



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 01:27 AM UTC

PDB ID : 9U58 / pdb_00009u58
EMDB ID : EMD-63866
Title : Cryo-EM structure of AZ-GS bound AtABCC2
Authors : Dong, J.; Yang, T.-L.; Yang, G.-F.
Deposited on : 2025-03-20
Resolution : 3.36 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

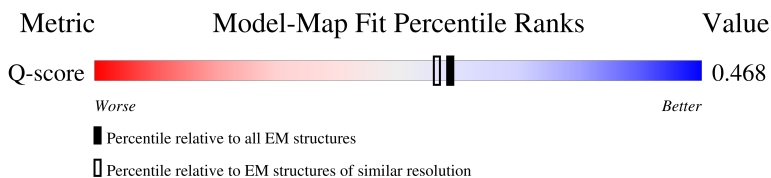
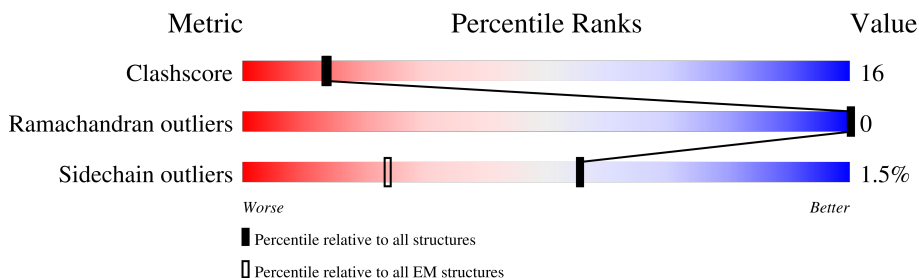
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.36 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	14332 (2.86 - 3.86)

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	1464	<p>64% 30% • 6%</p>

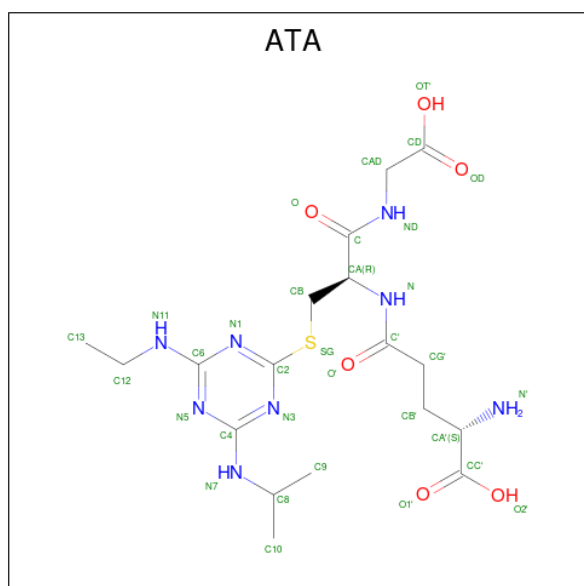
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In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ABC transporter C family member 2.

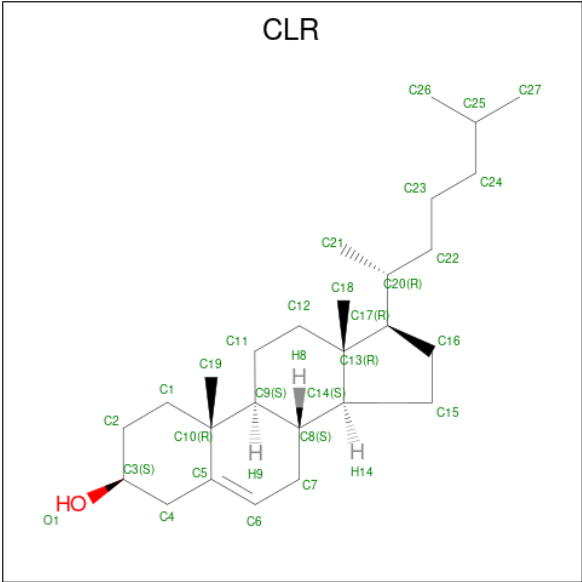
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1379	Total	C	N	O	S	0	0
			10915	7068	1839	1956	52		

- Molecule 2 is ATRAZINE GLUTATHIONE CONJUGATE (CCD ID: ATA) (formula: $C_{18}H_{30}N_8O_6S$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			33	18	8	6	1	

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: $\text{C}_{27}\text{H}_{46}\text{O}$).

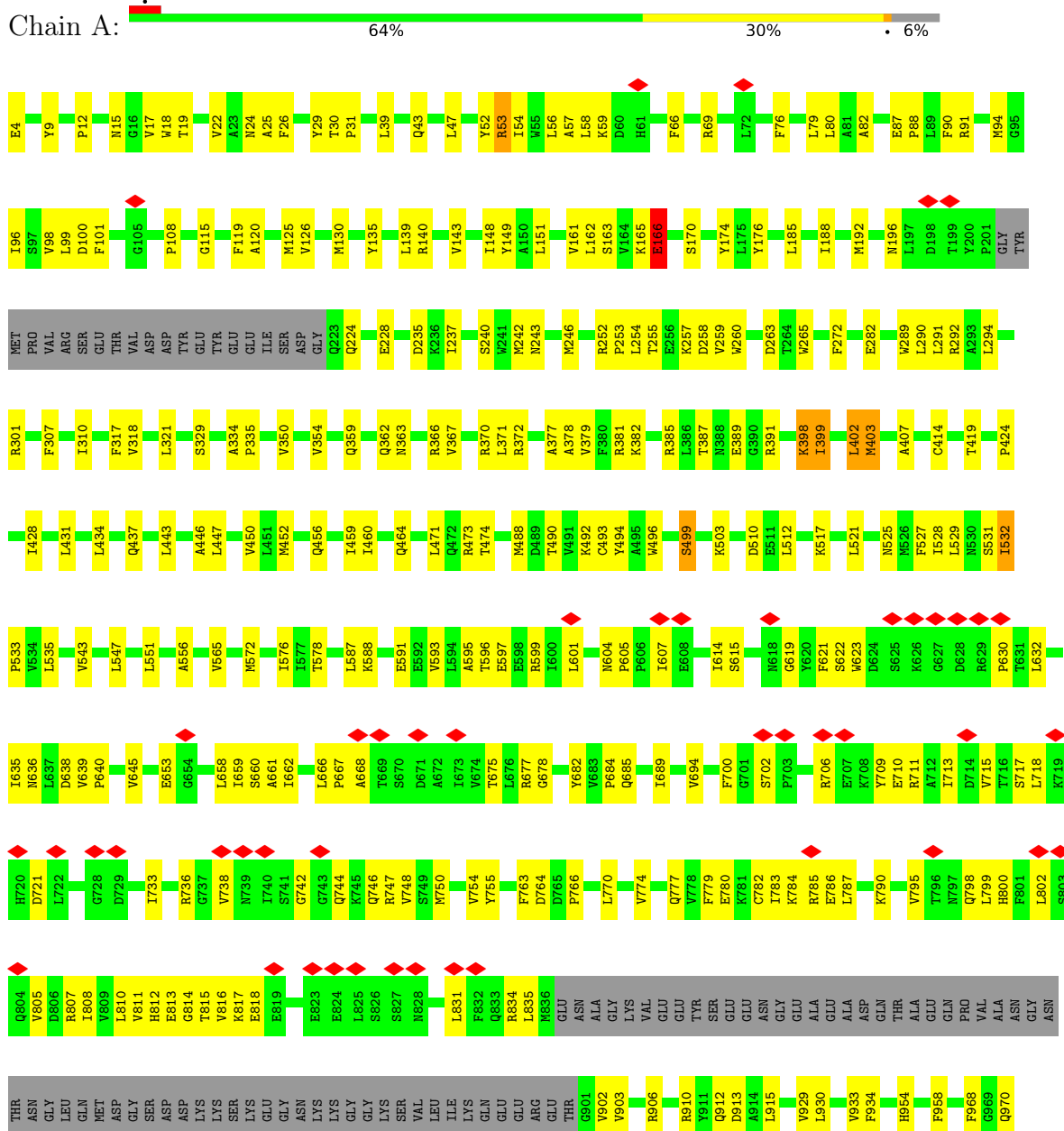


Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	

3 Residue-property plots

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

• Molecule 1: ABC transporter C family member 2



I1441	L1388	T1278	Y971
D1444	D1389	G1279	E1170
K1445		A1280	T974
	F1377	G1281	Y1185
V1448	N1378	K1282	K990
L1449	F1379	S1283	K991
D1450	S1380	S1284	L992
S1451		L1285	K996
G1452	Q1383	R1291	L1192
R1453	R1384	I1292	L1193
V1454	Q1385		T1194
Q1455	L1386	R1299	L1001
	L1387		R1002
S1459	S1388	I1302	F1008
N1462	S1390	D1306	D1023
		V1307	
N1466	L1393	G1308	T1027
E1467	L1394	K1309	
	R1395	F1310	V1033
	R1396	G1311	P1224
	S1397	L1312	P1225
			M1037
	L1400	L1315	
	V1401	R1316	L1051
	L1402		
	D1403	P1323	I1054
	E1404	P1326	S1056
	A1405	V1327	
	T1406		T1063
	A1407	T1332	M1064
	A1408	V1333	
	V1409	R1334	F1070
	D1410	F1335	
	V1411	M1336	Y1074
	R1412	L1337	
	T1413	D1338	E1083
		P1339	P1094
	I1417	F1340	
	Q1418		Q1098
	K1419	H1343	
	T1420	M1344	R1110
	I1421	D1345	
	R1422	A1346	R1117
	E1423		
		M1349	I1121
	K1426	E1350	
			F1132
	M1430	E1353	
	L1431	R1354	
	I1432		L1147
	I1433	L1357	E1148
	A1434	K1358	
	H1435	D1359	G1151
	R1436	T1360	
	L1437	I1361	M1154
	N1438	R1362	I1155
	T1439	R1363	W1156
	I1440		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135841	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 ($e^-/\text{\AA}^2$)	49.79	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.088	Depositor
Minimum map value	-1.215	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	296.0, 296.0, 296.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.74, 0.74, 0.74	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: CLR, ATA

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	0.60	1/11160 (0.0%)	0.70	9/15159 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	499	SER	CA-C	-5.15	1.45	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1339	PRO	CA-N-CD	-11.31	96.16	112.00
1	A	1225	PRO	N-CA-CB	-6.59	96.33	103.25
1	A	166	GLU	CA-C-N	-6.10	114.08	123.17
1	A	166	GLU	C-N-CA	-6.10	114.08	123.17
1	A	503	LYS	N-CA-C	-5.63	108.20	114.62
1	A	1192	LEU	N-CA-C	-5.51	106.23	113.17
1	A	1193	LEU	N-CA-C	-5.25	107.00	113.41
1	A	496	TRP	CA-CB-CG	5.21	123.49	113.60
1	A	1339	PRO	N-CD-CG	-5.10	95.55	103.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	53	ARG	Sidechain

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	10915	0	11098	345	0
2	A	33	0	28	1	0
3	A	196	0	322	28	0
All	All	11144	0	11448	355	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 16.

All (355) 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:A:929:VAL:HG22	3:A:1505:CLR:C26	1.38	1.48
1:A:929:VAL:CG2	3:A:1505:CLR:H262	1.73	1.18
1:A:929:VAL:CG2	3:A:1505:CLR:C26	2.23	1.13
1:A:929:VAL:HA	3:A:1505:CLR:H263	1.41	0.99
1:A:82:ALA:HA	1:A:125:MET:HE2	1.52	0.92
1:A:290:LEU:HD22	1:A:591:GLU:HB3	1.53	0.89
1:A:929:VAL:HG22	3:A:1505:CLR:H261	1.57	0.86
1:A:621:PHE:HB2	1:A:632:LEU:HB2	1.62	0.82
1:A:1353:GLU:HB3	1:A:1358:LYS:HD2	1.64	0.79
1:A:1280:ALA:HB1	1:A:1451:SER:H	1.47	0.79
1:A:929:VAL:CG2	3:A:1505:CLR:H261	2.12	0.79
1:A:929:VAL:HG22	3:A:1505:CLR:H262	0.77	0.76
1:A:596:THR:HG22	1:A:597:GLU:H	1.50	0.75
1:A:929:VAL:HA	3:A:1505:CLR:C26	2.17	0.75
1:A:39:LEU:O	1:A:43:GLN:NE2	2.20	0.74
1:A:721:ASP:OD2	1:A:747:ARG:NH1	2.21	0.73
1:A:91:ARG:HG3	1:A:96:ILE:HB	1.71	0.73
1:A:1054:ILE:HG12	3:A:1507:CLR:H72	1.70	0.73
1:A:1395:ARG:HD2	1:A:1397:SER:HB3	1.71	0.73
1:A:91:ARG:HH12	1:A:176:TYR:HD2	1.35	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:ASN:ND2	1:A:678:GLY:O	2.22	0.71
1:A:1357:LEU:HD21	1:A:1386:LEU:HB3	1.70	0.71
1:A:653:GLU:OE2	1:A:812:HIS:ND1	2.24	0.70
1:A:402:LEU:HB3	1:A:403:MET:HE2	1.73	0.69
1:A:69:ARG:HH21	1:A:196:ASN:HB2	1.55	0.69
1:A:713:ILE:HG13	1:A:718:LEU:HD23	1.73	0.68
3:A:1506:CLR:H71	3:A:1507:CLR:H71	1.74	0.68
1:A:666:LEU:HD12	1:A:667:PRO:HD2	1.75	0.68
1:A:263:ASP:HB3	1:A:265:TRP:HD1	1.57	0.68
1:A:902:VAL:HG12	1:A:903:VAL:H	1.57	0.68
1:A:289:TRP:HH2	3:A:1508:CLR:H191	1.59	0.68
1:A:605:PRO:HG2	1:A:677:ARG:HG3	1.77	0.67
1:A:492:LYS:O	1:A:1316:ARG:NH1	2.27	0.67
1:A:787:LEU:HD23	1:A:790:LYS:HG3	1.77	0.67
1:A:235:ASP:OD1	1:A:240:SER:HB2	1.95	0.66
1:A:15:ASN:HA	1:A:19:THR:HG21	1.77	0.66
1:A:228:GLU:OE2	1:A:362:GLN:NE2	2.27	0.66
1:A:291:LEU:HG	1:A:587:LEU:HD21	1.77	0.66
1:A:379:VAL:HG11	1:A:403:MET:HE1	1.77	0.66
1:A:90:PHE:HB3	1:A:94:MET:HE2	1.77	0.66
1:A:659:ILE:HA	1:A:662:ILE:HD12	1.78	0.66
1:A:834:ARG:NE	1:A:834:ARG:O	2.30	0.65
1:A:1450:ASP:O	1:A:1453:ARG:NH2	2.29	0.65
1:A:1390:SER:HA	1:A:1393:LEU:HB2	1.79	0.65
1:A:1245:GLU:OE1	1:A:1299:ARG:NH1	2.30	0.64
1:A:1232:PRO:HB3	1:A:1236:TRP:HE3	1.62	0.64
1:A:1422:ARG:O	1:A:1426:LYS:NZ	2.20	0.63
1:A:1236:TRP:HH2	1:A:1307:VAL:HG23	1.62	0.63
1:A:473:ARG:NH1	1:A:510:ASP:OD2	2.32	0.62
1:A:1074:TYR:HB2	1:A:1197:LEU:HD21	1.80	0.62
1:A:1230:ASN:HB3	1:A:1310:PHE:CD1	2.35	0.62
1:A:543:VAL:O	1:A:547:LEU:HG	2.00	0.62
1:A:1248:VAL:HG22	1:A:1261:GLY:H	1.65	0.61
1:A:1249:LEU:HD23	1:A:1284:SER:HB3	1.83	0.61
1:A:263:ASP:HB3	1:A:265:TRP:CD1	2.36	0.60
1:A:1291:ARG:NH1	1:A:1308:GLY:O	2.34	0.60
1:A:621:PHE:HB3	1:A:666:LEU:HG	1.82	0.60
1:A:702:SER:HB2	1:A:755:TYR:CE1	2.36	0.60
1:A:100:ASP:OD1	1:A:101:PHE:N	2.35	0.60
1:A:385:ARG:HH21	1:A:601:LEU:HD12	1.67	0.60
1:A:387:THR:HG22	1:A:599:ARG:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1359:ASP:OD1	1:A:1360:THR:N	2.35	0.59
1:A:1054:ILE:CG1	3:A:1507:CLR:H72	2.32	0.59
1:A:185:LEU:HA	1:A:188:ILE:HG22	1.85	0.58
1:A:1198:ARG:HH21	2:A:1501:ATA:HA'2	1.68	0.58
1:A:747:ARG:HA	1:A:750:MET:HE2	1.85	0.58
1:A:1436:ARG:O	1:A:1439:THR:OG1	2.20	0.58
1:A:623:TRP:CD2	1:A:666:LEU:HD13	2.38	0.58
1:A:802:LEU:HD22	1:A:808:ILE:HD11	1.85	0.58
1:A:1242:ILE:HD13	1:A:1431:LEU:HD11	1.84	0.58
1:A:1437:LEU:HD12	1:A:1440:ILE:HB	1.86	0.57
1:A:17:VAL:HG11	1:A:101:PHE:CD2	2.40	0.57
1:A:255:THR:O	1:A:257:LYS:N	2.38	0.57
1:A:659:ILE:HG21	1:A:795:VAL:HG21	1.86	0.57
1:A:661:ALA:HB2	1:A:666:LEU:HD23	1.86	0.57
1:A:529:LEU:O	1:A:533:PRO:HD2	2.04	0.57
1:A:1312:LEU:HD21	1:A:1316:ARG:NH2	2.20	0.57
1:A:1350:GLU:OE2	1:A:1354:ARG:NH2	2.37	0.57
1:A:115:GLY:O	1:A:119:PHE:HD1	1.88	0.56
1:A:1051:LEU:HD22	1:A:1185:TYR:CD2	2.40	0.56
1:A:1434:ALA:HB3	1:A:1440:ILE:HD11	1.87	0.56
1:A:607:ILE:HG13	1:A:677:ARG:HH12	1.69	0.56
1:A:1236:TRP:CD1	1:A:1237:PRO:HA	2.41	0.56
1:A:431:LEU:HD11	1:A:446:ALA:HB2	1.88	0.56
1:A:366:ARG:HD3	1:A:370:ARG:NH1	2.20	0.56
1:A:1151:GLY:HA3	1:A:1190:THR:HG23	1.88	0.55
1:A:1232:PRO:HB3	1:A:1236:TRP:CE3	2.42	0.55
1:A:1241:SER:OG	1:A:1268:PRO:HG3	2.07	0.55
1:A:1282:LYS:HB3	1:A:1433:ILE:HD11	1.87	0.55
1:A:494:TYR:HD1	1:A:1395:ARG:HH21	1.53	0.55
1:A:709:TYR:O	1:A:713:ILE:HD12	2.07	0.55
1:A:24:ASN:HB3	1:A:30:THR:HG21	1.87	0.55
1:A:1306:ASP:O	1:A:1309:LYS:HG2	2.07	0.55
1:A:359:GLN:O	1:A:363:ASN:ND2	2.39	0.54
1:A:623:TRP:NE1	1:A:666:LEU:HD22	2.22	0.54
1:A:135:TYR:OH	1:A:140:ARG:NH1	2.39	0.54
1:A:1349:TRP:HZ3	1:A:1361:ILE:HG21	1.72	0.54
1:A:1332:THR:HG23	1:A:1335:PHE:H	1.73	0.54
3:A:1505:CLR:H112	3:A:1506:CLR:H112	1.89	0.54
1:A:254:LEU:N	1:A:1083:GLU:OE1	2.34	0.54
1:A:126:VAL:O	1:A:130:MET:HG2	2.07	0.54
1:A:805:VAL:HG12	1:A:807:ARG:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1346:ALA:HA	1:A:1349:TRP:HD1	1.73	0.54
1:A:1383:GLN:NE2	1:A:1384:ARG:HG2	2.23	0.54
1:A:974:THR:HG22	1:A:974:THR:O	2.09	0.53
1:A:399:ILE:O	1:A:403:MET:HG2	2.08	0.53
1:A:689:ILE:O	1:A:689:ILE:HG13	2.08	0.53
1:A:968:PHE:O	1:A:970:GLN:N	2.41	0.53
1:A:228:GLU:OE1	1:A:366:ARG:NH2	2.41	0.53
1:A:1466:ASN:OD1	1:A:1467:GLU:N	2.41	0.53
1:A:954:HIS:HB3	1:A:958:PHE:CD2	2.44	0.53
1:A:1228:GLU:O	1:A:1231:ARG:HG2	2.08	0.53
1:A:494:TYR:HD1	1:A:1395:ARG:NH2	2.07	0.53
1:A:488:MET:O	1:A:492:LYS:HB2	2.09	0.53
1:A:968:PHE:O	1:A:971:VAL:N	2.20	0.53
1:A:933:VAL:HA	3:A:1505:CLR:H151	1.90	0.53
1:A:253:PRO:HB3	1:A:1083:GLU:OE2	2.09	0.53
1:A:1117:ARG:O	1:A:1121:ILE:HG12	2.09	0.53
1:A:954:HIS:HB3	1:A:958:PHE:HD2	1.73	0.52
1:A:1070:PHE:CE1	1:A:1197:LEU:HD22	2.43	0.52
1:A:447:LEU:O	1:A:450:VAL:HG12	2.10	0.52
1:A:471:LEU:O	1:A:474:THR:HG22	2.10	0.52
1:A:512:LEU:HD12	1:A:990:LYS:HG3	1.91	0.52
1:A:488:MET:HG2	1:A:1008:PHE:CE2	2.44	0.52
1:A:1419:LYS:HG2	1:A:1423:GLU:HG3	1.91	0.52
1:A:623:TRP:CZ2	1:A:666:LEU:HB2	2.44	0.52
1:A:1230:ASN:HB3	1:A:1310:PHE:HD1	1.73	0.52
1:A:294:LEU:HD21	1:A:371:LEU:HD11	1.90	0.52
1:A:307:PHE:O	1:A:310:ILE:HG22	2.10	0.52
1:A:98:VAL:HG13	1:A:99:LEU:HD22	1.91	0.52
1:A:282:GLU:OE2	1:A:292:ARG:NH2	2.43	0.52
1:A:1345:ASP:OD1	1:A:1349:TRP:NE1	2.42	0.51
1:A:252:ARG:NH2	1:A:258:ASP:OD1	2.41	0.51
1:A:452:MET:SD	1:A:532:ILE:HB	2.51	0.51
1:A:906:ARG:HA	1:A:906:ARG:NE	2.25	0.51
1:A:22:VAL:HG12	1:A:24:ASN:H	1.74	0.51
1:A:709:TYR:CE2	1:A:713:ILE:HD11	2.46	0.51
1:A:1380:SER:O	1:A:1383:GLN:HG3	2.10	0.51
1:A:623:TRP:HZ2	1:A:660:SER:HB3	1.74	0.51
1:A:224:GLN:N	1:A:224:GLN:OE1	2.43	0.51
1:A:490:THR:HG21	1:A:1327:VAL:HG21	1.93	0.51
1:A:1361:ILE:HG23	1:A:1362:ARG:HE	1.76	0.51
1:A:259:VAL:HG21	1:A:1132:PHE:HE1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:HIS:H	1:A:817:LYS:HG2	1.75	0.50
1:A:1419:LYS:O	1:A:1423:GLU:HG2	2.11	0.50
1:A:317:PHE:HE1	1:A:565:VAL:HG11	1.76	0.50
1:A:1225:PRO:HA	1:A:1312:LEU:N	2.26	0.50
1:A:1074:TYR:HB2	1:A:1197:LEU:HD11	1.94	0.50
1:A:1360:THR:O	1:A:1363:ARG:HG2	2.12	0.50
1:A:700:PHE:HB3	1:A:1117:ARG:CD	2.42	0.50
1:A:1225:PRO:HA	1:A:1312:LEU:H	1.76	0.49
1:A:1233:PRO:HG2	1:A:1236:TRP:HB2	1.94	0.49
1:A:694:VAL:HG13	1:A:733:ILE:HD11	1.94	0.49
1:A:39:LEU:HB3	1:A:43:GLN:HE22	1.77	0.49
1:A:607:ILE:HG13	1:A:677:ARG:NH1	2.28	0.49
1:A:1147:LEU:HD11	1:A:1197:LEU:HD23	1.93	0.49
1:A:52:TYR:CD2	1:A:139:LEU:HD11	2.47	0.49
1:A:607:ILE:HA	1:A:677:ARG:NH1	2.27	0.49
1:A:166:GLU:H	1:A:166:GLU:HG2	1.34	0.49
1:A:685:GLN:HB2	1:A:764:ASP:OD2	2.12	0.49
1:A:1264:PHE:HZ	1:A:1285:LEU:HD11	1.77	0.49
1:A:774:VAL:HA	1:A:777:GLN:HG2	1.95	0.48
1:A:996:MET:O	1:A:996:MET:HG2	2.11	0.48
1:A:350:VAL:O	1:A:354:VAL:HG23	2.13	0.48
1:A:929:VAL:HG23	3:A:1505:CLR:H261	1.95	0.48
1:A:1402:LEU:HD23	1:A:1403:ASP:N	2.27	0.48
1:A:334:ALA:HB1	1:A:335:PRO:HD2	1.95	0.48
1:A:934:PHE:HB3	1:A:970:GLN:HB2	1.96	0.48
1:A:1437:LEU:HA	1:A:1440:ILE:HD13	1.95	0.48
1:A:1448:VAL:HB	1:A:1455:GLN:HB2	1.95	0.48
1:A:622:SER:HB2	1:A:630:PRO:HA	1.95	0.48
1:A:1236:TRP:HZ2	1:A:1302:ILE:HB	1.78	0.48
1:A:1437:LEU:O	1:A:1441:ILE:HG13	2.13	0.48
1:A:17:VAL:HG11	1:A:101:PHE:CE2	2.49	0.48
1:A:742:GLY:O	1:A:746:GLN:HG2	2.14	0.48
1:A:750:MET:O	1:A:754:VAL:HG22	2.14	0.48
1:A:787:LEU:CD2	1:A:790:LYS:HG3	2.42	0.48
1:A:1459:SER:OG	1:A:1462:ASN:OD1	2.31	0.48
1:A:700:PHE:HB3	1:A:1117:ARG:HD2	1.95	0.48
1:A:69:ARG:NH2	1:A:196:ASN:HB2	2.26	0.48
1:A:1242:ILE:HD11	1:A:1266:ILE:HG13	1.96	0.47
1:A:398:LYS:HB2	1:A:398:LYS:HE2	1.37	0.47
1:A:1063:ILE:HD12	1:A:1154:MET:HG2	1.95	0.47
1:A:460:ILE:O	1:A:464:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:GLU:OE1	1:A:785:ARG:NE	2.48	0.47
1:A:810:LEU:O	1:A:817:LYS:HB2	2.14	0.47
1:A:779:PHE:HA	1:A:783:ILE:HD13	1.95	0.47
1:A:66:PHE:HD2	1:A:135:TYR:CD2	2.33	0.47
1:A:799:LEU:HA	1:A:802:LEU:HG	1.96	0.47
1:A:1337:LEU:HD11	1:A:1387:LEU:HD11	1.96	0.47
1:A:619:GLY:HA3	1:A:635:ILE:HB	1.97	0.47
1:A:831:LEU:O	1:A:835:LEU:HG	2.15	0.47
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.75	0.46
1:A:596:THR:HG22	1:A:597:GLU:N	2.25	0.46
1:A:24:ASN:OD1	1:A:25:ALA:N	2.49	0.46
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.67	0.46
1:A:488:MET:O	1:A:492:LYS:CB	2.63	0.46
1:A:317:PHE:CE1	1:A:565:VAL:HG11	2.49	0.46
1:A:402:LEU:HD11	1:A:593:VAL:HB	1.97	0.46
1:A:414:CYS:SG	3:A:1508:CLR:H271	2.55	0.46
1:A:621:PHE:CE2	1:A:668:ALA:HB2	2.51	0.46
1:A:639:VAL:HG22	1:A:645:VAL:HG21	1.95	0.46
1:A:1343:HIS:CG	1:A:1394:LEU:HD11	2.50	0.46
1:A:424:PRO:O	1:A:428:ILE:HG12	2.16	0.46
1:A:1361:ILE:HG23	1:A:1362:ARG:HH21	1.81	0.46
1:A:1420:THR:HA	1:A:1423:GLU:HB2	1.98	0.46
1:A:499:SER:HB2	1:A:1340:PHE:CE1	2.50	0.46
1:A:512:LEU:CD1	1:A:990:LYS:HG3	2.45	0.46
1:A:1056:SER:O	1:A:1056:SER:OG	2.31	0.46
1:A:614:ILE:HB	1:A:639:VAL:HB	1.98	0.46
1:A:992:LEU:HD23	1:A:1027:ILE:HG21	1.98	0.45
1:A:372:ARG:HG2	1:A:407:ALA:HB1	1.99	0.45
1:A:1094:PRO:O	1:A:1098:GLN:HG2	2.17	0.45
1:A:1402:LEU:HB3	1:A:1432:ILE:HD13	1.97	0.45
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.71	0.45
1:A:532:ILE:O	1:A:535:LEU:N	2.50	0.45
1:A:1312:LEU:HD21	1:A:1316:ARG:CZ	2.46	0.45
1:A:593:VAL:C	1:A:595:ALA:H	2.24	0.45
1:A:715:VAL:HG21	1:A:786:GLU:OE1	2.17	0.45
1:A:389:GLU:OE1	1:A:389:GLU:N	2.50	0.45
1:A:715:VAL:HB	1:A:782:CYS:HB2	1.99	0.45
1:A:763:PHE:CD2	1:A:766:PRO:HG3	2.52	0.45
1:A:1334:ARG:NH2	1:A:1369:ASP:OD1	2.42	0.45
1:A:1402:LEU:O	1:A:1433:ILE:HG22	2.17	0.45
1:A:1231:ARG:HD2	1:A:1231:ARG:HA	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLU:N	1:A:4:GLU:OE1	2.50	0.45
1:A:391:ARG:HG2	1:A:391:ARG:HH21	1.82	0.45
1:A:784:LYS:HA	1:A:784:LYS:HD3	1.84	0.45
1:A:1323:PRO:HG2	1:A:1326:PRO:HA	1.99	0.45
1:A:1386:LEU:HD23	1:A:1417:ILE:HG22	1.99	0.45
1:A:459:ILE:HG23	1:A:521:LEU:HD21	1.99	0.45
3:A:1502:CLR:H221	3:A:1502:CLR:H162	1.27	0.45
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.82	0.44
1:A:329:SER:O	1:A:334:ALA:HB3	2.17	0.44
1:A:713:ILE:HA	1:A:718:LEU:HB3	1.99	0.44
1:A:517:LYS:HE3	1:A:517:LYS:HB2	1.70	0.44
1:A:1413:THR:O	1:A:1417:ILE:HG23	2.18	0.44
3:A:1505:CLR:H211	3:A:1505:CLR:H232	1.76	0.44
1:A:706:ARG:O	1:A:710:GLU:CB	2.66	0.44
1:A:811:VAL:HG13	1:A:815:THR:O	2.18	0.44
1:A:998:HIS:CG	1:A:998:HIS:O	2.71	0.44
3:A:1503:CLR:H221	3:A:1503:CLR:H162	1.38	0.44
1:A:243:ASN:O	1:A:246:MET:N	2.50	0.44
1:A:929:VAL:CA	3:A:1505:CLR:C26	2.93	0.44
1:A:1023:ASP:O	1:A:1027:ILE:HG12	2.18	0.44
1:A:1236:TRP:NE1	1:A:1302:ILE:O	2.45	0.44
1:A:87:GLU:HB3	1:A:88:PRO:HD3	2.00	0.44
1:A:711:ARG:O	1:A:715:VAL:HG22	2.18	0.44
1:A:1417:ILE:HG13	1:A:1418:GLN:N	2.32	0.44
1:A:493:CYS:SG	1:A:1292:ILE:HD11	2.58	0.44
1:A:658:LEU:O	1:A:662:ILE:HG13	2.16	0.44
1:A:1272:VAL:HG12	1:A:1273:GLY:N	2.33	0.44
3:A:1508:CLR:H221	3:A:1508:CLR:H162	1.32	0.44
1:A:9:TYR:O	1:A:108:PRO:HG2	2.18	0.43
1:A:47:LEU:HD23	1:A:120:ALA:HB2	2.00	0.43
1:A:76:PHE:O	1:A:79:LEU:HD23	2.18	0.43
1:A:527:PHE:O	1:A:528:ILE:C	2.61	0.43
1:A:812:HIS:HD2	1:A:813:GLU:HB2	1.83	0.43
1:A:1051:LEU:HD12	1:A:1051:LEU:HA	1.82	0.43
3:A:1506:CLR:H71	3:A:1507:CLR:C7	2.45	0.43
1:A:294:LEU:HD21	1:A:371:LEU:CD1	2.48	0.43
1:A:638:ASP:OD1	1:A:640:PRO:HD3	2.17	0.43
1:A:1333:VAL:HB	1:A:1368:LEU:O	2.18	0.43
1:A:460:ILE:HG21	1:A:578:THR:HG21	2.00	0.43
1:A:636:ASN:O	1:A:816:VAL:HG11	2.18	0.43
1:A:968:PHE:C	1:A:970:GLN:N	2.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1208:ASN:O	1:A:1211:GLU:HG2	2.18	0.43
1:A:149:TYR:HA	1:A:1064:MET:HE1	2.01	0.43
1:A:434:LEU:O	1:A:437:GLN:N	2.48	0.43
1:A:1291:ARG:HE	1:A:1315:LEU:HD13	1.83	0.43
1:A:318:VAL:HG12	1:A:318:VAL:O	2.19	0.43
1:A:615:SER:HB3	1:A:675:THR:HB	2.01	0.43
1:A:54:ILE:O	1:A:57:ALA:HB3	2.18	0.43
1:A:301:ARG:HB2	1:A:367:VAL:HG23	2.01	0.43
1:A:632:LEU:HA	1:A:814:GLY:O	2.19	0.43
1:A:736:ARG:O	1:A:738:VAL:N	2.51	0.43
1:A:812:HIS:CD2	1:A:813:GLU:HB2	2.53	0.43
1:A:1230:ASN:ND2	1:A:1309:LYS:O	2.52	0.43
3:A:1502:CLR:H213	3:A:1502:CLR:H231	1.78	0.43
3:A:1507:CLR:H221	3:A:1507:CLR:H162	1.29	0.43
1:A:532:ILE:O	1:A:533:PRO:C	2.61	0.43
1:A:1358:LYS:O	1:A:1362:ARG:HG2	2.18	0.43
1:A:744:GLN:O	1:A:748:VAL:HG23	2.18	0.43
1:A:812:HIS:O	1:A:817:LYS:HE2	2.18	0.43
1:A:717:SER:HB2	1:A:747:ARG:HE	1.84	0.42
1:A:1418:GLN:HG3	1:A:1422:ARG:NH2	2.34	0.42
1:A:798:GLN:HB3	1:A:800:HIS:CE1	2.54	0.42
1:A:1224:PRO:HG2	1:A:1227:ILE:HD11	2.02	0.42
1:A:148:ILE:HD13	1:A:148:ILE:HA	1.83	0.42
1:A:237:ILE:HG21	1:A:237:ILE:HD13	1.77	0.42
1:A:1332:THR:O	1:A:1335:PHE:HB3	2.19	0.42
1:A:161:VAL:O	1:A:162:LEU:C	2.63	0.42
1:A:1389:LEU:HB3	1:A:1393:LEU:HD23	2.01	0.42
1:A:140:ARG:O	1:A:143:VAL:HG12	2.19	0.42
1:A:188:ILE:O	1:A:192:MET:HG2	2.20	0.42
1:A:593:VAL:C	1:A:595:ALA:N	2.78	0.42
1:A:1361:ILE:HD12	1:A:1361:ILE:HA	1.94	0.42
1:A:30:THR:N	1:A:31:PRO:HD2	2.35	0.42
1:A:289:TRP:CH2	3:A:1508:CLR:H191	2.47	0.42
1:A:588:LYS:HA	1:A:588:LYS:HD3	1.73	0.42
1:A:1063:ILE:HD13	1:A:1063:ILE:HA	1.80	0.42
1:A:82:ALA:HA	1:A:125:MET:CE	2.37	0.42
1:A:272:PHE:HE1	1:A:378:ALA:HB2	1.85	0.42
1:A:770:LEU:HD23	1:A:770:LEU:HA	1.90	0.42
1:A:902:VAL:HG12	1:A:903:VAL:N	2.29	0.42
1:A:1074:TYR:CG	1:A:1197:LEU:HD11	2.55	0.42
1:A:512:LEU:HA	1:A:512:LEU:HD23	1.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1278:THR:HA	1:A:1282:LYS:HE2	2.01	0.41
1:A:1394:LEU:O	1:A:1394:LEU:HD12	2.18	0.41
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.75	0.41
1:A:1033:VAL:O	1:A:1037:MET:HG3	2.20	0.41
1:A:1156:TRP:CH2	3:A:1503:CLR:H262	2.55	0.41
1:A:115:GLY:O	1:A:119:PHE:CD1	2.72	0.41
1:A:419:THR:HB	1:A:576:ILE:HD13	2.03	0.41
3:A:1508:CLR:H211	3:A:1508:CLR:H242	2.02	0.41
1:A:354:VAL:HG21	1:A:1148:GLU:CB	2.49	0.41
1:A:456:GLN:NE2	1:A:525:ASN:OD1	2.53	0.41
1:A:910:ARG:HA	1:A:913:ASP:OD2	2.21	0.41
1:A:12:PRO:HG3	1:A:29:TYR:CE1	2.55	0.41
1:A:26:PHE:CE1	3:A:1503:CLR:H112	2.55	0.41
1:A:434:LEU:HA	1:A:434:LEU:HD23	1.62	0.41
1:A:572:MET:O	1:A:572:MET:HG3	2.20	0.41
1:A:623:TRP:CZ2	1:A:660:SER:HB3	2.54	0.41
1:A:689:ILE:HD12	1:A:736:ARG:C	2.46	0.41
1:A:1451:SER:HB2	1:A:1453:ARG:NH2	2.35	0.41
1:A:224:GLN:HG2	1:A:260:TRP:HA	2.02	0.41
1:A:551:LEU:HD21	1:A:556:ALA:HB2	2.02	0.41
1:A:958:PHE:O	1:A:958:PHE:CG	2.73	0.41
1:A:968:PHE:C	1:A:970:GLN:H	2.27	0.41
1:A:17:VAL:HG13	1:A:18:TRP:N	2.36	0.41
1:A:682:TYR:CE2	1:A:684:PRO:HB3	2.56	0.41
1:A:1358:LYS:O	1:A:1361:ILE:HG22	2.20	0.41
1:A:1227:ILE:HD12	1:A:1311:GLY:HA2	2.02	0.41
1:A:1246:ASP:H	1:A:1263:SER:HB2	1.86	0.41
1:A:1273:GLY:O	1:A:1274:ILE:HD13	2.21	0.41
1:A:255:THR:C	1:A:257:LYS:H	2.27	0.41
1:A:391:ARG:HG2	1:A:391:ARG:NH2	2.36	0.41
1:A:593:VAL:O	1:A:595:ALA:N	2.54	0.41
1:A:912:GLN:HA	1:A:915:LEU:HD12	2.03	0.41
1:A:1170:GLU:HA	1:A:1170:GLU:OE2	2.21	0.41
1:A:1343:HIS:ND1	1:A:1394:LEU:HD11	2.36	0.41
1:A:379:VAL:CG1	1:A:403:MET:HE1	2.48	0.40
1:A:1224:PRO:HA	1:A:1225:PRO:HD3	1.90	0.40
1:A:1378:ASN:OD1	1:A:1378:ASN:N	2.45	0.40
1:A:170:SER:O	1:A:174:TYR:HB2	2.20	0.40
1:A:377:ALA:O	1:A:381:ARG:HD3	2.22	0.40
1:A:52:TYR:CE2	1:A:56:LEU:HD22	2.56	0.40
1:A:1256:PRO:HA	1:A:1257:PRO:HD2	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1400:LEU:HD22	1:A:1430:MET:HE2	2.02	0.40
1:A:242:MET:HG2	1:A:242:MET:O	2.21	0.40
1:A:599:ARG:HH21	1:A:1110:ARG:NH1	2.19	0.40
1:A:930:LEU:HD12	1:A:930:LEU:HA	1.54	0.40
1:A:1444:ASP:C	1:A:1445:LYS:HD2	2.46	0.40
1:A:58:LEU:HG	1:A:59:LYS:HE3	2.04	0.40
1:A:810:LEU:HB3	1:A:818:GLU:OE1	2.22	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	1373/1464 (94%)	1259 (92%)	114 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1193/1264 (94%)	1175 (98%)	18 (2%)	57	68

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	163	SER
1	A	165	LYS
1	A	166	GLU
1	A	382	LYS
1	A	398	LYS
1	A	399	ILE
1	A	402	LEU
1	A	403	MET
1	A	531	SER
1	A	532	ILE
1	A	1001	LEU
1	A	1002	ARG
1	A	1189	ILE
1	A	1190	THR
1	A	1193	LEU
1	A	1194	THR
1	A	1222	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	183	GLN
1	A	230	HIS
1	A	456	GLN
1	A	773	HIS
1	A	1205	ASN
1	A	1383	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

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CLR	A	1506	-	31,31,31	0.31	0	48,48,48	0.51	0
3	CLR	A	1507	-	31,31,31	0.32	0	48,48,48	0.42	0
3	CLR	A	1503	-	31,31,31	0.29	0	48,48,48	0.44	0
3	CLR	A	1504	-	31,31,31	0.35	0	48,48,48	0.81	1 (2%)
3	CLR	A	1508	-	31,31,31	0.31	0	48,48,48	0.46	0
3	CLR	A	1505	-	31,31,31	0.33	0	48,48,48	0.65	0
3	CLR	A	1502	-	31,31,31	0.33	0	48,48,48	0.56	0
2	ATA	A	1501	-	32,33,33	2.56	7 (21%)	40,43,43	4.84	14 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLR	A	1506	-	-	2/10/68/68	0/4/4/4
3	CLR	A	1507	-	-	10/10/68/68	0/4/4/4
3	CLR	A	1503	-	-	8/10/68/68	0/4/4/4
3	CLR	A	1504	-	-	9/10/68/68	0/4/4/4
3	CLR	A	1508	-	-	8/10/68/68	0/4/4/4
3	CLR	A	1505	-	-	9/10/68/68	0/4/4/4
3	CLR	A	1502	-	-	8/10/68/68	0/4/4/4
2	ATA	A	1501	-	-	14/34/34/34	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	ATA	C4-N7	8.52	1.44	1.34
2	A	1501	ATA	C6-N11	7.03	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	ATA	C'-N	5.05	1.44	1.34
2	A	1501	ATA	C-ND	4.44	1.44	1.33
2	A	1501	ATA	C2-SG	2.99	1.81	1.75
2	A	1501	ATA	O-C	-2.54	1.18	1.23
2	A	1501	ATA	O'-C'	-2.31	1.18	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501	ATA	C2-N1-C6	24.94	130.65	113.42
2	A	1501	ATA	N1-C6-N5	-7.69	113.66	126.26
2	A	1501	ATA	N3-C2-N1	-7.08	114.08	127.00
2	A	1501	ATA	C4-N7-C8	-6.65	119.50	124.55
2	A	1501	ATA	CB-SG-C2	6.03	107.32	102.65
2	A	1501	ATA	C2-N3-C4	5.22	117.03	113.42
2	A	1501	ATA	N11-C6-N5	3.61	123.40	117.16
2	A	1501	ATA	N11-C6-N1	3.35	122.94	117.16
2	A	1501	ATA	CD-CAD-ND	-3.24	102.99	113.06
2	A	1501	ATA	CG'-CB'-CA'	-3.13	106.68	113.86
2	A	1501	ATA	C12-N11-C6	-2.74	120.31	124.35
2	A	1501	ATA	CG'-C'-N	2.70	120.63	115.86
3	A	1504	CLR	C17-C13-C14	2.56	103.03	100.10
2	A	1501	ATA	OT'-CD-CAD	2.23	121.28	112.81
2	A	1501	ATA	CB-CA-C	-2.15	104.61	109.46

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1501	ATA	N5-C6-N11-C12
2	A	1501	ATA	N1-C6-N11-C12
2	A	1501	ATA	N1-C2-SG-CB
2	A	1501	ATA	N3-C2-SG-CB
2	A	1501	ATA	N5-C4-N7-C8
2	A	1501	ATA	N3-C4-N7-C8
3	A	1503	CLR	C13-C17-C20-C21
3	A	1503	CLR	C16-C17-C20-C22
3	A	1504	CLR	C13-C17-C20-C21
3	A	1508	CLR	C16-C17-C20-C21
3	A	1502	CLR	C16-C17-C20-C21
3	A	1503	CLR	C16-C17-C20-C21
3	A	1504	CLR	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
3	A	1507	CLR	C16-C17-C20-C21
3	A	1502	CLR	C13-C17-C20-C21
3	A	1507	CLR	C13-C17-C20-C21
3	A	1508	CLR	C13-C17-C20-C21
3	A	1504	CLR	C16-C17-C20-C22
3	A	1508	CLR	C16-C17-C20-C22
3	A	1503	CLR	C13-C17-C20-C22
3	A	1508	CLR	C13-C17-C20-C22
3	A	1504	CLR	C21-C20-C22-C23
3	A	1505	CLR	C21-C20-C22-C23
3	A	1507	CLR	C21-C20-C22-C23
3	A	1508	CLR	C21-C20-C22-C23
3	A	1507	CLR	C16-C17-C20-C22
3	A	1502	CLR	C13-C17-C20-C22
3	A	1504	CLR	C13-C17-C20-C22
3	A	1507	CLR	C13-C17-C20-C22
3	A	1503	CLR	C21-C20-C22-C23
3	A	1502	CLR	C16-C17-C20-C22
3	A	1505	CLR	C17-C20-C22-C23
3	A	1507	CLR	C17-C20-C22-C23
3	A	1508	CLR	C17-C20-C22-C23
3	A	1502	CLR	C17-C20-C22-C23
3	A	1504	CLR	C17-C20-C22-C23
3	A	1502	CLR	C21-C20-C22-C23
3	A	1505	CLR	C16-C17-C20-C21
3	A	1505	CLR	C13-C17-C20-C21
3	A	1505	CLR	C16-C17-C20-C22
3	A	1505	CLR	C13-C17-C20-C22
3	A	1503	CLR	C17-C20-C22-C23
3	A	1503	CLR	C22-C23-C24-C25
3	A	1506	CLR	C20-C22-C23-C24
3	A	1506	CLR	C22-C23-C24-C25
3	A	1502	CLR	C20-C22-C23-C24
3	A	1505	CLR	C20-C22-C23-C24
3	A	1507	CLR	C22-C23-C24-C25
2	A	1501	ATA	N'-CA'-CC'-O2'
3	A	1504	CLR	C20-C22-C23-C24
3	A	1505	CLR	C23-C24-C25-C26
3	A	1504	CLR	C23-C24-C25-C27
3	A	1507	CLR	C20-C22-C23-C24
2	A	1501	ATA	O-C-CA-N
2	A	1501	ATA	ND-C-CA-N

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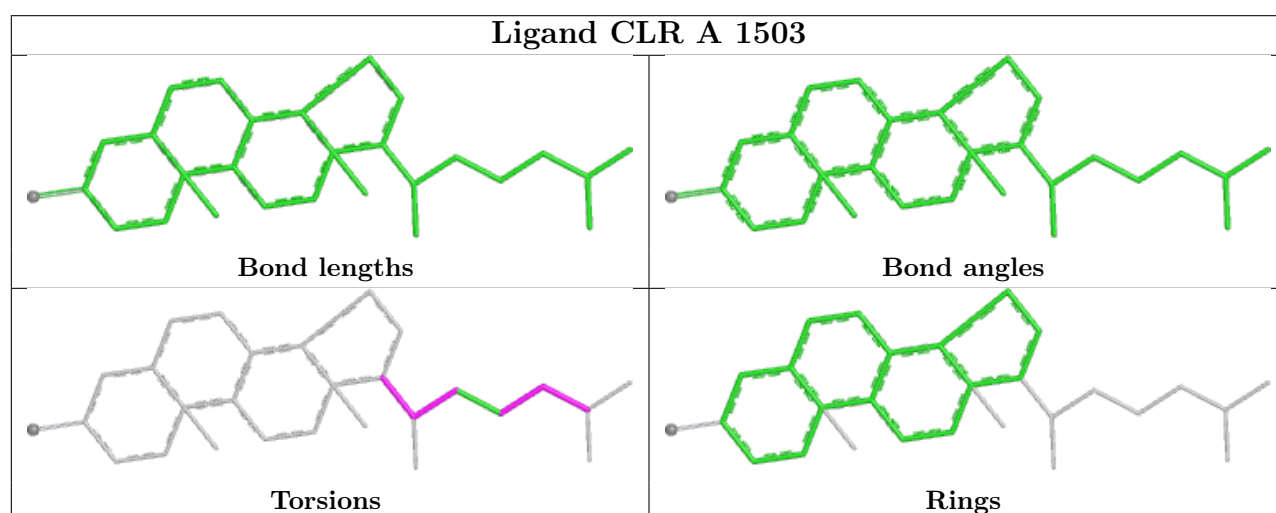
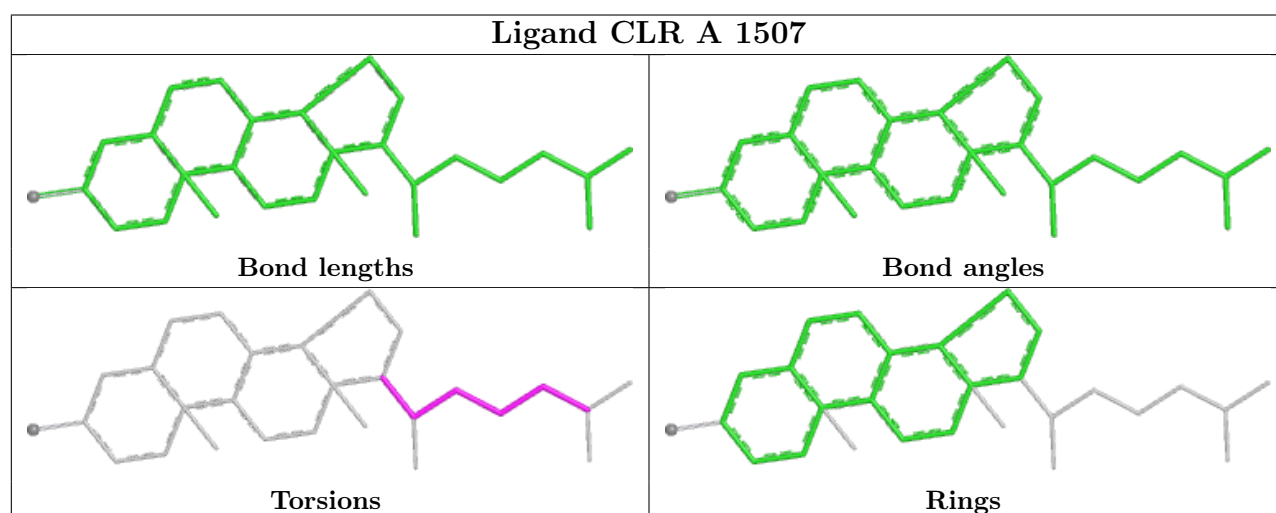
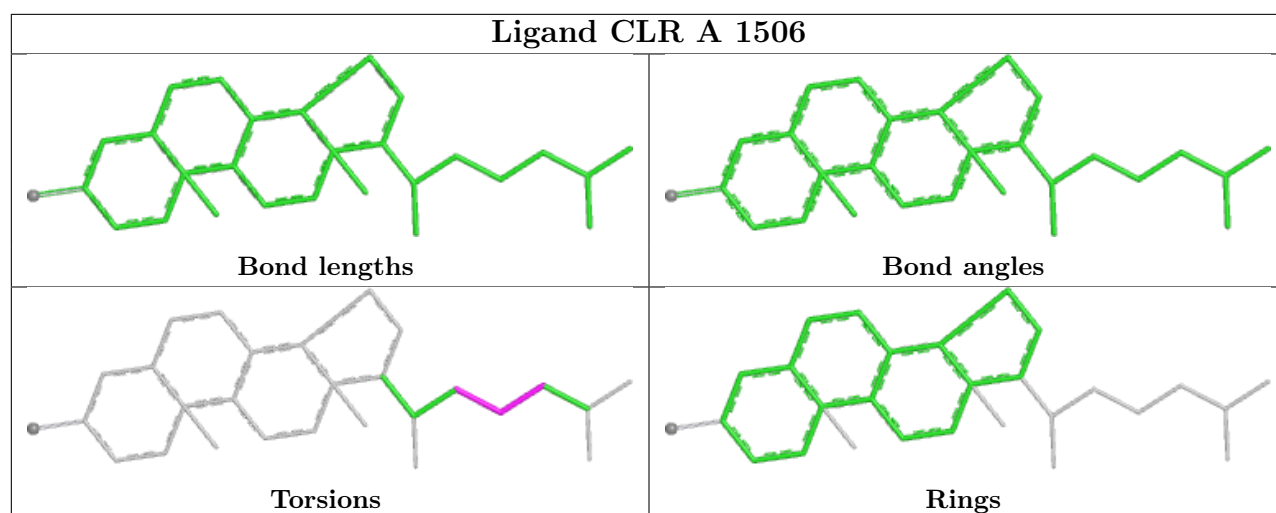
Mol	Chain	Res	Type	Atoms
2	A	1501	ATA	N'-CA'-CC'-O1'
3	A	1505	CLR	C23-C24-C25-C27
3	A	1504	CLR	C23-C24-C25-C26
3	A	1508	CLR	C22-C23-C24-C25
3	A	1507	CLR	C23-C24-C25-C27
2	A	1501	ATA	O'-C'-CG'-CB'
3	A	1508	CLR	C20-C22-C23-C24
3	A	1503	CLR	C23-C24-C25-C27
2	A	1501	ATA	N-C'-CG'-CB'
3	A	1507	CLR	C23-C24-C25-C26
2	A	1501	ATA	C13-C12-N11-C6
2	A	1501	ATA	CA-CB-SG-C2
3	A	1502	CLR	C22-C23-C24-C25

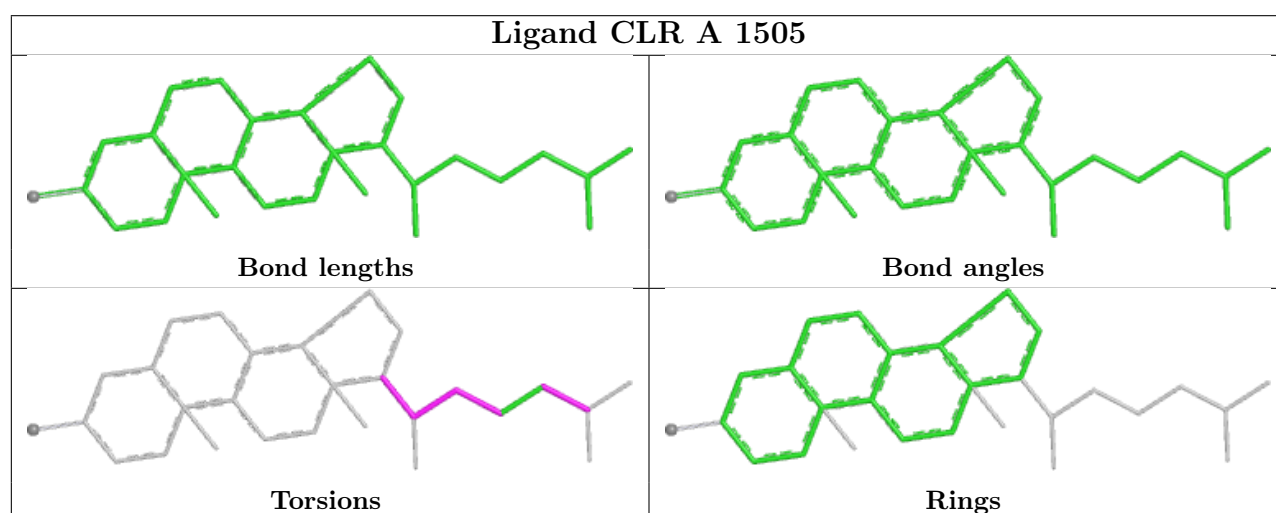
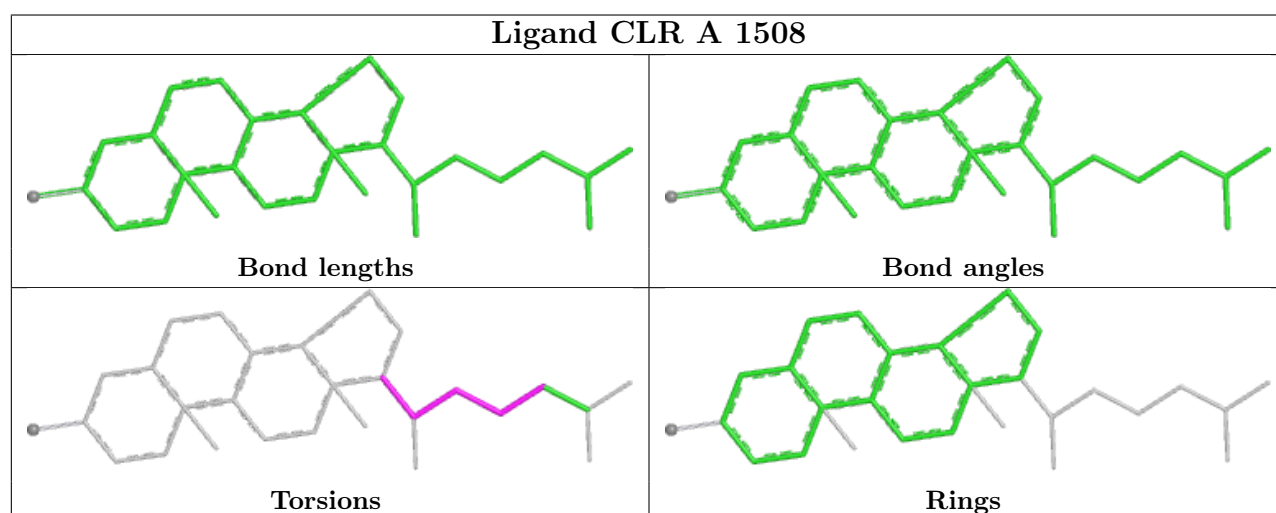
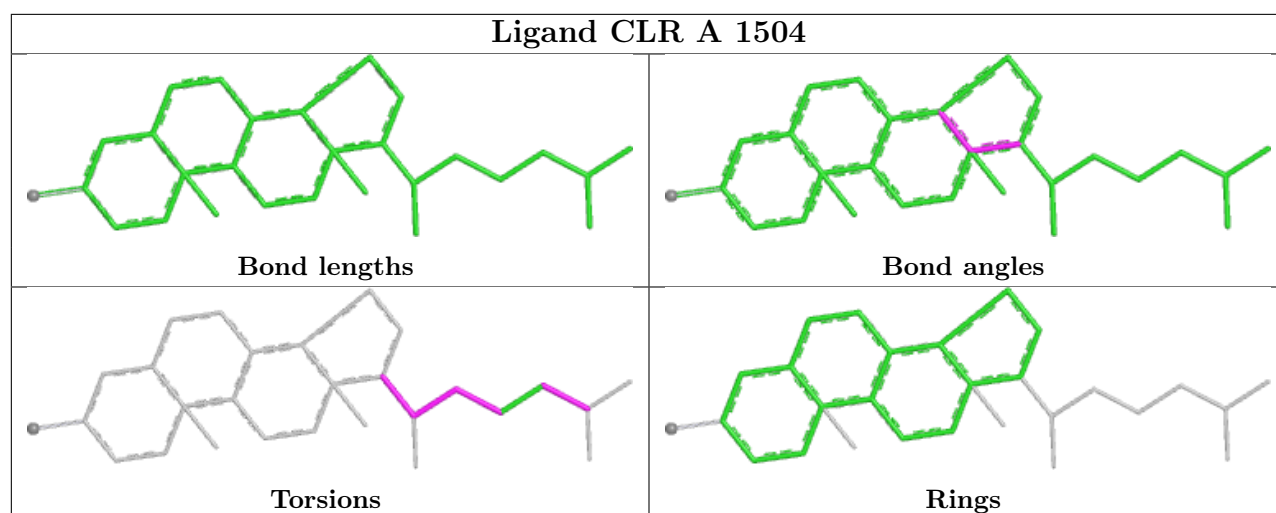
There are no ring outliers.

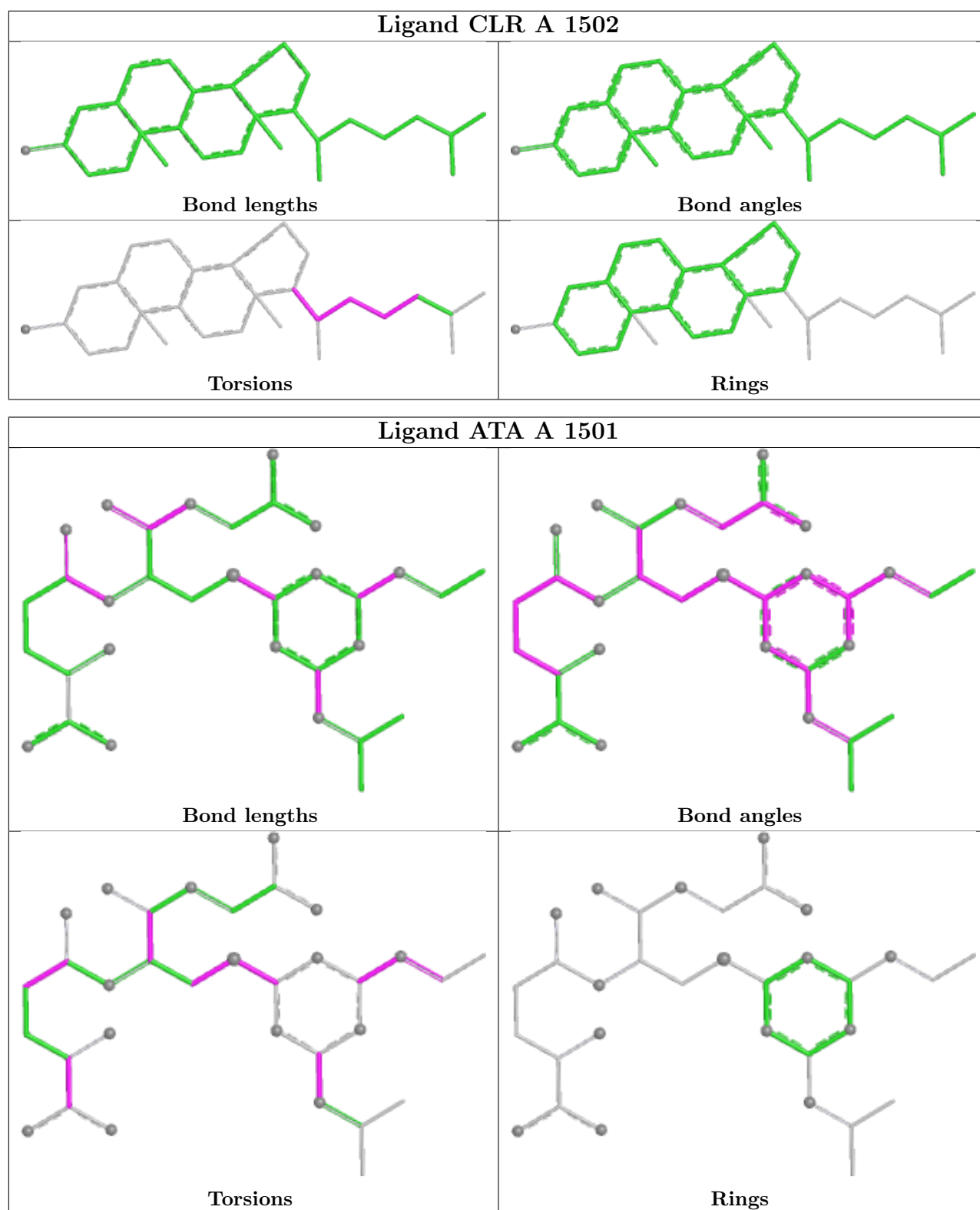
7 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1506	CLR	3	0
3	A	1507	CLR	5	0
3	A	1503	CLR	3	0
3	A	1508	CLR	5	0
3	A	1505	CLR	13	0
3	A	1502	CLR	2	0
2	A	1501	ATA	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

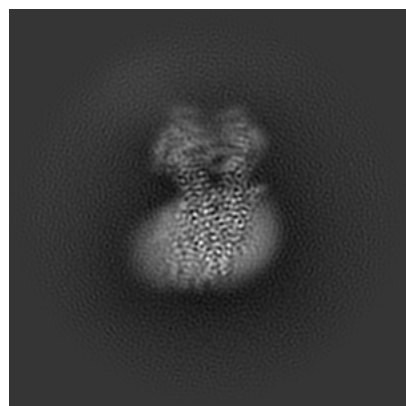
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63866. These allow visual inspection of the internal detail of the map and identification of artifacts.

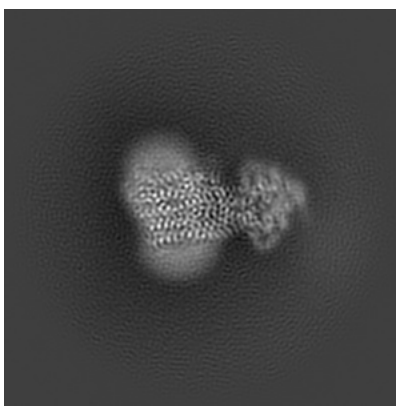
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

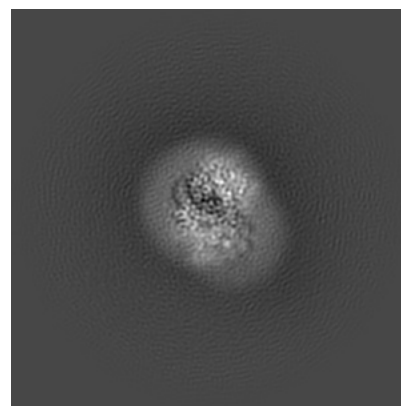
6.1.1 Primary map



X

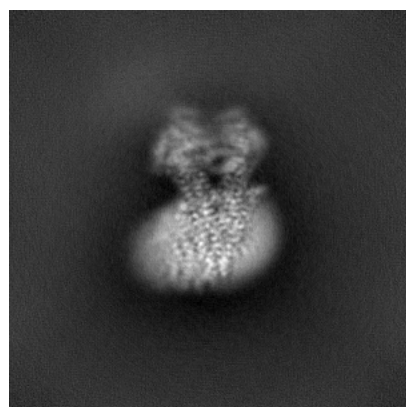


Y

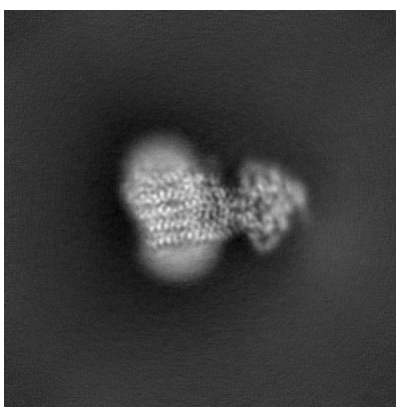


Z

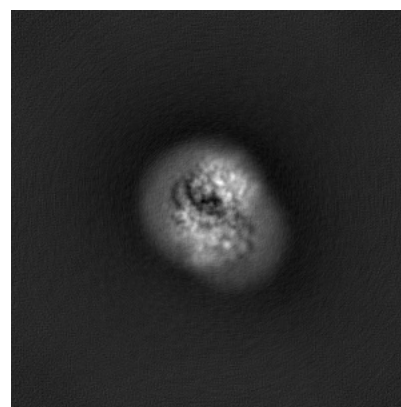
6.1.2 Raw map



X



Y

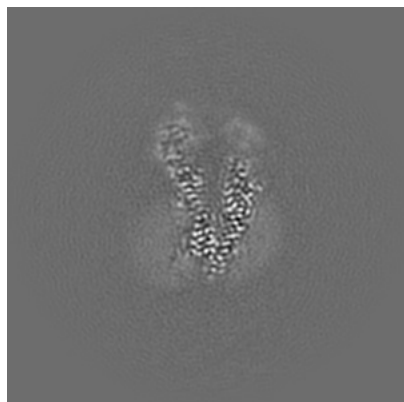


Z

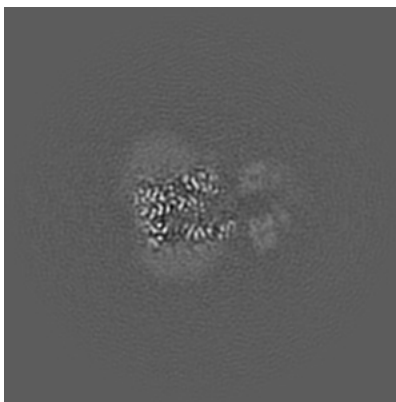
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

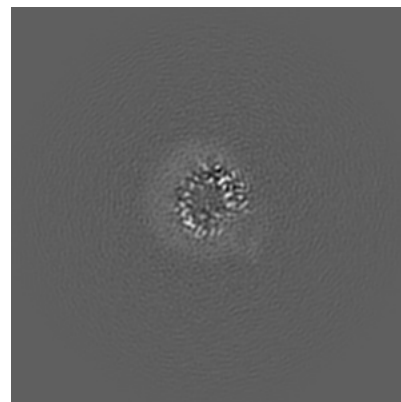
6.2.1 Primary map



X Index: 200

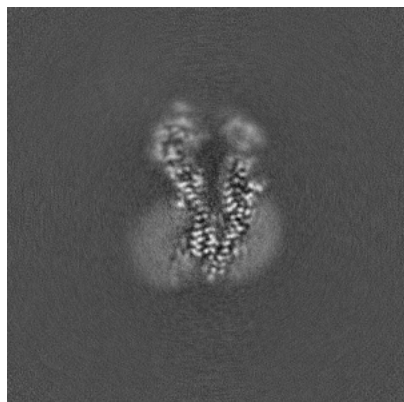


Y Index: 200

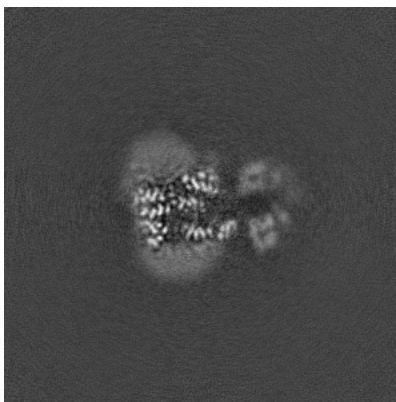


Z Index: 200

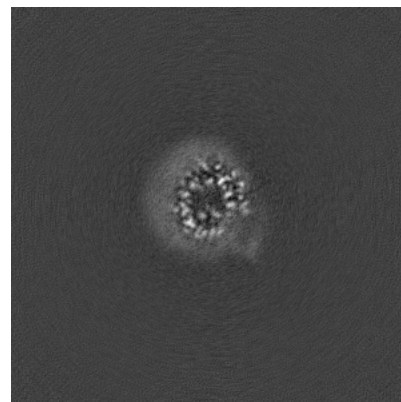
6.2.2 Raw map



X Index: 200



Y Index: 200

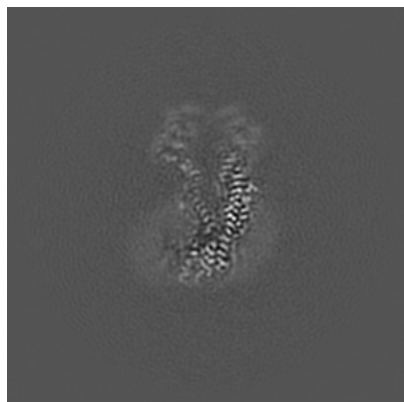


Z Index: 200

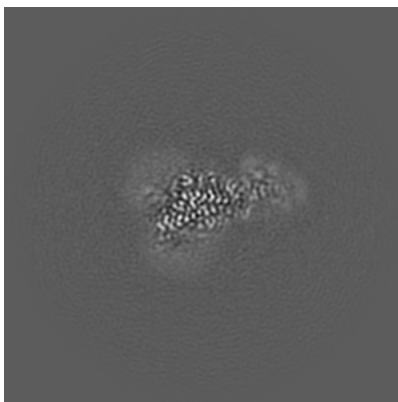
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

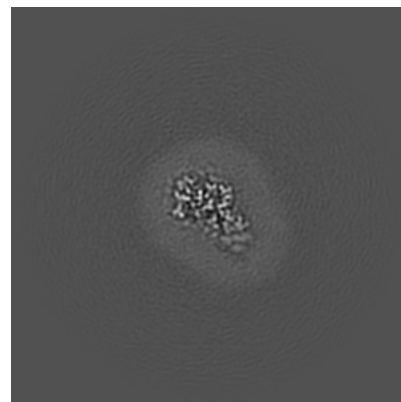
6.3.1 Primary map



X Index: 208

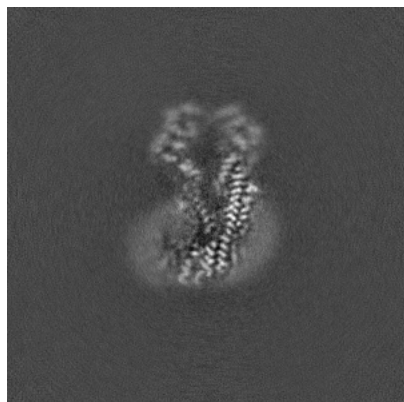


Y Index: 225

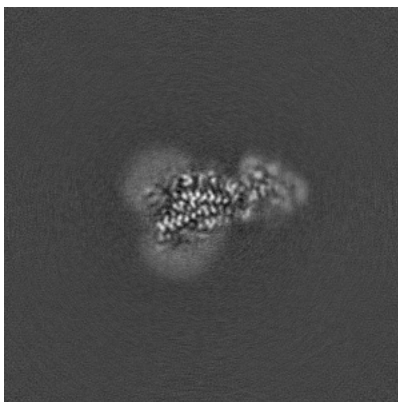


Z Index: 157

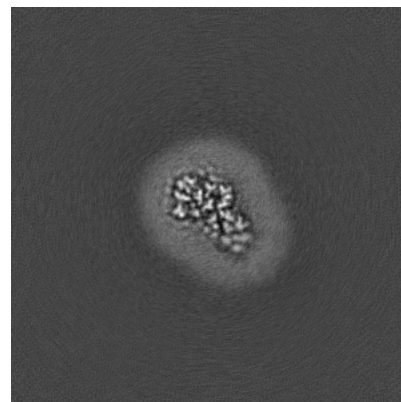
6.3.2 Raw map



X Index: 208



Y Index: 225

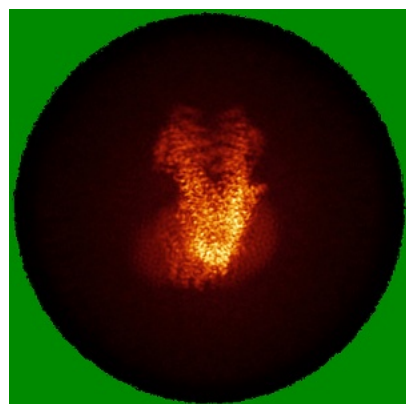


Z Index: 157

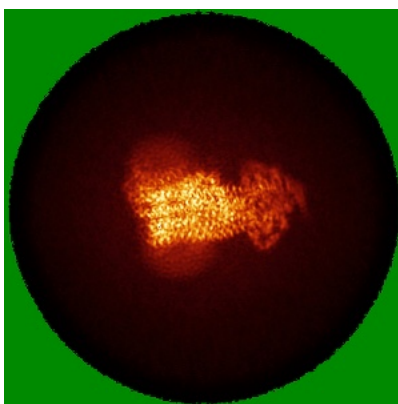
The images above show the largest variance slices of the map in three orthogonal directions.

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

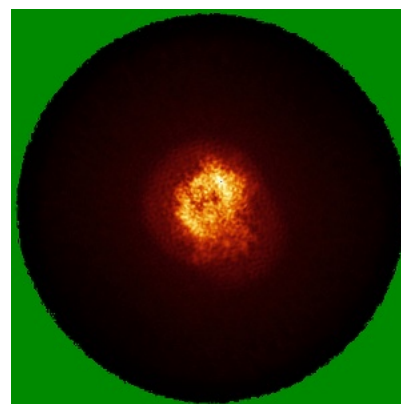
6.4.1 Primary map



X

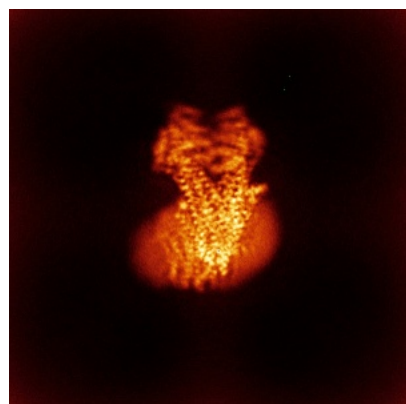


Y

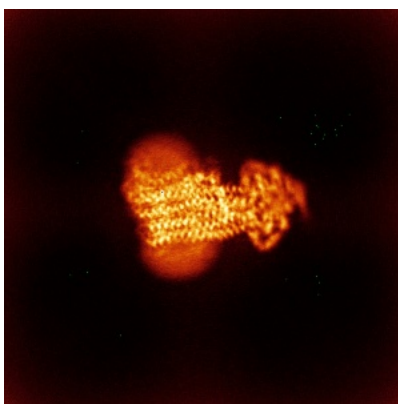


Z

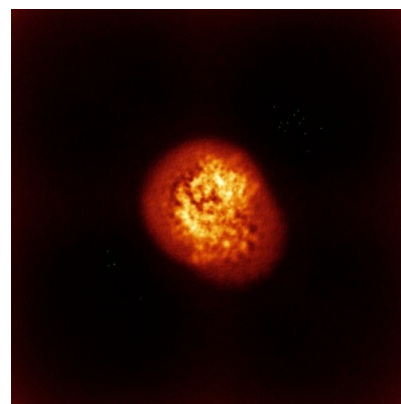
6.4.2 Raw map



X



Y

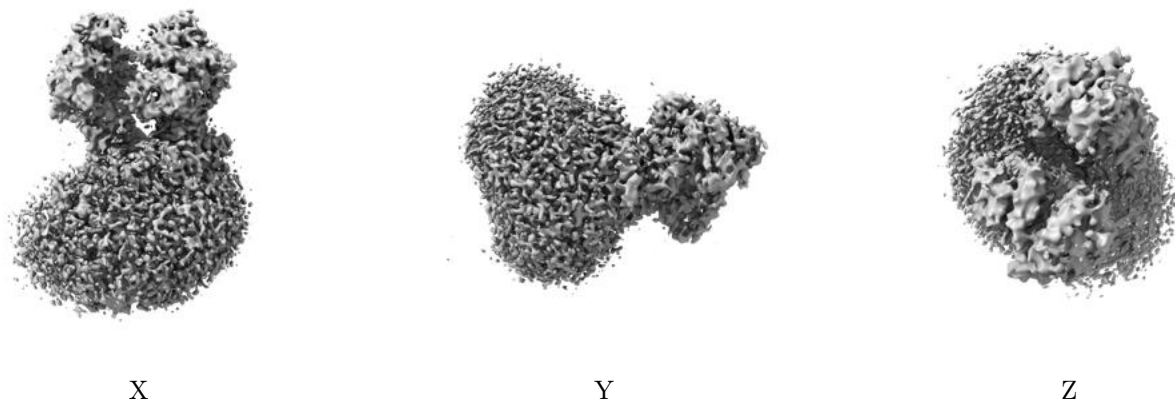


Z

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.

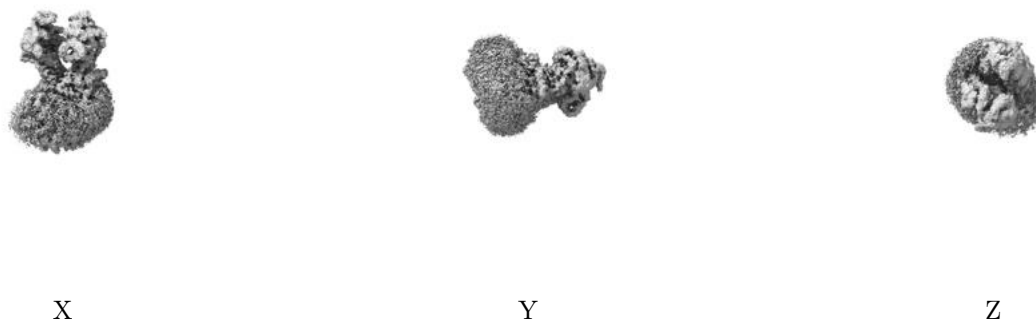
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

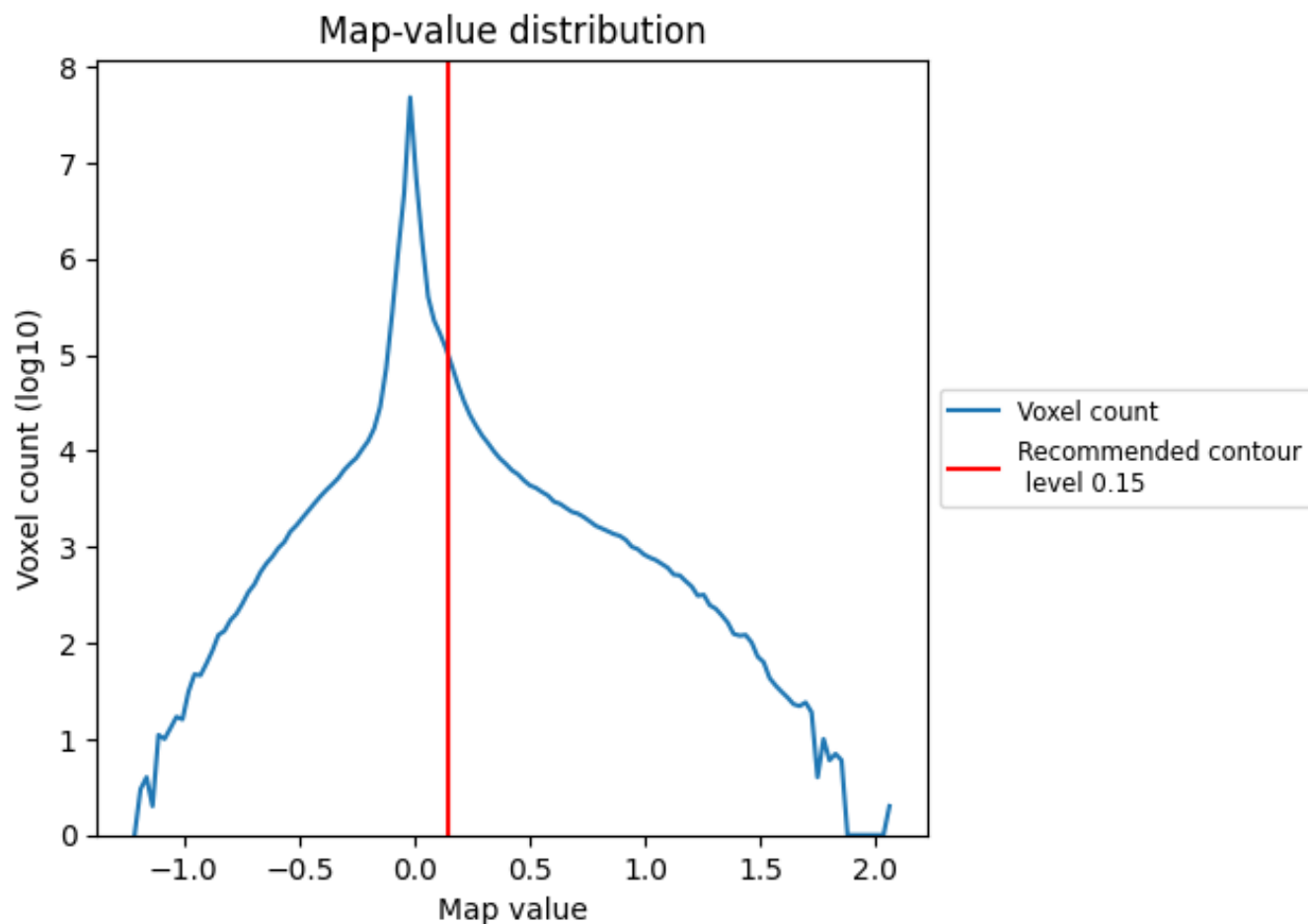
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

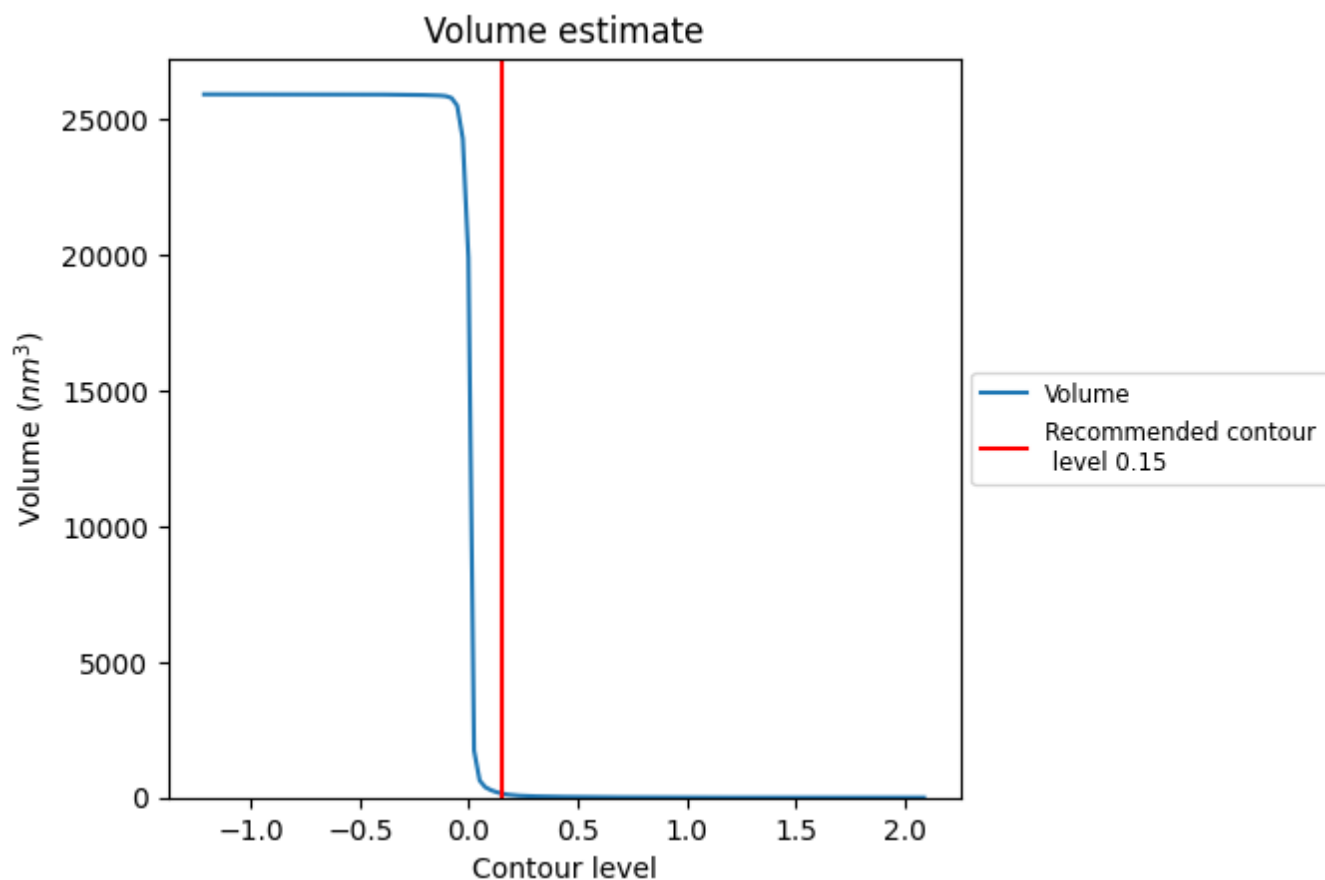
This section contains the results of statistical analysis of the map.

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.

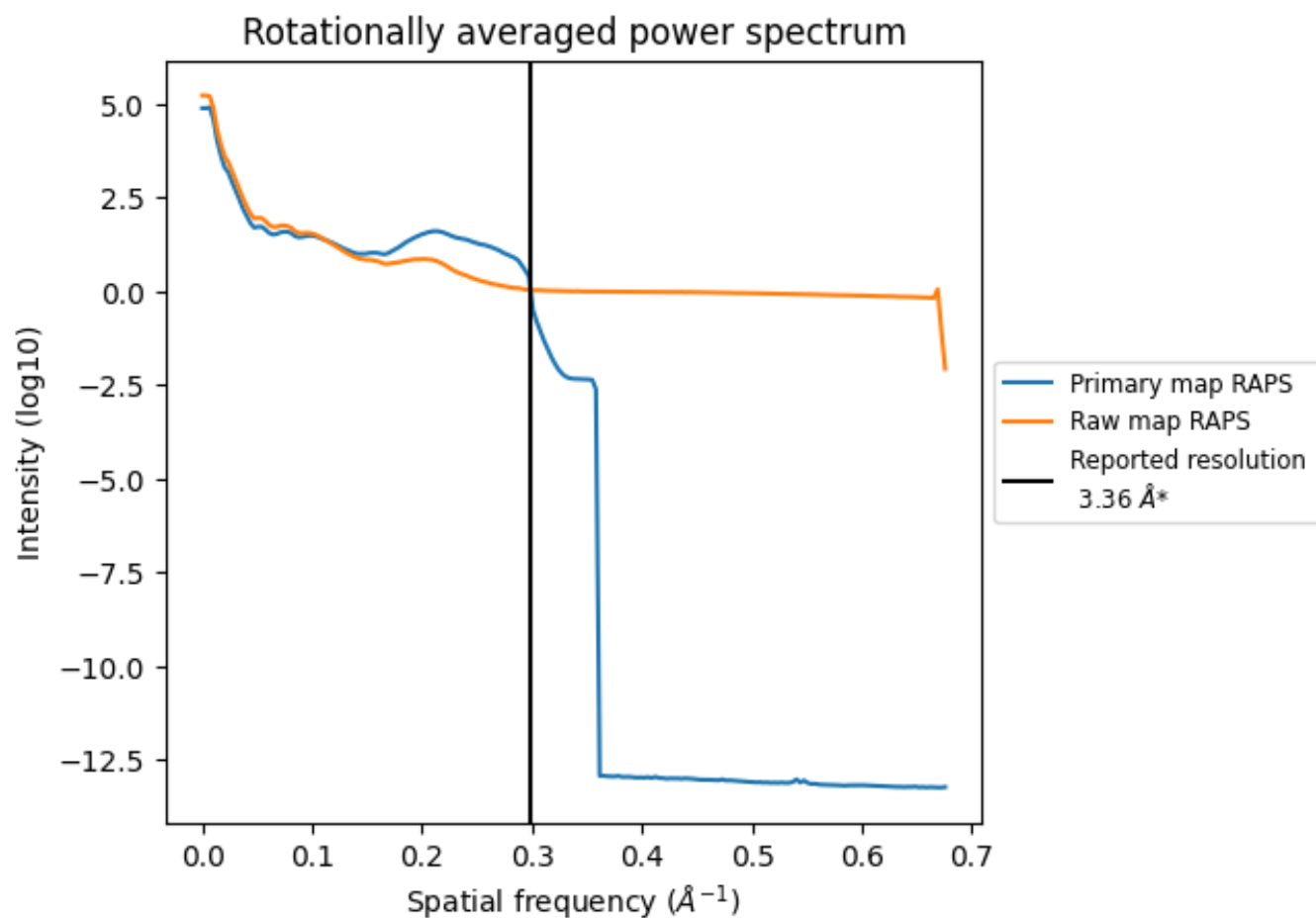
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 152 nm³; this corresponds to an approximate mass of 137 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 ⓘ

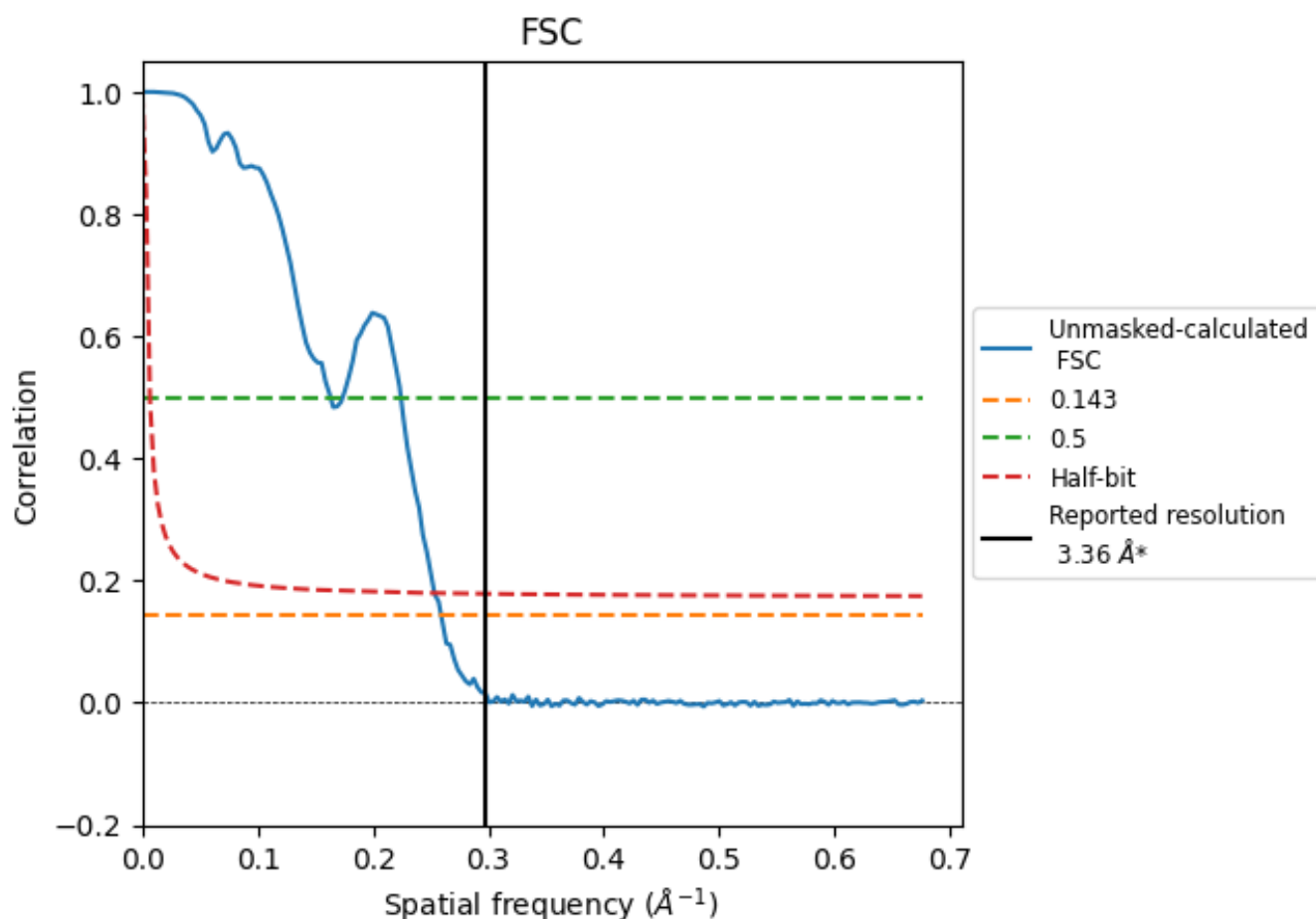


*Reported resolution corresponds to spatial frequency of 0.298 Å⁻¹

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 0.298 \AA^{-1}

8.2 Resolution estimates [i](#)

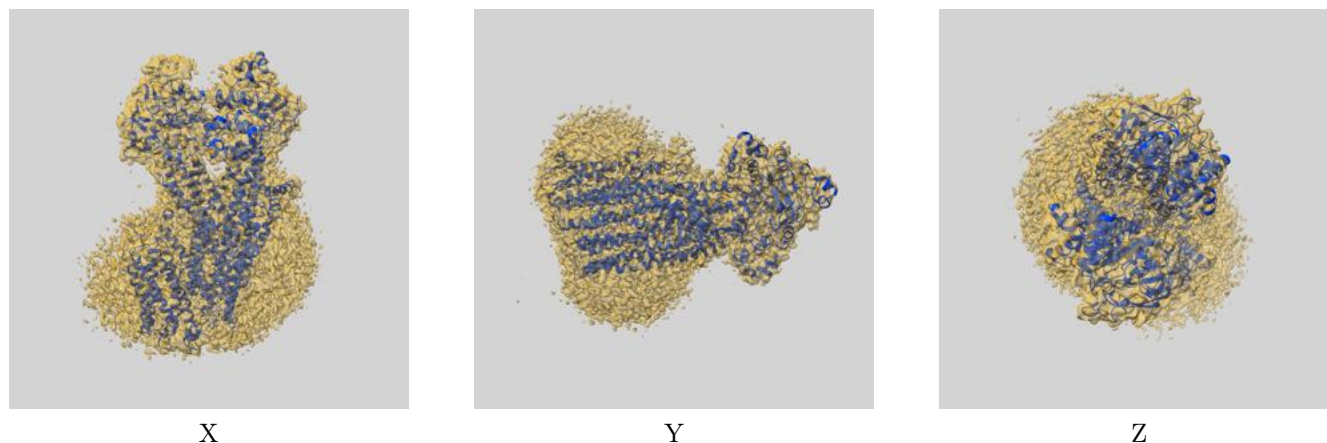
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.86	6.13	3.95

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.86 differs from the reported value 3.36 by more than 10 %

9 Map-model fit [i](#)

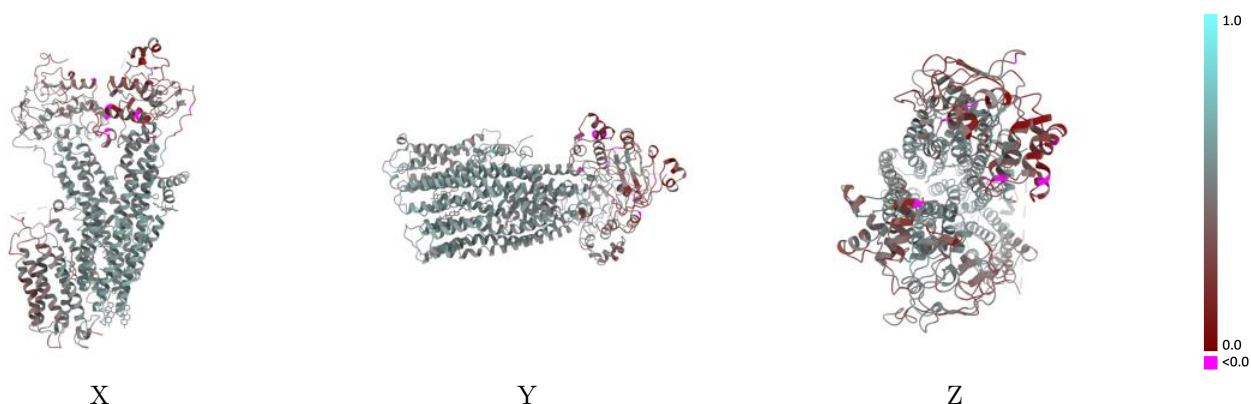
This section contains information regarding the fit between EMDB map EMD-63866 and PDB model 9U58. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



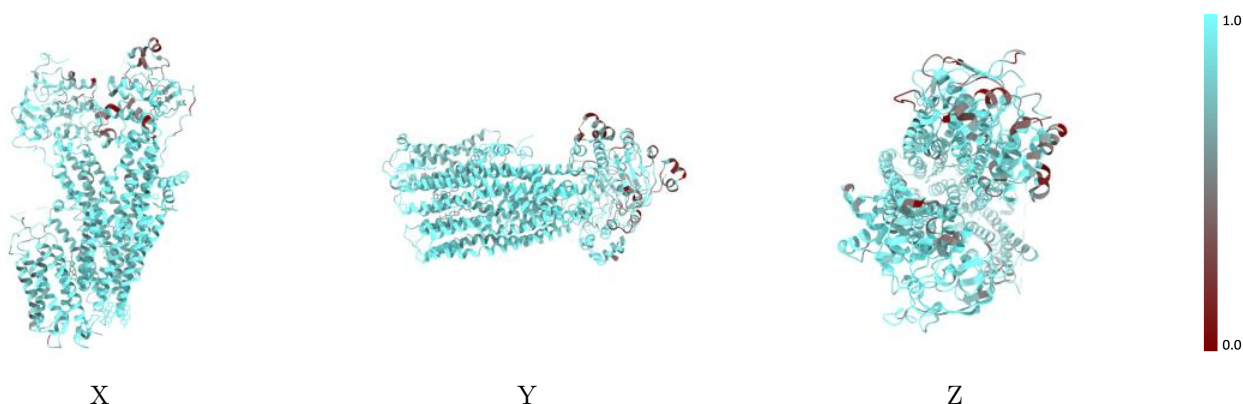
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



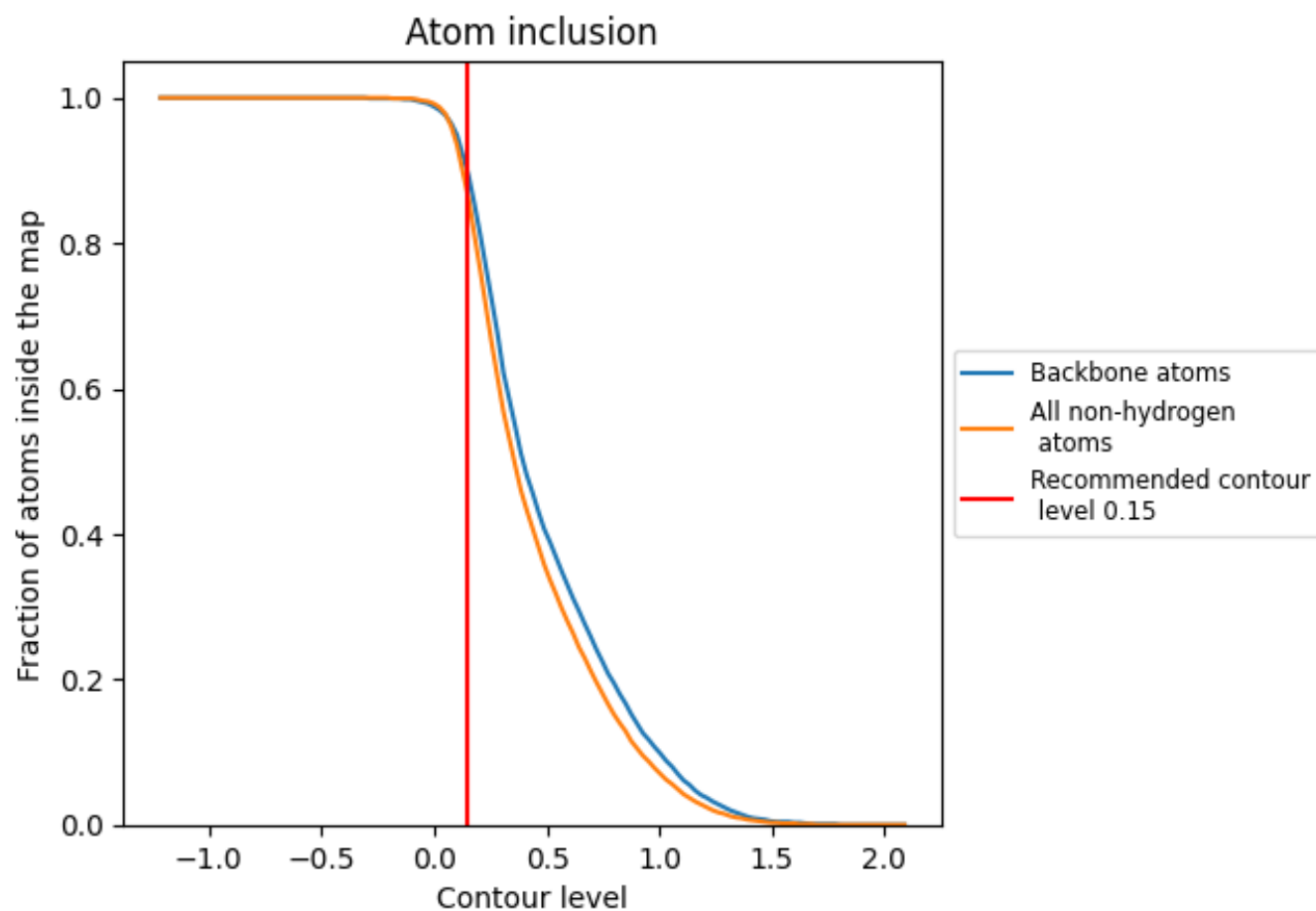
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8660	<div><div></div></div> 0.4680
A	<div><div></div></div> 0.8660	<div><div></div></div> 0.4680

