



Full wwPDB EM Validation Report ⓘ

Nov 17, 2025 – 01:47 PM EST

PDB ID : 9YX1 / pdb_00009yx1
EMDB ID : EMD-73575
Title : Structure of the long chain acyl-CoA carboxylase complex from Mycobacterium smegmatis
Authors : Liang, Y.; Rubinstein, J.L.
Deposited on : 2025-10-26
Resolution : 3.50 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:

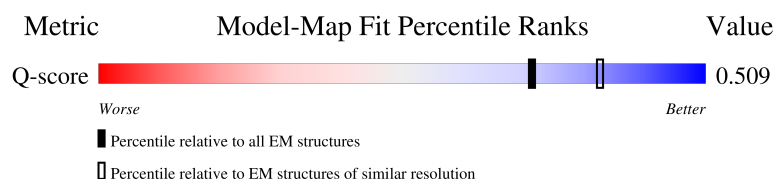
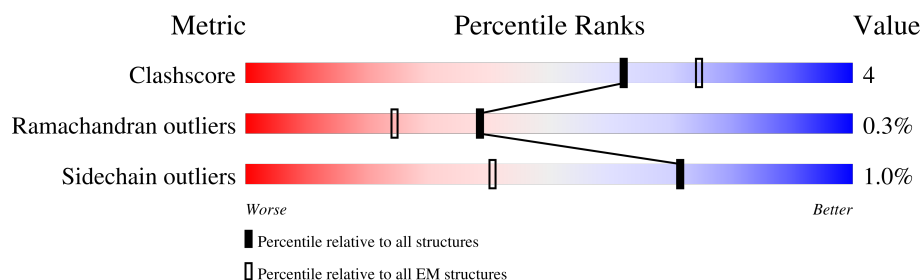
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive 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) : 2.46

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	F	517	
1	O	517	
2	G	542	
2	H	542	

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Mol	Chain	Length	Quality of chain
2	M	542	
2	N	542	
3	A	598	
3	B	598	
3	C	598	
3	D	598	
3	I	598	
3	J	598	
3	K	598	
3	L	598	
3	Q	598	
3	R	598	
3	S	598	
3	T	598	
4	E	94	
4	P	94	

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
5	BTN	I	601	-	-	X	-
5	BTN	L	601	-	-	X	-
6	BCT	Q	602	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 48731 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 Propionyl-CoA carboxylase beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	515	Total	C	N	O	S	0	0
			3719	2376	672	657	14		
1	O	515	Total	C	N	O	S	0	0
			3718	2377	666	660	15		

- Molecule 2 is a protein called Propionyl-CoA carboxylase beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	530	Total	C	N	O	S	0	0
			3880	2468	676	722	14		
2	H	539	Total	C	N	O	S	0	0
			3929	2502	687	725	15		
2	M	530	Total	C	N	O	S	0	0
			3888	2472	678	723	15		
2	N	532	Total	C	N	O	S	0	0
			3881	2472	679	716	14		

- Molecule 3 is a protein called Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	67	Total	C	N	O	S	0	0
			415	257	71	84	3		
3	I	67	Total	C	N	O	S	0	0
			390	243	70	75	2		
3	J	67	Total	C	N	O	S	0	0
			392	244	70	76	2		
3	L	67	Total	C	N	O	S	0	0
			396	246	70	78	2		
3	A	512	Total	C	N	O	S	0	0
			3409	2175	632	597	5		
3	D	410	Total	C	N	O	S	0	0
			2781	1772	506	499	4		
3	B	415	Total	C	N	O	S	0	0
			2859	1830	525	500	4		

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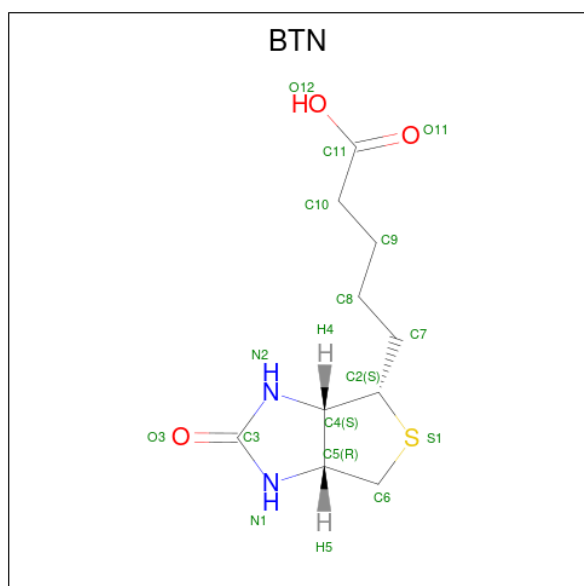
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	409	Total	C	N	O	S	0	0
			2822	1802	518	498	4		
3	Q	512	Total	C	N	O	S	0	0
			3564	2266	652	639	7		
3	S	410	Total	C	N	O	S	0	0
			2420	1515	450	454	1		
3	R	414	Total	C	N	O	S	0	0
			2817	1795	519	499	4		
3	T	406	Total	C	N	O	S	0	0
			2401	1501	442	456	2		

- Molecule 4 is a protein called Acetyl-/propionyl-coenzyme A carboxylase AccE5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	61	Total	C	N	O	S	0	0
			473	299	96	76	2		
4	P	62	Total	C	N	O	S	0	0
			479	303	91	81	4		

- Molecule 5 is BIOTIN (CCD ID: BTN) (formula: $C_{10}H_{16}N_2O_3S$) (labeled as "Ligand of Interest" by depositor).



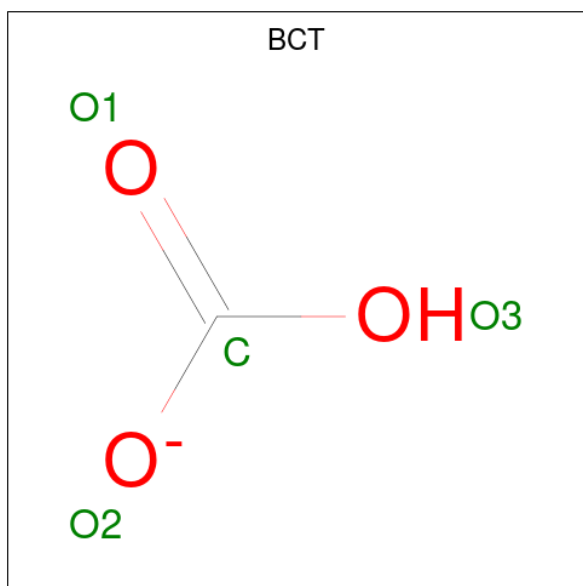
Mol	Chain	Residues	Atoms					AltConf
5	K	1	Total	C	N	O	S	0
			15	10	2	2	1	
5	I	1	Total	C	N	O	S	0
			15	10	2	2	1	

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Mol	Chain	Residues	Atoms					AltConf
5	J	1	Total	C	N	O	S	0
			15	10	2	2	1	
5	L	1	Total	C	N	O	S	0
			15	10	2	2	1	
5	A	1	Total	C	N	O	S	0
			15	10	2	2	1	
5	Q	1	Total	C	N	O	S	0
			15	10	2	2	1	

- Molecule 6 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



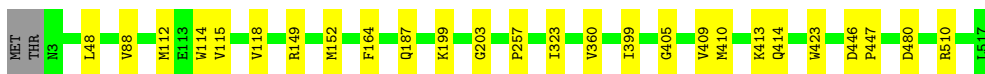
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			4	1	3	
6	Q	1	Total	C	O	0
			4	1	3	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

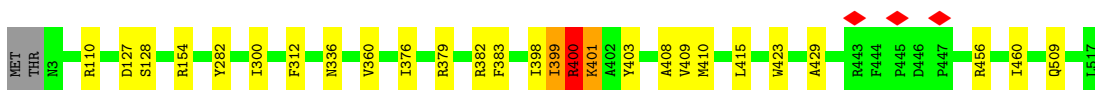
- Molecule 1: Propionyl-CoA carboxylase beta chain

Chain F: 



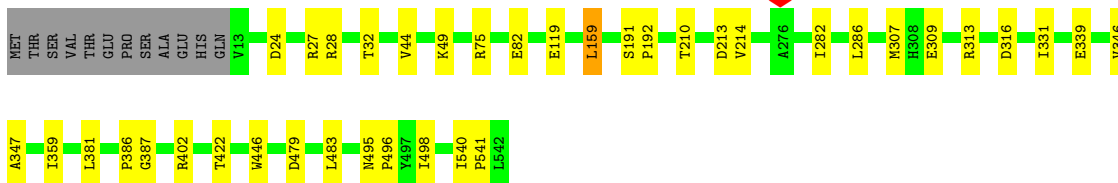
- Molecule 1: Propionyl-CoA carboxylase beta chain

Chain O: 



- Molecule 2: Propionyl-CoA carboxylase beta chain

Chain G: 




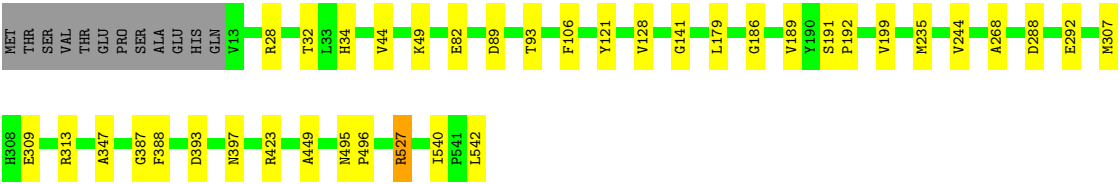
- Molecule 2: Propionyl-CoA carboxylase beta chain

Chain H: 




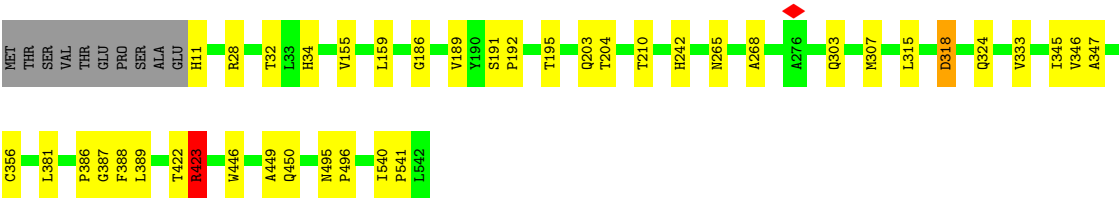
- Molecule 2: Propionyl-CoA carboxylase beta chain

Chain M:  91% 7%



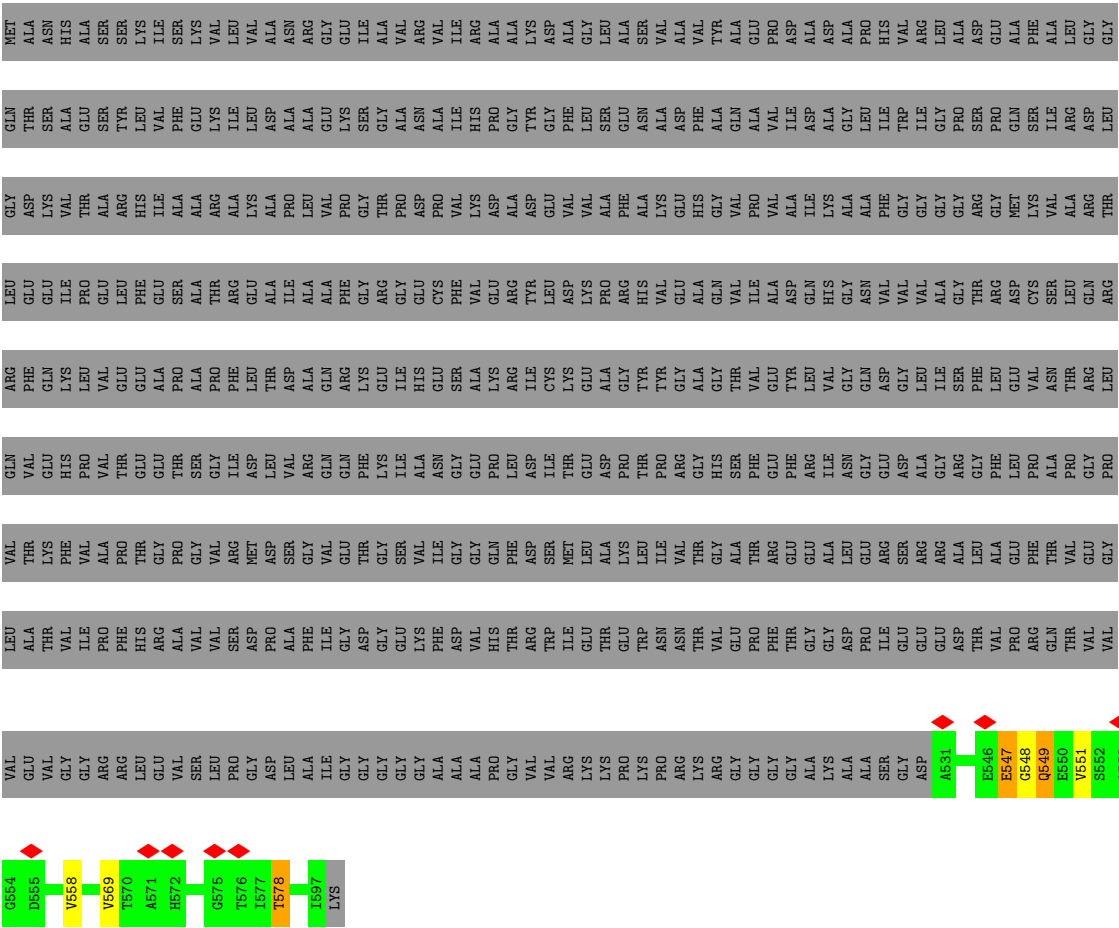
• Molecule 2: Propionyl-CoA carboxylase beta chain

Chain N:  91% 7%

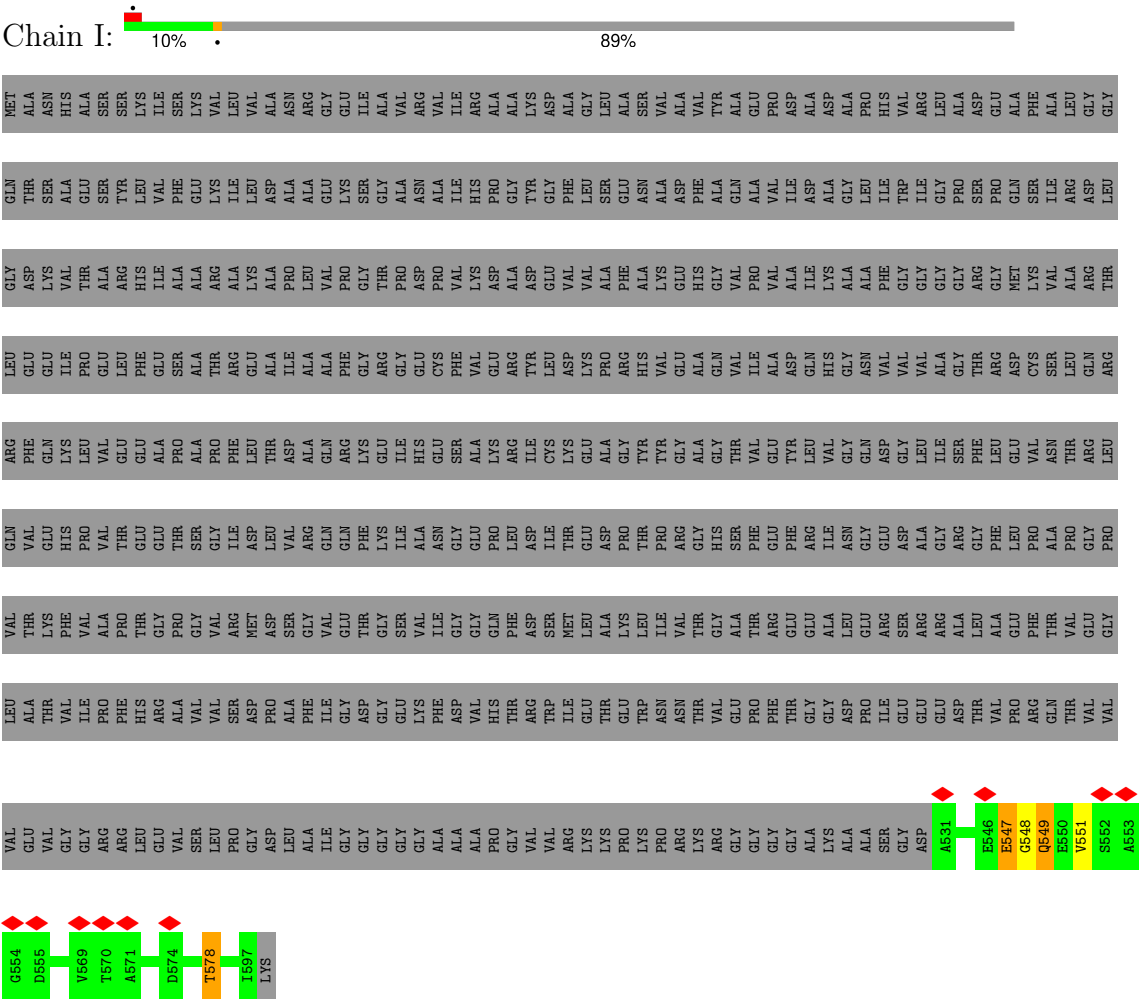


• Molecule 3: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

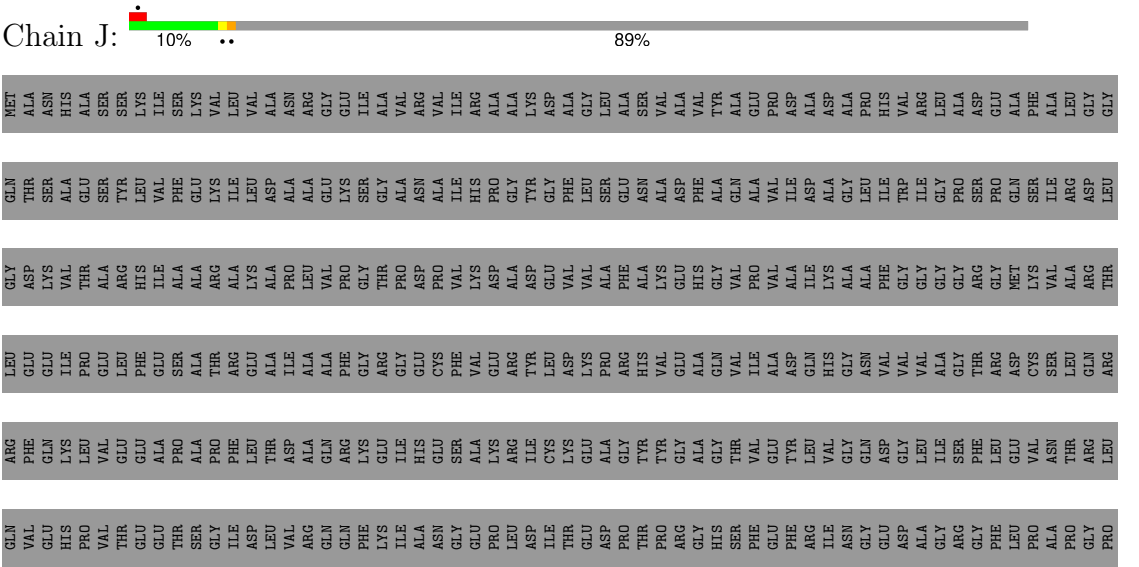
Chain K:  10% 89%

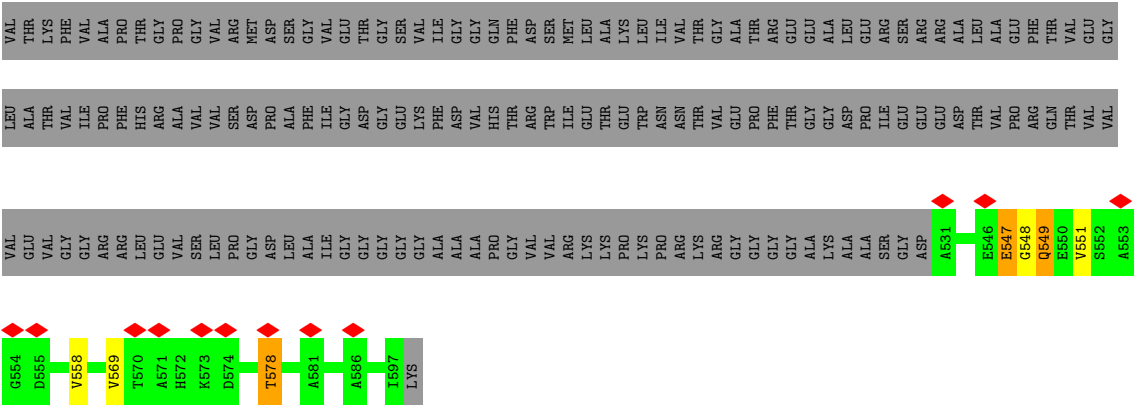


• Molecule 3: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit



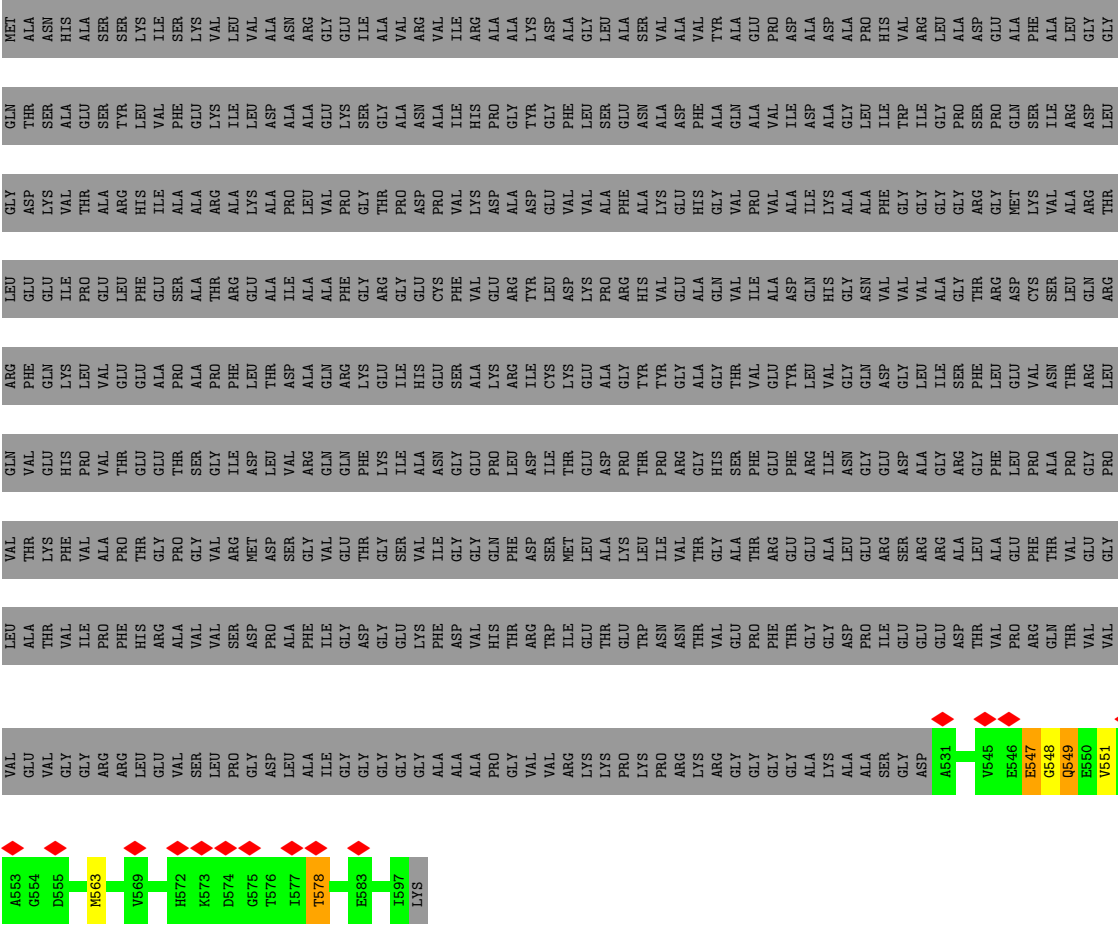
• Molecule 3: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit





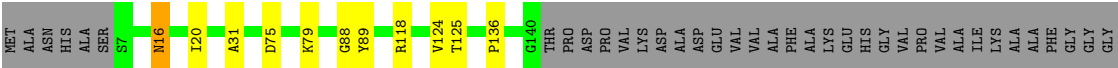
• Molecule 3: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

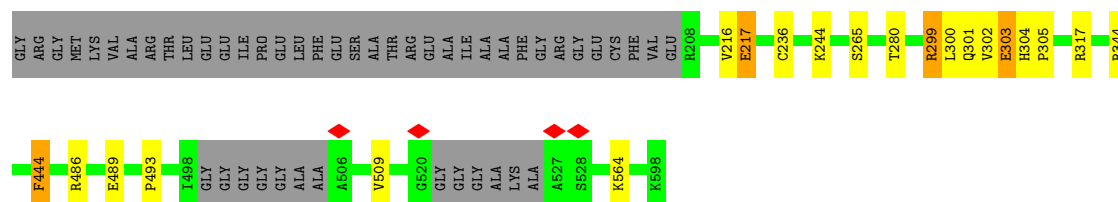
Chain L: 10% 89%



• Molecule 3: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

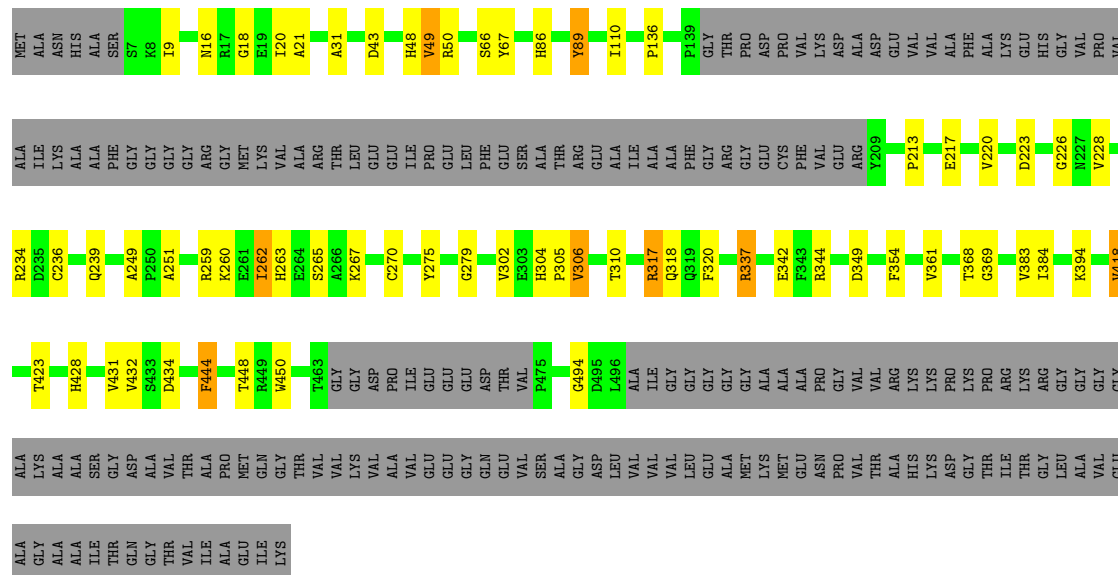
Chain A: 80% 5% 14%





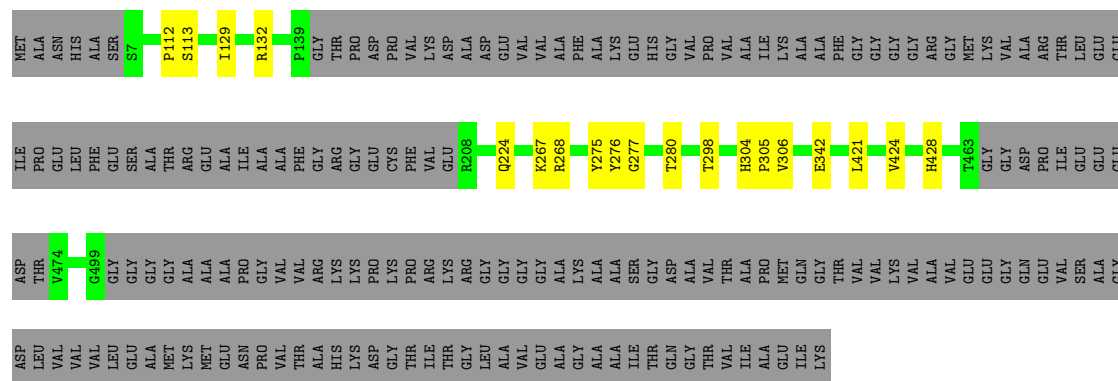
• Molecule 3: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

Chain D: 58% 10% 31%



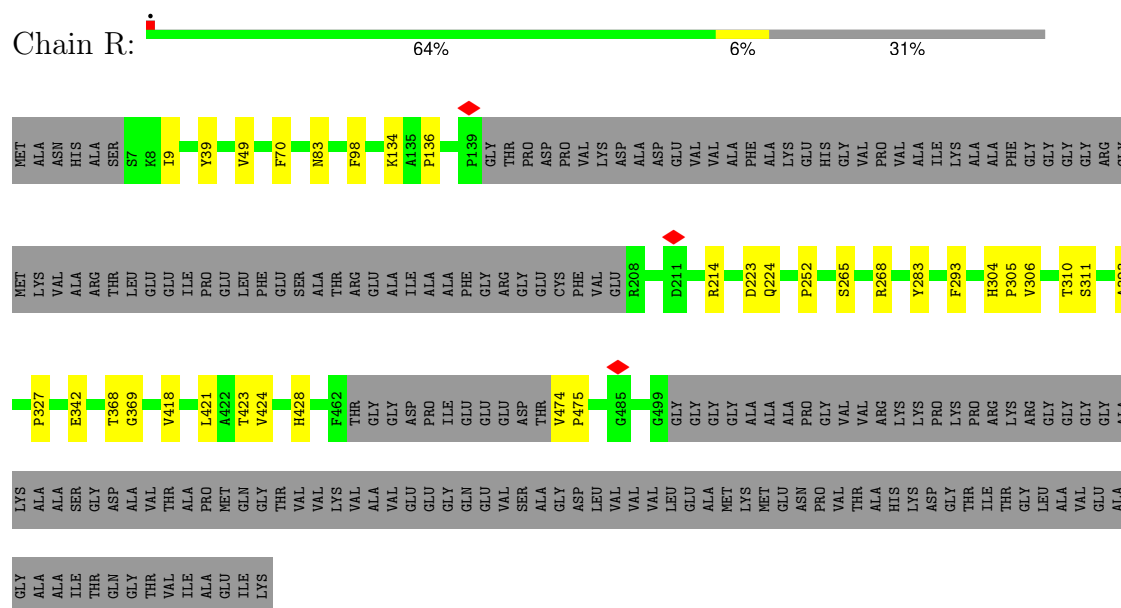
• Molecule 3: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

Chain B: 66% 31%

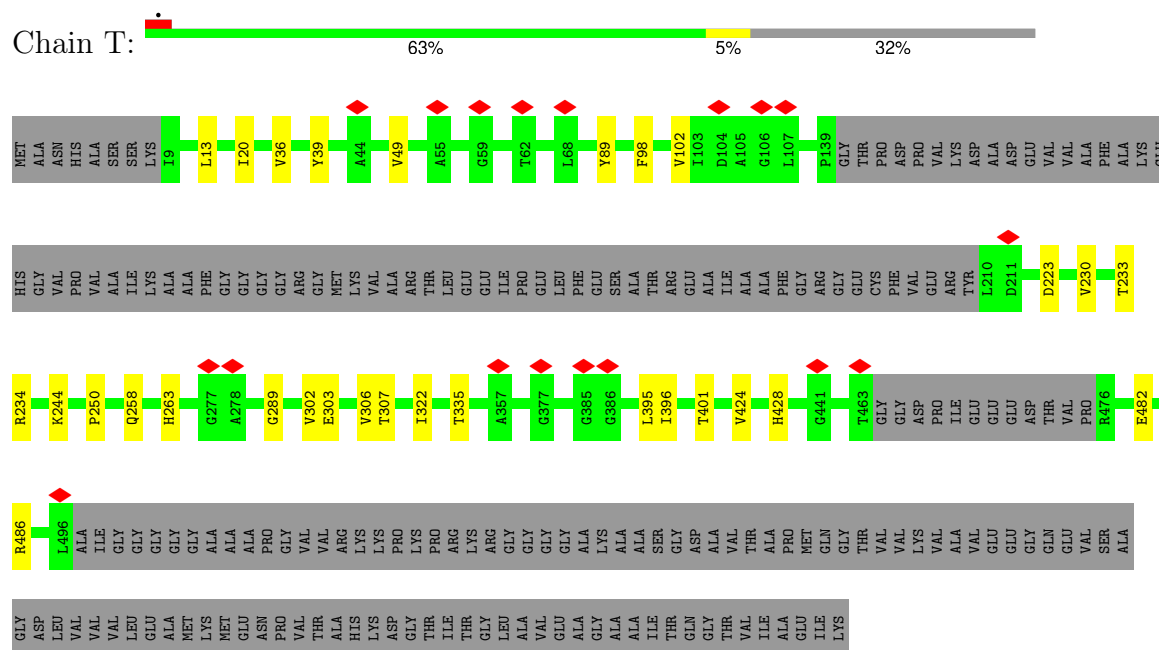


• Molecule 3: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

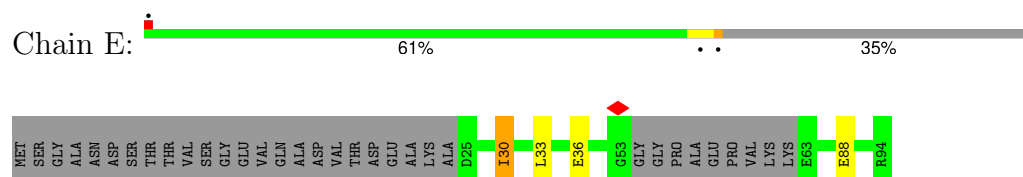
Chain C: 61% 6% 32%



- Molecule 3: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit



- Molecule 4: Acetyl-/propionyl-coenzyme A carboxylase AccE5



- Molecule 4: Acetyl-/propionyl-coenzyme A carboxylase AccE5



MET	SER	GLY	ALA	ASN	ASP	SER	THR	THR	VAL	SER	GLY	GLU	VAL	GLN	ALA	ASP	VAL	THR	ASP	GLU	ALA	LYS	ALA	D25	I30	G53	GLY	GLY	PRO	ALA	GLU	PRO	VAL	LYS	K62	E63	R64	R94
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11174	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	20000	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.996	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	446.4, 446.4, 446.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, 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	F	0.17	0/3798	0.50	0/5176
1	O	0.19	0/3798	0.51	1/5178 (0.0%)
2	G	0.16	0/3956	0.47	0/5397
2	H	0.17	0/4007	0.49	0/5468
2	M	0.17	0/3964	0.48	0/5407
2	N	0.17	0/3958	0.49	0/5400
3	A	0.21	0/3475	0.55	0/4776
3	B	0.19	0/2919	0.53	0/4001
3	C	0.24	0/2882	0.56	0/3950
3	D	0.23	0/2840	0.60	1/3897 (0.0%)
3	I	0.47	0/391	0.78	0/540
3	J	0.47	0/393	0.78	0/543
3	K	0.45	0/416	0.76	0/571
3	L	0.47	0/397	0.78	0/548
3	Q	0.17	0/3632	0.51	1/4968 (0.0%)
3	R	0.16	0/2877	0.50	0/3947
3	S	0.23	0/2462	0.57	0/3414
3	T	0.24	0/2440	0.60	0/3390
4	E	0.25	0/484	0.65	1/655 (0.2%)
4	P	0.27	0/490	0.51	0/663
All	All	0.21	0/49579	0.53	4/67889 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	O	0	2
2	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	1
All	All	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	241	ARG	CB-CA-C	-6.00	101.52	111.41
3	D	317	ARG	N-CA-C	-5.38	105.10	110.97
1	O	400	ARG	CB-CA-C	-5.36	99.75	110.42
4	E	30	ILE	N-CA-C	-5.19	104.40	110.05

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	510	ARG	Sidechain
2	H	402	ARG	Sidechain
2	M	527	ARG	Sidechain
1	O	382	ARG	Sidechain
1	O	398	ILE	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3719	0	3618	16	0
1	O	3718	0	3621	17	0
2	G	3880	0	3808	25	0
2	H	3929	0	3855	20	0
2	M	3888	0	3825	22	0
2	N	3881	0	3808	39	0
3	A	3409	0	3172	35	0
3	B	2859	0	2714	14	0
3	C	2822	0	2664	29	0
3	D	2781	0	2551	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	390	0	343	7	0
3	J	392	0	348	8	0
3	K	415	0	379	8	0
3	L	396	0	352	9	0
3	Q	3564	0	3442	42	0
3	R	2817	0	2609	19	0
3	S	2420	0	1897	13	0
3	T	2401	0	1919	19	0
4	E	473	0	461	4	0
4	P	479	0	461	4	0
5	A	15	0	15	3	0
5	I	15	0	15	7	0
5	J	15	0	15	1	0
5	K	15	0	15	2	0
5	L	15	0	15	15	0
5	Q	15	0	15	3	0
6	A	4	0	0	0	0
6	Q	4	0	0	4	0
All	All	48731	0	45937	383	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 4.

All (383) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:387:GLY:HA3	5:L:601:BTN:H5	1.33	1.10
3:Q:302:VAL:HG23	6:Q:602:BCT:O1	1.64	0.97
3:Q:241:ARG:HH12	3:Q:565:MET:CE	1.81	0.93
2:G:387:GLY:HA3	5:I:601:BTN:H5	1.51	0.90
3:B:112:PRO:HB3	3:B:275:TYR:CE2	2.07	0.88
3:Q:122:ASP:OD2	3:Q:125:THR:OG1	1.91	0.88
2:N:387:GLY:CA	5:L:601:BTN:H5	2.03	0.86
3:Q:241:ARG:HH12	3:Q:565:MET:HE1	1.40	0.86
2:N:388:PHE:N	5:L:601:BTN:HN1	1.74	0.83
3:A:236:CYS:HB3	3:A:244:LYS:HD3	1.60	0.82
3:B:275:TYR:HE1	3:B:298:THR:HA	1.45	0.81
3:Q:239:GLN:O	3:Q:240:ARG:HG2	1.81	0.80
1:O:400:ARG:O	1:O:401:LYS:HB2	1.81	0.79
3:L:547:GLU:O	3:L:578:THR:HA	1.83	0.79
3:J:547:GLU:O	3:J:578:THR:HA	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:387:GLY:HA3	5:L:601:BTN:C5	2.13	0.79
3:I:547:GLU:O	3:I:578:THR:HA	1.83	0.78
3:A:217:GLU:HG2	3:A:280:THR:CG2	2.13	0.78
3:C:138:VAL:HG22	3:C:139:PRO:HD2	1.66	0.77
3:K:547:GLU:O	3:K:578:THR:HA	1.83	0.76
3:Q:240:ARG:HH21	3:Q:241:ARG:NH1	1.85	0.75
5:Q:601:BTN:H5	6:Q:602:BCT:C	2.18	0.74
3:Q:240:ARG:HG3	3:Q:241:ARG:H	1.53	0.73
3:Q:241:ARG:NH1	3:Q:565:MET:CE	2.51	0.73
2:N:386:PRO:HG2	5:L:601:BTN:H61	1.70	0.73
3:B:275:TYR:CE1	3:B:298:THR:HA	2.23	0.72
3:Q:241:ARG:NH1	3:Q:565:MET:HE2	2.04	0.72
3:T:244:LYS:HE3	3:T:302:VAL:HB	1.73	0.70
3:K:548:GLY:O	3:K:549:GLN:C	2.35	0.70
3:J:548:GLY:O	3:J:549:GLN:C	2.35	0.70
3:I:548:GLY:O	3:I:549:GLN:C	2.34	0.70
3:Q:240:ARG:CG	3:Q:241:ARG:N	2.52	0.70
2:G:24:ASP:OD1	2:G:27:ARG:NH1	2.26	0.69
3:L:548:GLY:O	3:L:549:GLN:C	2.35	0.68
2:N:356:CYS:SG	5:L:601:BTN:C6	2.80	0.68
2:G:210:THR:HG21	5:L:601:BTN:O3	1.94	0.68
2:M:393:ASP:O	2:M:397:ASN:ND2	2.28	0.67
3:D:20:ILE:HB	3:D:89:TYR:CE2	2.29	0.67
3:Q:240:ARG:HG3	3:Q:241:ARG:N	2.09	0.67
3:S:112:PRO:HG3	3:S:275:TYR:CE1	2.30	0.66
2:N:356:CYS:SG	5:L:601:BTN:S1	2.93	0.66
3:D:217:GLU:OE2	3:D:234:ARG:NH1	2.29	0.66
1:O:127:ASP:OD1	1:O:128:SER:N	2.28	0.66
2:N:422:THR:O	2:N:423:ARG:HB2	1.94	0.66
3:A:75:ASP:O	3:A:79:LYS:HG3	1.97	0.65
2:N:388:PHE:H	5:L:601:BTN:HN1	1.42	0.65
3:D:302:VAL:HG11	3:D:344:ARG:NH2	2.11	0.64
3:Q:230:VAL:HG23	3:Q:267:LYS:HE2	1.78	0.64
2:N:28:ARG:O	2:N:32:THR:HG23	1.97	0.64
3:C:213:PRO:HB2	3:C:284:LEU:HG	1.79	0.64
2:G:387:GLY:HA3	5:I:601:BTN:C5	2.27	0.64
2:G:28:ARG:O	2:G:32:THR:HG23	1.98	0.63
2:N:210:THR:CG2	5:I:601:BTN:O3	2.47	0.62
3:A:216:VAL:HG12	3:A:217:GLU:H	1.65	0.62
3:T:223:ASP:CG	3:T:322:ILE:HG12	2.25	0.61
2:H:28:ARG:O	2:H:32:THR:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:129:ILE:O	3:Q:132:ARG:HG3	2.00	0.61
3:D:31:ALA:HB2	3:D:317:ARG:HH12	1.65	0.61
3:C:20:ILE:HB	3:C:89:TYR:CE2	2.36	0.61
3:S:240:ARG:N	3:S:243:GLN:O	2.34	0.60
2:N:210:THR:HG22	5:I:601:BTN:O3	2.01	0.60
3:A:31:ALA:HA	3:A:317:ARG:NH2	2.16	0.60
3:C:138:VAL:HG22	3:C:139:PRO:CD	2.31	0.60
3:A:217:GLU:CG	3:A:280:THR:CG2	2.79	0.60
3:C:223:ASP:OD2	3:C:227:ASN:ND2	2.29	0.60
3:A:31:ALA:HA	3:A:317:ARG:HH21	1.67	0.60
1:O:282:TYR:HE1	1:O:400:ARG:HH21	1.48	0.59
3:D:43:ASP:OD2	3:D:67:TYR:OH	2.18	0.59
3:T:223:ASP:OD2	3:T:322:ILE:HG12	2.02	0.59
2:N:356:CYS:SG	5:L:601:BTN:H62	2.43	0.59
2:G:386:PRO:HG2	5:I:601:BTN:H61	1.85	0.58
3:T:303:GLU:O	3:T:306:VAL:HG22	2.04	0.57
3:D:337:ARG:HB2	3:D:337:ARG:CZ	2.34	0.57
3:Q:239:GLN:O	3:Q:240:ARG:C	2.45	0.57
3:Q:301:GLN:NE2	6:Q:602:BCT:C	2.67	0.57
3:Q:301:GLN:HE22	6:Q:602:BCT:C	2.17	0.57
2:N:389:LEU:CD1	3:L:563:MET:HE1	2.35	0.57
3:A:216:VAL:HG12	3:A:217:GLU:N	2.20	0.57
3:C:462:PHE:CG	3:C:463:THR:N	2.67	0.57
3:B:129:ILE:HG12	3:B:132:ARG:HH21	1.69	0.56
2:N:265:ASN:OD1	2:N:268:ALA:N	2.33	0.56
3:R:134:LYS:O	3:R:268:ARG:NH1	2.36	0.56
3:C:223:ASP:OD1	3:C:226:GLY:N	2.39	0.55
3:Q:229:VAL:HA	3:Q:267:LYS:NZ	2.22	0.55
2:H:265:ASN:OD1	2:H:268:ALA:N	2.37	0.55
2:N:389:LEU:HD11	3:L:563:MET:HE1	1.89	0.55
3:Q:303:GLU:C	3:Q:305:PRO:HD2	2.32	0.55
2:G:210:THR:CG2	5:L:601:BTN:O3	2.54	0.55
2:G:495:ASN:HB2	2:G:496:PRO:HD2	1.87	0.55
3:I:547:GLU:C	3:I:578:THR:HA	2.32	0.55
3:S:46:ALA:O	3:S:49:VAL:HG22	2.07	0.55
2:H:119:GLU:HA	2:H:159:LEU:CD1	2.37	0.54
3:L:547:GLU:C	3:L:578:THR:HA	2.31	0.54
3:D:259:ARG:O	3:D:262:ILE:HG22	2.07	0.54
3:B:113:SER:HB3	3:B:276:TYR:HE1	1.71	0.54
3:B:275:TYR:HD2	3:B:276:TYR:N	2.06	0.54
2:N:303:GLN:O	2:N:423:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:9:ILE:HD12	3:D:9:ILE:H	1.72	0.54
3:C:138:VAL:HG23	3:C:292:SER:OG	2.07	0.54
3:Q:214:ARG:NH2	3:Q:252:PRO:O	2.38	0.54
3:J:547:GLU:C	3:J:578:THR:HA	2.32	0.54
3:K:547:GLU:C	3:K:578:THR:HA	2.31	0.54
3:A:299:ARG:O	3:A:300:LEU:C	2.47	0.54
3:J:549:GLN:O	3:J:551:VAL:HG23	2.09	0.53
3:D:31:ALA:CB	3:D:317:ARG:HH12	2.20	0.53
3:A:20:ILE:HB	3:A:89:TYR:CE2	2.43	0.53
3:C:89:TYR:CD1	3:C:89:TYR:C	2.86	0.53
1:O:399:ILE:O	1:O:400:ARG:HB2	2.07	0.53
3:K:549:GLN:O	3:K:551:VAL:HG23	2.09	0.53
3:A:303:GLU:C	3:A:305:PRO:HD2	2.34	0.53
3:S:490:VAL:HA	3:T:482:GLU:O	2.08	0.53
3:L:549:GLN:O	3:L:551:VAL:HG23	2.08	0.53
2:M:268:ALA:HA	4:P:64:ARG:O	2.09	0.53
2:N:387:GLY:CA	5:L:601:BTN:C5	2.80	0.53
3:Q:229:VAL:HA	3:Q:267:LYS:HZ3	1.72	0.53
3:I:549:GLN:O	3:I:551:VAL:HG23	2.09	0.52
3:D:31:ALA:N	3:D:317:ARG:HH22	2.07	0.52
2:G:387:GLY:CA	5:I:601:BTN:H5	2.31	0.52
2:M:527:ARG:HD3	4:P:94:ARG:HD3	1.92	0.52
2:N:388:PHE:N	5:L:601:BTN:N1	2.53	0.52
3:A:299:ARG:O	3:A:299:ARG:HG3	2.09	0.52
3:Q:564:LYS:HG3	5:Q:601:BTN:O11	2.10	0.52
1:F:446:ASP:N	1:F:447:PRO:HD2	2.24	0.52
1:O:403:TYR:HA	1:O:429:ALA:O	2.10	0.52
2:G:359:ILE:HG21	2:G:402:ARG:CZ	2.39	0.51
1:F:446:ASP:N	1:F:447:PRO:CD	2.73	0.51
2:M:34:HIS:O	2:M:34:HIS:ND1	2.41	0.51
1:F:164:PHE:O	1:F:187:GLN:HG2	2.10	0.51
3:A:217:GLU:HG2	3:A:280:THR:HG23	1.90	0.51
3:B:113:SER:HB3	3:B:276:TYR:CE1	2.45	0.51
3:Q:128:HIS:O	3:Q:132:ARG:HG2	2.11	0.51
3:Q:241:ARG:HH12	3:Q:565:MET:HE2	1.61	0.51
3:R:283:TYR:CD1	3:R:293:PHE:HA	2.46	0.51
1:O:400:ARG:O	1:O:401:LYS:CB	2.53	0.51
3:A:564:LYS:NZ	5:A:601:BTN:H102	2.26	0.51
3:Q:223:ASP:OD2	3:Q:327:PRO:HA	2.11	0.51
3:Q:239:GLN:C	3:Q:240:ARG:O	2.54	0.51
3:A:136:PRO:HD3	3:A:265:SER:OG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:108:ILE:N	3:Q:108:ILE:HD12	2.26	0.50
2:G:75:ARG:NH2	2:G:119:GLU:OE2	2.42	0.50
2:N:540:ILE:HG13	2:N:541:PRO:HD2	1.94	0.50
3:T:13:LEU:HA	3:T:36:VAL:HG13	1.93	0.50
3:K:547:GLU:O	3:K:578:THR:CA	2.59	0.50
3:C:9:ILE:HG13	3:C:324:ASN:OD1	2.12	0.50
3:D:249:ALA:HB3	3:D:306:VAL:CG1	2.42	0.50
1:F:257:PRO:CD	3:A:509:VAL:HG13	2.42	0.50
2:M:44:VAL:HG12	2:M:49:LYS:O	2.12	0.50
3:D:317:ARG:O	3:D:320:PHE:N	2.45	0.50
2:M:309:GLU:O	2:M:313:ARG:NH1	2.41	0.49
2:N:423:ARG:O	2:N:450:GLN:N	2.44	0.49
1:O:383:PHE:CD2	1:O:409:VAL:HG11	2.47	0.49
3:Q:492:LEU:HD23	4:P:30:ILE:HG23	1.93	0.49
1:F:360:VAL:HG22	1:F:410:MET:HB3	1.95	0.49
1:O:336:ASN:OD1	1:O:376:ILE:HD13	2.13	0.49
3:D:251:ALA:O	3:D:259:ARG:NH2	2.45	0.49
3:Q:301:GLN:HB3	3:Q:303:GLU:OE1	2.13	0.49
3:C:216:VAL:HG22	3:C:233:THR:CG2	2.43	0.49
3:Q:564:LYS:CD	5:Q:601:BTN:O11	2.60	0.49
3:R:418:VAL:HG21	3:R:423:THR:HG21	1.95	0.49
5:K:601:BTN:H5	2:M:387:GLY:HA3	1.95	0.49
2:M:179:LEU:HD23	2:M:199:VAL:HB	1.95	0.49
2:M:423:ARG:O	2:M:449:ALA:HA	2.12	0.49
2:H:275:VAL:HG11	2:H:339:GLU:HA	1.95	0.48
3:C:462:PHE:O	3:C:463:THR:C	2.56	0.48
2:M:307:MET:HG2	2:M:347:ALA:HB1	1.96	0.48
3:D:368:THR:HG22	3:D:369:GLY:N	2.28	0.48
3:Q:241:ARG:NH1	3:Q:565:MET:HE1	2.17	0.48
2:H:202:ASP:OD2	2:H:203:GLN:NE2	2.38	0.48
1:O:399:ILE:HG23	1:O:423:TRP:CE3	2.48	0.48
3:D:337:ARG:CZ	3:C:337:ARG:HB2	2.43	0.48
3:Q:303:GLU:O	3:Q:306:VAL:HG22	2.14	0.48
3:I:547:GLU:O	3:I:578:THR:CA	2.59	0.48
2:H:36:VAL:HG12	2:H:36:VAL:O	2.13	0.48
3:L:548:GLY:HA2	3:L:578:THR:CG2	2.44	0.48
3:C:7:SER:HB2	3:C:108:ILE:HD12	1.95	0.48
3:T:233:THR:O	3:T:250:PRO:HA	2.14	0.48
3:T:234:ARG:CG	3:T:307:THR:HG23	2.44	0.48
1:F:48:LEU:HD21	1:F:88:VAL:HG21	1.95	0.48
3:B:267:LYS:O	3:B:268:ARG:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:548:GLY:HA2	3:J:578:THR:CG2	2.44	0.48
3:B:112:PRO:HB3	3:B:275:TYR:CD2	2.48	0.48
3:K:548:GLY:HA2	3:K:578:THR:CG2	2.44	0.48
2:N:210:THR:HG21	5:I:601:BTN:O3	2.14	0.48
3:C:318:GLN:HA	3:C:321:LYS:HZ2	1.79	0.47
2:H:384:ASP:OD2	2:H:423:ARG:NH1	2.47	0.47
3:I:548:GLY:HA2	3:I:578:THR:CG2	2.44	0.47
2:G:422:THR:HG22	2:G:446:TRP:CD2	2.48	0.47
2:M:191:SER:HB3	2:M:192:PRO:HD3	1.97	0.47
3:A:304:HIS:N	3:A:305:PRO:CD	2.77	0.47
3:K:558:VAL:HG22	3:K:569:VAL:HB	1.97	0.47
3:J:547:GLU:O	3:J:578:THR:CA	2.59	0.47
3:A:217:GLU:CD	3:A:217:GLU:C	2.82	0.47
3:A:303:GLU:C	3:A:305:PRO:CD	2.88	0.47
3:D:259:ARG:HA	3:D:262:ILE:HG22	1.96	0.47
3:D:306:VAL:O	3:D:310:THR:HG23	2.14	0.47
3:Q:303:GLU:C	3:Q:305:PRO:CD	2.87	0.47
3:R:214:ARG:NH1	3:R:252:PRO:O	2.48	0.47
3:A:136:PRO:CD	3:A:265:SER:OG	2.63	0.47
3:A:564:LYS:HZ1	5:A:601:BTN:H102	1.79	0.47
2:H:14:ASP:OD1	2:H:16:HIS:ND1	2.33	0.47
3:C:223:ASP:OD1	3:C:223:ASP:C	2.58	0.47
3:Q:136:PRO:HD3	3:Q:265:SER:OG	2.15	0.47
1:F:405:GLY:O	1:F:409:VAL:HG22	2.14	0.46
3:D:349:ASP:O	3:D:354:PHE:N	2.48	0.46
3:C:424:VAL:HG12	3:C:424:VAL:O	2.15	0.46
3:D:136:PRO:HD3	3:D:265:SER:OG	2.16	0.46
1:F:199:LYS:O	1:F:203:GLY:N	2.46	0.46
3:J:558:VAL:HG22	3:J:569:VAL:HB	1.97	0.46
3:Q:304:HIS:N	3:Q:305:PRO:CD	2.78	0.46
3:K:548:GLY:HA2	3:K:578:THR:HG22	1.98	0.46
3:R:223:ASP:OD2	3:R:327:PRO:HA	2.15	0.46
3:T:230:VAL:HG11	3:T:263:HIS:CE1	2.51	0.46
1:O:456:ARG:O	1:O:460:ILE:HD13	2.15	0.46
3:R:39:TYR:HB3	3:R:49:VAL:HG22	1.97	0.46
3:C:125:THR:O	3:C:129:ILE:HG13	2.16	0.46
3:Q:388:PHE:HA	3:Q:564:LYS:HE3	1.98	0.46
3:A:302:VAL:HG21	3:A:344:ARG:CZ	2.46	0.46
3:J:548:GLY:HA2	3:J:578:THR:HG22	1.98	0.46
3:B:275:TYR:HD2	3:B:277:GLY:H	1.62	0.46
2:M:82:GLU:OE1	2:M:82:GLU:N	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:297:ASN:ND2	3:Q:301:GLN:OE1	2.35	0.45
1:O:509:GLN:NE2	4:E:88:GLU:OE2	2.37	0.45
2:N:186:GLY:O	2:N:189:VAL:HG22	2.15	0.45
2:N:422:THR:HG22	2:N:446:TRP:CD2	2.51	0.45
3:A:304:HIS:CG	3:A:305:PRO:HD3	2.52	0.45
3:A:444:PHE:CD1	3:A:444:PHE:C	2.94	0.45
3:D:306:VAL:HG23	3:D:342:GLU:HB2	1.97	0.45
3:S:86:HIS:CB	3:S:110:ILE:HD12	2.47	0.45
3:S:351:GLY:HA3	3:S:461:PRO:HA	1.97	0.45
3:L:547:GLU:O	3:L:578:THR:CA	2.59	0.45
3:A:217:GLU:OE2	3:A:280:THR:HG23	2.17	0.45
3:D:228:VAL:HB	3:D:267:LYS:NZ	2.32	0.45
3:C:321:LYS:O	3:C:324:ASN:HB2	2.17	0.45
3:D:259:ARG:O	3:D:260:LYS:C	2.59	0.45
3:D:418:VAL:HG21	3:D:423:THR:HG21	1.99	0.45
3:I:548:GLY:HA2	3:I:578:THR:HG22	1.98	0.45
3:L:548:GLY:HA2	3:L:578:THR:HG22	1.98	0.45
3:A:217:GLU:CG	3:A:280:THR:HG21	2.47	0.45
3:D:86:HIS:HB2	3:D:110:ILE:HD12	1.99	0.45
3:D:428:HIS:O	3:D:432:VAL:HG23	2.17	0.45
3:S:275:TYR:CD2	3:S:276:TYR:N	2.85	0.45
3:R:136:PRO:CD	3:R:265:SER:HB3	2.47	0.45
2:M:186:GLY:O	2:M:189:VAL:HG22	2.17	0.45
3:T:424:VAL:HG23	3:T:428:HIS:NE2	2.32	0.45
2:N:315:LEU:HD21	2:N:345:ILE:HD11	1.98	0.45
3:Q:303:GLU:H	3:Q:303:GLU:CD	2.25	0.45
3:D:236:CYS:O	3:D:239:GLN:CG	2.65	0.44
3:B:306:VAL:CG1	3:B:342:GLU:HB2	2.47	0.44
2:N:191:SER:HB3	2:N:192:PRO:HD3	1.98	0.44
2:H:305:TYR:HE1	2:H:423:ARG:NH1	2.16	0.44
2:H:495:ASN:HB2	2:H:496:PRO:HD2	1.99	0.44
2:M:288:ASP:O	2:M:292:GLU:HG3	2.17	0.44
2:N:307:MET:HG2	2:N:347:ALA:HB1	1.99	0.44
2:N:540:ILE:CG1	2:N:541:PRO:HD2	2.47	0.44
1:F:413:LYS:HE3	1:F:480:ASP:OD1	2.18	0.44
3:R:304:HIS:CG	3:R:305:PRO:HD3	2.53	0.44
2:M:495:ASN:HB2	2:M:496:PRO:HD2	1.98	0.44
3:D:368:THR:CG2	3:D:369:GLY:N	2.80	0.44
3:S:231:ALA:O	3:S:311:SER:OG	2.31	0.44
3:A:564:LYS:NZ	5:A:601:BTN:O11	2.51	0.44
3:D:305:PRO:HG2	3:D:394:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:224:GLN:HG2	3:B:276:TYR:CD2	2.53	0.44
2:G:316:ASP:OD2	2:G:339:GLU:N	2.50	0.44
3:S:39:TYR:CD2	3:S:44:ALA:HA	2.53	0.44
1:O:110:ARG:HG3	1:O:110:ARG:HH11	1.83	0.44
3:D:317:ARG:O	3:D:318:GLN:C	2.60	0.44
3:Q:293:PHE:CZ	3:Q:295:GLU:HA	2.53	0.44
3:T:335:THR:HG23	3:T:335:THR:O	2.17	0.44
3:A:124:VAL:HG23	3:A:125:THR:N	2.33	0.43
3:D:337:ARG:HH21	3:C:337:ARG:HH21	1.64	0.43
1:F:414:GLN:CD	1:F:414:GLN:H	2.27	0.43
3:D:444:PHE:C	3:D:444:PHE:CD1	2.95	0.43
1:F:323:ILE:N	1:F:323:ILE:HD12	2.32	0.43
3:C:284:LEU:HD12	3:C:284:LEU:HA	1.79	0.43
3:S:66:SER:OG	3:S:67:TYR:N	2.51	0.43
3:T:39:TYR:HB3	3:T:49:VAL:HG22	2.00	0.43
1:F:149:ARG:O	1:F:152:MET:HG2	2.19	0.43
1:F:257:PRO:HD2	3:A:509:VAL:HG13	2.00	0.43
3:A:493:PRO:HD2	4:E:30:ILE:HD13	2.00	0.43
3:D:213:PRO:O	3:D:448:THR:HG23	2.17	0.43
3:D:383:VAL:C	3:D:384:ILE:HD12	2.43	0.43
2:G:346:VAL:O	2:G:381:LEU:HA	2.19	0.43
3:D:50:ARG:CZ	3:D:50:ARG:HB3	2.49	0.43
3:D:262:ILE:HG23	3:D:263:HIS:HD2	1.83	0.43
3:D:304:HIS:CG	3:D:305:PRO:HD3	2.53	0.43
3:R:223:ASP:OD1	3:R:224:GLN:N	2.52	0.43
2:H:186:GLY:O	2:H:189:VAL:HG22	2.19	0.43
3:D:228:VAL:HB	3:D:267:LYS:HZ2	1.84	0.43
2:M:106:PHE:CZ	2:M:141:GLY:HA3	2.54	0.43
3:A:16:ASN:CG	3:A:88:GLY:HA3	2.44	0.43
3:R:474:VAL:N	3:R:475:PRO:HD2	2.34	0.43
2:N:356:CYS:HG	5:L:601:BTN:C6	2.31	0.43
2:N:388:PHE:O	5:L:601:BTN:N1	2.52	0.43
1:O:360:VAL:HG22	1:O:410:MET:HB3	2.01	0.43
3:A:118:ARG:HB2	3:A:118:ARG:CZ	2.49	0.43
2:G:44:VAL:HG12	2:G:49:LYS:O	2.19	0.43
2:G:119:GLU:HA	2:G:159:LEU:HD13	2.00	0.43
2:N:318:ASP:OD1	2:N:318:ASP:N	2.49	0.43
3:A:299:ARG:O	3:A:301:GLN:N	2.52	0.43
3:C:126:ALA:HA	3:C:129:ILE:HD12	2.01	0.43
3:Q:496:LEU:HD21	4:P:30:ILE:HD11	2.00	0.43
3:R:9:ILE:HD11	3:R:323:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:98:PHE:O	3:T:102:VAL:HG23	2.19	0.43
3:B:304:HIS:CG	3:B:305:PRO:HD3	2.54	0.42
3:T:258:GLN:HE21	3:T:289:GLY:HA3	1.83	0.42
5:K:601:BTN:N1	2:M:388:PHE:O	2.52	0.42
2:M:28:ARG:O	2:M:32:THR:HG23	2.20	0.42
2:N:191:SER:O	2:N:195:THR:HG23	2.19	0.42
3:C:423:THR:O	3:C:426:PRO:HD2	2.19	0.42
2:G:282:ILE:HG22	2:G:286:LEU:HD21	2.02	0.42
2:H:307:MET:HG2	2:H:347:ALA:HB1	2.02	0.42
3:D:66:SER:OG	3:D:67:TYR:N	2.51	0.42
3:R:136:PRO:CG	3:R:265:SER:OG	2.67	0.42
3:D:48:HIS:CE1	3:D:49:VAL:HG13	2.55	0.42
2:G:213:ASP:OD1	2:G:214:VAL:N	2.53	0.42
3:D:220:VAL:N	3:D:279:GLY:O	2.52	0.42
3:R:306:VAL:HG13	3:R:342:GLU:HB2	2.02	0.42
3:R:306:VAL:O	3:R:310:THR:HG23	2.19	0.42
3:T:20:ILE:HB	3:T:89:TYR:CE2	2.54	0.42
3:T:258:GLN:NE2	3:T:289:GLY:HA3	2.35	0.42
2:M:235:MET:HE2	2:M:244:VAL:HG23	2.02	0.42
3:B:424:VAL:HG23	3:B:428:HIS:NE2	2.34	0.42
3:S:304:HIS:N	3:S:305:PRO:CD	2.82	0.42
3:T:482:GLU:HA	3:T:486:ARG:O	2.20	0.42
2:G:307:MET:HG2	2:G:347:ALA:HB1	2.02	0.42
2:N:423:ARG:O	2:N:449:ALA:HA	2.19	0.42
1:O:154:ARG:HA	1:O:154:ARG:NE	2.35	0.42
2:M:540:ILE:HG23	2:M:542:LEU:HG	2.01	0.41
3:A:489:GLU:O	4:E:33:LEU:N	2.53	0.41
3:D:223:ASP:OD1	3:D:226:GLY:N	2.46	0.41
3:C:234:ARG:CG	3:C:307:THR:HG23	2.50	0.41
2:G:479:ASP:O	2:G:483:LEU:HD23	2.21	0.41
2:G:495:ASN:OD1	2:G:498:ILE:HG12	2.20	0.41
3:Q:233:THR:O	3:Q:250:PRO:HA	2.20	0.41
3:R:424:VAL:HG23	3:R:428:HIS:NE2	2.35	0.41
1:F:112:MET:HA	1:F:115:VAL:HG22	2.02	0.41
2:G:309:GLU:O	2:G:313:ARG:NH1	2.41	0.41
2:H:234:HIS:HA	2:H:238:SER:HG	1.86	0.41
2:N:242:HIS:HA	2:N:324:GLN:HG2	2.02	0.41
3:D:31:ALA:HB2	3:D:317:ARG:NH1	2.34	0.41
2:H:191:SER:HB3	2:H:192:PRO:HD3	2.03	0.41
1:O:300:ILE:HD11	1:O:312:PHE:CE2	2.55	0.41
2:N:346:VAL:O	2:N:381:LEU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:337:ARG:NH2	3:R:311:SER:O	2.53	0.41
1:F:399:ILE:HD12	1:F:423:TRP:CD2	2.56	0.41
2:G:191:SER:HB3	2:G:192:PRO:HD3	2.02	0.41
3:A:486:ARG:NH2	4:E:36:GLU:O	2.51	0.41
2:H:60:LEU:HD13	2:H:96:GLY:HA3	2.02	0.41
2:H:72:ALA:HB1	2:H:120:VAL:HG11	2.02	0.41
2:H:387:GLY:HA3	5:J:601:BTN:H5	2.02	0.41
3:S:234:ARG:NH2	3:S:307:THR:OG1	2.54	0.41
3:D:89:TYR:CD1	3:D:89:TYR:C	2.99	0.41
3:D:270:CYS:SG	3:D:275:TYR:HB3	2.61	0.41
3:S:425:ILE:N	3:S:426:PRO:CD	2.84	0.41
2:M:89:ASP:OD2	2:M:121:TYR:N	2.50	0.41
2:M:93:THR:HB	2:M:128:VAL:HG21	2.03	0.41
1:O:336:ASN:HB3	1:O:379:ARG:NE	2.36	0.41
3:C:304:HIS:CG	3:C:305:PRO:HD3	2.56	0.41
2:H:101:ARG:NH2	2:H:259:LEU:O	2.46	0.41
2:N:203:GLN:C	2:N:204:THR:HG23	2.46	0.41
1:O:408:ALA:O	1:O:415:LEU:HD12	2.21	0.41
3:D:361:VAL:O	3:D:361:VAL:HG12	2.21	0.41
3:R:70:PHE:CZ	3:R:98:PHE:HB2	2.55	0.41
2:G:82:GLU:OE1	2:G:82:GLU:N	2.47	0.40
2:N:155:VAL:O	2:N:159:LEU:HD23	2.20	0.40
3:C:39:TYR:HB3	3:C:49:VAL:CG2	2.51	0.40
3:T:396:ILE:N	3:T:396:ILE:HD12	2.36	0.40
2:G:540:ILE:HG13	2:G:541:PRO:HD2	2.03	0.40
3:D:18:GLY:O	3:D:21:ALA:HB3	2.21	0.40
3:C:84:ALA:HB2	3:C:108:ILE:CG2	2.51	0.40
3:C:349:ASP:O	3:C:354:PHE:N	2.52	0.40
3:R:136:PRO:HD2	3:R:265:SER:HB3	2.04	0.40
3:R:368:THR:HG22	3:R:369:GLY:N	2.36	0.40
1:F:114:TRP:O	1:F:118:VAL:HG22	2.22	0.40
2:H:149:ARG:NH1	2:H:152:GLU:OE2	2.54	0.40
2:N:495:ASN:HB2	2:N:496:PRO:HD2	2.04	0.40
3:Q:304:HIS:CG	3:Q:305:PRO:HD3	2.56	0.40
3:T:234:ARG:HD3	3:T:307:THR:HG23	2.03	0.40
2:H:410:TYR:CE2	2:H:434:GLY:HA2	2.57	0.40
3:D:434:ASP:OD2	3:D:450:TRP:CZ2	2.75	0.40
3:C:9:ILE:HD11	3:C:323:ALA:HB3	2.02	0.40
2:N:34:HIS:O	2:N:34:HIS:ND1	2.51	0.40
3:D:361:VAL:HG23	3:D:384:ILE:HD13	2.04	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	F	513/517 (99%)	492 (96%)	21 (4%)	0	100	100
1	O	513/517 (99%)	493 (96%)	18 (4%)	2 (0%)	30	64
2	G	528/542 (97%)	508 (96%)	20 (4%)	0	100	100
2	H	537/542 (99%)	515 (96%)	21 (4%)	1 (0%)	44	75
2	M	528/542 (97%)	511 (97%)	17 (3%)	0	100	100
2	N	530/542 (98%)	513 (97%)	16 (3%)	1 (0%)	44	75
3	A	504/598 (84%)	484 (96%)	19 (4%)	1 (0%)	44	75
3	B	409/598 (68%)	389 (95%)	20 (5%)	0	100	100
3	C	403/598 (67%)	381 (94%)	21 (5%)	1 (0%)	44	75
3	D	404/598 (68%)	388 (96%)	15 (4%)	1 (0%)	44	75
3	I	65/598 (11%)	57 (88%)	5 (8%)	3 (5%)	2	18
3	J	65/598 (11%)	57 (88%)	5 (8%)	3 (5%)	2	18
3	K	65/598 (11%)	57 (88%)	5 (8%)	3 (5%)	2	18
3	L	65/598 (11%)	57 (88%)	5 (8%)	3 (5%)	2	18
3	Q	504/598 (84%)	483 (96%)	21 (4%)	0	100	100
3	R	408/598 (68%)	386 (95%)	22 (5%)	0	100	100
3	S	404/598 (68%)	385 (95%)	18 (4%)	1 (0%)	44	75
3	T	400/598 (67%)	386 (96%)	14 (4%)	0	100	100
4	E	57/94 (61%)	55 (96%)	2 (4%)	0	100	100
4	P	58/94 (62%)	52 (90%)	6 (10%)	0	100	100
All	All	6960/10566 (66%)	6649 (96%)	291 (4%)	20 (0%)	38	68

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	423	ARG

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Mol	Chain	Res	Type
1	O	400	ARG
1	O	401	LYS
3	K	549	GLN
3	I	549	GLN
3	J	549	GLN
3	L	549	GLN
3	A	299	ARG
3	D	494	GLY
2	H	423	ARG
3	K	547	GLU
3	I	547	GLU
3	J	547	GLU
3	L	547	GLU
3	C	461	PRO
3	K	578	THR
3	I	578	THR
3	J	578	THR
3	L	578	THR
3	S	110	ILE

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	F	348/412 (84%)	348 (100%)	0	100	100
1	O	351/412 (85%)	350 (100%)	1 (0%)	91	96
2	G	387/436 (89%)	385 (100%)	2 (0%)	86	93
2	H	389/436 (89%)	384 (99%)	5 (1%)	65	81
2	M	390/436 (89%)	390 (100%)	0	100	100
2	N	384/436 (88%)	380 (99%)	4 (1%)	73	84
3	A	281/453 (62%)	277 (99%)	4 (1%)	62	79
3	B	251/453 (55%)	249 (99%)	2 (1%)	79	88
3	C	249/453 (55%)	241 (97%)	8 (3%)	34	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	235/453 (52%)	226 (96%)	9 (4%)	28	57
3	I	26/453 (6%)	26 (100%)	0	100	100
3	J	27/453 (6%)	27 (100%)	0	100	100
3	K	33/453 (7%)	33 (100%)	0	100	100
3	L	28/453 (6%)	28 (100%)	0	100	100
3	Q	326/453 (72%)	322 (99%)	4 (1%)	67	82
3	R	240/453 (53%)	238 (99%)	2 (1%)	79	88
3	S	143/453 (32%)	142 (99%)	1 (1%)	81	89
3	T	151/453 (33%)	149 (99%)	2 (1%)	65	81
4	E	45/76 (59%)	45 (100%)	0	100	100
4	P	47/76 (62%)	47 (100%)	0	100	100
All	All	4331/8156 (53%)	4287 (99%)	44 (1%)	71	84

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	159	LEU
2	G	331	ILE
2	H	128	VAL
2	H	156	SER
2	H	188	HIS
2	H	423	ARG
2	H	424	LYS
2	N	11	HIS
2	N	318	ASP
2	N	333	VAL
2	N	423	ARG
1	O	399	ILE
3	A	16	ASN
3	A	217	GLU
3	A	303	GLU
3	A	444	PHE
3	D	16	ASN
3	D	49	VAL
3	D	89	TYR
3	D	262	ILE
3	D	306	VAL
3	D	337	ARG

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Mol	Chain	Res	Type
3	D	418	VAL
3	D	431	VAL
3	D	444	PHE
3	B	280	THR
3	B	421	LEU
3	C	8	LYS
3	C	138	VAL
3	C	210	LEU
3	C	216	VAL
3	C	321	LYS
3	C	337	ARG
3	C	417	THR
3	C	444	PHE
3	Q	108	ILE
3	Q	240	ARG
3	Q	241	ARG
3	Q	245	LEU
3	S	333	ASP
3	R	83	ASN
3	R	421	LEU
3	T	395	LEU
3	T	401	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	235	GLN
1	F	484	GLN
2	G	34	HIS
2	G	143	ASN
2	G	188	HIS
2	H	167	ASN
2	M	167	ASN
2	M	394	GLN
2	N	45	HIS
2	N	167	ASN
2	N	450	GLN
1	O	93	GLN
1	O	177	GLN
3	L	537	GLN
3	A	297	ASN
3	A	339	HIS

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Mol	Chain	Res	Type
3	D	263	HIS
3	C	83	ASN
3	C	100	GLN
4	E	29	HIS
3	Q	100	GLN
3	Q	225	HIS
3	Q	387	GLN
3	S	263	HIS
3	R	100	GLN
3	R	215	HIS
3	R	239	GLN
3	T	215	HIS
3	T	263	HIS
4	P	82	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
5	BTN	A	601	-	15,16,17	0.48	0	20,21,23	1.02	2 (10%)
6	BCT	A	602	-	3,3,3	1.04	0	2,3,3	1.80	1 (50%)
6	BCT	Q	602	-	3,3,3	1.03	0	2,3,3	1.63	1 (50%)
5	BTN	Q	601	-	15,16,17	6.57	11 (73%)	20,21,23	3.00	10 (50%)
5	BTN	K	601	-	15,16,17	6.51	11 (73%)	20,21,23	2.64	7 (35%)
5	BTN	I	601	-	15,16,17	6.51	11 (73%)	20,21,23	2.64	7 (35%)
5	BTN	J	601	-	15,16,17	6.50	11 (73%)	20,21,23	2.64	7 (35%)
5	BTN	L	601	-	15,16,17	6.50	11 (73%)	20,21,23	2.64	7 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BTN	A	601	-	-	0/6/27/28	0/2/2/2
5	BTN	Q	601	-	-	0/6/27/28	0/2/2/2
5	BTN	K	601	-	-	3/6/27/28	0/2/2/2
5	BTN	I	601	-	-	3/6/27/28	0/2/2/2
5	BTN	J	601	-	-	3/6/27/28	0/2/2/2
5	BTN	L	601	-	-	3/6/27/28	0/2/2/2

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	601	BTN	C6-S1	-13.49	1.43	1.81
5	I	601	BTN	C6-S1	-13.35	1.44	1.81
5	K	601	BTN	C6-S1	-13.35	1.44	1.81
5	J	601	BTN	C6-S1	-13.35	1.44	1.81
5	L	601	BTN	C6-S1	-13.34	1.44	1.81
5	Q	601	BTN	C3-N1	12.79	1.58	1.35
5	K	601	BTN	C3-N1	12.60	1.58	1.35
5	I	601	BTN	C3-N1	12.59	1.58	1.35
5	J	601	BTN	C3-N1	12.57	1.58	1.35
5	L	601	BTN	C3-N1	12.56	1.58	1.35
5	Q	601	BTN	C5-N1	-8.93	1.32	1.46
5	Q	601	BTN	C3-N2	8.80	1.51	1.35
5	L	601	BTN	C5-N1	-8.76	1.33	1.46
5	I	601	BTN	C5-N1	-8.74	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	601	BTN	C5-N1	-8.74	1.33	1.46
5	J	601	BTN	C5-N1	-8.72	1.33	1.46
5	I	601	BTN	C3-N2	8.68	1.51	1.35
5	J	601	BTN	C3-N2	8.67	1.51	1.35
5	K	601	BTN	C3-N2	8.65	1.51	1.35
5	L	601	BTN	C3-N2	8.62	1.51	1.35
5	L	601	BTN	C2-S1	-7.23	1.71	1.82
5	I	601	BTN	C2-S1	-7.21	1.71	1.82
5	K	601	BTN	C2-S1	-7.21	1.71	1.82
5	J	601	BTN	C2-S1	-7.19	1.71	1.82
5	Q	601	BTN	C2-S1	-7.04	1.71	1.82
5	J	601	BTN	C6-C5	5.40	1.64	1.53
5	Q	601	BTN	C6-C5	5.39	1.64	1.53
5	K	601	BTN	C6-C5	5.38	1.64	1.53
5	L	601	BTN	C6-C5	5.38	1.64	1.53
5	I	601	BTN	C6-C5	5.36	1.64	1.53
5	L	601	BTN	C7-C2	4.27	1.63	1.52
5	I	601	BTN	C7-C2	4.25	1.63	1.52
5	K	601	BTN	C7-C2	4.25	1.63	1.52
5	J	601	BTN	C7-C2	4.23	1.63	1.52
5	Q	601	BTN	C7-C2	4.10	1.63	1.52
5	I	601	BTN	C4-N2	-4.08	1.38	1.45
5	J	601	BTN	C4-N2	-4.08	1.38	1.45
5	L	601	BTN	C4-N2	-4.07	1.38	1.45
5	K	601	BTN	C4-N2	-4.06	1.38	1.45
5	Q	601	BTN	C2-C4	-4.00	1.42	1.53
5	Q	601	BTN	C4-N2	-3.94	1.38	1.45
5	L	601	BTN	C2-C4	-3.69	1.43	1.53
5	K	601	BTN	C2-C4	-3.69	1.43	1.53
5	Q	601	BTN	C5-C4	3.67	1.66	1.55
5	I	601	BTN	C2-C4	-3.66	1.43	1.53
5	J	601	BTN	C2-C4	-3.65	1.43	1.53
5	L	601	BTN	C5-C4	3.61	1.66	1.55
5	I	601	BTN	C5-C4	3.61	1.66	1.55
5	K	601	BTN	C5-C4	3.61	1.66	1.55
5	J	601	BTN	C5-C4	3.59	1.66	1.55
5	I	601	BTN	O3-C3	-2.21	1.18	1.23
5	J	601	BTN	O3-C3	-2.19	1.18	1.23
5	K	601	BTN	O3-C3	-2.17	1.18	1.23
5	L	601	BTN	O3-C3	-2.16	1.18	1.23
5	Q	601	BTN	O3-C3	-2.13	1.18	1.23

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	601	BTN	C6-S1-C2	7.47	105.51	89.98
5	I	601	BTN	C6-S1-C2	6.50	103.50	89.98
5	J	601	BTN	C6-S1-C2	6.49	103.49	89.98
5	L	601	BTN	C6-S1-C2	6.49	103.47	89.98
5	K	601	BTN	C6-S1-C2	6.49	103.47	89.98
5	K	601	BTN	C4-C5-N1	5.74	108.80	102.43
5	J	601	BTN	C4-C5-N1	5.73	108.79	102.43
5	L	601	BTN	C4-C5-N1	5.72	108.78	102.43
5	I	601	BTN	C4-C5-N1	5.70	108.76	102.43
5	Q	601	BTN	C4-C5-N1	5.70	108.75	102.43
5	Q	601	BTN	C5-C4-N2	4.31	107.54	102.68
5	I	601	BTN	C5-C4-N2	4.01	107.20	102.68
5	J	601	BTN	C5-C4-N2	3.99	107.18	102.68
5	K	601	BTN	C5-C4-N2	3.98	107.17	102.68
5	L	601	BTN	C5-C4-N2	3.98	107.17	102.68
5	Q	601	BTN	C6-C5-N1	-3.88	108.18	113.18
5	Q	601	BTN	C4-N2-C3	-3.63	108.05	112.56
5	L	601	BTN	C4-N2-C3	-3.21	108.57	112.56
5	I	601	BTN	C4-N2-C3	-3.20	108.58	112.56
5	K	601	BTN	C4-N2-C3	-3.20	108.59	112.56
5	A	601	BTN	C6-S1-C2	-3.19	83.34	89.98
5	J	601	BTN	C4-N2-C3	-3.19	108.60	112.56
5	Q	601	BTN	C5-N1-C3	-3.18	107.72	112.38
5	K	601	BTN	C5-N1-C3	-3.14	107.77	112.38
5	L	601	BTN	C5-N1-C3	-3.13	107.78	112.38
5	J	601	BTN	C5-N1-C3	-3.12	107.79	112.38
5	I	601	BTN	C5-N1-C3	-3.11	107.81	112.38
5	I	601	BTN	C2-C4-C5	-2.92	105.31	108.89
5	J	601	BTN	C2-C4-C5	-2.91	105.34	108.89
5	L	601	BTN	C2-C4-C5	-2.90	105.34	108.89
5	K	601	BTN	C2-C4-C5	-2.89	105.35	108.89
5	Q	601	BTN	C8-C7-C2	-2.74	107.73	114.04
5	K	601	BTN	C6-C5-C4	-2.43	105.22	109.06
5	L	601	BTN	C6-C5-C4	-2.43	105.22	109.06
5	J	601	BTN	C6-C5-C4	-2.40	105.26	109.06
5	I	601	BTN	C6-C5-C4	-2.40	105.26	109.06
6	A	602	BCT	O2-C-O1	2.35	125.69	119.68
5	Q	601	BTN	C2-C4-C5	-2.27	106.12	108.89
5	Q	601	BTN	C6-C5-C4	-2.19	105.60	109.06
6	Q	602	BCT	O2-C-O1	2.13	125.11	119.68
5	A	601	BTN	C2-C4-C5	-2.07	106.36	108.89
5	Q	601	BTN	O11-C11-C10	-2.03	109.33	126.30

There are no chirality outliers.

All (12) torsion outliers are listed below:

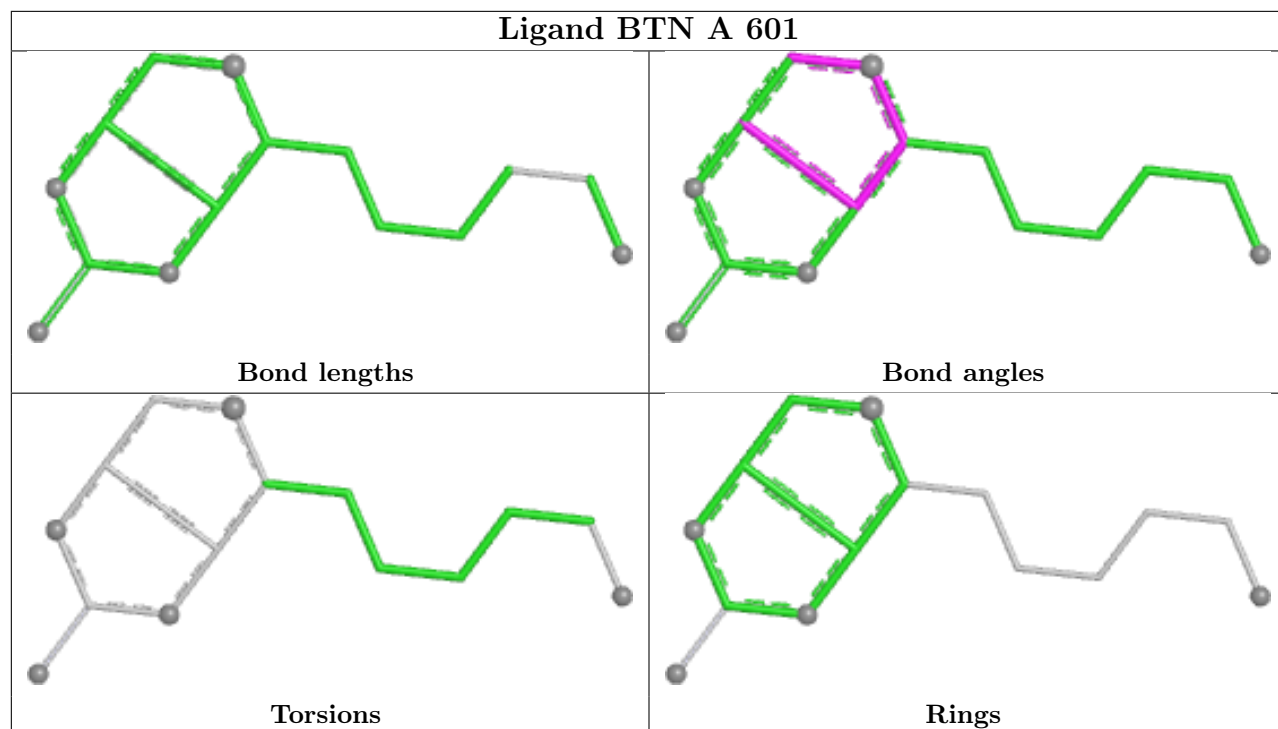
Mol	Chain	Res	Type	Atoms
5	K	601	BTN	C4-C2-C7-C8
5	I	601	BTN	C4-C2-C7-C8
5	J	601	BTN	C4-C2-C7-C8
5	L	601	BTN	C4-C2-C7-C8
5	I	601	BTN	C7-C8-C9-C10
5	K	601	BTN	C7-C8-C9-C10
5	J	601	BTN	C7-C8-C9-C10
5	L	601	BTN	C7-C8-C9-C10
5	K	601	BTN	C2-C7-C8-C9
5	I	601	BTN	C2-C7-C8-C9
5	J	601	BTN	C2-C7-C8-C9
5	L	601	BTN	C2-C7-C8-C9

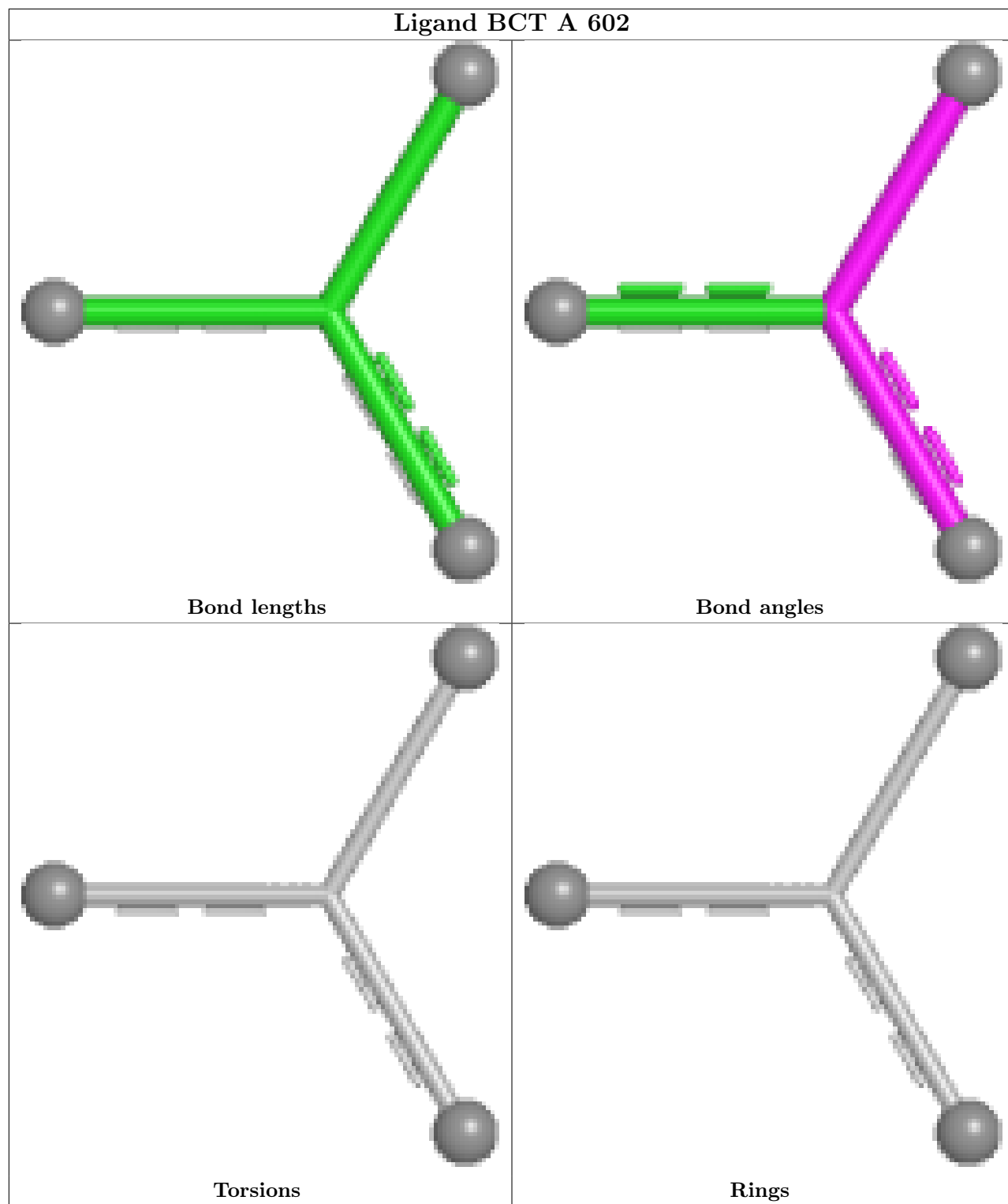
There are no ring outliers.

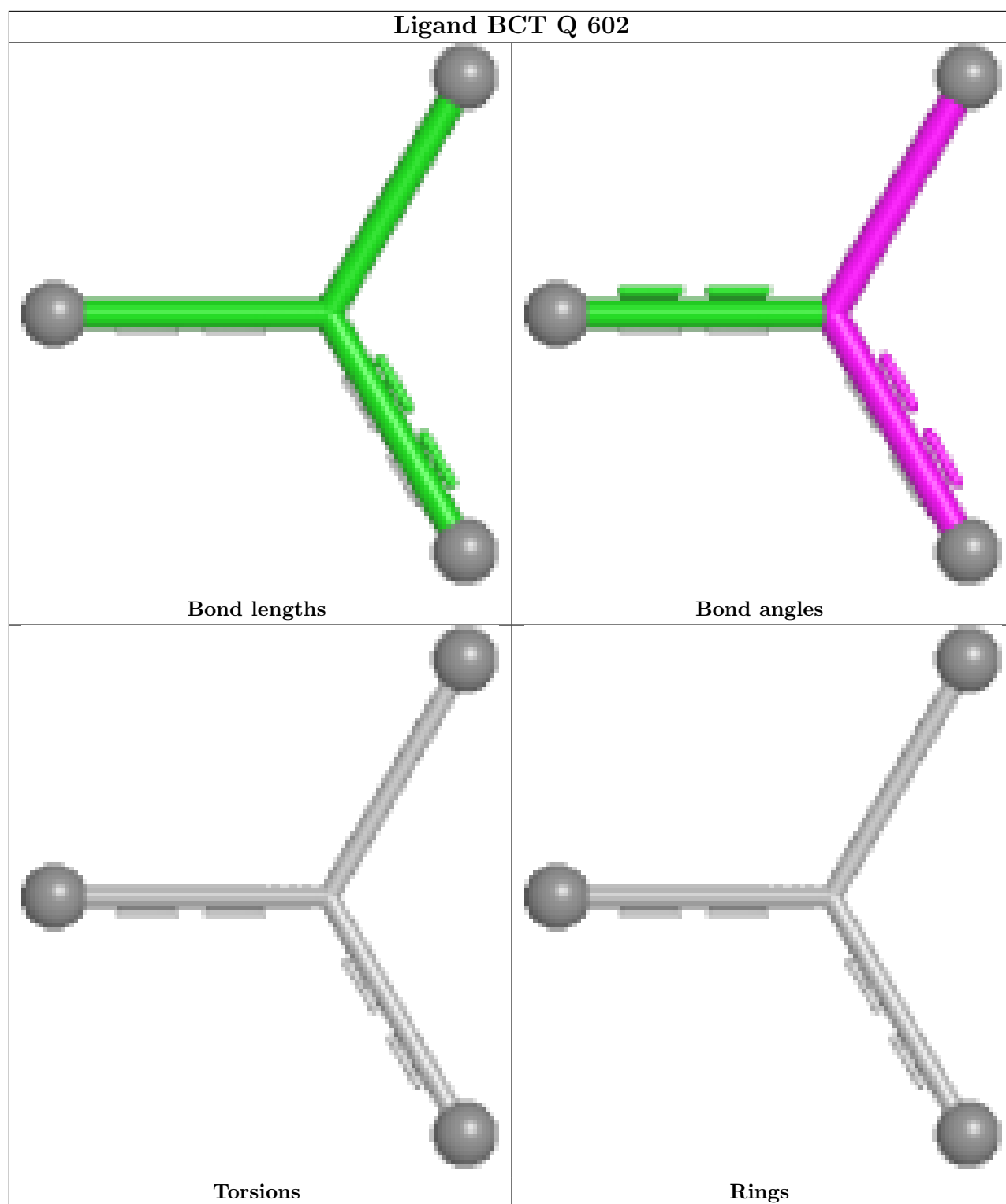
7 monomers are involved in 34 short contacts:

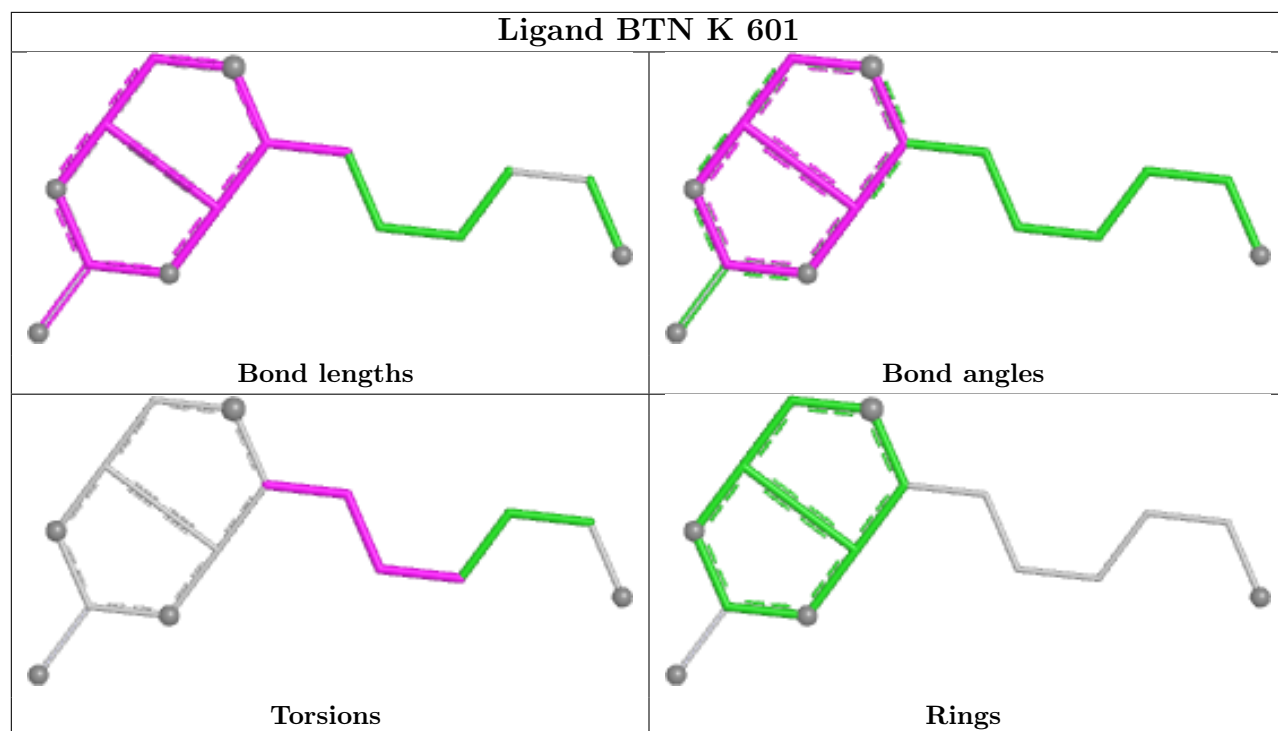
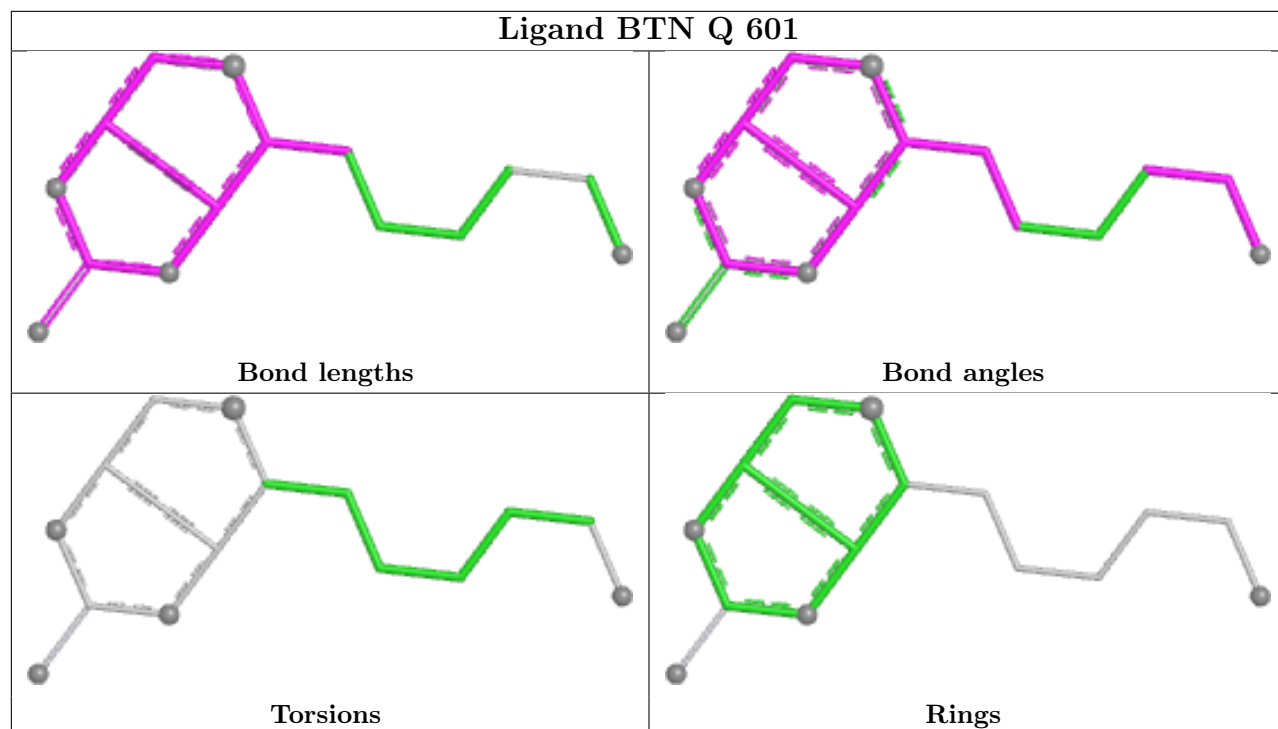
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	BTN	3	0
6	Q	602	BCT	4	0
5	Q	601	BTN	3	0
5	K	601	BTN	2	0
5	I	601	BTN	7	0
5	J	601	BTN	1	0
5	L	601	BTN	15	0

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.

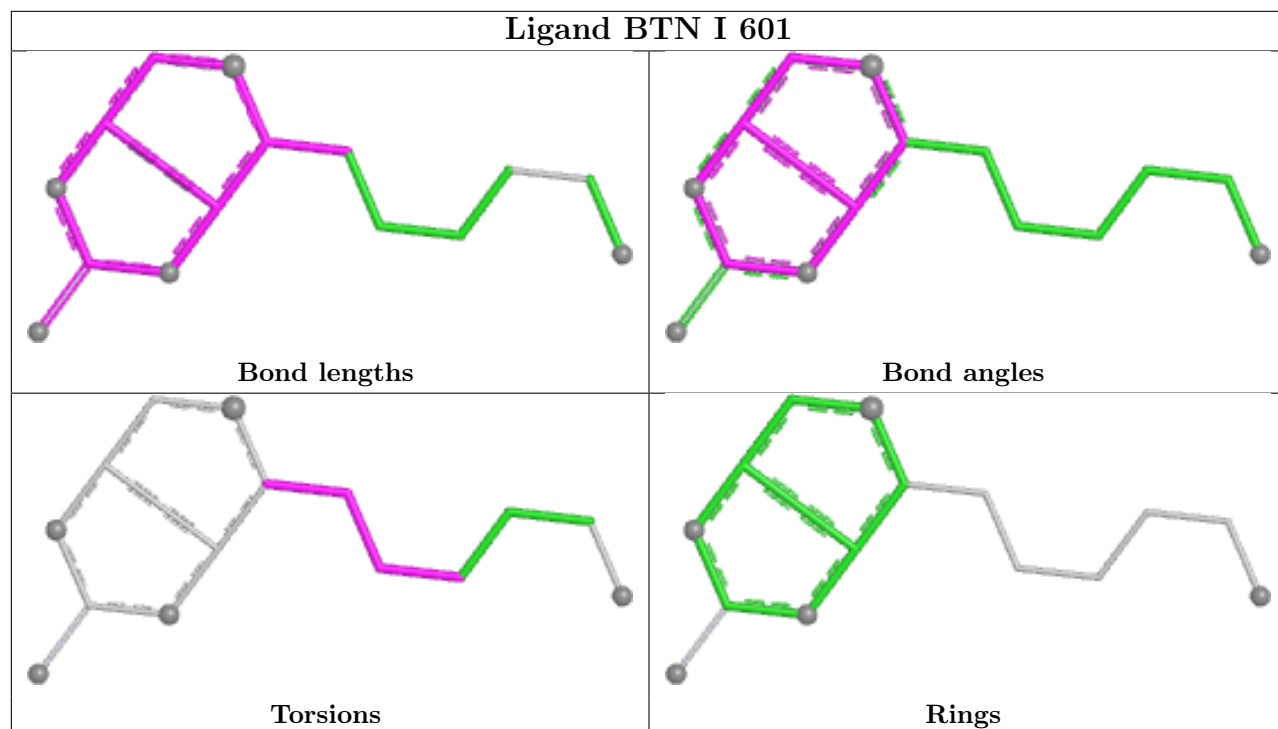




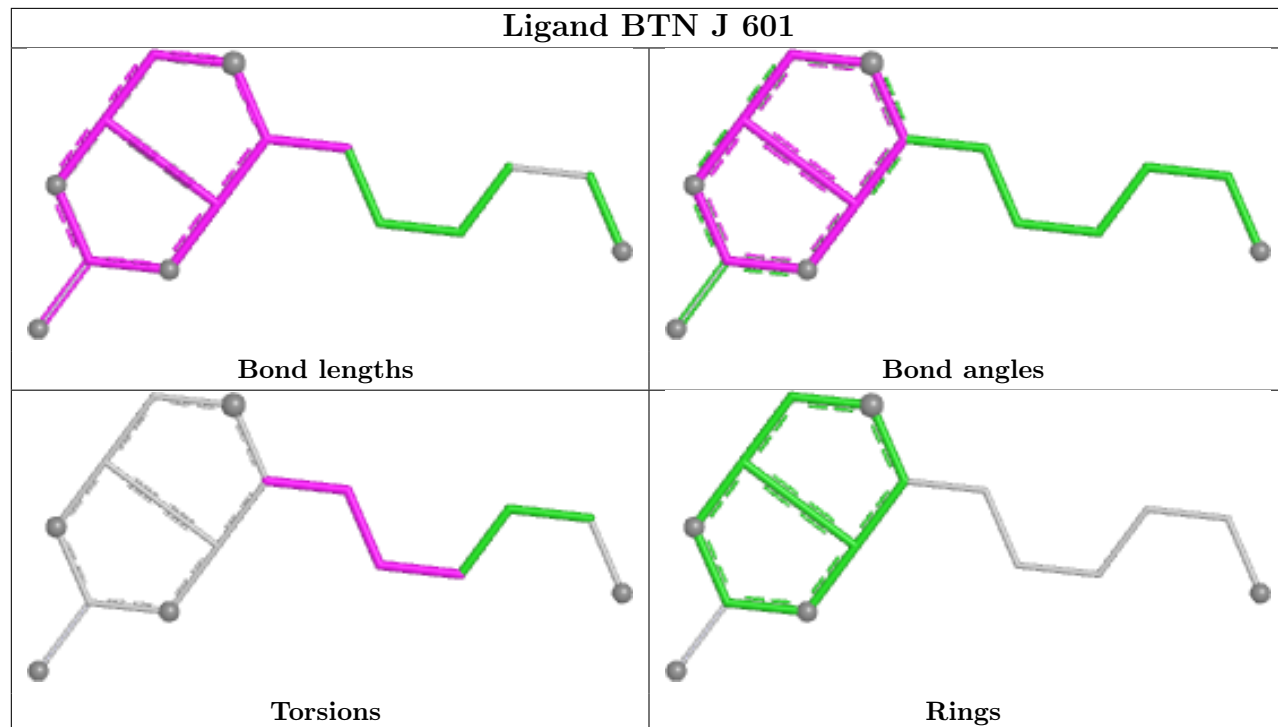


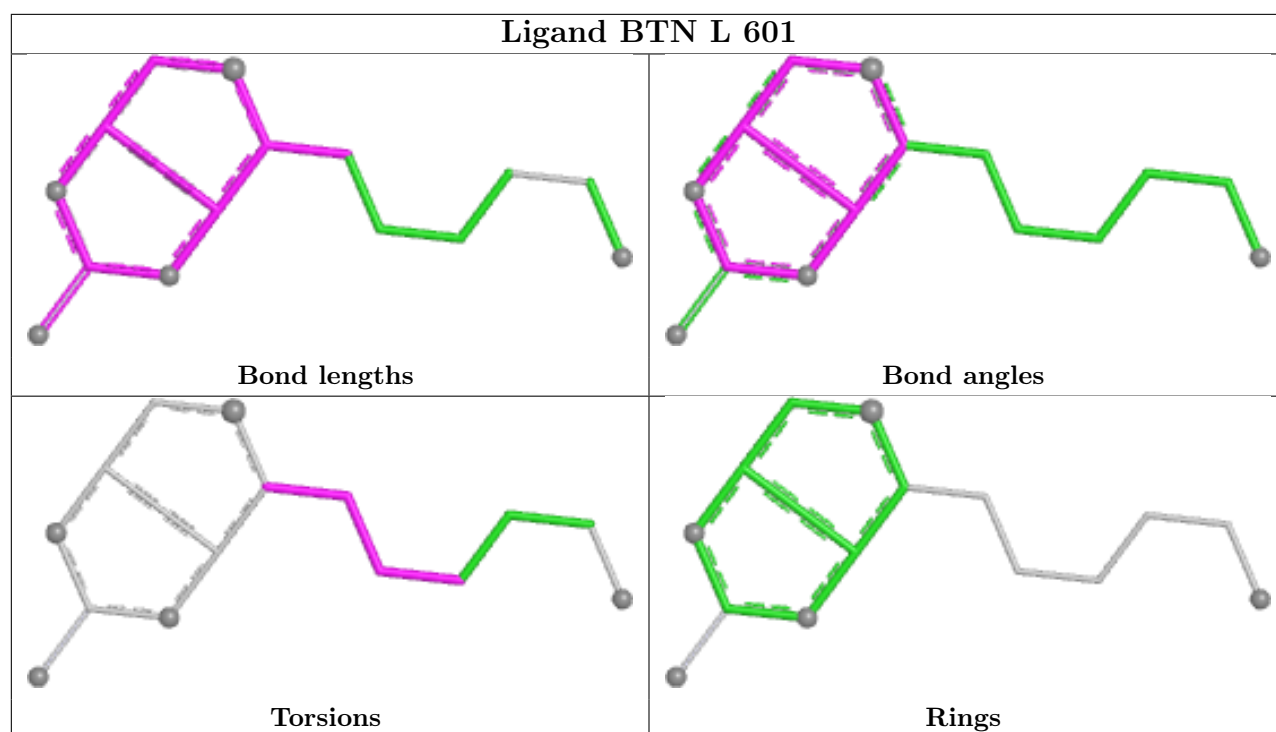


Ligand BTN I 601



Ligand BTN J 601





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.

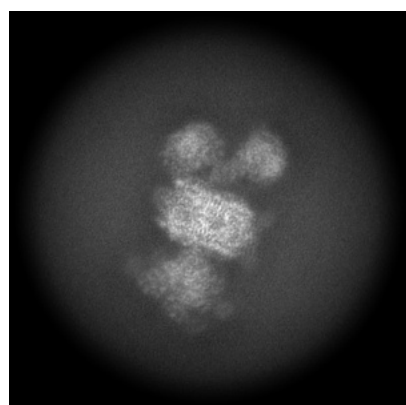
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73575. These allow visual inspection of the internal detail of the map and identification of artifacts.

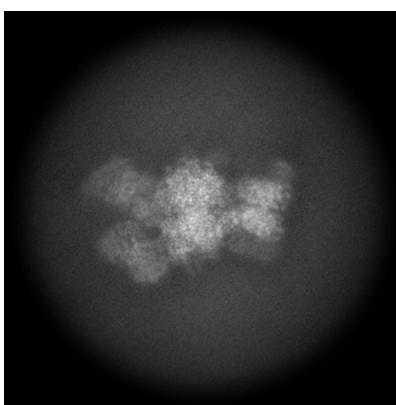
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

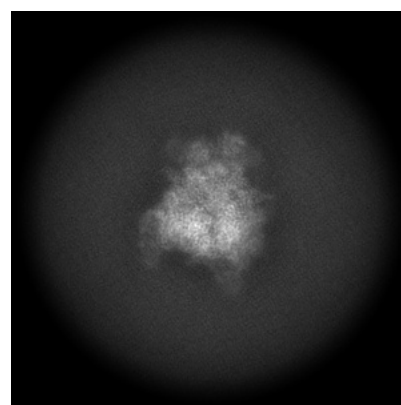
6.1.1 Primary map



X



Y

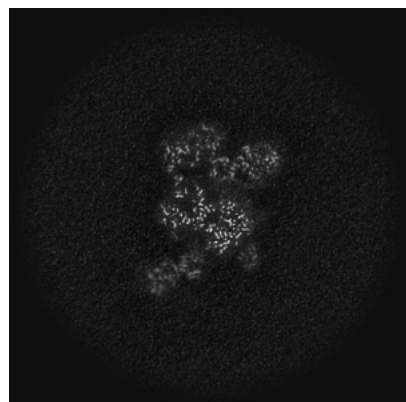


Z

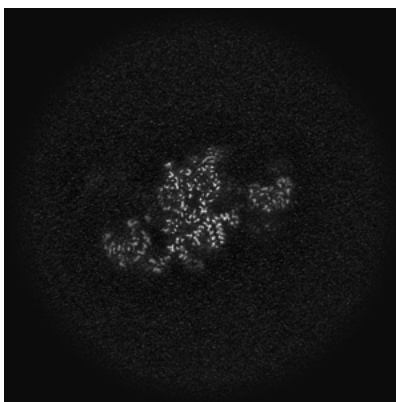
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

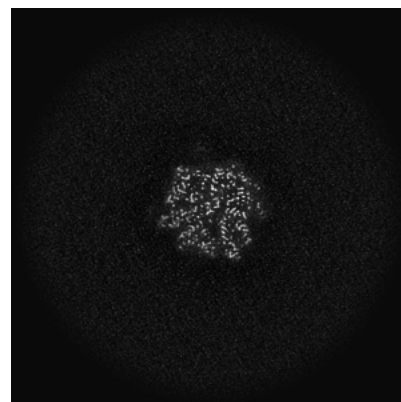
6.2.1 Primary map



X Index: 240



Y Index: 240

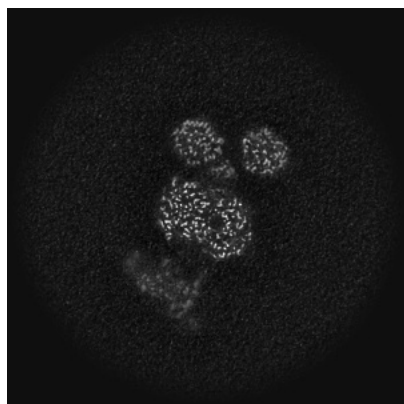


Z Index: 240

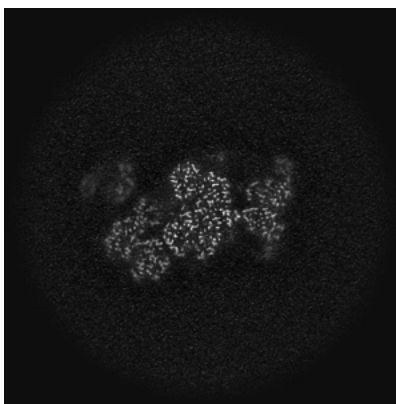
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

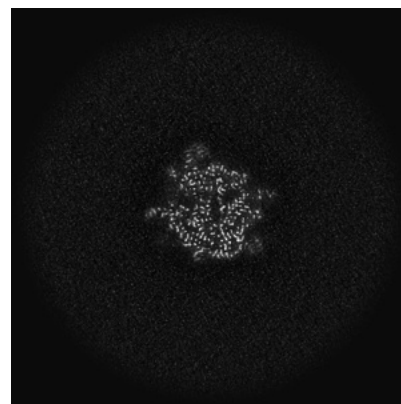
6.3.1 Primary map



X Index: 257



Y Index: 224

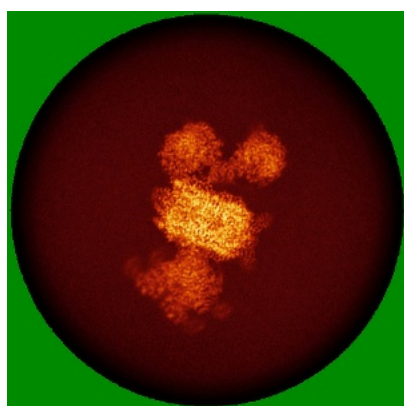


Z Index: 223

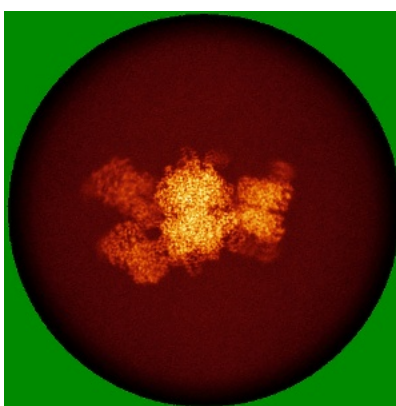
The images above show the largest variance slices of the map in three orthogonal directions.

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

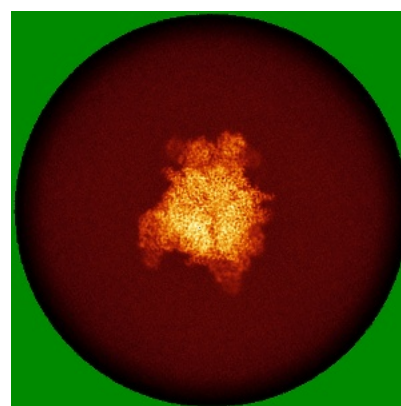
6.4.1 Primary map



X



Y

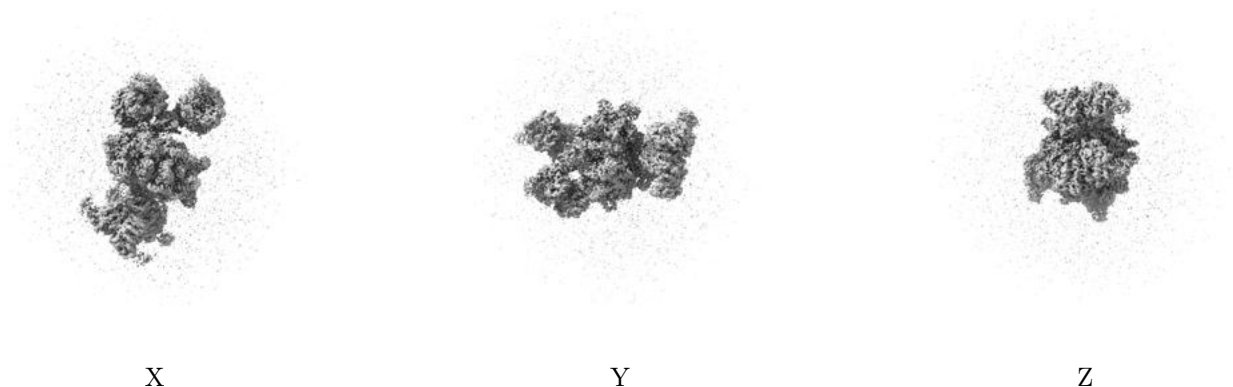


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

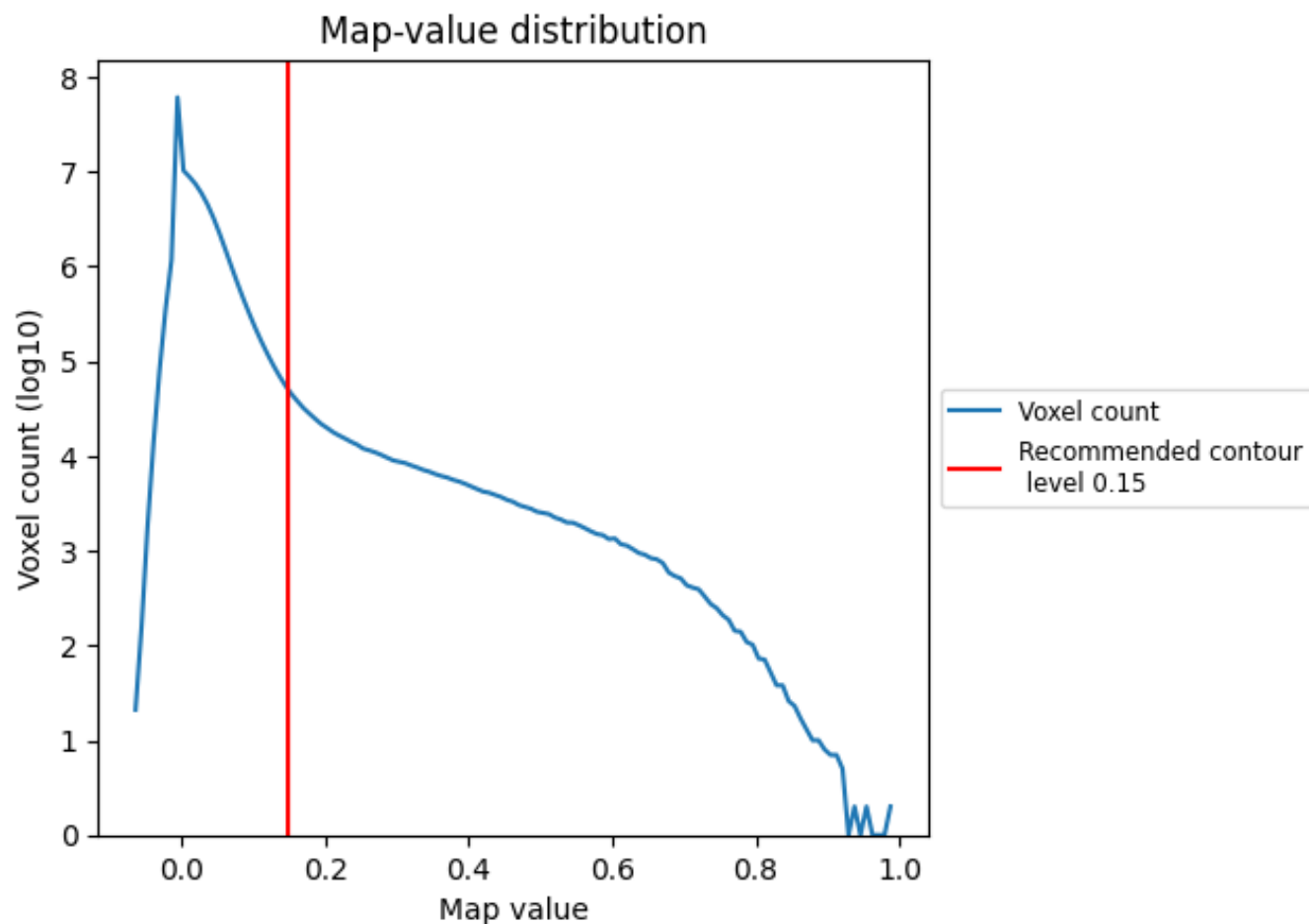
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

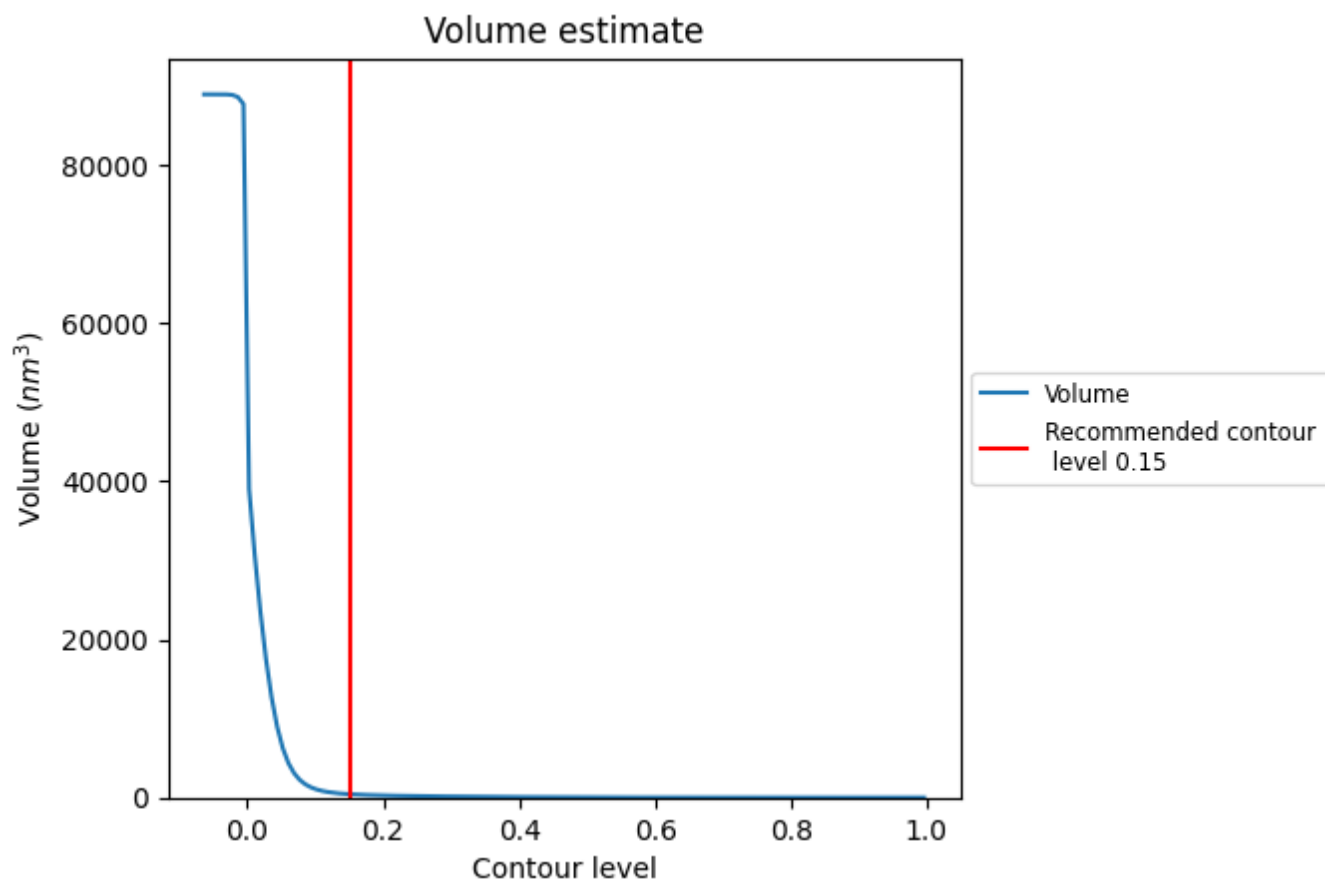
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

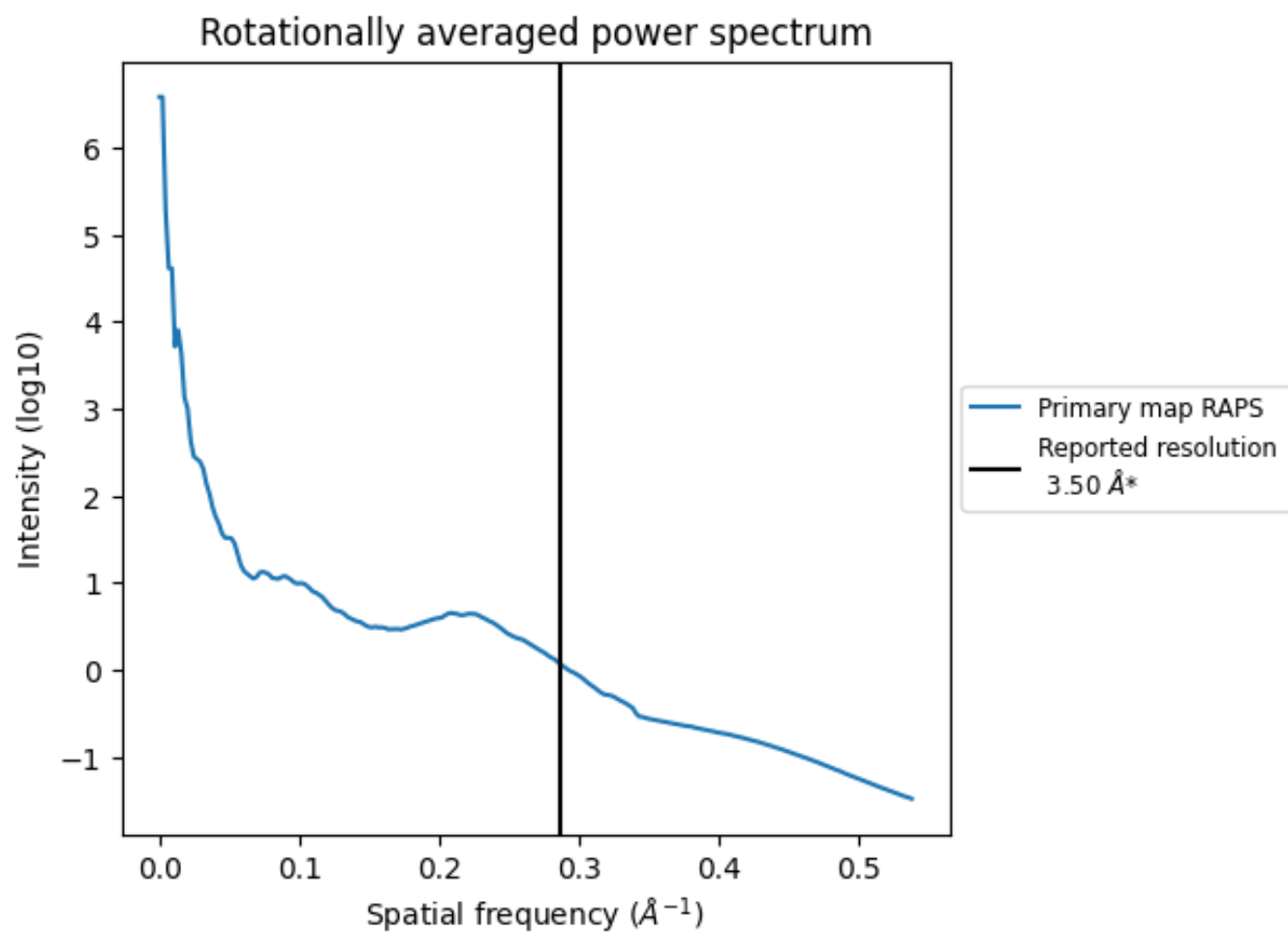
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 429 nm³; this corresponds to an approximate mass of 387 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 0.286 Å⁻¹

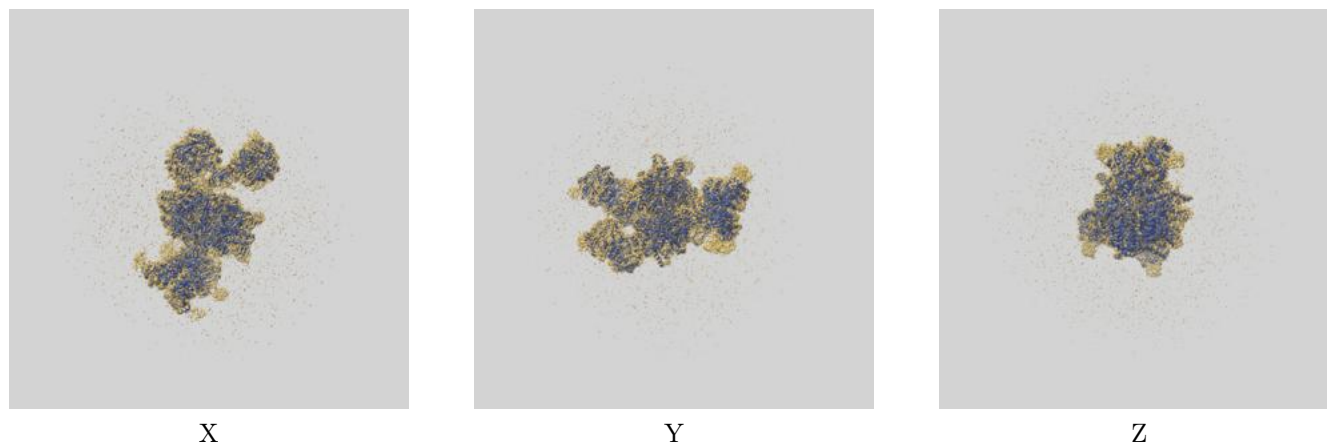
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

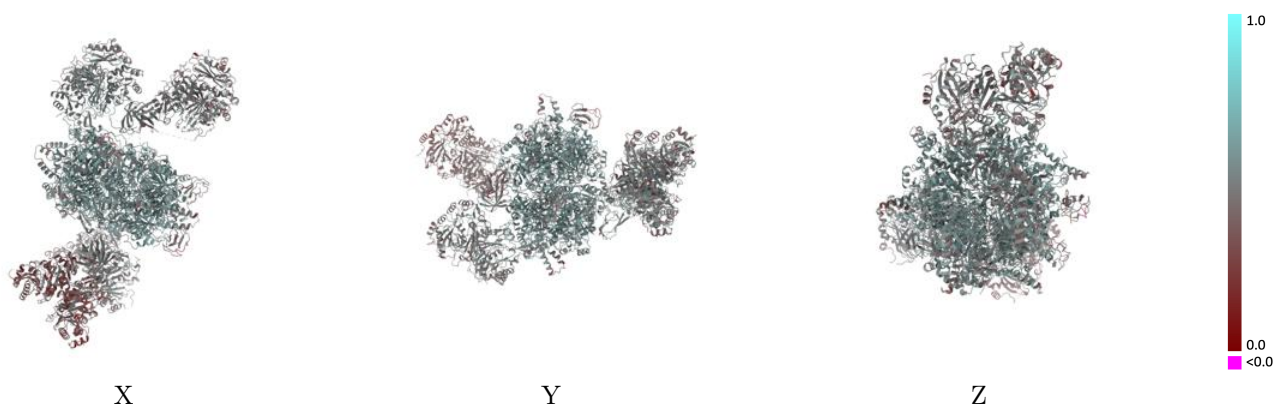
This section contains information regarding the fit between EMDB map EMD-73575 and PDB model 9YX1. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



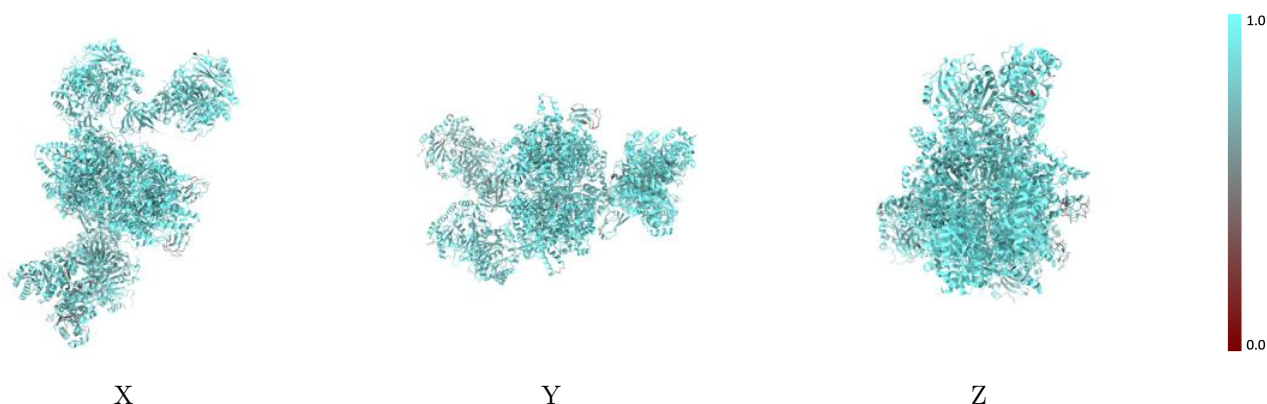
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



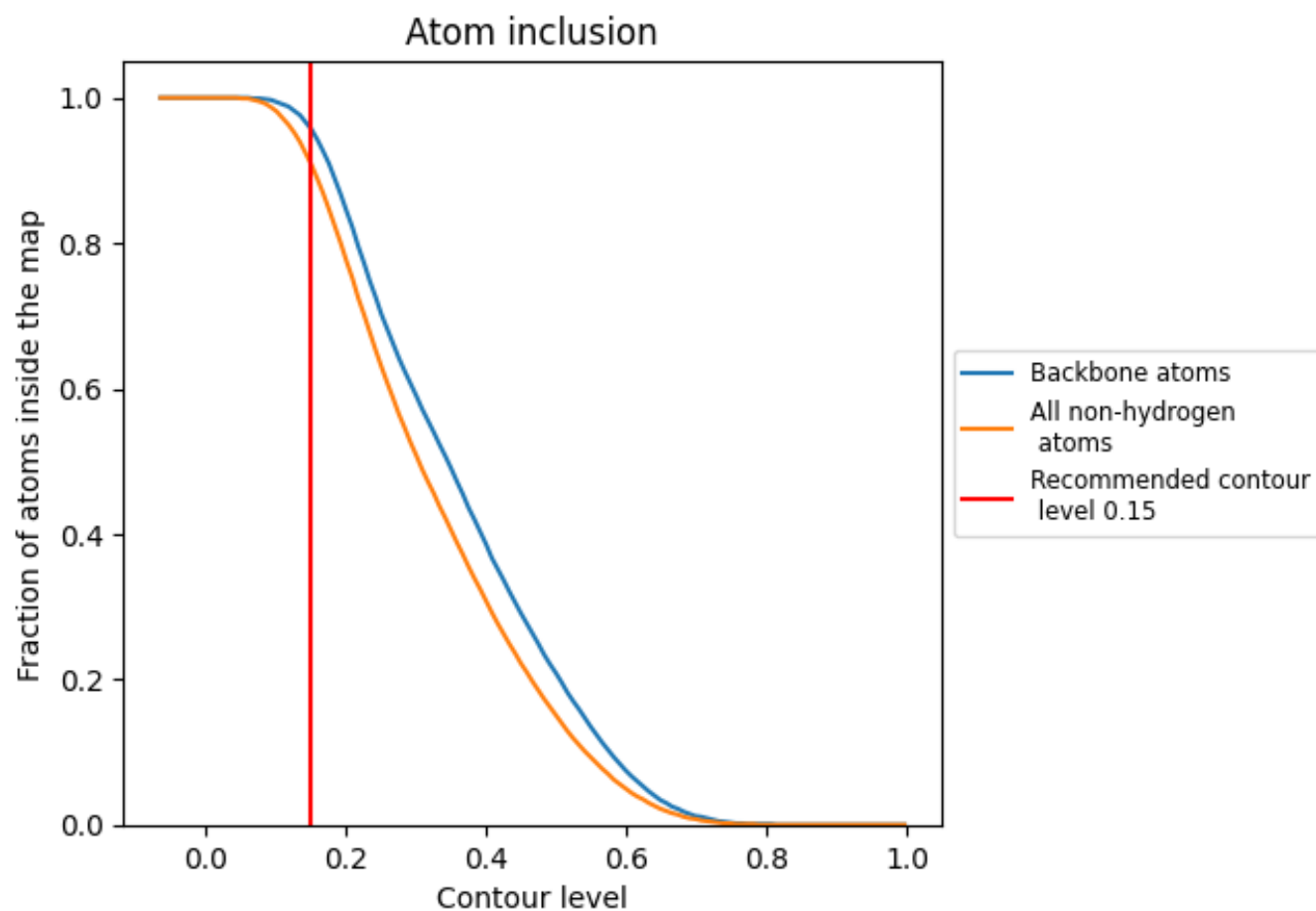
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 91% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9100	 0.5090
A	 0.9370	 0.5140
B	 0.9220	 0.4920
C	 0.8910	 0.4630
D	 0.9100	 0.4680
E	 0.9230	 0.5340
F	 0.9610	 0.5600
G	 0.9650	 0.5680
H	 0.9550	 0.5670
I	 0.6960	 0.4230
J	 0.6490	 0.3970
K	 0.7160	 0.4540
L	 0.6520	 0.3780
M	 0.9630	 0.5680
N	 0.9560	 0.5620
O	 0.9580	 0.5630
P	 0.9100	 0.5270
Q	 0.8910	 0.4870
R	 0.8750	 0.4720
S	 0.8030	 0.3660
T	 0.7560	 0.3590

