



## Full wwPDB EM Validation Report ⓘ

Dec 8, 2025 – 12:16 PM EST

PDB ID : 9O81 / pdb\_00009o81  
EMDB ID : EMD-70214  
Title : Cryo-EM structure of apo rabbit TRPM3 having 2 resting and 2 activated subunits (ortho position) at 37 degrees Celsius  
Authors : Kumar, S.; Lu, W.; Du, J.  
Deposited on : 2025-04-15  
Resolution : 3.96 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](mailto: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) : 2.47

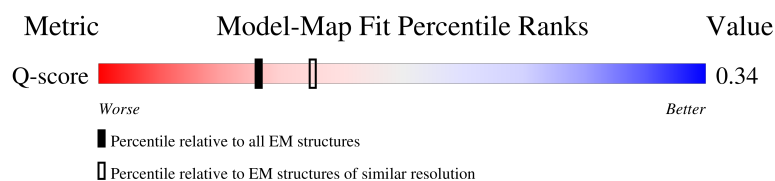
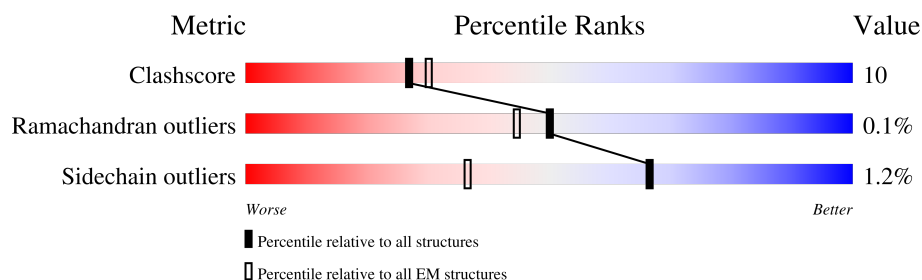
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.96 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	7646 ( 3.46 - 4.46 )

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  $\geq 3$ , 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.

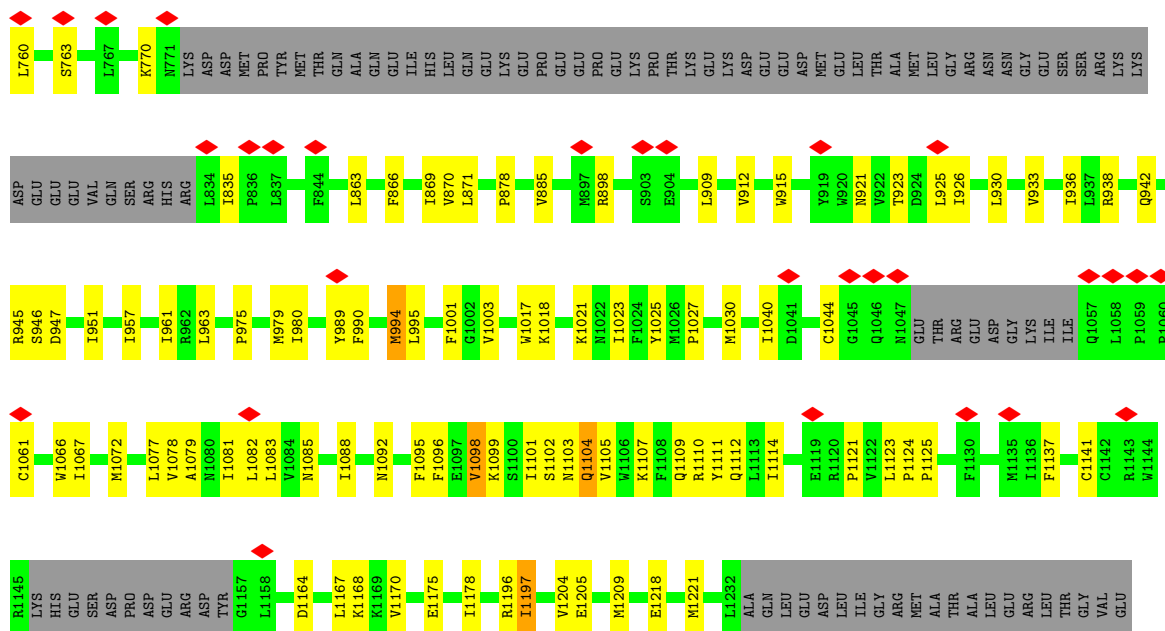
Mol	Chain	Length	Quality of chain
1	A	1306	<div> <div>22%</div> <div>63%</div> <div>15%</div> <div>21%</div> </div>
1	B	1306	<div> <div>17%</div> <div>63%</div> <div>16%</div> <div>21%</div> </div>
1	C	1306	<div> <div>15%</div> <div>61%</div> <div>17%</div> <div>21%</div> </div>
1	D	1306	<div> <div>23%</div> <div>64%</div> <div>14%</div> <div>20%</div> </div>



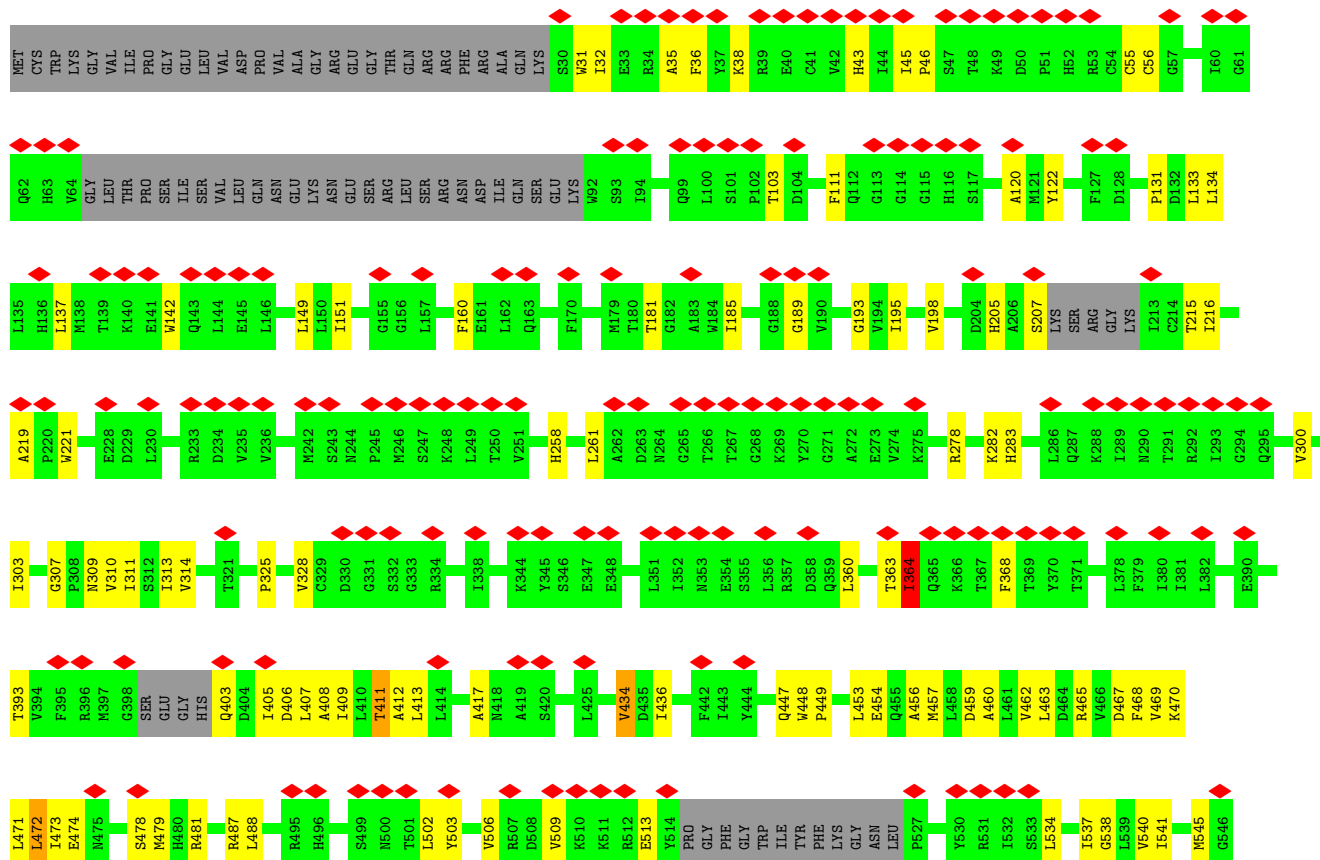
*Continued from previous page...*

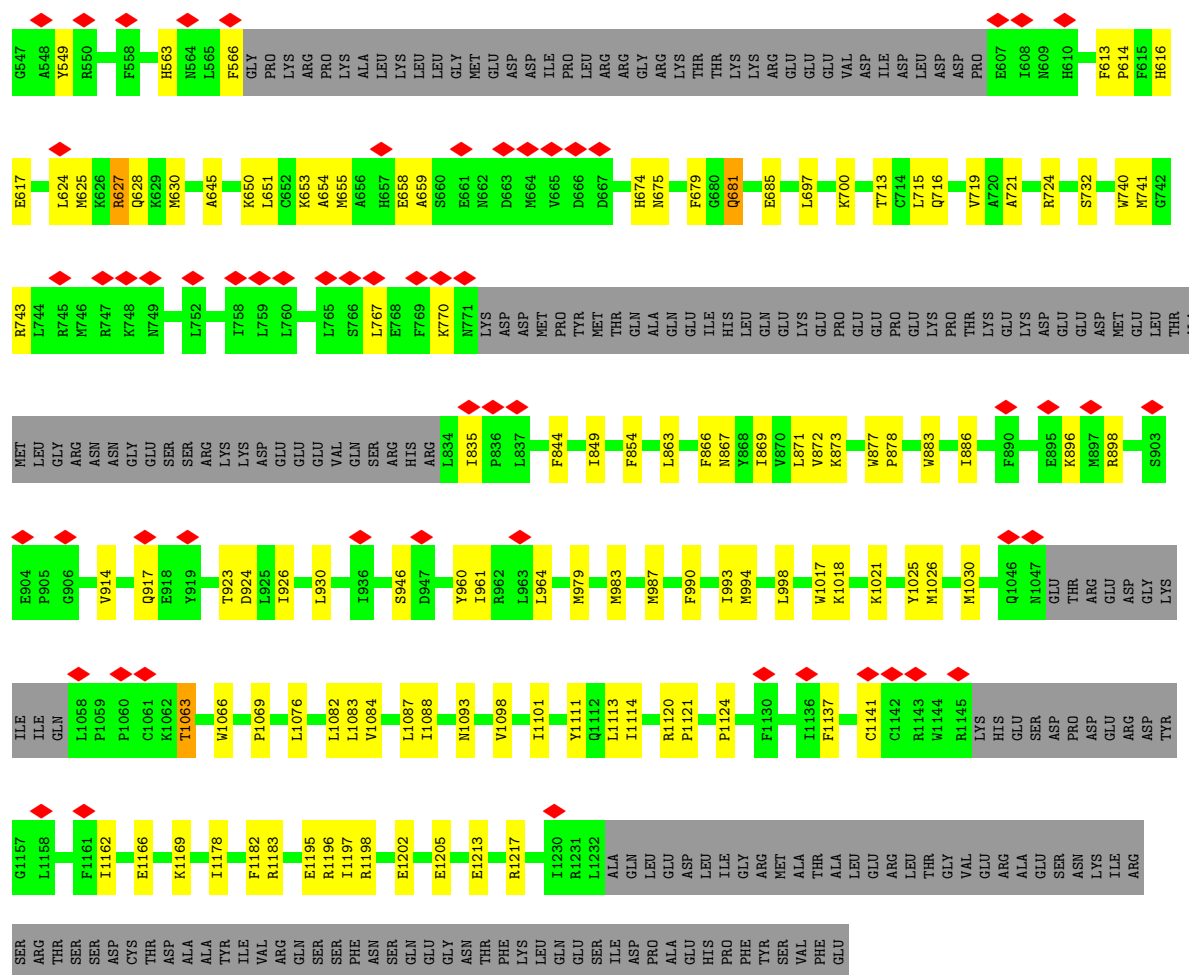
Mol	Chain	Residues	Atoms			AltConf
2	B	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	D	1	Total	C	O	0
			35	31	4	
2	D	1	Total	C	O	0
			35	31	4	
2	D	1	Total	C	O	0
			35	31	4	



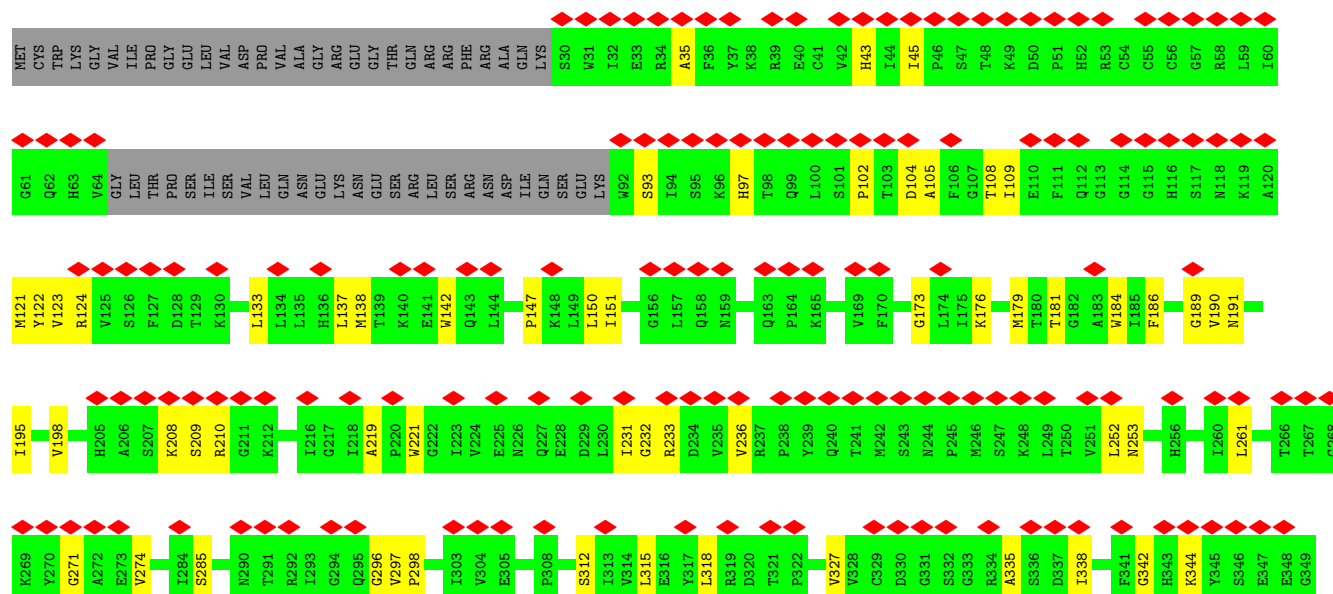


• Molecule 1: TRPM3



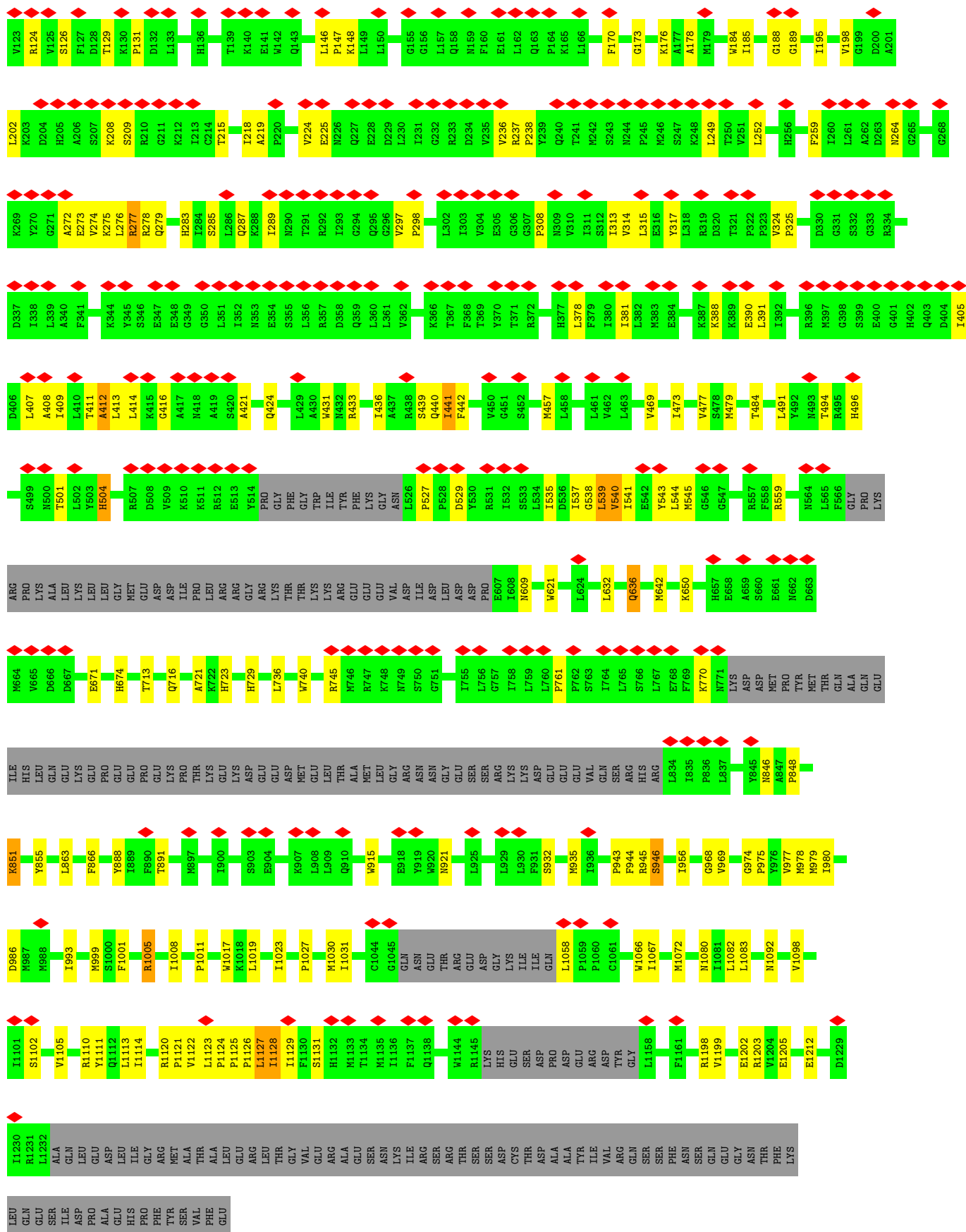


• Molecule 1: TRPM3









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	84256	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.009	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.0025	Depositor
Map size (Å)	317.184, 317.184, 317.184	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: Y01

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	0.44	1/8000 (0.0%)	0.91	8/10896 (0.1%)
1	B	0.50	2/8009 (0.0%)	0.97	13/10891 (0.1%)
1	C	0.49	1/8039 (0.0%)	0.95	9/10932 (0.1%)
1	D	0.49	1/7919 (0.0%)	0.95	14/10793 (0.1%)
All	All	0.48	5/31967 (0.0%)	0.95	44/43512 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	835	ILE	C-N	6.55	1.43	1.33
1	D	761	PRO	C-N	6.22	1.41	1.34
1	B	1026	MET	C-N	5.53	1.42	1.33
1	A	904	GLU	C-N	5.49	1.40	1.33
1	C	835	ILE	C-N	5.32	1.41	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1031	ILE	N-CA-C	-7.60	105.31	112.83
1	A	441	ILE	N-CA-C	-7.50	105.40	112.83
1	A	941	ASP	N-CA-C	7.48	120.18	110.53
1	D	1067	ILE	CA-C-N	7.20	124.78	120.24
1	D	1067	ILE	C-N-CA	7.20	124.78	120.24
1	D	413	LEU	N-CA-C	-6.61	105.75	113.88
1	A	1124	PRO	CB-CA-C	6.42	118.76	110.92
1	A	966	ILE	N-CA-C	-6.37	105.48	112.80
1	A	864	MET	N-CA-C	-6.35	106.16	114.04
1	A	440	GLN	N-CA-C	6.27	124.15	110.80
1	B	627	ARG	CA-C-N	6.04	128.65	120.38
1	B	627	ARG	C-N-CA	6.04	128.65	120.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1125	PRO	N-CA-C	5.92	117.92	110.70
1	B	411	THR	N-CA-C	-5.79	104.88	111.07
1	B	1063	THR	N-CA-C	-5.76	100.76	108.19
1	D	537	ILE	N-CA-C	-5.74	104.76	110.62
1	B	406	ASP	N-CA-C	-5.70	104.76	110.97
1	B	364	ILE	N-CA-C	-5.69	104.33	112.35
1	C	731	CYS	CB-CA-C	-5.68	101.96	110.88
1	C	627	ARG	CA-C-N	5.67	129.32	120.82
1	C	627	ARG	C-N-CA	5.67	129.32	120.82
1	B	45	ILE	N-CA-C	5.61	121.00	108.88
1	B	741	MET	N-CA-C	-5.56	106.45	113.18
1	D	729	HIS	CA-C-N	5.53	127.96	120.38
1	D	729	HIS	C-N-CA	5.53	127.96	120.38
1	B	434	VAL	CA-C-N	5.46	127.86	120.38
1	B	434	VAL	C-N-CA	5.46	127.86	120.38
1	B	479	MET	CA-C-N	5.37	127.73	120.38
1	B	479	MET	C-N-CA	5.37	127.73	120.38
1	D	1082	LEU	N-CA-C	5.36	116.81	110.97
1	C	723	HIS	CA-C-N	5.35	127.45	120.28
1	C	723	HIS	C-N-CA	5.35	127.45	120.28
1	C	1067	ILE	CA-C-N	5.35	123.61	120.24
1	C	1067	ILE	C-N-CA	5.35	123.61	120.24
1	D	439	SER	N-CA-C	-5.35	107.30	113.88
1	D	723	HIS	CA-C-N	5.34	127.75	120.54
1	D	723	HIS	C-N-CA	5.34	127.75	120.54
1	A	636	GLN	N-CA-C	-5.27	106.82	113.20
1	D	412	ALA	N-CA-C	-5.16	106.95	113.20
1	D	851	LYS	CB-CG-CD	-5.10	99.57	111.30
1	D	313	ILE	N-CA-C	-5.07	104.64	111.44
1	D	539	LEU	N-CA-C	-5.07	105.66	111.14
1	B	681	GLN	N-CA-C	-5.03	105.88	111.36
1	C	621	TRP	N-CA-C	5.02	117.40	111.33

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	7818	0	7458	155	0
1	B	7835	0	7473	163	0
1	C	7863	0	7557	169	0
1	D	7740	0	7291	145	0
2	A	105	0	147	8	0
2	B	105	0	147	5	0
2	C	105	0	147	5	0
2	D	105	0	147	9	0
All	All	31676	0	30367	603	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 10.

All (603) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:VAL:CG2	1:B:471:LEU:HD11	1.67	1.24
1:D:237:ARG:CD	1:D:238:PRO:HD2	1.75	1.17
1:D:237:ARG:HD3	1:D:238:PRO:HD2	1.23	1.14
1:D:1124:PRO:HB2	1:D:1127:LEU:HB2	1.40	1.02
1:D:440:GLN:HG3	1:D:441:ILE:H	1.21	1.02
1:C:541:ILE:O	1:C:545:MET:HB3	1.61	1.00
1:C:170:PHE:HE1	1:C:302:LEU:HD21	1.26	0.98
1:D:851:LYS:HD3	1:D:1122:VAL:HG13	1.47	0.96
1:B:434:VAL:CG2	1:B:471:LEU:CD1	2.43	0.95
1:D:237:ARG:HD3	1:D:238:PRO:CD	1.97	0.94
1:C:1197:ILE:HD11	1:B:1197:ILE:HD12	1.49	0.93
1:B:434:VAL:HG22	1:B:471:LEU:HD11	1.47	0.93
1:A:1199:VAL:CG1	1:A:1203:ARG:HE	1.83	0.91
1:B:867:ASN:HD22	2:A:1403:Y01:HAO1	1.32	0.90
1:D:424:GLN:HB3	1:D:441:ILE:HD12	1.52	0.89
1:B:407:LEU:HB3	1:B:436:ILE:HG12	1.56	0.88
1:B:434:VAL:HG23	1:B:471:LEU:CD1	2.04	0.87
1:B:405:ILE:HA	1:B:408:ALA:HB3	1.57	0.87
1:C:1082:LEU:HD23	1:C:1083:LEU:HD23	1.57	0.87
1:C:994:MET:HE1	1:C:1079:ALA:CB	2.07	0.83
1:A:1199:VAL:O	1:A:1203:ARG:HG3	1.80	0.81
1:D:1123:LEU:HD12	1:D:1131:SER:HB3	1.64	0.80
1:A:1123:LEU:HD12	1:A:1130:PHE:HB2	1.62	0.79
1:C:994:MET:CE	1:C:1079:ALA:HB1	2.12	0.79
1:B:31:TRP:O	1:B:35:ALA:HB3	1.83	0.78
1:D:440:GLN:HG3	1:D:441:ILE:N	1.99	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:LEU:HD21	1:D:436:ILE:HB	1.65	0.76
1:A:208:LYS:O	1:A:208:LYS:HG2	1.87	0.75
1:C:994:MET:HE1	1:C:1079:ALA:HA	1.69	0.74
1:C:170:PHE:CE1	1:C:302:LEU:HD21	2.18	0.74
1:C:1003:VAL:HG11	1:D:956:ILE:HD13	1.71	0.73
1:C:31:TRP:O	1:C:35:ALA:HB3	1.89	0.73
1:C:1077:LEU:HD12	1:C:1081:ILE:HD12	1.71	0.73
1:C:560:THR:O	1:C:564:ASN:HB2	1.89	0.72
1:B:413:LEU:O	1:B:417:ALA:HB3	1.90	0.71
1:D:208:LYS:O	1:D:208:LYS:HG2	1.91	0.71
1:A:1138:GLN:HA	1:A:1142:CYS:H	1.55	0.71
1:A:1029:TRP:HB2	1:A:1036:PHE:HE2	1.55	0.71
1:A:1085:ASN:HA	1:A:1088:ILE:HG12	1.71	0.71
1:C:646:LEU:HD11	1:C:726:PHE:HE2	1.56	0.70
1:B:681:GLN:HE21	1:B:685:GLU:HG3	1.57	0.69
1:A:433:ARG:O	1:A:436:ILE:HG12	1.92	0.69
1:D:414:LEU:HB3	1:D:440:GLN:HG2	1.75	0.69
1:C:479:MET:HE3	1:C:483:LEU:HB2	1.75	0.68
1:D:412:ALA:O	1:D:416:GLY:HA3	1.94	0.68
1:D:846:ASN:HA	1:D:1122:VAL:HG11	1.75	0.68
1:C:898:ARG:HH22	1:C:1121:PRO:HD3	1.59	0.68
1:C:534:LEU:HA	1:C:537:ILE:HG12	1.76	0.68
1:B:743:ARG:HE	1:B:770:LYS:HB2	1.59	0.68
1:B:149:LEU:HD21	1:B:409:ILE:HG21	1.76	0.68
1:B:403:GLN:HA	1:B:407:LEU:HD21	1.75	0.67
1:B:454:GLU:HB3	1:B:487:ARG:HH12	1.59	0.67
1:C:994:MET:HE1	1:C:1079:ALA:CA	2.24	0.67
1:B:624:LEU:HA	1:B:655:MET:HE1	1.77	0.67
1:C:565:LEU:HD13	1:C:608:ILE:HD12	1.75	0.67
1:B:434:VAL:HG23	1:B:471:LEU:HD12	1.73	0.66
1:D:848:PRO:HA	1:D:851:LYS:HE2	1.77	0.66
1:C:1017:TRP:HB3	2:C:1401:Y01:HAR2	1.77	0.66
1:B:871:LEU:HD21	1:A:1023:ILE:HD11	1.78	0.65
1:A:636:GLN:HG2	1:A:1182:PHE:CZ	2.31	0.65
1:A:636:GLN:HG2	1:A:1182:PHE:CE2	2.31	0.65
1:B:987:MET:HE1	1:A:1081:ILE:HG22	1.79	0.65
1:D:740:TRP:HB2	1:D:1114:ILE:HD12	1.79	0.65
1:A:1199:VAL:HG12	1:A:1203:ARG:HE	1.58	0.65
1:D:314:VAL:HA	1:D:317:TYR:HB2	1.78	0.64
1:C:1196:ARG:NH1	1:B:1198:ARG:HG3	2.12	0.64
1:B:993:ILE:HG22	1:B:1083:LEU:HD21	1.80	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:ASP:O	1:C:463:LEU:HB2	1.98	0.64
1:C:668:ILE:O	1:C:672:LEU:HB2	1.97	0.64
1:B:1069:PRO:HB2	2:B:1401:Y01:HAE3	1.79	0.64
1:D:440:GLN:CG	1:D:441:ILE:H	2.04	0.64
1:B:360:LEU:O	1:B:364:ILE:HB	1.97	0.63
1:A:1129:ILE:O	1:A:1132:HIS:N	2.27	0.63
1:B:133:LEU:O	1:B:137:LEU:HB2	1.97	0.63
1:C:151:ILE:HD11	1:C:302:LEU:HB2	1.80	0.63
1:C:488:LEU:HD12	1:C:491:LEU:HD11	1.81	0.63
1:B:46:PRO:HD2	1:B:55:CYS:HB2	1.79	0.63
1:A:465:ARG:HB3	1:A:468:PHE:HB2	1.80	0.63
1:A:1199:VAL:HG13	1:A:1203:ARG:HE	1.62	0.63
1:B:1088:ILE:HD12	1:A:1088:ILE:HG13	1.80	0.63
1:B:434:VAL:HG21	1:B:471:LEU:HD11	1.77	0.63
1:B:471:LEU:O	1:B:472:LEU:C	2.40	0.63
1:C:493:ASN:HD21	1:C:531:ARG:HH11	1.47	0.62
1:C:479:MET:HE2	1:C:618:LEU:HD11	1.82	0.62
1:C:1082:LEU:CD2	1:C:1083:LEU:HD23	2.29	0.62
1:C:1095:PHE:HE2	1:B:1093:ASN:HB2	1.63	0.62
1:D:538:GLY:O	1:D:541:ILE:HB	2.00	0.62
1:B:1021:LYS:O	1:B:1025:TYR:HB2	1.99	0.62
1:A:1129:ILE:O	1:A:1130:PHE:C	2.42	0.62
1:C:289:ILE:HG23	1:C:292:ARG:H	1.65	0.62
1:A:505:LEU:HD23	1:A:544:LEU:HD21	1.82	0.62
1:C:500:ASN:HB3	1:C:502:LEU:H	1.64	0.61
1:A:1029:TRP:HB2	1:A:1036:PHE:CE2	2.35	0.61
1:D:237:ARG:HD2	1:D:238:PRO:HD2	1.80	0.61
1:B:1017:TRP:HB3	2:B:1402:Y01:HAR2	1.81	0.61
1:D:433:ARG:O	1:D:436:ILE:HG12	2.00	0.61
1:A:1210:ARG:HH12	1:D:1212:GLU:HA	1.65	0.61
1:D:866:PHE:HD1	1:D:956:ILE:HD12	1.64	0.61
1:A:1127:LEU:O	1:A:1129:ILE:N	2.34	0.61
1:C:994:MET:HE3	1:C:1079:ALA:HB1	1.82	0.60
1:C:1085:ASN:HA	1:C:1088:ILE:HG12	1.83	0.60
1:A:655:MET:HB2	1:A:672:LEU:HD21	1.84	0.60
1:B:541:ILE:O	1:B:545:MET:HB3	2.01	0.60
1:A:1127:LEU:C	1:A:1129:ILE:N	2.57	0.60
1:B:216:ILE:HG13	1:B:258:HIS:HB2	1.84	0.60
1:C:994:MET:CE	1:C:1079:ALA:CB	2.75	0.59
1:C:619:MET:HE3	1:C:644:LYS:HD2	1.84	0.59
1:D:1066:TRP:HB2	2:D:1401:Y01:HAD1	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:GLU:H	1:A:938:ARG:HH22	1.48	0.58
1:B:960:TYR:HD2	1:A:1000:SER:HA	1.66	0.58
1:A:509:VAL:HG21	1:A:540:VAL:HG22	1.85	0.58
1:A:1093:ASN:C	1:A:1095:PHE:H	2.11	0.58
1:D:126:SER:HB3	1:D:129:THR:HG23	1.85	0.58
1:C:550:ARG:HH12	1:C:554:THR:C	2.12	0.58
1:C:1066:TRP:HB2	2:C:1403:Y01:HAD1	1.84	0.58
1:C:1137:PHE:O	1:C:1141:CYS:HB3	2.02	0.58
1:C:560:THR:O	1:C:564:ASN:CB	2.52	0.58
1:D:237:ARG:CG	1:D:238:PRO:HD2	2.31	0.58
1:B:654:ALA:O	1:B:658:GLU:HB2	2.04	0.58
1:A:1128:ILE:O	1:A:1129:ILE:C	2.47	0.58
1:B:1197:ILE:HD11	1:A:1197:ILE:HG12	1.84	0.58
1:D:713:THR:HB	1:D:716:GLN:HG3	1.86	0.58
1:B:650:LYS:HB2	1:B:721:ALA:HB2	1.86	0.57
1:A:1129:ILE:O	1:A:1131:SER:N	2.37	0.57
1:C:754:VAL:O	1:C:758:ILE:HB	2.03	0.57
1:A:1124:PRO:HG2	1:A:1127:LEU:HD13	1.87	0.57
1:B:407:LEU:O	1:B:411:THR:N	2.25	0.57
1:A:866:PHE:HA	1:A:869:ILE:HG22	1.86	0.57
1:D:264:ASN:HB3	1:D:272:ALA:HB2	1.87	0.57
1:C:149:LEU:HB3	1:C:183:ALA:HB2	1.86	0.57
1:C:361:LEU:HD22	1:C:375:ALA:HB1	1.86	0.57
1:A:862:TYR:HH	1:A:959:TRP:CG	2.23	0.57
1:D:424:GLN:HB3	1:D:441:ILE:CD1	2.32	0.57
1:A:410:LEU:HA	1:A:413:LEU:HD12	1.87	0.57
1:C:142:TRP:HZ3	1:C:258:HIS:HB3	1.69	0.56
1:B:462:VAL:HA	1:B:627:ARG:HH12	1.70	0.56
1:B:405:ILE:HA	1:B:408:ALA:CB	2.32	0.56
1:C:915:TRP:HH2	1:C:925:LEU:HB2	1.70	0.56
1:C:1204:VAL:HG12	1:D:1203:ARG:NH1	2.20	0.56
1:A:108:THR:HB	1:A:236:VAL:HG22	1.88	0.56
1:C:327:VAL:HG21	1:C:408:ALA:HB1	1.86	0.56
1:D:891:THR:HB	1:D:1128:ILE:HG13	1.87	0.56
1:A:650:LYS:HD3	1:A:721:ALA:HA	1.86	0.56
1:B:471:LEU:O	1:B:474:GLU:N	2.39	0.56
2:B:1402:Y01:HBFB	2:A:1401:Y01:HAS1	1.87	0.56
1:A:485:ILE:HG12	1:A:609:ASN:HA	1.86	0.56
1:A:935:MET:HG3	1:A:939:LEU:HD23	1.87	0.56
1:C:410:LEU:HB2	1:C:436:ILE:HD13	1.88	0.55
1:C:1205:GLU:HA	1:D:1203:ARG:HH12	1.70	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:994:MET:HE1	1:C:1079:ALA:HB1	1.74	0.55
1:B:403:GLN:HB3	1:B:407:LEU:HD11	1.88	0.55
1:C:1001:PHE:HD2	1:C:1027:PRO:HB3	1.71	0.55
1:D:745:ARG:HH21	1:D:770:LYS:HA	1.71	0.55
1:D:888:TYR:HD2	1:D:1126:PRO:HB3	1.71	0.55
1:D:484:THR:HB	1:D:609:ASN:HB3	1.89	0.55
1:D:632:LEU:HD23	1:D:636:GLN:HE21	1.72	0.55
1:C:691:TYR:HD2	1:C:731:CYS:SG	2.30	0.54
1:A:998:LEU:HA	1:A:1075:TYR:HE2	1.71	0.54
1:C:1123:LEU:HD12	1:C:1124:PRO:HD2	1.89	0.54
1:A:1138:GLN:O	1:A:1139:HIS:C	2.49	0.54
1:D:494:THR:HG22	1:D:496:HIS:H	1.72	0.54
1:C:699:MET:HE1	1:C:731:CYS:SG	2.48	0.54
1:B:137:LEU:HD23	1:B:142:TRP:CZ3	2.42	0.54
1:B:456:ALA:O	1:B:460:ALA:HB2	2.07	0.54
1:D:1017:TRP:HB3	2:D:1402:Y01:HAR2	1.88	0.54
1:C:187:THR:HB	1:C:195:ILE:HD12	1.90	0.54
1:B:38:LYS:HB3	1:B:103:THR:HA	1.89	0.54
1:B:724:ARG:HH12	1:B:1101:ILE:HG13	1.72	0.54
1:D:979:MET:HG3	1:D:1098:VAL:HG12	1.89	0.54
1:C:1102:SER:HA	1:C:1105:VAL:HG12	1.90	0.54
1:C:1218:GLU:O	1:C:1221:MET:HB2	2.08	0.54
1:D:440:GLN:O	1:D:442:PHE:N	2.41	0.54
1:A:1093:ASN:C	1:A:1095:PHE:N	2.63	0.54
1:C:946:SER:HB3	1:B:1063:THR:HG23	1.89	0.54
1:B:447:GLN:HG3	1:B:449:PRO:HD3	1.90	0.54
1:D:308:PRO:HB3	1:D:378:LEU:HD21	1.89	0.54
1:D:436:ILE:O	1:D:440:GLN:HB3	2.08	0.53
1:C:226:ASN:HB3	1:C:229:ASP:HB3	1.89	0.53
1:C:691:TYR:HD2	1:C:731:CYS:HG	1.55	0.53
1:A:271:GLY:HA2	1:A:274:VAL:HG22	1.90	0.53
1:A:1134:THR:OG1	1:A:1135:MET:N	2.41	0.53
1:D:195:ILE:HA	1:D:198:VAL:HG22	1.88	0.53
1:B:509:VAL:O	1:B:513:GLU:CB	2.56	0.53
1:A:147:PRO:HG2	1:A:297:VAL:HG11	1.90	0.53
1:A:895:GLU:HA	1:A:1132:HIS:HE1	1.73	0.53
1:C:1078:VAL:O	1:C:1082:LEU:HB3	2.09	0.53
1:C:1082:LEU:HD21	1:D:980:ILE:HG23	1.90	0.53
1:B:645:ALA:HA	1:B:679:PHE:HE1	1.74	0.53
1:A:189:GLY:HA3	1:A:219:ALA:HB2	1.90	0.53
1:A:285:SER:O	1:A:296:GLY:HA3	2.09	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ILE:HA	1:C:198:VAL:HG12	1.91	0.53
1:C:435:ASP:HA	1:C:438:ARG:HG2	1.91	0.53
1:B:502:LEU:HD13	1:B:625:MET:HG2	1.90	0.53
1:A:404:ASP:HB3	1:A:407:LEU:HB2	1.91	0.53
1:D:650:LYS:HD3	1:D:721:ALA:HA	1.90	0.53
1:C:757:GLY:HA2	1:C:763:SER:HB3	1.90	0.53
1:C:220:PRO:HB2	1:C:223:ILE:HG12	1.90	0.52
1:A:1127:LEU:C	1:A:1129:ILE:H	2.17	0.52
1:D:993:ILE:HG22	1:D:1083:LEU:HD21	1.91	0.52
1:C:1092:ASN:HD22	1:D:1092:ASN:HD21	1.55	0.52
1:C:541:ILE:O	1:C:545:MET:CB	2.47	0.52
1:C:424:GLN:HB3	1:C:441:ILE:HD12	1.92	0.52
1:A:687:LEU:HD13	1:A:702:LEU:HD21	1.91	0.52
1:A:871:LEU:HB3	1:D:1019:LEU:HD13	1.92	0.52
1:D:275:LYS:O	1:D:279:GLN:N	2.30	0.52
1:B:195:ILE:HA	1:B:198:VAL:HG22	1.92	0.52
1:D:1027:PRO:HA	1:D:1030:MET:HG3	1.92	0.52
1:D:1199:VAL:HG22	1:D:1203:ARG:HD2	1.91	0.52
1:B:407:LEU:O	1:B:411:THR:HG23	2.10	0.52
1:D:1128:ILE:HG22	1:D:1131:SER:HB2	1.92	0.52
1:A:318:LEU:HD11	1:A:392:ILE:HD11	1.92	0.52
1:D:105:ALA:HB3	1:D:124:ARG:HD2	1.91	0.52
1:D:148:LYS:HA	1:D:289:ILE:HD11	1.91	0.52
1:A:221:TRP:HA	1:A:261:LEU:HD12	1.92	0.51
1:B:946:SER:HB2	1:A:1063:THR:HG21	1.91	0.51
1:C:149:LEU:HD13	1:C:413:LEU:HD12	1.92	0.51
1:C:1110:ARG:O	1:C:1114:ILE:HG12	2.11	0.51
1:B:871:LEU:HD23	1:A:1019:LEU:HB3	1.93	0.51
1:B:310:VAL:HG12	1:B:313:ILE:HD12	1.91	0.51
1:B:325:PRO:HB2	1:B:412:ALA:HB1	1.91	0.51
1:A:484:THR:HG22	1:A:609:ASN:HD22	1.74	0.51
1:C:994:MET:SD	1:C:1083:LEU:HD12	2.51	0.51
1:D:178:ALA:HB2	1:D:185:ILE:HD11	1.92	0.51
1:C:1082:LEU:CD2	1:C:1083:LEU:CD2	2.88	0.51
1:B:1183:ARG:NH1	1:A:209:SER:N	2.59	0.51
1:C:933:VAL:HA	1:C:936:ILE:HG22	1.90	0.51
1:B:1018:LYS:HE2	2:B:1402:Y01:HAR1	1.93	0.51
1:B:467:ASP:O	1:B:471:LEU:HG	2.11	0.51
1:B:1213:GLU:O	1:B:1217:ARG:HB2	2.11	0.51
1:C:308:PRO:HD3	1:C:368:PHE:HE1	1.76	0.51
1:B:459:ASP:O	1:B:463:LEU:HB2	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:987:MET:SD	1:B:1087:LEU:HD11	2.51	0.51
1:A:871:LEU:HD11	1:D:1023:ILE:HD11	1.93	0.50
1:D:408:ALA:O	1:D:412:ALA:HB2	2.11	0.50
1:D:1110:ARG:O	1:D:1114:ILE:HG12	2.11	0.50
1:B:465:ARG:HB3	1:B:468:PHE:HB2	1.92	0.50
1:C:433:ARG:HG2	1:C:436:ILE:HD12	1.92	0.50
1:A:891:THR:HA	1:A:894:ILE:HG12	1.93	0.50
1:B:478:SER:HB3	1:B:481:ARG:HG2	1.93	0.50
1:B:990:PHE:HE1	1:B:1083:LEU:HB3	1.77	0.50
1:A:105:ALA:HB2	1:A:231:ILE:HD13	1.94	0.50
1:B:189:GLY:HA3	1:B:219:ALA:HB2	1.94	0.50
1:C:760:LEU:HD22	1:C:763:SER:HB2	1.93	0.50
1:B:867:ASN:ND2	2:A:1403:Y01:HAO1	2.13	0.50
1:B:898:ARG:HH22	1:B:1121:PRO:HD3	1.77	0.50
1:A:195:ILE:HA	1:A:198:VAL:HG22	1.92	0.50
1:D:325:PRO:HG2	1:D:416:GLY:HA2	1.93	0.50
1:C:1040:ILE:HG21	1:C:1072:MET:HE1	1.92	0.50
1:D:1120:ARG:HD3	1:D:1121:PRO:HD2	1.93	0.50
1:C:106:PHE:HB3	1:C:123:VAL:HG23	1.93	0.50
1:A:121:MET:HE2	1:A:142:TRP:CD1	2.47	0.50
1:A:123:VAL:HG21	1:A:137:LEU:HD11	1.94	0.50
1:D:538:GLY:HA2	1:D:541:ILE:HD12	1.95	0.49
1:D:1001:PHE:CZ	1:D:1005:ARG:HB2	2.47	0.49
1:B:122:TYR:HB2	1:B:261:LEU:HD23	1.94	0.49
1:B:681:GLN:NE2	1:B:685:GLU:HG3	2.26	0.49
1:D:275:LYS:O	1:D:276:LEU:C	2.55	0.49
1:D:736:LEU:HD21	1:D:1111:TYR:HD1	1.77	0.49
1:C:1204:VAL:HG12	1:D:1203:ARG:HH11	1.76	0.49
1:A:121:MET:HE2	1:A:142:TRP:HD1	1.77	0.49
1:B:654:ALA:O	1:B:658:GLU:CB	2.61	0.49
1:B:456:ALA:O	1:B:460:ALA:CB	2.61	0.49
1:B:713:THR:HB	1:B:716:GLN:HG3	1.94	0.49
1:C:942:GLN:HG2	1:C:945:ARG:HD3	1.94	0.49
1:C:354:GLU:HA	1:C:357:ARG:HB3	1.94	0.49
1:A:706:LEU:HD11	1:A:717:LEU:HD21	1.95	0.49
1:C:1077:LEU:CD1	1:C:1081:ILE:HD12	2.42	0.49
1:B:131:PRO:HB3	1:B:134:LEU:HD12	1.95	0.49
1:A:1138:GLN:O	1:A:1142:CYS:N	2.46	0.49
1:B:960:TYR:CD2	1:A:1000:SER:HA	2.47	0.48
1:A:1078:VAL:O	1:A:1082:LEU:HB3	2.12	0.48
1:A:949:ARG:NH2	1:D:1011:PRO:HA	2.29	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:ILE:HD12	1:C:297:VAL:HA	1.94	0.48
1:B:563:HIS:HA	1:B:566:PHE:HD1	1.78	0.48
1:B:1098:VAL:HA	1:B:1101:ILE:HG22	1.95	0.48
1:A:545:MET:HG3	1:A:650:LYS:HG2	1.94	0.48
1:D:457:MET:HE1	1:D:469:VAL:HG13	1.95	0.48
1:C:915:TRP:CE2	1:C:921:ASN:HB3	2.47	0.48
1:C:1167:LEU:HA	1:C:1170:VAL:HG22	1.96	0.48
1:B:740:TRP:CE3	1:B:1114:ILE:HG12	2.48	0.48
1:D:851:LYS:HD3	1:D:1122:VAL:CG1	2.32	0.48
1:A:899:GLU:HG3	1:A:915:TRP:HE1	1.78	0.48
1:C:687:LEU:HD22	1:C:726:PHE:CE1	2.49	0.48
1:B:413:LEU:O	1:B:417:ALA:CB	2.59	0.48
1:D:173:GLY:HA2	1:D:176:LYS:HZ2	1.78	0.48
1:C:866:PHE:HA	1:C:869:ILE:HG22	1.96	0.48
1:B:715:LEU:HD11	1:B:732:SER:HB2	1.96	0.48
1:B:896:LYS:HE3	1:B:924:ASP:HB3	1.96	0.48
1:A:190:VAL:HG12	1:A:252:LEU:HD23	1.96	0.48
1:B:630:MET:HB3	1:B:630:MET:HE2	1.72	0.47
1:C:407:LEU:HA	1:C:436:ILE:HD11	1.97	0.47
1:A:342:GLY:HA3	1:A:382:LEU:HD11	1.96	0.47
1:D:969:VAL:HG12	1:D:1113:LEU:HD21	1.96	0.47
1:C:146:LEU:HD12	1:C:147:PRO:HD2	1.96	0.47
1:B:867:ASN:HD22	2:A:1403:Y01:CAO	2.15	0.47
1:B:1166:GLU:HA	1:B:1169:LYS:HB3	1.97	0.47
1:D:388:LYS:HD2	1:D:391:LEU:HD13	1.96	0.47
1:C:646:LEU:HD11	1:C:726:PHE:CE2	2.43	0.47
1:C:930:LEU:HA	1:C:933:VAL:HG12	1.95	0.47
1:B:994:MET:HE3	1:B:998:LEU:HB2	1.96	0.47
1:B:149:LEU:HD22	1:B:181:THR:HG21	1.97	0.47
1:C:56:CYS:HA	1:C:266:THR:HG22	1.96	0.47
1:C:1175:GLU:HA	1:C:1178:ILE:HG12	1.95	0.47
1:B:697:LEU:HA	1:B:700:LYS:HE2	1.97	0.47
1:D:285:SER:HA	1:D:297:VAL:HG22	1.95	0.47
1:D:409:ILE:HA	1:D:412:ALA:HB3	1.96	0.47
1:C:736:LEU:HD21	1:C:1111:TYR:HD2	1.79	0.47
1:C:909:LEU:HA	1:C:912:VAL:HG12	1.96	0.47
1:B:873:LYS:HE3	1:A:1012:ASN:HA	1.96	0.47
1:B:393:THR:HG21	1:B:412:ALA:HA	1.97	0.47
1:B:1030:MET:HE2	1:B:1076:LEU:HD21	1.97	0.47
1:A:1130:PHE:O	1:A:1134:THR:HG23	2.15	0.47
1:C:1021:LYS:O	1:C:1025:TYR:HB2	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:LEU:O	1:A:1129:ILE:HG23	2.15	0.46
1:C:144:LEU:HB3	1:C:184:TRP:HZ2	1.80	0.46
1:A:179:MET:HE3	1:A:179:MET:HB3	1.79	0.46
1:D:457:MET:HG3	1:D:477:VAL:HG11	1.97	0.46
1:C:733:GLN:CD	1:C:1107:LYS:HD2	2.40	0.46
1:C:975:PRO:HB3	1:C:1102:SER:HB2	1.97	0.46
1:B:278:ARG:HG3	1:B:282:LYS:HE2	1.98	0.46
1:B:613:PHE:HB3	1:B:616:HIS:ND1	2.31	0.46
1:A:1196:ARG:HH12	1:D:1198:ARG:HG3	1.80	0.46
2:A:1403:Y01:HAJ1	2:A:1403:Y01:HAC2	1.77	0.46
1:D:1001:PHE:CE1	1:D:1072:MET:HB2	2.50	0.46
1:D:932:SER:HA	1:D:935:MET:HG3	1.98	0.46
1:A:978:MET:HB3	1:A:1102:SER:HB2	1.97	0.46
1:D:1001:PHE:CZ	1:D:1072:MET:HB2	2.50	0.46
1:D:1125:PRO:HG2	1:D:1126:PRO:HD3	1.98	0.46
1:D:539:LEU:O	1:D:540:VAL:C	2.59	0.46
1:B:413:LEU:HD12	1:B:417:ALA:HB2	1.98	0.46
1:A:619:MET:HE2	1:A:619:MET:HB2	1.75	0.46
1:A:1138:GLN:O	1:A:1142:CYS:HB3	2.16	0.46
1:D:421:ALA:HA	1:D:424:GLN:HB2	1.97	0.46
1:D:1031:ILE:HA	1:D:1080:ASN:HD21	1.80	0.46
1:A:147:PRO:HB3	1:A:184:TRP:CE2	2.51	0.46
1:A:736:LEU:HD21	1:A:1111:TYR:HD1	1.81	0.46
1:C:1104:GLN:HE21	1:C:1104:GLN:HB2	1.55	0.46
1:C:1205:GLU:HA	1:D:1203:ARG:HH22	1.81	0.46
1:A:1167:LEU:HG	1:A:1171:HIS:CE1	2.51	0.46
1:D:999:MET:HE2	1:D:999:MET:HB3	1.76	0.46
1:C:744:LEU:HA	1:C:770:LYS:H	1.80	0.46
1:B:863:LEU:HD12	1:B:863:LEU:HA	1.69	0.46
1:A:1017:TRP:HB3	2:A:1402:Y01:HAR2	1.97	0.46
1:C:1018:LYS:HE2	2:C:1401:Y01:HAR1	1.98	0.45
1:C:1109:GLN:HE21	1:C:1112:GLN:NE2	2.14	0.45
1:A:1021:LYS:HG3	2:D:1401:Y01:HBF	1.97	0.45
1:C:866:PHE:HD1	1:C:885:VAL:HG11	1.81	0.45
1:B:303:ILE:HB	1:B:328:VAL:HG23	1.97	0.45
1:D:224:VAL:O	1:D:249:LEU:HD23	2.17	0.45
1:D:671:GLU:HA	1:D:674[A]:HIS:HB3	1.98	0.45
1:A:1124:PRO:HG2	1:A:1127:LEU:CD1	2.45	0.45
1:D:977:VAL:HA	1:D:980:ILE:HD12	1.98	0.45
1:C:625:MET:HB2	1:C:625:MET:HE3	1.41	0.45
1:C:646:LEU:HD12	1:C:714:CYS:HB2	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:767:LEU:HD23	1:B:844:PHE:HE2	1.81	0.45
1:D:527:PRO:C	1:D:529:ASP:H	2.24	0.45
2:D:1402:Y01:HAP1	2:D:1402:Y01:HAO2	1.75	0.45
1:C:467:ASP:HA	1:C:470:LYS:HB3	1.98	0.45
1:B:111:PHE:HE2	1:B:120:ALA:HB3	1.80	0.45
1:A:138:MET:HA	1:A:142:TRP:HB2	1.98	0.45
1:A:1140:LEU:HD12	1:A:1140:LEU:HA	1.82	0.45
1:A:1009:LEU:HD11	1:A:1068:VAL:HG11	1.97	0.45
1:D:407:LEU:HA	1:D:411:THR:HG23	1.99	0.45
1:A:1001:PHE:CE2	1:A:1072:MET:HB2	2.52	0.45
1:A:1030:MET:HB3	1:A:1076:LEU:HD21	1.97	0.45
1:D:469:VAL:O	1:D:473:ILE:HG12	2.16	0.45
1:D:539:LEU:C	1:D:541:ILE:N	2.74	0.45
1:C:284:ILE:HG22	1:C:297:VAL:HG21	1.99	0.45
1:B:923:THR:HA	1:B:926:ILE:HG22	1.99	0.45
1:C:144:LEU:HB3	1:C:184:TRP:CZ2	2.52	0.45
1:C:240:GLN:HG3	1:C:242:MET:HB3	1.99	0.45
1:D:543:TYR:HD2	1:D:544:LEU:HD22	1.82	0.45
1:C:311:ILE:HD11	1:C:335:ALA:HB1	1.99	0.45
1:C:1001:PHE:CD2	1:C:1027:PRO:HB3	2.52	0.45
1:B:854:PHE:HB3	1:B:1124:PRO:HG3	1.99	0.45
1:A:888:TYR:HD2	1:A:889:ILE:HD13	1.82	0.45
1:D:915:TRP:HE1	1:D:921:ASN:HD22	1.63	0.45
2:C:1403:Y01:HAS1	2:D:1402:Y01:HBF	1.99	0.44
1:B:1183:ARG:NH1	1:A:209:SER:H	2.15	0.44
1:D:283:HIS:CE1	1:D:287:GLN:HE22	2.34	0.44
1:D:473:ILE:HD12	1:D:479:MET:HE3	1.99	0.44
1:D:535:ILE:HD13	1:D:559:ARG:NH1	2.33	0.44
1:D:943:PRO:O	1:D:946:SER:OG	2.35	0.44
2:D:1403:Y01:HAC2	2:D:1403:Y01:HAJ2	1.77	0.44
1:C:870:VAL:HG13	1:C:871:LEU:HG	1.99	0.44
1:B:43:HIS:CD2	1:B:55:CYS:HB3	2.52	0.44
1:B:151:ILE:CG2	1:B:185:ILE:HD13	2.48	0.44
1:B:488:LEU:HD21	1:B:617:GLU:HG3	1.99	0.44
1:D:108:THR:HB	1:D:236:VAL:HA	1.98	0.44
1:C:687:LEU:HD11	1:C:702:LEU:HD11	2.00	0.44
1:B:221:TRP:HA	1:B:261:LEU:HD12	1.99	0.44
1:D:855:TYR:HD1	1:D:1125:PRO:HB3	1.83	0.44
1:D:944:PHE:O	1:D:945:ARG:C	2.60	0.44
1:C:554:THR:HG22	1:C:554:THR:O	2.18	0.44
1:B:979:MET:O	1:B:983:MET:HG2	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:VAL:HG12	1:A:1108:PHE:HE1	1.82	0.44
1:A:1129:ILE:C	1:A:1131:SER:N	2.74	0.44
1:D:545:MET:C	1:D:650:LYS:HZ1	2.24	0.44
1:C:898:ARG:HH12	1:C:1121:PRO:HG3	1.83	0.44
1:A:1133:MET:HB3	1:A:1133:MET:HE3	1.66	0.44
1:C:224:VAL:HG11	1:C:261:LEU:HD23	1.99	0.44
1:B:307:GLY:HA2	1:B:368:PHE:HE2	1.83	0.44
1:B:866:PHE:HA	1:B:869:ILE:HG22	1.99	0.44
1:A:1125:PRO:O	1:A:1126:PRO:C	2.60	0.44
1:C:325:PRO:HG3	1:C:416:GLY:HA3	2.00	0.44
1:C:479:MET:HE2	1:C:618:LEU:HD21	2.00	0.44
1:A:1123:LEU:CD1	1:A:1130:PHE:HB2	2.41	0.44
1:A:1200:THR:O	1:A:1204:VAL:HG23	2.18	0.44
1:D:170:PHE:HA	1:D:405:ILE:HD13	2.00	0.44
1:D:491:LEU:HB3	1:D:621:TRP:HE1	1.83	0.44
1:B:448:TRP:HZ3	1:B:453:LEU:HD21	1.82	0.44
1:A:754:VAL:HG13	1:A:850:VAL:HG22	2.00	0.44
1:A:1193:ASN:O	1:A:1197:ILE:HD12	2.17	0.44
1:C:619:MET:HE2	1:C:619:MET:HB2	1.50	0.43
1:B:409:ILE:O	1:B:413:LEU:N	2.51	0.43
1:A:1131:SER:O	1:A:1132:HIS:C	2.61	0.43
1:D:273:GLU:HA	1:D:276:LEU:HB3	1.99	0.43
1:C:648:ALA:O	1:C:652:CYS:HB2	2.19	0.43
1:C:650:LYS:HD3	1:C:721:ALA:HA	1.99	0.43
1:B:1202:GLU:O	1:B:1205:GLU:HB2	2.18	0.43
1:A:252:LEU:HD21	1:A:261:LEU:HD11	2.00	0.43
1:D:315:LEU:HD13	1:D:381:ILE:HG23	2.00	0.43
1:C:979:MET:HG2	1:C:1098:VAL:HG23	2.00	0.43
1:A:335:ALA:HA	1:A:338:ILE:HG12	2.00	0.43
1:D:866:PHE:CE1	1:D:956:ILE:HB	2.53	0.43
1:D:999:MET:HE1	2:D:1403:Y01:HAB1	2.00	0.43
1:C:650:LYS:O	1:C:654:ALA:HB2	2.19	0.43
1:C:989:TYR:O	1:C:990:PHE:C	2.59	0.43
1:B:151:ILE:HD12	1:B:300:VAL:HG13	2.00	0.43
1:B:1178:ILE:HG13	1:B:1182:PHE:CE2	2.53	0.43
1:C:480:HIS:CE1	1:C:610:HIS:HB3	2.54	0.43
1:C:957:ILE:O	1:C:961:ILE:HG12	2.19	0.43
1:B:311:ILE:HA	1:B:314:VAL:HG12	2.00	0.43
1:C:650:LYS:O	1:C:654:ALA:CB	2.67	0.43
1:B:309:ASN:O	1:B:313:ILE:HG13	2.18	0.43
1:A:210:ARG:HA	1:A:210:ARG:HD3	1.86	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:PRO:HB2	1:A:413:LEU:HD22	1.99	0.43
1:D:1128:ILE:H	1:D:1128:ILE:HG12	1.66	0.43
1:C:980:ILE:HG23	1:B:1082:LEU:HD21	2.00	0.43
1:C:1096:PHE:HB2	1:B:1093:ASN:HD21	1.84	0.43
1:B:43:HIS:CE1	1:B:56:CYS:HB2	2.54	0.43
1:B:1088:ILE:HG23	1:A:1088:ILE:HG21	2.01	0.43
1:A:35:ALA:HB1	1:A:133:LEU:HD11	2.01	0.43
1:D:43:HIS:CD2	1:D:45:ILE:H	2.36	0.43
1:D:131:PRO:HG2	1:D:283:HIS:CD2	2.54	0.43
1:C:1209:MET:HE2	1:C:1209:MET:HB3	1.89	0.43
1:A:327:VAL:HG11	1:A:409:ILE:HG22	2.00	0.43
1:D:540:VAL:O	1:D:544:LEU:HD23	2.18	0.43
1:B:1137:PHE:O	1:B:1141:CYS:HB2	2.19	0.43
1:A:102:PRO:HB2	1:A:233:ARG:HH22	1.83	0.43
1:A:1017:TRP:CD1	2:A:1403:Y01:HAT1	2.54	0.43
1:C:32:ILE:HA	1:C:36:PHE:HD2	1.83	0.42
1:C:144:LEU:HD21	1:C:258:HIS:CE1	2.54	0.42
1:C:406:ASP:HB3	1:C:433:ARG:HH12	1.84	0.42
1:B:360:LEU:HA	1:B:363:THR:HG22	2.00	0.42
1:B:990:PHE:CE1	1:B:1083:LEU:HB3	2.53	0.42
1:A:173:GLY:HA2	1:A:176:LYS:HG2	2.01	0.42
1:A:635:TRP:CZ3	1:A:1182:PHE:HZ	2.37	0.42
1:A:764:ILE:HD11	1:A:841:ILE:HA	2.00	0.42
1:A:1127:LEU:HD12	1:A:1127:LEU:H	1.83	0.42
2:D:1403:Y01:HAP1	2:D:1403:Y01:HAO2	1.85	0.42
1:C:863:LEU:HD22	1:C:963:LEU:HD21	2.00	0.42
1:C:923:THR:HA	1:C:926:ILE:HG22	2.01	0.42
1:B:1066:TRP:HB3	2:B:1401:Y01:HAD2	2.01	0.42
1:B:1162:ILE:HD12	1:B:1162:ILE:HA	1.93	0.42
1:B:1183:ARG:HD2	1:A:210:ARG:NH1	2.34	0.42
1:A:181:THR:HG1	1:A:431:TRP:CD1	2.37	0.42
1:A:1128:ILE:HD13	1:A:1130:PHE:CE2	2.54	0.42
1:D:851:LYS:HB2	1:D:1122:VAL:HG13	2.01	0.42
1:C:93:SER:HA	1:C:97:HIS:HA	2.01	0.42
1:D:189:GLY:HA3	1:D:219:ALA:HB2	2.02	0.42
1:D:289:ILE:HD13	1:D:297:VAL:HA	2.00	0.42
1:D:298:PRO:HG3	1:D:431:TRP:HZ2	1.84	0.42
1:B:1113:LEU:HD12	1:B:1113:LEU:HA	1.81	0.42
1:A:105:ALA:HA	1:A:232:GLY:H	1.84	0.42
1:A:534:LEU:HA	1:A:537:ILE:HG22	2.01	0.42
1:A:982:LYS:HA	1:A:982:LYS:HD3	1.79	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:TRP:O	1:B:35:ALA:CB	2.63	0.42
1:B:740:TRP:NE1	1:B:849:ILE:HD13	2.35	0.42
1:B:1197:ILE:CD1	1:A:1197:ILE:HG12	2.49	0.42
1:A:312:SER:HA	1:A:315:LEU:HB3	2.01	0.42
1:D:93:SER:HA	1:D:97:HIS:HA	2.00	0.42
1:D:968:GLY:HA2	1:D:974:GLY:HA2	2.02	0.42
1:D:975:PRO:O	1:D:978:MET:HB2	2.20	0.42
1:C:314:VAL:HG23	1:C:326:VAL:HG11	2.01	0.42
1:D:1128:ILE:O	1:D:1129:ILE:C	2.61	0.42
1:C:434:VAL:HA	1:C:468:PHE:CE1	2.55	0.42
1:C:715:LEU:HD11	1:C:732:SER:HB2	2.00	0.42
1:B:877:TRP:HE3	1:B:878:PRO:HD3	1.85	0.42
1:D:273:GLU:HA	1:D:276:LEU:CB	2.50	0.42
1:D:863:LEU:HD12	1:D:863:LEU:HA	1.91	0.42
1:C:1021:LYS:O	1:C:1025:TYR:CB	2.68	0.42
1:B:472:LEU:HD12	1:B:472:LEU:HA	1.65	0.42
1:B:545:MET:HG2	1:B:549:TYR:CD2	2.55	0.42
1:A:719:VAL:HG11	1:A:1111:TYR:CD2	2.54	0.42
1:D:202:LEU:HD21	1:D:215:THR:HG21	2.02	0.42
1:D:218:ILE:HD12	1:D:277:ARG:HD2	2.00	0.42
1:A:151:ILE:HD13	1:A:151:ILE:HG21	1.87	0.42
1:A:979:MET:HG2	1:A:1098:VAL:HG12	2.02	0.42
1:C:123:VAL:HG12	1:C:142:TRP:HZ2	1.85	0.42
1:C:278:ARG:HG3	1:C:282:LYS:HE2	2.02	0.42
1:C:501:THR:HG23	1:C:626:LYS:HE2	2.02	0.42
1:A:758:ILE:HG23	1:A:854:PHE:HD1	1.84	0.42
1:A:853:TRP:HA	1:A:856:THR:HG22	2.02	0.42
1:A:862:TYR:HH	1:A:959:TRP:CD1	2.38	0.42
1:A:1130:PHE:O	1:A:1131:SER:C	2.63	0.42
1:C:308:PRO:HD3	1:C:368:PHE:CE1	2.55	0.41
1:A:104:ASP:H	1:A:124:ARG:NH2	2.17	0.41
1:D:559:ARG:HA	1:D:559:ARG:HD2	1.83	0.41
1:B:545:MET:HE2	1:B:545:MET:HB2	1.83	0.41
1:B:651:LEU:HD23	1:B:651:LEU:HA	1.86	0.41
1:B:1195:GLU:O	1:B:1196:ARG:C	2.62	0.41
1:D:1058:LEU:HD12	1:D:1058:LEU:HA	1.93	0.41
1:C:687:LEU:HD22	1:C:726:PHE:HE1	1.85	0.41
1:A:43:HIS:CD2	1:A:45:ILE:H	2.38	0.41
1:A:109:ILE:HG12	1:A:122:TYR:CE1	2.56	0.41
1:A:1123:LEU:HD23	1:A:1123:LEU:HA	1.79	0.41
1:D:188:GLY:H	1:D:195:ILE:HD11	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:668:ILE:HB	1:C:672:LEU:HD23	2.01	0.41
1:C:748:LYS:O	1:C:749:ASN:C	2.62	0.41
2:C:1403:Y01:HAR1	2:D:1402:Y01:HBC	2.02	0.41
1:B:914:VAL:HA	1:B:917:GLN:HG2	2.01	0.41
1:A:1137:PHE:O	1:A:1141:CYS:N	2.36	0.41
1:D:642:MET:HE2	1:D:642:MET:HB2	1.89	0.41
1:C:36:PHE:CZ	1:C:137:LEU:HD13	2.55	0.41
1:C:613:PHE:HB3	1:C:616:HIS:CE1	2.56	0.41
1:B:509:VAL:HG21	1:B:540:VAL:HA	2.03	0.41
1:A:748:LYS:O	1:A:749:ASN:C	2.64	0.41
1:D:501:THR:HA	1:D:504:HIS:CE1	2.55	0.41
1:D:1102:SER:HA	1:D:1105:VAL:HB	2.03	0.41
1:C:484:THR:HA	1:C:609:ASN:HB3	2.02	0.41
1:C:626:LYS:HE3	1:C:626:LYS:HB3	1.87	0.41
1:C:1164:ASP:HB2	1:C:1168:LYS:NZ	2.35	0.41
1:B:538:GLY:HA2	1:B:541:ILE:HD12	2.02	0.41
1:B:655:MET:O	1:B:659:ALA:CB	2.69	0.41
1:B:961:ILE:HG23	1:B:964:LEU:HD12	2.02	0.41
1:A:93:SER:HA	1:A:97:HIS:HA	2.02	0.41
1:A:1182:PHE:O	1:A:1185:LYS:HB3	2.21	0.41
1:A:1209:MET:HE3	1:A:1210:ARG:HB2	2.02	0.41
1:B:469:VAL:O	1:B:470:LYS:C	2.62	0.41
1:B:613:PHE:HA	1:B:614:PRO:HD3	1.91	0.41
1:A:150:LEU:HD11	1:A:186:PHE:CD2	2.55	0.41
1:A:1183:ARG:HH12	1:D:209:SER:N	2.19	0.41
1:B:205:HIS:CE1	1:B:207:SER:HB2	2.55	0.41
1:B:872:VAL:HG13	1:A:1015:PRO:HD3	2.01	0.41
1:A:950:VAL:HG22	1:D:1008:ILE:HD12	2.03	0.41
1:D:273:GLU:O	1:D:274:VAL:C	2.64	0.41
1:C:149:LEU:HB3	1:C:183:ALA:CB	2.50	0.41
1:C:509:VAL:HG21	1:C:540:VAL:HG22	2.03	0.41
1:C:531:ARG:HD2	1:C:531:ARG:HA	1.81	0.41
1:C:878:PRO:HG3	1:C:938:ARG:HH12	1.84	0.41
1:C:994:MET:O	1:C:995:LEU:C	2.62	0.41
1:C:1044:CYS:HB3	1:C:1061:CYS:HB3	1.61	0.41
1:C:1092:ASN:ND2	1:D:1092:ASN:HD21	2.19	0.41
1:B:32:ILE:HA	1:B:36:PHE:CE2	2.56	0.41
1:B:151:ILE:HG22	1:B:185:ILE:HD13	2.01	0.41
1:B:160:PHE:H	1:B:193:GLY:HA2	1.86	0.41
1:B:185:ILE:HB	1:B:215:THR:HG22	2.02	0.41
1:B:503:TYR:HA	1:B:506:VAL:HG12	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:LEU:HA	1:B:537:ILE:HG12	2.03	0.41
1:B:628:GLN:HG3	1:B:675:ASN:OD1	2.21	0.41
1:B:1084:VAL:O	1:B:1088:ILE:HG12	2.21	0.41
1:A:744:LEU:HD21	1:A:844:PHE:HD1	1.86	0.41
1:A:951:ILE:HA	1:A:954:VAL:HG12	2.03	0.41
1:D:146:LEU:HG	1:D:147:PRO:HD2	2.03	0.41
1:D:278:ARG:HH22	1:D:324:VAL:HG21	1.85	0.41
1:D:1128:ILE:O	1:D:1131:SER:N	2.54	0.41
1:C:181:THR:OG1	1:C:183:ALA:HB2	2.21	0.41
1:C:390:GLU:HG2	1:C:391:LEU:HD22	2.03	0.41
1:B:719:VAL:HG11	1:B:1111:TYR:CD2	2.56	0.41
1:A:191:ASN:HB2	1:A:253:ASN:HA	2.03	0.41
1:A:344:LYS:HE2	1:A:344:LYS:HB2	1.87	0.41
1:A:618:LEU:HA	1:A:621:TRP:HB3	2.02	0.41
1:B:883:TRP:HA	1:B:886:ILE:HG22	2.01	0.40
2:A:1402:Y01:HAE2	2:A:1402:Y01:HBB	1.97	0.40
1:D:38:LYS:HB3	1:D:103:THR:HG22	2.03	0.40
1:C:669:SER:O	1:C:673:ASN:HB2	2.22	0.40
1:C:758:ILE:HD13	1:C:758:ILE:HG21	1.85	0.40
1:B:651:LEU:O	1:B:655:MET:HG3	2.21	0.40
1:B:653:LYS:HA	1:B:653:LYS:HD2	1.90	0.40
1:B:1120:ARG:HA	1:B:1121:PRO:HD3	1.95	0.40
1:A:449:PRO:HD2	1:A:452:SER:HB3	2.04	0.40
1:D:225:GLU:HA	1:D:249:LEU:HB3	2.04	0.40
1:D:390:GLU:HG2	1:D:391:LEU:HD12	2.03	0.40
1:D:1202:GLU:O	1:D:1205:GLU:HB2	2.21	0.40
1:C:429:LEU:HA	1:C:468:PHE:CE2	2.55	0.40
1:C:464:ASP:OD1	1:C:627:ARG:HD3	2.22	0.40
1:C:1030:MET:HE3	1:C:1072:MET:HE3	2.03	0.40
1:B:151:ILE:HG22	1:B:185:ILE:HA	2.02	0.40
1:A:104:ASP:H	1:A:124:ARG:HH21	1.69	0.40
1:A:863:LEU:HD12	1:A:863:LEU:HA	1.76	0.40
1:D:915:TRP:NE1	1:D:921:ASN:HD22	2.19	0.40
1:C:138:MET:HA	1:C:142:TRP:HB2	2.03	0.40
1:C:947:ASP:O	1:C:951:ILE:HG12	2.22	0.40
1:B:613:PHE:HB3	1:B:616:HIS:CE1	2.57	0.40
1:B:863:LEU:HD11	1:B:960:TYR:HD1	1.86	0.40
1:A:1008:ILE:HD13	1:A:1008:ILE:HA	1.92	0.40
1:B:131:PRO:HG2	1:B:283:HIS:CG	2.56	0.40
1:B:930:LEU:HA	1:B:930:LEU:HD12	1.85	0.40
1:B:987:MET:HE1	1:A:1081:ILE:O	2.22	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:CYS:SG	1:D:56:CYS:HB3	2.61	0.40
1:D:147:PRO:HB3	1:D:184:TRP:CD2	2.57	0.40
1:D:252:LEU:HD13	1:D:259:PHE:CG	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1024/1306 (78%)	947 (92%)	75 (7%)	2 (0%)	44	76
1	B	1014/1306 (78%)	936 (92%)	78 (8%)	0	100	100
1	C	1015/1306 (78%)	944 (93%)	71 (7%)	0	100	100
1	D	1026/1306 (79%)	954 (93%)	71 (7%)	1 (0%)	48	81
All	All	4079/5224 (78%)	3781 (93%)	295 (7%)	3 (0%)	50	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1130	PHE
1	A	1128	ILE
1	D	441	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	771/1162 (66%)	756 (98%)	15 (2%)	52	69
1	B	779/1162 (67%)	774 (99%)	5 (1%)	84	88
1	C	788/1162 (68%)	779 (99%)	9 (1%)	70	79
1	D	749/1162 (64%)	740 (99%)	9 (1%)	67	78
All	All	3087/4648 (66%)	3049 (99%)	38 (1%)	66	78

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	43	HIS
1	C	994	MET
1	C	1023	ILE
1	C	1098	VAL
1	C	1099	LYS
1	C	1101	ILE
1	C	1103	ASN
1	C	1104	GLN
1	C	1197	ILE
1	B	364	ILE
1	B	457	MET
1	B	472	LEU
1	B	473	ILE
1	B	674	HIS
1	A	674	HIS
1	A	706	LEU
1	A	1083	LEU
1	A	1114	ILE
1	A	1122	VAL
1	A	1128	ILE
1	A	1129	ILE
1	A	1130	PHE
1	A	1131	SER
1	A	1132	HIS
1	A	1133	MET
1	A	1134	THR
1	A	1136	ILE
1	A	1160	LEU
1	A	1162	ILE
1	D	277	ARG
1	D	504	HIS
1	D	540	VAL
1	D	636	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	946	SER
1	D	986	ASP
1	D	1005	ARG
1	D	1127	LEU
1	D	1128	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	118	ASN
1	C	256	HIS
1	C	353	ASN
1	C	440	GLN
1	C	446	GLN
1	C	493	ASN
1	C	636	GLN
1	C	674	HIS
1	C	1092	ASN
1	C	1093	ASN
1	C	1104	GLN
1	C	1109	GLN
1	B	353	ASN
1	B	424	GLN
1	B	432	ASN
1	B	440	GLN
1	B	447	GLN
1	B	616	HIS
1	B	681	GLN
1	B	771	ASN
1	B	867	ASN
1	B	1085	ASN
1	B	1093	ASN
1	A	43	HIS
1	A	283	HIS
1	A	353	ASN
1	A	480	HIS
1	A	716	GLN
1	A	723	HIS
1	A	1006	GLN
1	A	1171	HIS
1	D	112	GLN
1	D	253	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	283	HIS
1	D	402	HIS
1	D	610	HIS
1	D	921	ASN
1	D	1138	GLN
1	D	1206	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	$\# Z  > 2$
2	Y01	A	1401	-	38,38,38	0.41	0	57,57,57	0.82	1 (1%)
2	Y01	C	1403	-	38,38,38	0.41	0	57,57,57	0.52	0
2	Y01	D	1402	-	38,38,38	0.40	0	57,57,57	0.48	0
2	Y01	C	1402	-	38,38,38	0.37	0	57,57,57	0.57	0
2	Y01	D	1403	-	38,38,38	0.39	0	57,57,57	0.65	0
2	Y01	B	1403	-	38,38,38	0.40	0	57,57,57	0.53	0
2	Y01	A	1403	-	38,38,38	0.40	0	57,57,57	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	Y01	B	1401	-	38,38,38	0.37	0	57,57,57	0.66	1 (1%)
2	Y01	C	1401	-	38,38,38	0.42	0	57,57,57	0.67	0
2	Y01	B	1402	-	38,38,38	0.44	0	57,57,57	0.65	0
2	Y01	A	1402	-	38,38,38	0.40	0	57,57,57	0.52	0
2	Y01	D	1401	-	38,38,38	0.40	0	57,57,57	0.48	0

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
2	Y01	A	1401	-	-	7/19/77/77	0/4/4/4
2	Y01	C	1403	-	-	8/19/77/77	0/4/4/4
2	Y01	D	1402	-	-	9/19/77/77	0/4/4/4
2	Y01	C	1402	-	-	9/19/77/77	0/4/4/4
2	Y01	D	1403	-	-	10/19/77/77	0/4/4/4
2	Y01	B	1403	-	-	9/19/77/77	0/4/4/4
2	Y01	A	1403	-	-	9/19/77/77	0/4/4/4
2	Y01	B	1401	-	-	8/19/77/77	0/4/4/4
2	Y01	C	1401	-	-	3/19/77/77	0/4/4/4
2	Y01	B	1402	-	-	1/19/77/77	0/4/4/4
2	Y01	A	1402	-	-	9/19/77/77	0/4/4/4
2	Y01	D	1401	-	-	10/19/77/77	0/4/4/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	Y01	CBD-CAK-CAI	-2.44	109.38	112.76
2	B	1401	Y01	OAW-CBC-CAV	-2.19	103.52	108.04

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1401	Y01	CAO-CBB-CBE-CBI
2	C	1401	Y01	CAJ-CAO-CBB-CAC

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	C	1402	Y01	CAJ-CAO-CBB-CAC
2	B	1401	Y01	CAJ-CAO-CBB-CAC
2	B	1403	Y01	CAJ-CAO-CBB-CAC
2	B	1401	Y01	CAC-CBB-CBE-CBI
2	A	1403	Y01	CAJ-CAO-CBB-CAC
2	B	1403	Y01	CAJ-CAO-CBB-CBE
2	A	1402	Y01	CAJ-CAO-CBB-CBE
2	A	1403	Y01	CAJ-CAO-CBB-CBE
2	D	1402	Y01	CAJ-CAO-CBB-CBE
2	B	1401	Y01	CAC-CBB-CBE-CAP
2	C	1403	Y01	CAJ-CAO-CBB-CAC
2	D	1401	Y01	CAJ-CAO-CBB-CAC
2	D	1402	Y01	CAJ-CAO-CBB-CAC
2	A	1402	Y01	CAO-CAJ-CAN-CBA
2	B	1401	Y01	CAO-CBB-CBE-CAP
2	D	1402	Y01	CAO-CAJ-CAN-CBA
2	B	1401	Y01	CAJ-CAO-CBB-CBE
2	A	1402	Y01	CAJ-CAO-CBB-CAC
2	C	1402	Y01	CAO-CBB-CBE-CBI
2	A	1403	Y01	CAO-CAJ-CAN-CBA
2	A	1403	Y01	CAX-CAL-CAM-CAY
2	D	1402	Y01	CAO-CBB-CBE-CBI
2	A	1401	Y01	CAO-CBB-CBE-CBI
2	A	1402	Y01	CAO-CBB-CBE-CBI
2	D	1403	Y01	CAN-CAJ-CAO-CBB
2	C	1402	Y01	CAO-CBB-CBE-CAP
2	C	1402	Y01	CAC-CBB-CBE-CAP
2	D	1402	Y01	CAC-CBB-CBE-CAP
2	C	1402	Y01	CAC-CBB-CBE-CBI
2	B	1402	Y01	CAJ-CAO-CBB-CAC
2	D	1402	Y01	CAO-CBB-CBE-CAP
2	A	1402	Y01	CAC-CBB-CBE-CAP
2	D	1402	Y01	CAC-CBB-CBE-CBI
2	C	1402	Y01	CAJ-CAO-CBB-CBE
2	D	1403	Y01	CAJ-CAO-CBB-CBE
2	A	1401	Y01	CAC-CBB-CBE-CAP
2	A	1401	Y01	CAC-CBB-CBE-CBI
2	A	1403	Y01	CAN-CAJ-CAO-CBB
2	A	1402	Y01	CAO-CBB-CBE-CAP
2	A	1401	Y01	CAO-CBB-CBE-CAP
2	A	1402	Y01	CAC-CBB-CBE-CBI
2	B	1403	Y01	CAL-CAM-CAY-OAW

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	1403	Y01	CAN-CAJ-CAO-CBB
2	D	1401	Y01	CAO-CBB-CBE-CBI
2	D	1401	Y01	CAO-CBB-CBE-CAP
2	C	1402	Y01	CAN-CAJ-CAO-CBB
2	D	1401	Y01	CAC-CBB-CBE-CBI
2	D	1401	Y01	CAC-CBB-CBE-CAP
2	D	1401	Y01	CAN-CAJ-CAO-CBB
2	C	1403	Y01	CAO-CBB-CBE-CAP
2	D	1401	Y01	CAM-CAL-CAX-OAH
2	B	1403	Y01	CAO-CBB-CBE-CAP
2	D	1403	Y01	CAX-CAL-CAM-CAY
2	D	1403	Y01	CAO-CBB-CBE-CAP
2	D	1401	Y01	CAM-CAL-CAX-OAF
2	B	1401	Y01	CAM-CAL-CAX-OAH
2	B	1401	Y01	CAM-CAL-CAX-OAF
2	A	1401	Y01	CAM-CAL-CAX-OAF
2	C	1403	Y01	CAN-CAJ-CAO-CBB
2	A	1402	Y01	CAM-CAL-CAX-OAH
2	A	1402	Y01	CAM-CAL-CAX-OAF
2	A	1401	Y01	CAM-CAL-CAX-OAH
2	D	1403	Y01	CAM-CAL-CAX-OAH
2	C	1403	Y01	CAM-CAL-CAX-OAH
2	D	1402	Y01	CAM-CAL-CAX-OAH
2	A	1403	Y01	CAM-CAL-CAX-OAH
2	C	1403	Y01	CAM-CAL-CAX-OAF
2	D	1402	Y01	CAM-CAL-CAX-OAF
2	C	1402	Y01	CAM-CAL-CAX-OAH
2	B	1403	Y01	CAM-CAL-CAX-OAH
2	C	1403	Y01	CAO-CBB-CBE-CBI
2	D	1403	Y01	CAM-CAL-CAX-OAF
2	C	1403	Y01	CAC-CBB-CBE-CBI
2	C	1402	Y01	CAM-CAL-CAX-OAF
2	A	1403	Y01	CAM-CAL-CAX-OAF
2	B	1403	Y01	CAM-CAL-CAX-OAF
2	A	1401	Y01	CAJ-CAO-CBB-CAC
2	D	1401	Y01	CAL-CAM-CAY-OAW
2	D	1403	Y01	CAJ-CAN-CBA-CAA
2	C	1401	Y01	CAL-CAM-CAY-OAW
2	D	1403	Y01	CAL-CAM-CAY-OAW
2	A	1403	Y01	CAL-CAM-CAY-OAW
2	D	1403	Y01	CAC-CBB-CBE-CBI
2	B	1403	Y01	CAL-CAM-CAY-OAG

*Continued on next page...*

*Continued from previous page...*

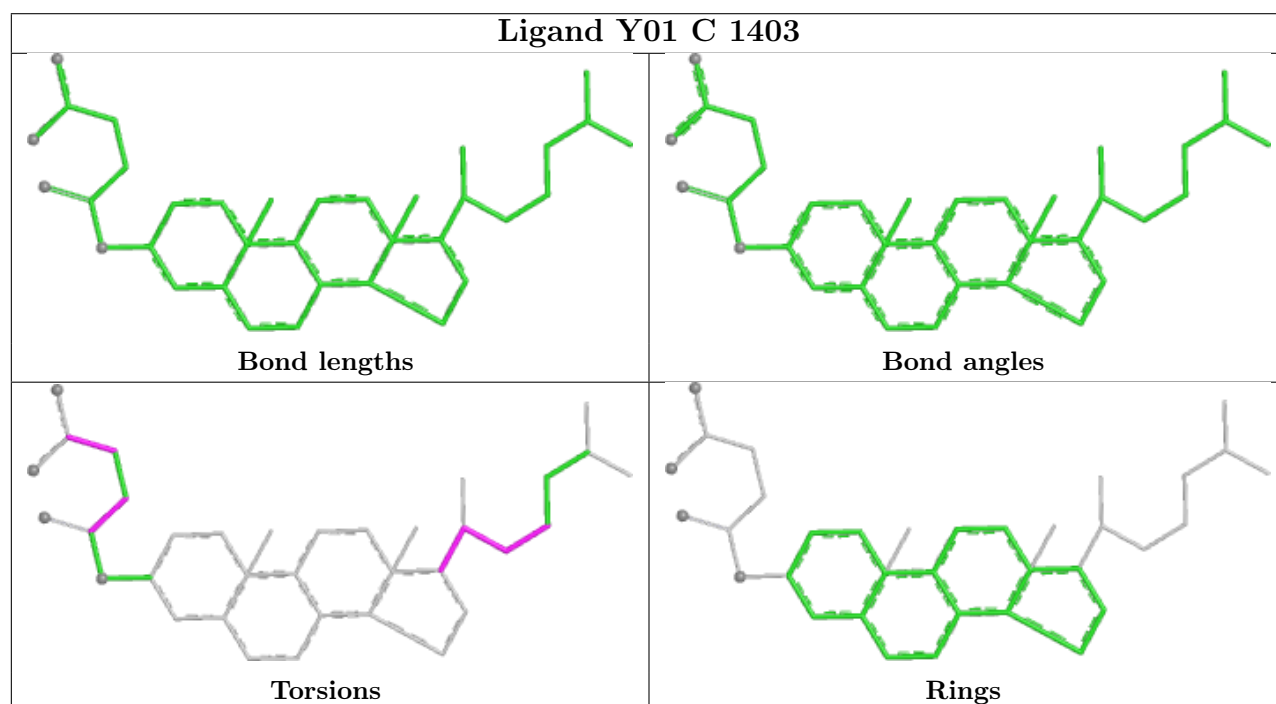
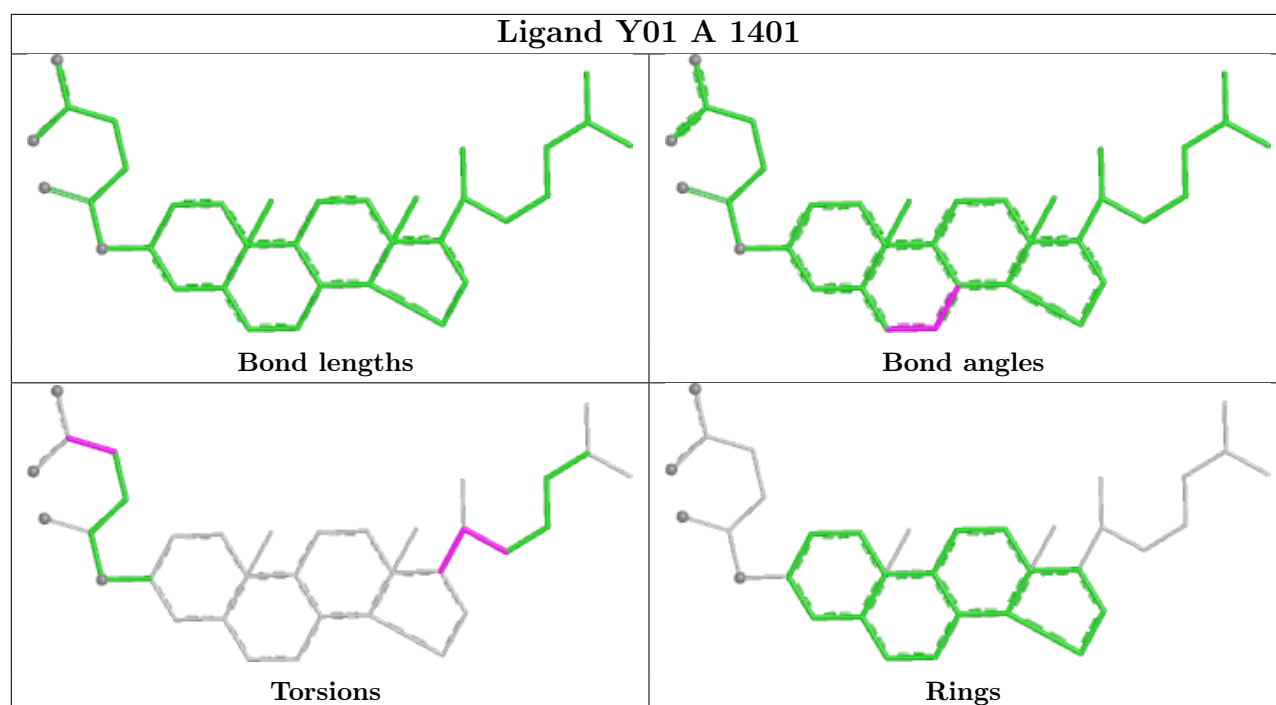
Mol	Chain	Res	Type	Atoms
2	D	1403	Y01	CAL-CAM-CAY-OAG
2	D	1401	Y01	CAL-CAM-CAY-OAG
2	A	1403	Y01	CAL-CAM-CAY-OAG
2	B	1403	Y01	CAO-CBB-CBE-CBI
2	C	1403	Y01	CAL-CAM-CAY-OAW
2	C	1401	Y01	CAL-CAM-CAY-OAG

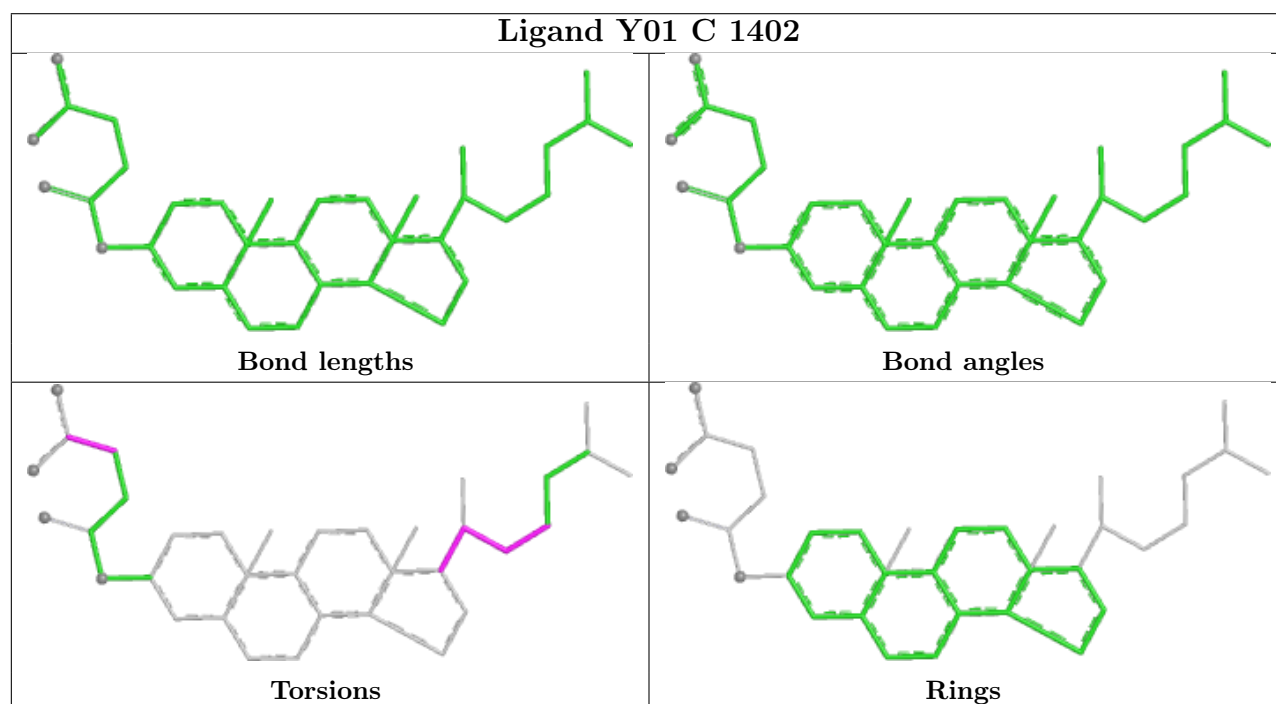
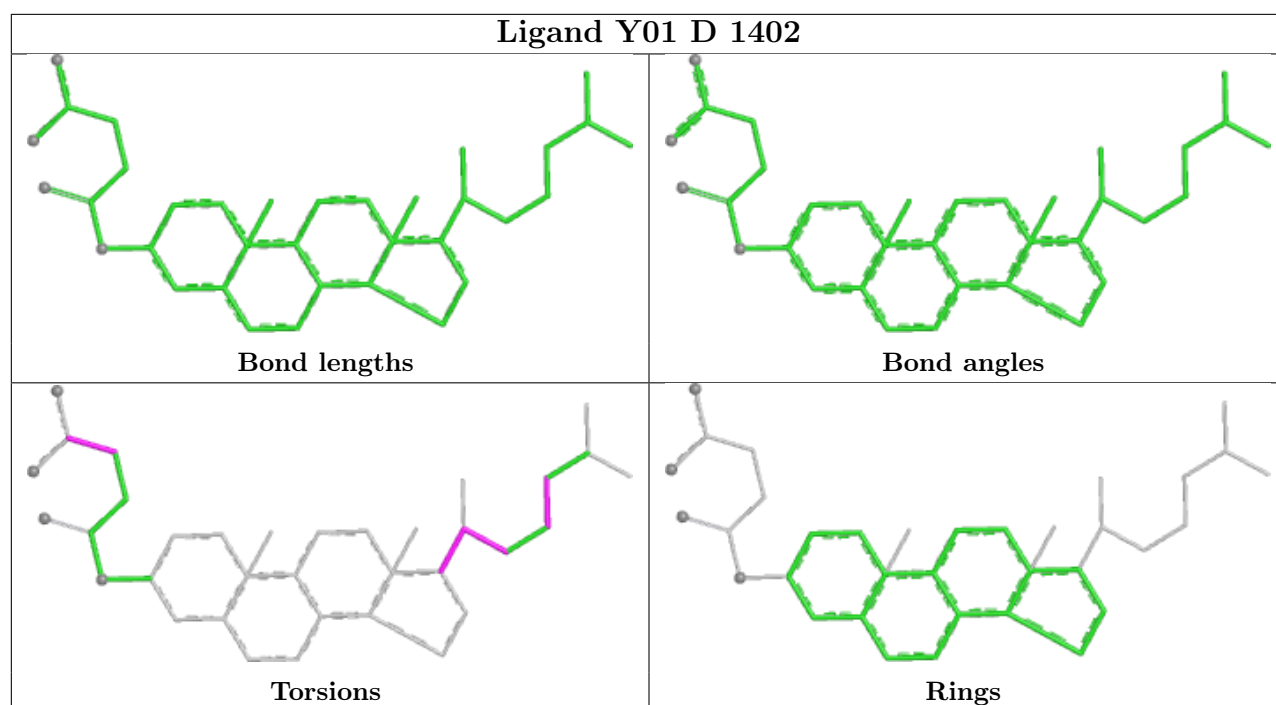
There are no ring outliers.

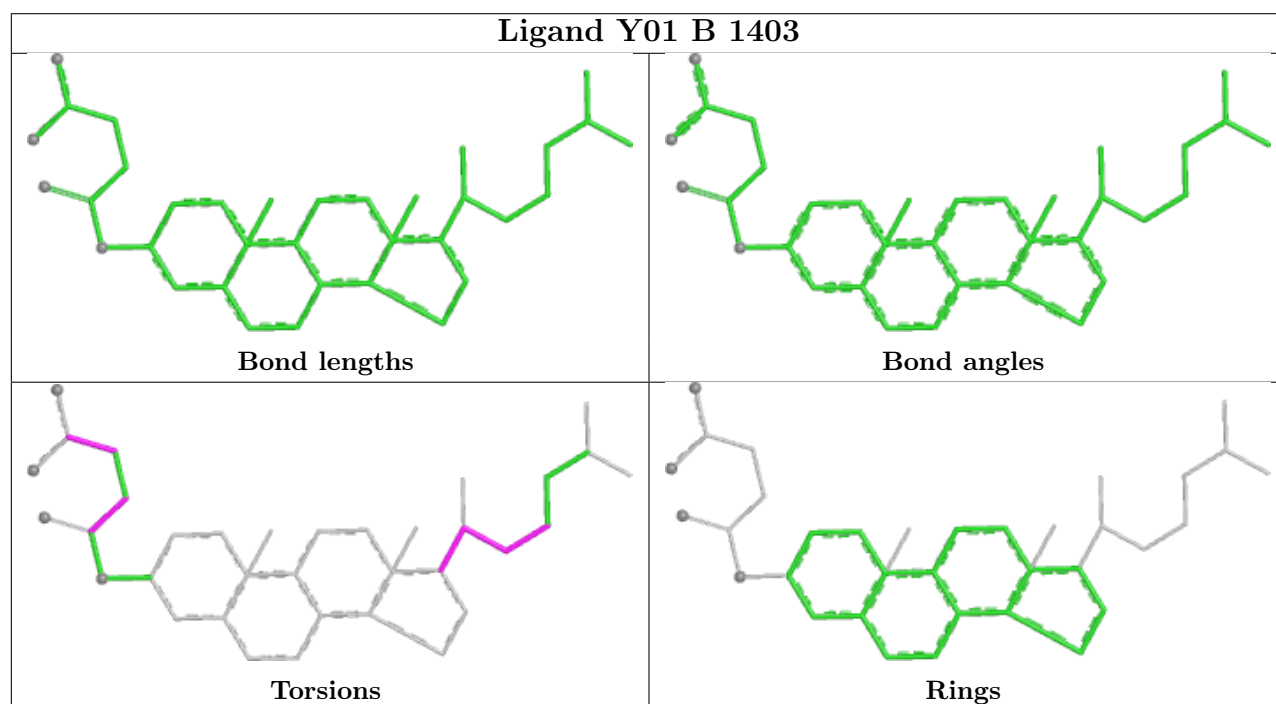
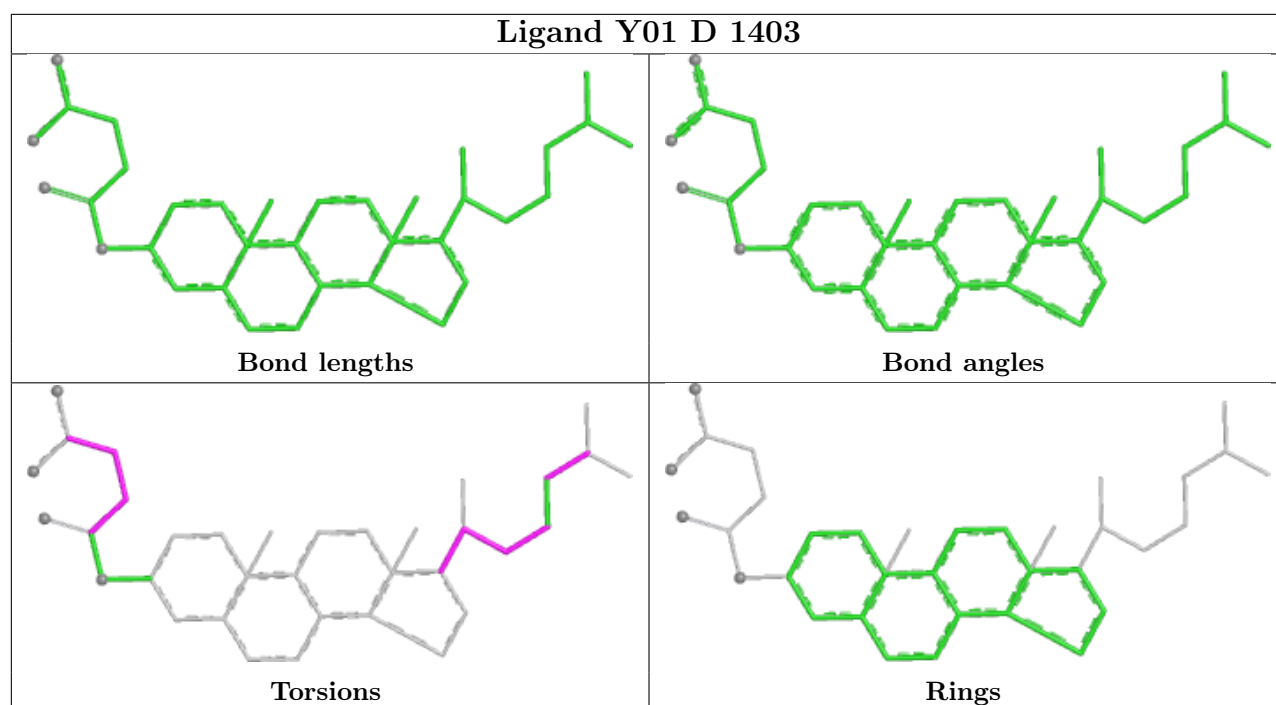
10 monomers are involved in 24 short contacts:

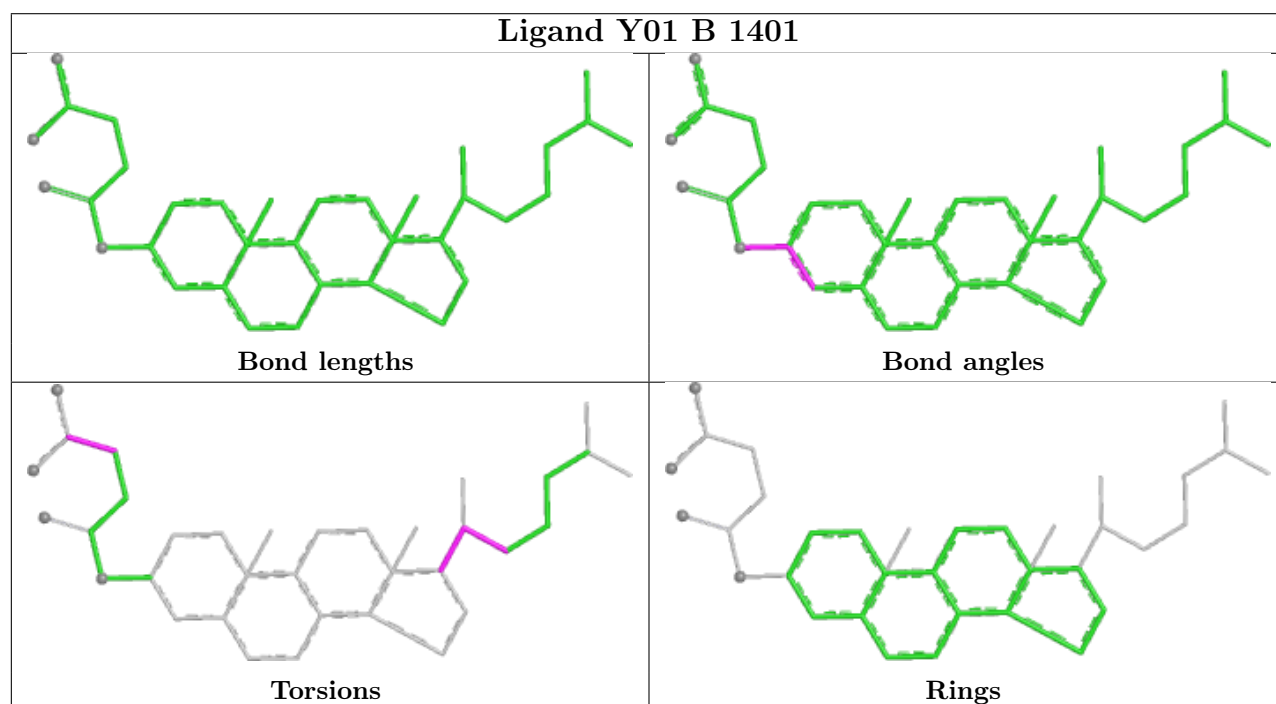
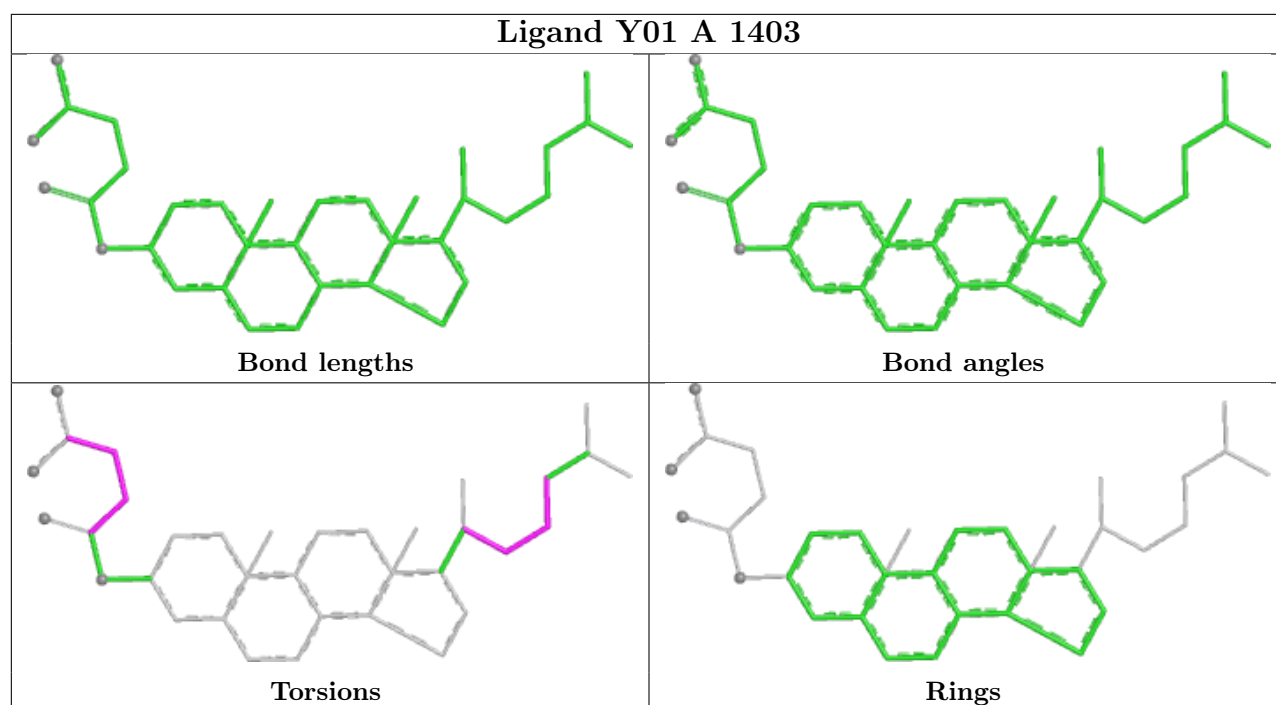
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1401	Y01	1	0
2	C	1403	Y01	3	0
2	D	1402	Y01	4	0
2	D	1403	Y01	3	0
2	A	1403	Y01	5	0
2	B	1401	Y01	2	0
2	C	1401	Y01	2	0
2	B	1402	Y01	3	0
2	A	1402	Y01	2	0
2	D	1401	Y01	2	0

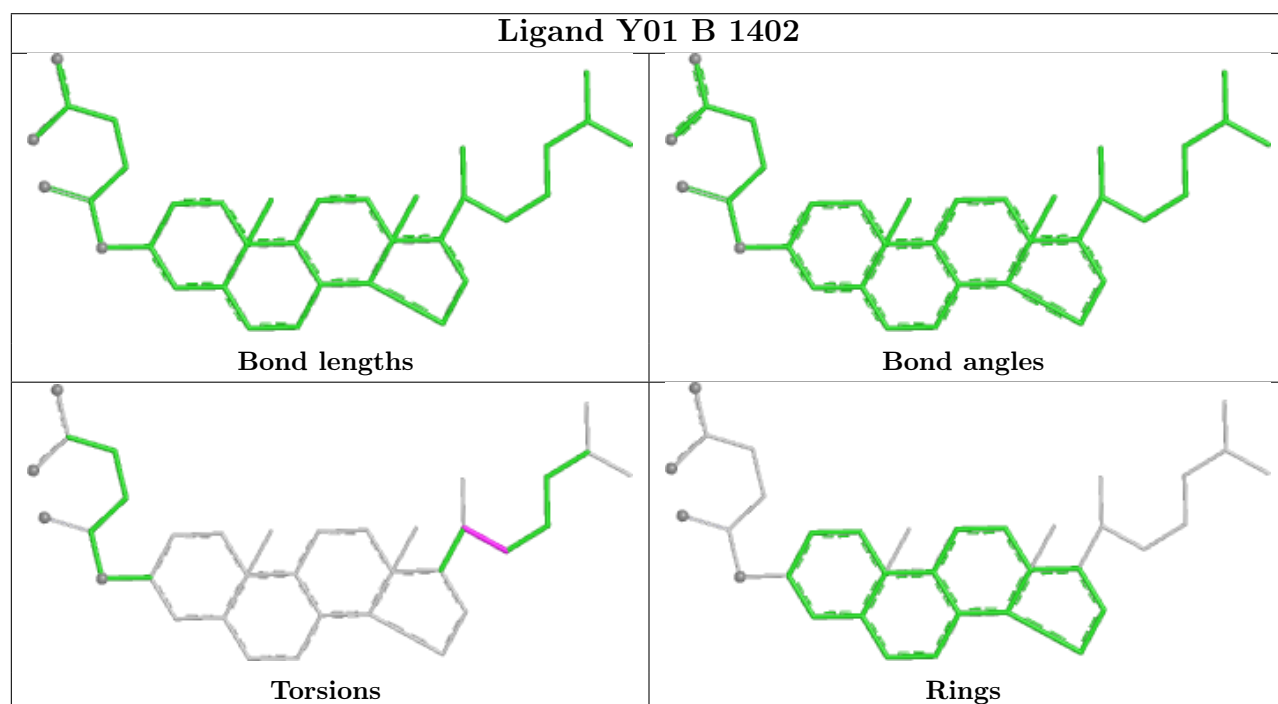
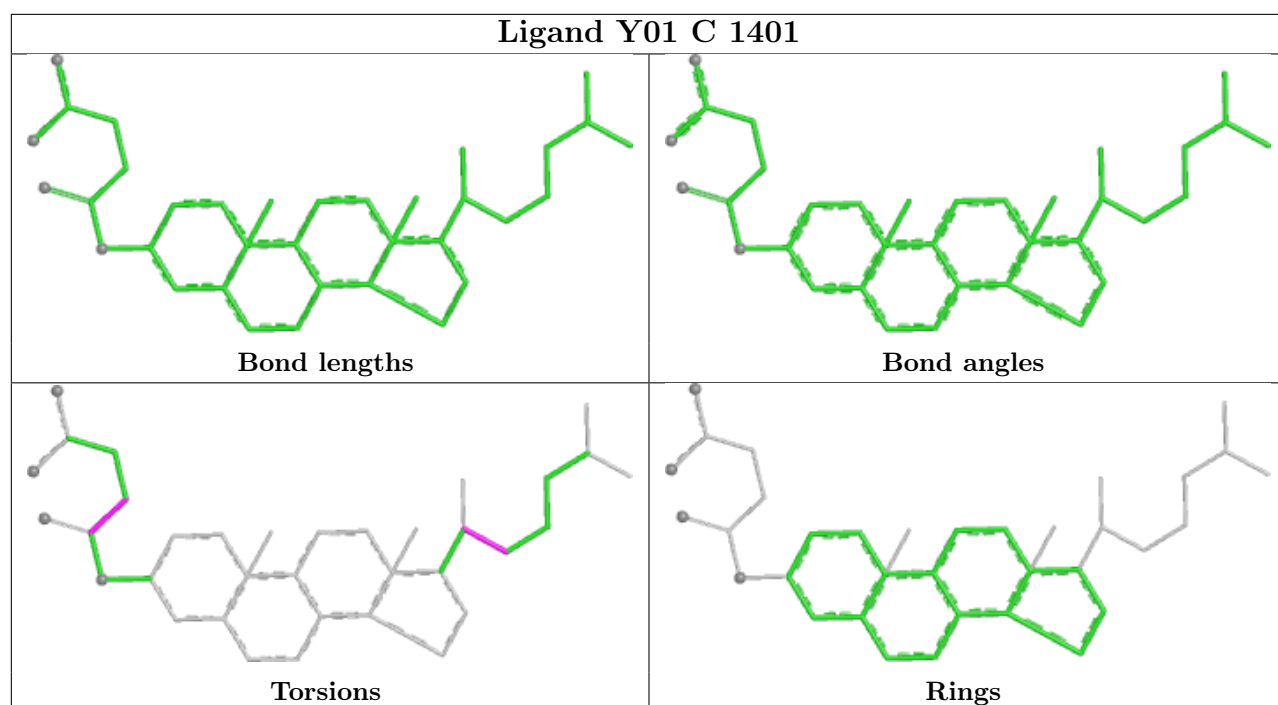
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



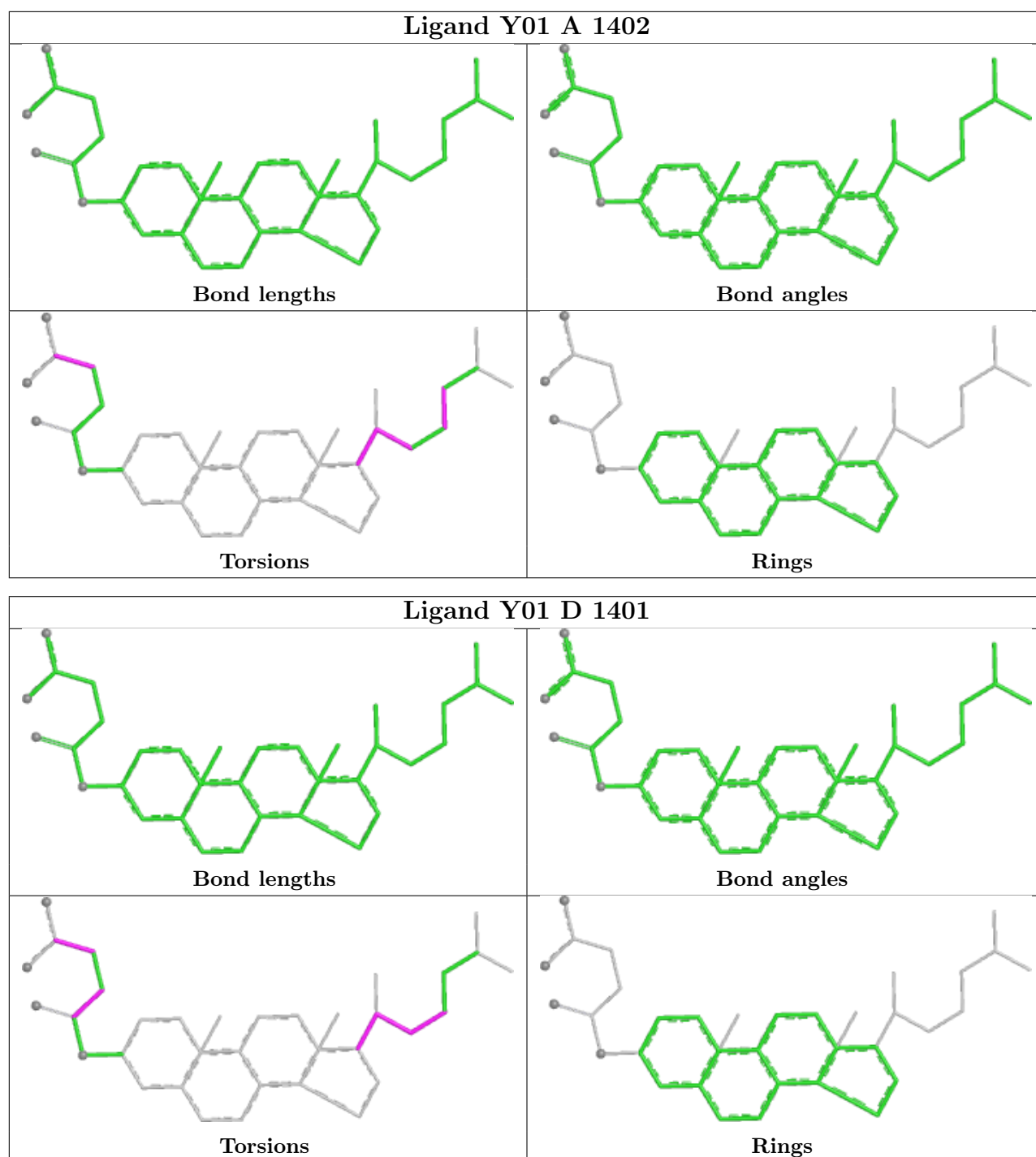












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

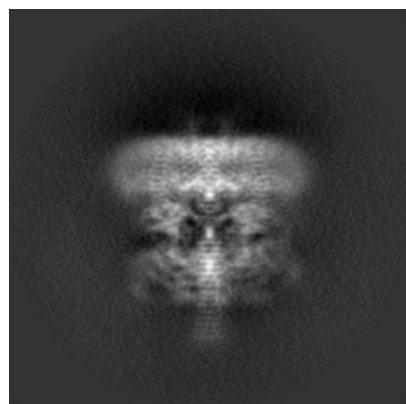
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70214. These allow visual inspection of the internal detail of the map and identification of artifacts.

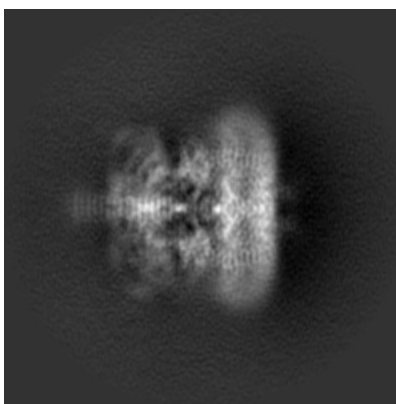
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

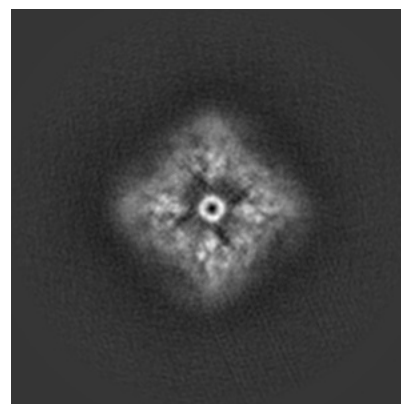
#### 6.1.1 Primary map



X

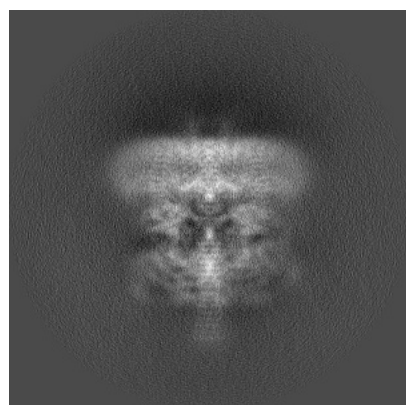


Y

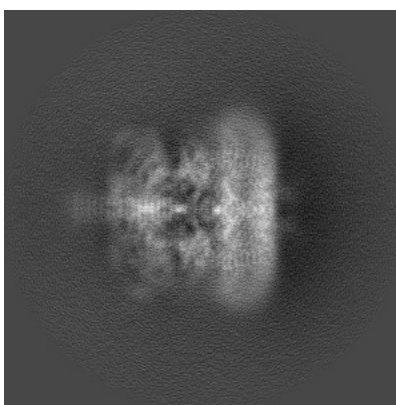


Z

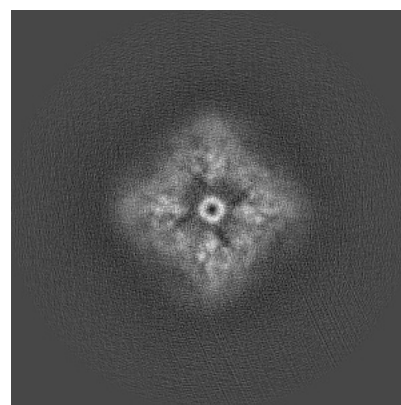
#### 6.1.2 Raw map



X



Y

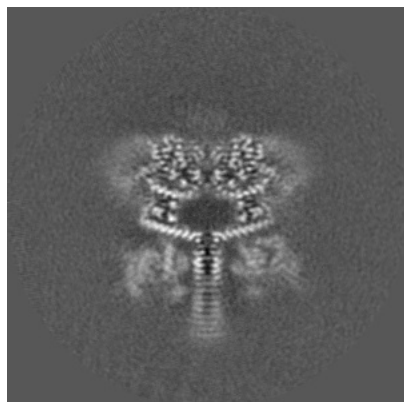


Z

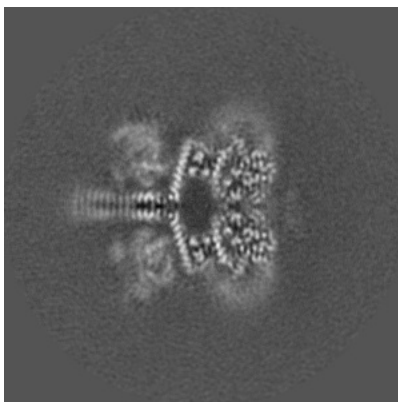
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

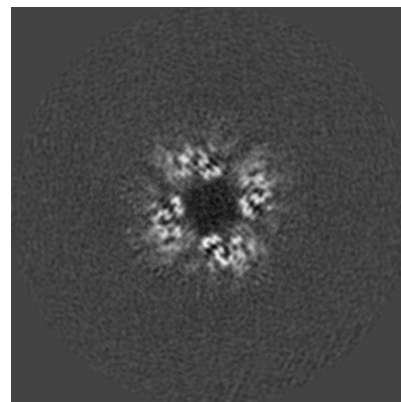
### 6.2.1 Primary map



X Index: 192

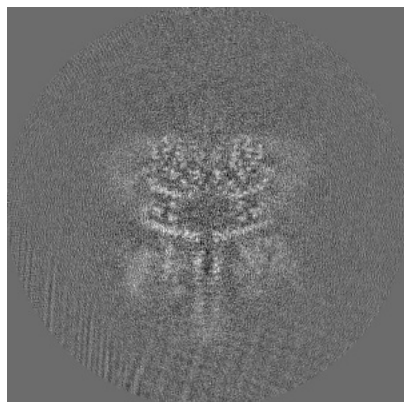


Y Index: 192

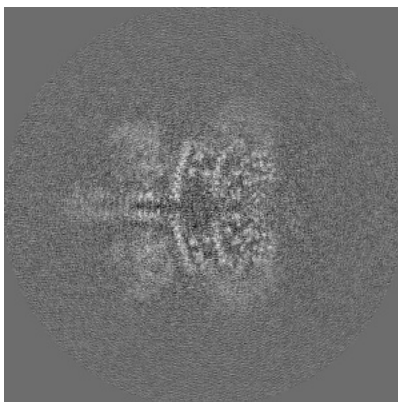


Z Index: 192

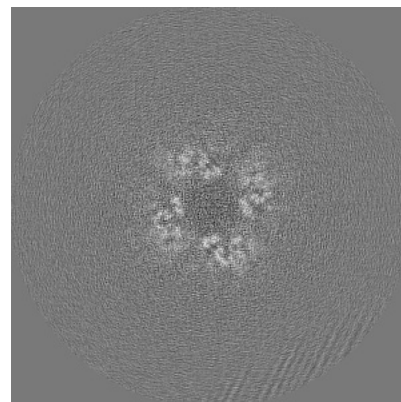
### 6.2.2 Raw map



X Index: 192



Y Index: 192

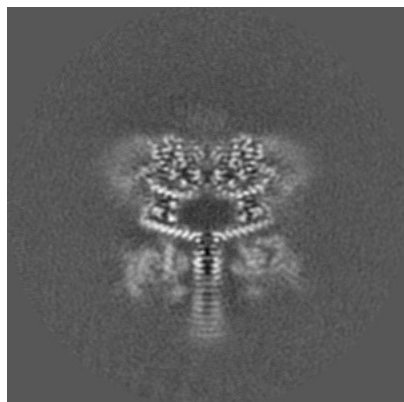


Z Index: 192

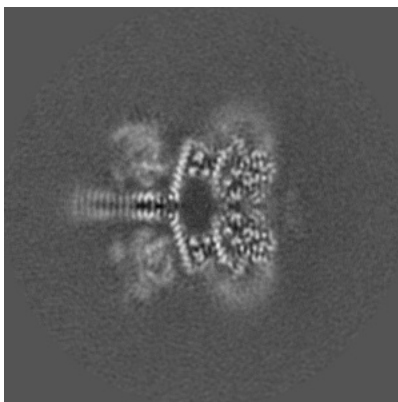
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

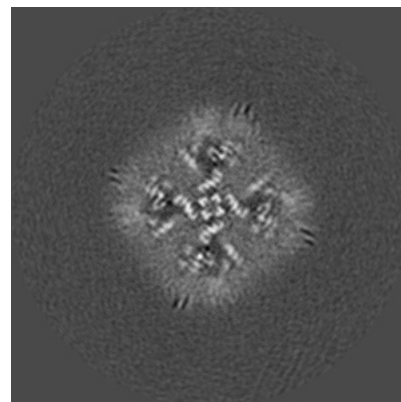
### 6.3.1 Primary map



X Index: 192

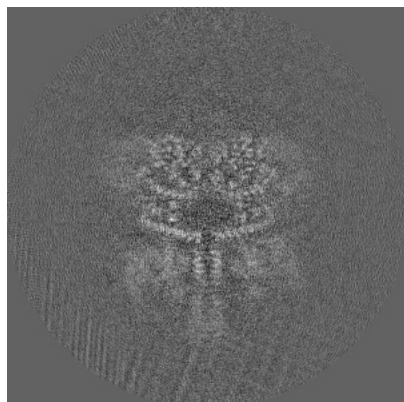


Y Index: 192

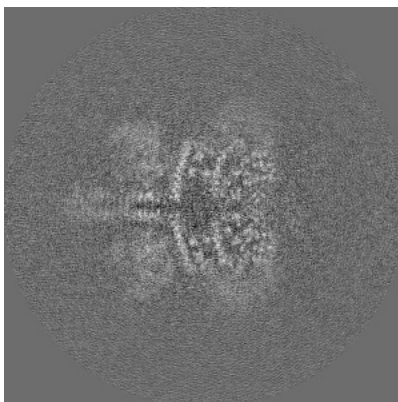


Z Index: 214

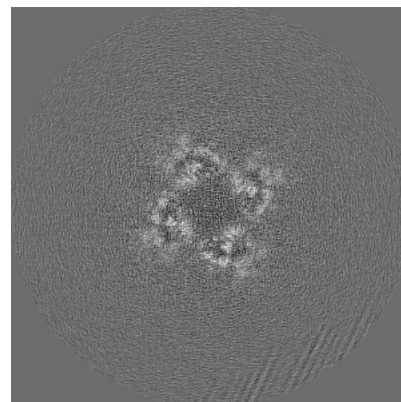
### 6.3.2 Raw map



X Index: 193



Y Index: 192



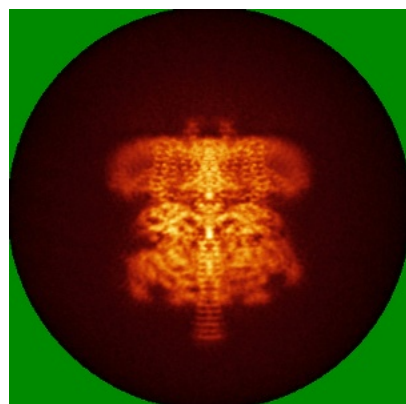
Z Index: 186

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

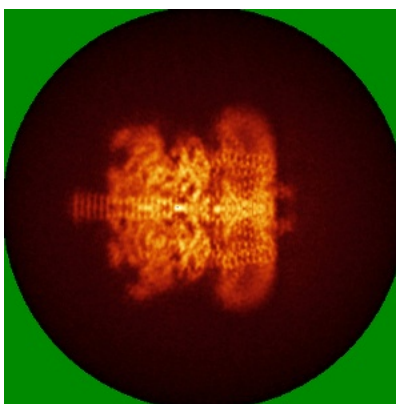


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

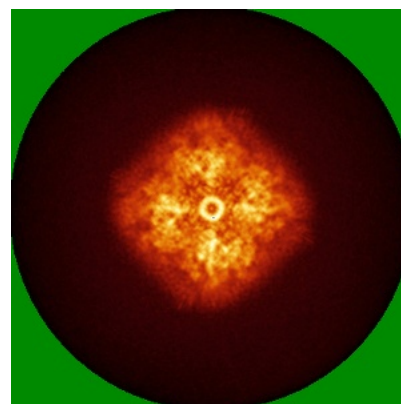
### 6.4.1 Primary map



X

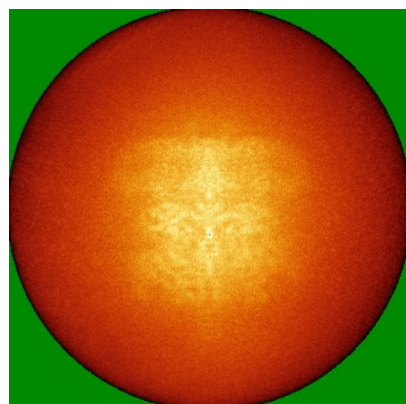


Y

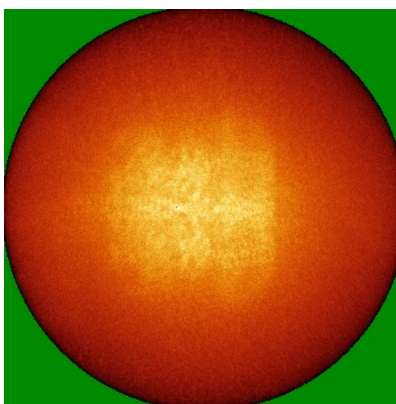


Z

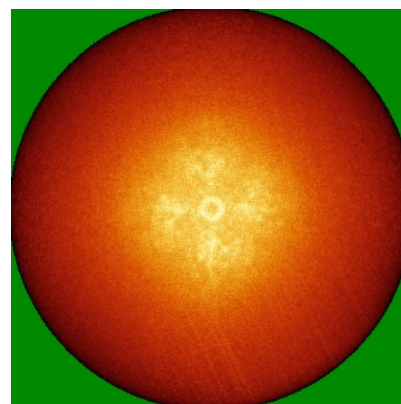
### 6.4.2 Raw map



X



Y

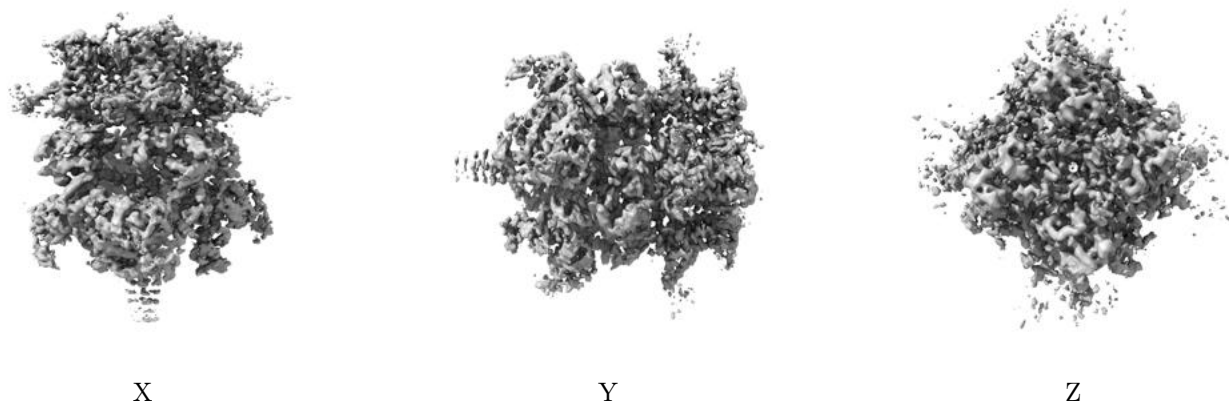


Z

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

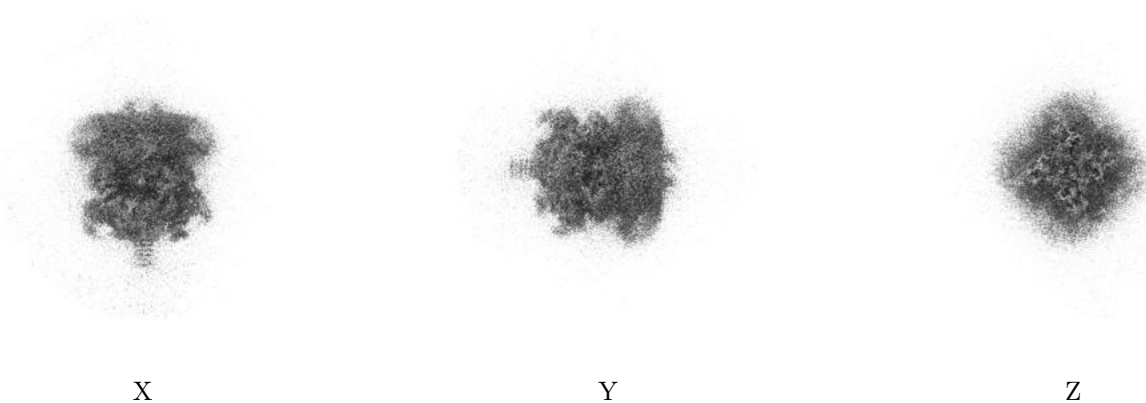
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

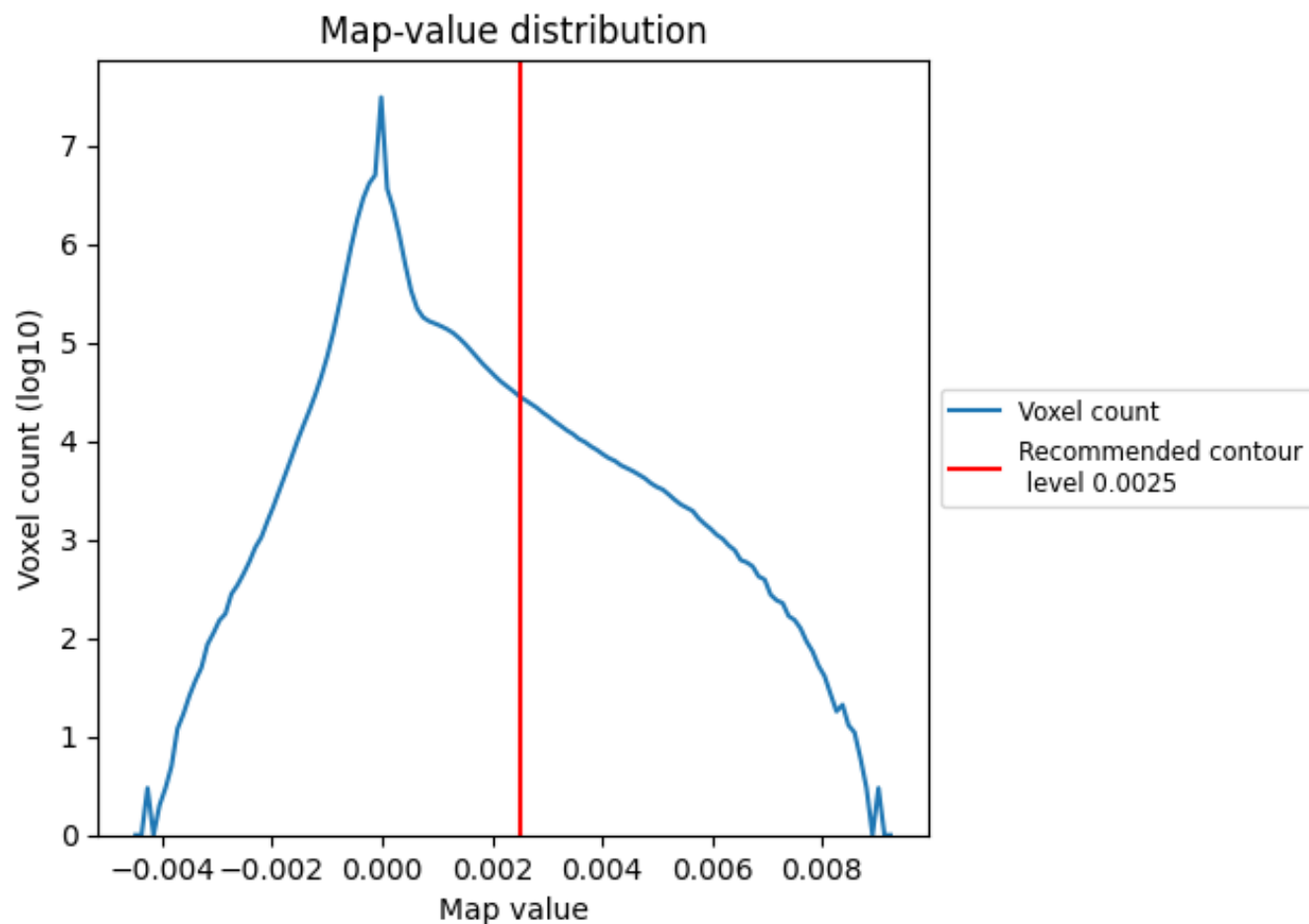
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

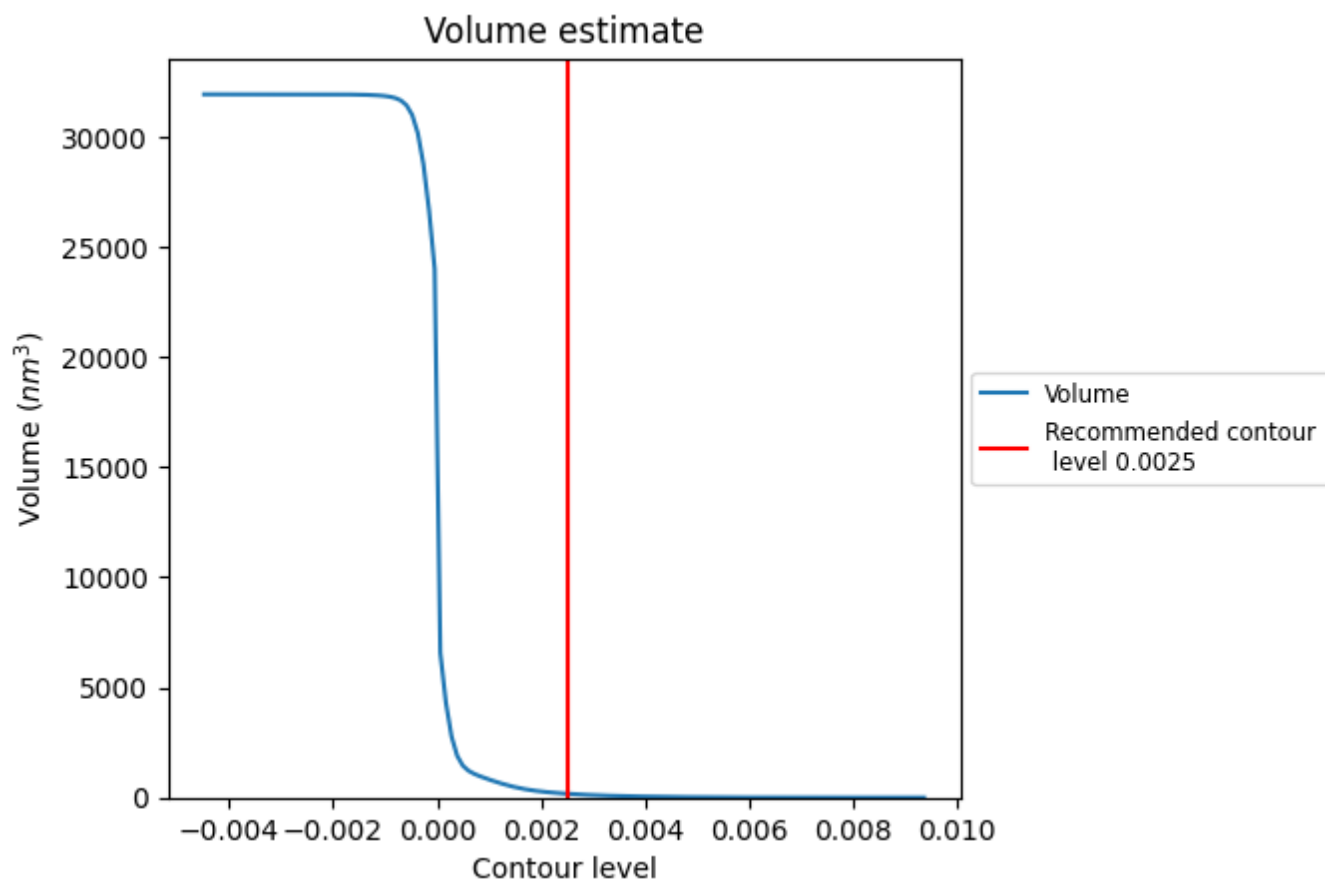
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

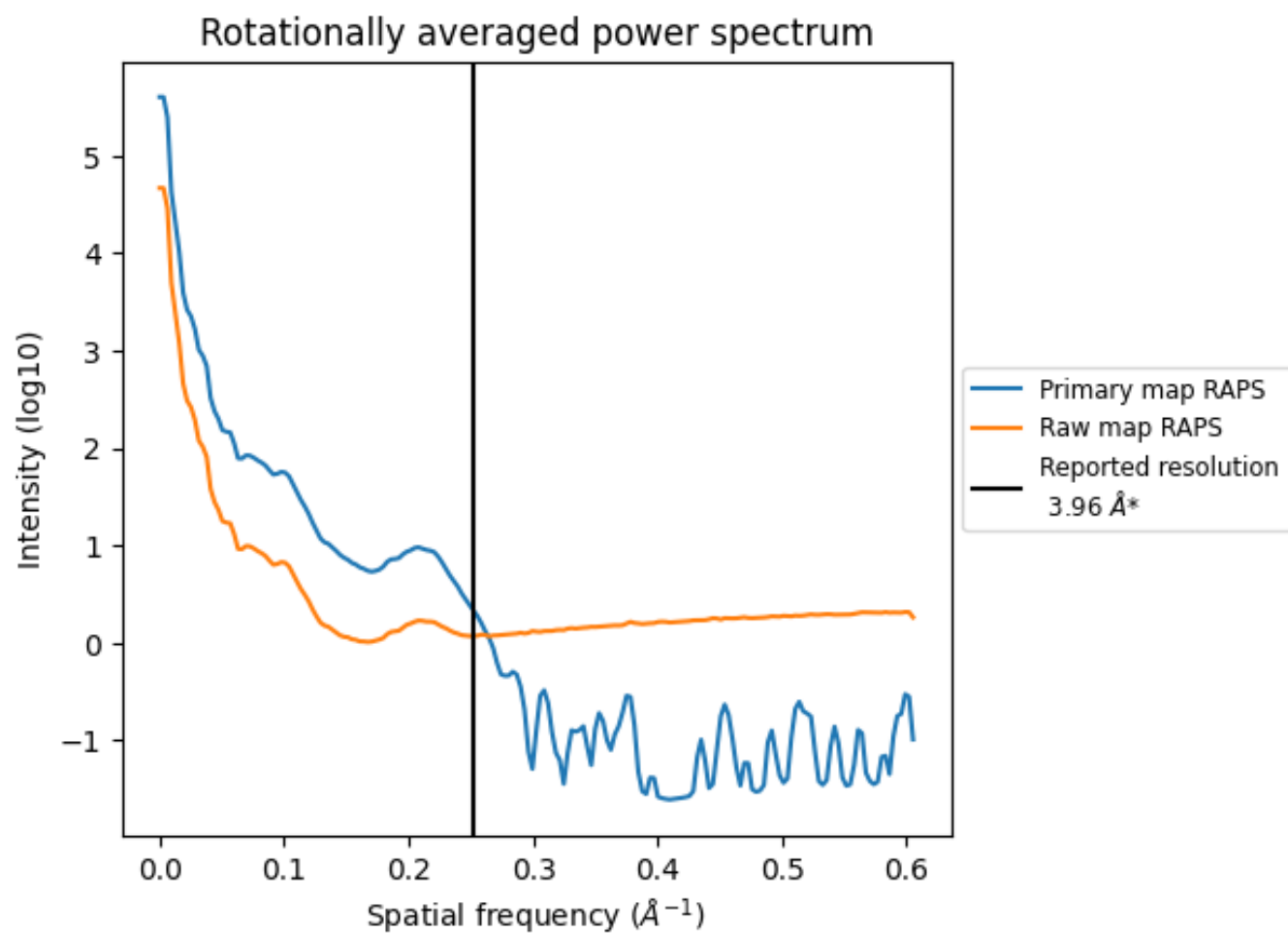


The volume at the recommended contour level is 172 nm<sup>3</sup>; this corresponds to an approximate mass of 155 kDa.

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 ⓘ

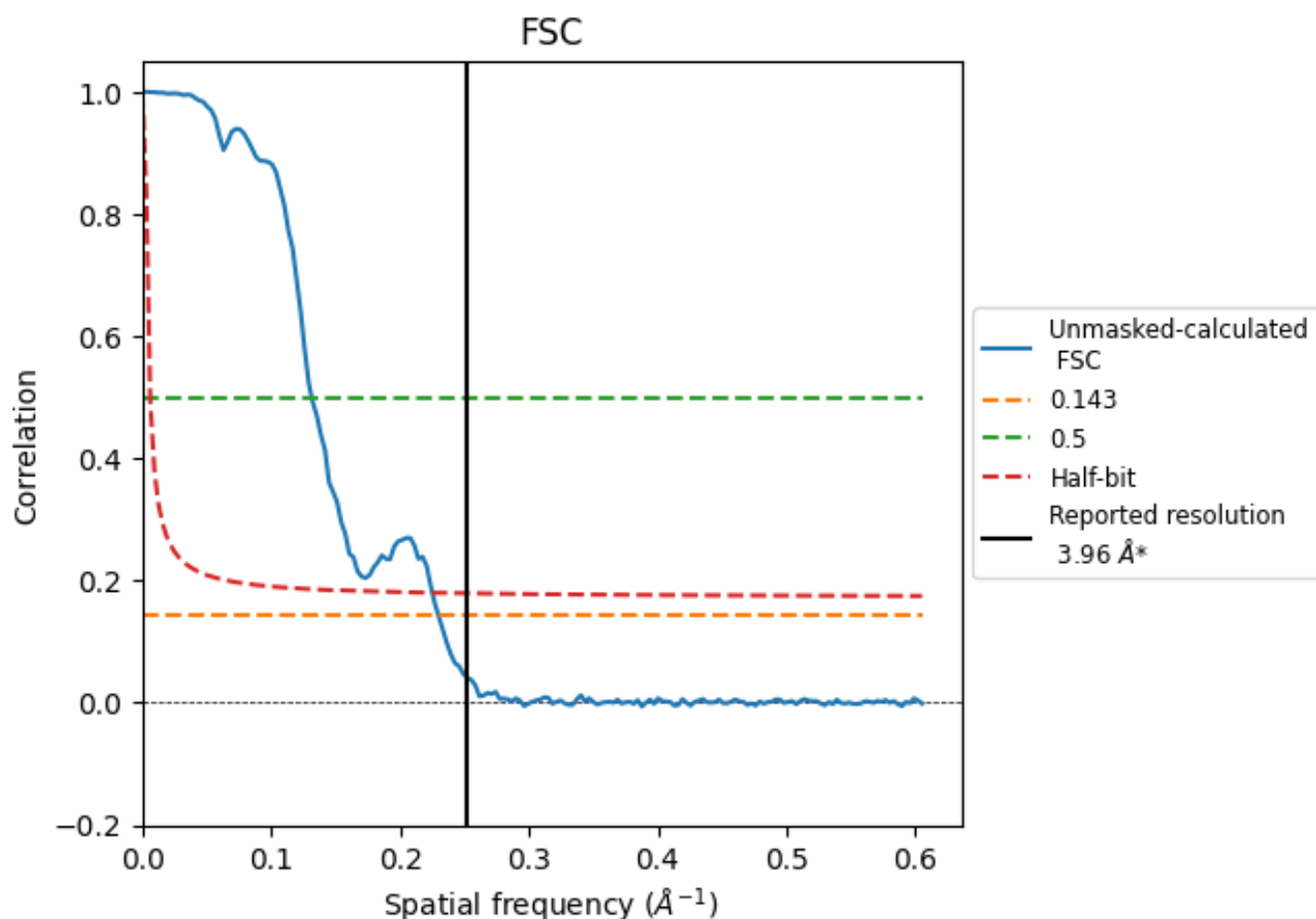


\*Reported resolution corresponds to spatial frequency of 0.253  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.253 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

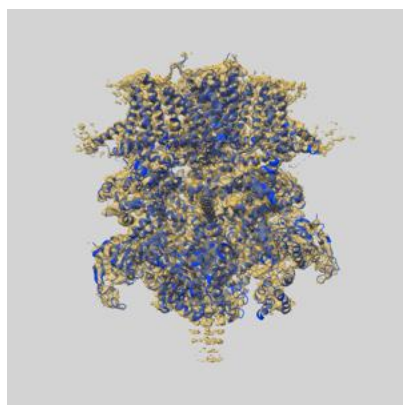
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.96	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.35	7.60	4.44

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

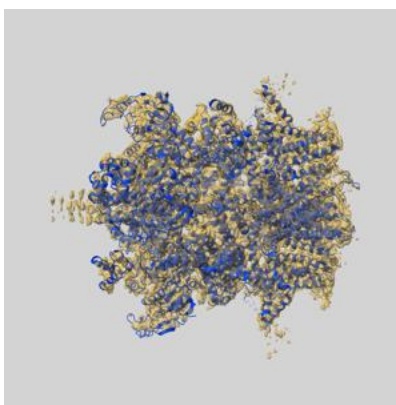
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70214 and PDB model 9O81. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

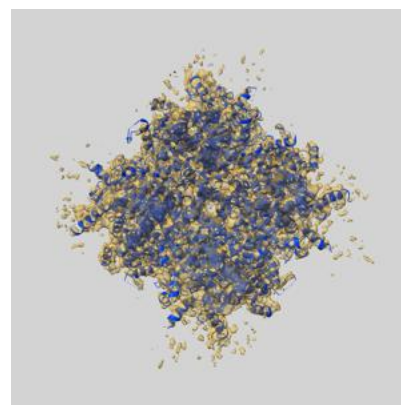
### 9.1 Map-model overlay [i](#)



X



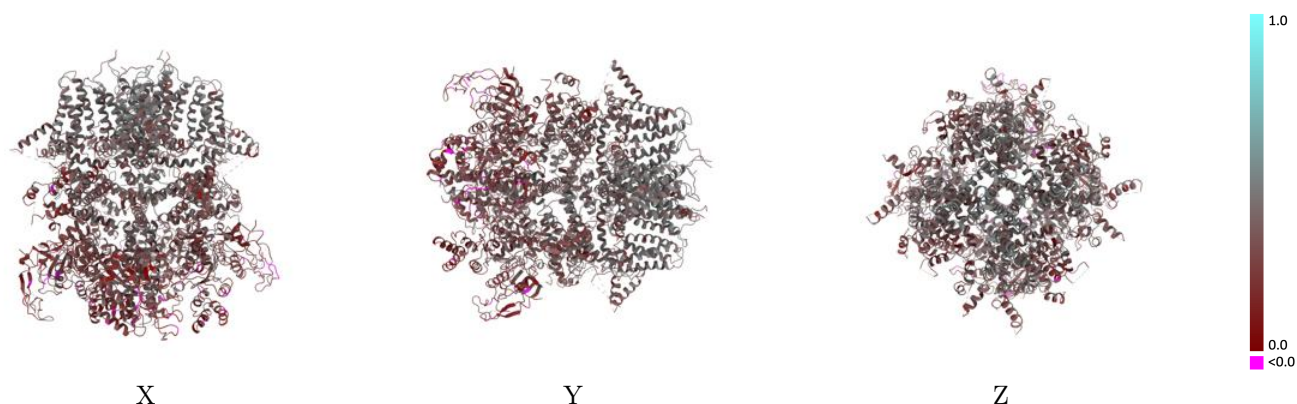
Y



Z

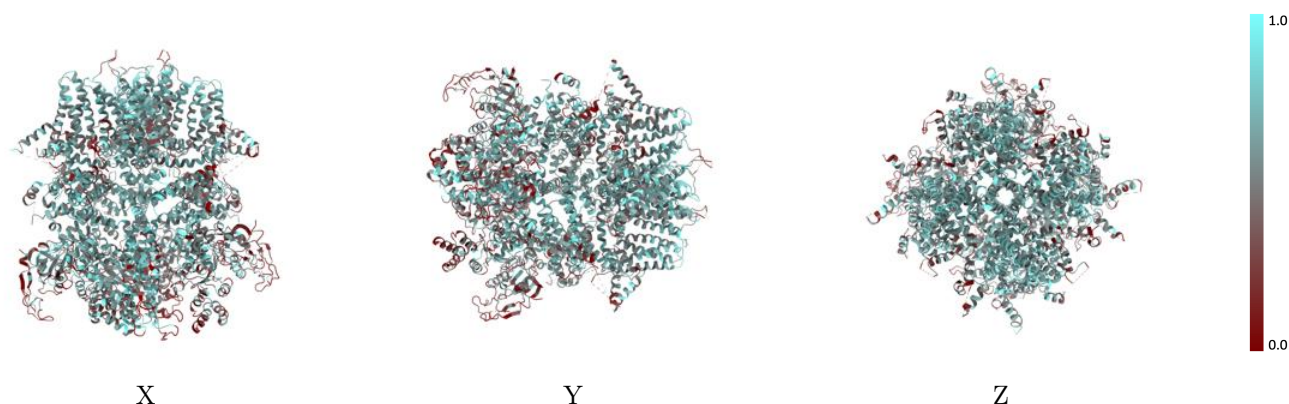
The images above show the 3D surface view of the map at the recommended contour level 0.0025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



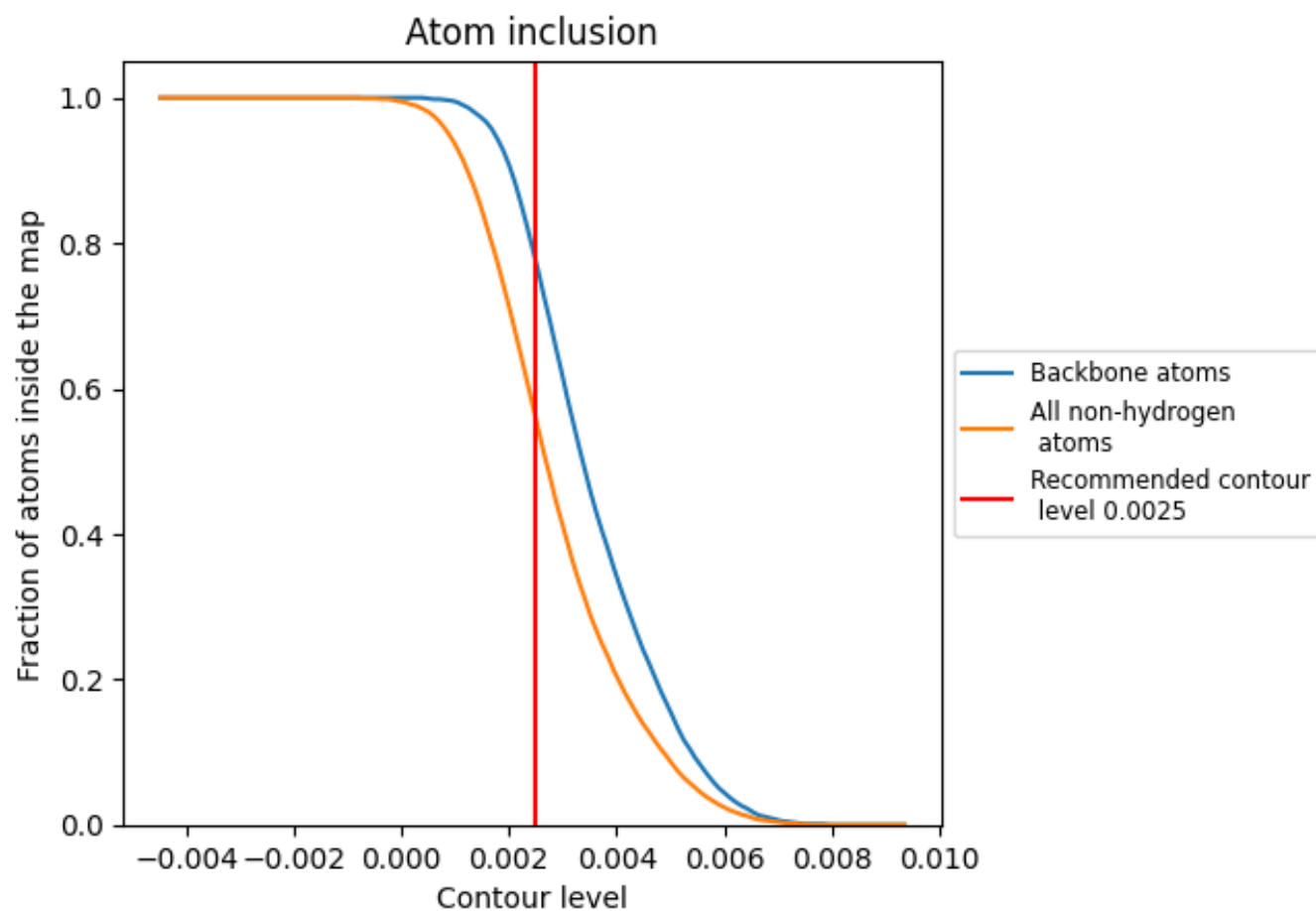
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0025).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 56% 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 (0.0025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5580	<div></div> 0.3400
A	<div></div> 0.5350	<div></div> 0.3480
B	<div></div> 0.5760	<div></div> 0.3350
C	<div></div> 0.5800	<div></div> 0.3380
D	<div></div> 0.5390	<div></div> 0.3390

