:HD12	2.03	0.41
2:F:414:GLU:OE2	2:L:241:LEU:CB	2.68	0.41
1:G:263:ASP:OD1	1:G:263:ASP:C	2.63	0.41
1:G:707:ARG:HH11	1:G:707:ARG:HG3	1.86	0.41
2:H:408:MET:SD	1:I:653:MET:HG3	2.49	0.41
2:J:226:MET:HE3	2:J:226:MET:HB3	1.89	0.41
1:K:651:ALA:O	1:K:707:ARG:HA	2.21	0.41
2:B:409:VAL:HG21	2:H:250:ALA:HB3	2.03	0.41
1:E:590:TYR:HH	1:E:608:LYS:CD	2.18	0.41
2:F:409:VAL:HG21	2:L:250:ALA:HB3	2.03	0.41
2:H:476:GLU:O	2:H:480:ASN:ND2	2.53	0.41
1:K:663:LYS:HE2	1:K:663:LYS:HB2	1.95	0.41
2:F:241:LEU:CB	2:L:414:GLU:OE2	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:333:GLU:O	2:F:337:ARG:NH1	2.49	0.41
2:F:476:GLU:O	2:F:480:ASN:ND2	2.53	0.41
2:H:288:ARG:NH2	2:L:23:TYR:HD2	2.19	0.41
2:H:300:LEU:HA	2:H:300:LEU:HD23	1.86	0.41
2:J:476:GLU:O	2:J:480:ASN:ND2	2.53	0.41
1:A:707:ARG:NE	1:A:708:HIS:NE2	2.69	0.41
2:D:178:LEU:HD22	2:J:482:LEU:CD1	2.49	0.41
1:E:590:TYR:OH	1:E:608:LYS:CE	2.68	0.41
1:E:707:ARG:HH11	1:E:707:ARG:HG3	1.86	0.41
2:F:187:ASP:CG	2:L:527:TRP:CD1	2.99	0.41
2:F:245:PRO:HB3	2:L:484:THR:HG23	2.01	0.41
1:I:263:ASP:OD1	1:I:263:ASP:C	2.63	0.41
1:I:590:TYR:OH	1:I:608:LYS:CE	2.68	0.41
1:K:707:ARG:HG3	1:K:707:ARG:HH11	1.86	0.41
1:A:707:ARG:HG3	1:A:707:ARG:HH11	1.86	0.41
1:C:651:ALA:O	1:C:707:ARG:HA	2.21	0.41
2:D:193:ARG:NH1	2:J:456:ALA:O	2.54	0.41
2:D:456:ALA:O	2:J:193:ARG:NH1	2.54	0.41
1:G:651:ALA:O	1:G:707:ARG:HA	2.21	0.41
2:H:23:TYR:HB2	2:J:92:ASP:OD2	2.21	0.41
1:I:663:LYS:HE2	1:I:663:LYS:HB2	1.95	0.41
2:J:485:ILE:HD11	4:J:601:ACO:OAP	2.21	0.41
1:K:288:GLU:HG2	1:K:382:PHE:CE2	2.56	0.41
1:K:707:ARG:NE	1:K:708:HIS:NE2	2.69	0.41
1:A:654:THR:CG2	2:D:413:TYR:HE2	2.34	0.40
2:B:241:LEU:HB2	2:H:414:GLU:OE2	2.21	0.40
2:B:445:TYR:HB2	3:E:801:BTN:O11	2.19	0.40
1:E:651:ALA:O	1:E:707:ARG:HA	2.21	0.40
2:F:445:TYR:CE1	2:F:473:MET:O	2.72	0.40
1:G:288:GLU:HG2	1:G:382:PHE:CE2	2.56	0.40
1:G:682:MET:HE2	1:G:684:HIS:CD2	2.54	0.40
2:J:177:TYR:O	2:J:179:PRO:HD2	2.21	0.40
2:L:476:GLU:O	2:L:480:ASN:ND2	2.53	0.40
2:B:405:THR:HG22	1:E:681:LYS:HG3	2.03	0.40
4:B:602:ACO:HH32	2:H:178:LEU:HD12	2.01	0.40
2:D:218:ALA:HB1	3:K:801:BTN:H5	2.03	0.40
1:I:651:ALA:O	1:I:707:ARG:HA	2.21	0.40
1:I:707:ARG:NE	1:I:708:HIS:NE2	2.69	0.40
2:B:187:ASP:CB	2:B:190:HIS:ND1	2.80	0.40
2:B:251:THR:HG22	1:I:653:MET:HE2	2.02	0.40
1:C:680:MET:HE1	2:F:407:PHE:N	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:706:ASN:O	1:E:709:THR:HB	2.20	0.40
1:E:707:ARG:NE	1:E:708:HIS:NE2	2.69	0.40
2:H:348:LYS:HE3	2:J:274:ASP:OD1	2.22	0.40
2:H:452:MET:HB3	2:H:452:MET:HE3	1.80	0.40
1:I:76:VAL:HA	1:I:94:GLU:O	2.22	0.40
2:J:177:TYR:O	2:J:178:LEU:CB	2.70	0.40
1:K:681:LYS:HE3	3:K:801:BTN:H102	1.86	0.40
2:L:452:MET:HE3	2:L:452:MET:HB3	1.80	0.40
2:B:325:LEU:HD23	2:B:325:LEU:HA	1.89	0.40
2:B:473:MET:O	2:B:474:GLY:O	2.40	0.40
1:G:590:TYR:OH	1:G:608:LYS:CE	2.68	0.40
1:G:681:LYS:HG3	2:L:405:THR:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	206/725 (28%)	191 (93%)	14 (7%)	1 (0%)	24	42
1	C	206/725 (28%)	191 (93%)	14 (7%)	1 (0%)	24	42
1	E	206/725 (28%)	191 (93%)	14 (7%)	1 (0%)	24	42
1	G	578/725 (80%)	557 (96%)	20 (4%)	1 (0%)	43	62
1	I	656/725 (90%)	632 (96%)	23 (4%)	1 (0%)	43	62
1	K	578/725 (80%)	557 (96%)	20 (4%)	1 (0%)	43	62
2	B	539/563 (96%)	500 (93%)	34 (6%)	5 (1%)	14	28
2	D	539/563 (96%)	499 (93%)	36 (7%)	4 (1%)	18	35
2	F	539/563 (96%)	499 (93%)	35 (6%)	5 (1%)	14	28
2	H	539/563 (96%)	497 (92%)	37 (7%)	5 (1%)	14	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	539/563 (96%)	496 (92%)	36 (7%)	7 (1%)	9	21
2	L	539/563 (96%)	501 (93%)	34 (6%)	4 (1%)	18	35
All	All	5664/7728 (73%)	5311 (94%)	317 (6%)	36 (1%)	23	38

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	187	ASP
2	B	191	PHE
2	D	187	ASP
2	D	191	PHE
2	F	187	ASP
2	F	191	PHE
2	H	176	ALA
2	H	187	ASP
2	H	191	PHE
2	J	178	LEU
2	J	187	ASP
2	J	191	PHE
2	L	187	ASP
2	L	191	PHE
2	H	473	MET
2	B	177	TYR
2	D	177	TYR
2	F	177	TYR
2	J	176	ALA
2	J	473	MET
2	L	177	TYR
1	A	707	ARG
1	C	707	ARG
1	E	707	ARG
1	G	707	ARG
1	I	707	ARG
1	K	707	ARG
2	F	473	MET
2	J	476	GLU
2	B	186	PRO
2	D	186	PRO
2	F	186	PRO
2	H	186	PRO
2	J	186	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	186	PRO
2	B	474	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	179/609 (29%)	172 (96%)	7 (4%)	28	54
1	C	179/609 (29%)	173 (97%)	6 (3%)	32	58
1	E	179/609 (29%)	173 (97%)	6 (3%)	32	58
1	G	490/609 (80%)	483 (99%)	7 (1%)	59	78
1	I	553/609 (91%)	547 (99%)	6 (1%)	65	81
1	K	490/609 (80%)	484 (99%)	6 (1%)	63	80
2	B	430/445 (97%)	426 (99%)	4 (1%)	70	84
2	D	430/445 (97%)	425 (99%)	5 (1%)	63	80
2	F	430/445 (97%)	426 (99%)	4 (1%)	70	84
2	H	430/445 (97%)	427 (99%)	3 (1%)	76	87
2	J	430/445 (97%)	425 (99%)	5 (1%)	63	80
2	L	430/445 (97%)	426 (99%)	4 (1%)	70	84
All	All	4650/6324 (74%)	4587 (99%)	63 (1%)	57	78

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	672	ASP
1	A	677	MET
1	A	678	ILE
1	A	682	MET
1	A	707	ARG
1	A	709	THR
1	A	712	VAL
2	B	140	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	187	ASP
2	B	301	ASP
2	B	326	LYS
1	C	672	ASP
1	C	677	MET
1	C	678	ILE
1	C	682	MET
1	C	707	ARG
1	C	709	THR
2	D	140	VAL
2	D	187	ASP
2	D	301	ASP
2	D	473	MET
2	D	485	ILE
1	E	672	ASP
1	E	677	MET
1	E	678	ILE
1	E	707	ARG
1	E	709	THR
1	E	712	VAL
2	F	140	VAL
2	F	187	ASP
2	F	301	ASP
2	F	473	MET
1	G	672	ASP
1	G	677	MET
1	G	678	ILE
1	G	682	MET
1	G	707	ARG
1	G	709	THR
1	G	712	VAL
2	H	140	VAL
2	H	187	ASP
2	H	301	ASP
1	I	672	ASP
1	I	677	MET
1	I	678	ILE
1	I	682	MET
1	I	707	ARG
1	I	709	THR
2	J	140	VAL
2	J	180	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	187	ASP
2	J	301	ASP
2	J	326	LYS
1	K	672	ASP
1	K	677	MET
1	K	678	ILE
1	K	682	MET
1	K	707	ARG
1	K	709	THR
2	L	140	VAL
2	L	187	ASP
2	L	301	ASP
2	L	485	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	531	HIS
1	A	552	ASN
1	A	561	ASN
1	A	706	ASN
2	B	24	HIS
2	B	43	GLN
2	B	230	ASN
2	B	281	HIS
2	B	389	GLN
2	B	449	ASN
2	B	480	ASN
2	B	489	GLN
1	C	531	HIS
1	C	552	ASN
1	C	561	ASN
1	C	706	ASN
2	D	24	HIS
2	D	198	GLN
2	D	230	ASN
2	D	281	HIS
2	D	389	GLN
2	D	449	ASN
2	D	480	ASN
2	D	489	GLN
1	E	531	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	552	ASN
1	E	561	ASN
1	E	706	ASN
2	F	24	HIS
2	F	43	GLN
2	F	198	GLN
2	F	230	ASN
2	F	281	HIS
2	F	389	GLN
2	F	449	ASN
2	F	480	ASN
2	F	489	GLN
1	G	264	HIS
1	G	337	ASN
1	G	459	ASN
1	G	531	HIS
1	G	552	ASN
1	G	561	ASN
1	G	706	ASN
2	H	24	HIS
2	H	43	GLN
2	H	230	ASN
2	H	281	HIS
2	H	285	HIS
2	H	389	GLN
2	H	449	ASN
2	H	480	ASN
2	H	489	GLN
1	I	264	HIS
1	I	337	ASN
1	I	459	ASN
1	I	531	HIS
1	I	552	ASN
1	I	561	ASN
1	I	706	ASN
2	J	24	HIS
2	J	43	GLN
2	J	198	GLN
2	J	230	ASN
2	J	281	HIS
2	J	389	GLN
2	J	449	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	480	ASN
2	J	489	GLN
1	K	264	HIS
1	K	337	ASN
1	K	459	ASN
1	K	531	HIS
1	K	552	ASN
1	K	706	ASN
2	L	24	HIS
2	L	43	GLN
2	L	198	GLN
2	L	230	ASN
2	L	281	HIS
2	L	293	ASN
2	L	389	GLN
2	L	449	ASN
2	L	480	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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
3	BTN	A	801	1	15,16,17	3.31	2 (13%)	20,21,23	1.71	3 (15%)
4	ACO	F	601	-	51,53,53	1.11	5 (9%)	73,79,79	1.49	11 (15%)
4	ACO	L	601	-	51,53,53	1.06	5 (9%)	73,79,79	1.56	13 (17%)
3	BTN	I	801	1	15,16,17	3.31	2 (13%)	20,21,23	1.71	3 (15%)
3	BTN	G	801	1	15,16,17	3.31	2 (13%)	20,21,23	1.71	3 (15%)
4	ACO	B	602	-	51,53,53	1.11	5 (9%)	73,79,79	1.51	9 (12%)
3	BTN	E	801	1	15,16,17	3.30	2 (13%)	20,21,23	1.71	3 (15%)
3	BTN	C	801	1	15,16,17	3.33	2 (13%)	20,21,23	1.71	3 (15%)
3	BTN	K	801	1	15,16,17	3.31	2 (13%)	20,21,23	1.71	3 (15%)
4	ACO	J	601	-	51,53,53	1.11	5 (9%)	73,79,79	1.50	10 (13%)
4	ACO	B	601	-	51,53,53	1.11	5 (9%)	73,79,79	1.47	10 (13%)
4	ACO	J	602	-	51,53,53	1.09	5 (9%)	73,79,79	1.58	11 (15%)

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
3	BTN	A	801	1	-	4/6/27/28	0/2/2/2
4	ACO	F	601	-	-	20/51/67/67	0/3/3/3
4	ACO	L	601	-	-	14/51/67/67	0/3/3/3
3	BTN	I	801	1	-	4/6/27/28	0/2/2/2
3	BTN	G	801	1	-	4/6/27/28	0/2/2/2
4	ACO	B	602	-	-	15/51/67/67	0/3/3/3
3	BTN	E	801	1	-	4/6/27/28	0/2/2/2
3	BTN	C	801	1	-	4/6/27/28	0/2/2/2
3	BTN	K	801	1	-	4/6/27/28	0/2/2/2
4	ACO	J	601	-	-	20/51/67/67	0/3/3/3
4	ACO	B	601	-	-	21/51/67/67	0/3/3/3
4	ACO	J	602	-	-	28/51/67/67	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	801	BTN	C2-S1	-9.32	1.67	1.82
3	I	801	BTN	C2-S1	-9.26	1.68	1.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	BTN	C2-S1	-9.26	1.68	1.82
3	K	801	BTN	C2-S1	-9.26	1.68	1.82
3	G	801	BTN	C2-S1	-9.26	1.68	1.82
3	E	801	BTN	C2-S1	-9.24	1.68	1.82
3	C	801	BTN	O3-C3	8.34	1.41	1.23
3	G	801	BTN	O3-C3	8.34	1.41	1.23
3	A	801	BTN	O3-C3	8.33	1.41	1.23
3	I	801	BTN	O3-C3	8.33	1.41	1.23
3	K	801	BTN	O3-C3	8.32	1.41	1.23
3	E	801	BTN	O3-C3	8.31	1.41	1.23
4	F	601	ACO	C5A-C4A	4.41	1.46	1.39
4	B	601	ACO	C5A-C4A	4.29	1.46	1.39
4	B	602	ACO	C5A-C4A	4.13	1.46	1.39
4	L	601	ACO	C5A-C4A	4.06	1.46	1.39
4	J	602	ACO	C5A-C4A	4.03	1.46	1.39
4	J	601	ACO	C5A-C4A	4.02	1.46	1.39
4	B	601	ACO	C5A-N7A	-2.66	1.34	1.39
4	J	602	ACO	C5A-C6A	2.64	1.48	1.41
4	F	601	ACO	C5A-C6A	2.60	1.48	1.41
4	B	602	ACO	C5A-C6A	2.57	1.48	1.41
4	F	601	ACO	C8A-N7A	2.49	1.36	1.31
4	J	602	ACO	C5A-N7A	-2.47	1.34	1.39
4	L	601	ACO	C5A-C6A	2.46	1.47	1.41
4	B	601	ACO	C5A-C6A	2.45	1.47	1.41
4	J	601	ACO	C5A-C6A	2.44	1.47	1.41
4	B	602	ACO	C5A-N7A	-2.42	1.34	1.39
4	F	601	ACO	C5A-N7A	-2.40	1.34	1.39
4	B	601	ACO	C8A-N7A	2.29	1.36	1.31
4	L	601	ACO	C5A-N7A	-2.29	1.34	1.39
4	L	601	ACO	C4A-N9A	-2.23	1.33	1.37
4	J	601	ACO	C5A-N7A	-2.22	1.35	1.39
4	J	601	ACO	C4A-N9A	-2.21	1.33	1.37
4	F	601	ACO	C4A-N9A	-2.17	1.33	1.37
4	J	602	ACO	C8A-N7A	2.15	1.35	1.31
4	J	601	ACO	C8A-N7A	2.14	1.35	1.31
4	B	602	ACO	C8A-N7A	2.14	1.35	1.31
4	B	601	ACO	C4A-N9A	-2.13	1.33	1.37
4	L	601	ACO	C8A-N7A	2.09	1.35	1.31
4	B	602	ACO	C4A-N9A	-2.09	1.33	1.37
4	J	602	ACO	C4A-N9A	-2.02	1.33	1.37

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	602	ACO	C5A-C4A-N3A	-5.98	118.48	126.72
4	F	601	ACO	C5A-C4A-N3A	-5.66	118.92	126.72
4	J	601	ACO	C5A-C4A-N3A	-5.63	118.97	126.72
4	B	602	ACO	C5A-C4A-N3A	-5.63	118.97	126.72
4	B	601	ACO	C5A-C4A-N3A	-5.45	119.22	126.72
4	L	601	ACO	C5A-C4A-N3A	-5.44	119.23	126.72
3	G	801	BTN	C4-C2-S1	5.27	111.01	105.03
3	C	801	BTN	C4-C2-S1	5.26	111.00	105.03
3	E	801	BTN	C4-C2-S1	5.26	111.00	105.03
3	I	801	BTN	C4-C2-S1	5.26	111.00	105.03
3	K	801	BTN	C4-C2-S1	5.26	111.00	105.03
3	A	801	BTN	C4-C2-S1	5.22	110.97	105.03
4	J	601	ACO	N3A-C4A-N9A	4.59	134.97	127.17
4	J	602	ACO	N3A-C4A-N9A	4.49	134.81	127.17
4	B	602	ACO	N3A-C4A-N9A	4.47	134.77	127.17
4	L	601	ACO	N3A-C4A-N9A	4.31	134.49	127.17
4	B	601	ACO	N3A-C4A-N9A	4.19	134.29	127.17
4	F	601	ACO	N3A-C4A-N9A	4.17	134.26	127.17
4	J	602	ACO	C2A-N3A-C4A	3.99	121.57	111.83
4	F	601	ACO	C4A-C5A-N7A	-3.92	106.10	110.58
4	J	602	ACO	C4A-C5A-N7A	-3.82	106.22	110.58
4	B	602	ACO	C2A-N3A-C4A	3.77	121.04	111.83
4	L	601	ACO	C2A-N3A-C4A	3.75	120.99	111.83
4	L	601	ACO	C4A-C5A-N7A	-3.71	106.34	110.58
4	B	601	ACO	C4A-C5A-N7A	-3.71	106.34	110.58
4	J	601	ACO	C4A-C5A-N7A	-3.69	106.37	110.58
4	B	601	ACO	C2A-N3A-C4A	3.68	120.83	111.83
4	J	601	ACO	C4A-N9A-C8A	3.67	109.59	105.74
4	F	601	ACO	C2A-N3A-C4A	3.64	120.71	111.83
4	B	601	ACO	N3A-C2A-N1A	-3.62	123.10	128.58
4	L	601	ACO	N3A-C2A-N1A	-3.62	123.11	128.58
4	J	601	ACO	C2A-N3A-C4A	3.57	120.56	111.83
4	J	602	ACO	N3A-C2A-N1A	-3.56	123.20	128.58
4	B	602	ACO	C4A-C5A-N7A	-3.47	106.62	110.58
4	B	602	ACO	N3A-C2A-N1A	-3.44	123.38	128.58
4	L	601	ACO	C4A-N9A-C8A	3.31	109.22	105.74
4	F	601	ACO	N3A-C2A-N1A	-3.24	123.68	128.58
4	J	601	ACO	N3A-C2A-N1A	-3.04	123.98	128.58
3	E	801	BTN	C5-C6-S1	3.04	110.25	106.06
3	K	801	BTN	C5-C6-S1	3.04	110.24	106.06
3	A	801	BTN	C5-C6-S1	3.03	110.23	106.06
3	I	801	BTN	C5-C6-S1	3.03	110.23	106.06
3	G	801	BTN	C5-C6-S1	3.02	110.22	106.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	801	BTN	C5-C6-S1	3.02	110.22	106.06
4	J	602	ACO	CEP-CBP-CAP	2.97	113.83	108.77
4	B	602	ACO	C4A-N9A-C8A	2.95	108.83	105.74
4	J	601	ACO	C5A-N7A-C8A	2.86	107.94	103.45
4	B	601	ACO	C4A-N9A-C8A	2.83	108.71	105.74
4	L	601	ACO	C5A-N7A-C8A	2.79	107.83	103.45
4	J	602	ACO	C5A-N7A-C8A	2.78	107.82	103.45
4	B	601	ACO	C5A-N7A-C8A	2.78	107.81	103.45
4	J	601	ACO	N9A-C8A-N7A	-2.76	110.03	113.94
4	F	601	ACO	C4A-N9A-C8A	2.75	108.62	105.74
4	F	601	ACO	C5A-N7A-C8A	2.73	107.74	103.45
4	J	602	ACO	C4A-N9A-C8A	2.62	108.49	105.74
4	B	602	ACO	C5A-N7A-C8A	2.61	107.55	103.45
4	L	601	ACO	C6A-C5A-N7A	2.59	137.09	132.09
4	L	601	ACO	N9A-C8A-N7A	-2.54	110.33	113.94
4	J	602	ACO	C6A-C5A-N7A	2.46	136.83	132.09
4	F	601	ACO	C6A-C5A-N7A	2.45	136.82	132.09
4	B	601	ACO	C6A-C5A-N7A	2.44	136.79	132.09
4	J	601	ACO	O6A-CCP-CBP	-2.40	106.69	110.55
3	G	801	BTN	C6-C5-N1	-2.33	110.18	113.18
4	B	602	ACO	C6A-C5A-N7A	2.32	136.57	132.09
4	B	601	ACO	N9A-C8A-N7A	-2.32	110.64	113.94
3	C	801	BTN	C6-C5-N1	-2.32	110.19	113.18
3	A	801	BTN	C6-C5-N1	-2.31	110.20	113.18
3	E	801	BTN	C6-C5-N1	-2.30	110.21	113.18
3	I	801	BTN	C6-C5-N1	-2.30	110.22	113.18
4	L	601	ACO	C3B-C2B-C1B	2.29	104.93	99.89
3	K	801	BTN	C6-C5-N1	-2.28	110.25	113.18
4	L	601	ACO	O5A-P2A-O4A	2.27	122.99	112.44
4	F	601	ACO	N9A-C8A-N7A	-2.26	110.72	113.94
4	B	602	ACO	N9A-C8A-N7A	-2.25	110.74	113.94
4	J	602	ACO	N9A-C8A-N7A	-2.23	110.77	113.94
4	J	601	ACO	C6A-C5A-N7A	2.21	136.35	132.09
4	L	601	ACO	C2A-N1A-C6A	2.19	122.33	118.73
4	B	601	ACO	C2A-N1A-C6A	2.14	122.24	118.73
4	F	601	ACO	O3B-C3B-C2B	-2.07	104.24	111.68
4	L	601	ACO	O9A-P3B-O8A	2.07	115.55	107.80
4	F	601	ACO	C2A-N1A-C6A	2.06	122.11	118.73
4	J	602	ACO	CDP-CBP-CCP	2.04	111.59	108.22

There are no chirality outliers.

All (142) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	BTN	C9-C10-C11-O11
3	A	801	BTN	C2-C7-C8-C9
3	A	801	BTN	S1-C2-C7-C8
3	C	801	BTN	C9-C10-C11-O11
3	C	801	BTN	C2-C7-C8-C9
3	C	801	BTN	S1-C2-C7-C8
3	E	801	BTN	C9-C10-C11-O11
3	E	801	BTN	C2-C7-C8-C9
3	E	801	BTN	S1-C2-C7-C8
3	G	801	BTN	C9-C10-C11-O11
3	G	801	BTN	C2-C7-C8-C9
3	G	801	BTN	S1-C2-C7-C8
3	I	801	BTN	C9-C10-C11-O11
3	I	801	BTN	C2-C7-C8-C9
3	I	801	BTN	S1-C2-C7-C8
3	K	801	BTN	C9-C10-C11-O11
3	K	801	BTN	C2-C7-C8-C9
3	K	801	BTN	S1-C2-C7-C8
4	B	601	ACO	C4B-C3B-O3B-P3B
4	B	601	ACO	C5B-O5B-P1A-O1A
4	B	601	ACO	C5B-O5B-P1A-O2A
4	B	601	ACO	C5B-O5B-P1A-O3A
4	B	601	ACO	CCP-O6A-P2A-O4A
4	B	601	ACO	O9P-C9P-CAP-OAP
4	B	601	ACO	O-C-S1P-C2P
4	B	601	ACO	CH3-C-S1P-C2P
4	B	602	ACO	C5B-O5B-P1A-O3A
4	B	602	ACO	O9P-C9P-CAP-OAP
4	B	602	ACO	S1P-C2P-C3P-N4P
4	B	602	ACO	O-C-S1P-C2P
4	B	602	ACO	CH3-C-S1P-C2P
4	F	601	ACO	CDP-CBP-CCP-O6A
4	F	601	ACO	CEP-CBP-CCP-O6A
4	F	601	ACO	CAP-CBP-CCP-O6A
4	F	601	ACO	CAP-C9P-N8P-C7P
4	F	601	ACO	O9P-C9P-N8P-C7P
4	F	601	ACO	C5P-C6P-C7P-N8P
4	F	601	ACO	C6P-C5P-N4P-C3P
4	F	601	ACO	O5P-C5P-N4P-C3P
4	F	601	ACO	C3P-C2P-S1P-C
4	F	601	ACO	O-C-S1P-C2P
4	F	601	ACO	CH3-C-S1P-C2P
4	J	601	ACO	CCP-O6A-P2A-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	J	601	ACO	CCP-O6A-P2A-O4A
4	J	601	ACO	CCP-O6A-P2A-O5A
4	J	601	ACO	O9P-C9P-CAP-CBP
4	J	601	ACO	N8P-C9P-CAP-CBP
4	J	601	ACO	N8P-C9P-CAP-OAP
4	J	601	ACO	CAP-C9P-N8P-C7P
4	J	601	ACO	C6P-C5P-N4P-C3P
4	J	601	ACO	O5P-C5P-N4P-C3P
4	J	601	ACO	S1P-C2P-C3P-N4P
4	J	601	ACO	C3P-C2P-S1P-C
4	J	601	ACO	O-C-S1P-C2P
4	J	601	ACO	CH3-C-S1P-C2P
4	J	602	ACO	C3B-C4B-C5B-O5B
4	J	602	ACO	O4B-C4B-C5B-O5B
4	J	602	ACO	C5B-O5B-P1A-O3A
4	J	602	ACO	CBP-CCP-O6A-P2A
4	J	602	ACO	CDP-CBP-CCP-O6A
4	J	602	ACO	CEP-CBP-CCP-O6A
4	J	602	ACO	CAP-CBP-CCP-O6A
4	J	602	ACO	OAP-CAP-CBP-CCP
4	J	602	ACO	C9P-CAP-CBP-CCP
4	J	602	ACO	OAP-CAP-CBP-CDP
4	J	602	ACO	C9P-CAP-CBP-CDP
4	J	602	ACO	OAP-CAP-CBP-CEP
4	J	602	ACO	C9P-CAP-CBP-CEP
4	J	602	ACO	O9P-C9P-CAP-OAP
4	J	602	ACO	CAP-C9P-N8P-C7P
4	J	602	ACO	O9P-C9P-N8P-C7P
4	J	602	ACO	C5P-C6P-C7P-N8P
4	J	602	ACO	C6P-C5P-N4P-C3P
4	J	602	ACO	C2P-C3P-N4P-C5P
4	J	602	ACO	S1P-C2P-C3P-N4P
4	J	602	ACO	O-C-S1P-C2P
4	J	602	ACO	CH3-C-S1P-C2P
4	L	601	ACO	C5B-O5B-P1A-O1A
4	L	601	ACO	CAP-C9P-N8P-C7P
4	L	601	ACO	C6P-C5P-N4P-C3P
4	L	601	ACO	O5P-C5P-N4P-C3P
4	L	601	ACO	C3P-C2P-S1P-C
4	J	601	ACO	O9P-C9P-N8P-C7P
4	L	601	ACO	O9P-C9P-N8P-C7P
4	J	602	ACO	O5P-C5P-N4P-C3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	J	601	ACO	C4B-C3B-O3B-P3B
4	L	601	ACO	C4B-C3B-O3B-P3B
4	F	601	ACO	C3B-C4B-C5B-O5B
4	F	601	ACO	O4B-C4B-C5B-O5B
4	L	601	ACO	C3B-C4B-C5B-O5B
4	L	601	ACO	O4B-C4B-C5B-O5B
4	J	602	ACO	C2B-C3B-O3B-P3B
4	J	602	ACO	C4B-C3B-O3B-P3B
3	A	801	BTN	C7-C8-C9-C10
3	C	801	BTN	C7-C8-C9-C10
3	E	801	BTN	C7-C8-C9-C10
3	G	801	BTN	C7-C8-C9-C10
3	I	801	BTN	C7-C8-C9-C10
3	K	801	BTN	C7-C8-C9-C10
4	L	601	ACO	C5P-C6P-C7P-N8P
4	J	601	ACO	O9P-C9P-CAP-OAP
4	J	601	ACO	OAP-CAP-CBP-CDP
4	L	601	ACO	S1P-C2P-C3P-N4P
4	B	601	ACO	N8P-C9P-CAP-CBP
4	F	601	ACO	N8P-C9P-CAP-CBP
4	B	601	ACO	N8P-C9P-CAP-OAP
4	B	602	ACO	C2P-C3P-N4P-C5P
4	B	602	ACO	C5P-C6P-C7P-N8P
4	B	601	ACO	C6P-C7P-N8P-C9P
4	F	601	ACO	CBP-CCP-O6A-P2A
4	B	601	ACO	CDP-CBP-CCP-O6A
4	B	602	ACO	C3P-C2P-S1P-C
4	F	601	ACO	C3B-O3B-P3B-O7A
4	L	601	ACO	O-C-S1P-C2P
4	B	601	ACO	CCP-O6A-P2A-O3A
4	B	601	ACO	CCP-O6A-P2A-O5A
4	B	602	ACO	C5B-O5B-P1A-O1A
4	F	601	ACO	C5B-O5B-P1A-O1A
4	J	601	ACO	OAP-CAP-CBP-CCP
4	J	602	ACO	C5B-O5B-P1A-O1A
4	B	601	ACO	P2A-O3A-P1A-O2A
4	F	601	ACO	P1A-O3A-P2A-O4A
4	B	601	ACO	O9P-C9P-CAP-CBP
4	F	601	ACO	O9P-C9P-CAP-CBP
4	B	602	ACO	C4B-C3B-O3B-P3B
4	L	601	ACO	CH3-C-S1P-C2P
4	B	602	ACO	N8P-C9P-CAP-OAP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	602	ACO	C2B-C3B-O3B-P3B
4	B	601	ACO	C3B-O3B-P3B-O7A
4	F	601	ACO	P1A-O3A-P2A-O5A
4	B	601	ACO	O5P-C5P-N4P-C3P
4	J	601	ACO	P2A-O3A-P1A-O1A
4	B	602	ACO	CBP-CCP-O6A-P2A
4	B	602	ACO	O5P-C5P-C6P-C7P
4	B	601	ACO	CEP-CBP-CCP-O6A
4	B	601	ACO	C5P-C6P-C7P-N8P
4	J	602	ACO	C3B-O3B-P3B-O7A
4	B	601	ACO	C6P-C5P-N4P-C3P
4	J	602	ACO	N8P-C9P-CAP-OAP
4	L	601	ACO	N8P-C9P-CAP-OAP
4	B	602	ACO	N4P-C5P-C6P-C7P
4	J	601	ACO	P2A-O3A-P1A-O2A

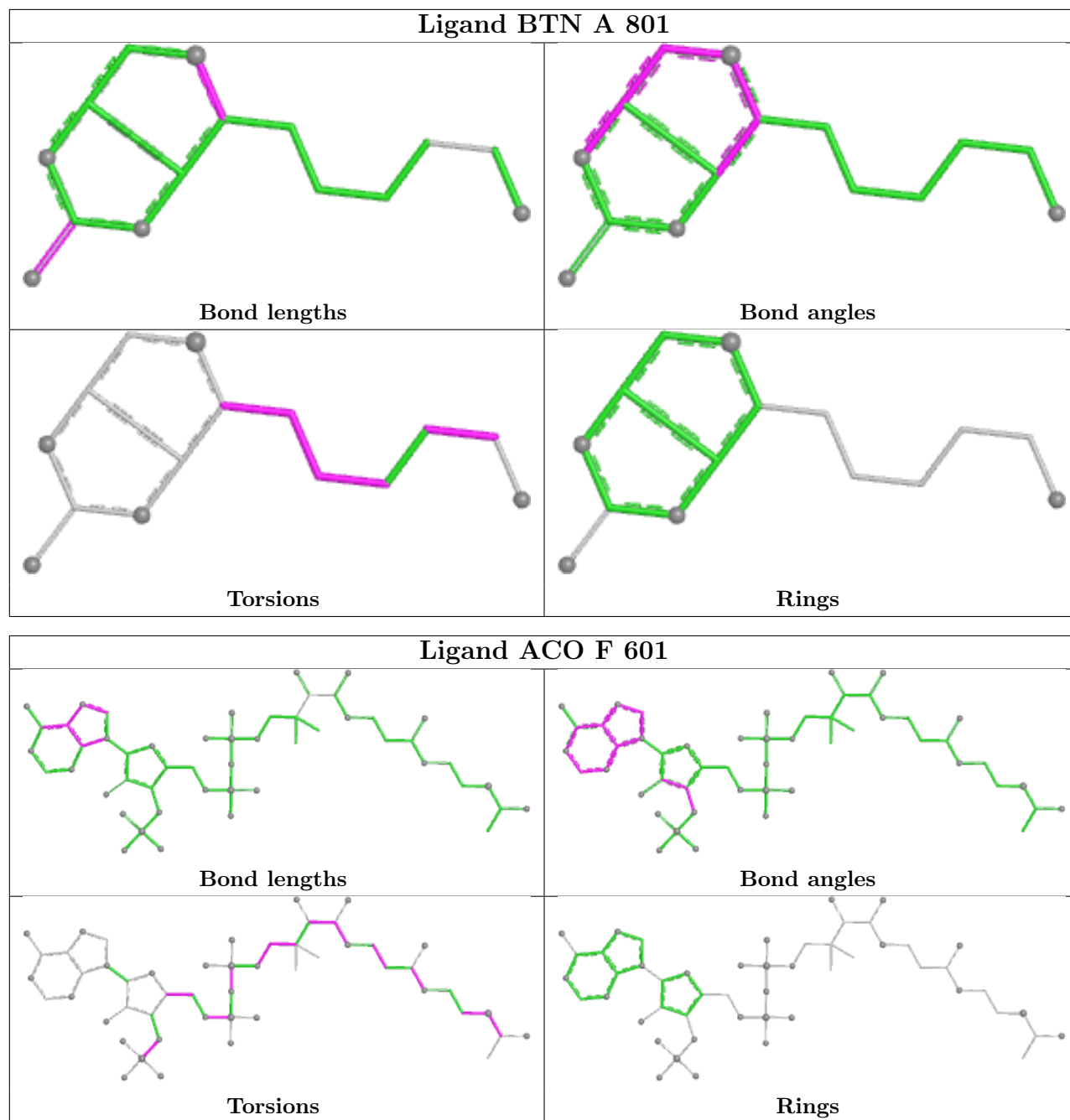
There are no ring outliers.

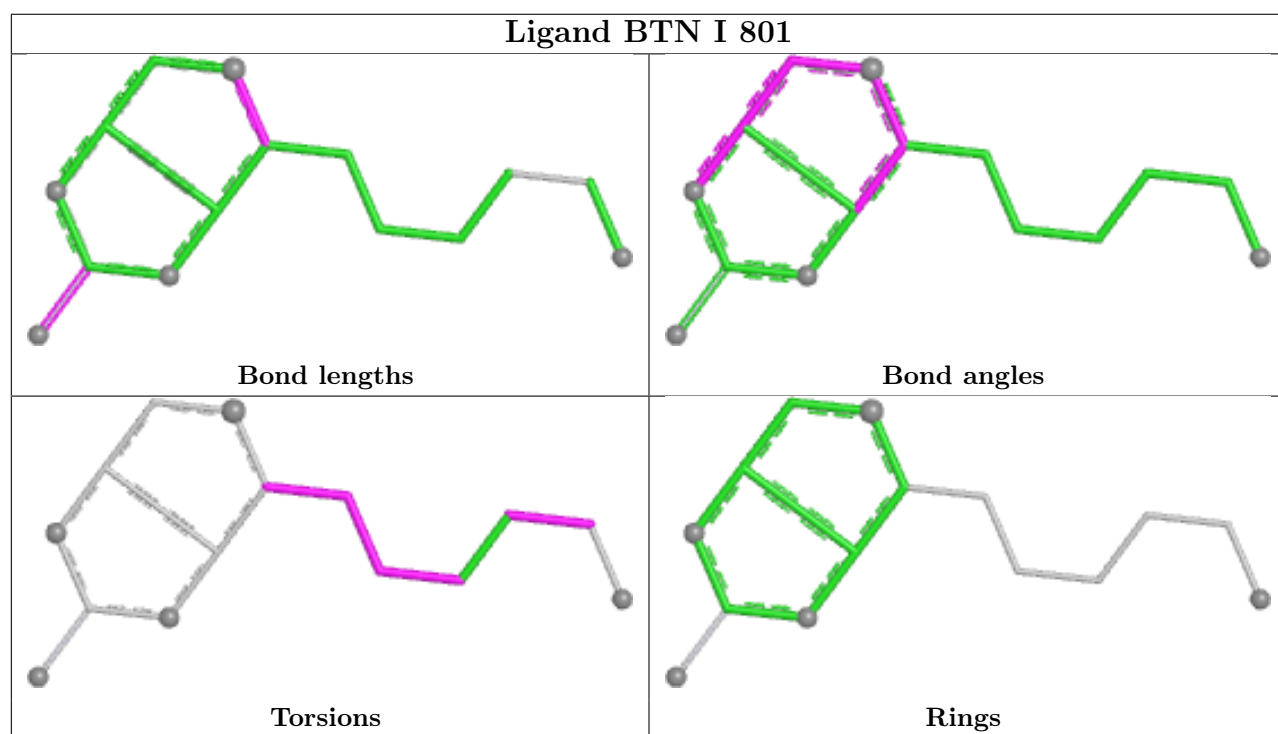
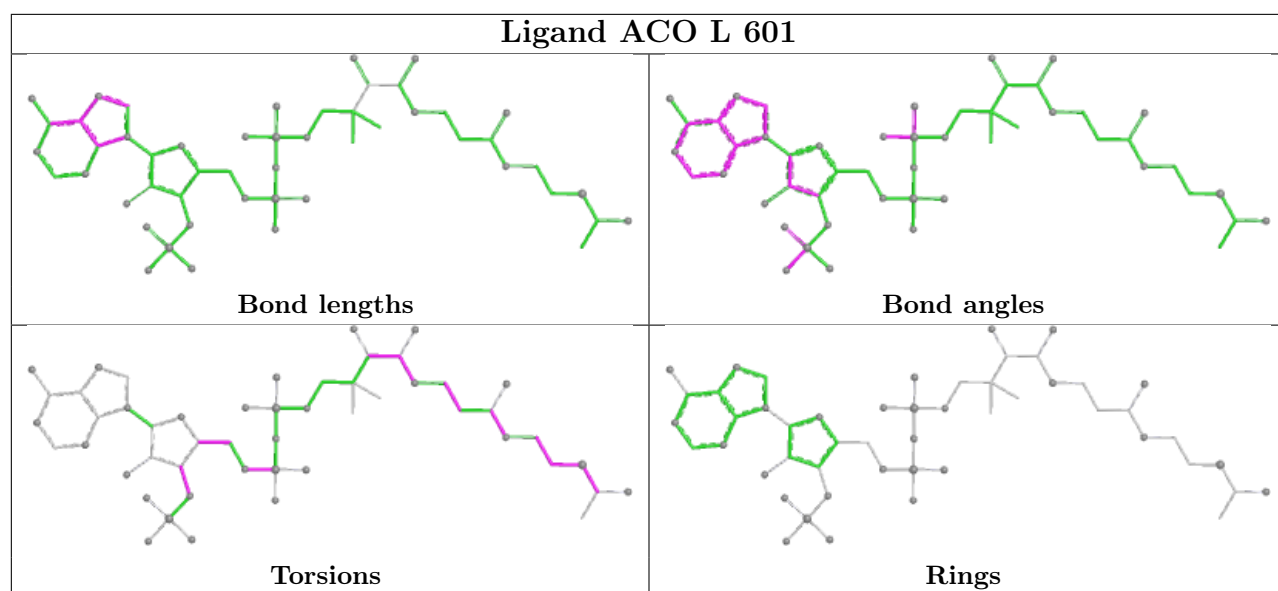
12 monomers are involved in 166 short contacts:

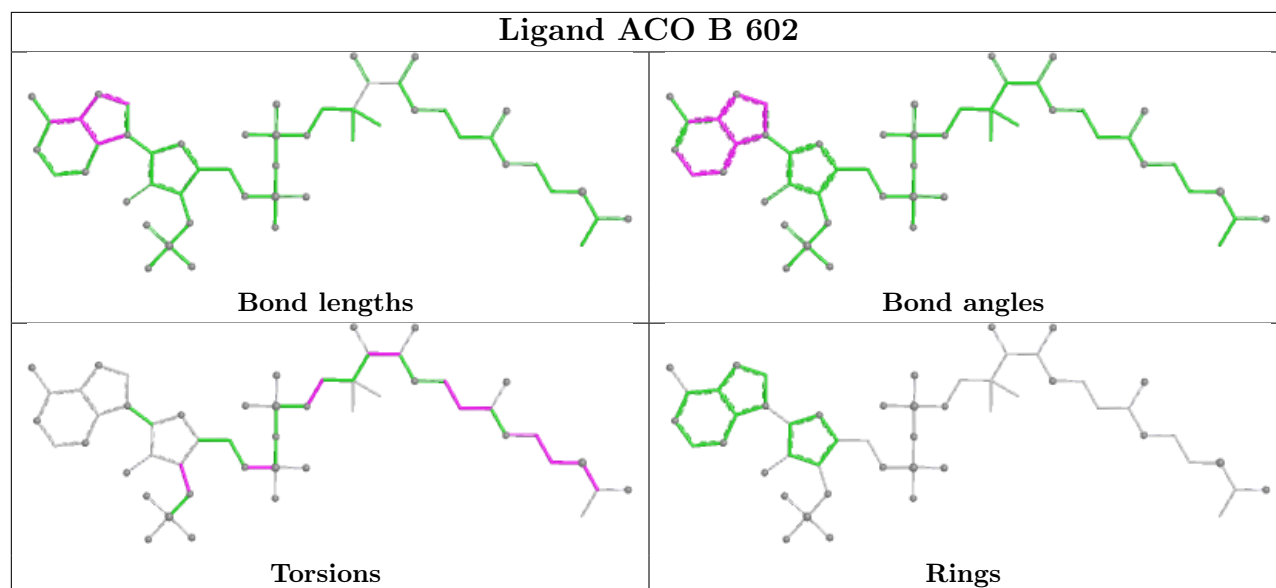
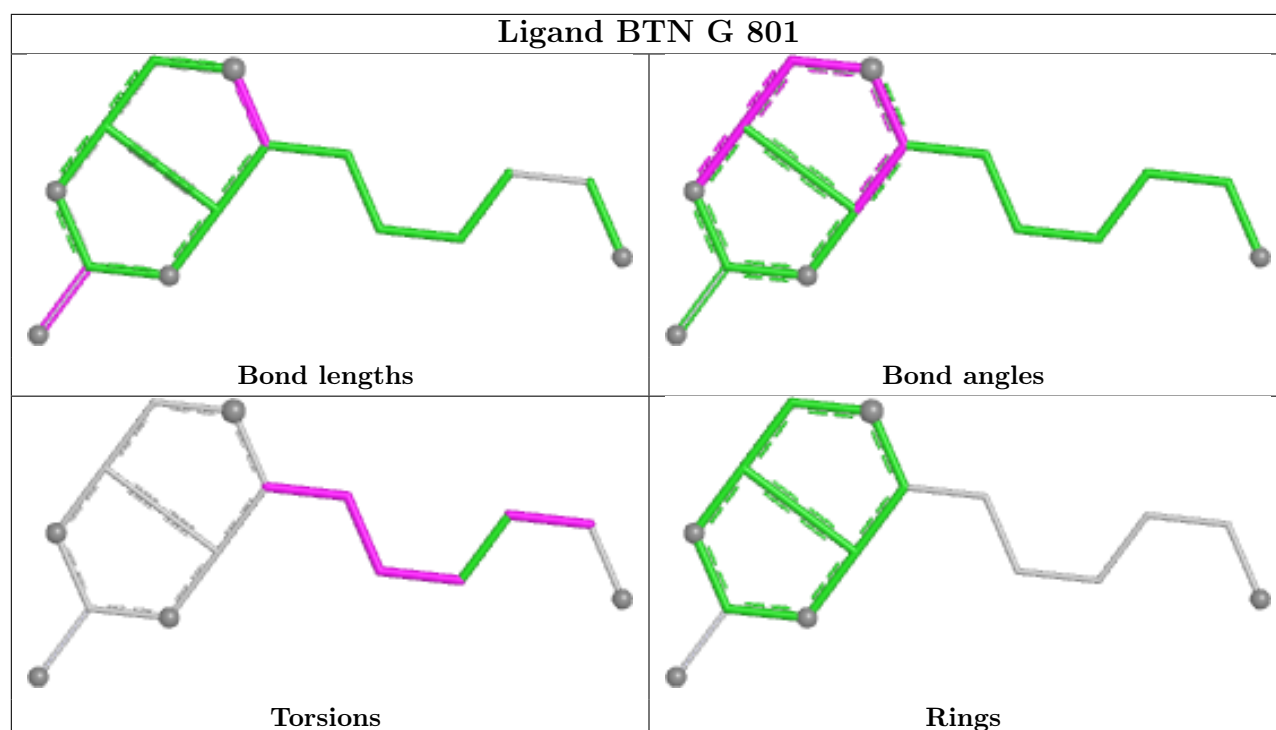
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	BTN	8	0
4	F	601	ACO	17	0
4	L	601	ACO	24	0
3	I	801	BTN	9	0
3	G	801	BTN	8	0
4	B	602	ACO	18	0
3	E	801	BTN	5	0
3	C	801	BTN	6	0
3	K	801	BTN	7	0
4	J	601	ACO	32	0
4	B	601	ACO	9	0
4	J	602	ACO	23	0

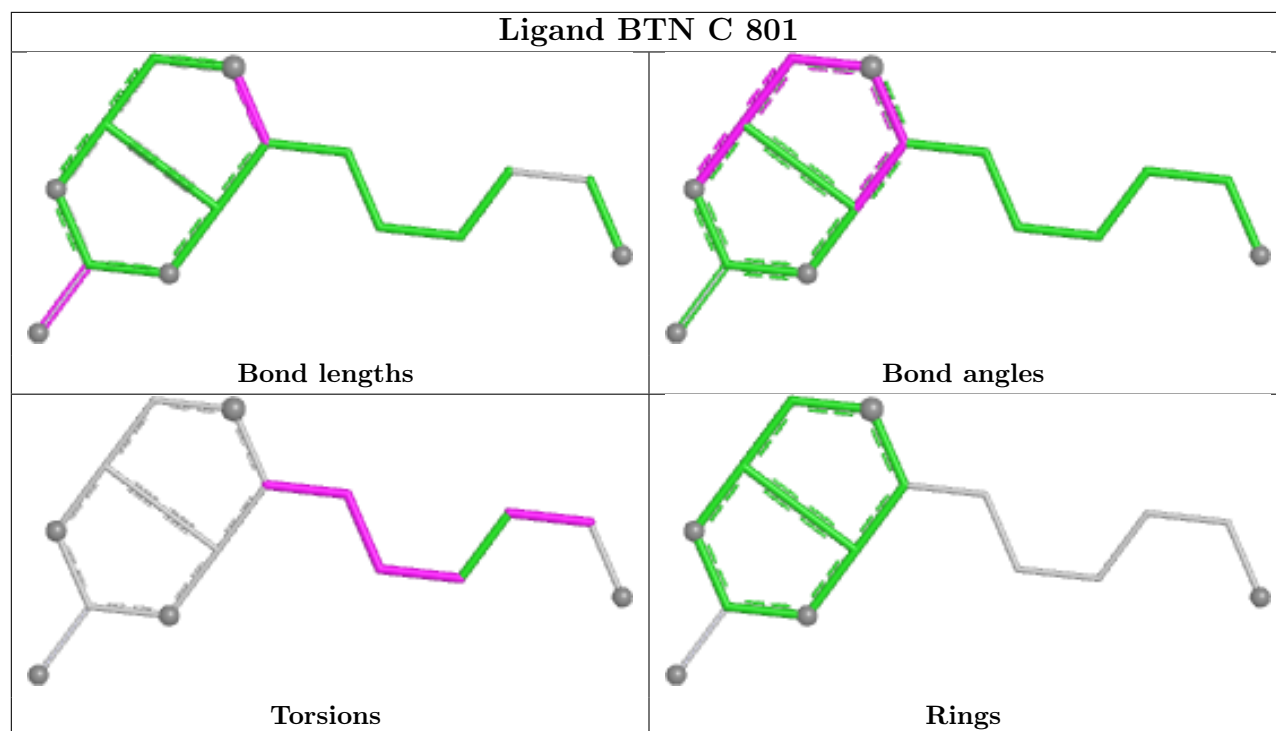
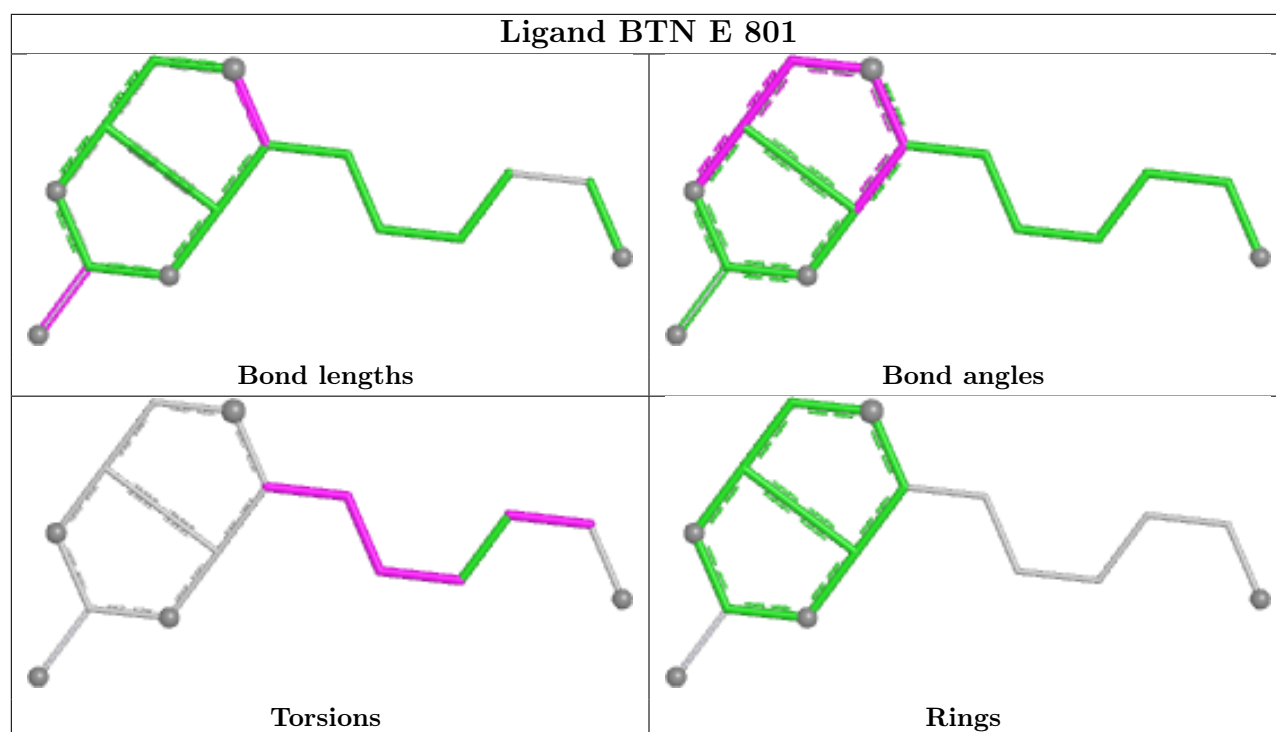
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

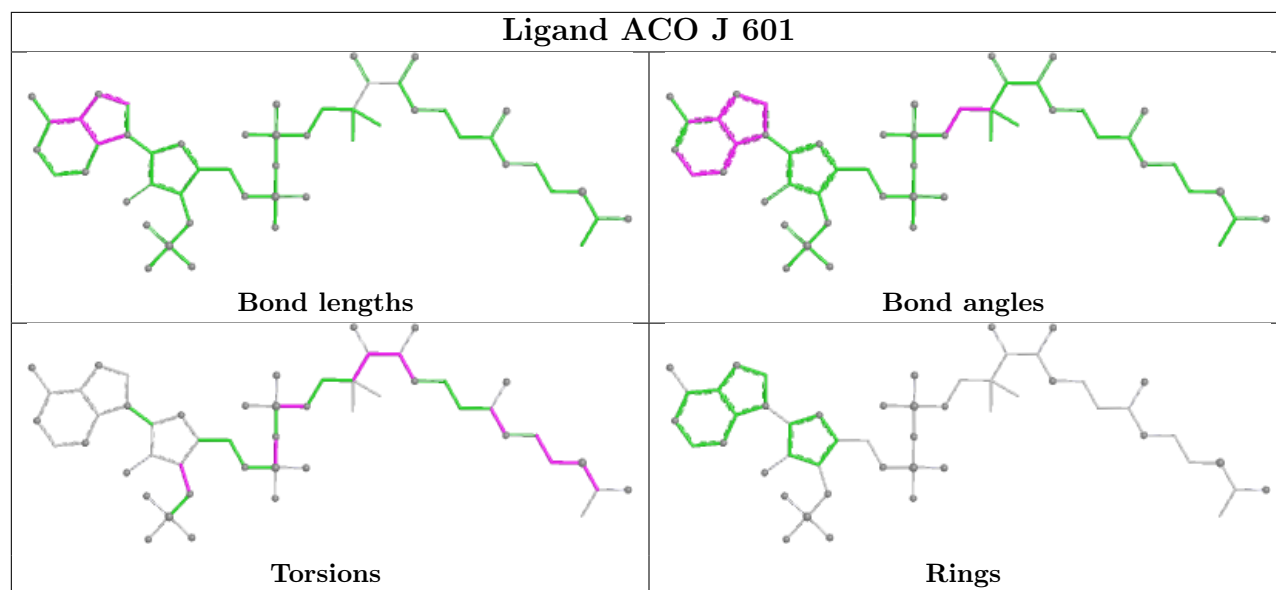
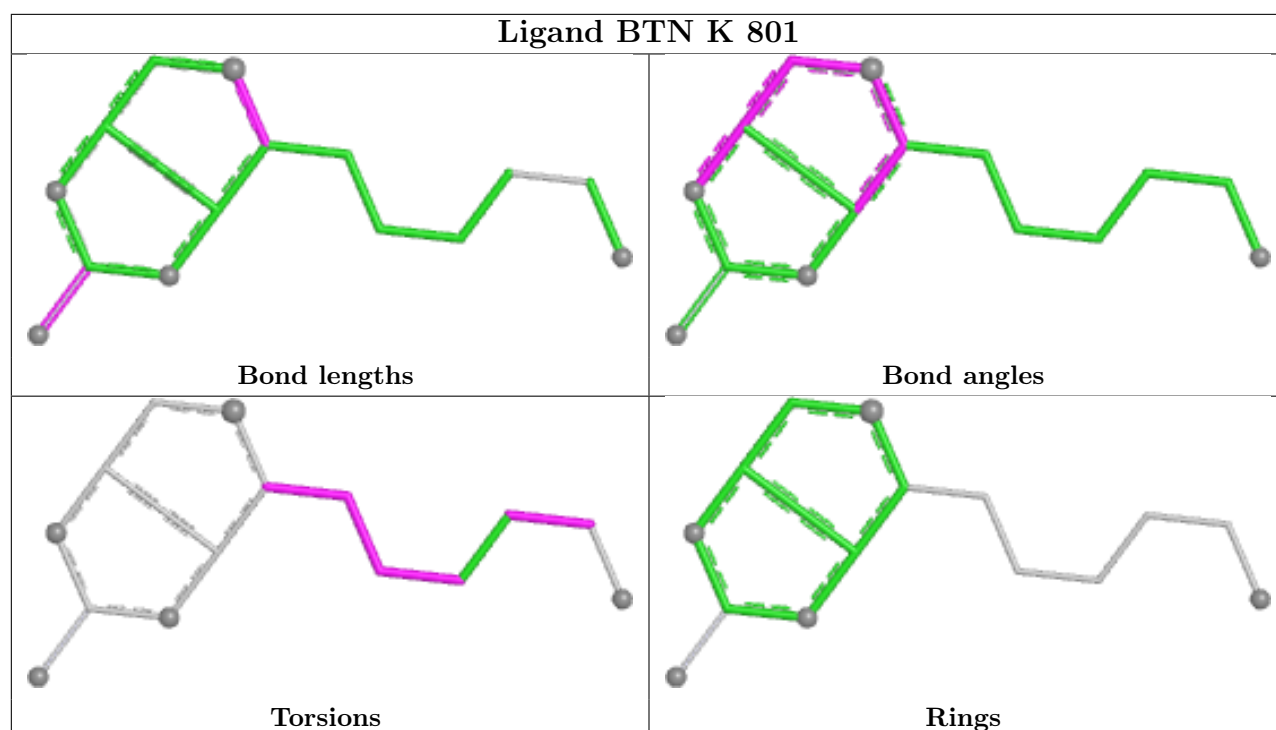
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

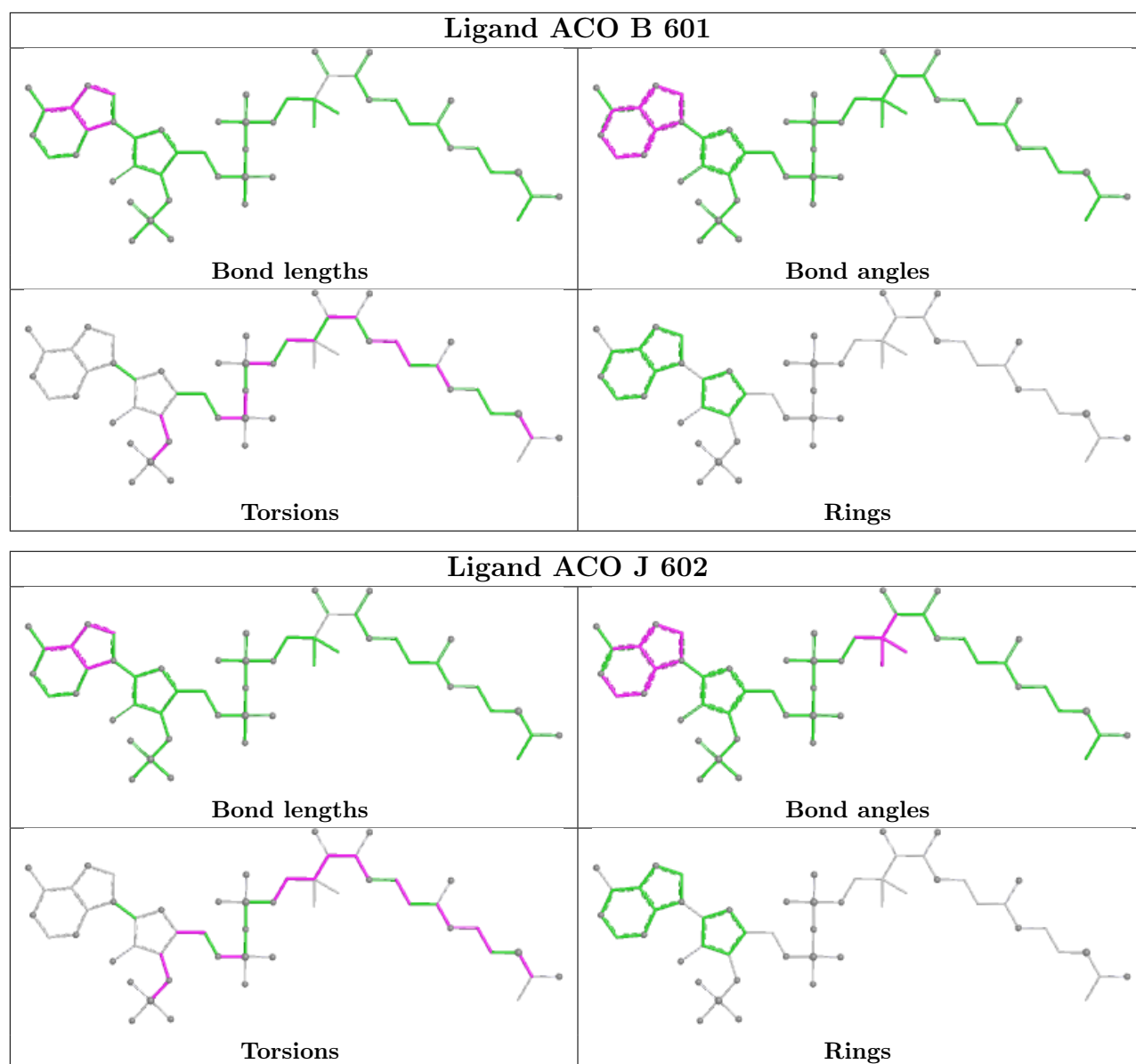












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

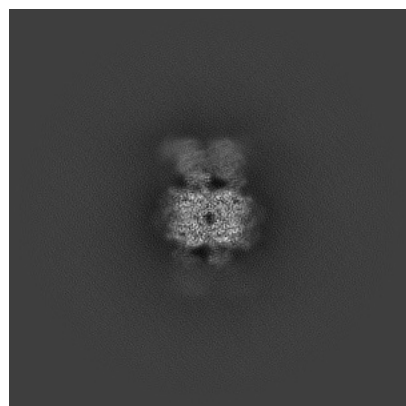
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38440. These allow visual inspection of the internal detail of the map and identification of artifacts.

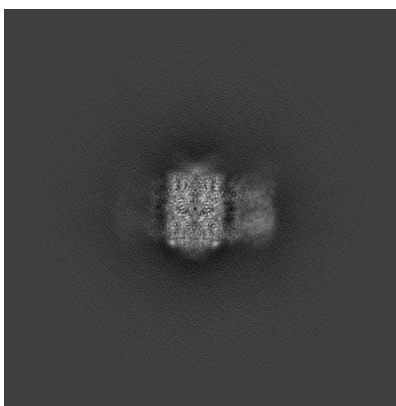
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

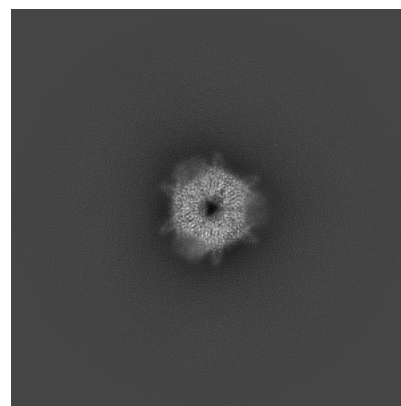
6.1.1 Primary map



X

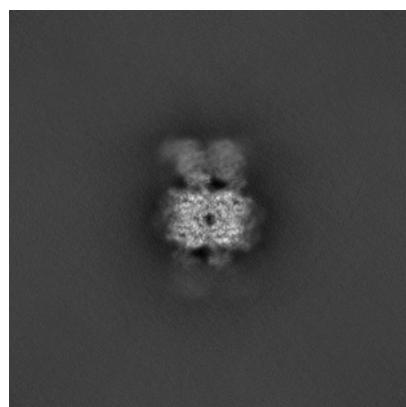


Y

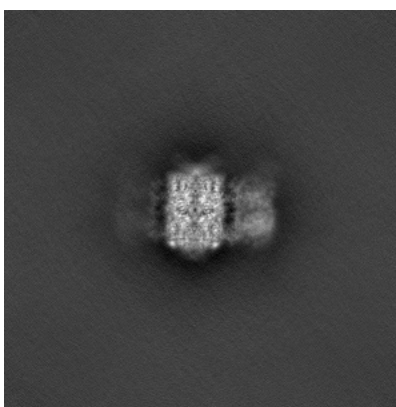


Z

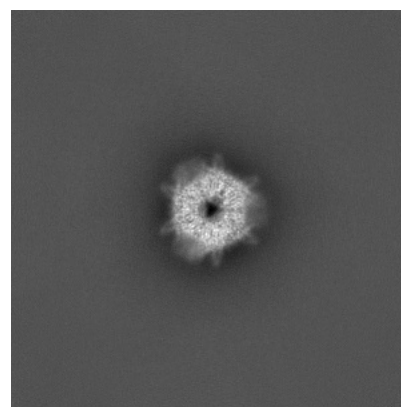
6.1.2 Raw map



X



Y



Z

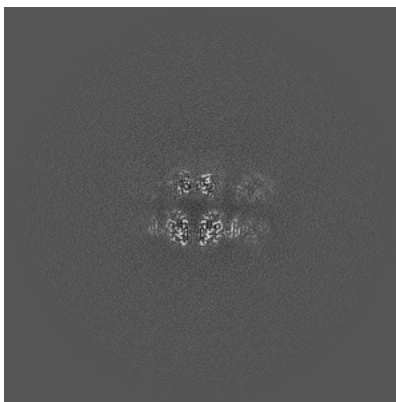
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

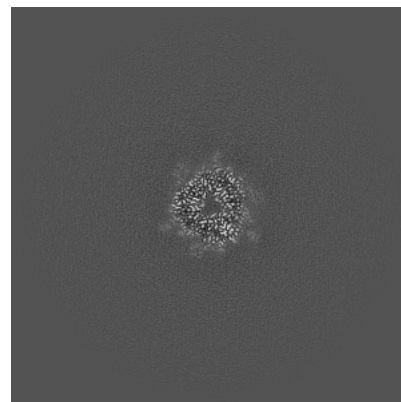
6.2.1 Primary map



X Index: 240



Y Index: 240

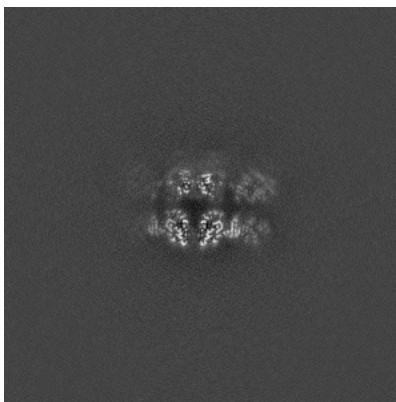


Z Index: 240

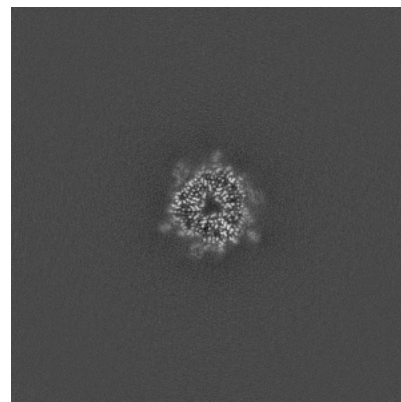
6.2.2 Raw map



X Index: 240



Y Index: 240

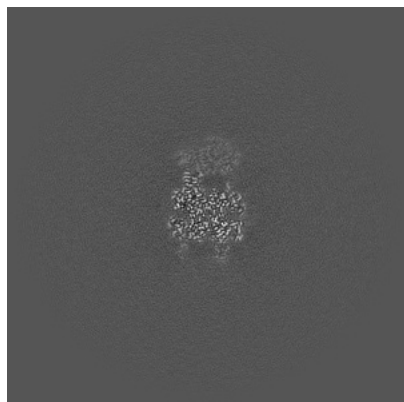


Z Index: 240

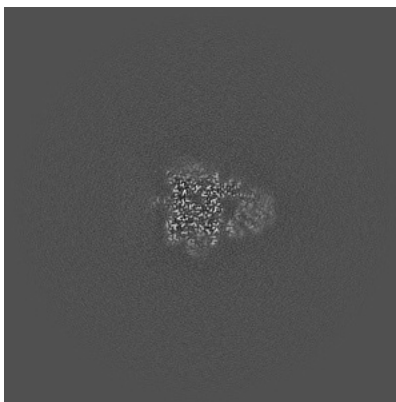
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

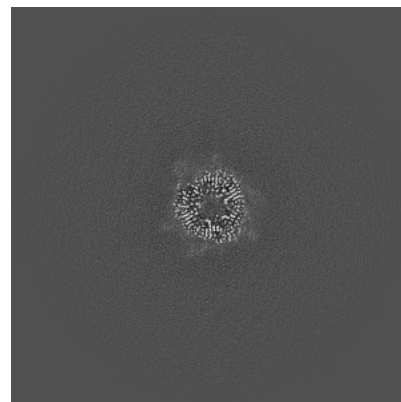
6.3.1 Primary map



X Index: 258

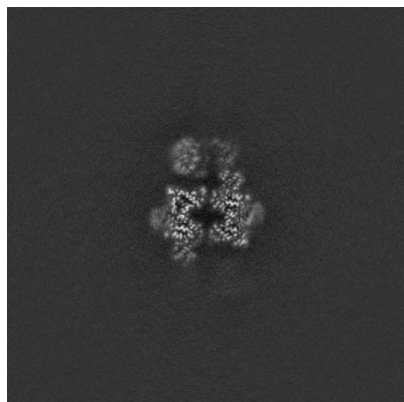


Y Index: 220

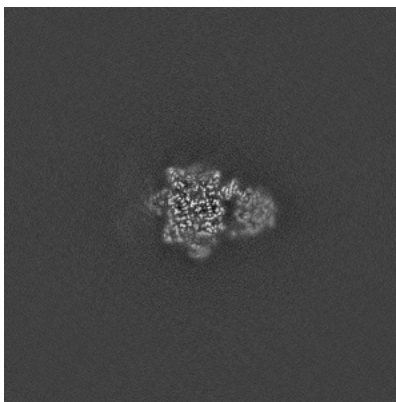


Z Index: 244

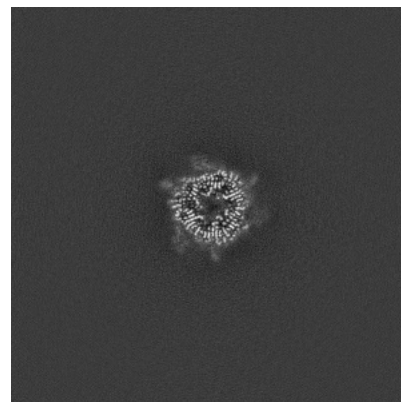
6.3.2 Raw map



X Index: 246



Y Index: 215

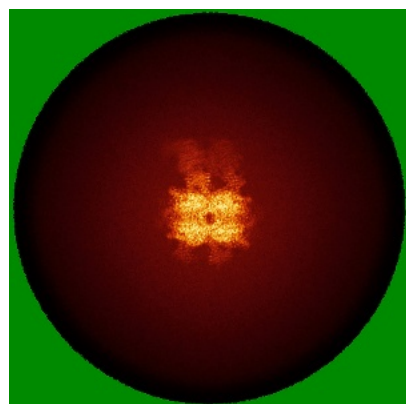


Z Index: 214

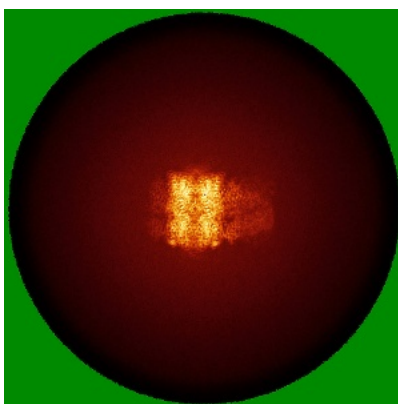
The images above show the largest variance slices of the map in three orthogonal directions.

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

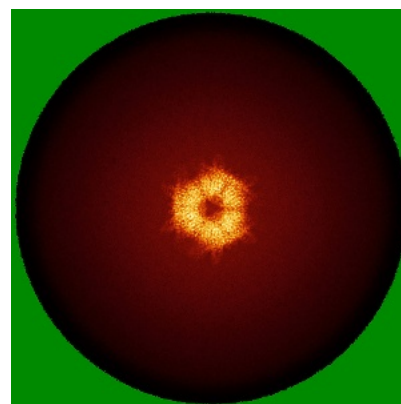
6.4.1 Primary map



X

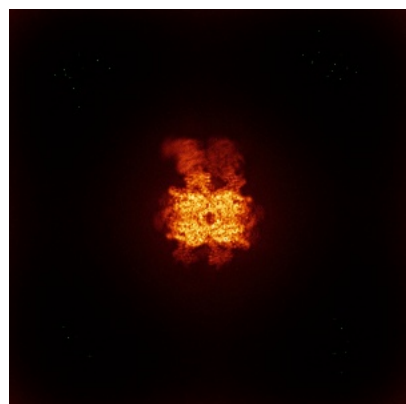


Y

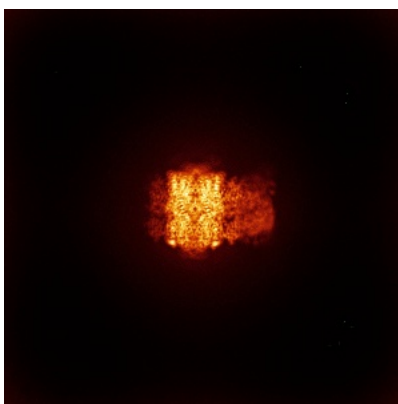


Z

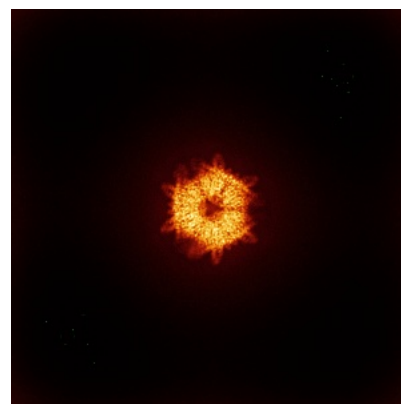
6.4.2 Raw map



X



Y

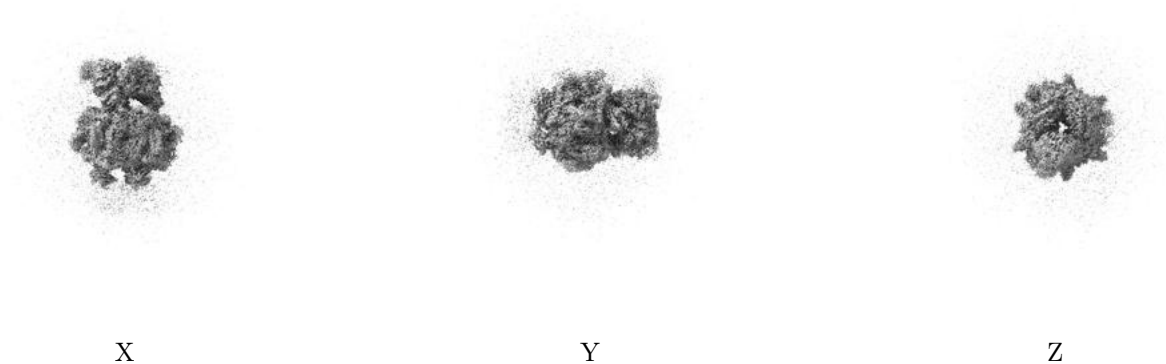


Z

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.

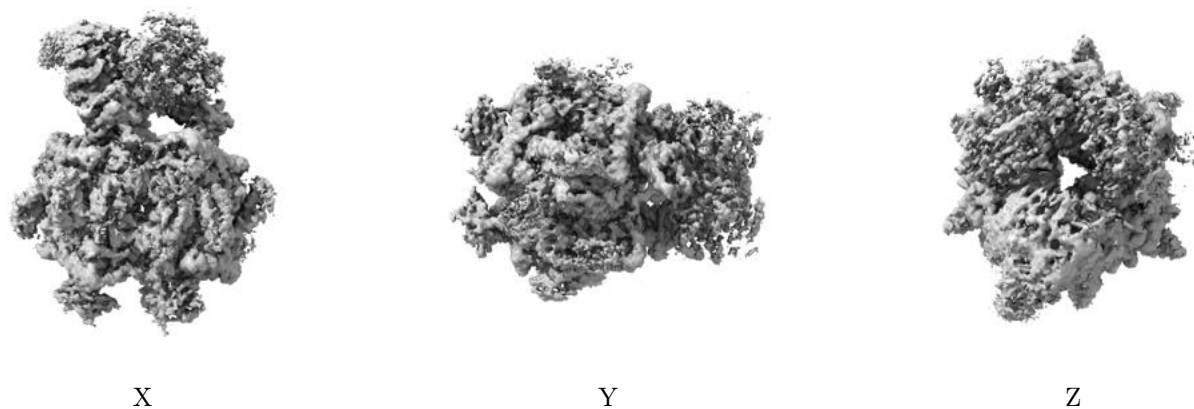
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

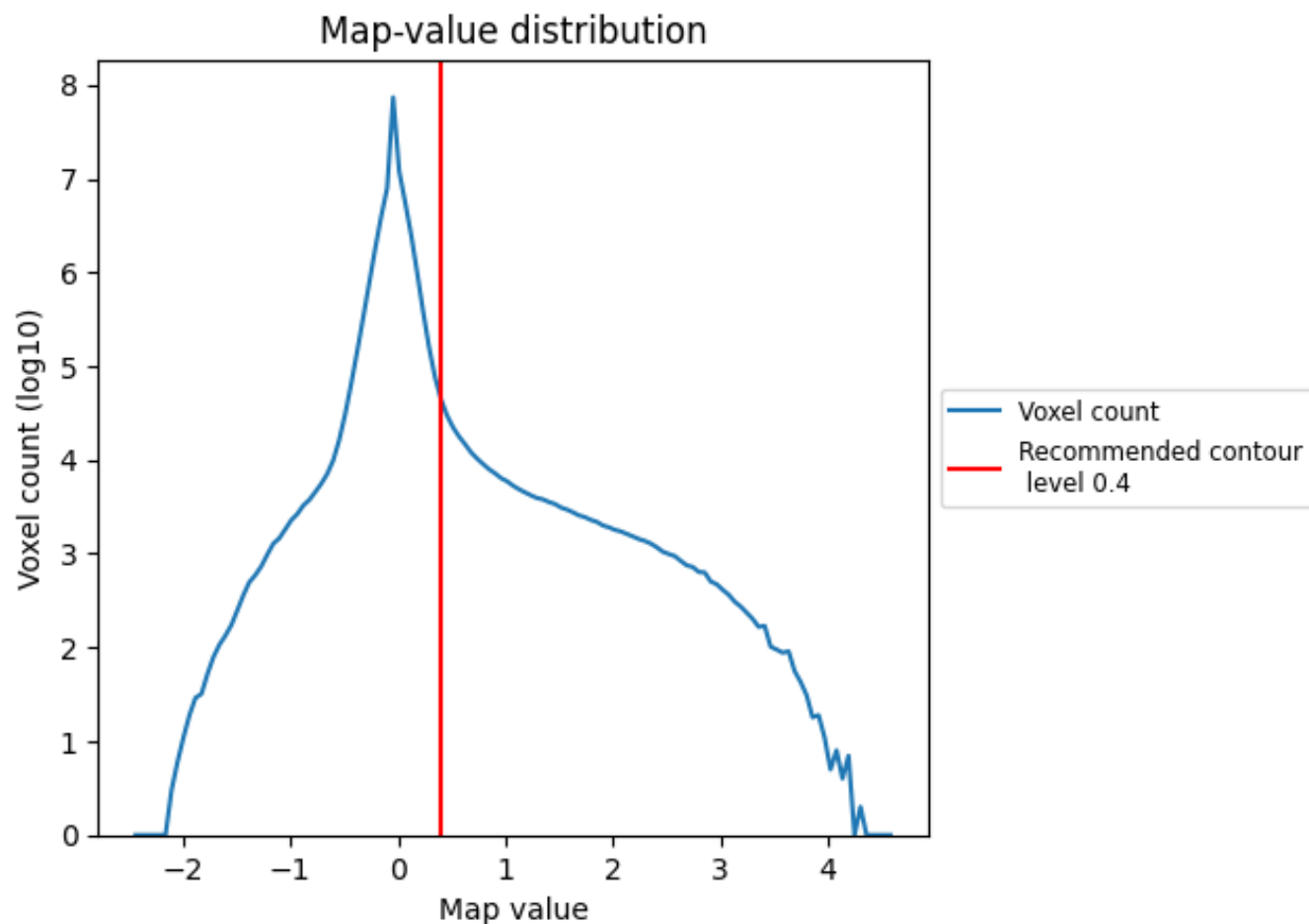
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

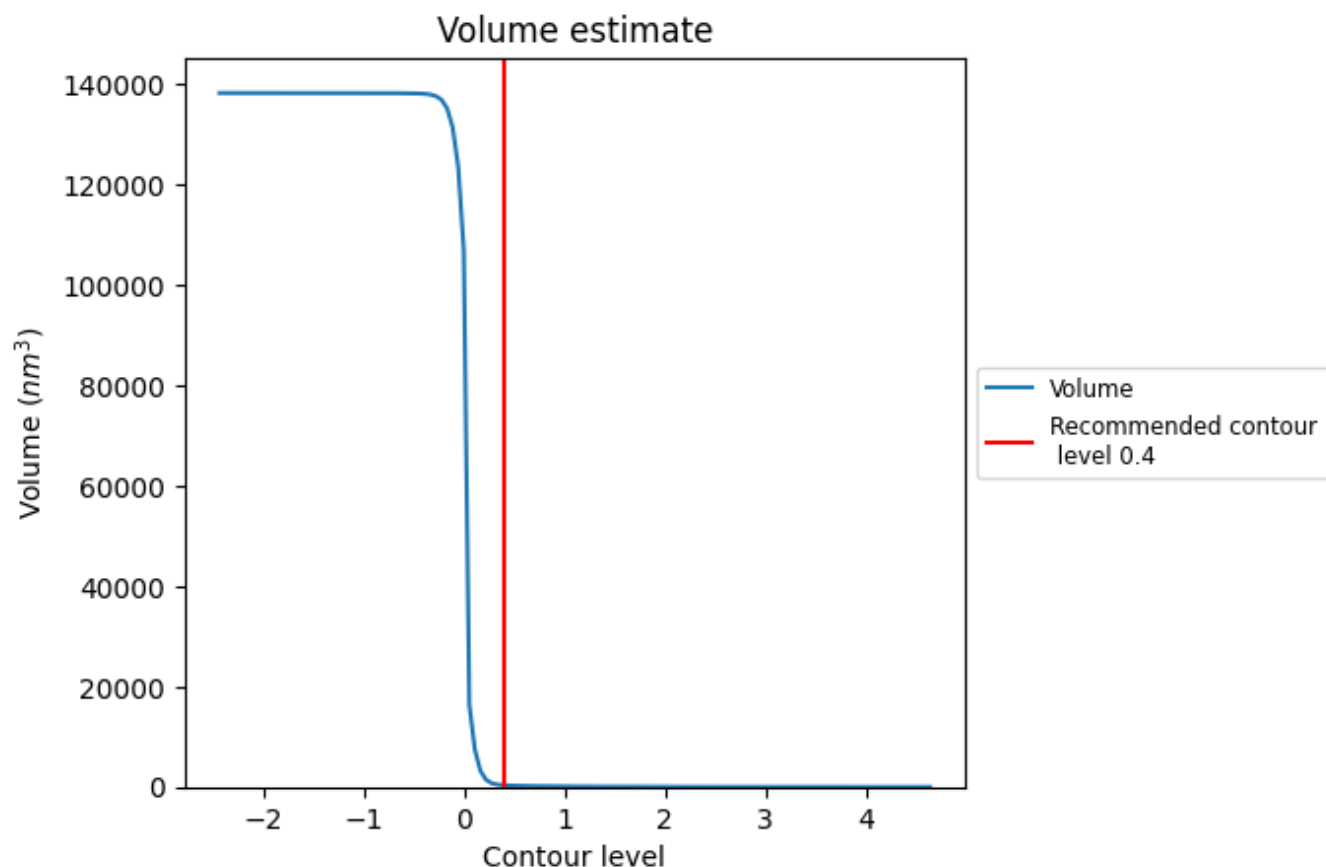
This section contains the results of statistical analysis of the map.

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.

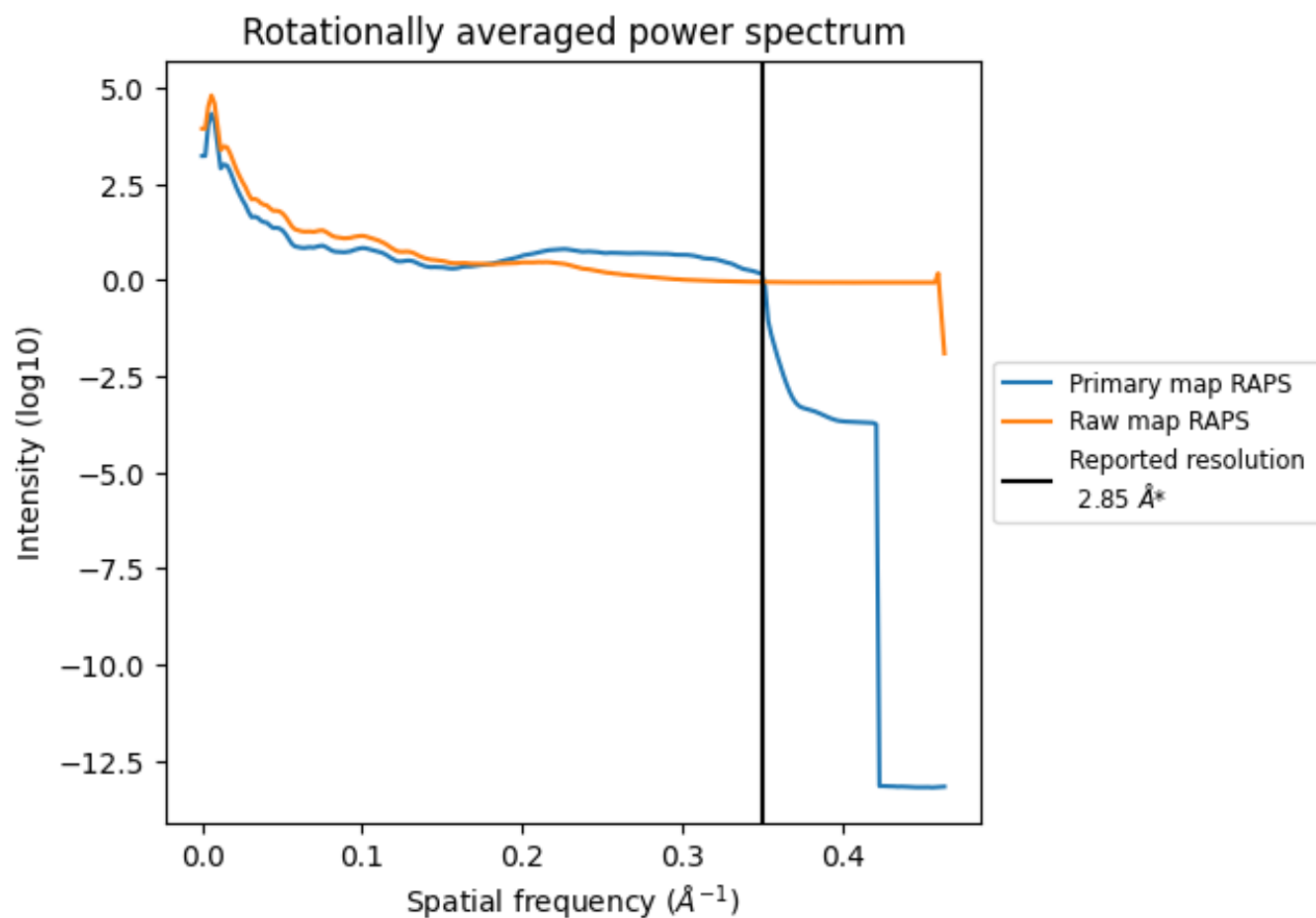
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 339 nm³; this corresponds to an approximate mass of 306 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 ⓘ

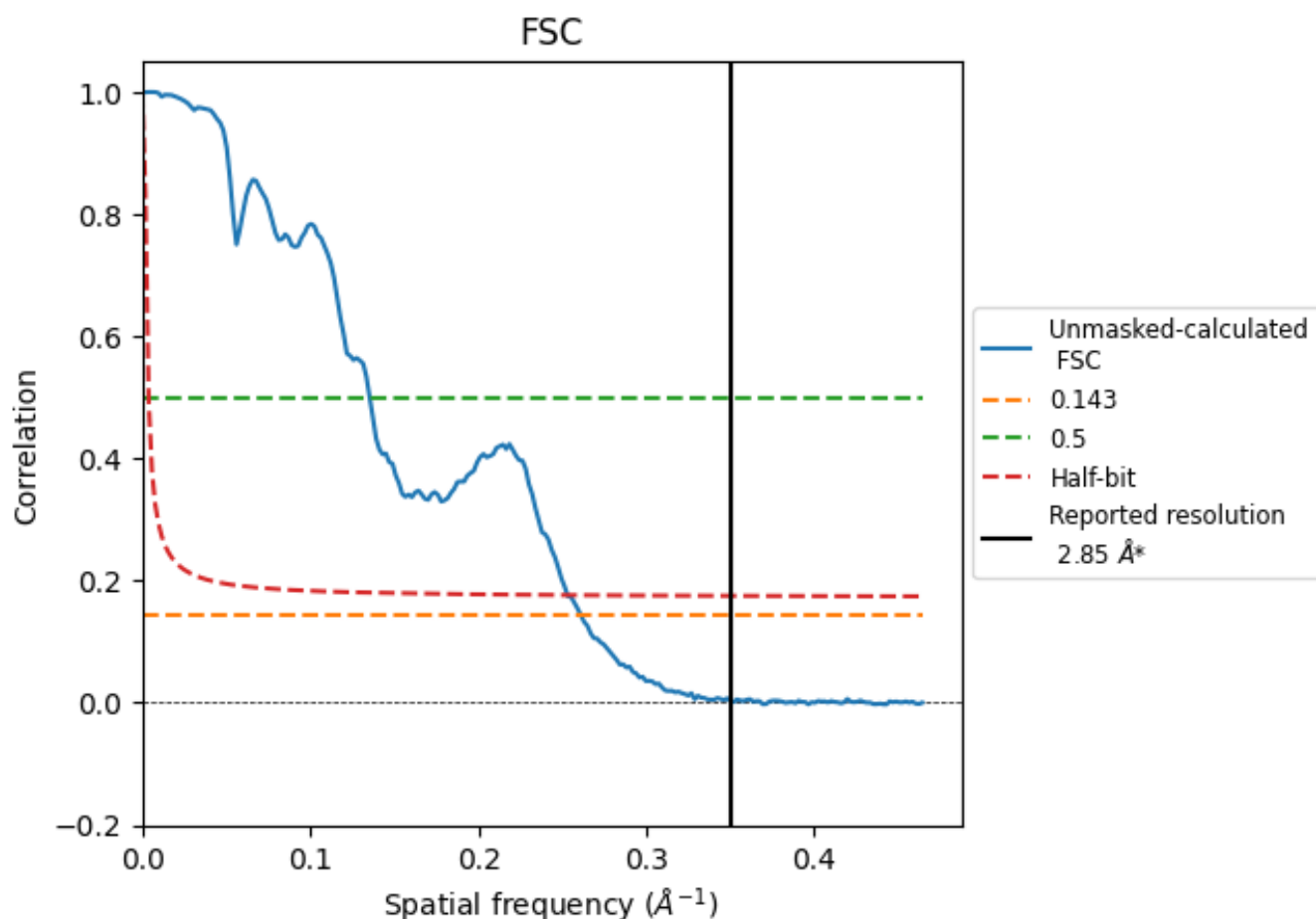


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

8.2 Resolution estimates [i](#)

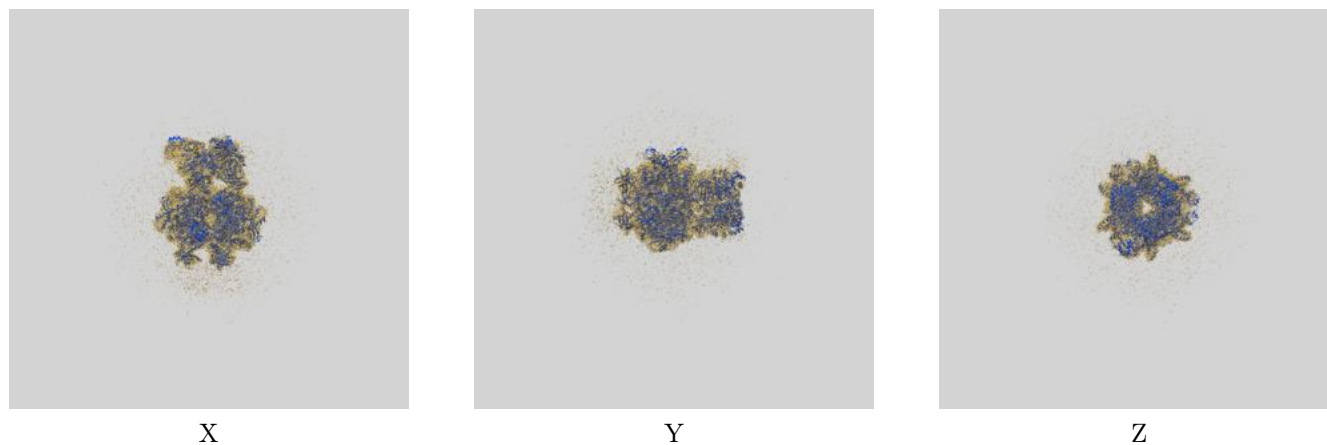
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.83	7.39	3.95

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 2.85 by more than 10 %

9 Map-model fit [i](#)

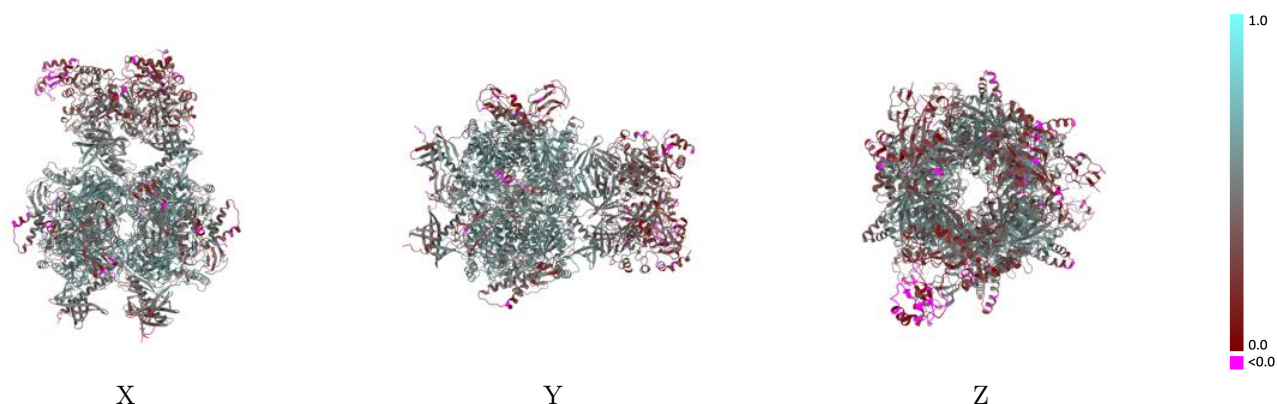
This section contains information regarding the fit between EMDB map EMD-38440 and PDB model 8XL7. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



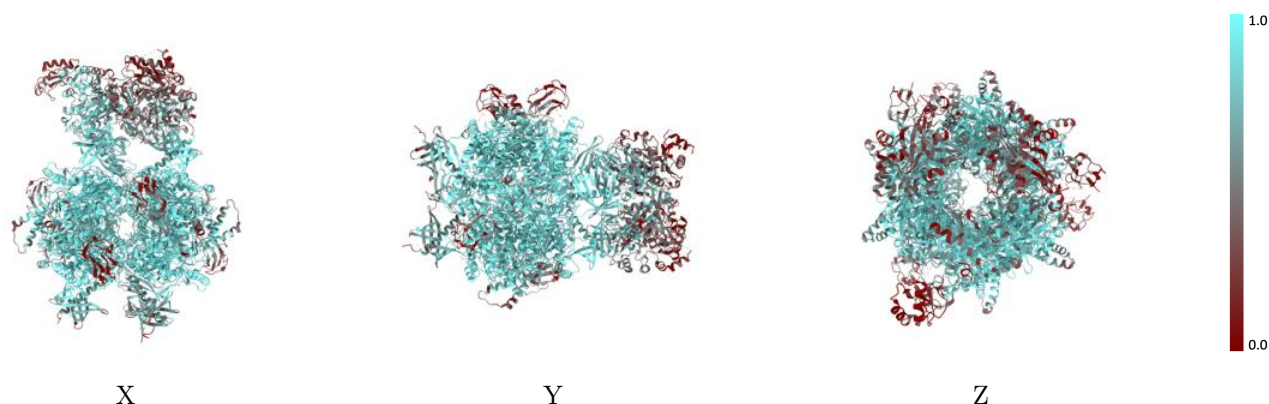
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



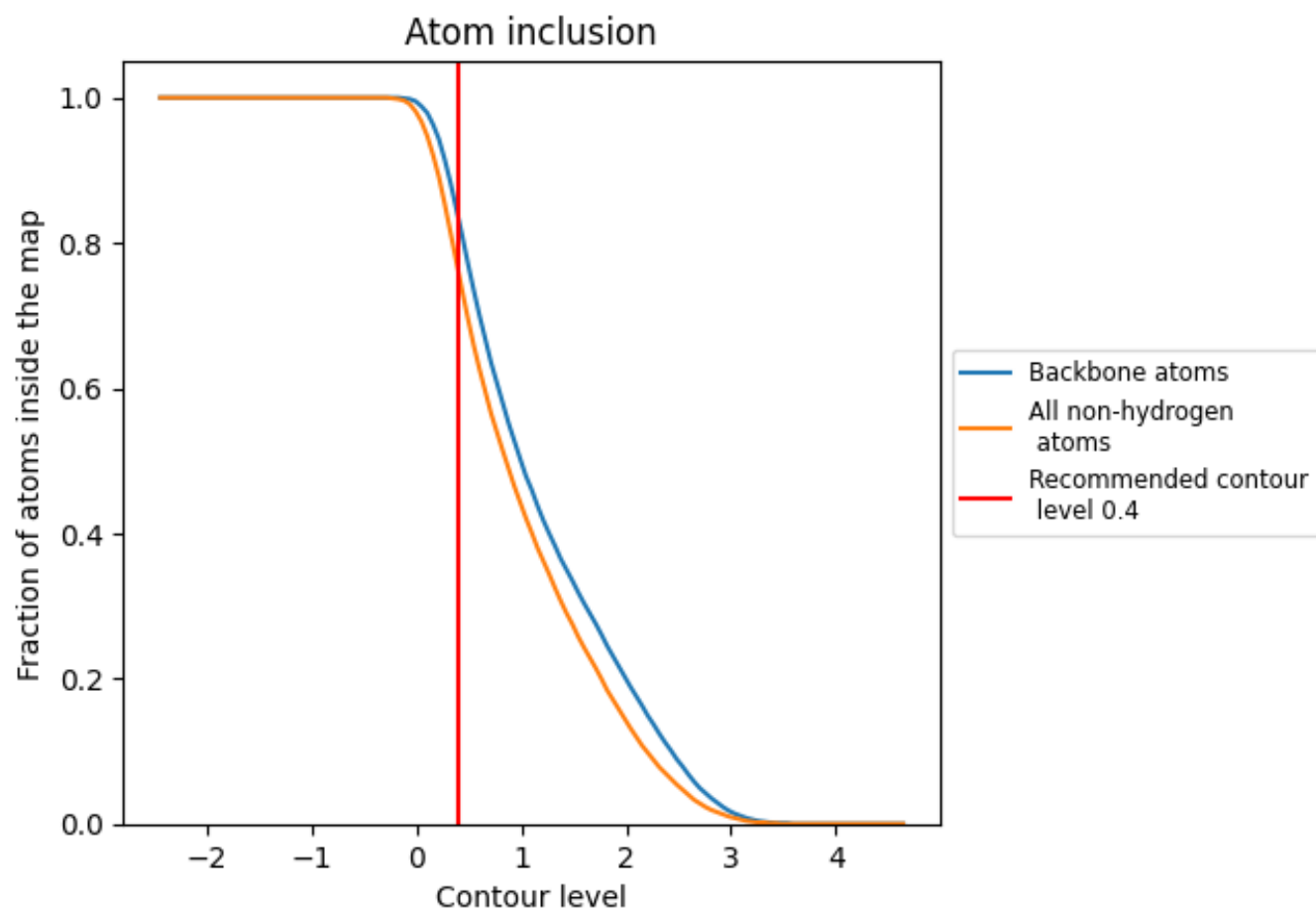
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7600	0.4690
A	0.5530	0.3660
B	0.9150	0.5530
C	0.5750	0.3890
D	0.9470	0.5910
E	0.4580	0.3490
F	0.9140	0.5500
G	0.4870	0.3320
H	0.9260	0.5560
I	0.6370	0.3370
J	0.9210	0.5610
K	0.5200	0.3560
L	0.9110	0.5520

1.0

0.0

<0.0