



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:29 PM UTC

PDB ID : 8Z3S / pdb_00008z3s
EMDB ID : EMD-39753
Title : Activation mechanism and novel binding site of the BKCa channel activator CTIBD
Authors : Lee, N.; Kim, S.; Jo, H.; Lee, N.Y.; Jin, M.S.; Park, C.S.
Deposited on : 2024-04-16
Resolution : 3.90 Å(reported)
Based on initial model : 6V38

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

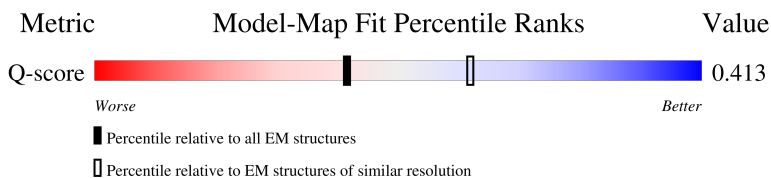
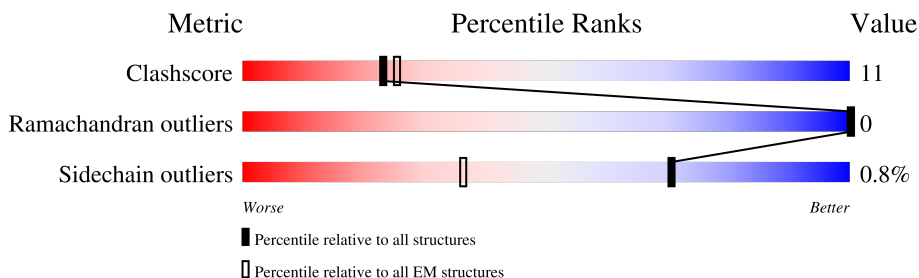
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	1114	 5% 57% 24% 19%
1	B	1114	 5% 58% 23% 19%
1	C	1114	 5% 58% 23% 19%
1	D	1114	 5% 61% 19% 19%

2 Entry composition [i](#)

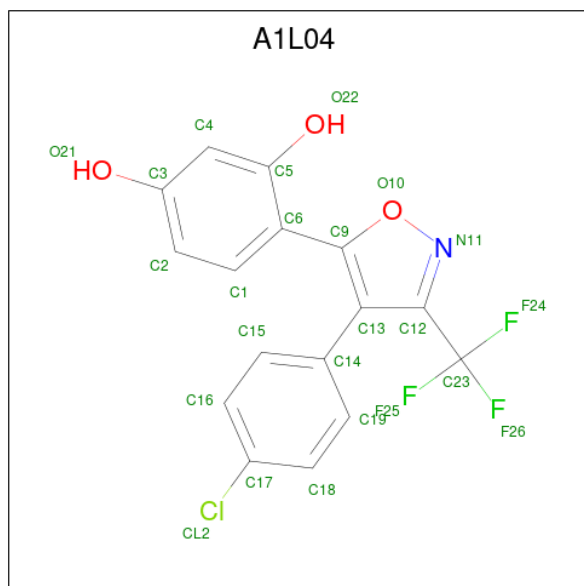
There are 5 unique types of molecules in this entry. The entry contains 29005 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Calcium-activated potassium channel subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	900	Total	C	N	O	S	0	0
			7168	4657	1171	1294	46		
1	B	900	Total	C	N	O	S	0	0
			7170	4657	1171	1296	46		
1	C	900	Total	C	N	O	S	0	0
			7158	4651	1168	1293	46		
1	D	900	Total	C	N	O	S	0	0
			7165	4654	1171	1295	45		

- Molecule 2 is 4-[4-(4-chlorophenyl)-3-(trifluoromethyl)-1,2-oxazol-5-yl]benzene-1,3-diol (CCD ID: A1L04) (formula: C₁₆H₉ClF₃NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	Cl	F	N	O
			24	16	1	3	1	3
2	A	1	Total	C	Cl	F	N	O
			24	16	1	3	1	3

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Mol	Chain	Residues	Atoms						AltConf
2	B	1	Total 24	C 16	Cl 1	F 3	N 1	O 3	0
2	B	1	Total 24	C 16	Cl 1	F 3	N 1	O 3	0
2	C	1	Total 24	C 16	Cl 1	F 3	N 1	O 3	0
2	C	1	Total 24	C 16	Cl 1	F 3	N 1	O 3	0
2	D	1	Total 24	C 16	Cl 1	F 3	N 1	O 3	0
2	D	1	Total 24	C 16	Cl 1	F 3	N 1	O 3	0

- # Y01

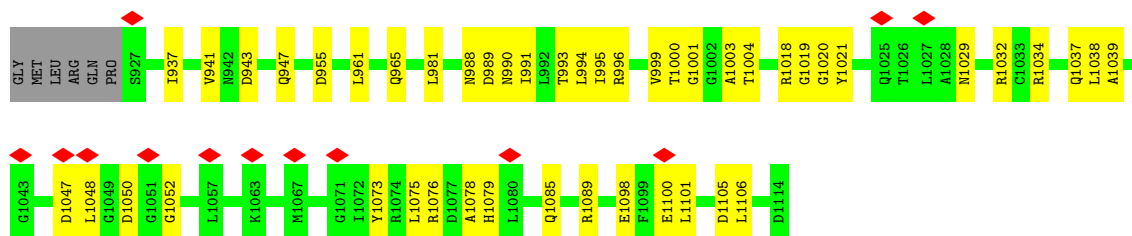
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total 35	C 31	O 4	0
3	B	1	Total 35	C 31	O 4	0
3	C	1	Total 35	C 31	O 4	0
3	D	1	Total 35	C 31	O 4	0

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- WORLD WIDE
PDB
PROTEIN DATA BANK

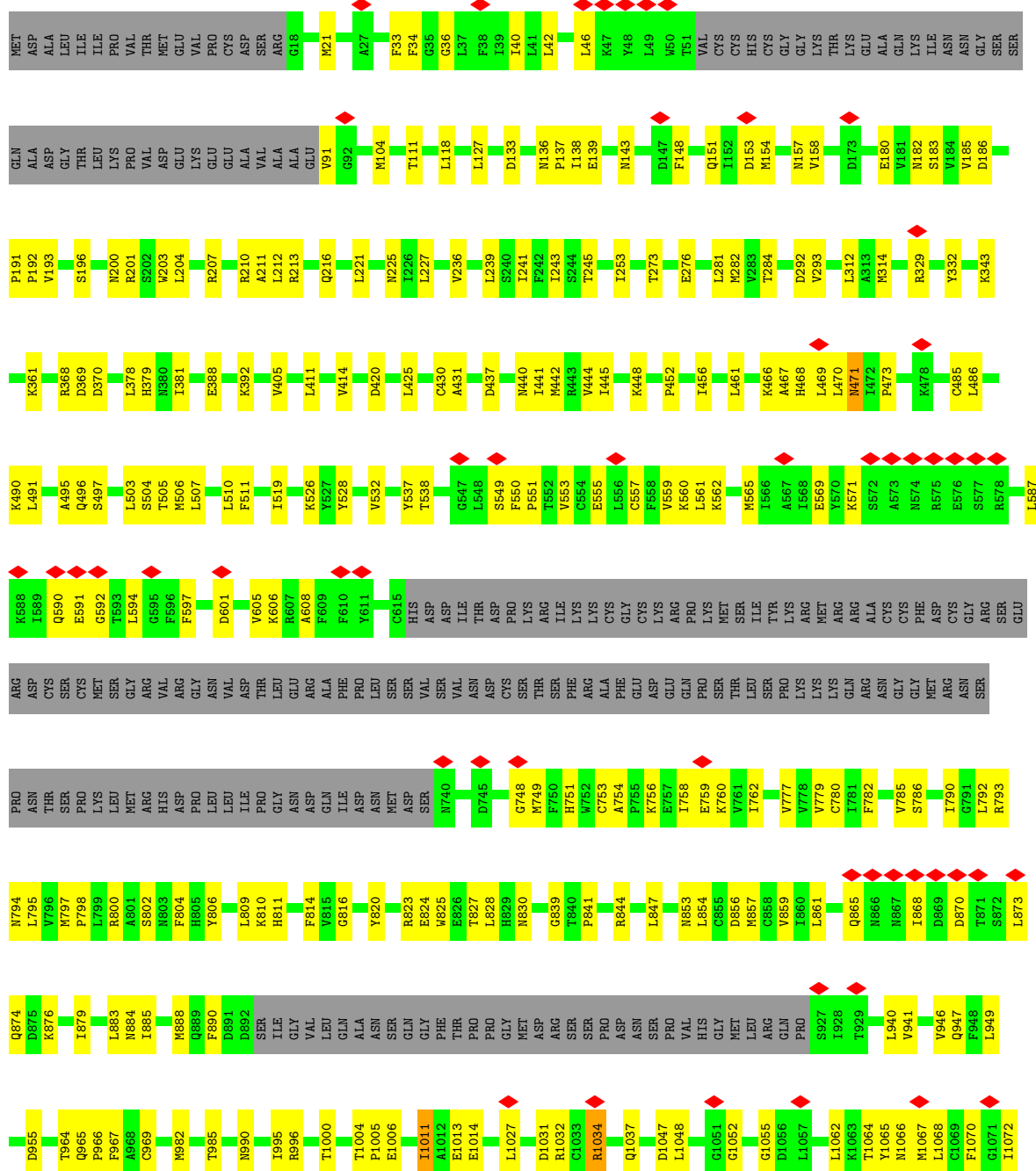
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Mg 1	0
4	B	1	Total 1	Mg 1	0
4	C	1	Total 1	Mg 1	0
4	D	1	Total 1	Mg 1	0

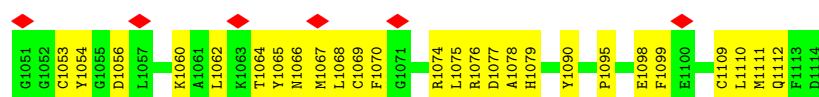
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total 2	Ca 2	0
5	B	2	Total 2	Ca 2	0
5	C	2	Total 2	Ca 2	0
5	D	2	Total 2	Ca 2	0



• Molecule 1: Calcium-activated potassium channel subunit alpha-1







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	288878	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	73000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.891	Depositor
Minimum map value	-0.757	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.0829	Depositor
Map size (Å)	282.0, 282.0, 282.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.41, 1.41, 1.41	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1L04, MG, CA, 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	0.38	0/7335	0.67	5/9958 (0.1%)
1	B	0.34	0/7337	0.58	7/9960 (0.1%)
1	C	0.24	0/7325	0.43	0/9946
1	D	0.26	0/7332	0.47	3/9955 (0.0%)
All	All	0.31	0/29329	0.55	15/39819 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	473	PRO	N-CA-C	8.33	124.89	113.65
1	D	473	PRO	N-CA-C	6.80	122.68	113.84
1	B	473	PRO	CB-CA-C	-6.16	102.60	112.21
1	A	996	ARG	N-CA-C	-5.78	105.53	113.56
1	A	37	LEU	N-CA-C	-5.62	105.15	111.28
1	A	28	SER	N-CA-C	-5.47	105.32	111.28
1	D	473	PRO	CB-CA-C	-5.35	104.25	111.85
1	B	466	LYS	CB-CA-C	-5.24	102.09	110.79
1	B	1031	ASP	N-CA-C	-5.22	106.14	112.88
1	B	473	PRO	CA-C-N	-5.22	114.46	122.60
1	B	473	PRO	C-N-CA	-5.22	114.46	122.60
1	D	790	ILE	N-CA-C	-5.17	108.80	113.71
1	A	1003	ALA	N-CA-C	-5.14	105.31	112.30
1	A	991	ILE	N-CA-C	-5.08	105.03	110.36
1	B	471	ASN	N-CA-C	5.04	116.86	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7168	0	7150	172	0
1	B	7170	0	7163	169	0
1	C	7158	0	7142	170	0
1	D	7165	0	7151	143	0
2	A	48	0	0	1	0
2	B	48	0	0	1	0
2	C	48	0	0	0	0
2	D	48	0	0	0	0
3	A	35	0	49	1	0
3	B	35	0	49	0	0
3	C	35	0	49	1	0
3	D	35	0	49	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
All	All	29005	0	28802	640	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 11.

All (640) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:LEU:O	1:C:46:LEU:HB2	1.71	0.90
1:C:558:PHE:HA	1:C:561:LEU:HB2	1.60	0.83
1:B:557:CYS:O	1:B:561:LEU:HB2	1.77	0.83
1:D:800:ARG:HH12	1:D:810:LYS:H	1.28	0.81
1:C:824:GLU:O	1:C:827:THR:HG22	1.79	0.81
1:A:473:PRO:HD3	1:B:883:LEU:HD21	1.65	0.78
1:A:865:GLN:HG3	1:A:941:VAL:HG11	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:GLY:HA3	1:A:1029:ASN:HD22	1.49	0.77
1:B:865:GLN:HG3	1:B:941:VAL:HG11	1.67	0.76
1:B:1062:LEU:HG	1:B:1066:ASN:HA	1.68	0.76
1:C:186:ASP:OD1	1:C:213:ARG:NH2	2.20	0.75
1:A:427:ASN:N	1:A:436:GLU:OE2	2.20	0.75
1:A:557:CYS:HA	1:A:561:LEU:HB2	1.69	0.74
1:B:559:VAL:HG23	1:B:560:LYS:HG2	1.68	0.74
1:C:582:ASN:HD22	1:C:1068:LEU:HG	1.52	0.74
1:C:813:VAL:HG12	1:C:835:SER:HB2	1.68	0.74
1:A:133:ASP:OD2	1:A:207:ARG:NH1	2.20	0.73
1:A:803:ASN:OD1	1:A:1032:ARG:NH1	2.21	0.73
1:D:167:ARG:NH2	1:D:182:ASN:OD1	2.21	0.72
1:A:392:LYS:HG2	1:D:223:PHE:HE1	1.54	0.72
1:D:785:VAL:O	1:D:823:ARG:NH1	2.23	0.71
1:B:571:LYS:HE2	1:B:587:LEU:HD11	1.72	0.71
1:C:785:VAL:O	1:C:823:ARG:NH2	2.24	0.71
1:A:855:CYS:SG	1:A:856:ASP:N	2.64	0.70
1:C:827:THR:HG23	1:C:828:LEU:N	2.06	0.70
1:C:133:ASP:OD2	1:C:207:ARG:NH1	2.25	0.70
1:C:865:GLN:HG3	1:C:941:VAL:HG21	1.72	0.70
1:D:1089:ARG:HH22	1:D:1106:LEU:HG	1.55	0.70
1:D:561:LEU:HD22	1:D:607:ARG:HD3	1.72	0.70
1:D:571:LYS:NZ	1:D:591:GLU:O	2.25	0.70
1:C:167:ARG:NH2	1:C:182:ASN:OD1	2.25	0.69
1:C:411:LEU:HD22	1:C:416:ILE:HD11	1.74	0.69
1:D:744:TYR:OH	1:D:1030:ARG:NH1	2.25	0.69
1:A:448:LYS:NZ	1:A:452:PRO:O	2.25	0.69
1:C:837:LEU:HD12	1:C:838:PRO:HD2	1.74	0.69
1:A:284:THR:HG21	1:A:304:MET:HE1	1.73	0.69
1:D:1075:LEU:HB2	1:D:1078:ALA:HB2	1.76	0.68
1:B:538:THR:HB	1:B:594:LEU:HD11	1.74	0.68
1:C:752:TRP:NE1	1:C:830:ASN:OD1	2.26	0.67
1:B:1062:LEU:HA	1:B:1067:MET:H	1.59	0.67
1:C:800:ARG:HH12	1:C:810:LYS:H	1.42	0.67
1:D:1062:LEU:HA	1:D:1066:ASN:HA	1.75	0.67
1:B:870:ASP:HB2	1:B:873:LEU:HB2	1.76	0.67
1:A:498:CYS:SG	1:A:499:LEU:N	2.67	0.67
1:A:965:GLN:OE1	1:A:1076:ARG:NH1	2.27	0.67
1:D:444:VAL:HG11	1:D:475:TRP:HZ3	1.60	0.67
1:D:553:VAL:HG23	1:D:565:MET:HE1	1.76	0.67
1:B:186:ASP:OD1	1:B:213:ARG:NH1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:PRO:HB2	1:D:462:GLN:HE22	1.61	0.66
1:D:139:GLU:OE1	1:D:201:ARG:NH2	2.29	0.66
1:D:1062:LEU:O	1:D:1066:ASN:ND2	2.28	0.66
1:A:563:LEU:HD11	1:A:597:PHE:HB3	1.78	0.66
1:C:491:LEU:HD12	1:C:795:LEU:HD12	1.76	0.66
1:A:857:MET:HE2	1:A:937:ILE:HD13	1.78	0.66
1:D:292:ASP:OD1	1:D:293:VAL:N	2.29	0.66
1:C:378:LEU:HD22	1:C:414:VAL:HG21	1.79	0.65
1:D:559:VAL:HG23	1:D:560:LYS:HG2	1.78	0.65
1:D:1048:LEU:HD11	1:D:1060:LYS:HD3	1.77	0.65
1:A:442:MET:HE1	1:B:876:LYS:HA	1.79	0.65
1:D:186:ASP:OD1	1:D:213:ARG:NH2	2.29	0.65
1:B:138:ILE:HG22	1:B:139:GLU:HG3	1.79	0.65
1:C:262:PRO:HA	1:C:266:PHE:HE1	1.61	0.65
1:C:488:GLU:OE2	1:C:996:ARG:NH2	2.30	0.64
1:A:491:LEU:HD11	1:A:861:LEU:HD21	1.78	0.64
1:D:133:ASP:OD2	1:D:207:ARG:NH1	2.31	0.64
1:C:448:LYS:NZ	1:C:452:PRO:O	2.30	0.64
1:B:571:LYS:HG3	1:B:587:LEU:HD21	1.79	0.64
1:A:441:ILE:HG12	1:A:469:LEU:HD11	1.80	0.64
1:C:1001:GLY:O	1:C:1032:ARG:NH1	2.31	0.64
1:B:785:VAL:O	1:B:823:ARG:NH1	2.31	0.64
1:C:459:GLN:NE2	1:C:982:MET:SD	2.66	0.64
1:C:402:GLN:O	1:C:413:ARG:NH2	2.30	0.63
1:C:513:MET:HG2	1:C:535:GLU:HG2	1.80	0.63
1:D:1075:LEU:HA	1:D:1089:ARG:HG2	1.78	0.63
1:D:868:ILE:HD12	1:D:873:LEU:HB3	1.81	0.63
1:C:292:ASP:OD1	1:C:293:VAL:N	2.31	0.63
1:A:550:PHE:CD1	1:A:551:PRO:HD3	2.33	0.63
1:C:405:VAL:HG23	1:C:411:LEU:HD21	1.79	0.63
1:B:104:MET:SD	1:B:111:THR:OG1	2.58	0.62
1:C:522:ASP:O	1:C:1079:HIS:NE2	2.26	0.62
1:D:153:ASP:OD1	1:D:157:ASN:ND2	2.33	0.62
1:D:740:ASN:HA	1:D:743:LYS:HZ3	1.63	0.62
1:B:793:ARG:O	1:B:797:MET:HG3	1.99	0.62
1:C:308:ILE:HG23	1:C:312:LEU:HD13	1.82	0.62
1:C:342:ARG:NH2	1:C:374:GLU:OE2	2.32	0.62
1:D:965:GLN:OE1	1:D:1076:ARG:NH1	2.33	0.62
1:A:1052:GLY:HA2	1:A:1101:LEU:HB2	1.82	0.61
1:B:800:ARG:HH12	1:B:810:LYS:H	1.48	0.61
1:A:955:ASP:OD2	1:D:449:ASN:ND2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:LEU:HD11	1:B:414:VAL:HG21	1.82	0.61
1:B:792:LEU:HD22	1:B:814:PHE:HE2	1.65	0.61
1:B:965:GLN:NE2	1:B:969:CYS:SG	2.72	0.61
1:A:1075:LEU:HB2	1:A:1078:ALA:HB2	1.83	0.60
1:C:476:ASN:N	1:C:481:ASP:OD2	2.30	0.60
1:D:813:VAL:HG12	1:D:835:SER:HB2	1.83	0.60
1:D:868:ILE:HB	1:D:873:LEU:HD13	1.83	0.60
1:D:253:ILE:HD12	1:D:304:MET:HE1	1.82	0.60
1:A:793:ARG:O	1:A:797:MET:HG3	2.02	0.60
1:C:449:ASN:ND2	1:D:955:ASP:OD2	2.33	0.60
1:D:844:ARG:HG3	1:D:888:MET:HE2	1.82	0.60
1:B:491:LEU:HD12	1:B:795:LEU:HB2	1.83	0.59
1:C:853:ASN:OD1	1:C:854:LEU:N	2.35	0.59
1:B:853:ASN:ND2	1:B:854:LEU:HD23	2.18	0.59
1:B:777:VAL:HG23	1:B:857:MET:HB2	1.84	0.59
1:C:491:LEU:HD11	1:C:861:LEU:HD21	1.84	0.59
1:B:1075:LEU:HB2	1:B:1078:ALA:HB2	1.85	0.59
1:D:501:GLN:HE22	1:D:935:PRO:HB3	1.67	0.59
1:A:186:ASP:HA	1:A:189:THR:HG22	1.84	0.59
1:A:522:ASP:O	1:A:1079:HIS:NE2	2.35	0.59
1:B:425:LEU:HD13	1:B:982:MET:HE1	1.84	0.59
1:C:748:GLY:HA3	1:C:1029:ASN:HB3	1.84	0.58
1:A:402:GLN:O	1:A:413:ARG:NH2	2.36	0.58
1:D:491:LEU:HD12	1:D:795:LEU:HD12	1.84	0.58
1:B:292:ASP:OD1	1:B:293:VAL:N	2.36	0.58
1:A:437:ASP:OD1	1:A:465:ASN:ND2	2.35	0.58
1:D:378:LEU:HD12	1:D:414:VAL:HG21	1.84	0.58
1:A:517:ILE:HD12	1:A:529:LEU:HD21	1.86	0.58
1:A:449:ASN:OD1	1:A:450:TYR:N	2.36	0.58
1:A:864:ASN:OD1	1:A:867:ASN:ND2	2.37	0.58
1:C:477:TRP:HA	1:C:481:ASP:HB2	1.86	0.58
1:C:23:TRP:H	1:C:23:TRP:CD1	2.22	0.57
1:B:245:THR:HG21	1:B:314:MET:HE2	1.84	0.57
1:C:525:GLN:N	1:C:525:GLN:OE1	2.37	0.57
1:A:182:ASN:ND2	1:A:216:GLN:OE1	2.37	0.57
1:B:485:CYS:SG	1:B:486:LEU:N	2.77	0.57
1:B:1109:CYS:SG	1:B:1110:LEU:N	2.77	0.57
1:D:1064:THR:HG23	1:D:1065:TYR:HD1	1.69	0.57
1:A:153:ASP:O	1:A:157:ASN:ND2	2.38	0.57
1:A:491:LEU:HD12	1:A:795:LEU:HD12	1.86	0.57
1:C:499:LEU:HD21	1:C:804:PHE:HZ	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:430:CYS:SG	1:D:431:ALA:N	2.78	0.57
1:B:1013:GLU:O	1:C:845:ALA:HB2	2.05	0.57
1:C:496:GLN:O	1:C:496:GLN:NE2	2.38	0.57
1:D:488:GLU:HG3	1:D:794:ASN:HD21	1.69	0.57
1:B:847:LEU:HD13	1:B:885:ILE:HD11	1.87	0.56
1:B:332:TYR:OH	1:B:388:GLU:OE2	2.22	0.56
1:A:126:ALA:HB1	1:A:210:ARG:HD3	1.87	0.56
1:C:281:LEU:O	1:C:284:THR:HG22	2.05	0.56
1:D:21:MET:HE3	1:D:24:ALA:HB2	1.87	0.56
1:D:604:GLU:O	1:D:607:ARG:HG2	2.05	0.56
1:A:797:MET:HB2	1:A:798:PRO:HD3	1.87	0.56
1:C:797:MET:HB3	1:C:798:PRO:HD3	1.88	0.56
1:A:837:LEU:HD12	1:A:838:PRO:HD2	1.86	0.56
1:C:368:ARG:NH1	1:C:513:MET:HE1	2.21	0.56
1:C:749:MET:HG3	1:C:750:PHE:CE1	2.40	0.56
1:C:888:MET:HE3	1:C:890:PHE:HZ	1.70	0.56
1:C:827:THR:CG2	1:C:828:LEU:N	2.69	0.56
1:C:262:PRO:HA	1:C:266:PHE:CE1	2.41	0.55
1:C:803:ASN:O	1:C:1034:ARG:NH1	2.39	0.55
1:A:559:VAL:O	1:A:562:LYS:NZ	2.40	0.55
1:D:490:LYS:HG2	1:D:491:LEU:HD22	1.88	0.55
1:D:844:ARG:HD3	1:D:888:MET:HG3	1.88	0.55
1:D:870:ASP:HB3	1:D:873:LEU:HG	1.87	0.55
1:B:448:LYS:NZ	1:B:452:PRO:O	2.39	0.55
1:C:749:MET:HE1	1:C:1001:GLY:C	2.31	0.55
1:C:332:TYR:OH	1:C:388:GLU:OE2	2.25	0.55
1:D:347:VAL:HG22	1:D:423:LEU:HB2	1.87	0.55
1:A:92:GLY:O	1:A:95:THR:OG1	2.22	0.55
1:A:305:VAL:HG13	1:B:282:MET:HG2	1.88	0.55
1:A:879:ILE:O	1:A:883:LEU:HD12	2.07	0.55
1:C:568:ILE:HA	1:C:595:GLY:HA2	1.88	0.55
1:B:825:TRP:HD1	1:B:828:LEU:HB2	1.72	0.55
1:B:1052:GLY:HA2	1:B:1101:LEU:H	1.71	0.55
1:C:120:PHE:HB2	1:C:220:ILE:HD12	1.89	0.55
1:C:1038:LEU:HD11	1:C:1067:MET:HE3	1.88	0.55
1:A:342:ARG:NH2	1:A:374:GLU:OE2	2.40	0.55
1:A:848:ARG:NH2	1:D:1013:GLU:OE2	2.40	0.55
1:C:779:VAL:HG23	1:C:859:VAL:HG13	1.89	0.54
1:C:1075:LEU:HB2	1:C:1078:ALA:HB2	1.89	0.54
1:B:868:ILE:O	1:B:874:GLN:NE2	2.40	0.54
1:D:982:MET:O	1:D:985:THR:OG1	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:LEU:HA	1:A:607:ARG:HH21	1.70	0.54
1:B:506:MET:HE2	1:B:1070:PHE:HE2	1.73	0.54
1:A:430:CYS:SG	1:A:431:ALA:N	2.80	0.54
1:A:602:ALA:HA	1:A:605:VAL:HG12	1.88	0.54
1:A:847:LEU:HD22	1:A:888:MET:HE1	1.88	0.54
1:C:888:MET:HE3	1:C:890:PHE:CZ	2.42	0.54
1:B:440:ASN:O	1:B:444:VAL:HG23	2.07	0.54
1:D:464:HIS:NE2	1:D:465:ASN:OD1	2.41	0.54
1:C:994:LEU:O	1:C:997:THR:HB	2.08	0.54
1:D:870:ASP:H	1:D:873:LEU:HD12	1.73	0.54
1:A:542:SER:HB2	1:A:609:PHE:H	1.73	0.54
1:A:877:GLU:HG2	1:A:878:CYS:N	2.23	0.54
1:A:1098:GLU:N	1:A:1098:GLU:OE1	2.41	0.54
1:A:514:ARG:O	1:A:533:SER:OG	2.27	0.53
1:A:784:ASP:HA	1:A:820:TYR:HB2	1.89	0.53
1:B:127:LEU:HD21	1:B:211:ALA:HB2	1.90	0.53
1:D:847:LEU:HD22	1:D:852:ILE:HD11	1.90	0.53
1:A:379:HIS:CG	1:A:380:ASN:H	2.26	0.53
1:A:446:SER:HA	1:A:449:ASN:ND2	2.24	0.53
1:C:105:ILE:HD11	1:C:166:LEU:HB3	1.90	0.53
1:D:787:SER:O	1:D:823:ARG:NH2	2.42	0.53
1:B:528:TYR:O	1:B:532:VAL:HG23	2.09	0.53
1:D:362:ASP:OD2	1:D:980:SER:OG	2.23	0.53
1:B:497:SER:OG	1:B:504:SER:N	2.42	0.53
1:B:1066:ASN:ND2	1:B:1112:GLN:OE1	2.35	0.53
1:A:798:PRO:HG3	1:A:1000:THR:HA	1.90	0.53
1:B:405:VAL:HG23	1:B:411:LEU:HD21	1.90	0.53
1:A:888:MET:HG2	1:A:890:PHE:HE1	1.73	0.52
1:B:253:ILE:HG13	1:B:281:LEU:HD21	1.91	0.52
1:B:569:GLU:HG2	1:B:594:LEU:HB3	1.91	0.52
1:D:497:SER:OG	1:D:504:SER:N	2.43	0.52
1:A:989:ASP:OD1	1:A:990:ASN:N	2.42	0.52
1:C:245:THR:HG21	1:C:314:MET:HE1	1.91	0.52
1:D:484:ILE:HD11	1:D:985:THR:HG21	1.91	0.52
1:B:947:GLN:HB2	1:B:955:ASP:CG	2.35	0.52
1:C:368:ARG:HG2	1:C:369:ASP:H	1.74	0.52
1:B:758:ILE:HB	1:B:825:TRP:HZ3	1.74	0.52
1:B:856:ASP:O	1:B:857:MET:HE2	2.10	0.52
1:D:874:GLN:OE1	1:D:874:GLN:N	2.40	0.52
1:A:411:LEU:HD21	1:A:416:ILE:HG21	1.92	0.52
1:C:741:VAL:O	1:C:743:LYS:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:764:THR:OG1	1:C:767:GLU:OE1	2.20	0.52
1:C:1062:LEU:HA	1:C:1066:ASN:HA	1.91	0.52
1:D:120:PHE:O	1:D:123:SER:OG	2.26	0.52
1:A:144:PHE:O	1:A:151:GLN:NE2	2.43	0.52
1:C:284:THR:HG23	1:C:285:MET:N	2.24	0.52
1:A:538:THR:HB	1:A:988:ASN:HD21	1.75	0.51
1:C:870:ASP:OD2	1:C:872:SER:OG	2.28	0.51
1:A:223:PHE:HE1	1:B:392:LYS:HG2	1.75	0.51
1:B:368:ARG:HG3	1:B:369:ASP:N	2.25	0.51
1:B:157:ASN:HD22	1:B:193:VAL:HG21	1.74	0.51
1:B:830:ASN:O	1:B:830:ASN:ND2	2.41	0.51
1:C:610:PHE:HE1	1:C:614:ALA:HB3	1.75	0.51
1:A:871:THR:HA	1:A:874:GLN:HE22	1.75	0.51
1:B:153:ASP:OD1	1:B:157:ASN:ND2	2.44	0.51
1:B:437:ASP:O	1:B:441:ILE:HG13	2.11	0.51
1:D:550:PHE:HA	1:D:553:VAL:HG22	1.91	0.51
1:A:228:LYS:O	1:A:229:THR:HG23	2.11	0.51
1:A:804:PHE:HA	1:A:1034:ARG:HH11	1.74	0.51
1:C:368:ARG:CZ	1:C:513:MET:HE1	2.40	0.51
1:D:837:LEU:HD12	1:D:838:PRO:HD2	1.92	0.51
1:A:888:MET:HG2	1:A:890:PHE:CE1	2.45	0.51
1:D:853:ASN:HB3	1:D:890:PHE:CE2	2.45	0.51
1:A:215:ILE:HD12	1:A:241:ILE:HD13	1.93	0.51
1:A:773:LEU:HB3	1:A:776:HIS:ND1	2.26	0.51
1:B:42:LEU:O	1:B:46:LEU:N	2.33	0.51
1:C:253:ILE:HG13	1:C:281:LEU:HD21	1.93	0.51
1:C:430:CYS:SG	1:C:431:ALA:N	2.84	0.51
1:C:589:ILE:HG22	1:C:590:GLN:O	2.11	0.51
1:D:756:LYS:HD3	1:D:760:LYS:HD2	1.92	0.51
1:A:153:ASP:OD1	1:A:157:ASN:ND2	2.44	0.50
1:A:747:THR:HG23	1:A:749:MET:H	1.75	0.50
1:D:460:MET:HE2	1:D:465:ASN:HB3	1.92	0.50
1:A:369:ASP:OD1	1:A:370:ASP:N	2.41	0.50
1:B:490:LYS:HG2	1:B:491:LEU:HD22	1.92	0.50
1:B:844:ARG:HG2	1:B:884:ASN:HD21	1.76	0.50
1:B:982:MET:O	1:B:985:THR:HB	2.11	0.50
1:A:272:LEU:HA	1:A:276:GLU:OE1	2.12	0.50
1:D:1062:LEU:HD12	1:D:1066:ASN:HA	1.93	0.50
1:B:143:ASN:HA	1:B:200:ASN:HD21	1.77	0.50
1:C:506:MET:HE1	1:C:1070:PHE:O	2.11	0.50
1:A:147:ASP:OD1	1:A:149:THR:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:ILE:O	1:A:590:GLN:HG3	2.11	0.50
1:B:221:LEU:HD13	1:B:227:LEU:HD11	1.94	0.50
1:B:800:ARG:NH1	1:B:810:LYS:H	2.09	0.50
1:A:947:GLN:HB2	1:A:955:ASP:CG	2.37	0.50
1:D:853:ASN:OD1	1:D:854:LEU:N	2.44	0.50
1:A:203:TRP:CH2	1:A:205:GLY:HA3	2.47	0.49
1:C:857:MET:HE1	1:C:937:ILE:HG13	1.93	0.49
1:B:868:ILE:HD12	1:B:873:LEU:HB3	1.93	0.49
1:D:193:VAL:O	1:D:196:SER:OG	2.24	0.49
1:C:504:SER:OG	1:C:505:THR:N	2.45	0.49
1:A:1037:GLN:O	1:A:1038:LEU:HD23	2.13	0.49
1:B:1047:ASP:OD1	1:B:1048:LEU:N	2.45	0.49
1:A:368:ARG:HH22	1:A:513:MET:HE3	1.77	0.49
1:A:566:ILE:HD11	1:A:598:ILE:HD11	1.93	0.49
1:A:800:ARG:NH1	1:A:809:LEU:HB2	2.27	0.49
1:C:363:PHE:HD2	1:C:364:LEU:HD22	1.78	0.49
1:D:428:LYS:NZ	1:D:979:ASP:OD2	2.45	0.49
1:A:378:LEU:HD12	1:A:414:VAL:HG21	1.94	0.49
1:A:826:GLU:O	1:A:829:HIS:ND1	2.40	0.49
1:D:203:TRP:CD1	1:D:204:LEU:N	2.81	0.49
1:D:229:THR:HG23	1:D:231:ASN:H	1.78	0.49
1:A:469:LEU:HD23	1:A:475:TRP:CH2	2.48	0.49
1:A:1073:TYR:CE1	1:A:1089:ARG:HB2	2.47	0.49
1:B:284:THR:OG1	1:C:290:TYR:OH	2.20	0.49
1:B:888:MET:HG2	1:B:890:PHE:CE1	2.48	0.49
1:D:262:PRO:HG2	1:D:263:TRP:CE3	2.47	0.49
1:D:491:LEU:HD11	1:D:861:LEU:HD21	1.95	0.49
1:A:780:CYS:HB3	1:A:841:PRO:CG	2.43	0.48
1:A:1089:ARG:HH21	1:A:1105:ASP:HA	1.77	0.48
1:B:550:PHE:HA	1:B:553:VAL:HG12	1.93	0.48
1:C:368:ARG:HG2	1:C:369:ASP:N	2.27	0.48
1:A:572:SER:OG	1:A:574:ASN:O	2.26	0.48
1:B:491:LEU:HD11	1:B:861:LEU:HD21	1.95	0.48
1:B:758:ILE:HG23	1:B:759:GLU:OE2	2.13	0.48
1:C:1074:ARG:NH2	1:C:1090:TYR:OH	2.46	0.48
1:B:203:TRP:CD1	1:B:204:LEU:N	2.81	0.48
1:B:442:MET:HA	1:B:445:ILE:HD12	1.94	0.48
1:B:780:CYS:HB3	1:B:841:PRO:HG3	1.95	0.48
1:B:888:MET:HG2	1:B:890:PHE:HE1	1.78	0.48
1:C:1034:ARG:O	1:C:1110:LEU:HD12	2.12	0.48
1:D:319:VAL:HA	1:D:322:ILE:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:SER:OG	1:A:819:GLU:OE1	2.32	0.48
1:B:753:CYS:SG	1:B:754:ALA:N	2.74	0.48
1:B:1112:GLN:HG3	1:B:1113:PHE:N	2.29	0.48
1:C:930:THR:HG22	1:C:932:VAL:H	1.77	0.48
1:C:1098:GLU:O	1:C:1098:GLU:HG2	2.13	0.48
1:D:332:TYR:OH	1:D:388:GLU:OE2	2.31	0.48
1:A:1047:ASP:OD1	1:A:1048:LEU:N	2.46	0.48
1:B:559:VAL:O	1:B:562:LYS:NZ	2.36	0.48
1:B:565:MET:HB3	1:B:597:PHE:CE2	2.49	0.48
1:B:1072:ILE:CG2	1:B:1092:ILE:HB	2.43	0.48
1:D:740:ASN:HA	1:D:743:LYS:NZ	2.27	0.48
1:B:378:LEU:HD21	1:B:414:VAL:HG21	1.95	0.48
1:C:1076:ARG:NE	1:C:1077:ASP:OD1	2.43	0.48
1:D:448:LYS:NZ	1:D:452:PRO:O	2.44	0.48
1:D:778:VAL:HG23	1:D:813:VAL:HG23	1.95	0.48
1:B:369:ASP:OD1	1:B:370:ASP:N	2.45	0.48
1:B:196:SER:O	1:B:200:ASN:N	2.44	0.48
1:B:495:ALA:HB2	1:B:795:LEU:HD12	1.96	0.48
1:B:1073:TYR:HB3	1:B:1106:LEU:HB2	1.94	0.48
1:A:387:LEU:HD21	1:A:391:PHE:CE2	2.49	0.48
1:A:746:SER:H	1:A:1019:GLY:HA3	1.78	0.48
1:B:241:ILE:O	1:B:245:THR:HG22	2.14	0.48
1:A:438:ALA:HA	1:A:441:ILE:HD12	1.94	0.48
1:A:565:MET:HB3	1:A:597:PHE:CE1	2.49	0.48
1:A:851:ASN:OD1	1:A:853:ASN:HB2	2.14	0.48
1:D:983:SER:OG	1:D:984:ALA:N	2.47	0.48
1:C:938:THR:OG1	1:C:939:GLU:N	2.46	0.47
1:D:876:LYS:O	1:D:880:LEU:HD12	2.14	0.47
1:B:748:GLY:O	1:B:749:MET:HE2	2.14	0.47
1:D:103:VAL:HG13	1:D:108:GLN:HB2	1.95	0.47
1:A:506:MET:HE3	1:A:506:MET:O	2.13	0.47
1:C:245:THR:HG21	1:C:314:MET:CE	2.45	0.47
1:A:437:ASP:O	1:A:441:ILE:HG13	2.13	0.47
1:D:1098:GLU:N	1:D:1098:GLU:OE1	2.47	0.47
1:B:33:PHE:HD2	1:B:34:PHE:HD1	1.61	0.47
1:B:797:MET:HB2	1:B:798:PRO:HD3	1.95	0.47
1:D:549:SER:O	1:D:552:THR:OG1	2.28	0.47
1:C:203:TRP:CD1	1:C:204:LEU:N	2.82	0.47
1:D:369:ASP:OD1	1:D:370:ASP:N	2.46	0.47
1:A:147:ASP:OD1	1:A:148:PHE:N	2.48	0.47
1:B:343:LYS:HD2	1:B:420:ASP:OD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ILE:HD11	1:C:258:ASN:HB3	1.97	0.47
1:C:464:HIS:ND1	1:C:465:ASN:OD1	2.46	0.47
1:D:1050:ASP:OD1	1:D:1050:ASP:N	2.45	0.47
1:C:383:PRO:HB3	1:C:387:LEU:HD23	1.96	0.47
1:D:749:MET:SD	1:D:1032:ARG:NH1	2.86	0.47
1:D:1067:MET:HE3	1:D:1109:CYS:HB3	1.95	0.47
1:A:363:PHE:HD2	1:A:364:LEU:HD22	1.79	0.47
1:C:455:ARG:HH21	1:C:457:ILE:HD11	1.79	0.47
1:D:748:GLY:O	1:D:749:MET:HE2	2.14	0.47
1:A:815:VAL:HG22	1:A:837:LEU:HB3	1.96	0.46
1:B:1062:LEU:HD12	1:B:1068:LEU:HB2	1.97	0.46
1:A:223:PHE:CE1	1:B:392:LYS:HG2	2.49	0.46
1:B:549:SER:OG	1:B:551:PRO:HD2	2.14	0.46
1:B:879:ILE:HD12	1:B:879:ILE:H	1.79	0.46
1:C:154:MET:SD	1:C:197:VAL:HG21	2.55	0.46
1:A:29:SER:O	1:A:30:MET:C	2.57	0.46
1:A:203:TRP:CZ3	1:A:205:GLY:HA3	2.50	0.46
1:A:1050:ASP:OD1	1:A:1050:ASP:N	2.48	0.46
1:B:467:ALA:O	1:B:470:LEU:HB2	2.16	0.46
1:B:786:SER:O	1:B:786:SER:OG	2.29	0.46
1:C:461:LEU:HD23	1:C:461:LEU:HA	1.75	0.46
1:D:1006:GLU:OE1	1:D:1006:GLU:N	2.40	0.46
1:A:27:ALA:O	1:A:28:SER:C	2.58	0.46
1:A:157:ASN:ND2	1:A:193:VAL:HG21	2.31	0.46
1:B:804:PHE:HD1	1:B:1034:ARG:HH21	1.62	0.46
1:A:143:ASN:OD1	1:A:200:ASN:ND2	2.43	0.46
1:A:782:PHE:CD2	1:A:877:GLU:HG3	2.50	0.46
1:B:1074:ARG:NH1	1:B:1105:ASP:OD2	2.49	0.46
1:C:794:ASN:O	1:C:794:ASN:ND2	2.46	0.46
1:D:319:VAL:O	1:D:322:ILE:HG22	2.15	0.46
1:C:33:PHE:HD2	1:C:34:PHE:HD1	1.64	0.46
1:D:437:ASP:O	1:D:441:ILE:HG13	2.16	0.46
1:A:253:ILE:HG13	1:A:281:LEU:HD21	1.98	0.46
1:A:989:ASP:OD2	1:A:990:ASN:ND2	2.48	0.46
1:B:312:LEU:CD1	1:C:286:SER:HB2	2.46	0.46
1:B:368:ARG:HG3	1:B:369:ASP:H	1.81	0.46
1:B:430:CYS:SG	1:B:431:ALA:N	2.89	0.46
1:A:516:PHE:CZ	1:A:518:LYS:HE3	2.51	0.45
1:A:1076:ARG:C	1:A:1076:ARG:HD2	2.41	0.45
1:C:201:ARG:HG2	1:C:202:SER:H	1.81	0.45
1:C:756:LYS:HD3	1:C:760:LYS:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:760:LYS:HB2	1:D:760:LYS:HE2	1.64	0.45
1:B:273:THR:OG1	1:B:276:GLU:OE1	2.20	0.45
1:B:468:HIS:HB3	1:C:880:LEU:HD11	1.98	0.45
1:B:571:LYS:HZ2	1:B:590:GLN:H	1.64	0.45
1:A:196:SER:O	1:A:200:ASN:N	2.46	0.45
1:A:1020:GLY:C	1:A:1021:TYR:HD1	2.24	0.45
1:B:511:PHE:HZ	1:B:995:ILE:HD11	1.81	0.45
1:B:782:PHE:HE1	1:B:841:PRO:HG2	1.82	0.45
1:C:212:LEU:HD12	1:C:244:SER:OG	2.17	0.45
1:D:1023:THR:HG1	1:D:1026:THR:HG1	1.57	0.45
1:A:273:THR:H	1:A:276:GLU:CD	2.25	0.45
1:B:467:ALA:HA	1:B:470:LEU:HD23	1.98	0.45
1:B:793:ARG:NH2	1:B:797:MET:HE2	2.31	0.45
1:C:437:ASP:O	1:C:441:ILE:HG13	2.16	0.45
1:C:511:PHE:HZ	1:C:995:ILE:HD11	1.81	0.45
1:C:540:TYR:CD1	1:C:594:LEU:HD13	2.52	0.45
1:C:550:PHE:CZ	1:C:582:ASN:HA	2.51	0.45
1:C:1067:MET:HE1	1:C:1111:MET:HE3	1.98	0.45
1:D:351:ILE:HB	1:D:379:HIS:CD2	2.50	0.45
1:D:442:MET:HA	1:D:445:ILE:HD12	1.99	0.45
1:D:555:GLU:C	1:D:557:CYS:H	2.25	0.45
1:A:390:LEU:HD23	1:A:393:ARG:NH1	2.32	0.45
1:B:133:ASP:OD2	1:B:207:ARG:NH1	2.50	0.45
1:D:1074:ARG:HD2	1:D:1090:TYR:OH	2.16	0.45
1:B:794:ASN:O	1:B:798:PRO:HD3	2.16	0.45
1:C:441:ILE:O	1:C:445:ILE:HG13	2.17	0.45
1:D:550:PHE:CZ	1:D:583:PRO:HD2	2.52	0.45
1:D:1061:ALA:O	1:D:1066:ASN:N	2.50	0.45
1:A:245:THR:HG21	1:A:314:MET:HE1	1.98	0.45
1:A:742:LYS:HG2	1:A:752:TRP:CZ3	2.51	0.45
1:A:804:PHE:HA	1:A:1034:ARG:NH1	2.32	0.45
1:B:557:CYS:HA	1:B:561:LEU:HD12	1.99	0.45
1:B:136:ASN:OD1	1:B:137:PRO:HD2	2.17	0.45
1:B:154:MET:O	1:B:158:VAL:HG23	2.17	0.45
1:C:304:MET:HE3	1:C:304:MET:HB3	1.75	0.45
1:C:746:SER:HB3	1:C:1020:GLY:H	1.81	0.45
1:D:136:ASN:OD1	1:D:137:PRO:HD2	2.17	0.45
1:D:33:PHE:HD2	1:D:34:PHE:HD1	1.64	0.45
1:D:488:GLU:HA	1:D:794:ASN:HD22	1.81	0.45
1:D:817:SER:HB3	1:D:819:GLU:OE1	2.16	0.45
1:C:127:LEU:HD12	1:C:127:LEU:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:LEU:HD23	1:D:30:MET:HG2	1.99	0.44
1:C:139:GLU:OE2	1:C:201:ARG:NH2	2.50	0.44
1:C:499:LEU:HD21	1:C:804:PHE:CZ	2.50	0.44
1:C:938:THR:HG21	1:C:949:LEU:HD11	1.99	0.44
1:A:1001:GLY:O	1:A:1032:ARG:NH2	2.50	0.44
1:C:385:LEU:O	1:C:388:GLU:HB3	2.17	0.44
1:D:500:ALA:HB1	1:D:1037:GLN:HG3	1.99	0.44
1:A:200:ASN:C	1:A:201:ARG:HD2	2.42	0.44
2:A:1202:A1L04:F26	2:A:1202:A1L04:C19	2.55	0.44
1:D:363:PHE:HD2	1:D:364:LEU:HD22	1.82	0.44
1:D:460:MET:HG3	1:D:461:LEU:H	1.82	0.44
1:B:591:GLU:OE2	1:B:592:GLY:N	2.51	0.44
1:D:19:GLN:OE1	1:D:19:GLN:N	2.44	0.44
1:C:262:PRO:HG2	1:C:263:TRP:CE3	2.52	0.44
1:B:940:LEU:HD11	1:B:949:LEU:HD21	1.98	0.44
1:C:29:SER:HB3	1:C:188:PHE:CD1	2.53	0.44
1:C:840:THR:HG22	1:C:842:LEU:H	1.83	0.44
1:A:341:GLY:HA3	1:D:91:VAL:N	2.33	0.44
1:A:511:PHE:HE2	1:A:995:ILE:HG13	1.83	0.44
1:B:33:PHE:HD2	1:B:34:PHE:CD1	2.36	0.44
1:C:760:LYS:HB2	1:C:760:LYS:HE2	1.69	0.44
1:D:196:SER:O	1:D:200:ASN:N	2.43	0.44
1:D:511:PHE:HZ	1:D:995:ILE:HD11	1.82	0.44
1:C:36:GLY:O	1:C:40:ILE:HG12	2.17	0.44
1:C:806:TYR:CD1	1:C:809:LEU:HD11	2.53	0.44
1:C:365:HIS:CE1	1:C:367:ASP:HB2	2.53	0.43
1:C:519:ILE:O	1:C:526:LYS:HE2	2.18	0.43
1:D:554:CYS:HA	1:D:565:MET:HE2	2.00	0.43
1:D:752:TRP:HE1	1:D:830:ASN:HD21	1.65	0.43
1:B:756:LYS:HD2	1:B:760:LYS:NZ	2.33	0.43
1:B:996:ARG:O	1:B:1000:THR:HG22	2.18	0.43
1:C:451:HIS:HE1	1:C:453:LYS:HB2	1.83	0.43
1:D:438:ALA:HA	1:D:441:ILE:HD12	1.99	0.43
1:D:503:LEU:HG	1:D:507:LEU:HD13	2.00	0.43
1:B:191:PRO:N	1:B:192:PRO:HD2	2.33	0.43
1:B:312:LEU:HD11	1:C:286:SER:HB2	2.00	0.43
1:C:345:ILE:O	1:C:376:VAL:HG22	2.18	0.43
1:C:467:ALA:HA	1:C:470:LEU:HD23	2.01	0.43
1:C:927:SER:OG	1:C:928:ILE:N	2.48	0.43
1:D:101:ALA:O	1:D:105:ILE:HG12	2.18	0.43
1:D:471:ASN:O	1:D:472:ILE:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:CYS:HB3	1:A:201:ARG:HG3	2.00	0.43
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.83	0.43
1:A:379:HIS:CG	1:A:380:ASN:N	2.87	0.43
1:A:773:LEU:HB3	1:A:776:HIS:CE1	2.53	0.43
1:A:779:VAL:HG13	1:A:859:VAL:HG23	2.00	0.43
1:C:246:TRP:CE2	1:C:282:MET:HE2	2.53	0.43
1:A:404:SER:N	1:A:410:ASP:OD2	2.38	0.43
1:B:1052:GLY:HA2	1:B:1101:LEU:N	2.33	0.43
1:C:498:CYS:HA	1:C:857:MET:SD	2.58	0.43
1:A:147:ASP:OD1	1:A:149:THR:N	2.51	0.43
1:A:519:ILE:HD11	1:A:526:LYS:N	2.34	0.43
1:A:888:MET:HE3	1:A:890:PHE:CE1	2.54	0.43
1:B:1085:GLN:N	1:B:1085:GLN:OE1	2.51	0.43
1:A:186:ASP:O	1:A:190:VAL:HG22	2.19	0.43
1:A:221:LEU:HD13	1:A:227:LEU:HD11	1.99	0.43
1:A:392:LYS:HG2	1:D:223:PHE:CE1	2.44	0.43
1:A:550:PHE:HZ	1:A:583:PRO:HD3	1.83	0.43
1:C:21:MET:O	1:C:21:MET:HG3	2.18	0.43
1:C:546:VAL:HB	1:C:591:GLU:HA	2.00	0.43
1:C:877:GLU:HG2	1:C:878:CYS:N	2.33	0.43
1:C:1054:TYR:OH	1:C:1069:CYS:O	2.36	0.43
1:B:225:ASN:OD1	1:C:393:ARG:NH1	2.52	0.43
1:B:964:THR:OG1	1:B:966:PRO:HD2	2.18	0.43
2:B:1202:A1L04:C19	2:B:1202:A1L04:F24	2.56	0.43
1:C:496:GLN:HG3	1:C:503:LEU:HD23	2.00	0.43
1:C:1054:TYR:CD2	1:C:1095:PRO:HG2	2.54	0.43
1:D:964:THR:HG23	1:D:966:PRO:HD2	1.99	0.43
1:A:604:GLU:O	1:A:607:ARG:HD3	2.18	0.43
1:A:850:VAL:O	1:A:852:ILE:N	2.51	0.43
1:A:865:GLN:HE21	1:A:866:ASN:CG	2.26	0.43
1:C:1065:TYR:O	1:C:1112:GLN:NE2	2.51	0.43
1:A:610:PHE:CE1	1:A:613:LYS:HB3	2.54	0.43
1:D:461:LEU:HA	1:D:461:LEU:HD23	1.75	0.43
1:D:797:MET:HB3	1:D:798:PRO:HD3	2.00	0.43
1:A:343:LYS:HD2	1:A:420:ASP:OD2	2.19	0.42
1:C:92:GLY:O	1:C:95:THR:OG1	2.33	0.42
1:C:1013:GLU:OE2	1:D:848:ARG:NH2	2.52	0.42
1:C:1067:MET:SD	1:C:1109:CYS:HB3	2.59	0.42
1:D:752:TRP:NE1	1:D:830:ASN:HD21	2.17	0.42
1:D:860:ILE:C	1:D:861:LEU:HD12	2.43	0.42
1:D:1014:GLU:OE1	1:D:1018:ARG:NH2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ASP:HA	1:A:437:ASP:OD2	2.19	0.42
1:B:496:GLN:HG3	1:B:503:LEU:CD2	2.49	0.42
1:B:779:VAL:HG22	1:B:859:VAL:HB	2.00	0.42
1:C:273:THR:O	1:C:276:GLU:N	2.50	0.42
1:D:221:LEU:HD12	1:D:221:LEU:HA	1.89	0.42
1:D:865:GLN:HG3	1:D:941:VAL:HG21	2.01	0.42
1:A:190:VAL:CG2	1:A:191:PRO:HD3	2.49	0.42
1:A:256:VAL:HG11	1:A:299:LEU:HB3	2.01	0.42
1:A:556:LEU:HG	1:A:560:LYS:HE3	2.01	0.42
1:B:91:VAL:N	1:C:341:GLY:HA3	2.34	0.42
1:B:555:GLU:O	1:B:559:VAL:HG22	2.19	0.42
1:B:806:TYR:CD1	1:B:809:LEU:HD11	2.54	0.42
1:B:816:GLY:O	1:B:839:GLY:N	2.52	0.42
1:A:498:CYS:HA	1:A:857:MET:SD	2.59	0.42
1:A:752:TRP:NE1	1:A:1018:ARG:HA	2.34	0.42
1:D:153:ASP:OD2	1:D:210:ARG:NH2	2.43	0.42
1:D:441:ILE:O	1:D:445:ILE:HG13	2.19	0.42
1:B:844:ARG:HB3	1:B:888:MET:SD	2.60	0.42
1:C:393:ARG:HE	1:C:393:ARG:HB2	1.68	0.42
1:C:784:ASP:O	1:C:787:SER:OG	2.25	0.42
1:D:469:LEU:HD13	1:D:475:TRP:CH2	2.55	0.42
1:A:557:CYS:O	1:A:562:LYS:N	2.52	0.42
1:C:165:GLY:O	1:C:169:ILE:HG12	2.20	0.42
1:C:275:TRP:O	1:C:278:VAL:HG12	2.19	0.42
1:C:301:ARG:O	1:C:305:VAL:HG23	2.20	0.42
1:C:782:PHE:CE2	1:C:877:GLU:HB2	2.55	0.42
1:A:469:LEU:HD23	1:A:475:TRP:HH2	1.85	0.42
1:B:751:HIS:CD2	1:B:802:SER:HA	2.54	0.42
1:A:22:TRP:CG	1:A:23:TRP:N	2.88	0.42
1:A:796:VAL:HA	1:A:799:LEU:HD12	2.01	0.42
1:B:1004:THR:O	1:B:1005:PRO:C	2.63	0.42
3:D:1203:Y01:HAP1	3:D:1203:Y01:HAO2	1.38	0.42
1:A:871:THR:HA	1:A:874:GLN:NE2	2.35	0.42
1:A:943:ASP:HB2	1:A:961:LEU:HD12	2.01	0.42
1:B:118:LEU:HD23	1:B:118:LEU:HA	1.76	0.42
1:B:329:ARG:HE	1:B:329:ARG:HB2	1.72	0.42
1:B:503:LEU:HG	1:B:507:LEU:HD23	2.01	0.42
1:B:1013:GLU:HG3	1:B:1014:GLU:N	2.35	0.42
1:D:404:SER:OG	1:D:405:VAL:N	2.51	0.42
1:A:1039:ALA:HA	1:A:1106:LEU:HD22	2.01	0.42
1:B:153:ASP:OD2	1:B:210:ARG:NH2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1006:GLU:H	1:B:1006:GLU:HG2	1.61	0.42
1:C:286:SER:O	1:C:287:THR:OG1	2.32	0.42
1:C:422:CYS:O	1:C:423:LEU:HD12	2.20	0.42
1:C:503:LEU:HG	1:C:507:LEU:HD13	2.01	0.42
1:D:147:ASP:OD1	1:D:148:PHE:N	2.53	0.42
1:C:220:ILE:HG13	1:C:221:LEU:N	2.35	0.41
1:C:476:ASN:N	1:C:476:ASN:OD1	2.53	0.41
1:D:557:CYS:SG	1:D:558:PHE:N	2.93	0.41
1:A:467:ALA:HA	1:A:470:LEU:HD23	2.02	0.41
1:B:444:VAL:HG13	1:B:456:ILE:HD13	2.01	0.41
1:B:946:VAL:HG22	1:B:966:PRO:HG2	2.02	0.41
1:C:235:LEU:HD11	1:C:326:ILE:HG13	2.02	0.41
1:C:469:LEU:HD23	1:C:475:TRP:CH2	2.55	0.41
1:C:565:MET:HB3	1:C:597:PHE:CE2	2.55	0.41
1:D:486:LEU:HD23	1:D:486:LEU:HA	1.78	0.41
1:D:578:ARG:O	1:D:579:ILE:HD13	2.20	0.41
1:D:795:LEU:O	1:D:798:PRO:HD2	2.20	0.41
1:A:517:ILE:C	1:A:518:LYS:HD2	2.44	0.41
1:B:227:LEU:HD21	1:B:236:VAL:HG21	2.02	0.41
1:C:154:MET:HE3	1:C:154:MET:HB3	1.86	0.41
1:C:1053:CYS:HB3	1:C:1056:ASP:OD2	2.20	0.41
1:A:550:PHE:CG	1:A:551:PRO:HD3	2.56	0.41
1:B:36:GLY:O	1:B:40:ILE:HG12	2.21	0.41
1:B:537:TYR:HD2	1:B:605:VAL:HG21	1.84	0.41
1:C:803:ASN:OD1	1:C:1032:ARG:NH2	2.53	0.41
1:A:42:LEU:O	1:A:46:LEU:HB2	2.20	0.41
1:A:99:ASP:O	1:A:103:VAL:HG22	2.20	0.41
1:B:148:PHE:O	1:B:151:GLN:HB2	2.20	0.41
1:C:794:ASN:C	1:C:794:ASN:HD22	2.25	0.41
1:D:806:TYR:CD1	1:D:809:LEU:HD11	2.55	0.41
1:D:825:TRP:HD1	1:D:828:LEU:HB2	1.84	0.41
1:D:1063:LYS:HA	1:D:1063:LYS:HD3	1.89	0.41
1:B:182:ASN:ND2	1:B:216:GLN:OE1	2.53	0.41
1:B:825:TRP:O	1:B:825:TRP:CD1	2.74	0.41
1:C:1060:LYS:O	1:C:1064:THR:HG22	2.20	0.41
1:D:504:SER:OG	1:D:505:THR:N	2.51	0.41
1:A:404:SER:OG	1:A:405:VAL:N	2.52	0.41
1:A:567:ALA:HB1	1:A:578:ARG:O	2.21	0.41
1:A:990:ASN:HB3	1:A:993:THR:HB	2.03	0.41
1:B:185:VAL:HG11	1:B:212:LEU:HD23	2.03	0.41
1:B:239:LEU:O	1:B:243:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:LYS:HE3	1:B:361:LYS:HB2	1.93	0.41
1:B:441:ILE:O	1:B:445:ILE:HG13	2.21	0.41
1:C:743:LYS:O	1:C:751:HIS:HA	2.20	0.41
1:C:1014:GLU:C	1:C:1016:ALA:H	2.29	0.41
1:D:1038:LEU:HD21	1:D:1067:MET:HE2	2.03	0.41
1:A:550:PHE:CD2	1:A:581:ILE:HB	2.56	0.41
1:B:606:LYS:C	1:B:608:ALA:N	2.77	0.41
1:B:758:ILE:O	1:B:762:ILE:HG12	2.20	0.41
1:B:1066:ASN:HB2	1:B:1112:GLN:OE1	2.20	0.41
1:C:933:ASN:O	1:C:933:ASN:ND2	2.51	0.41
1:D:947:GLN:HB2	1:D:955:ASP:CG	2.45	0.41
1:D:981:LEU:O	1:D:982:MET:C	2.63	0.41
1:A:212:LEU:HD12	1:A:244:SER:OG	2.21	0.41
1:A:323:ILE:HD13	1:A:323:ILE:HA	1.93	0.41
1:A:529:LEU:HD12	1:A:532:VAL:HG11	2.03	0.41
1:B:379:HIS:CE1	1:B:381:ILE:HB	2.56	0.41
1:B:785:VAL:HG23	1:B:823:ARG:HD2	2.03	0.41
1:B:790:ILE:HG12	1:B:820:TYR:OH	2.21	0.41
1:B:990:ASN:OD1	1:B:990:ASN:N	2.53	0.41
1:B:1055:GLY:HA3	1:B:1097:TYR:CE1	2.56	0.41
1:D:521:GLU:O	1:D:523:THR:HG22	2.21	0.41
1:D:891:ASP:OD1	1:D:891:ASP:N	2.53	0.41
1:A:513:MET:SD	1:A:513:MET:N	2.94	0.41
1:A:538:THR:OG1	1:A:594:LEU:HD11	2.21	0.41
1:B:824:GLU:O	1:B:827:THR:HG22	2.21	0.41
1:C:937:ILE:HD13	1:C:971:THR:HA	2.02	0.41
1:A:753:CYS:O	1:A:830:ASN:ND2	2.50	0.40
1:A:981:LEU:HA	1:A:981:LEU:HD23	1.78	0.40
1:B:21:MET:SD	1:B:201:ARG:NE	2.94	0.40
1:C:280:LEU:HD12	1:C:293:VAL:HG23	2.03	0.40
1:C:284:THR:CG2	1:C:285:MET:N	2.83	0.40
1:C:1074:ARG:HH12	1:C:1099:PHE:HE2	1.67	0.40
1:D:36:GLY:O	1:D:40:ILE:HG12	2.21	0.40
1:B:1064:THR:HG23	1:B:1065:TYR:CD2	2.56	0.40
1:C:101:ALA:O	1:C:105:ILE:HG12	2.21	0.40
1:C:227:LEU:HD21	1:C:236:VAL:HG21	2.03	0.40
3:C:1203:Y01:HAA2	3:C:1203:Y01:HAJ1	1.91	0.40
1:D:889:GLN:C	1:D:890:PHE:HD1	2.29	0.40
1:D:1067:MET:HE1	1:D:1111:MET:HB2	2.01	0.40
1:B:448:LYS:HA	1:B:448:LYS:HD2	1.68	0.40
1:B:505:THR:HG23	1:B:967:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1074:ARG:HD2	1:B:1090:TYR:OH	2.21	0.40
1:C:161:LEU:HD13	1:C:190:VAL:HG11	2.04	0.40
1:C:1076:ARG:HE	1:C:1077:ASP:CG	2.29	0.40
1:D:130:TYR:OH	1:D:208:PHE:HB3	2.22	0.40
1:A:361:LYS:HE3	1:A:361:LYS:HB2	1.96	0.40
1:A:376:VAL:HA	1:A:399:GLU:O	2.21	0.40
1:A:1052:GLY:HA3	1:A:1100:GLU:OE2	2.22	0.40
3:A:1203:Y01:HAC3	3:A:1203:Y01:HAJ1	1.82	0.40
1:B:239:LEU:HD23	1:B:239:LEU:HA	1.92	0.40
1:B:510:LEU:HA	1:B:510:LEU:HD23	1.86	0.40
1:A:449:ASN:OD1	1:A:449:ASN:C	2.64	0.40
1:A:1085:GLN:N	1:A:1085:GLN:OE1	2.55	0.40
1:B:180:GLU:OE1	1:B:183:SER:N	2.46	0.40
1:B:519:ILE:O	1:B:526:LYS:HG3	2.21	0.40
1:B:777:VAL:HG12	1:B:811:HIS:O	2.21	0.40
1:B:1011:ILE:HD13	1:B:1011:ILE:HA	1.87	0.40
1:C:580:LEU:HD23	1:C:580:LEU:HA	1.91	0.40
1:C:1014:GLU:OE2	1:C:1018:ARG:HD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	892/1114 (80%)	838 (94%)	54 (6%)	0	100	100
1	B	892/1114 (80%)	829 (93%)	63 (7%)	0	100	100
1	C	892/1114 (80%)	835 (94%)	57 (6%)	0	100	100
1	D	892/1114 (80%)	829 (93%)	63 (7%)	0	100	100
All	All	3568/4456 (80%)	3331 (93%)	237 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	786/980 (80%)	773 (98%)	13 (2%)	53	68
1	B	789/980 (80%)	780 (99%)	9 (1%)	65	74
1	C	786/980 (80%)	786 (100%)	0	100	100
1	D	787/980 (80%)	784 (100%)	3 (0%)	84	83
All	All	3148/3920 (80%)	3123 (99%)	25 (1%)	70	77

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	ASP
1	A	272	LEU
1	A	285	MET
1	A	292	ASP
1	A	293	VAL
1	A	741	VAL
1	A	765	ARG
1	A	772	VAL
1	A	777	VAL
1	A	778	VAL
1	A	994	LEU
1	A	999	VAL
1	A	1004	THR
1	B	461	LEU
1	B	469	LEU
1	B	471	ASN
1	B	601	ASP
1	B	1011	ILE
1	B	1027	LEU
1	B	1032	ARG
1	B	1034	ARG
1	B	1037	GLN
1	D	471	ASN
1	D	476	ASN
1	D	479	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	ASN
1	A	270	GLN
1	A	394	HIS
1	A	496	GLN
1	A	534	ASN
1	A	794	ASN
1	A	853	ASN
1	A	990	ASN
1	A	1015	ASN
1	A	1029	ASN
1	B	157	ASN
1	B	464	HIS
1	C	19	GLN
1	C	216	GLN
1	C	344	HIS
1	C	471	ASN
1	C	805	HIS
1	C	965	GLN
1	D	157	ASN
1	D	200	ASN
1	D	216	GLN
1	D	402	GLN
1	D	496	GLN
1	D	501	GLN
1	D	794	ASN
1	D	1066	ASN
1	D	1112	GLN

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

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1L04	B	1202	-	26,26,26	0.41	0	36,39,39	0.80	1 (2%)
2	A1L04	A	1202	-	26,26,26	0.41	0	36,39,39	0.70	1 (2%)
2	A1L04	C	1201	-	26,26,26	0.32	0	36,39,39	0.61	1 (2%)
3	Y01	D	1203	-	38,38,38	0.47	0	57,57,57	0.65	0
2	A1L04	B	1201	-	26,26,26	0.34	0	36,39,39	0.70	1 (2%)
2	A1L04	D	1202	-	26,26,26	0.40	0	36,39,39	0.78	1 (2%)
3	Y01	C	1203	-	38,38,38	0.48	0	57,57,57	0.65	0
2	A1L04	C	1202	-	26,26,26	0.41	0	36,39,39	0.76	1 (2%)
3	Y01	B	1203	-	38,38,38	0.48	0	57,57,57	0.51	0
2	A1L04	A	1201	-	26,26,26	0.33	0	36,39,39	0.61	1 (2%)
3	Y01	A	1203	-	38,38,38	0.48	0	57,57,57	0.68	0
2	A1L04	D	1201	-	26,26,26	0.34	0	36,39,39	0.59	1 (2%)

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	A1L04	B	1202	-	-	7/14/14/14	0/3/3/3
2	A1L04	A	1202	-	-	3/14/14/14	0/3/3/3
2	A1L04	C	1201	-	-	5/14/14/14	0/3/3/3
3	Y01	D	1203	-	-	10/19/77/77	0/4/4/4
2	A1L04	B	1201	-	-	5/14/14/14	0/3/3/3
2	A1L04	D	1202	-	-	7/14/14/14	0/3/3/3
3	Y01	C	1203	-	-	1/19/77/77	0/4/4/4
2	A1L04	C	1202	-	-	4/14/14/14	0/3/3/3
3	Y01	B	1203	-	-	10/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1L04	A	1201	-	-	3/14/14/14	0/3/3/3
3	Y01	A	1203	-	-	11/19/77/77	0/4/4/4
2	A1L04	D	1201	-	-	2/14/14/14	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1202	A1L04	C14-C13-C12	-3.38	123.47	128.62
2	D	1202	A1L04	C14-C13-C12	-3.26	123.65	128.62
2	C	1202	A1L04	C14-C13-C12	-3.23	123.70	128.62
2	A	1202	A1L04	C14-C13-C12	-2.77	124.40	128.62
2	B	1201	A1L04	C14-C13-C12	-2.64	124.60	128.62
2	D	1201	A1L04	C13-C12-N11	-2.21	110.12	112.89
2	C	1201	A1L04	C13-C12-N11	-2.10	110.26	112.89
2	A	1201	A1L04	C13-C12-N11	-2.09	110.27	112.89

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1203	Y01	CAC-CBB-CBE-CBI
3	B	1203	Y01	CAO-CBB-CBE-CAP
3	B	1203	Y01	CAO-CBB-CBE-CBI
3	B	1203	Y01	CAC-CBB-CBE-CBI
3	D	1203	Y01	CAO-CBB-CBE-CAP
3	D	1203	Y01	CAC-CBB-CBE-CBI
3	A	1203	Y01	CAV-CBC-OAW-CAY
3	B	1203	Y01	CAJ-CAO-CBB-CAC
3	A	1203	Y01	CAC-CBB-CBE-CAP
3	B	1203	Y01	CAC-CBB-CBE-CAP
3	D	1203	Y01	CAC-CBB-CBE-CAP
3	D	1203	Y01	CAO-CBB-CBE-CBI
3	D	1203	Y01	CAR-CBC-OAW-CAY
3	D	1203	Y01	CAJ-CAO-CBB-CAC
3	A	1203	Y01	CAO-CBB-CBE-CBI
3	A	1203	Y01	CAO-CBB-CBE-CAP
3	D	1203	Y01	CAJ-CAO-CBB-CBE
3	B	1203	Y01	CAJ-CAO-CBB-CBE
3	A	1203	Y01	CAJ-CAO-CBB-CAC

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Mol	Chain	Res	Type	Atoms
3	C	1203	Y01	CAO-CAJ-CAN-CBA
3	B	1203	Y01	CAM-CAY-OAW-CBC
3	B	1203	Y01	OAG-CAY-OAW-CBC
2	A	1201	A1L04	C5-C6-C9-O10
2	A	1202	A1L04	C5-C6-C9-O10
3	A	1203	Y01	CAR-CBC-OAW-CAY
3	D	1203	Y01	CAV-CBC-OAW-CAY
3	A	1203	Y01	CAM-CAL-CAX-OAF
3	A	1203	Y01	CAM-CAL-CAX-OAH
2	D	1202	A1L04	C13-C12-C23-F25
3	B	1203	Y01	CAM-CAL-CAX-OAH
2	B	1201	A1L04	N11-C12-C23-F25
2	B	1201	A1L04	N11-C12-C23-F26
2	B	1202	A1L04	N11-C12-C23-F25
2	B	1202	A1L04	N11-C12-C23-F26
2	C	1201	A1L04	N11-C12-C23-F25
2	C	1201	A1L04	N11-C12-C23-F26
2	D	1202	A1L04	N11-C12-C23-F24
2	D	1202	A1L04	N11-C12-C23-F25
3	A	1203	Y01	CAJ-CAN-CBA-CAB
3	D	1203	Y01	CAM-CAL-CAX-OAH
2	D	1202	A1L04	C13-C12-C23-F24
3	A	1203	Y01	CAX-CAL-CAM-CAY
3	B	1203	Y01	CAM-CAL-CAX-OAF
2	B	1202	A1L04	C1-C6-C9-C13
2	C	1202	A1L04	C1-C6-C9-C13
2	D	1202	A1L04	C1-C6-C9-C13
3	D	1203	Y01	CAM-CAL-CAX-OAF
2	B	1201	A1L04	C13-C12-C23-F25
2	B	1201	A1L04	C13-C12-C23-F26
2	B	1202	A1L04	C13-C12-C23-F25
2	B	1202	A1L04	C13-C12-C23-F26
2	C	1201	A1L04	C13-C12-C23-F25
2	C	1201	A1L04	C13-C12-C23-F26
2	A	1201	A1L04	C13-C12-C23-F24
2	A	1202	A1L04	C13-C12-C23-F24
2	A	1202	A1L04	C13-C12-C23-F25
2	C	1202	A1L04	C13-C12-C23-F26
2	D	1201	A1L04	C13-C12-C23-F24
2	D	1202	A1L04	C13-C12-C23-F26
2	B	1201	A1L04	C13-C12-C23-F24
2	D	1201	A1L04	C13-C12-C23-F26

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Mol	Chain	Res	Type	Atoms
2	B	1202	A1L04	C5-C6-C9-O10
2	C	1202	A1L04	C5-C6-C9-O10
2	D	1202	A1L04	C5-C6-C9-O10
2	A	1201	A1L04	C13-C12-C23-F25
2	B	1202	A1L04	C13-C12-C23-F24
2	C	1201	A1L04	C13-C12-C23-F24
2	C	1202	A1L04	C13-C12-C23-F24

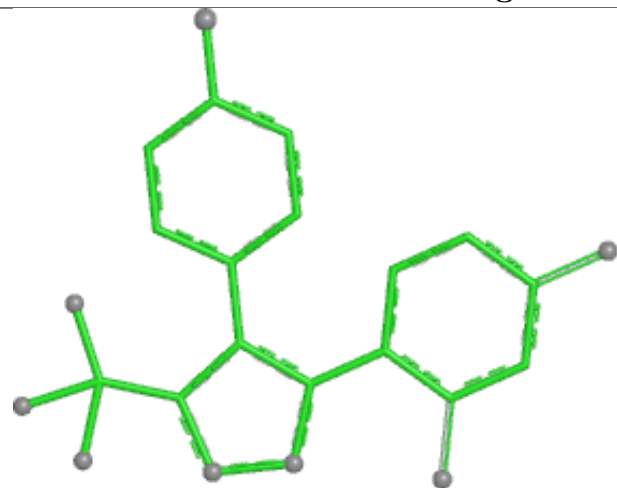
There are no ring outliers.

5 monomers are involved in 5 short contacts:

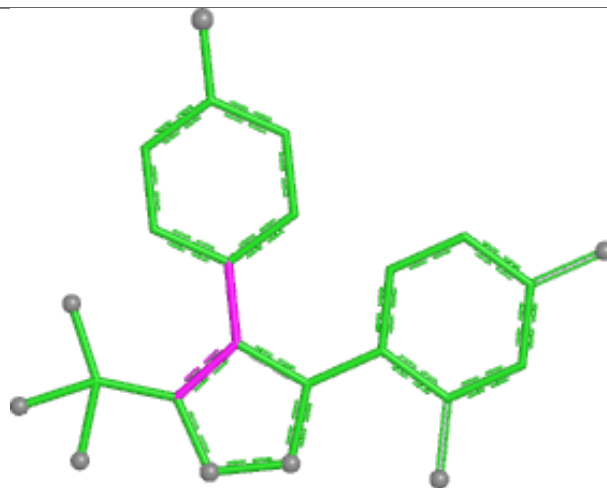
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1202	A1L04	1	0
2	A	1202	A1L04	1	0
3	D	1203	Y01	1	0
3	C	1203	Y01	1	0
3	A	1203	Y01	1	0

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.

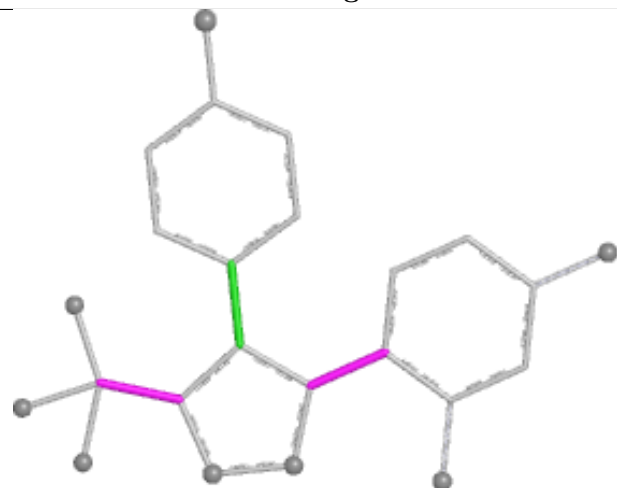
Ligand A1L04 B 1202



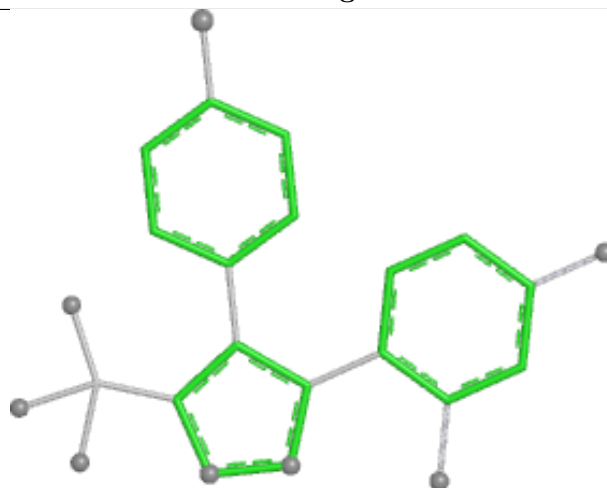
Bond lengths



Bond angles

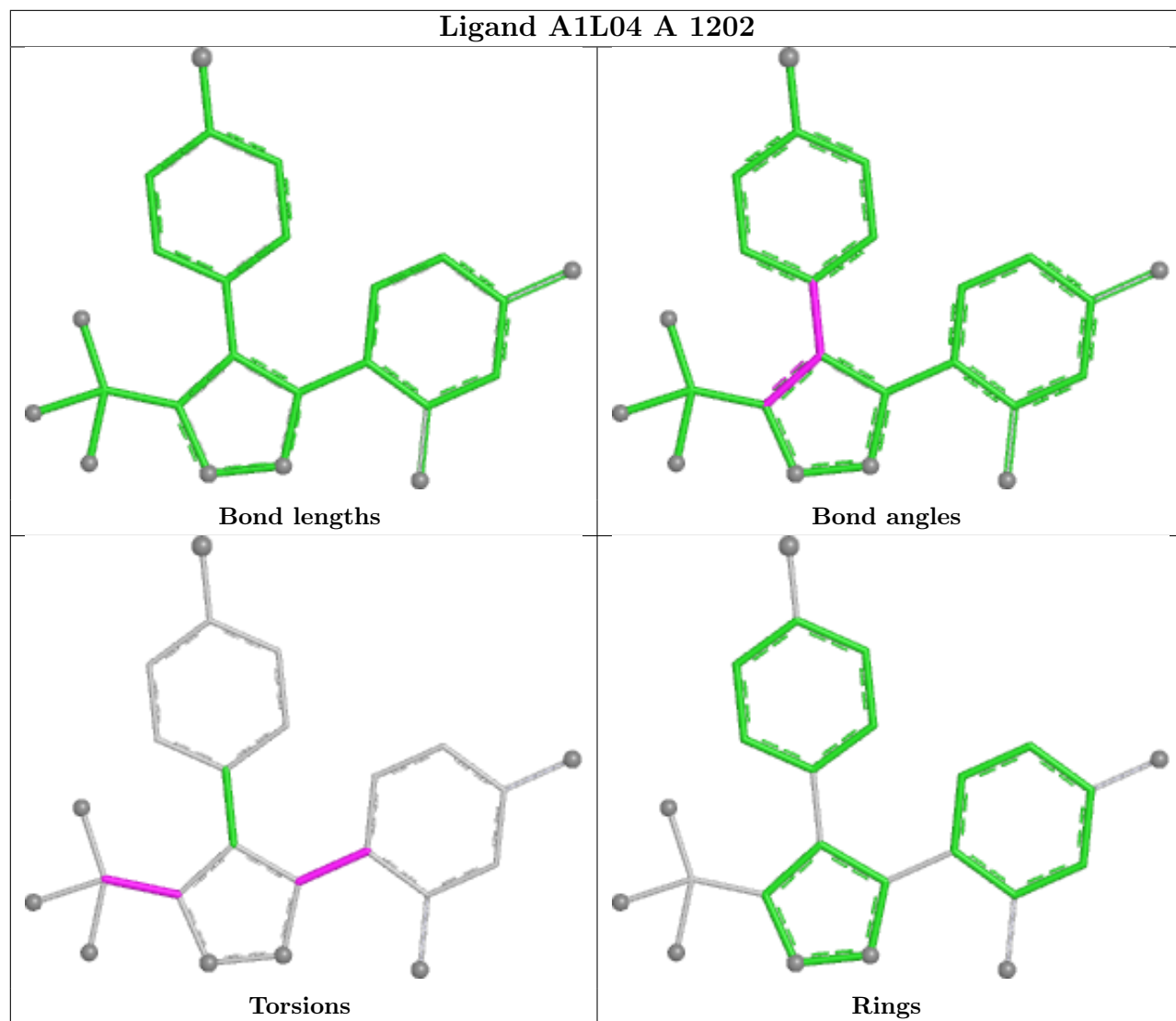


Torsions

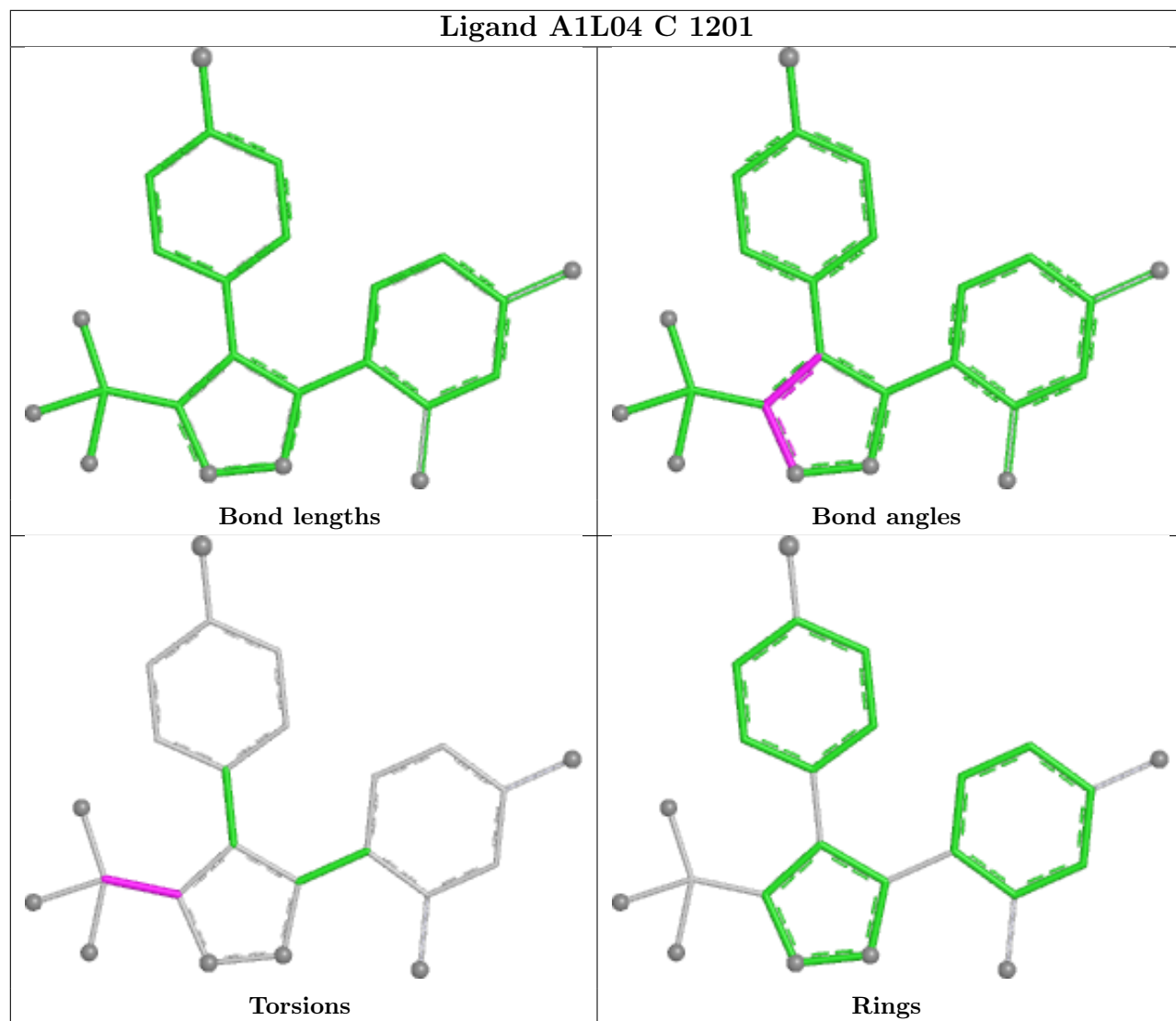


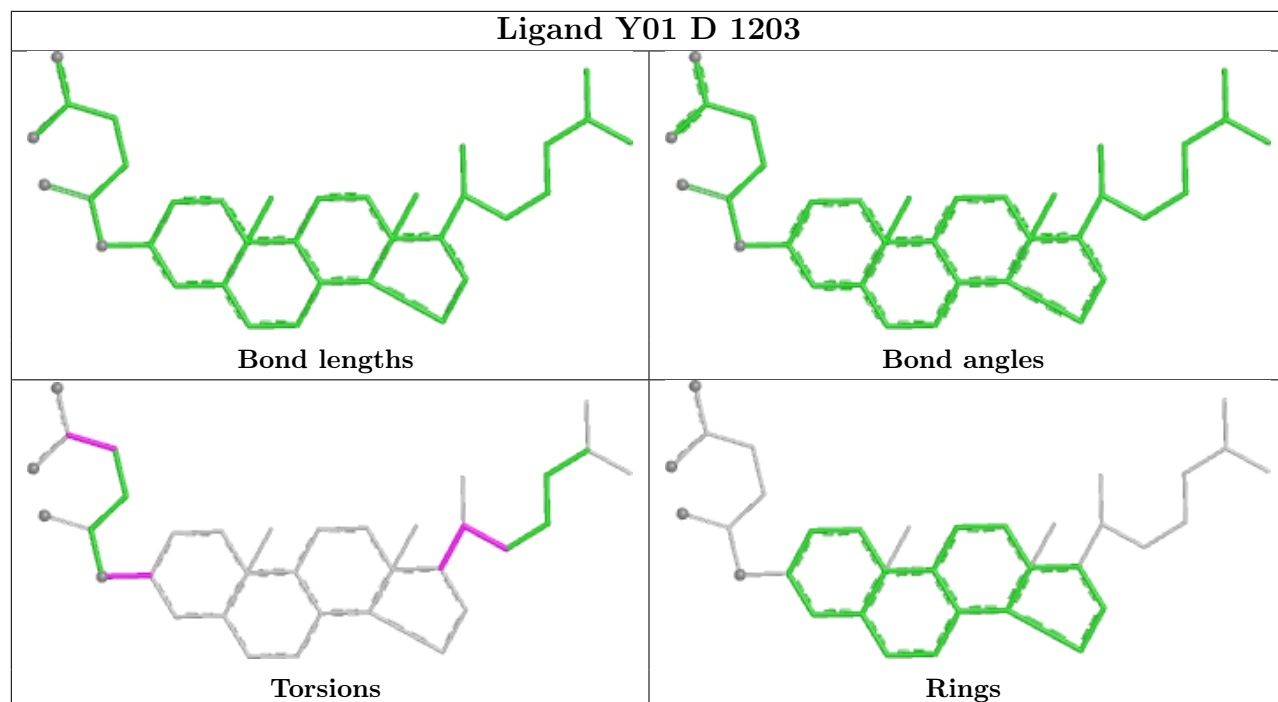
Rings

Ligand A1L04 A 1202

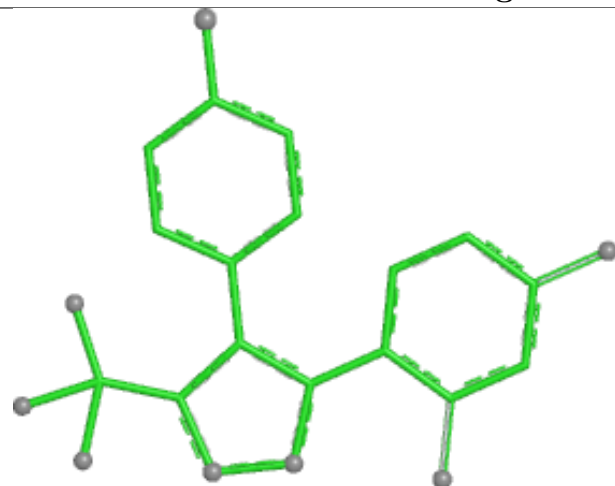


Ligand A1L04 C 1201

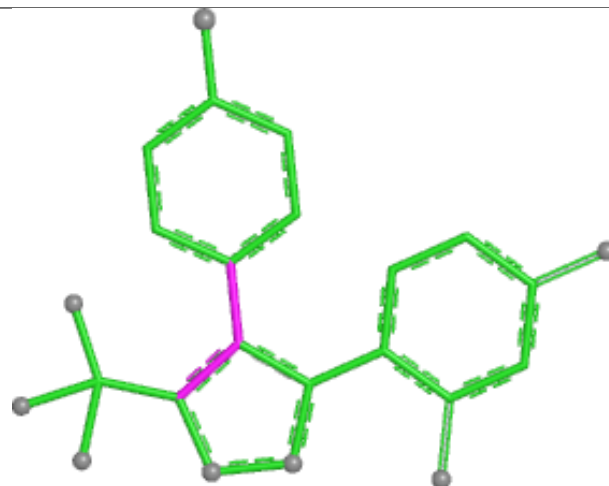




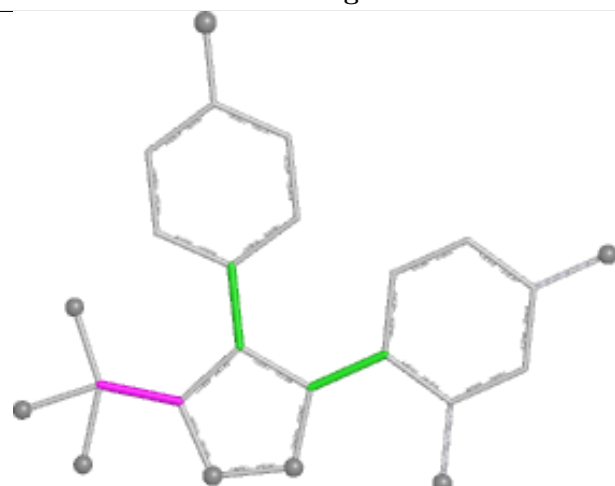
Ligand A1L04 B 1201



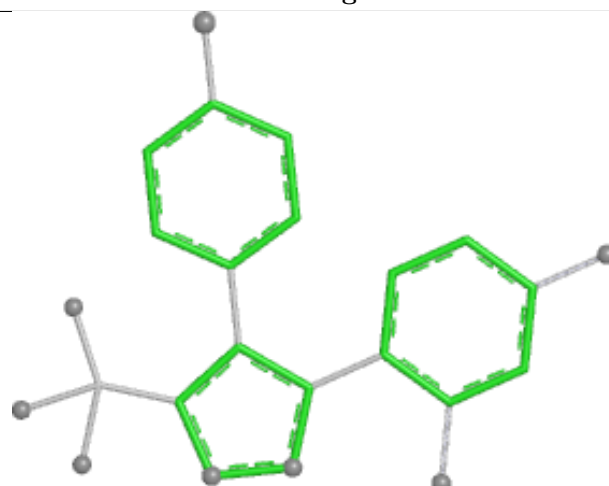
Bond lengths



Bond angles

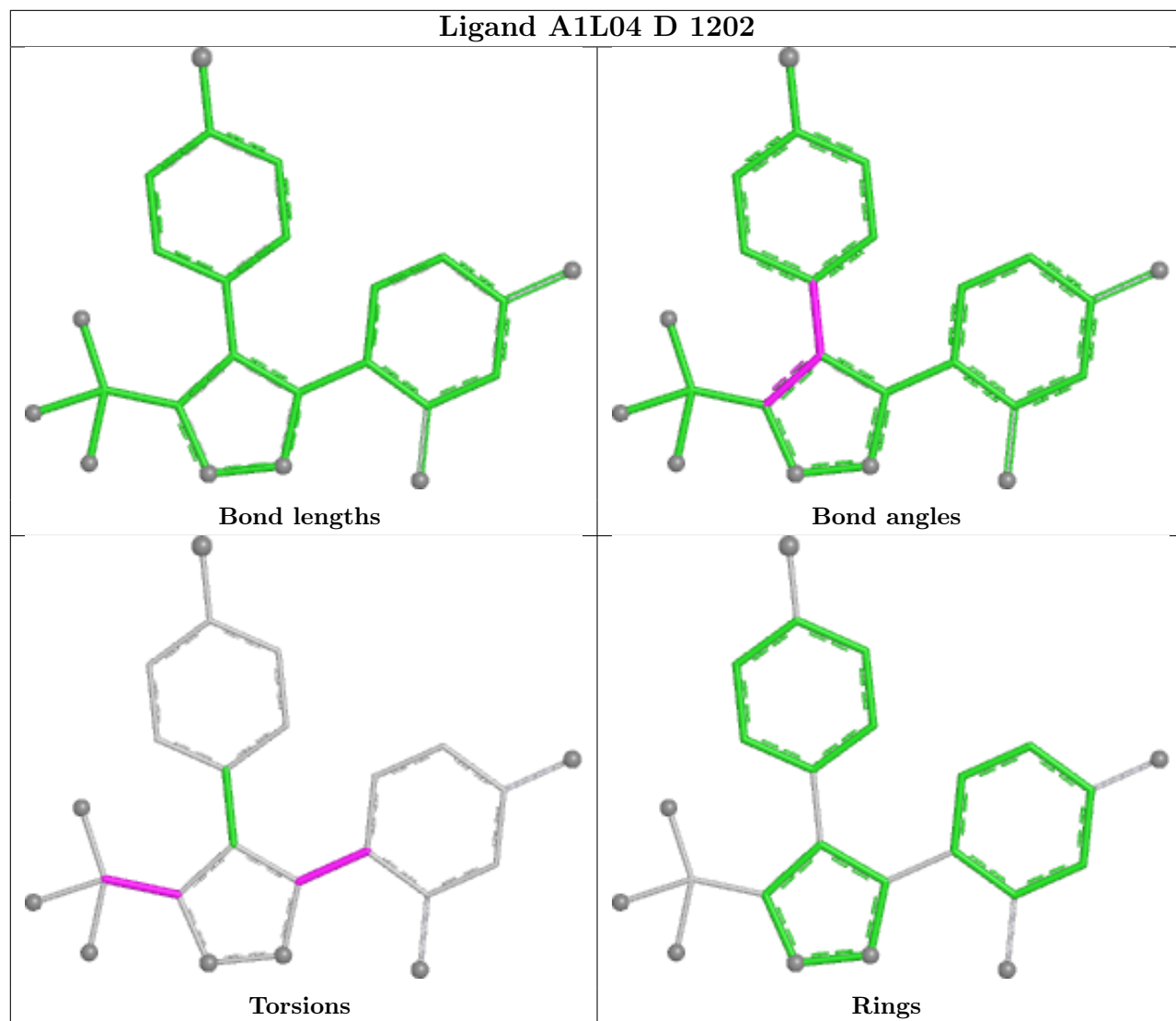


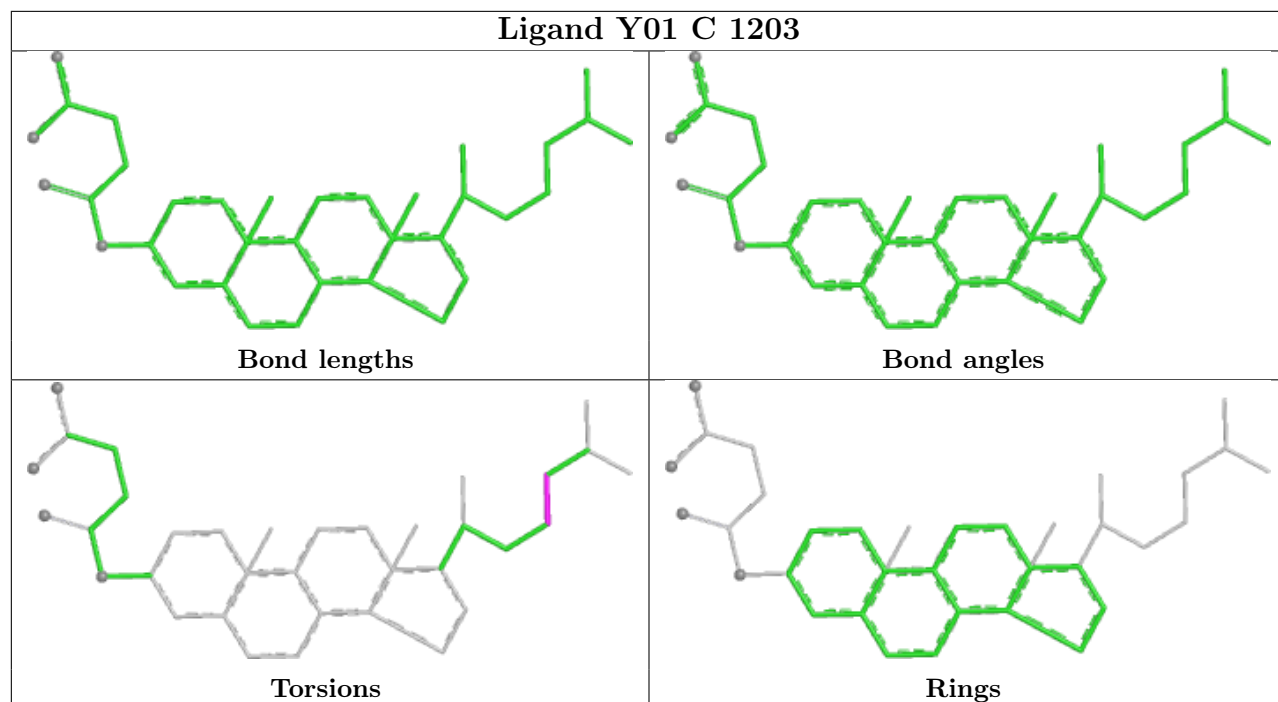
Torsions



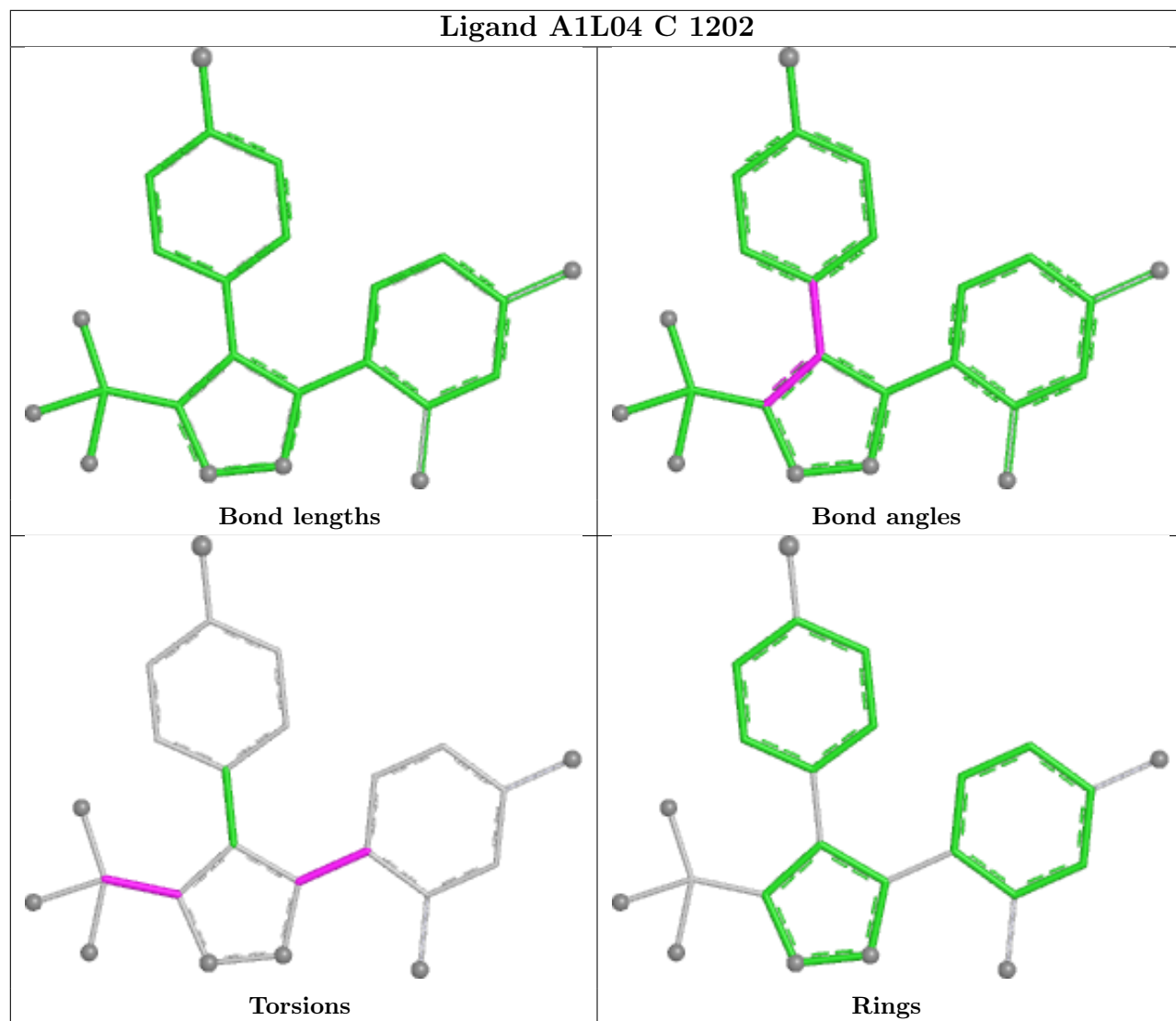
Rings

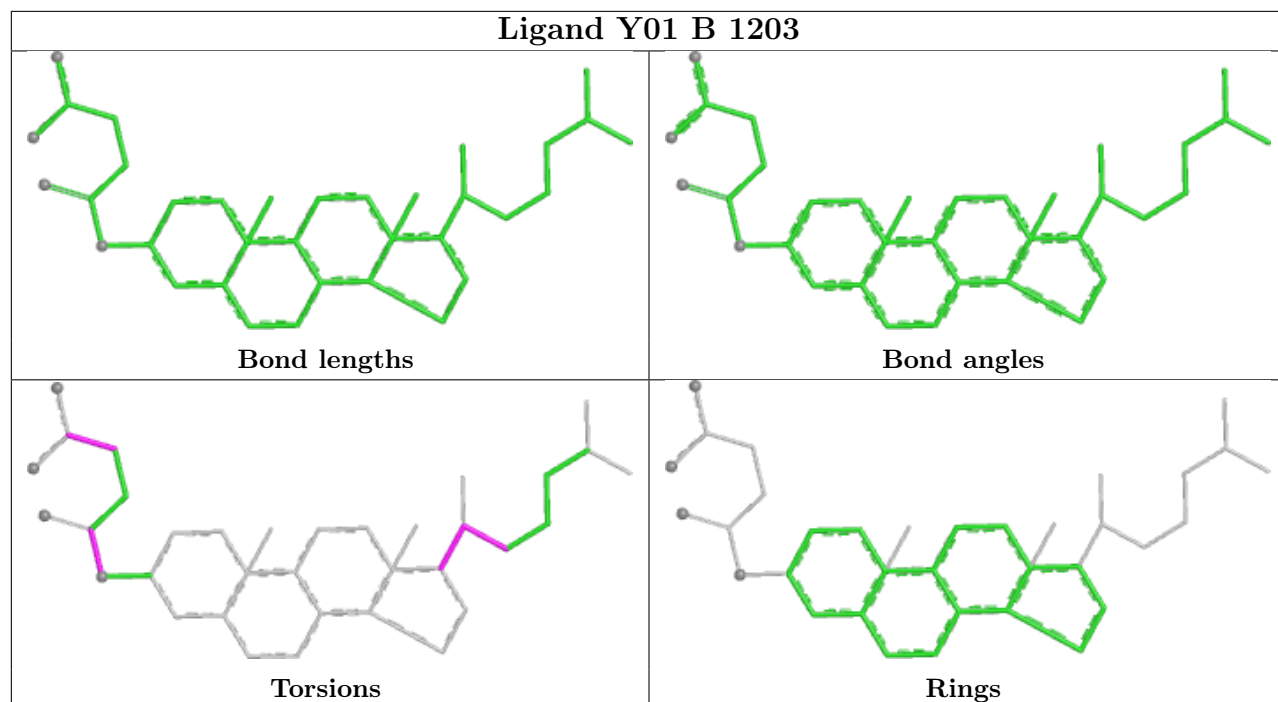
Ligand A1L04 D 1202



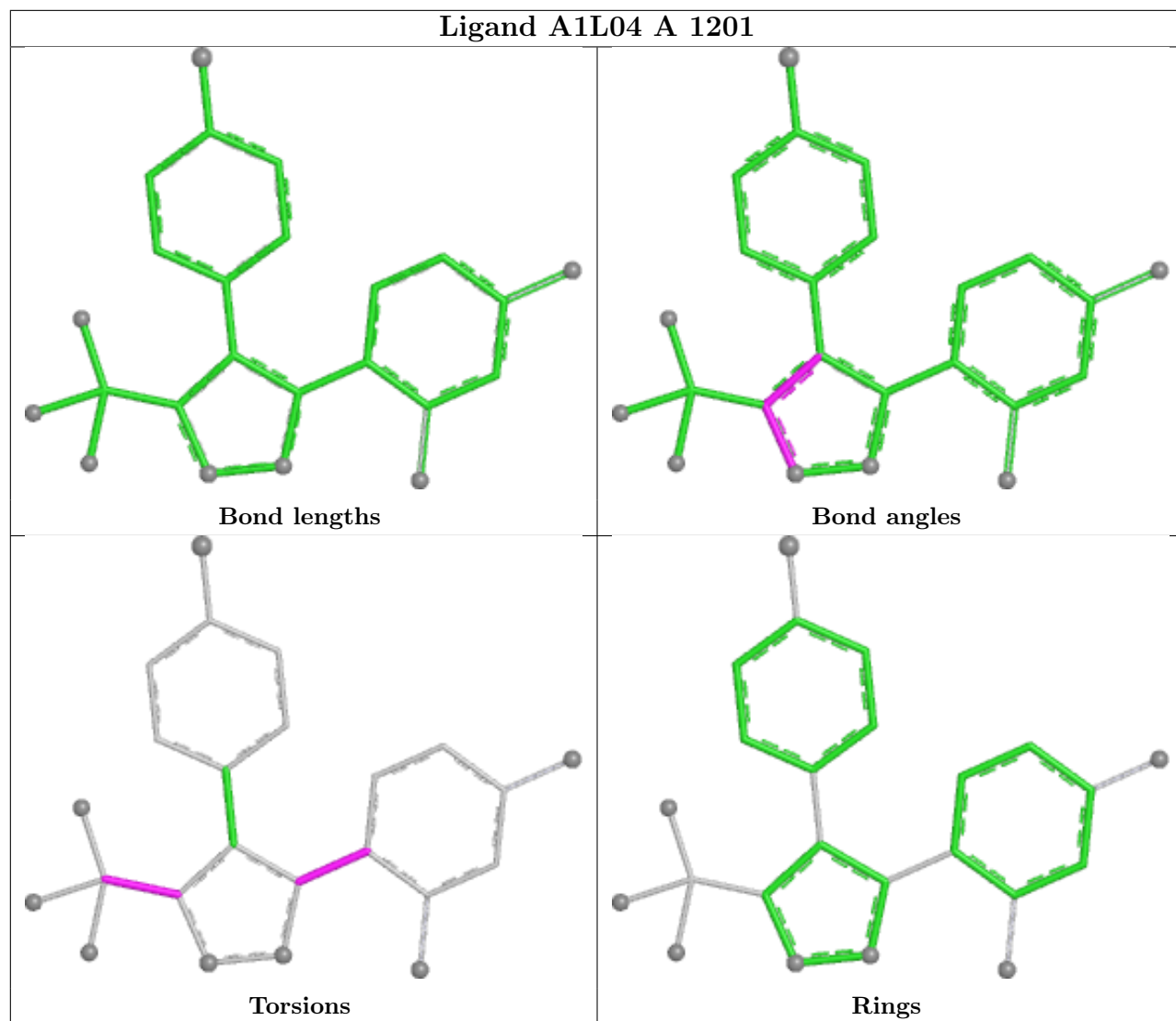


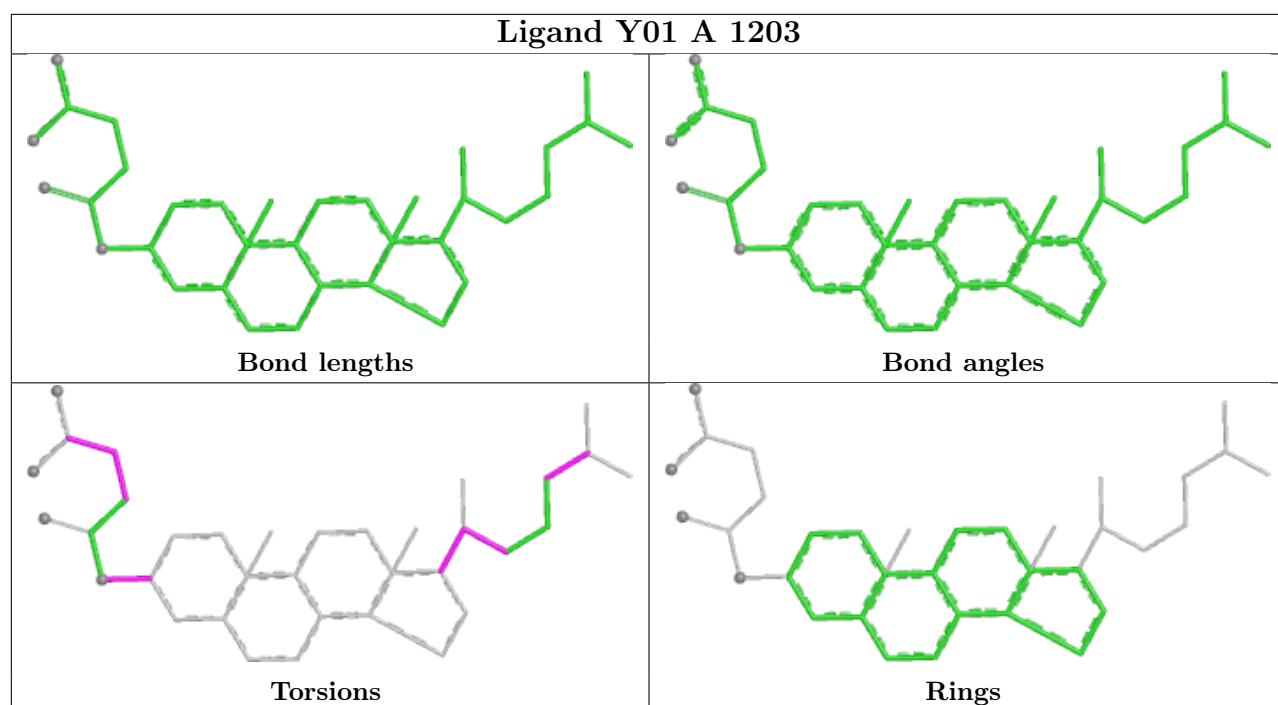
Ligand A1L04 C 1202

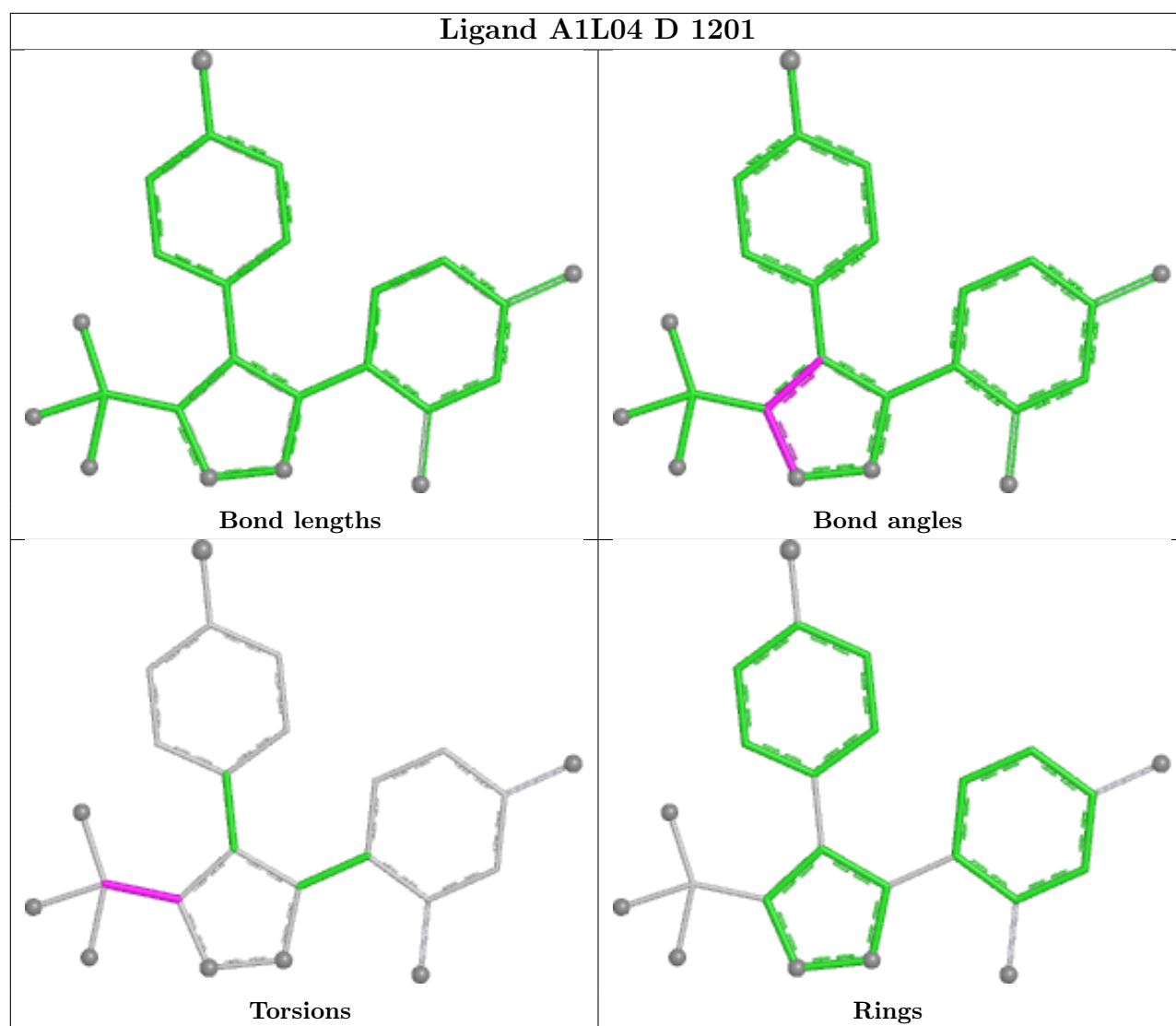




Ligand A1L04 A 1201







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.

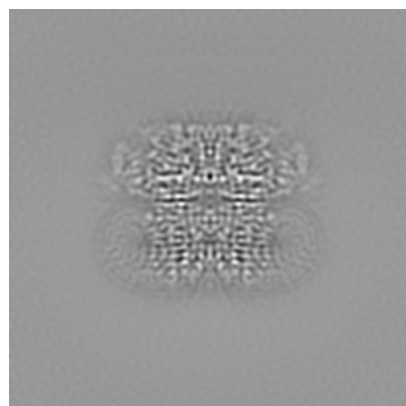
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39753. These allow visual inspection of the internal detail of the map and identification of artifacts.

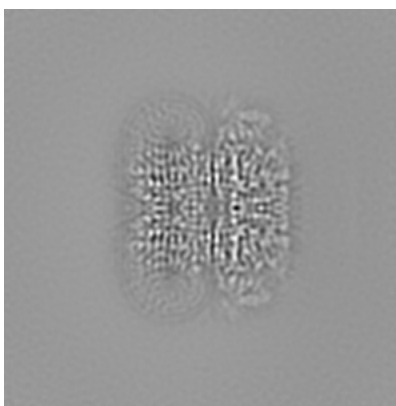
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

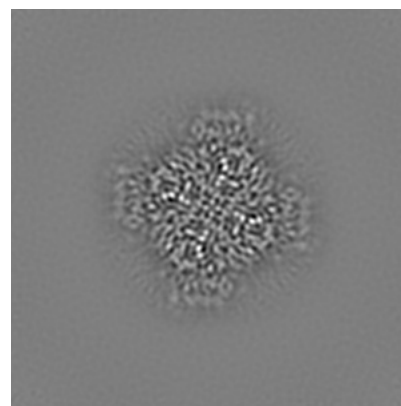
6.1.1 Primary map



X

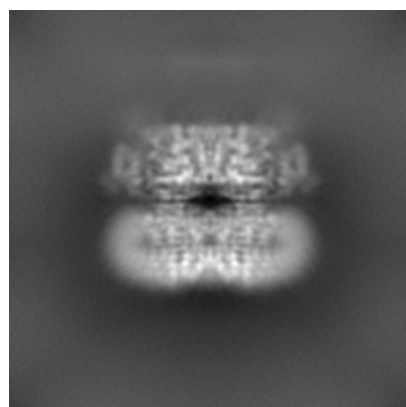


Y

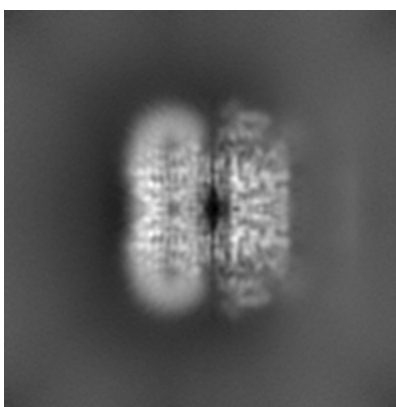


Z

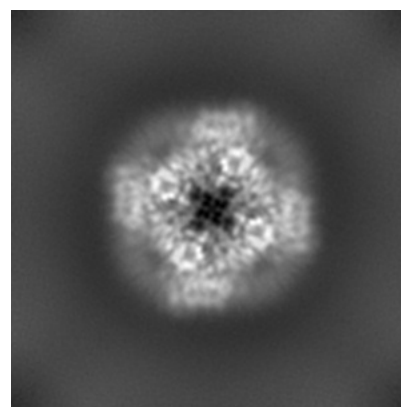
6.1.2 Raw map



X



Y

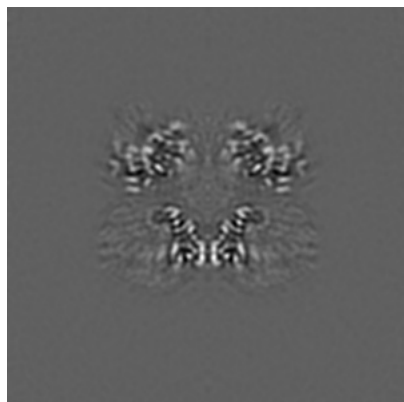


Z

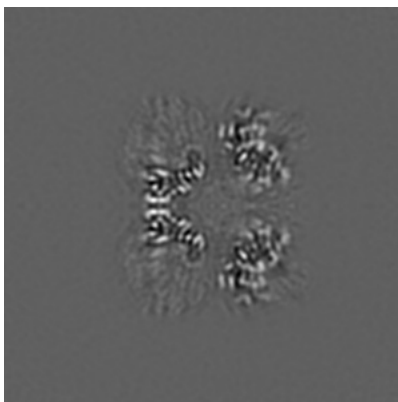
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

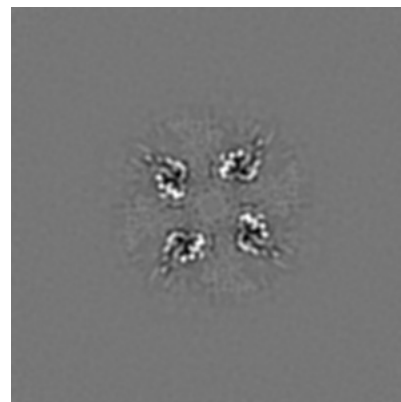
6.2.1 Primary map



X Index: 100

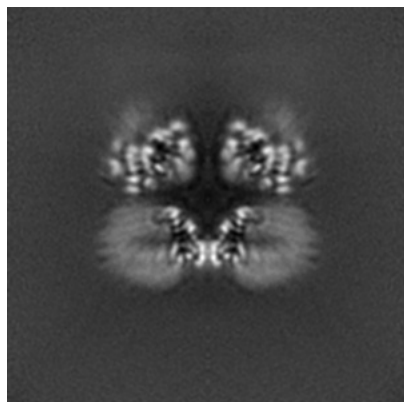


Y Index: 100

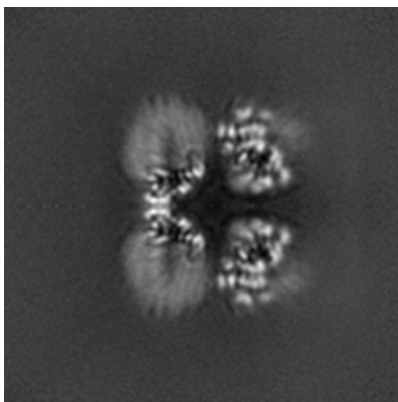


Z Index: 100

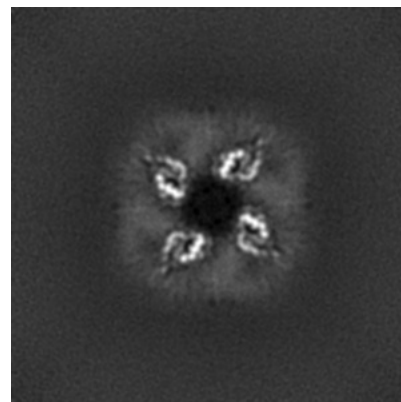
6.2.2 Raw map



X Index: 100



Y Index: 100

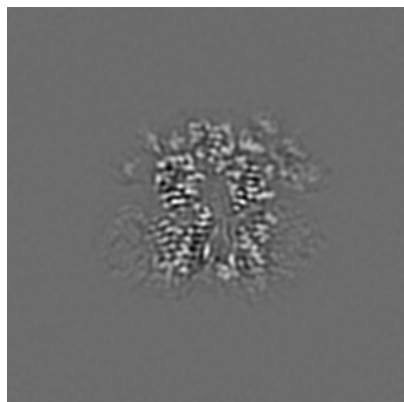


Z Index: 100

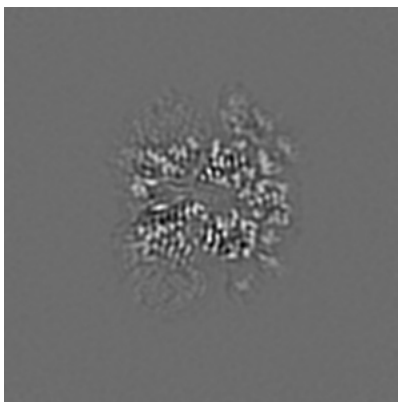
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

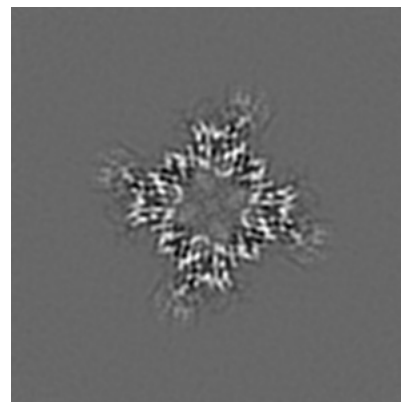
6.3.1 Primary map



X Index: 117

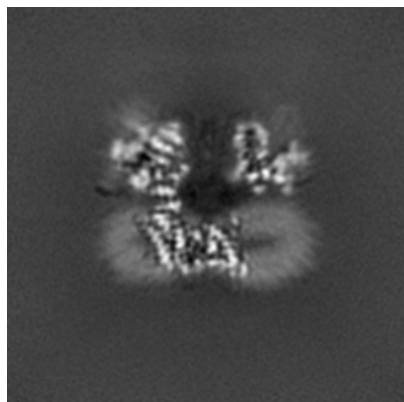


Y Index: 83

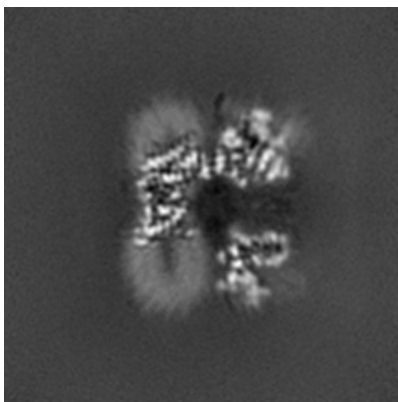


Z Index: 114

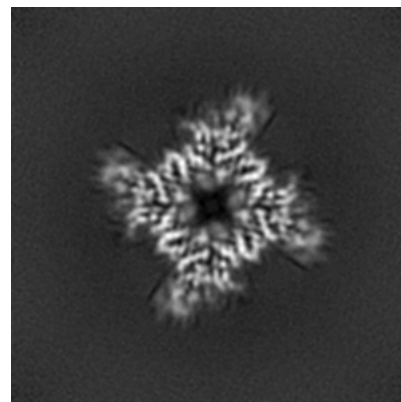
6.3.2 Raw map



X Index: 94



Y Index: 94

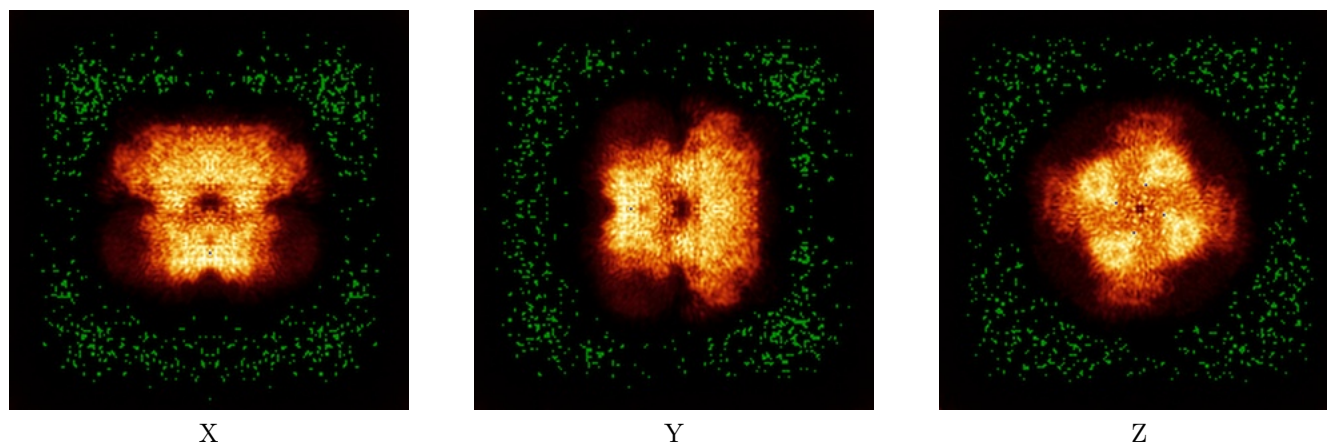


Z Index: 115

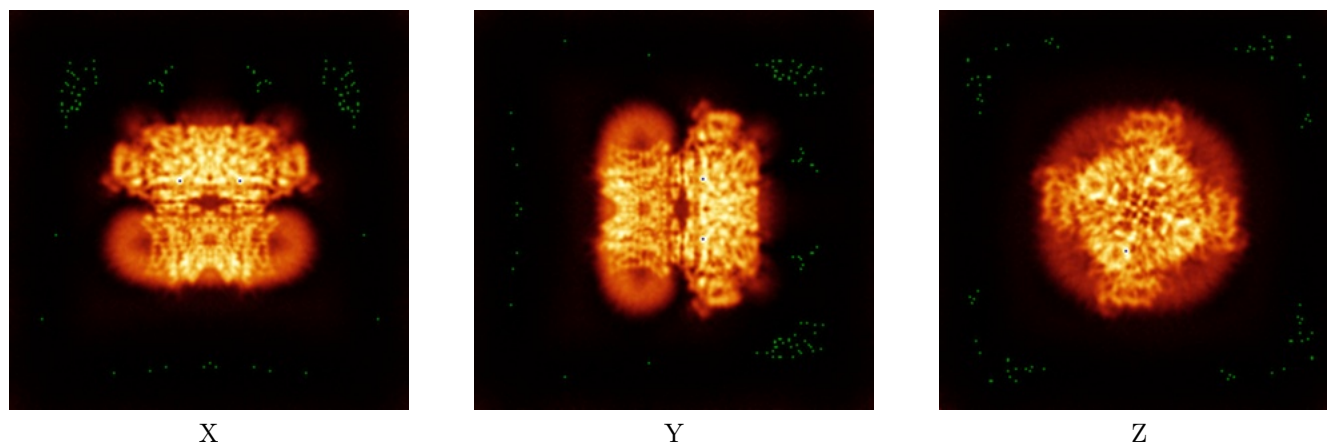
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

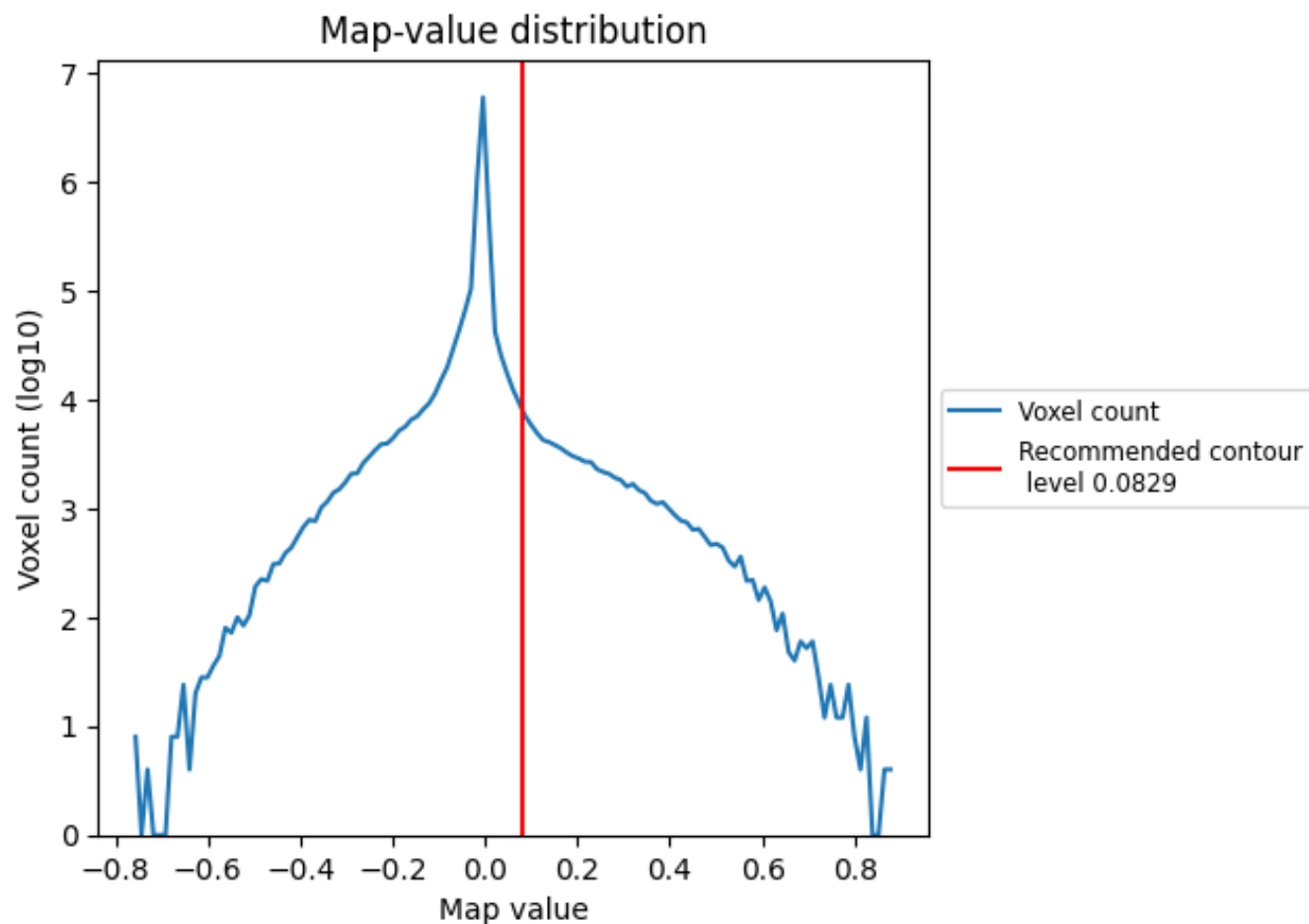
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

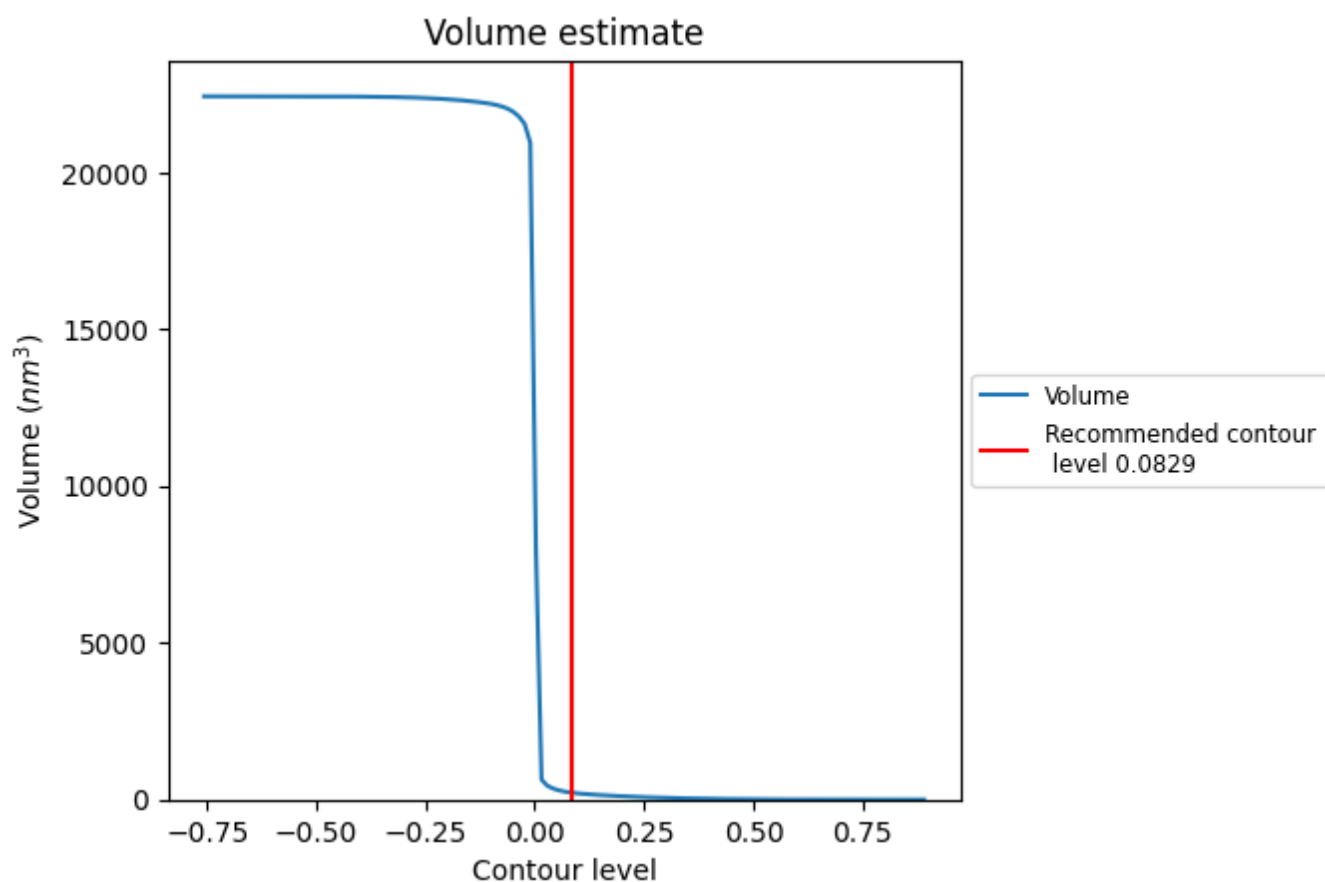
This section contains the results of statistical analysis of the map.

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.

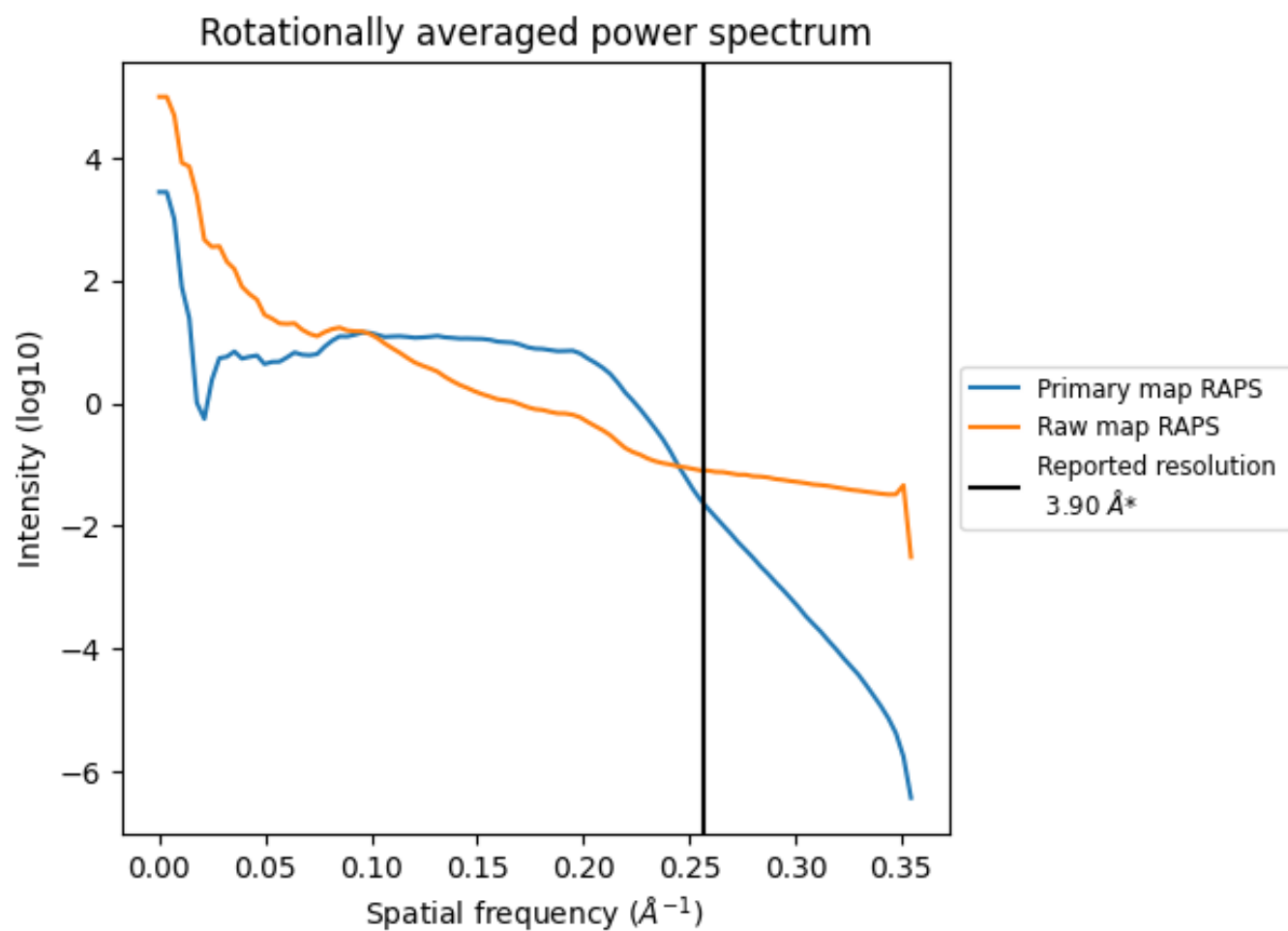
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 223 nm³; this corresponds to an approximate mass of 201 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 ⓘ

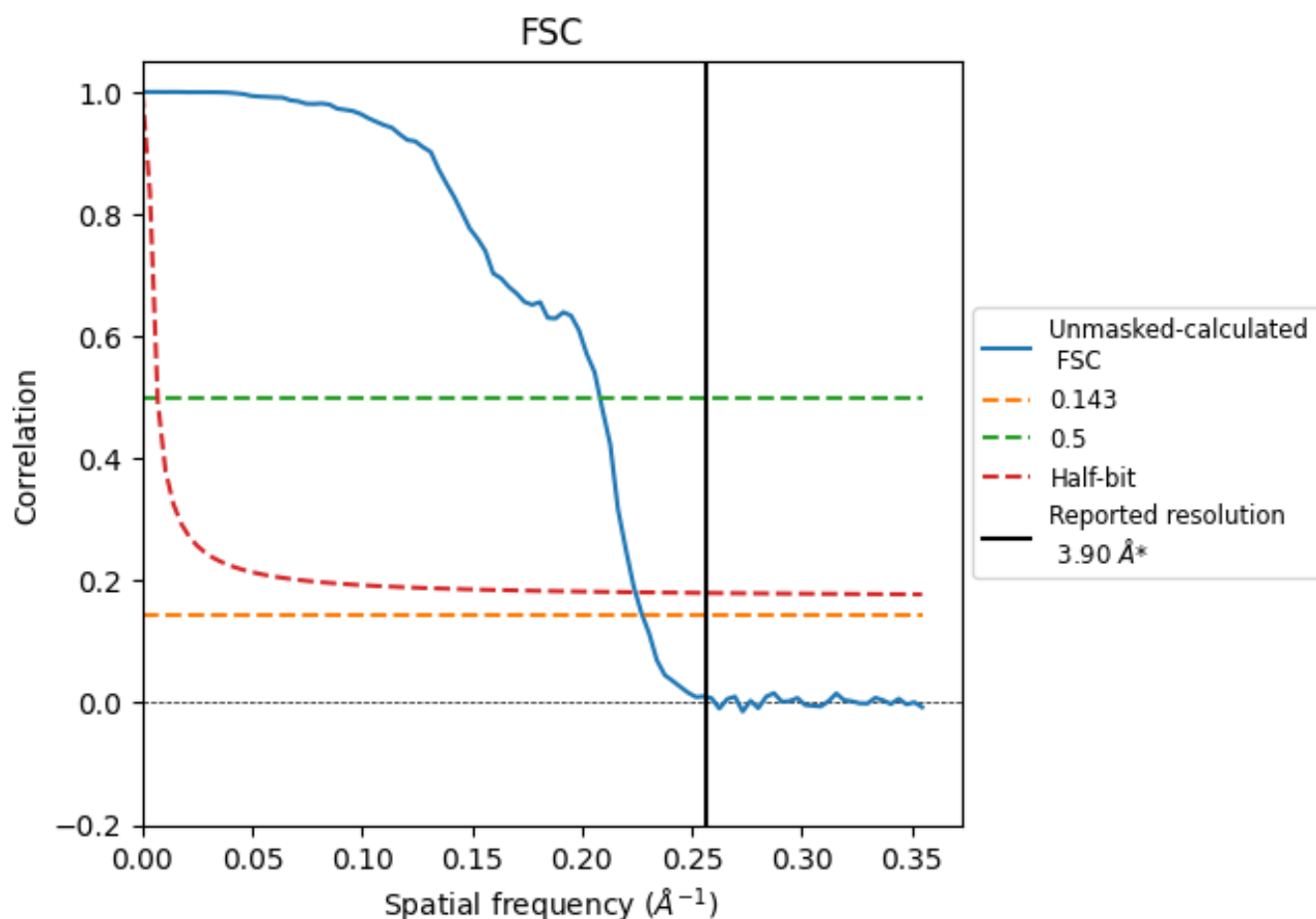


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.40	4.81	4.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.40 differs from the reported value 3.9 by more than 10 %

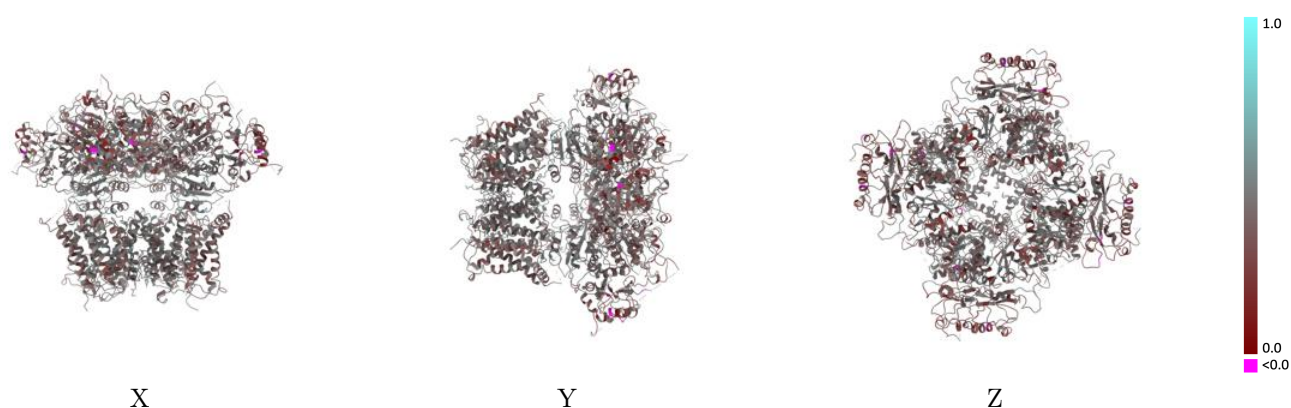
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-39753 and PDB model 8Z3S. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

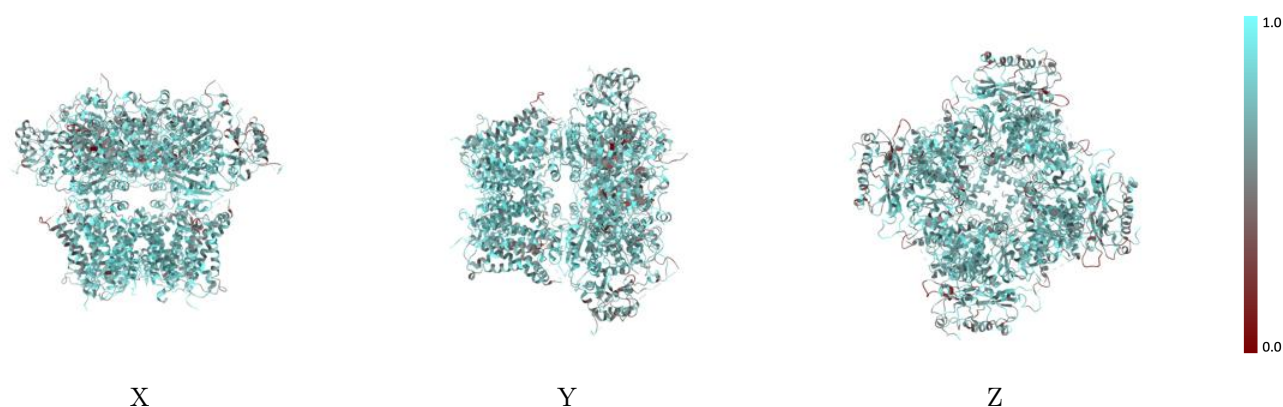
This section was not generated.

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



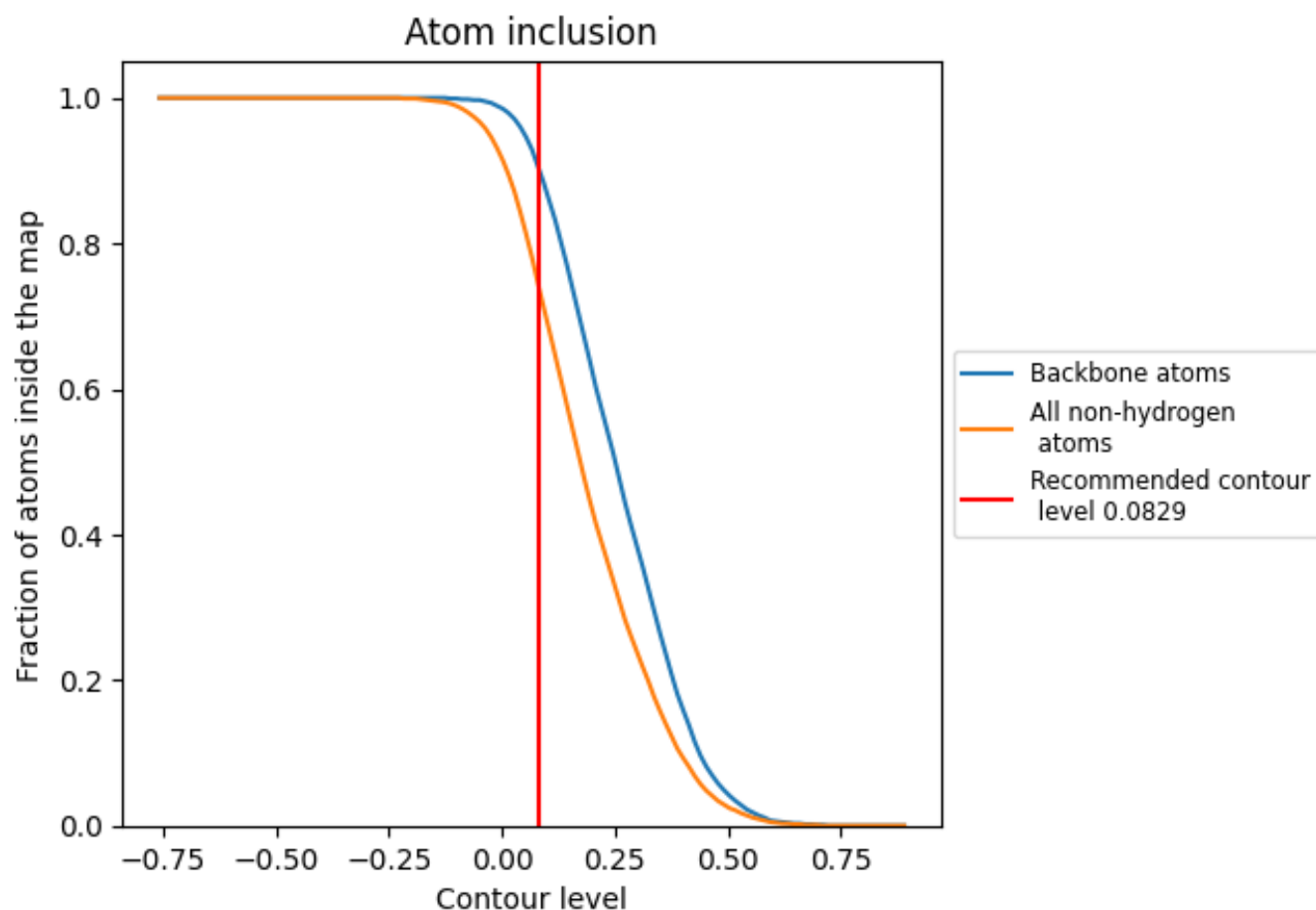
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0829).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 74% 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 (0.0829) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7380	0.4130
A	0.7410	0.4170
B	0.7360	0.4120
C	0.7410	0.4120
D	0.7360	0.4110

