



Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 08:46 am GMT

PDB ID : 6YBP
EMDB ID : EMD-10770
Title : Propionyl-CoA carboxylase of *Methylorubrum extorquens* with bound CoA
Authors : Schuller, J.M.; Schuller, S.K.; Zarzycki, J.; Scheffen, M.; Marchal, D.M.; Erb, T.J.
Deposited on : 2020-03-17
Resolution : 3.48 Å (reported)
Based on initial model : 3N6R

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:

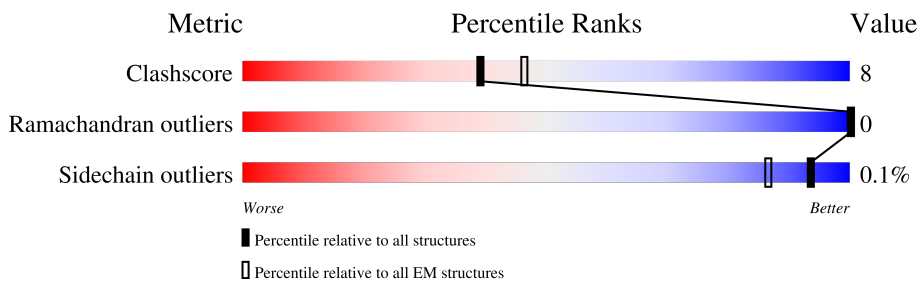
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.48 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



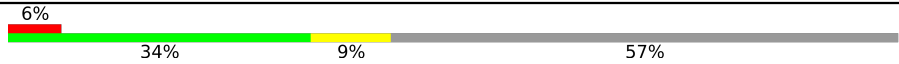

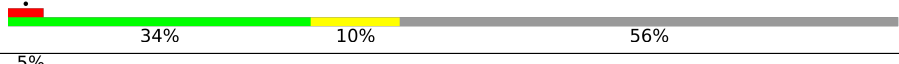

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	510	79% (green), 21% (yellow), 0% (red), 0% (grey)
1	B	510	82% (green), 17% (yellow), 0% (red), 0% (grey)
1	C	510	82% (green), 17% (yellow), 0% (red), 0% (grey)
1	D	510	84% (green), 16% (yellow), 0% (red), 0% (grey)
1	E	510	84% (green), 15% (yellow), 0% (red), 0% (grey)
1	F	510	86% (green), 14% (yellow), 0% (red), 0% (grey)
2	G	667	7% (red), 33% (green), 9% (yellow), 58% (grey)
2	H	667	5% (red), 24% (green), 7% (yellow), 69% (grey)

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	667	 6% 34% 9% 57%
2	J	667	 3% 35% 11% 55%
2	K	667	 3% 34% 10% 56%
2	L	667	 5% 33% 10% 56%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 36410 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
			Total	C	N	O	S		
1	A	506	3910	2483	684	727	16	0	0
1	B	506	3910	2483	684	727	16	0	0
1	C	506	3910	2483	684	727	16	0	0
1	D	506	3910	2483	684	727	16	0	0
1	E	506	3910	2483	684	727	16	0	0
1	F	506	3910	2483	684	727	16	0	0

- Molecule 2 is a protein called Propionyl-CoA carboxylase alpha subunit.

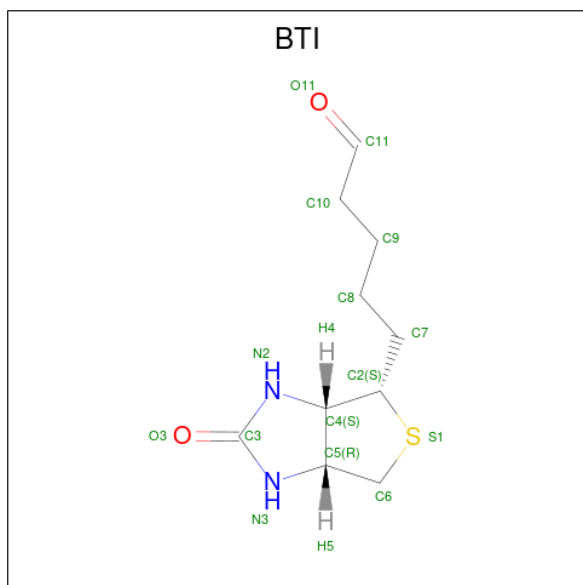
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	283	2135	1336	387	403	9	0	0
2	H	208	1565	978	285	295	7	0	0
2	I	288	2183	1371	389	414	9	0	0
2	J	303	2305	1449	414	433	9	0	0
2	K	293	2217	1390	399	419	9	0	0
2	L	291	2208	1385	397	417	9	0	0

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
3	A	1	48	21	7	16	3	1	0
3	B	1	48	21	7	16	3	1	0
3	C	1	36	15	5	13	3		0
3	D	1	36	15	5	13	3		0
3	E	1	31	10	5	13	3		0
3	F	1	48	21	7	16	3	1	0

- Molecule 4 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: C₁₀H₁₆N₂O₂S).

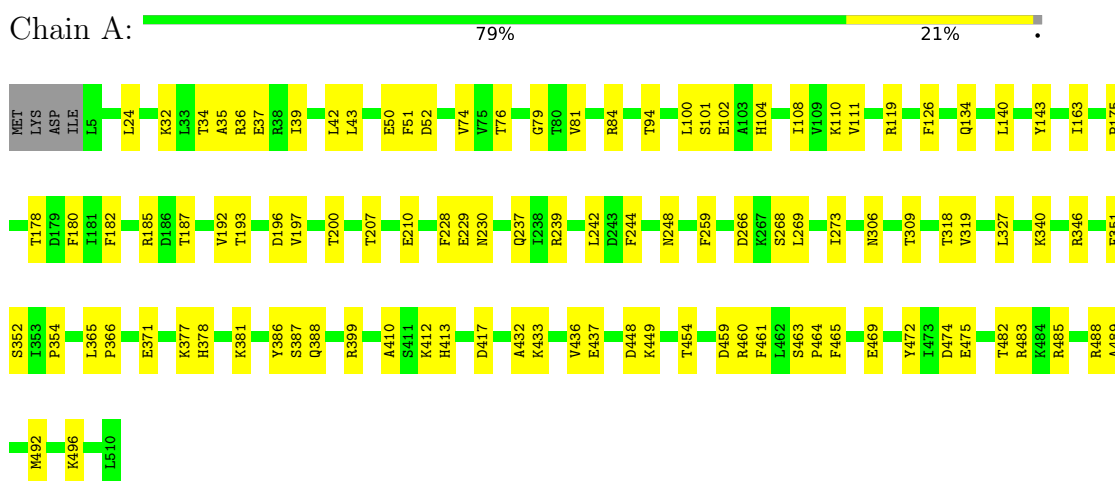


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
4	G	1	Total	C	N	O	S	0
			15	10	2	2	1	
4	H	1	Total	C	N	O	S	0
			15	10	2	2	1	
4	I	1	Total	C	N	O	S	0
			15	10	2	2	1	
4	J	1	Total	C	N	O	S	0
			15	10	2	2	1	
4	K	1	Total	C	N	O	S	0
			15	10	2	2	1	
4	L	1	Total	C	N	O	S	0
			15	10	2	2	1	

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.

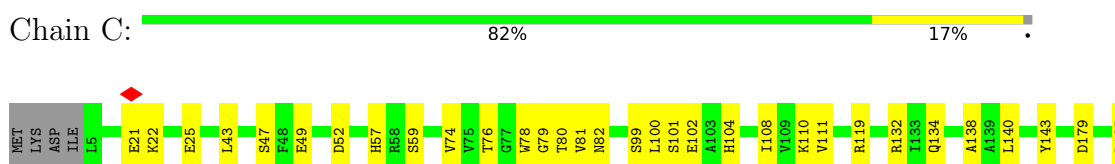
- Molecule 1: Propionyl-CoA carboxylase beta chain

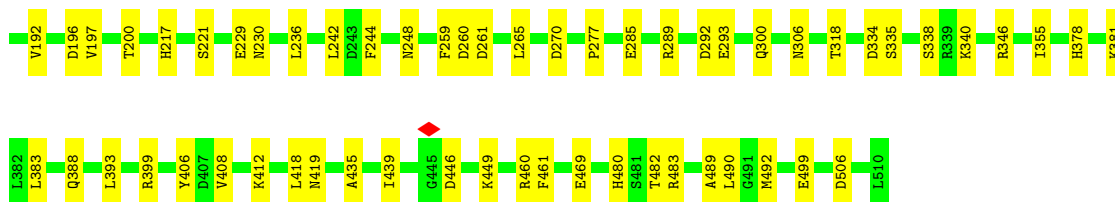


- Molecule 1: Propionyl-CoA carboxylase beta chain



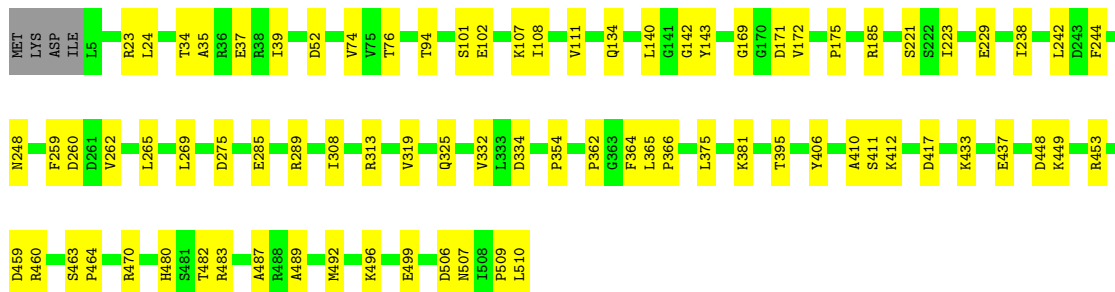
- Molecule 1: Propionyl-CoA carboxylase beta chain





- Molecule 1: Propionyl-CoA carboxylase beta chain

Chain D: 84% 16%



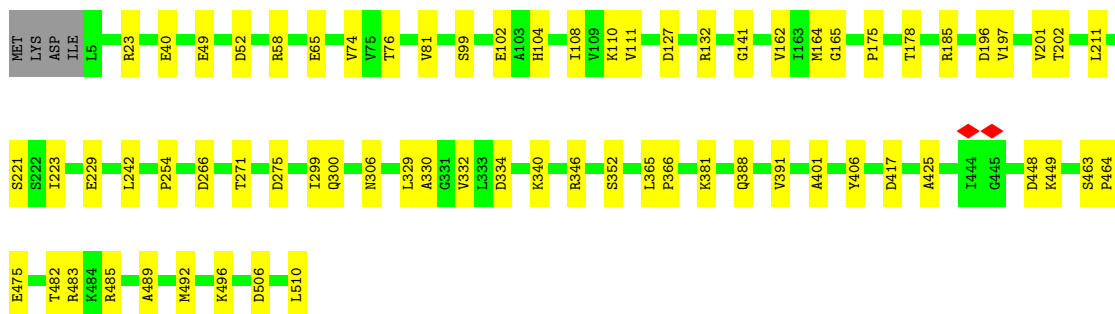
- Molecule 1: Propionyl-CoA carboxylase beta chain

Chain E: 84% 15%

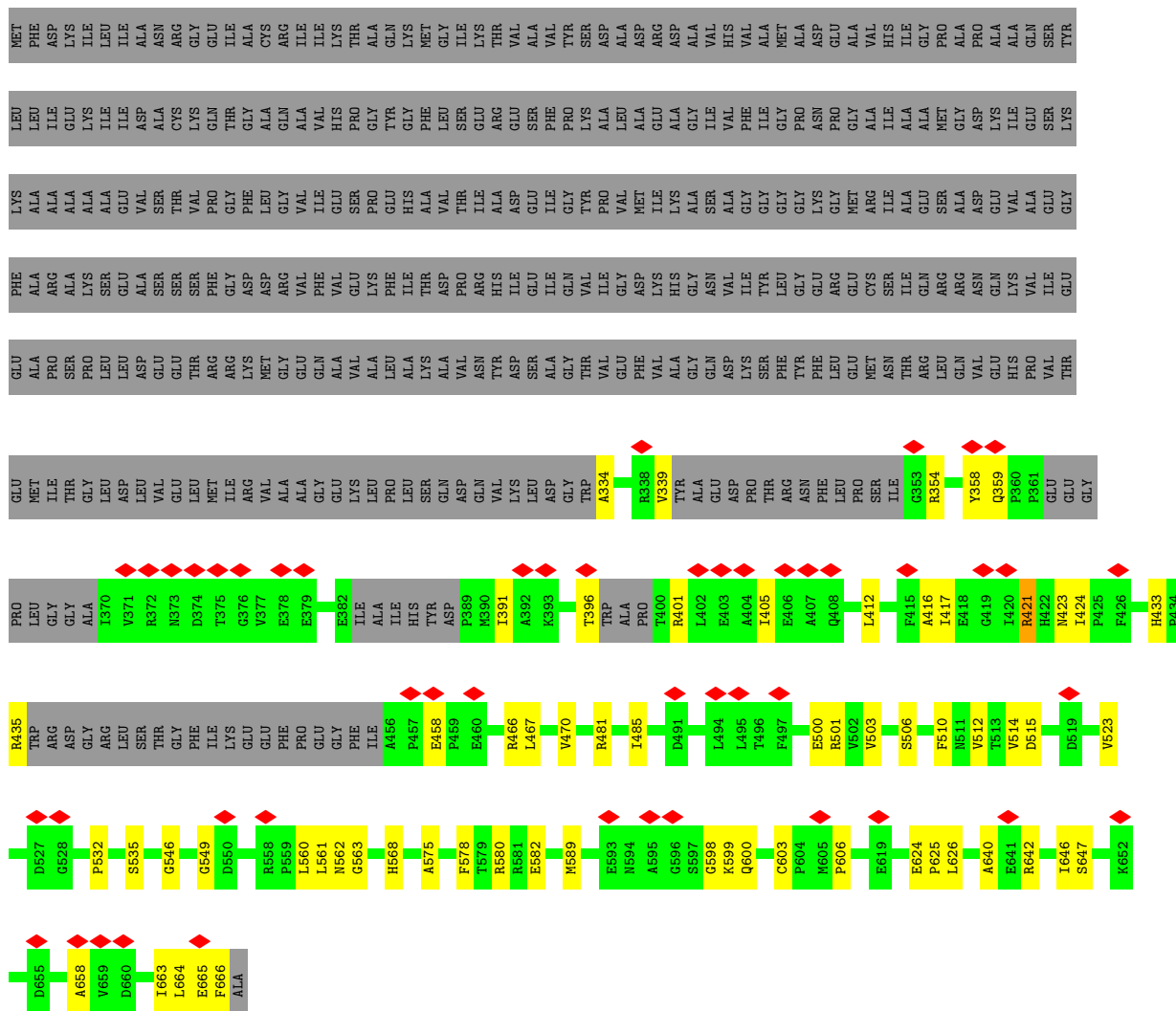
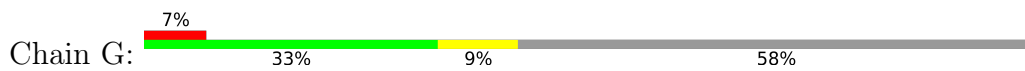


- Molecule 1: Propionyl-CoA carboxylase beta chain

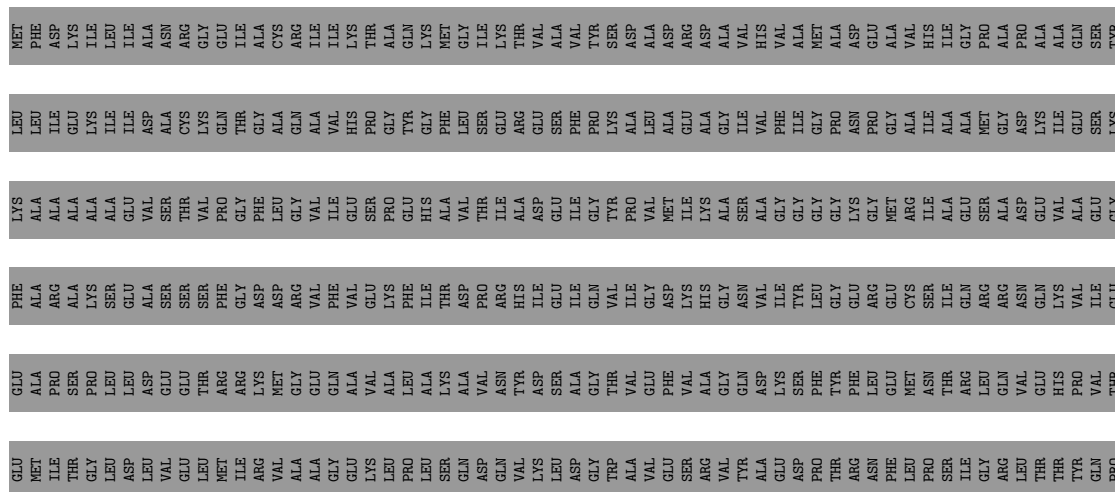
Chain F: 86% 14%

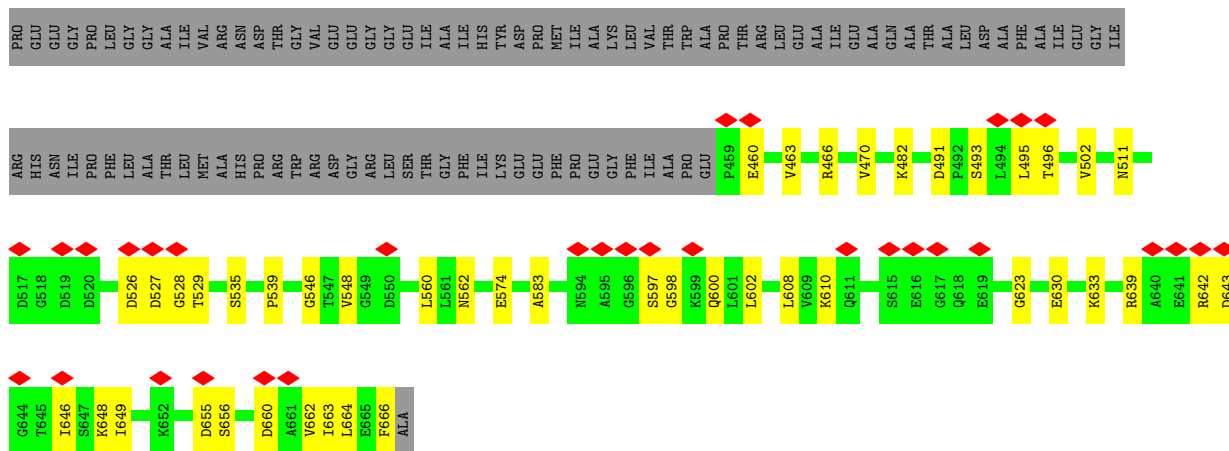


- Molecule 2: Propionyl-CoA carboxylase alpha subunit

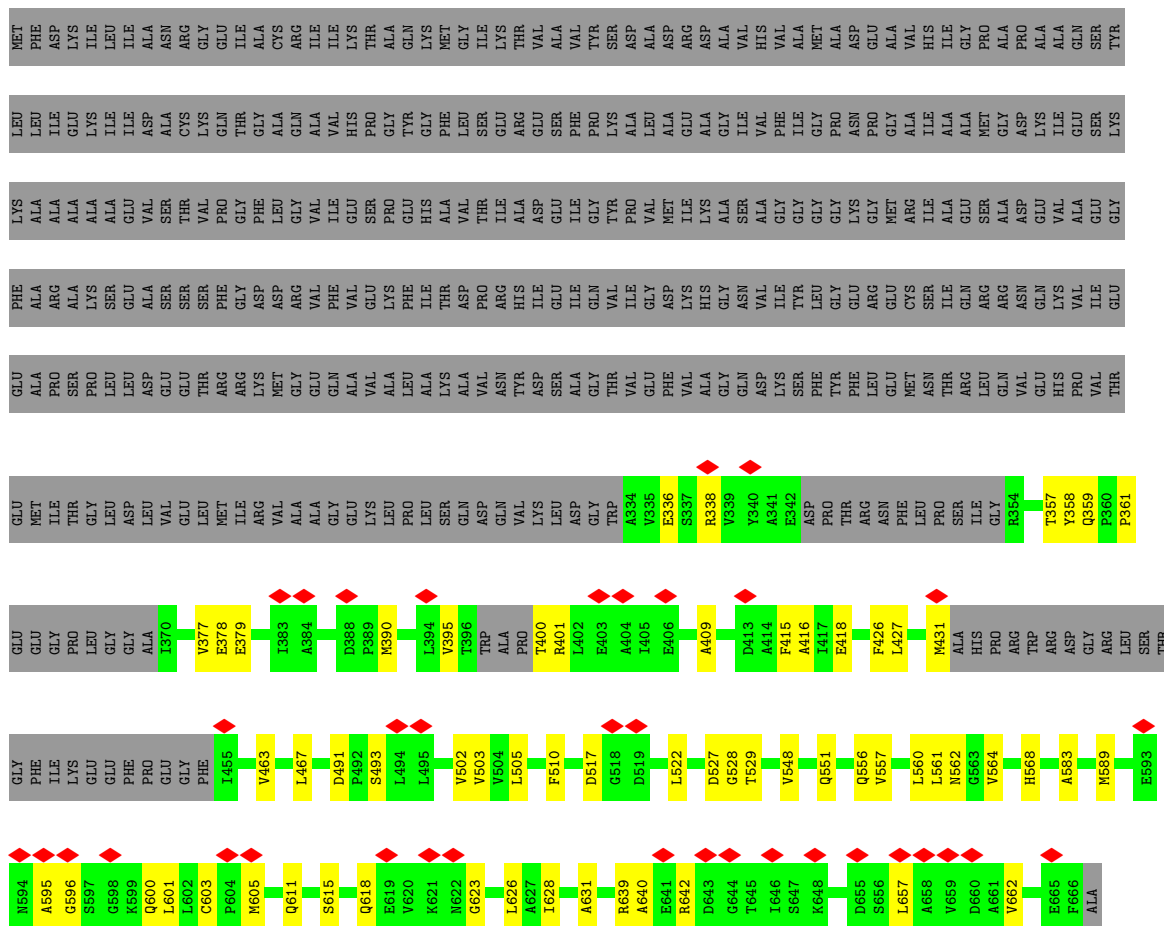
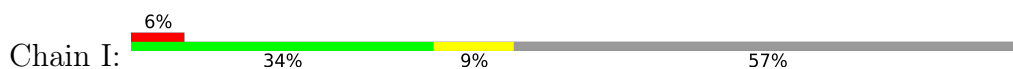


• Molecule 2: Propionyl-CoA carboxylase alpha subunit

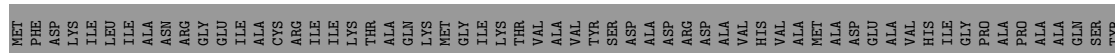
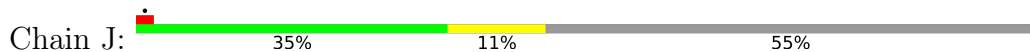


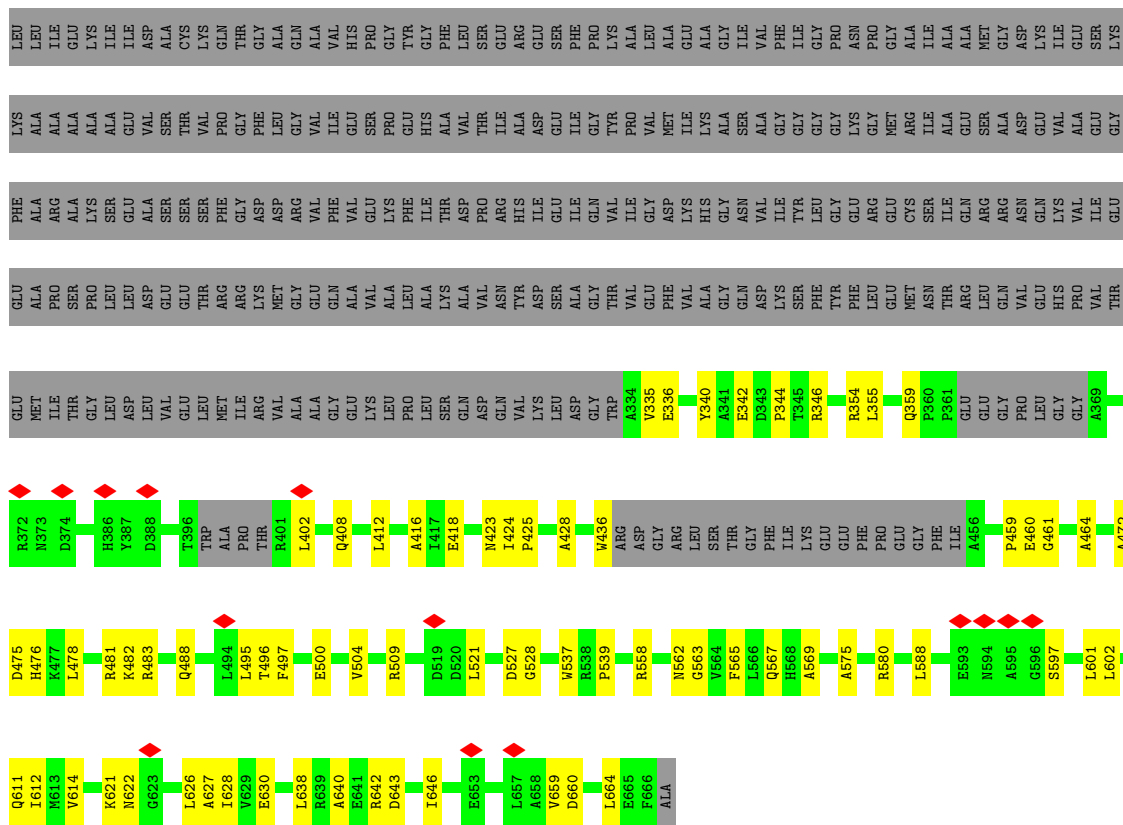


• Molecule 2: Propionyl-CoA carboxylase alpha subunit

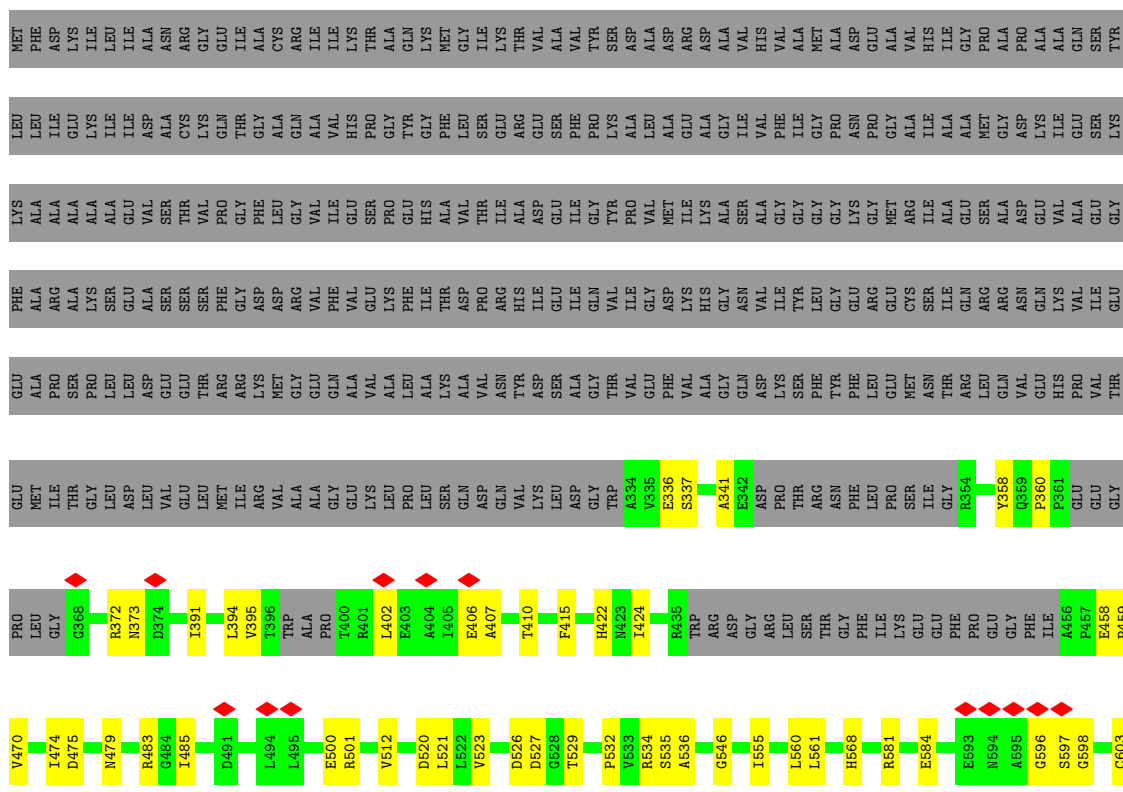
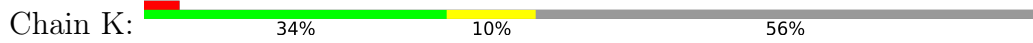


• Molecule 2: Propionyl-CoA carboxylase alpha subunit



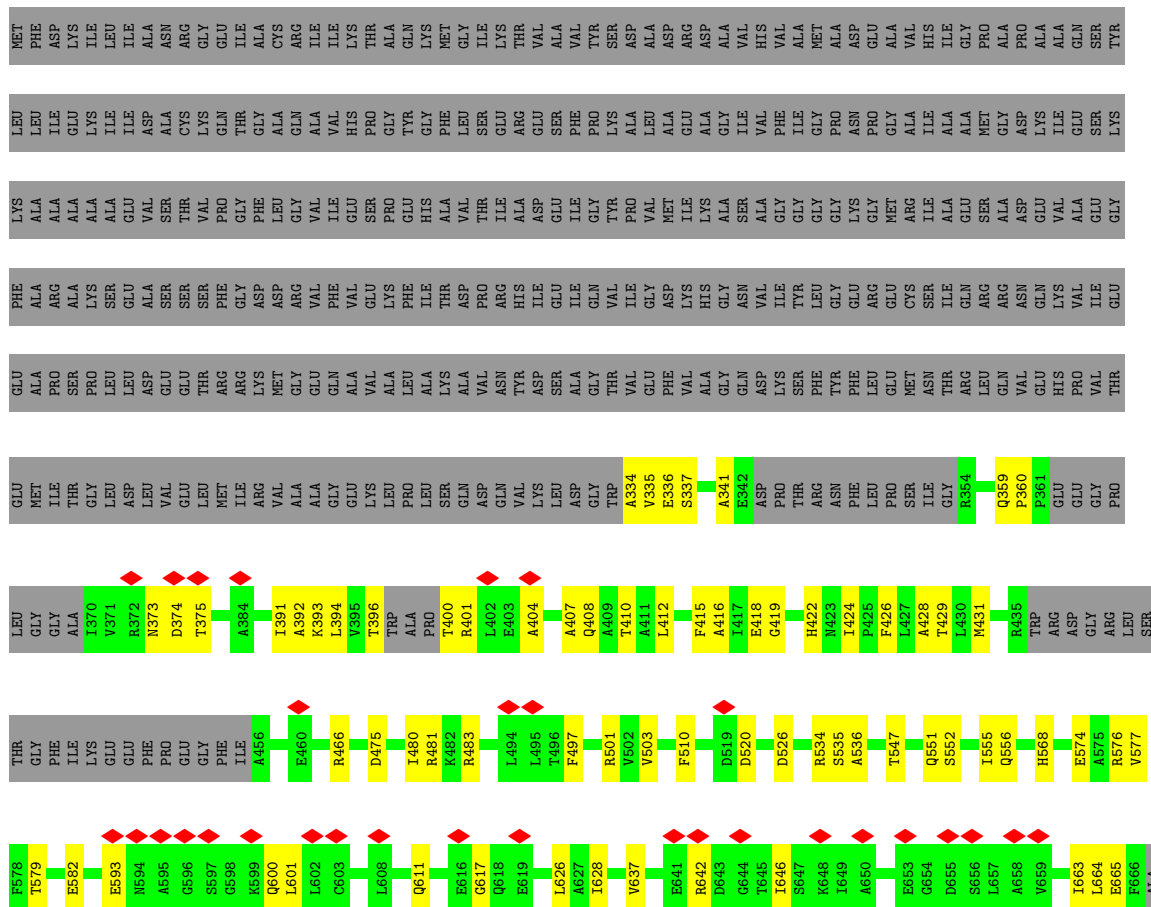
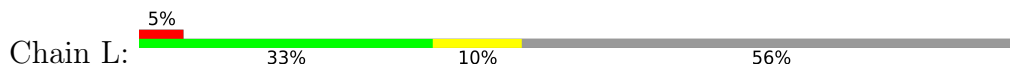


● Molecule 2: Propionyl-CoA carboxylase alpha subunit





• Molecule 2: Propionyl-CoA carboxylase alpha subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77714	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	1.289	Depositor
Minimum map value	-0.601	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.23	Depositor
Map size (\AA)	302.08, 302.08, 302.08	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.18, 1.18, 1.18	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.46	0/3986	0.52	0/5381
1	B	0.48	1/3986 (0.0%)	0.52	0/5381
1	C	0.45	0/3986	0.51	0/5381
1	D	0.46	0/3986	0.52	0/5381
1	E	0.46	0/3986	0.51	0/5381
1	F	0.46	0/3986	0.52	0/5381
2	G	0.32	0/2165	0.50	0/2930
2	H	0.31	0/1589	0.54	0/2152
2	I	0.32	0/2215	0.49	0/3002
2	J	0.33	0/2345	0.50	0/3183
2	K	0.34	0/2251	0.52	0/3051
2	L	0.32	0/2242	0.49	0/3039
All	All	0.42	1/36723 (0.0%)	0.51	0/49643

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	244	PHE	C-N	-5.72	1.21	1.34

There are no bond angle outliers.

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	3910	0	3913	70	0
1	B	3910	0	3913	58	0
1	C	3910	0	3913	65	0
1	D	3910	0	3913	54	0
1	E	3910	0	3913	53	0
1	F	3910	0	3913	47	0
2	G	2135	0	2164	41	0
2	H	1565	0	1592	30	0
2	I	2183	0	2207	41	0
2	J	2305	0	2320	44	0
2	K	2217	0	2236	42	0
2	L	2208	0	2228	44	0
3	A	48	0	32	0	0
3	B	48	0	32	0	0
3	C	36	0	19	1	0
3	D	36	0	19	1	0
3	E	31	0	11	1	0
3	F	48	0	32	4	0
4	G	15	0	15	0	0
4	H	15	0	15	0	0
4	I	15	0	15	0	0
4	J	15	0	15	1	0
4	K	15	0	15	4	0
4	L	15	0	15	5	0
All	All	36410	0	36460	565	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 8.

All (565) 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:L:466:ARG:HH11	2:L:551:GLN:HG2	1.45	0.80
2:K:596:GLY:HA2	2:K:642:ARG:HH11	1.50	0.77
1:C:236:LEU:HD12	2:H:562:ASN:HD21	1.52	0.74
1:B:381:LYS:NZ	1:B:510:LEU:OXT	2.20	0.73
1:E:475:GLU:OE1	1:E:485:ARG:NH1	2.21	0.73
2:L:334:ALA:HB1	2:L:396:THR:HG23	1.69	0.73
2:G:603:CYS:HB2	2:G:663:ILE:HD11	1.69	0.73
1:C:82:ASN:HD21	2:H:482:LYS:HE3	1.55	0.72
2:K:649:ILE:HG22	2:K:651:ALA:H	1.53	0.71
1:C:52:ASP:OD2	1:C:110:LYS:NZ	2.23	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:ARG:NH2	1:D:229:GLU:OE2	2.24	0.71
1:C:74:VAL:HG21	1:C:108:ILE:HD11	1.74	0.70
2:H:597:SER:HB3	2:H:642:ARG:HD3	1.74	0.70
1:E:233:GLU:OE1	2:I:562:ASN:ND2	2.26	0.69
2:L:600:GLN:NE2	2:L:665:GLU:OE2	2.26	0.69
1:B:475:GLU:OE1	1:B:485:ARG:NH1	2.26	0.69
2:J:627:ALA:HB3	2:J:638:LEU:HD12	1.75	0.69
2:K:336:GLU:HB3	2:K:395:VAL:HG12	1.74	0.69
2:J:418:GLU:OE2	2:J:558:ARG:NH2	2.26	0.68
1:B:346:ARG:HH11	1:B:388:GLN:HE22	1.40	0.68
2:L:497:PHE:HE2	2:L:501:ARG:HE	1.42	0.68
2:K:535:SER:HB2	2:K:546:GLY:HA3	1.75	0.68
1:C:285:GLU:OE1	1:C:289:ARG:NH2	2.24	0.68
2:G:334:ALA:N	2:G:396:THR:O	2.27	0.67
1:D:381:LYS:NZ	1:D:509:PRO:O	2.28	0.67
2:L:359:GLN:HG3	2:L:416:ALA:HB3	1.76	0.67
2:G:339:VAL:O	2:G:391:ILE:N	2.26	0.66
2:J:565:PHE:HE1	2:J:567:GLN:HE21	1.40	0.66
2:H:663:ILE:HG22	2:H:664:LEU:HG	1.77	0.66
1:F:185:ARG:NH2	1:F:229:GLU:OE2	2.28	0.66
2:L:601:LEU:HD11	2:L:626:LEU:HD13	1.75	0.66
1:C:138:ALA:HB2	1:D:470:ARG:HH12	1.60	0.66
2:K:581:ARG:NH1	2:K:584:GLU:OE1	2.28	0.65
1:A:81:VAL:HG11	1:A:242:LEU:HD23	1.78	0.65
1:F:475:GLU:OE1	1:F:485:ARG:NH1	2.30	0.64
2:G:359:GLN:HB2	2:G:416:ALA:HB3	1.79	0.64
1:E:365:LEU:HD12	1:E:366:PRO:HD2	1.80	0.64
2:L:337:SER:OG	2:L:408:GLN:NE2	2.30	0.64
1:B:401:ALA:HB1	1:B:406:TYR:HB2	1.79	0.64
2:I:502:VAL:HG11	2:I:583:ALA:HB2	1.79	0.64
2:L:335:VAL:HG21	2:L:404:ALA:HA	1.78	0.63
2:G:599:LYS:O	2:G:666:PHE:N	2.32	0.63
1:F:52:ASP:OD2	1:F:110:LYS:NZ	2.25	0.63
2:G:339:VAL:HG12	2:G:391:ILE:HD13	1.80	0.63
1:E:81:VAL:HG11	1:E:242:LEU:HD23	1.80	0.63
2:K:603:CYS:HB2	2:K:663:ILE:HD11	1.81	0.62
1:B:99:SER:HG	1:B:132:ARG:HE	1.45	0.62
1:B:488:ARG:NH2	1:F:49:GLU:OE1	2.30	0.62
1:C:99:SER:OG	1:C:132:ARG:NE	2.32	0.62
1:E:82:ASN:ND2	1:E:243:ASP:OD2	2.32	0.62
2:H:502:VAL:HG11	2:H:583:ALA:HB2	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:595:ALA:O	2:I:642:ARG:NH1	2.32	0.62
1:C:196:ASP:OD1	1:C:197:VAL:N	2.32	0.62
3:F:601:COA:HN8	3:F:601:COA:H31	1.65	0.61
1:B:99:SER:OG	1:B:132:ARG:NE	2.33	0.61
1:F:300:GLN:HB2	1:F:340:LYS:HE3	1.82	0.61
1:C:460:ARG:HE	1:C:461:PHE:HE1	1.49	0.61
2:K:626:LEU:HD11	2:K:640:ALA:HB2	1.83	0.61
1:B:74:VAL:HG21	1:B:108:ILE:HD11	1.82	0.61
1:C:101:SER:OG	1:C:102:GLU:N	2.33	0.61
2:G:598:GLY:O	2:G:642:ARG:NH2	2.33	0.61
1:C:185:ARG:NH2	1:C:229:GLU:OE2	2.34	0.60
1:D:260:ASP:OD1	1:D:483:ARG:NH2	2.32	0.60
2:J:335:VAL:HG11	2:J:408:GLN:HB2	1.83	0.60
2:J:483:ARG:HH22	2:J:497:PHE:HB2	1.66	0.60
1:D:433:LYS:O	1:D:437:GLU:HG2	2.01	0.60
1:A:268:SER:OG	2:G:354:ARG:NH2	2.34	0.60
2:H:642:ARG:HG2	2:H:643:ASP:H	1.64	0.60
1:C:49:GLU:OE1	1:C:78:TRP:NE1	2.34	0.60
2:H:495:LEU:HD12	2:H:496:THR:H	1.66	0.60
1:A:32:LYS:HD2	1:A:187:THR:HG21	1.83	0.60
1:B:417:ASP:OD2	1:B:496:LYS:NZ	2.26	0.60
2:I:527:ASP:OD1	2:I:528:GLY:N	2.35	0.60
1:A:365:LEU:HD12	1:A:366:PRO:HD2	1.85	0.59
1:D:448:ASP:OD1	1:D:449:LYS:N	2.35	0.59
1:F:381:LYS:NZ	1:F:510:LEU:OXT	2.28	0.59
1:B:233:GLU:OE1	2:J:562:ASN:ND2	2.36	0.59
1:B:119:ARG:HB3	1:B:248:ASN:HD22	1.68	0.59
2:K:620:VAL:HG21	2:K:626:LEU:HD21	1.85	0.59
1:B:266:ASP:OD1	1:B:266:ASP:N	2.36	0.58
2:I:336:GLU:HB3	2:I:395:VAL:HG23	1.84	0.58
1:B:76:THR:HB	1:B:111:VAL:HG21	1.85	0.58
3:C:601:COA:H8A	3:C:601:COA:H52A	1.84	0.58
2:I:338:ARG:HD3	2:I:390:MET:HB3	1.84	0.58
2:L:579:THR:HG22	2:L:582:GLU:OE1	2.04	0.58
1:B:381:LYS:NZ	1:B:509:PRO:O	2.34	0.58
1:C:469:GLU:OE2	1:E:56:GLN:NE2	2.37	0.57
2:K:535:SER:OG	2:K:536:ALA:N	2.37	0.57
2:I:409:ALA:HB2	2:I:431:MET:HG2	1.86	0.57
2:L:418:GLU:OE2	2:L:419:GLY:N	2.37	0.57
1:A:266:ASP:OD1	1:A:266:ASP:N	2.38	0.57
1:A:475:GLU:OE1	1:A:485:ARG:NH1	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:489:ALA:O	1:C:492:MET:HG3	2.04	0.57
2:G:626:LEU:HD11	2:G:640:ALA:HB2	1.86	0.57
2:H:623:GLY:O	2:H:639:ARG:NH1	2.38	0.57
2:I:467:LEU:HD11	2:I:568:HIS:HB3	1.85	0.57
2:K:422:HIS:CD2	2:K:424:ILE:HB	2.40	0.57
2:K:555:ILE:HG12	2:K:568:HIS:HB2	1.87	0.57
2:K:500:GLU:OE2	2:K:500:GLU:N	2.33	0.57
1:A:433:LYS:O	1:A:437:GLU:HG2	2.05	0.57
1:E:197:VAL:HA	1:E:200:THR:HG22	1.86	0.57
1:F:463:SER:OG	1:F:464:PRO:HD2	2.05	0.56
1:C:460:ARG:HB3	1:C:461:PHE:HD1	1.70	0.56
2:L:407:ALA:HA	2:L:410:THR:HG22	1.86	0.56
1:C:265:LEU:HD13	1:C:480:HIS:HD2	1.71	0.56
2:I:527:ASP:OD1	2:I:529:THR:HG22	2.06	0.56
2:I:623:GLY:O	2:I:639:ARG:NH1	2.39	0.56
1:C:346:ARG:HH11	1:C:388:GLN:HE22	1.52	0.56
2:I:626:LEU:HD11	2:I:640:ALA:HB2	1.88	0.56
2:G:503:VAL:HG22	2:G:510:PHE:HB2	1.86	0.56
2:H:535:SER:OG	2:H:546:GLY:HA3	2.05	0.56
2:J:588:LEU:HD23	2:J:588:LEU:H	1.70	0.56
1:A:76:THR:HB	1:A:111:VAL:HG21	1.87	0.56
2:I:596:GLY:HA2	2:I:642:ARG:HH11	1.71	0.56
1:C:81:VAL:HG11	1:C:242:LEU:HD23	1.88	0.55
2:J:402:LEU:HA	2:J:436:TRP:HH2	1.71	0.55
2:K:527:ASP:OD1	2:K:529:THR:HG23	2.06	0.55
1:D:259:PHE:CE2	2:L:481:ARG:HD3	2.42	0.55
2:K:623:GLY:O	2:K:639:ARG:NH1	2.39	0.55
2:G:515:ASP:OD1	2:G:515:ASP:N	2.39	0.55
1:D:76:THR:HB	1:D:111:VAL:HG21	1.88	0.55
2:L:628:ILE:HG12	2:L:637:VAL:HG22	1.88	0.55
2:G:535:SER:OG	2:G:546:GLY:HA3	2.06	0.55
2:H:527:ASP:OD1	2:H:529:THR:HG23	2.07	0.55
1:A:459:ASP:OD1	1:A:460:ARG:N	2.40	0.55
1:F:74:VAL:HG21	1:F:108:ILE:HD11	1.89	0.55
1:F:346:ARG:HH11	1:F:388:GLN:HE22	1.55	0.55
1:F:448:ASP:OD1	1:F:449:LYS:N	2.40	0.55
2:G:560:LEU:HG	2:G:561:LEU:H	1.72	0.55
1:C:300:GLN:HB2	1:C:340:LYS:HE3	1.89	0.54
1:D:23:ARG:HH21	3:D:601:COA:P3B	2.31	0.54
1:C:260:ASP:OD1	1:C:261:ASP:N	2.38	0.54
1:E:459:ASP:OD1	1:E:460:ARG:N	2.39	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:483:ARG:HH12	2:L:497:PHE:HE1	1.55	0.54
2:L:400:THR:OG1	2:L:401:ARG:N	2.40	0.54
2:J:626:LEU:HD11	2:J:640:ALA:HB2	1.89	0.54
2:K:597:SER:OG	2:K:598:GLY:N	2.40	0.54
1:B:299:ILE:HG22	1:B:300:GLN:HG3	1.90	0.54
1:E:266:ASP:N	1:E:266:ASP:OD1	2.40	0.54
1:F:334:ASP:OD1	1:F:334:ASP:N	2.38	0.54
1:F:266:ASP:OD1	1:F:266:ASP:N	2.41	0.54
1:F:506:ASP:OD1	1:F:506:ASP:N	2.41	0.54
1:A:417:ASP:OD1	1:A:496:LYS:NZ	2.40	0.54
1:F:275:ASP:OD1	1:F:275:ASP:N	2.38	0.54
2:K:337:SER:OG	2:K:394:LEU:HB3	2.08	0.54
1:A:197:VAL:HA	1:A:200:THR:HG22	1.89	0.53
1:C:99:SER:HG	1:C:132:ARG:HE	1.53	0.53
1:A:34:THR:OG1	1:A:37:GLU:OE1	2.21	0.53
1:B:499:GLU:OE1	1:B:499:GLU:N	2.41	0.53
1:C:43:LEU:HD13	1:C:79:GLY:HA3	1.90	0.53
2:K:526:ASP:OD1	2:K:527:ASP:N	2.41	0.53
2:K:560:LEU:HG	2:K:561:LEU:H	1.74	0.53
2:L:593:GLU:N	2:L:593:GLU:OE1	2.42	0.53
1:C:277:PRO:HA	1:C:399:ARG:HH21	1.73	0.53
2:J:500:GLU:OE2	2:J:580:ARG:NE	2.41	0.53
1:B:460:ARG:HB3	1:B:461:PHE:HD1	1.73	0.53
2:J:646:ILE:HD12	2:J:664:LEU:HD22	1.91	0.53
1:C:138:ALA:HB2	1:D:470:ARG:NH1	2.24	0.53
2:L:341:ALA:HB2	2:L:391:ILE:HD11	1.90	0.53
1:A:346:ARG:HH11	1:A:388:GLN:HE22	1.57	0.53
1:D:101:SER:OG	1:D:102:GLU:N	2.40	0.53
1:E:134:GLN:OE1	1:E:134:GLN:N	2.41	0.53
1:F:196:ASP:OD1	1:F:197:VAL:N	2.42	0.53
1:B:396:ILE:HD13	1:B:420:TYR:HB2	1.91	0.53
1:D:506:ASP:N	1:D:506:ASP:OD1	2.40	0.53
1:E:506:ASP:OD1	1:E:506:ASP:N	2.40	0.53
1:F:58:ARG:NH1	1:F:102:GLU:OE1	2.42	0.53
1:E:334:ASP:OD1	1:E:334:ASP:N	2.42	0.52
1:B:169:GLY:O	1:B:172:VAL:HG12	2.08	0.52
1:E:197:VAL:O	1:E:201:VAL:HG12	2.08	0.52
2:I:426:PHE:HD2	2:I:427:LEU:HD12	1.74	0.52
1:B:198:VAL:O	1:B:202:THR:HG22	2.09	0.52
2:J:346:ARG:HD2	2:J:621:LYS:HD3	1.91	0.52
2:J:359:GLN:HB3	2:J:416:ALA:HB3	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:701:BTI:N2	4:L:701:BTI:C8	2.73	0.52
1:F:489:ALA:O	1:F:492:MET:HG3	2.09	0.52
2:J:563:GLY:HA3	2:J:575:ALA:O	2.10	0.52
2:K:479:ASN:OD1	2:K:483:ARG:NH1	2.43	0.52
2:I:400:THR:OG1	2:I:401:ARG:N	2.43	0.52
1:A:193:THR:HG21	4:J:701:BTI:O3	2.10	0.52
2:H:527:ASP:OD1	2:H:528:GLY:N	2.42	0.52
2:I:615:SER:H	2:I:618:GLN:NE2	2.08	0.52
1:C:140:LEU:HD13	1:D:406:TYR:HD2	1.75	0.52
1:F:74:VAL:HB	1:F:104:HIS:CE1	2.45	0.52
2:H:646:ILE:HD11	2:H:664:LEU:HB3	1.90	0.52
1:D:417:ASP:OD2	1:D:496:LYS:NZ	2.32	0.51
1:F:254:PRO:HB2	2:K:485:ILE:HD11	1.92	0.51
2:L:555:ILE:HG23	2:L:568:HIS:HB2	1.92	0.51
1:A:460:ARG:HB3	1:A:461:PHE:HD1	1.74	0.51
1:E:171:ASP:OD1	1:E:171:ASP:O	2.28	0.51
2:L:535:SER:OG	2:L:536:ALA:N	2.42	0.51
1:D:334:ASP:N	1:D:334:ASP:OD1	2.41	0.51
1:A:465:PHE:O	1:A:469:GLU:HG3	2.10	0.51
1:B:43:LEU:HD13	1:B:79:GLY:HA3	1.93	0.51
2:G:646:ILE:HD11	2:G:664:LEU:HB3	1.91	0.51
2:J:476:HIS:ND1	2:J:521:LEU:HD21	2.26	0.51
1:C:335:SER:OG	1:C:378:HIS:ND1	2.42	0.51
1:D:169:GLY:O	1:D:172:VAL:HG12	2.10	0.51
2:K:605:MET:SD	2:K:606:PRO:HD2	2.51	0.51
2:K:615:SER:OG	2:K:616:GLU:N	2.44	0.51
2:I:361:PRO:HD3	2:I:415:PHE:CD1	2.45	0.51
2:J:622:ASN:N	2:J:643:ASP:OD1	2.44	0.51
1:B:82:ASN:ND2	1:B:243:ASP:OD2	2.44	0.51
1:C:506:ASP:OD1	1:C:506:ASP:N	2.42	0.51
2:I:415:PHE:O	2:I:556:GLN:NE2	2.43	0.51
2:J:482:LYS:HG2	2:J:482:LYS:O	2.11	0.51
1:F:162:VAL:HG12	1:F:164:MET:HG3	1.93	0.50
2:K:341:ALA:HB2	2:K:391:ILE:HD11	1.92	0.50
1:B:21:GLU:O	1:B:25:GLU:HG2	2.12	0.50
1:E:499:GLU:N	1:E:499:GLU:OE1	2.44	0.50
2:G:466:ARG:O	2:G:470:VAL:HG23	2.11	0.50
2:L:547:THR:HA	2:L:552:SER:HA	1.93	0.50
1:B:339:ARG:HH11	1:B:378:HIS:CD2	2.29	0.50
1:F:76:THR:HB	1:F:111:VAL:HG21	1.93	0.50
2:I:615:SER:H	2:I:618:GLN:HE21	1.59	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:VAL:HA	1:C:200:THR:HG22	1.93	0.50
1:A:244:PHE:O	1:A:318:THR:HG21	2.11	0.50
1:B:346:ARG:HH11	1:B:388:GLN:NE2	2.08	0.50
2:H:460:GLU:HB3	2:H:463:VAL:HG12	1.93	0.50
1:C:74:VAL:HB	1:C:104:HIS:CE1	2.47	0.50
2:G:500:GLU:OE2	2:G:580:ARG:NH1	2.44	0.50
1:B:51:PHE:HB3	1:B:52:ASP:OD1	2.12	0.50
1:B:259:PHE:HE2	2:J:481:ARG:HD2	1.76	0.50
1:D:489:ALA:O	1:D:492:MET:HG3	2.11	0.50
2:G:458:GLU:OE1	2:G:506:SER:OG	2.27	0.50
2:H:597:SER:OG	2:H:598:GLY:N	2.44	0.50
1:C:334:ASP:OD1	1:C:334:ASP:N	2.41	0.50
2:K:372:ARG:HG3	2:K:395:VAL:HG22	1.93	0.50
2:L:415:PHE:O	2:L:556:GLN:NE2	2.45	0.50
1:B:74:VAL:HB	1:B:104:HIS:CE1	2.47	0.49
1:E:74:VAL:HB	1:E:104:HIS:CE1	2.47	0.49
1:F:365:LEU:HD12	1:F:366:PRO:HD2	1.94	0.49
2:H:630:GLU:OE2	2:H:633:LYS:HA	2.12	0.49
2:L:503:VAL:HG13	2:L:510:PHE:HB2	1.94	0.49
1:B:460:ARG:HE	1:B:461:PHE:HE1	1.60	0.49
2:I:357:THR:CG2	2:I:418:GLU:HB3	2.43	0.49
1:C:179:ASP:OD1	1:D:507:ASN:ND2	2.44	0.49
2:H:602:LEU:HD12	2:H:660:ASP:HA	1.93	0.49
1:B:495:THR:O	1:B:497:GLU:HG3	2.13	0.49
1:F:175:PRO:O	1:F:178:THR:OG1	2.28	0.49
2:H:608:LEU:HD12	2:H:655:ASP:O	2.13	0.49
1:E:44:ASP:OD1	1:E:45:HIS:N	2.45	0.49
1:E:99:SER:OG	1:E:132:ARG:NE	2.36	0.49
1:E:399:ARG:O	1:E:425:ALA:HA	2.13	0.49
1:A:207:THR:HG23	1:A:210:GLU:H	1.77	0.49
1:D:74:VAL:HG21	1:D:108:ILE:HD11	1.94	0.49
2:I:517:ASP:OD1	2:I:517:ASP:N	2.46	0.49
2:I:603:CYS:SG	2:I:657:LEU:HD13	2.52	0.49
1:C:217:HIS:HA	1:C:221:SER:OG	2.12	0.49
1:C:355:ILE:HB	1:C:393:LEU:HD23	1.95	0.49
1:D:332:VAL:HG12	1:D:362:PRO:HG2	1.95	0.49
1:F:401:ALA:HB1	1:F:406:TYR:HB2	1.95	0.49
2:G:433:HIS:ND1	2:G:435:ARG:HG3	2.28	0.49
2:G:532:PRO:HD2	2:G:549:GLY:HA2	1.95	0.49
2:J:459:PRO:HB2	2:J:464:ALA:HB2	1.93	0.49
2:J:472:ALA:HA	2:J:475:ASP:OD2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:346:ARG:NH1	1:F:388:GLN:HE22	2.11	0.49
1:A:378:HIS:HD2	1:A:381:LYS:HE2	1.77	0.49
1:E:489:ALA:O	1:E:492:MET:HG3	2.13	0.49
2:G:514:VAL:HG12	2:G:523:VAL:HG22	1.95	0.49
2:L:375:THR:HA	2:L:392:ALA:HB1	1.95	0.49
1:D:275:ASP:OD1	1:D:275:ASP:N	2.46	0.48
2:L:428:ALA:O	2:L:431:MET:HG2	2.13	0.48
1:A:101:SER:OG	1:A:102:GLU:N	2.46	0.48
1:A:309:THR:HG22	1:A:340:LYS:HE2	1.95	0.48
1:B:61:ASP:OD1	1:B:61:ASP:N	2.42	0.48
1:A:230:ASN:HD22	2:G:589:MET:HB3	1.77	0.48
1:D:449:LYS:O	1:D:453:ARG:HG2	2.13	0.48
1:A:412:LYS:NZ	1:A:474:ASP:OD1	2.46	0.48
1:D:332:VAL:HG21	1:D:365:LEU:HD13	1.95	0.48
1:E:270:ASP:OD1	1:E:479:PRO:HG2	2.14	0.48
2:I:378:GLU:OE2	2:I:379:GLU:N	2.47	0.48
4:K:701:BTI:C8	4:K:701:BTI:H63	2.43	0.48
1:C:435:ALA:O	1:C:439:ILE:HG13	2.14	0.48
1:F:330:ALA:HB2	2:K:632:MET:HB2	1.94	0.48
2:L:412:LEU:HD11	2:L:424:ILE:HG23	1.96	0.48
1:A:51:PHE:HB3	1:A:52:ASP:OD1	2.14	0.48
1:B:259:PHE:CE2	2:J:481:ARG:HD2	2.49	0.48
1:A:273:ILE:HG23	1:A:399:ARG:HD2	1.96	0.48
1:A:460:ARG:HB3	1:A:461:PHE:CD1	2.48	0.48
1:B:196:ASP:OD1	1:B:197:VAL:N	2.47	0.48
1:D:24:LEU:HD23	1:D:94:THR:HG21	1.94	0.48
1:A:180:PHE:HB3	1:A:182:PHE:HE1	1.79	0.48
1:C:265:LEU:HD13	1:C:480:HIS:CD2	2.49	0.48
1:D:459:ASP:OD1	1:D:460:ARG:N	2.46	0.48
2:H:511:ASN:HB2	2:H:526:ASP:OD2	2.14	0.48
2:L:360:PRO:HB2	2:L:373:ASN:HD22	1.79	0.48
1:A:134:GLN:OE1	1:A:134:GLN:N	2.41	0.47
1:E:30:ARG:HH12	1:E:93:PHE:HE2	1.62	0.47
1:D:262:VAL:HG13	1:D:487:ALA:HB1	1.95	0.47
1:A:463:SER:OG	1:A:464:PRO:HD2	2.13	0.47
1:C:499:GLU:OE2	1:C:499:GLU:N	2.47	0.47
2:K:652:LYS:N	2:K:655:ASP:OD2	2.47	0.47
2:L:466:ARG:NH1	2:L:551:GLN:HG2	2.22	0.47
2:L:475:ASP:HB2	2:L:577:VAL:HG11	1.96	0.47
1:C:57:HIS:HD2	1:C:59:SER:H	1.63	0.47
2:G:624:GLU:HG3	2:G:625:PRO:HD2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:VAL:HB	1:A:104:HIS:CE1	2.49	0.47
1:B:52:ASP:OD2	1:B:110:LYS:NZ	2.48	0.47
2:J:612:ILE:HG22	2:J:614:VAL:HG22	1.96	0.47
2:K:520:ASP:HB3	2:K:534:ARG:HG3	1.96	0.47
1:A:351:PHE:O	1:A:352:SER:OG	2.30	0.47
1:A:488:ARG:HH21	1:C:49:GLU:HB2	1.80	0.47
1:B:346:ARG:NH1	1:B:388:GLN:HE22	2.10	0.47
1:C:381:LYS:HD3	1:D:510:LEU:HD13	1.96	0.47
1:D:381:LYS:HZ1	1:D:510:LEU:C	2.17	0.47
1:F:81:VAL:HG11	1:F:242:LEU:HD23	1.97	0.47
1:C:134:GLN:OE1	1:C:134:GLN:N	2.45	0.47
1:C:446:ASP:OD2	1:C:449:LYS:N	2.36	0.47
1:E:217:HIS:HA	1:E:221:SER:OG	2.15	0.47
2:K:358:TYR:CD1	2:K:360:PRO:HD3	2.50	0.47
1:C:285:GLU:O	1:C:289:ARG:HG2	2.15	0.47
2:K:475:ASP:OD2	2:K:501:ARG:NH2	2.48	0.47
2:H:560:LEU:HD13	2:H:574:GLU:OE1	2.15	0.47
4:K:701:BTI:H103	4:K:701:BTI:H73	1.64	0.47
1:A:192:VAL:HG23	1:A:193:THR:H	1.79	0.46
1:A:273:ILE:HD12	1:A:399:ARG:HD2	1.97	0.46
1:A:448:ASP:OD1	1:A:449:LYS:N	2.48	0.46
1:D:221:SER:OG	1:D:223:ILE:HG12	2.14	0.46
1:D:308:ILE:HD11	1:D:325:GLN:NE2	2.30	0.46
2:I:548:VAL:HG13	2:I:548:VAL:O	2.15	0.46
1:C:119:ARG:HB3	1:C:248:ASN:HD22	1.79	0.46
1:C:192:VAL:HG21	1:D:375:LEU:HD23	1.97	0.46
1:E:351:PHE:O	1:E:352:SER:OG	2.30	0.46
2:G:578:PHE:HB3	2:G:582:GLU:HG3	1.97	0.46
2:J:340:TYR:HB3	2:J:342:GLU:HG2	1.97	0.46
2:J:601:LEU:HD12	2:J:602:LEU:H	1.79	0.46
1:E:110:LYS:HB2	1:E:110:LYS:HE3	1.71	0.46
2:H:491:ASP:OD1	2:H:493:SER:OG	2.29	0.46
2:L:337:SER:O	2:L:394:LEU:HG	2.16	0.46
1:F:40:GLU:OE2	2:K:581:ARG:NE	2.34	0.46
2:L:617:GLY:H	2:L:646:ILE:HB	1.81	0.46
1:B:101:SER:OG	1:B:132:ARG:NH1	2.48	0.46
1:B:285:GLU:O	1:B:289:ARG:HG2	2.14	0.46
1:E:275:ASP:OD1	1:E:276:ASN:N	2.48	0.46
1:F:306:ASN:N	1:F:306:ASN:OD1	2.48	0.46
2:L:374:ASP:OD1	2:L:374:ASP:N	2.48	0.46
1:D:34:THR:OG1	1:D:37:GLU:OE1	2.21	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:GLY:O	1:E:172:VAL:HG12	2.16	0.46
2:I:605:MET:HE2	2:I:631:ALA:HB3	1.98	0.46
1:E:448:ASP:OD1	1:E:449:LYS:N	2.42	0.46
2:I:358:TYR:HB3	2:I:379:GLU:HB2	1.97	0.46
4:L:701:BTI:HN2	4:L:701:BTI:H83	1.79	0.46
2:I:361:PRO:HD3	2:I:415:PHE:HD1	1.81	0.46
2:J:460:GLU:HG3	2:J:461:GLY:H	1.81	0.46
2:L:611:GLN:HG3	2:L:628:ILE:HD12	1.97	0.46
1:A:175:PRO:O	1:A:178:THR:OG1	2.33	0.45
1:A:346:ARG:HH21	1:B:508:ILE:HG22	1.81	0.45
1:F:23:ARG:NH2	3:F:601:COA:O8A	2.50	0.45
2:K:470:VAL:O	2:K:474:ILE:HG13	2.15	0.45
1:A:432:ALA:O	1:A:436:VAL:HG23	2.15	0.45
1:B:306:ASN:OD1	1:B:337:ALA:HB2	2.16	0.45
1:D:364:PHE:O	4:L:701:BTI:N3	2.49	0.45
1:B:83:GLY:HA3	2:J:488:GLN:HG2	1.98	0.45
1:F:221:SER:OG	1:F:223:ILE:HG12	2.16	0.45
2:I:601:LEU:HD11	2:I:626:LEU:HD12	1.98	0.45
2:L:337:SER:OG	2:L:394:LEU:HD11	2.17	0.45
1:D:463:SER:OG	1:D:464:PRO:HD2	2.17	0.45
2:G:580:ARG:HD3	2:G:580:ARG:HA	1.82	0.45
2:L:663:ILE:HG22	2:L:664:LEU:HG	1.98	0.45
1:C:242:LEU:HD12	1:C:242:LEU:HA	1.77	0.45
1:E:201:VAL:HG11	1:F:366:PRO:HG2	1.99	0.45
1:E:217:HIS:HD2	1:E:221:SER:OG	2.00	0.45
2:J:424:ILE:HG22	2:J:425:PRO:HD3	1.98	0.45
1:C:248:ASN:N	1:C:248:ASN:OD1	2.45	0.45
2:G:358:TYR:CD2	2:G:417:ILE:HD11	2.52	0.45
2:J:504:VAL:HG12	2:J:509:ARG:HG2	1.99	0.45
1:A:24:LEU:HD23	1:A:94:THR:HG21	1.99	0.45
1:D:52:ASP:HB3	1:D:107:LYS:HE3	1.99	0.45
1:A:52:ASP:OD2	1:A:110:LYS:NZ	2.50	0.45
2:H:600:GLN:HB2	2:H:662:VAL:HG13	1.99	0.45
1:A:371:GLU:HG3	1:B:211:LEU:HD11	1.99	0.44
1:B:270:ASP:OD1	1:B:479:PRO:HG2	2.17	0.44
1:E:319:VAL:HG22	1:E:354:PRO:HG2	1.98	0.44
2:G:433:HIS:CE1	2:G:435:ARG:HG3	2.52	0.44
2:J:537:TRP:CZ2	2:J:539:PRO:HA	2.52	0.44
1:B:392:PRO:HB3	1:B:493:LEU:HD13	1.99	0.44
1:C:76:THR:HB	1:C:111:VAL:HG21	1.99	0.44
1:C:338:SER:OG	1:C:378:HIS:O	2.24	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:GLN:OE1	1:D:134:GLN:N	2.49	0.44
1:F:329:LEU:O	1:F:332:VAL:HG22	2.18	0.44
2:K:402:LEU:O	2:K:406:GLU:HG2	2.17	0.44
1:A:43:LEU:HD13	1:A:79:GLY:HA3	2.00	0.44
2:H:548:VAL:HG23	2:H:548:VAL:O	2.17	0.44
2:G:421:ARG:H	2:G:421:ARG:HD3	1.83	0.44
2:J:335:VAL:HG22	2:J:336:GLU:H	1.81	0.44
2:J:475:ASP:OD1	2:J:476:HIS:N	2.51	0.44
1:C:306:ASN:N	1:C:306:ASN:OD1	2.50	0.44
1:A:182:PHE:HD2	1:A:228:PHE:CE2	2.35	0.44
2:J:346:ARG:HB3	2:J:621:LYS:HD3	2.00	0.44
2:L:520:ASP:HB3	2:L:534:ARG:HG3	2.00	0.44
1:A:100:LEU:HD22	1:A:143:TYR:CD1	2.53	0.44
1:C:412:LYS:HD3	1:C:419:ASN:OD1	2.18	0.44
1:D:319:VAL:HG22	1:D:354:PRO:HG2	2.00	0.44
1:E:460:ARG:HB3	1:E:461:PHE:HD1	1.83	0.44
2:H:610:LYS:HD2	2:H:630:GLU:OE1	2.18	0.44
1:A:119:ARG:HB3	1:A:248:ASN:HD22	1.83	0.44
1:B:277:PRO:HA	1:B:399:ARG:NH2	2.33	0.44
1:D:238:ILE:HD13	1:D:238:ILE:HA	1.88	0.44
1:E:196:ASP:OD1	1:E:197:VAL:N	2.50	0.44
1:F:99:SER:OG	1:F:132:ARG:N	2.51	0.44
1:F:299:ILE:HG22	1:F:300:GLN:HG3	2.00	0.44
2:H:648:LYS:HG2	2:H:649:ILE:N	2.33	0.44
2:J:597:SER:HB3	2:J:642:ARG:HH21	1.83	0.44
1:D:35:ALA:O	1:D:39:ILE:HG12	2.18	0.44
3:E:601:COA:H52A	3:E:601:COA:H8A	1.99	0.44
2:J:611:GLN:O	2:J:628:ILE:HG22	2.18	0.44
2:I:359:GLN:HB2	2:I:416:ALA:HB3	1.99	0.43
2:J:527:ASP:OD1	2:J:528:GLY:N	2.51	0.43
1:A:126:PHE:HB2	1:A:163:ILE:HD13	2.00	0.43
1:A:185:ARG:NH2	1:A:229:GLU:OE2	2.51	0.43
1:A:489:ALA:O	1:A:492:MET:HG3	2.17	0.43
1:B:308:ILE:HD11	1:B:325:GLN:NE2	2.33	0.43
1:A:482:THR:HG23	1:A:483:ARG:N	2.33	0.43
1:E:106:ALA:O	1:E:109:VAL:HG12	2.18	0.43
1:E:326:PRO:HG3	1:E:360:ASP:OD2	2.17	0.43
2:J:412:LEU:HD22	2:J:424:ILE:HD11	1.99	0.43
2:K:521:LEU:O	2:K:532:PRO:HA	2.18	0.43
4:K:701:BTI:HN2	4:K:701:BTI:H72	1.75	0.43
2:L:642:ARG:HD3	2:L:642:ARG:HA	1.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:602:LEU:HD23	2:H:602:LEU:H	1.82	0.43
2:I:600:GLN:HG3	2:I:662:VAL:HG12	2.01	0.43
2:K:407:ALA:HA	2:K:410:THR:HG22	2.00	0.43
1:A:230:ASN:N	1:A:230:ASN:OD1	2.50	0.43
1:C:104:HIS:O	1:C:108:ILE:HG12	2.19	0.43
1:C:230:ASN:OD1	1:C:230:ASN:N	2.50	0.43
1:D:411:SER:OG	1:D:412:LYS:N	2.52	0.43
1:F:201:VAL:HG12	1:F:202:THR:HG23	2.00	0.43
2:K:402:LEU:HD12	2:K:402:LEU:H	1.83	0.43
2:K:458:GLU:HG2	2:K:459:PRO:HD2	2.00	0.43
1:A:35:ALA:O	1:A:39:ILE:HG12	2.19	0.43
1:E:371:GLU:HG3	1:F:211:LEU:HD11	2.01	0.43
1:B:244:PHE:O	1:B:318:THR:HG21	2.18	0.43
1:D:265:LEU:HD13	1:D:480:HIS:HD2	1.84	0.43
2:I:503:VAL:HG13	2:I:510:PHE:HB2	2.01	0.43
2:I:560:LEU:HG	2:I:561:LEU:H	1.82	0.43
2:L:374:ASP:OD1	2:L:393:LYS:HB2	2.18	0.43
1:E:306:ASN:OD1	1:E:306:ASN:N	2.52	0.43
2:G:501:ARG:HB2	2:G:512:VAL:HG23	2.00	0.43
2:I:357:THR:HG22	2:I:418:GLU:HB3	2.01	0.43
2:I:557:VAL:HG23	2:I:564:VAL:HG13	2.01	0.43
2:L:394:LEU:HD11	2:L:408:GLN:HE22	1.84	0.43
1:A:269:LEU:HA	1:A:269:LEU:HD23	1.75	0.43
1:C:383:LEU:HB2	1:C:408:VAL:HG12	2.01	0.43
1:E:482:THR:HG23	1:E:483:ARG:N	2.33	0.43
1:B:230:ASN:N	1:B:230:ASN:OD1	2.51	0.43
2:K:360:PRO:HB2	2:K:373:ASN:HD22	1.84	0.43
2:L:336:GLU:HG2	2:L:394:LEU:O	2.19	0.43
1:D:140:LEU:HD23	1:D:140:LEU:HA	1.90	0.42
1:D:285:GLU:O	1:D:289:ARG:HG2	2.19	0.42
1:F:425:ALA:O	1:F:464:PRO:HD3	2.19	0.42
3:F:601:COA:O8A	3:F:601:COA:H4B	2.17	0.42
1:E:74:VAL:HG21	1:E:108:ILE:HD11	2.00	0.42
1:F:482:THR:HG23	1:F:483:ARG:N	2.34	0.42
1:F:271:THR:O	1:F:271:THR:HG22	2.19	0.42
2:G:600:GLN:HA	2:G:665:GLU:HA	2.00	0.42
2:H:466:ARG:O	2:H:470:VAL:HG13	2.20	0.42
1:D:244:PHE:HE1	1:D:313:ARG:NH1	2.17	0.42
1:E:230:ASN:OD1	1:E:230:ASN:N	2.52	0.42
2:G:646:ILE:HG12	2:G:647:SER:H	1.84	0.42
1:A:74:VAL:HG21	1:A:108:ILE:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LEU:HA	1:A:327:LEU:HD23	1.82	0.42
1:B:499:GLU:HG2	1:B:499:GLU:O	2.18	0.42
1:E:465:PHE:O	1:E:469:GLU:HG3	2.19	0.42
1:F:417:ASP:OD1	1:F:496:LYS:NZ	2.52	0.42
2:G:606:PRO:HB3	2:G:658:ALA:HA	2.02	0.42
2:J:478:LEU:O	2:J:481:ARG:HG2	2.20	0.42
1:E:100:LEU:HD22	1:E:143:TYR:CD1	2.55	0.42
4:K:701:BTI:H63	4:K:701:BTI:H83	2.02	0.42
1:A:387:SER:OG	1:B:151:VAL:HG21	2.19	0.42
1:A:413:HIS:HE1	1:A:472:TYR:CE1	2.37	0.42
1:C:259:PHE:CD2	2:H:539:PRO:HD2	2.55	0.42
1:C:490:LEU:HA	1:C:490:LEU:HD23	1.79	0.42
2:G:401:ARG:O	2:G:405:ILE:HG22	2.19	0.42
2:G:412:LEU:HD23	2:G:412:LEU:HA	1.86	0.42
2:J:340:TYR:HB2	2:J:423:ASN:ND2	2.35	0.42
1:E:491:GLY:HA2	1:E:494:ARG:NH1	2.35	0.42
2:G:339:VAL:HG21	2:G:424:ILE:HD11	2.02	0.42
2:G:467:LEU:HD21	2:G:568:HIS:HB2	2.01	0.42
2:G:563:GLY:HA3	2:G:575:ALA:O	2.19	0.42
2:K:512:VAL:HG13	2:K:523:VAL:HG13	2.02	0.42
2:L:574:GLU:OE2	2:L:576:ARG:NH2	2.42	0.42
1:A:377:LYS:HG3	1:B:223:ILE:HD12	2.01	0.41
1:A:436:VAL:HG21	1:A:454:THR:HA	2.01	0.41
1:A:482:THR:HG23	1:A:483:ARG:H	1.85	0.41
1:C:482:THR:HG23	1:C:483:ARG:N	2.34	0.41
1:F:346:ARG:HH11	1:F:388:GLN:NE2	2.16	0.41
2:I:463:VAL:HG23	2:I:568:HIS:HD2	1.85	0.41
2:I:522:LEU:HD23	2:I:522:LEU:HA	1.87	0.41
1:B:463:SER:OG	1:B:464:PRO:HD2	2.19	0.41
3:F:601:COA:H31	3:F:601:COA:N8P	2.32	0.41
2:L:422:HIS:CE1	2:L:424:ILE:HB	2.56	0.41
1:A:100:LEU:HD22	1:A:143:TYR:CE1	2.56	0.41
1:A:196:ASP:OD1	1:A:197:VAL:N	2.54	0.41
1:A:306:ASN:OD1	1:A:306:ASN:N	2.48	0.41
1:B:456:GLU:HA	1:B:459:ASP:OD2	2.21	0.41
2:J:344:PRO:HG3	2:J:423:ASN:HA	2.01	0.41
2:J:428:ALA:HB1	2:J:569:ALA:O	2.19	0.41
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.92	0.41
1:C:100:LEU:HD13	1:C:143:TYR:CE1	2.55	0.41
1:E:417:ASP:O	1:E:418:LEU:HD23	2.20	0.41
2:J:610:LYS:NZ	2:J:630:GLU:OE1	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ILE:HD13	1:B:238:ILE:HA	1.88	0.41
1:C:21:GLU:OE2	1:C:25:GLU:HG2	2.19	0.41
1:D:269:LEU:HD23	1:D:269:LEU:HA	1.89	0.41
2:G:423:ASN:OD1	2:G:423:ASN:N	2.53	0.41
2:H:642:ARG:NH1	2:H:666:PHE:HB3	2.35	0.41
2:I:491:ASP:OD1	2:I:493:SER:OG	2.33	0.41
2:J:354:ARG:HG2	2:J:355:LEU:H	1.85	0.41
1:B:81:VAL:HG11	1:B:242:LEU:HD23	2.03	0.41
1:D:171:ASP:O	1:D:175:PRO:HD2	2.21	0.41
1:D:248:ASN:OD1	1:D:248:ASN:N	2.54	0.41
1:E:309:THR:HG22	1:E:340:LYS:HE2	2.03	0.41
2:L:426:PHE:O	2:L:429:THR:HG22	2.20	0.41
1:E:413:HIS:NE2	1:F:141:GLY:HA2	2.35	0.41
2:H:655:ASP:OD1	2:H:656:SER:N	2.53	0.41
2:J:659:VAL:HG22	2:J:660:ASP:OD1	2.21	0.41
2:K:337:SER:HG	2:K:394:LEU:HB3	1.84	0.41
2:K:642:ARG:HD3	2:K:642:ARG:HA	1.73	0.41
1:A:386:TYR:CE1	1:A:410:ALA:HB2	2.56	0.41
1:C:22:LYS:HE2	1:C:22:LYS:HB2	1.88	0.41
1:E:230:ASN:HB2	2:I:589:MET:HE2	2.03	0.41
2:L:480:ILE:HD12	2:L:480:ILE:HA	1.83	0.41
1:A:42:LEU:O	1:A:239:ARG:NH1	2.54	0.41
1:A:319:VAL:HG22	1:A:354:PRO:HG2	2.01	0.41
1:C:244:PHE:O	1:C:318:THR:HG21	2.20	0.41
1:C:292:ASP:OD1	1:C:293:GLU:N	2.48	0.41
1:E:65:GLU:OE1	1:E:65:GLU:N	2.29	0.41
1:E:82:ASN:HD22	1:E:243:ASP:CG	2.25	0.41
1:E:386:TYR:CE1	1:E:410:ALA:HB2	2.56	0.41
2:I:505:LEU:HD12	2:I:505:LEU:HA	1.92	0.41
2:K:623:GLY:O	2:K:639:ARG:HD2	2.21	0.41
2:L:526:ASP:OD1	2:L:526:ASP:N	2.53	0.41
4:L:701:BTI:C8	4:L:701:BTI:HN2	2.33	0.41
1:B:277:PRO:HA	1:B:399:ARG:HH21	1.85	0.41
1:D:499:GLU:OE2	1:D:499:GLU:N	2.54	0.41
1:F:352:SER:HA	1:F:391:VAL:HG11	2.03	0.41
2:H:646:ILE:CD1	2:H:664:LEU:HB3	2.52	0.41
1:B:106:ALA:O	1:B:109:VAL:HG12	2.20	0.40
1:B:275:ASP:OD1	1:B:276:ASN:N	2.54	0.40
1:B:332:VAL:HG12	1:B:362:PRO:HG2	2.03	0.40
1:C:418:LEU:HD23	1:C:418:LEU:HA	1.93	0.40
1:D:142:GLY:O	1:D:143:TYR:C	2.60	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:482:THR:HG23	1:D:483:ARG:N	2.36	0.40
1:F:65:GLU:OE1	1:F:65:GLU:N	2.30	0.40
2:G:599:LYS:HA	2:G:642:ARG:HH22	1.86	0.40
1:E:499:GLU:O	1:E:499:GLU:HG2	2.21	0.40
1:C:47:SER:CB	1:C:80:THR:HG22	2.51	0.40
2:I:551:GLN:OE1	2:I:551:GLN:HA	2.21	0.40
2:I:611:GLN:HB3	2:I:628:ILE:HB	2.02	0.40
2:K:360:PRO:HB3	2:K:415:PHE:CE1	2.56	0.40
1:A:36:ARG:NH2	1:A:50:GLU:OE2	2.49	0.40
1:A:84:ARG:HD2	2:G:485:ILE:HD13	2.04	0.40
1:D:242:LEU:HA	1:D:242:LEU:HD12	1.88	0.40
1:D:366:PRO:HD3	4:L:701:BTI:H63	2.04	0.40
1:D:395:THR:HG21	1:D:410:ALA:O	2.22	0.40
2:J:495:LEU:HD12	2:J:496:THR:H	1.87	0.40
1:A:237:GLN:HE21	2:G:562:ASN:HD21	1.69	0.40
1:A:259:PHE:CE2	2:G:481:ARG:HG3	2.57	0.40
1:C:270:ASP:OD1	1:C:480:HIS:HB3	2.22	0.40
1:C:406:TYR:HD2	1:D:140:LEU:HD13	1.87	0.40
1:E:201:VAL:HG11	1:F:366:PRO:CG	2.51	0.40
1:E:401:ALA:HB1	1:E:406:TYR:HB2	2.03	0.40
1:F:127:ASP:OD1	1:F:165:GLY:HA3	2.21	0.40
2:I:377:VAL:HG22	2:I:378:GLU:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	504/510 (99%)	487 (97%)	17 (3%)	0	100	100
1	B	504/510 (99%)	494 (98%)	10 (2%)	0	100	100
1	C	504/510 (99%)	486 (96%)	18 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	504/510 (99%)	484 (96%)	20 (4%)	0	100	100
1	E	504/510 (99%)	493 (98%)	11 (2%)	0	100	100
1	F	504/510 (99%)	484 (96%)	20 (4%)	0	100	100
2	G	271/667 (41%)	236 (87%)	35 (13%)	0	100	100
2	H	206/667 (31%)	191 (93%)	15 (7%)	0	100	100
2	I	278/667 (42%)	246 (88%)	32 (12%)	0	100	100
2	J	295/667 (44%)	248 (84%)	47 (16%)	0	100	100
2	K	283/667 (42%)	251 (89%)	32 (11%)	0	100	100
2	L	281/667 (42%)	243 (86%)	38 (14%)	0	100	100
All	All	4638/7062 (66%)	4343 (94%)	295 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/410 (99%)	406 (100%)	0	100	100
1	B	406/410 (99%)	405 (100%)	1 (0%)	93	98
1	C	406/410 (99%)	406 (100%)	0	100	100
1	D	406/410 (99%)	406 (100%)	0	100	100
1	E	406/410 (99%)	406 (100%)	0	100	100
1	F	406/410 (99%)	406 (100%)	0	100	100
2	G	224/523 (43%)	223 (100%)	1 (0%)	91	96
2	H	165/523 (32%)	165 (100%)	0	100	100
2	I	229/523 (44%)	229 (100%)	0	100	100
2	J	241/523 (46%)	241 (100%)	0	100	100
2	K	231/523 (44%)	231 (100%)	0	100	100
2	L	231/523 (44%)	231 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3757/5598 (67%)	3755 (100%)	2 (0%)	93 98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	386	TYR
2	G	421	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	217	HIS
1	A	237	GLN
1	A	325	GLN
1	A	349	ASN
1	A	378	HIS
1	A	388	GLN
1	A	413	HIS
1	A	480	HIS
1	B	57	HIS
1	B	104	HIS
1	B	217	HIS
1	B	325	GLN
1	B	378	HIS
1	B	388	GLN
1	B	480	HIS
1	C	57	HIS
1	C	104	HIS
1	C	217	HIS
1	C	278	ASN
1	C	325	GLN
1	C	388	GLN
1	C	413	HIS
1	C	480	HIS
1	D	217	HIS
1	D	278	ASN
1	D	325	GLN
1	D	349	ASN
1	D	413	HIS
1	D	480	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	57	HIS
1	E	104	HIS
1	E	217	HIS
1	E	278	ASN
1	F	27	GLN
1	F	57	HIS
1	F	217	HIS
1	F	278	ASN
1	F	388	GLN
1	F	413	HIS
1	F	480	HIS
2	G	611	GLN
2	H	479	ASN
2	H	562	ASN
2	I	386	HIS
2	I	488	GLN
2	I	556	GLN
2	I	618	GLN
2	J	359	GLN
2	J	386	HIS
2	J	567	GLN
2	J	622	ASN
2	K	373	ASN
2	K	562	ASN
2	L	408	GLN
2	L	488	GLN
2	L	556	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	COA	A	601	-	41,50,50	2.49	15 (36%)	52,75,75	1.61	10 (19%)
4	BTI	L	701	2	16,16,16	0.58	0	21,21,21	1.27	3 (14%)
4	BTI	J	701	2	16,16,16	0.60	0	21,21,21	1.33	2 (9%)
4	BTI	K	701	2	16,16,16	0.62	0	21,21,21	1.44	5 (23%)
3	COA	C	601	-	33,38,50	2.10	10 (30%)	40,60,75	1.55	7 (17%)
4	BTI	I	701	2	16,16,16	0.43	0	21,21,21	0.71	0
3	COA	E	601	-	28,33,50	2.36	11 (39%)	35,52,75	1.67	7 (20%)
3	COA	F	601	-	41,50,50	2.50	15 (36%)	52,75,75	1.56	9 (17%)
4	BTI	G	701	2	16,16,16	0.52	0	21,21,21	1.40	5 (23%)
4	BTI	H	701	2	16,16,16	0.50	0	21,21,21	1.12	2 (9%)
3	COA	D	601	-	33,38,50	2.10	9 (27%)	40,60,75	1.50	6 (15%)
3	COA	B	601	-	41,50,50	2.47	14 (34%)	52,75,75	1.50	10 (19%)

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	COA	A	601	-	-	21/44/64/64	0/3/3/3
4	BTI	L	701	2	-	4/5/27/27	0/2/2/2
4	BTI	J	701	2	-	4/5/27/27	0/2/2/2
4	BTI	K	701	2	-	4/5/27/27	0/2/2/2
3	COA	C	601	-	-	10/24/44/64	0/3/3/3
4	BTI	I	701	2	-	3/5/27/27	0/2/2/2
3	COA	E	601	-	-	9/17/37/64	0/3/3/3
3	COA	F	601	-	-	17/44/64/64	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTI	G	701	2	-	5/5/27/27	0/2/2/2
4	BTI	H	701	2	-	2/5/27/27	0/2/2/2
3	COA	D	601	-	-	14/24/44/64	0/3/3/3
3	COA	B	601	-	-	16/44/64/64	0/3/3/3

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	601	COA	O4B-C1B	7.16	1.51	1.41
3	A	601	COA	C9P-N8P	7.04	1.49	1.33
3	A	601	COA	O4B-C1B	6.94	1.50	1.41
3	B	601	COA	C9P-N8P	6.92	1.48	1.33
3	F	601	COA	C9P-N8P	6.90	1.48	1.33
3	D	601	COA	O4B-C1B	6.89	1.50	1.41
3	F	601	COA	O4B-C1B	6.86	1.50	1.41
3	C	601	COA	O4B-C1B	6.82	1.50	1.41
3	B	601	COA	O4B-C1B	6.55	1.50	1.41
3	F	601	COA	C5P-N4P	6.48	1.48	1.33
3	A	601	COA	C5P-N4P	6.40	1.47	1.33
3	B	601	COA	C5P-N4P	6.40	1.47	1.33
3	B	601	COA	C2B-C1B	-3.69	1.48	1.53
3	F	601	COA	C2B-C1B	-3.67	1.48	1.53
3	C	601	COA	C2B-C1B	-3.50	1.48	1.53
3	A	601	COA	C2B-C1B	-3.42	1.48	1.53
3	D	601	COA	C2B-C1B	-3.41	1.48	1.53
3	E	601	COA	C2B-C1B	-3.28	1.48	1.53
3	E	601	COA	P2A-O6A	3.27	1.67	1.54
3	C	601	COA	P3B-O3B	3.26	1.65	1.59
3	F	601	COA	C6A-N6A	3.25	1.45	1.34
3	F	601	COA	C2B-C3B	-3.23	1.45	1.52
3	B	601	COA	C6A-N6A	3.21	1.45	1.34
3	A	601	COA	C6A-N6A	3.19	1.45	1.34
3	D	601	COA	C6A-N6A	3.18	1.45	1.34
3	E	601	COA	P3B-O3B	3.18	1.65	1.59
3	D	601	COA	P3B-O3B	3.17	1.65	1.59
3	C	601	COA	C6A-N6A	3.17	1.45	1.34
3	E	601	COA	C6A-N6A	3.14	1.45	1.34
3	B	601	COA	P3B-O3B	3.12	1.65	1.59
3	B	601	COA	C2B-C3B	-3.12	1.46	1.52
3	A	601	COA	P3B-O3B	3.07	1.65	1.59
3	C	601	COA	C2B-C3B	-3.07	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	601	COA	P3B-O3B	3.05	1.65	1.59
3	E	601	COA	C2B-C3B	-3.05	1.46	1.52
3	D	601	COA	C2B-C3B	-2.97	1.46	1.52
3	A	601	COA	C2B-C3B	-2.84	1.46	1.52
3	F	601	COA	C4A-N3A	-2.67	1.32	1.35
3	A	601	COA	C4A-N3A	-2.60	1.32	1.35
3	E	601	COA	C4A-N3A	-2.59	1.32	1.35
3	D	601	COA	C4A-N3A	-2.50	1.32	1.35
3	B	601	COA	C4A-N3A	-2.47	1.32	1.35
3	C	601	COA	C4A-N3A	-2.43	1.32	1.35
3	F	601	COA	C6P-C5P	2.32	1.55	1.51
3	F	601	COA	O9P-C9P	-2.31	1.18	1.23
3	A	601	COA	P3B-O9A	-2.30	1.46	1.54
3	A	601	COA	C6P-C5P	2.30	1.55	1.51
3	C	601	COA	P3B-O9A	-2.29	1.46	1.54
3	B	601	COA	C6P-C5P	2.27	1.55	1.51
3	D	601	COA	P3B-O9A	-2.26	1.46	1.54
3	E	601	COA	P3B-O9A	-2.26	1.46	1.54
3	B	601	COA	O9P-C9P	-2.26	1.18	1.23
3	F	601	COA	P3B-O9A	-2.24	1.46	1.54
3	B	601	COA	P3B-O9A	-2.24	1.46	1.54
3	E	601	COA	P3B-O8A	-2.23	1.46	1.54
3	A	601	COA	O9P-C9P	-2.23	1.19	1.23
3	E	601	COA	P2A-O5A	-2.21	1.46	1.54
3	F	601	COA	P3B-O8A	-2.19	1.46	1.54
3	C	601	COA	P3B-O8A	-2.19	1.46	1.54
3	D	601	COA	P3B-O8A	-2.19	1.46	1.54
3	A	601	COA	P3B-O8A	-2.18	1.46	1.54
3	B	601	COA	P3B-O8A	-2.18	1.46	1.54
3	B	601	COA	OAP-CAP	-2.16	1.38	1.42
3	E	601	COA	O4B-C4B	2.09	1.49	1.45
3	F	601	COA	OAP-CAP	-2.08	1.38	1.42
3	F	601	COA	O4B-C4B	2.07	1.49	1.45
3	B	601	COA	O4B-C4B	2.07	1.49	1.45
3	A	601	COA	OAP-CAP	-2.07	1.38	1.42
3	D	601	COA	P2A-O6A	2.07	1.67	1.59
3	C	601	COA	O4B-C4B	2.06	1.49	1.45
3	C	601	COA	P2A-O6A	2.05	1.67	1.59
3	A	601	COA	P2A-O6A	2.02	1.67	1.59
3	A	601	COA	O4B-C4B	2.02	1.49	1.45
3	F	601	COA	P2A-O6A	2.02	1.67	1.59

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	601	COA	N3A-C2A-N1A	-4.14	122.20	128.68
3	C	601	COA	N3A-C2A-N1A	-4.13	122.23	128.68
3	B	601	COA	N3A-C2A-N1A	-4.08	122.30	128.68
3	D	601	COA	N3A-C2A-N1A	-4.02	122.39	128.68
3	C	601	COA	C4A-C5A-N7A	-3.96	105.27	109.40
3	E	601	COA	N3A-C2A-N1A	-3.96	122.49	128.68
3	A	601	COA	C4A-C5A-N7A	-3.95	105.28	109.40
3	A	601	COA	N3A-C2A-N1A	-3.94	122.51	128.68
3	F	601	COA	C4A-C5A-N7A	-3.94	105.29	109.40
3	E	601	COA	C4A-C5A-N7A	-3.89	105.35	109.40
3	B	601	COA	C4A-C5A-N7A	-3.86	105.38	109.40
3	D	601	COA	C4A-C5A-N7A	-3.85	105.39	109.40
4	K	701	BTI	C6-C5-C4	-3.68	105.46	108.66
3	A	601	COA	C3B-C2B-C1B	3.47	107.57	99.89
3	E	601	COA	P1A-O3A-P2A	-3.35	121.33	132.83
3	C	601	COA	C3B-C2B-C1B	3.25	107.09	99.89
3	D	601	COA	C3B-C2B-C1B	3.12	106.80	99.89
3	F	601	COA	C6P-C5P-N4P	3.09	121.63	116.42
4	G	701	BTI	C5-C6-S1	-3.08	103.67	106.31
3	F	601	COA	P2A-O3A-P1A	-3.07	122.30	132.83
3	E	601	COA	C3B-C2B-C1B	2.93	106.37	99.89
3	C	601	COA	P2A-O3A-P1A	-2.89	122.92	132.83
4	G	701	BTI	C5-N3-C3	-2.86	108.74	112.46
3	B	601	COA	C3B-C2B-C1B	2.79	106.07	99.89
4	J	701	BTI	C5-N3-C3	-2.79	108.83	112.46
3	F	601	COA	C3B-C2B-C1B	2.76	106.00	99.89
3	A	601	COA	P2A-O3A-P1A	-2.75	123.38	132.83
3	F	601	COA	C1B-N9A-C4A	-2.67	121.95	126.64
4	L	701	BTI	C6-C5-N3	2.62	116.36	113.03
3	A	601	COA	C2B-C3B-C4B	2.61	107.85	103.22
4	L	701	BTI	C4-N2-C3	-2.59	110.21	112.62
3	A	601	COA	O9P-C9P-N8P	-2.58	117.45	122.99
4	J	701	BTI	C4-C2-S1	2.53	107.62	105.20
3	A	601	COA	O5A-P2A-O4A	-2.53	99.72	112.24
4	K	701	BTI	C4-N2-C3	-2.49	110.30	112.62
4	K	701	BTI	C5-C6-S1	-2.47	104.19	106.31
3	D	601	COA	P2A-O3A-P1A	-2.46	124.39	132.83
3	A	601	COA	C6P-C5P-N4P	2.45	120.55	116.42
3	A	601	COA	O2A-P1A-O1A	-2.43	100.22	112.24
4	K	701	BTI	C4-C2-S1	2.42	107.51	105.20
3	A	601	COA	C1B-N9A-C4A	-2.34	122.53	126.64
3	C	601	COA	O5A-P2A-O4A	-2.34	100.68	112.24
4	G	701	BTI	N2-C3-N3	-2.33	106.57	108.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	COA	O5A-P2A-O4A	-2.32	100.75	112.24
3	E	601	COA	O5A-P2A-O4A	-2.32	101.61	110.68
3	B	601	COA	O9P-C9P-N8P	-2.31	118.02	122.99
3	B	601	COA	C1B-N9A-C4A	-2.31	122.58	126.64
4	G	701	BTI	C2-C4-N2	2.31	115.19	113.13
3	D	601	COA	O2A-P1A-O1A	-2.29	100.91	112.24
3	C	601	COA	C1B-N9A-C4A	-2.27	122.65	126.64
4	L	701	BTI	N2-C3-N3	-2.27	106.63	108.76
3	B	601	COA	O2A-P1A-O1A	-2.26	101.05	112.24
3	C	601	COA	O2A-P1A-O1A	-2.26	101.06	112.24
4	G	701	BTI	C4-N2-C3	-2.26	110.52	112.62
3	E	601	COA	O2A-P1A-O1A	-2.24	101.15	112.24
3	F	601	COA	O2A-P1A-O1A	-2.24	101.17	112.24
3	F	601	COA	O5A-P2A-O4A	-2.24	101.18	112.24
4	K	701	BTI	C6-S1-C2	-2.23	85.30	89.89
3	B	601	COA	O5A-P2A-O4A	-2.22	101.27	112.24
3	E	601	COA	C1B-N9A-C4A	-2.21	122.77	126.64
3	B	601	COA	P2A-O3A-P1A	-2.20	125.29	132.83
3	B	601	COA	C6P-C5P-N4P	2.14	120.02	116.42
4	H	701	BTI	C4-C2-S1	2.11	107.22	105.20
3	F	601	COA	O5P-C5P-N4P	-2.08	119.09	123.01
3	B	601	COA	C2B-C3B-C4B	2.06	106.88	103.22
4	H	701	BTI	C6-C5-N3	2.05	115.64	113.03

There are no chirality outliers.

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	COA	C3B-O3B-P3B-O7A
3	A	601	COA	C5B-O5B-P1A-O1A
3	A	601	COA	C5B-O5B-P1A-O3A
3	A	601	COA	CCP-O6A-P2A-O5A
3	A	601	COA	CDP-CBP-CCP-O6A
3	A	601	COA	CEP-CBP-CCP-O6A
3	A	601	COA	CAP-CBP-CCP-O6A
3	A	601	COA	O9P-C9P-CAP-CBP
3	A	601	COA	N8P-C9P-CAP-CBP
3	A	601	COA	O9P-C9P-CAP-OAP
3	A	601	COA	N8P-C9P-CAP-OAP
3	A	601	COA	CAP-C9P-N8P-C7P
3	B	601	COA	CDP-CBP-CCP-O6A
3	B	601	COA	CEP-CBP-CCP-O6A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	601	COA	CAP-CBP-CCP-O6A
3	B	601	COA	O9P-C9P-CAP-OAP
3	B	601	COA	CAP-C9P-N8P-C7P
3	B	601	COA	C5P-C6P-C7P-N8P
3	B	601	COA	S1P-C2P-C3P-N4P
3	C	601	COA	C3B-O3B-P3B-O7A
3	C	601	COA	C5B-O5B-P1A-O2A
3	C	601	COA	C5B-O5B-P1A-O3A
3	D	601	COA	C4B-C3B-O3B-P3B
3	D	601	COA	C3B-O3B-P3B-O7A
3	D	601	COA	C5B-O5B-P1A-O2A
3	D	601	COA	C5B-O5B-P1A-O3A
3	D	601	COA	CCP-O6A-P2A-O3A
3	D	601	COA	CCP-O6A-P2A-O5A
3	E	601	COA	C3B-O3B-P3B-O7A
3	E	601	COA	O4B-C4B-C5B-O5B
3	E	601	COA	P2A-O3A-P1A-O5B
3	F	601	COA	C3B-O3B-P3B-O8A
3	F	601	COA	P1A-O3A-P2A-O6A
3	F	601	COA	CCP-O6A-P2A-O4A
3	F	601	COA	CCP-O6A-P2A-O5A
3	F	601	COA	CDP-CBP-CCP-O6A
3	F	601	COA	CEP-CBP-CCP-O6A
3	F	601	COA	CAP-CBP-CCP-O6A
3	F	601	COA	S1P-C2P-C3P-N4P
4	G	701	BTI	S1-C2-C7-C8
4	G	701	BTI	C4-C2-C7-C8
4	I	701	BTI	S1-C2-C7-C8
4	I	701	BTI	C4-C2-C7-C8
4	J	701	BTI	C11-C10-C9-C8
4	J	701	BTI	S1-C2-C7-C8
4	J	701	BTI	C4-C2-C7-C8
4	K	701	BTI	S1-C2-C7-C8
4	K	701	BTI	C4-C2-C7-C8
4	L	701	BTI	C11-C10-C9-C8
3	A	601	COA	C6P-C5P-N4P-C3P
3	B	601	COA	C6P-C5P-N4P-C3P
3	F	601	COA	C6P-C5P-N4P-C3P
3	A	601	COA	O9P-C9P-N8P-C7P
3	B	601	COA	O9P-C9P-N8P-C7P
4	K	701	BTI	C7-C8-C9-C10
3	C	601	COA	C3B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	601	COA	O4B-C4B-C5B-O5B
3	D	601	COA	C3B-C4B-C5B-O5B
3	D	601	COA	O4B-C4B-C5B-O5B
3	E	601	COA	C3B-C4B-C5B-O5B
3	F	601	COA	C3B-C4B-C5B-O5B
3	A	601	COA	C4B-C3B-O3B-P3B
3	E	601	COA	C4B-C3B-O3B-P3B
3	F	601	COA	C4B-C3B-O3B-P3B
3	A	601	COA	O5P-C5P-N4P-C3P
3	B	601	COA	O5P-C5P-N4P-C3P
3	F	601	COA	O5P-C5P-N4P-C3P
4	L	701	BTI	C7-C8-C9-C10
3	F	601	COA	O4B-C4B-C5B-O5B
3	C	601	COA	C2B-C3B-O3B-P3B
3	C	601	COA	C4B-C3B-O3B-P3B
4	G	701	BTI	C7-C8-C9-C10
3	E	601	COA	C2B-C3B-O3B-P3B
3	D	601	COA	CDP-CBP-CCP-O6A
3	D	601	COA	CEP-CBP-CCP-O6A
3	D	601	COA	CAP-CBP-CCP-O6A
3	F	601	COA	C5P-C6P-C7P-N8P
4	I	701	BTI	C2-C7-C8-C9
4	K	701	BTI	C2-C7-C8-C9
3	B	601	COA	P1A-O3A-P2A-O6A
4	L	701	BTI	S1-C2-C7-C8
3	B	601	COA	N8P-C9P-CAP-OAP
3	F	601	COA	C3B-O3B-P3B-O7A
4	L	701	BTI	C2-C7-C8-C9
3	B	601	COA	CCP-O6A-P2A-O3A
3	D	601	COA	C3B-O3B-P3B-O8A
3	F	601	COA	CCP-O6A-P2A-O3A
3	A	601	COA	CBP-CCP-O6A-P2A
3	F	601	COA	CBP-CCP-O6A-P2A
3	A	601	COA	C5B-O5B-P1A-O2A
3	A	601	COA	CCP-O6A-P2A-O4A
3	B	601	COA	CCP-O6A-P2A-O4A
3	C	601	COA	C5B-O5B-P1A-O1A
3	D	601	COA	C5B-O5B-P1A-O1A
3	E	601	COA	C5B-O5B-P1A-O1A
4	G	701	BTI	C11-C10-C9-C8
4	H	701	BTI	C11-C10-C9-C8
4	G	701	BTI	C2-C7-C8-C9

Continued on next page...

Continued from previous page...

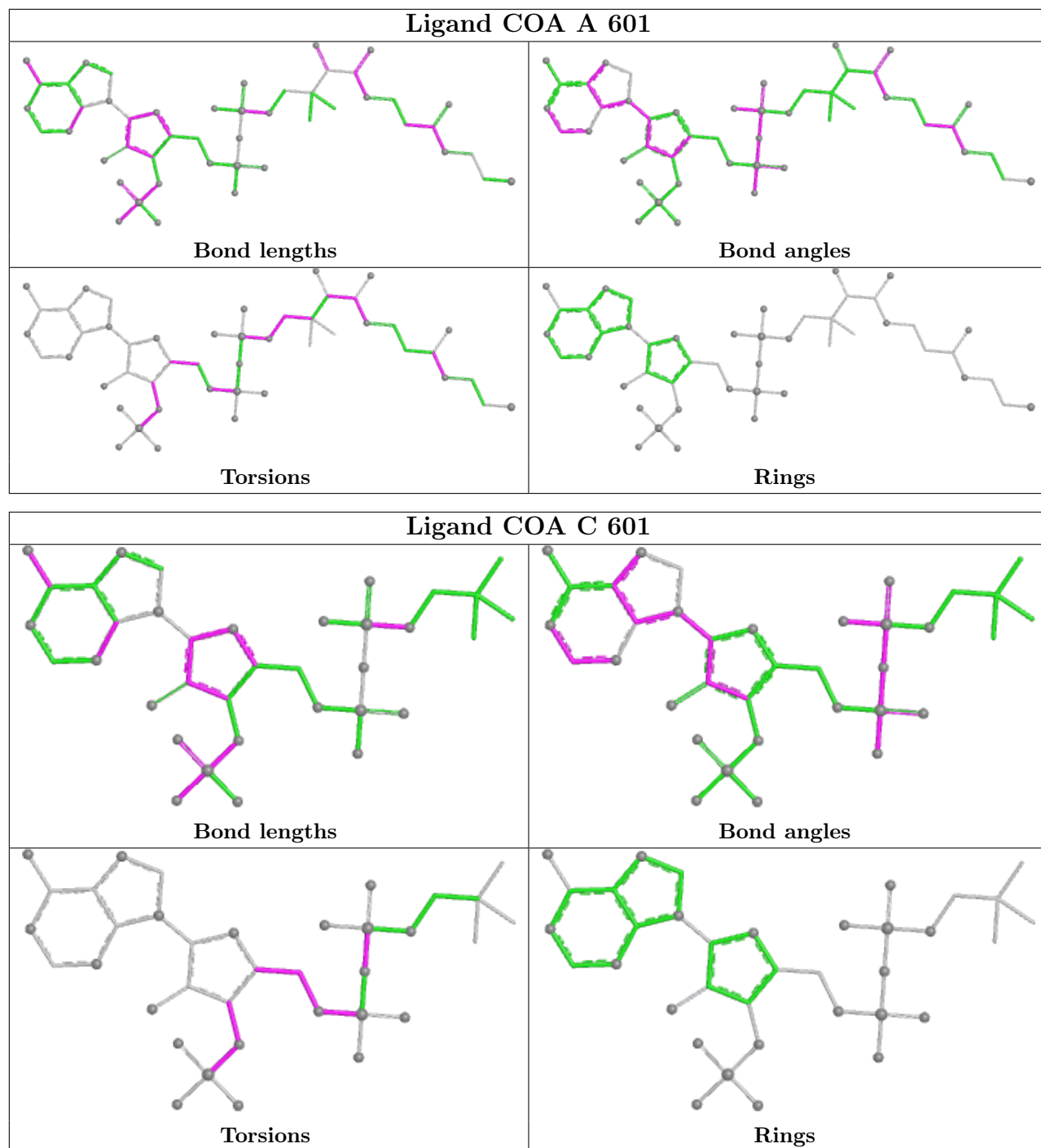
Mol	Chain	Res	Type	Atoms
3	E	601	COA	C4B-C5B-O5B-P1A
3	B	601	COA	O9P-C9P-CAP-CBP
4	H	701	BTI	C2-C7-C8-C9
3	B	601	COA	N8P-C9P-CAP-CBP
4	J	701	BTI	C7-C8-C9-C10
3	C	601	COA	P1A-O3A-P2A-O6A
3	A	601	COA	CCP-O6A-P2A-O3A
3	E	601	COA	C5B-O5B-P1A-O3A
3	C	601	COA	C4B-C5B-O5B-P1A
3	D	601	COA	CCP-O6A-P2A-O4A
3	A	601	COA	O4B-C4B-C5B-O5B

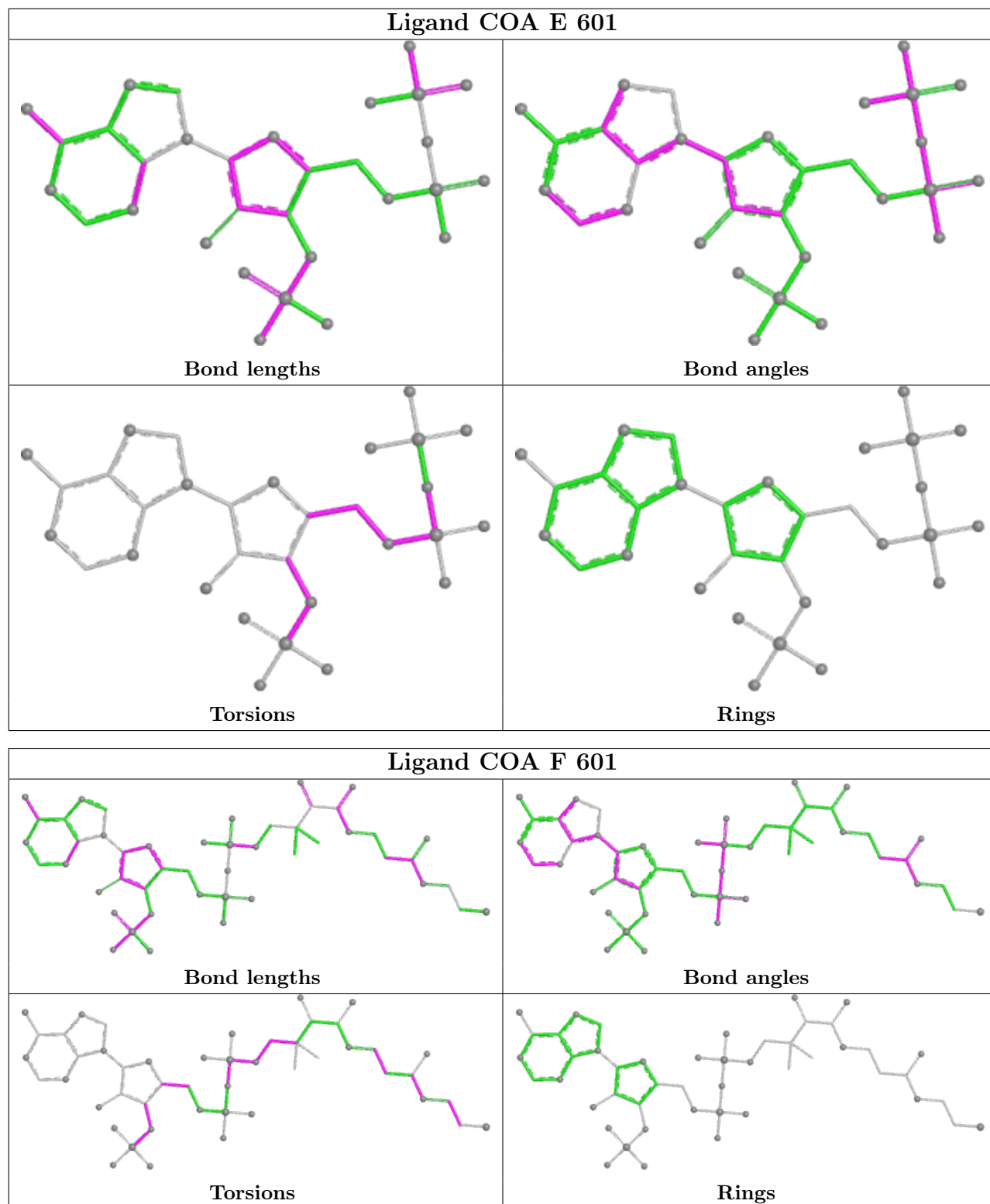
There are no ring outliers.

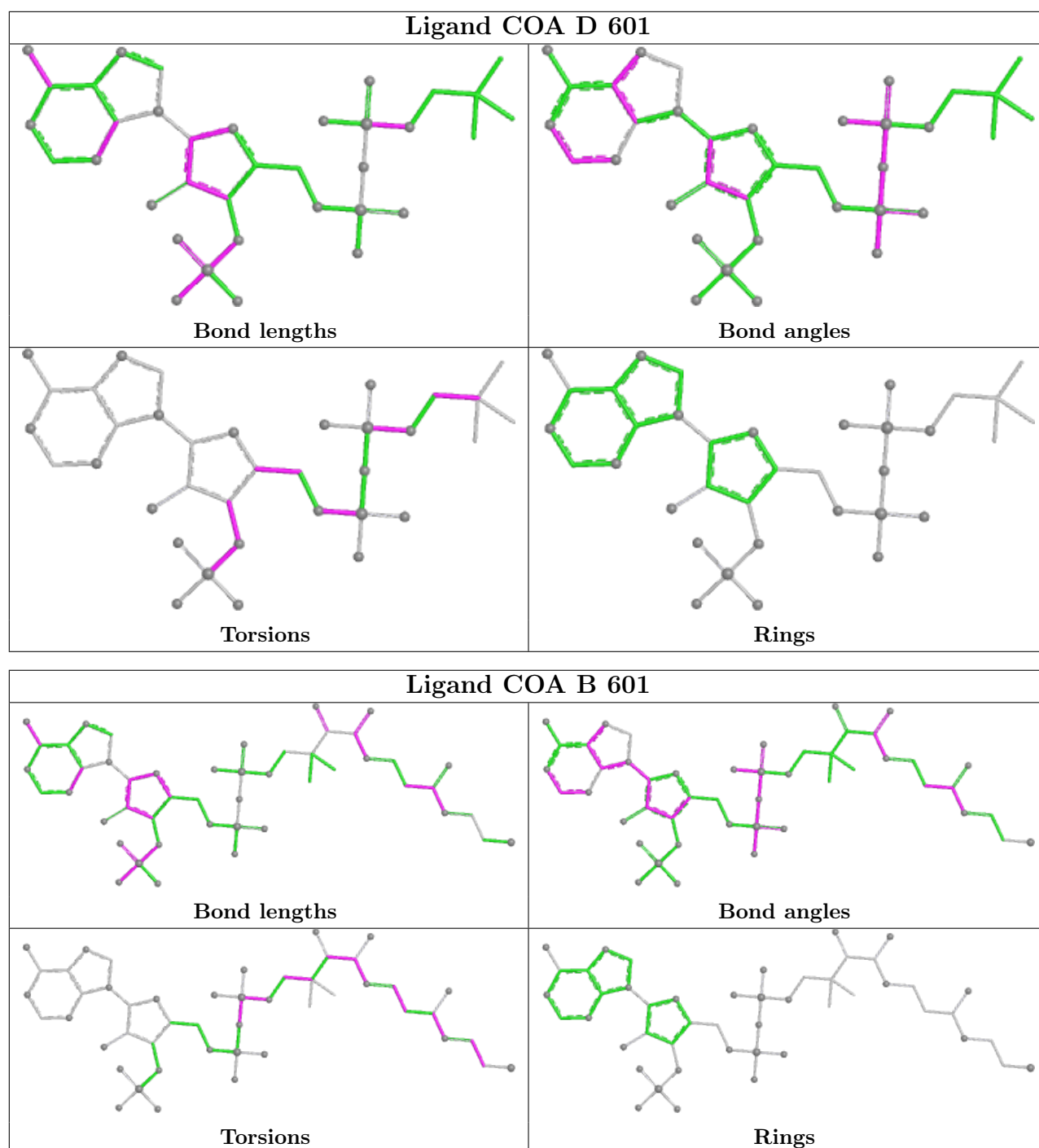
7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	701	BTI	5	0
4	J	701	BTI	1	0
4	K	701	BTI	4	0
3	C	601	COA	1	0
3	E	601	COA	1	0
3	F	601	COA	4	0
3	D	601	COA	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

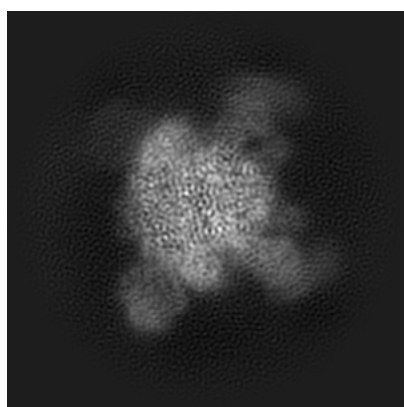
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10770. These allow visual inspection of the internal detail of the map and identification of artifacts.

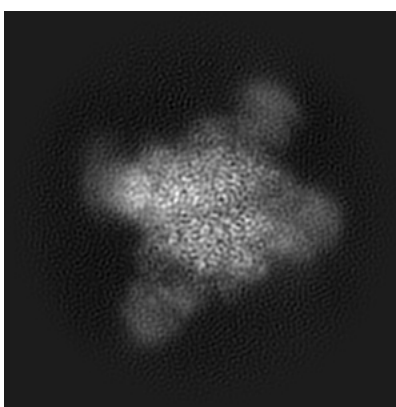
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

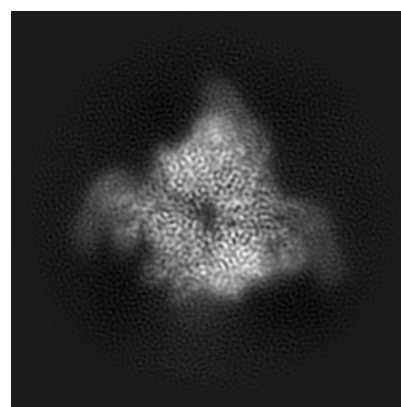
6.1.1 Primary map



X



Y

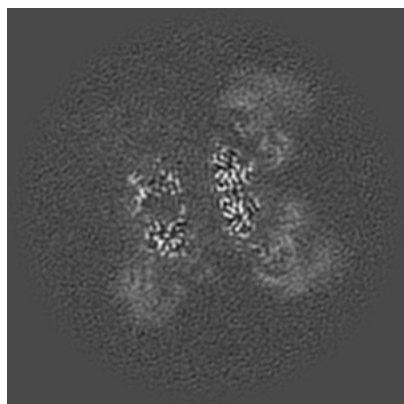


Z

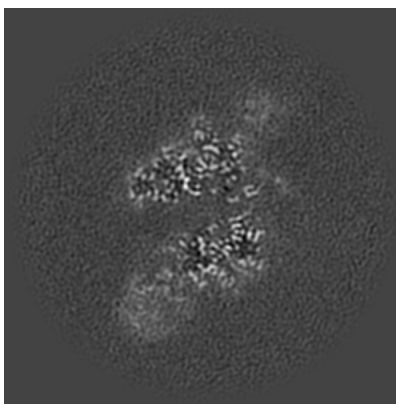
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

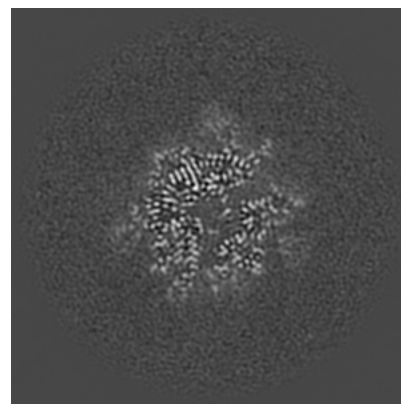
6.2.1 Primary map



X Index: 128



Y Index: 128

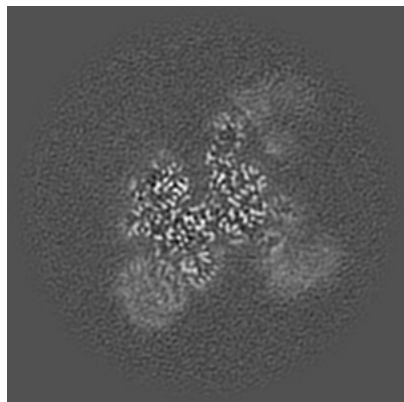


Z Index: 128

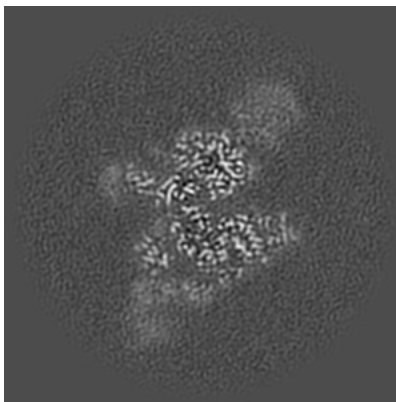
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

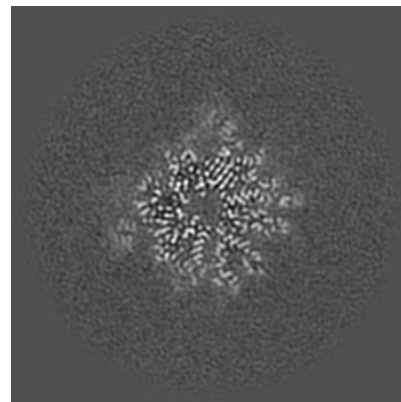
6.3.1 Primary map



X Index: 137



Y Index: 114



Z Index: 122

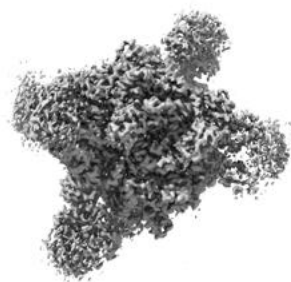
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.23. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

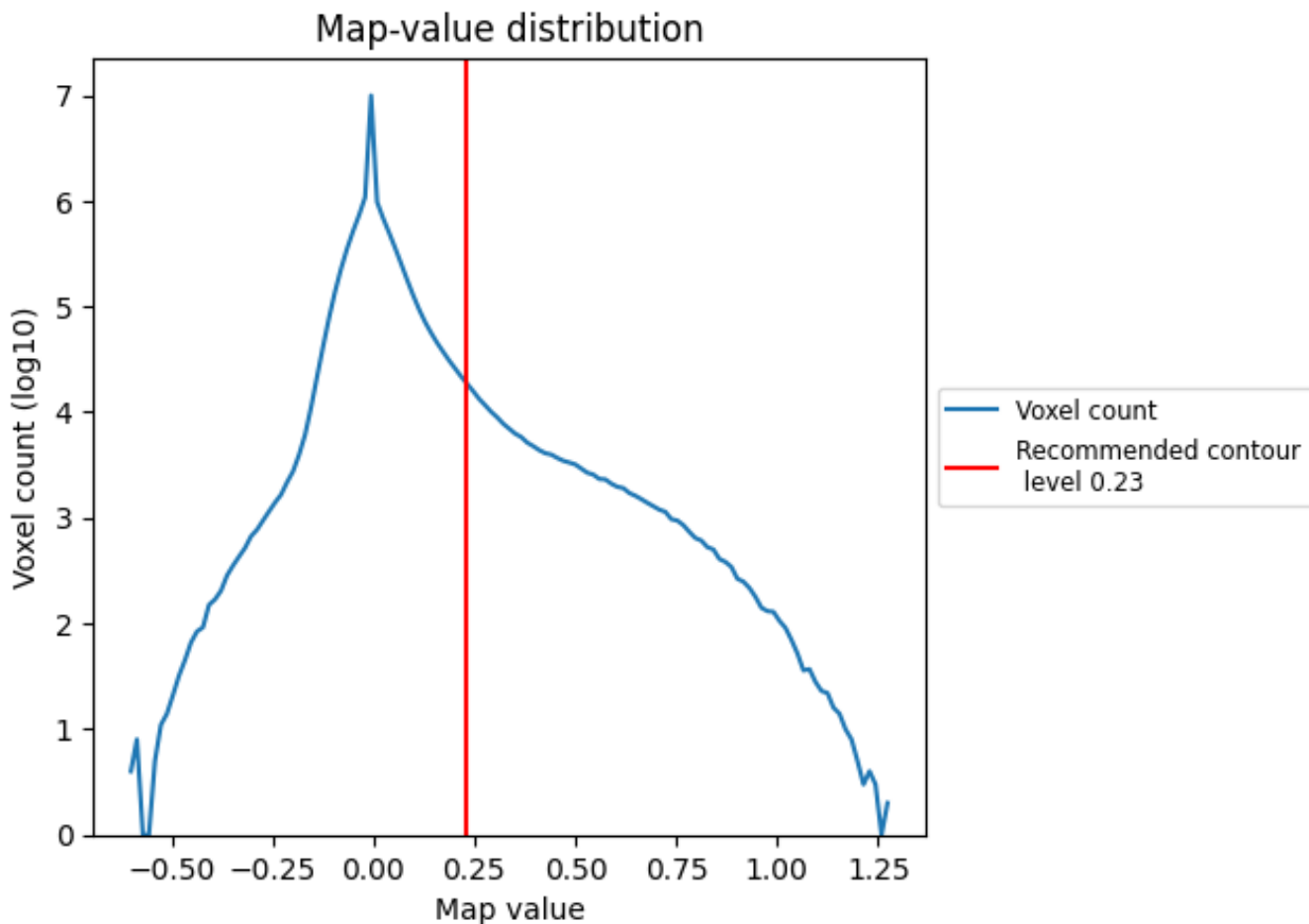
6.5 Mask visualisation

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

7 Map analysis [i](#)

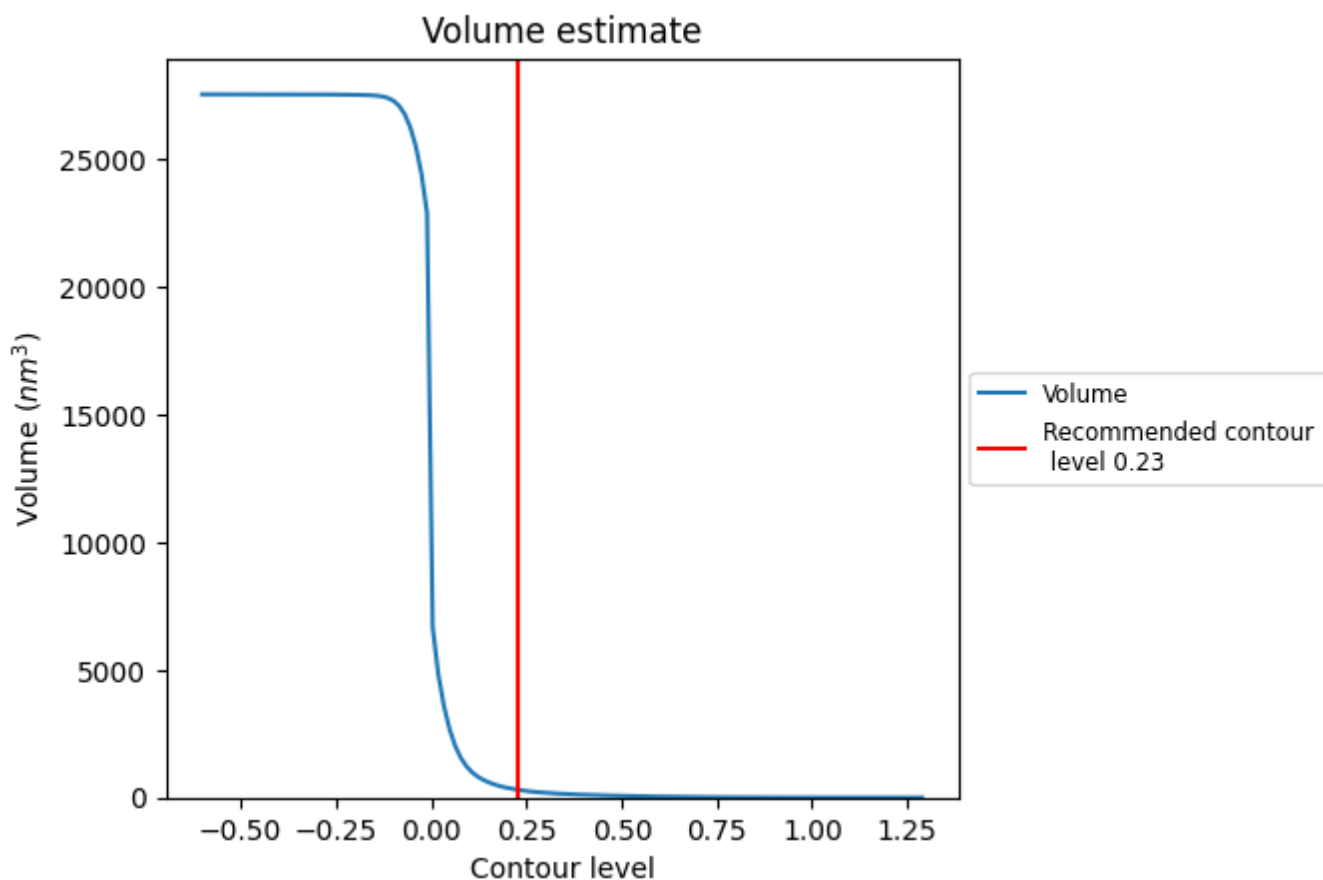
This section contains the results of statistical analysis of the map.

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.

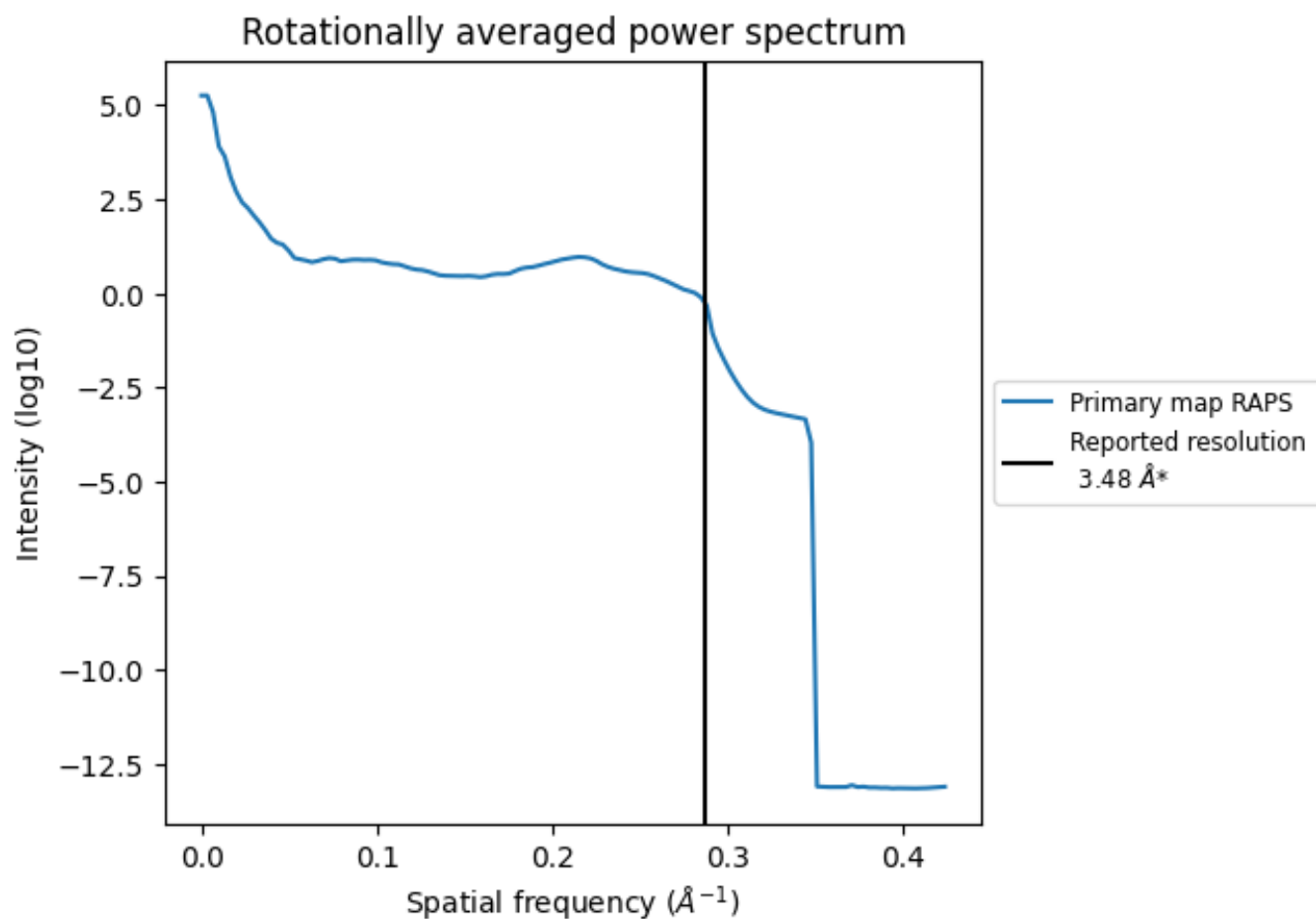
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 299 nm³; this corresponds to an approximate mass of 270 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.287 Å⁻¹

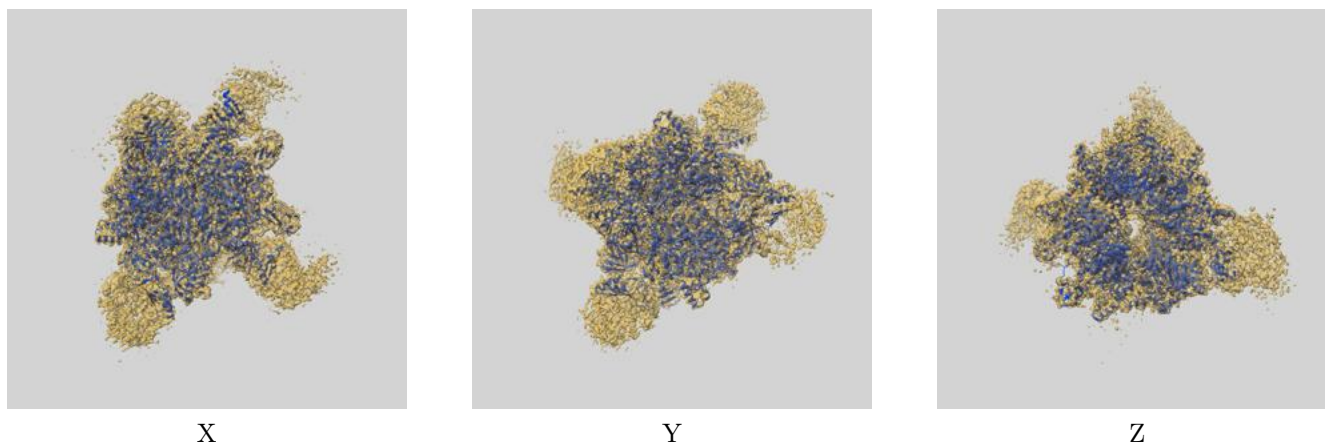
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

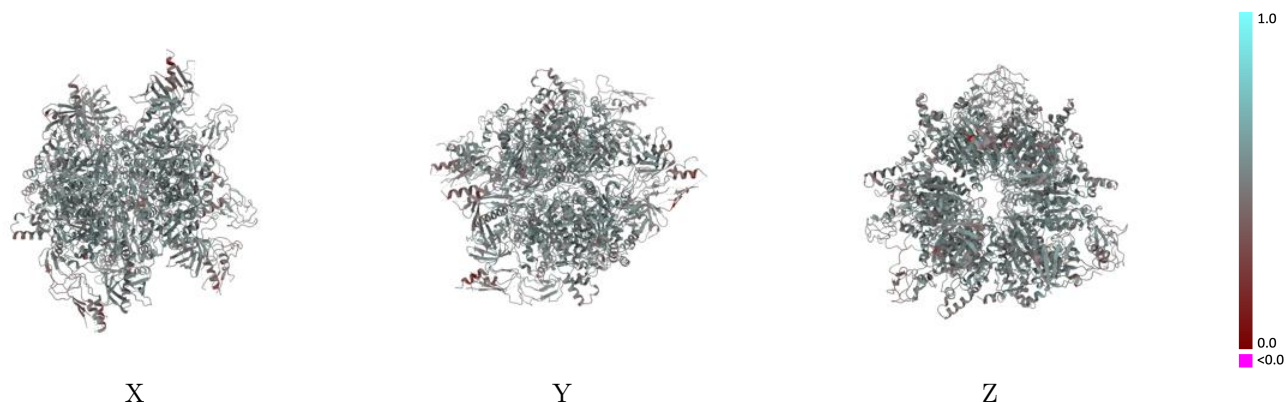
This section contains information regarding the fit between EMDB map EMD-10770 and PDB model 6YBP. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



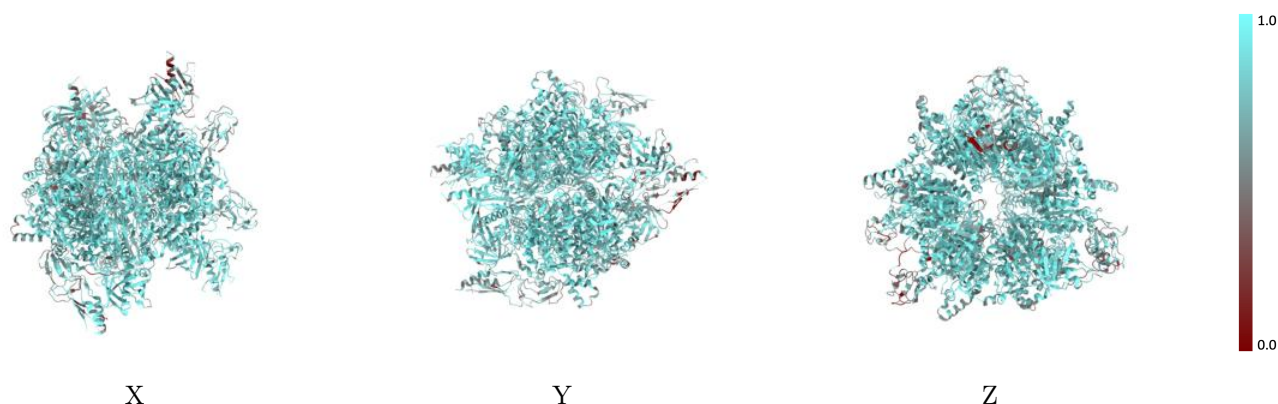
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



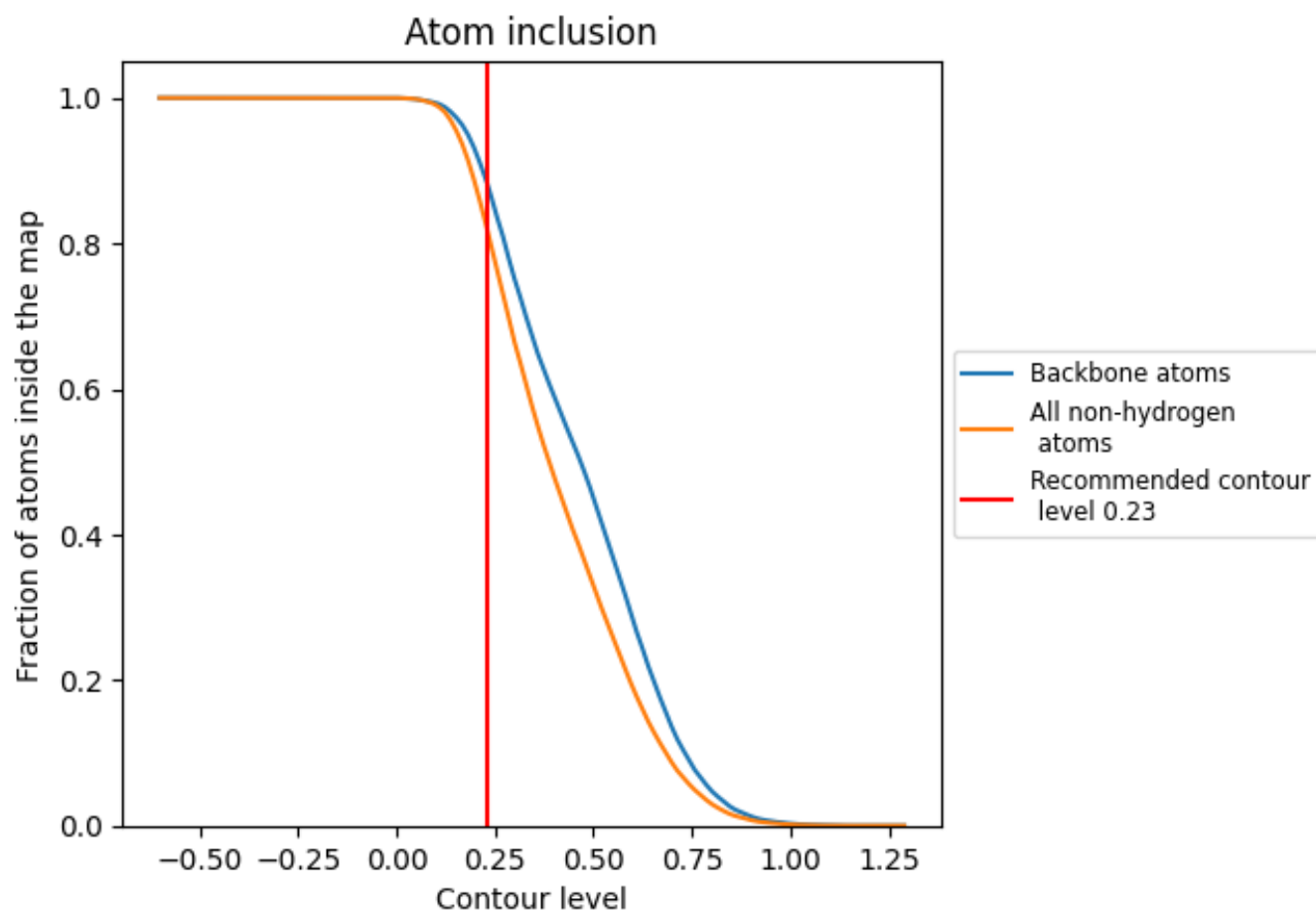
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.23).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 82% 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 (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8198	 0.5110
A	 0.8713	 0.5260
B	 0.8873	 0.5270
C	 0.8652	 0.5260
D	 0.8701	 0.5270
E	 0.8764	 0.5320
F	 0.8821	 0.5300
G	 0.6561	 0.4800
H	 0.6628	 0.4770
I	 0.6972	 0.4910
J	 0.7965	 0.4780
K	 0.7533	 0.4820
L	 0.7086	 0.4760

