



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:43 PM UTC

PDB ID : 6DM1 / pdb_00006dm1
EMDB ID : EMD-7961
Title : Open state GluA2 in complex with STZ and blocked by NASPM, after micelle signal subtraction
Authors : Twomey, E.C.; Yelshanskaya, M.V.; Vassilevski, A.A.; Sobolevsky, A.I.
Deposited on : 2018-06-04
Resolution : 4.20 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

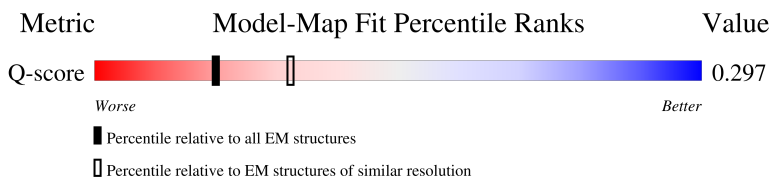
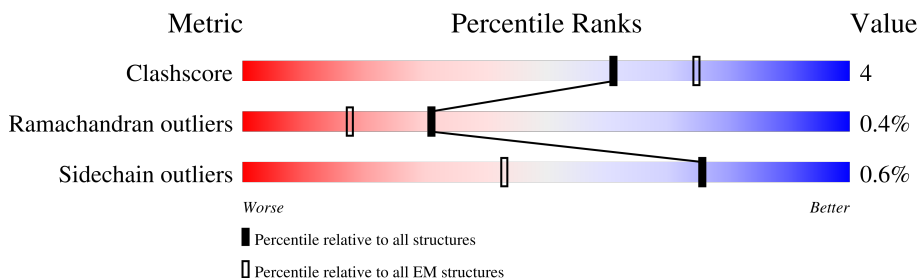
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	5410 (3.70 - 4.70)

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	1031	34% 84% 10% 5%
1	B	1031	36% 83% 12% .
1	C	1031	34% 84% 11% 5%
1	D	1031	36% 83% 13% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31131 atoms, of which 34 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 Glutamate receptor 2, Voltage-dependent calcium channel gamma-2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	983	Total	C	N	O	S	0	0
			7730	4978	1277	1434	41		
1	B	985	Total	C	N	O	S	0	0
			7735	4981	1279	1434	41		
1	C	984	Total	C	N	O	S	0	0
			7734	4980	1278	1435	41		
1	D	985	Total	C	N	O	S	0	0
			7735	4981	1279	1434	41		

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	999	GLY	-	linker	UNP P19491
A	1000	THR	-	linker	UNP P19491
A	1047	ASP	ASN	conflict	UNP Q9Y698
A	1208	THR	-	expression tag	UNP Q9Y698
A	1209	GLY	-	expression tag	UNP Q9Y698
A	1210	GLY	-	expression tag	UNP Q9Y698
A	1211	ALA	-	expression tag	UNP Q9Y698
A	1212	GLU	-	expression tag	UNP Q9Y698
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491

Continued on next page...

Continued from previous page...

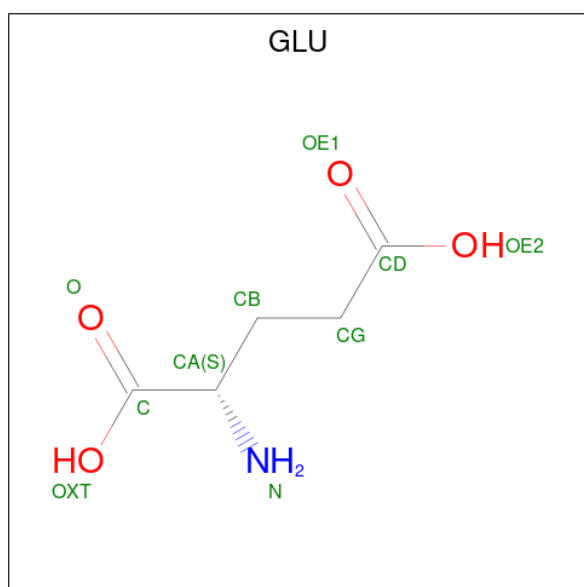
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	999	GLY	-	linker	UNP P19491
B	1000	THR	-	linker	UNP P19491
B	1047	ASP	ASN	conflict	UNP Q9Y698
B	1208	THR	-	expression tag	UNP Q9Y698
B	1209	GLY	-	expression tag	UNP Q9Y698
B	1210	GLY	-	expression tag	UNP Q9Y698
B	1211	ALA	-	expression tag	UNP Q9Y698
B	1212	GLU	-	expression tag	UNP Q9Y698
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	999	GLY	-	linker	UNP P19491
C	1000	THR	-	linker	UNP P19491
C	1047	ASP	ASN	conflict	UNP Q9Y698
C	1208	THR	-	expression tag	UNP Q9Y698
C	1209	GLY	-	expression tag	UNP Q9Y698
C	1210	GLY	-	expression tag	UNP Q9Y698
C	1211	ALA	-	expression tag	UNP Q9Y698
C	1212	GLU	-	expression tag	UNP Q9Y698
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491

Continued on next page...

Continued from previous page...

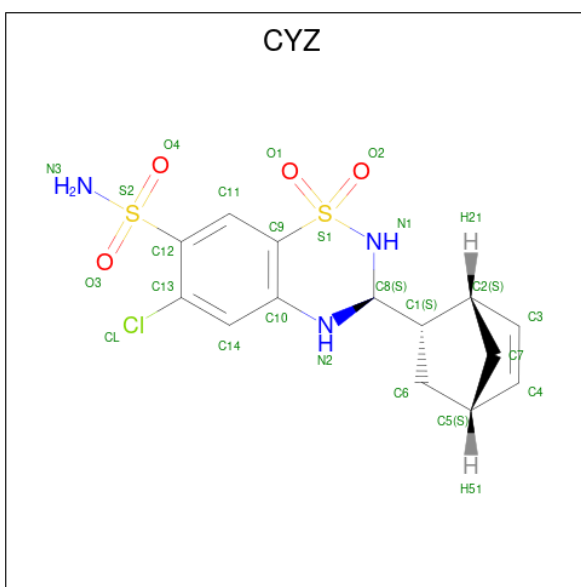
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	999	GLY	-	linker	UNP P19491
D	1000	THR	-	linker	UNP P19491
D	1047	ASP	ASN	conflict	UNP Q9Y698
D	1208	THR	-	expression tag	UNP Q9Y698
D	1209	GLY	-	expression tag	UNP Q9Y698
D	1210	GLY	-	expression tag	UNP Q9Y698
D	1211	ALA	-	expression tag	UNP Q9Y698
D	1212	GLU	-	expression tag	UNP Q9Y698

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$).



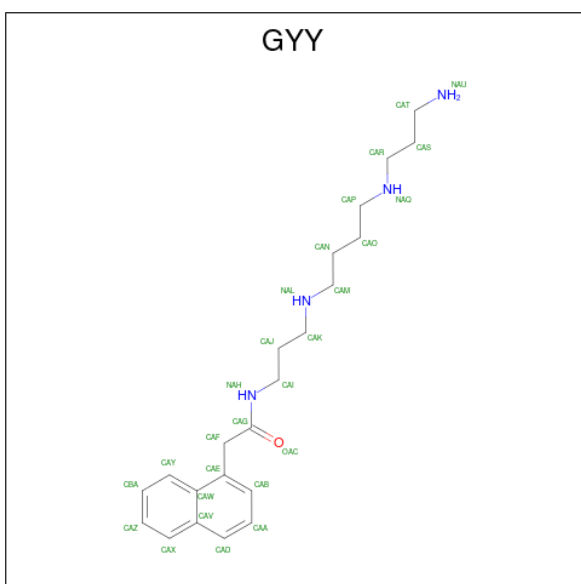
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			10	5	1	4	
2	B	1	Total	C	N	O	0
			10	5	1	4	
2	C	1	Total	C	N	O	0
			10	5	1	4	
2	D	1	Total	C	N	O	0
			10	5	1	4	

- Molecule 3 is CYCLOTHIAZIDE (CCD ID: CYZ) (formula: $C_{14}H_{16}ClN_3O_4S_2$).

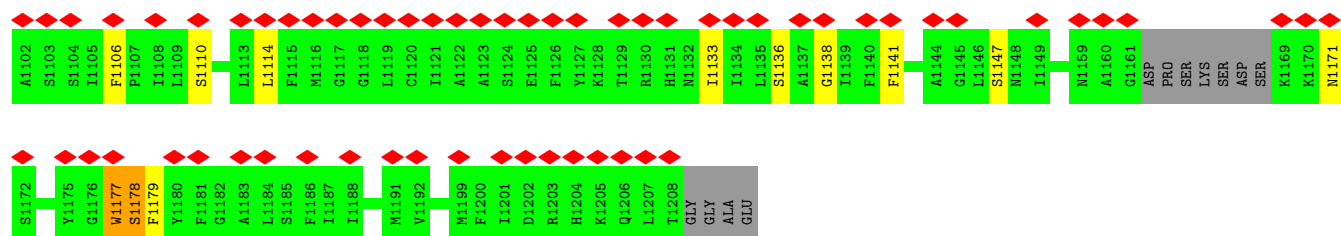


Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	0
3	B	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	0
3	C	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	0
3	D	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	0

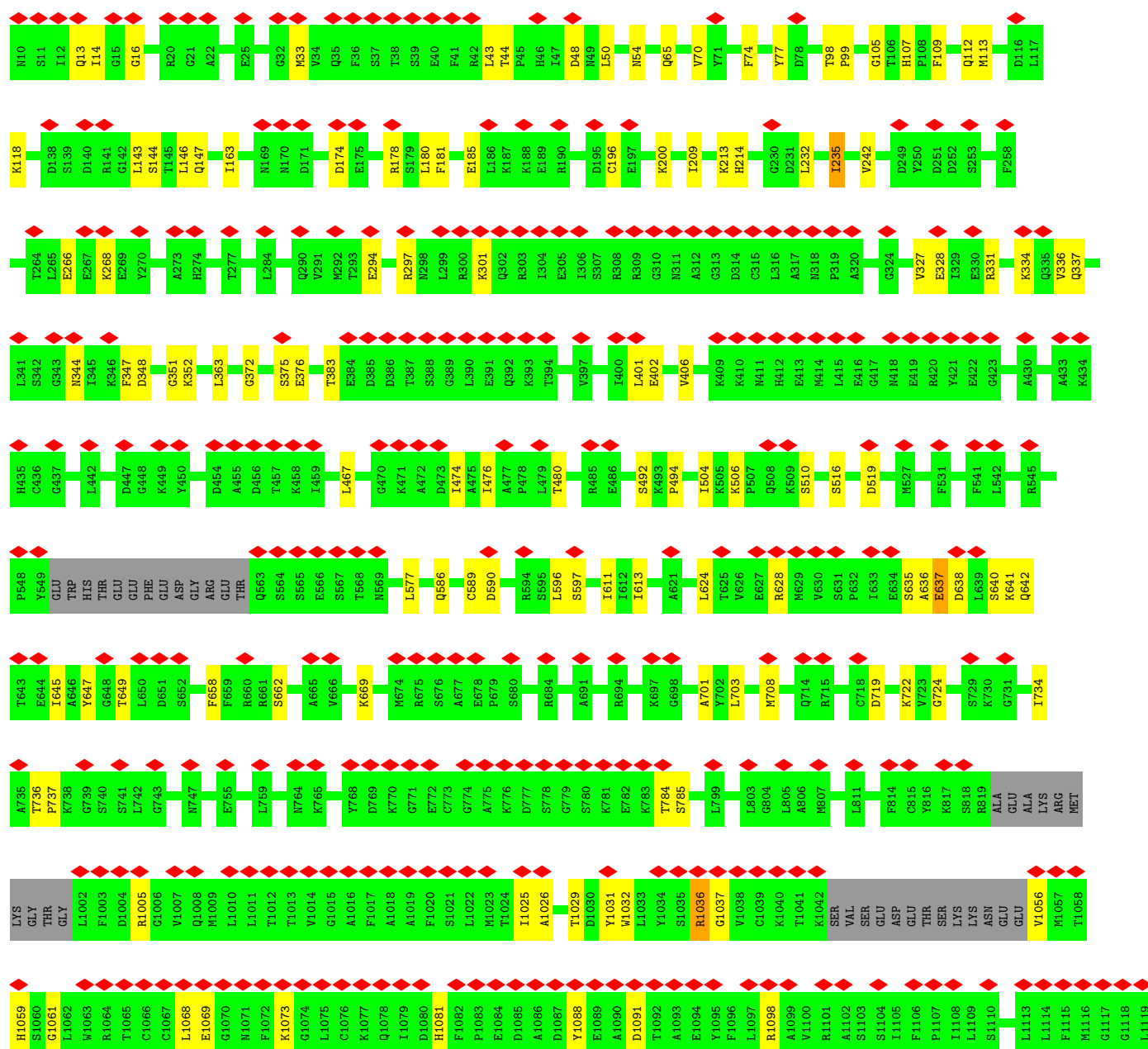
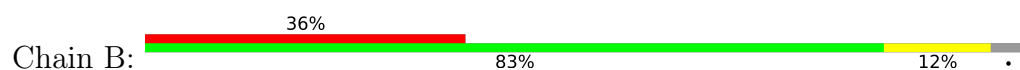
- Molecule 4 is N-[3-({4-[(3-aminopropyl)amino]butyl}amino)propyl]-2-(naphthalen-1-yl)acetamide (CCD ID: GYY) (formula: $C_{22}H_{34}N_4O$).

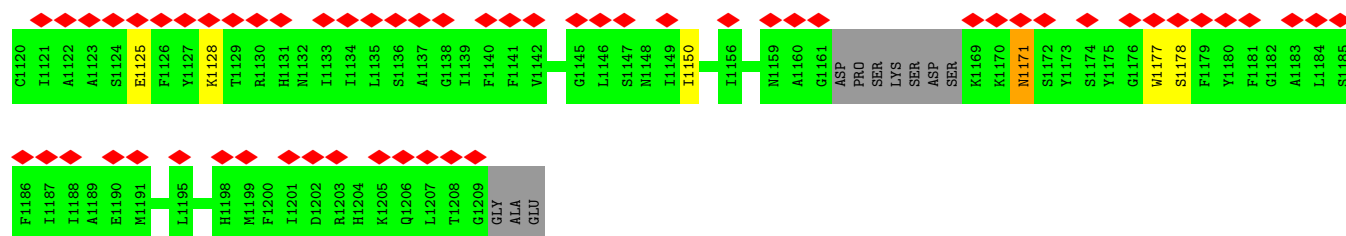


Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	H	N	O	0
			61	22	34	4	1	

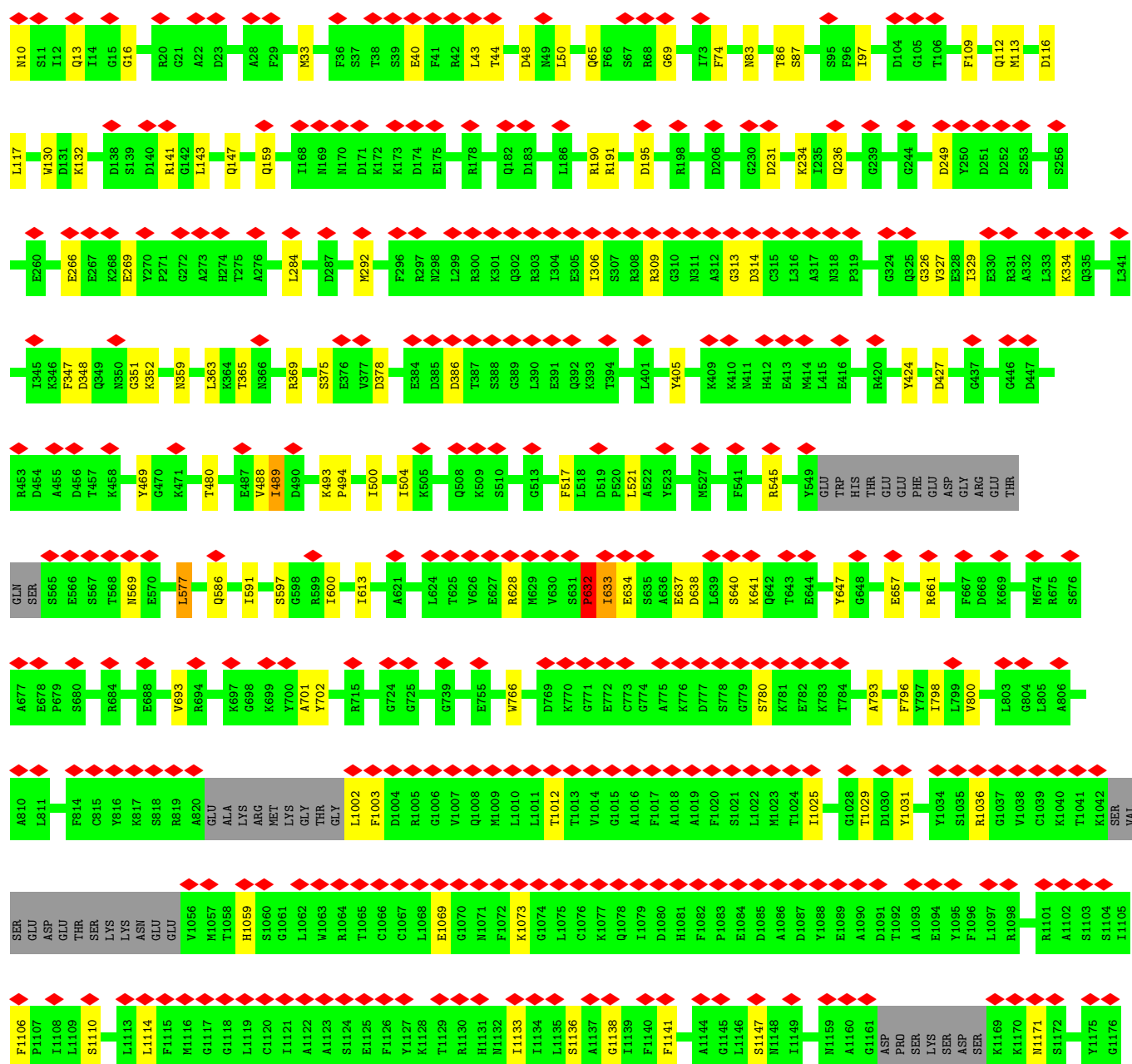
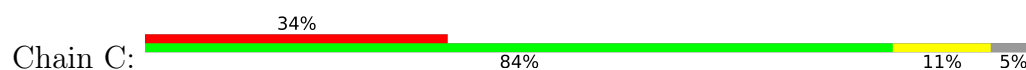


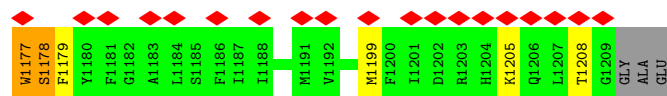
• Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-2 subunit



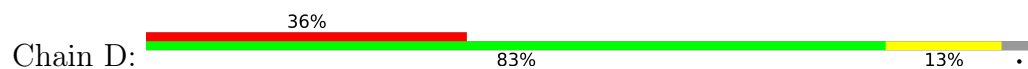


- Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-2 subunit





- Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-2 subunit



A1189	E1190	M1191	L1195	H1198	M1199	F1200	I1201	D1202	R1203	H1204	K1205	Q1206	L1207	T1208	G1209	GLY	ALA	GLU
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	39835	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 ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.134	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.33	0/7896	0.67	5/10665 (0.0%)
1	B	0.33	0/7901	0.65	4/10672 (0.0%)
1	C	0.33	0/7900	0.67	5/10670 (0.0%)
1	D	0.33	0/7901	0.65	5/10672 (0.0%)
All	All	0.33	0/31598	0.66	19/42679 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	3
1	D	0	3
All	All	0	11

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	577	LEU	CA-C-N	-7.14	109.91	122.26
1	A	577	LEU	C-N-CA	-7.14	109.91	122.26
1	C	577	LEU	CA-C-N	-7.07	110.03	122.26
1	C	577	LEU	C-N-CA	-7.07	110.03	122.26
1	A	632	PRO	CA-C-N	6.06	132.88	121.97
1	A	632	PRO	C-N-CA	6.06	132.88	121.97
1	C	632	PRO	CA-C-N	6.04	132.84	121.97
1	C	632	PRO	C-N-CA	6.04	132.84	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	818	SER	N-CA-C	-5.78	105.49	113.18
1	D	1036	ARG	CA-C-N	5.63	126.50	122.16
1	D	1036	ARG	C-N-CA	5.63	126.50	122.16
1	B	1036	ARG	CA-C-N	5.61	126.48	122.16
1	B	1036	ARG	C-N-CA	5.61	126.48	122.16
1	D	1171	ASN	CA-C-N	5.39	130.07	122.46
1	D	1171	ASN	C-N-CA	5.39	130.07	122.46
1	B	1171	ASN	CA-C-N	5.33	129.97	122.46
1	B	1171	ASN	C-N-CA	5.33	129.97	122.46
1	A	1178	SER	N-CA-C	5.28	122.06	110.80
1	C	1178	SER	N-CA-C	5.27	122.02	110.80

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1177	TRP	Peptide
1	A	313	GLY	Peptide
1	A	632	PRO	Peptide
1	B	1005	ARG	Peptide
1	B	635	SER	Peptide
1	C	1177	TRP	Peptide
1	C	313	GLY	Peptide
1	C	632	PRO	Peptide
1	D	1005	ARG	Peptide
1	D	38	THR	Peptide
1	D	635	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7730	0	7710	60	0
1	B	7735	0	7708	81	0
1	C	7734	0	7713	65	0
1	D	7735	0	7708	80	0
2	A	10	0	5	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	5	1	0
2	C	10	0	5	1	0
2	D	10	0	5	1	0
3	A	24	0	11	1	0
3	B	24	0	11	1	0
3	C	24	0	11	1	0
3	D	24	0	11	1	0
4	C	27	34	0	0	0
All	All	31097	34	30903	274	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (274) 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:D:480:THR:HG1	2:D:1301:GLU:N	1.79	0.81
1:B:480:THR:HG1	2:B:1301:GLU:N	1.83	0.77
1:B:1037:GLY:O	1:B:1056:VAL:HB	1.89	0.73
1:D:1037:GLY:O	1:D:1056:VAL:HB	1.91	0.71
1:B:586:GLN:NE2	1:B:613:ILE:HD11	2.08	0.68
1:D:586:GLN:NE2	1:D:613:ILE:HD11	2.09	0.67
1:B:586:GLN:HE21	1:B:613:ILE:HD11	1.60	0.66
1:C:480:THR:HG1	2:C:1301:GLU:N	1.93	0.66
1:D:586:GLN:HE21	1:D:613:ILE:HD11	1.60	0.66
1:B:33:MET:HE1	1:B:43:LEU:HB2	1.79	0.65
1:D:33:MET:HE1	1:D:43:LEU:HB2	1.79	0.63
1:C:375:SER:HB3	1:C:378:ASP:HB2	1.82	0.62
1:C:1025:ILE:O	1:C:1029:THR:OG1	2.17	0.61
1:A:480:THR:HG1	2:A:1301:GLU:N	1.98	0.61
1:A:375:SER:HB3	1:A:378:ASP:HB2	1.82	0.61
1:B:13:GLN:HA	1:B:44:THR:HB	1.83	0.61
1:D:372:GLY:HA2	1:D:383:THR:HG23	1.83	0.60
1:B:372:GLY:HA2	1:B:383:THR:HG23	1.83	0.60
1:B:589:CYS:SG	1:B:590:ASP:N	2.71	0.60
1:A:586:GLN:HE22	1:A:613:ILE:HG21	1.66	0.60
1:B:328:GLU:OE2	1:B:331:ARG:NH2	2.34	0.60
1:A:1036:ARG:HH11	1:A:1171:ASN:HA	1.67	0.60
1:C:693:VAL:HG21	1:C:702:TYR:HB2	1.83	0.59
1:D:13:GLN:HA	1:D:44:THR:HB	1.83	0.59
1:C:586:GLN:HE22	1:C:613:ILE:HG21	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ARG:HH12	1:A:386:ASP:HB2	1.67	0.58
1:D:328:GLU:OE2	1:D:331:ARG:NH2	2.35	0.58
1:A:112:GLN:HE21	1:A:352:LYS:HG2	1.68	0.58
1:D:185:GLU:OE2	1:D:213:LYS:NZ	2.36	0.58
1:C:112:GLN:HE21	1:C:352:LYS:HG2	1.68	0.58
1:C:236:GLN:HA	1:C:363:LEU:HD21	1.86	0.58
1:B:185:GLU:OE2	1:B:213:LYS:NZ	2.36	0.57
1:C:369:ARG:HH12	1:C:386:ASP:HB2	1.68	0.57
1:C:1036:ARG:HH11	1:C:1171:ASN:HA	1.69	0.57
1:B:476:ILE:HG12	1:B:734:ILE:HD12	1.87	0.57
1:A:693:VAL:HG21	1:A:702:TYR:HB2	1.86	0.56
1:A:236:GLN:HA	1:A:363:LEU:HD21	1.86	0.56
1:D:476:ILE:HG12	1:D:734:ILE:HD12	1.87	0.56
1:B:1026:ALA:O	1:B:1178:SER:OG	2.23	0.56
1:D:589:CYS:SG	1:D:590:ASP:N	2.71	0.56
1:B:586:GLN:HE21	1:B:613:ILE:CD1	2.18	0.56
1:A:405:TYR:HA	1:A:424:TYR:HB3	1.88	0.56
1:C:1029:THR:HG22	1:C:1031:TYR:H	1.70	0.55
1:B:337:GLN:HE21	1:B:344:ASN:HD21	1.54	0.55
1:C:405:TYR:HA	1:C:424:TYR:HB3	1.88	0.55
1:D:586:GLN:HE21	1:D:613:ILE:CD1	2.19	0.55
1:D:1026:ALA:O	1:D:1178:SER:OG	2.23	0.55
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.89	0.54
1:A:48:ASP:OD2	1:A:65:GLN:NE2	2.38	0.54
1:B:1088:TYR:HD2	1:B:1091:ASP:HB2	1.73	0.54
1:D:638:ASP:HA	1:D:641:LYS:HB2	1.90	0.54
1:C:48:ASP:OD2	1:C:65:GLN:NE2	2.38	0.54
1:C:1177:TRP:O	1:C:1179:PHE:N	2.41	0.54
1:C:48:ASP:HB3	1:C:50:LEU:HD13	1.90	0.54
1:C:236:GLN:NE2	1:C:365:THR:O	2.41	0.54
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.90	0.54
1:A:48:ASP:HB3	1:A:50:LEU:HD13	1.90	0.54
1:A:1177:TRP:O	1:A:1179:PHE:N	2.41	0.54
1:A:236:GLN:NE2	1:A:365:THR:O	2.41	0.53
1:A:249:ASP:OD1	1:A:359:ASN:ND2	2.42	0.53
1:D:1088:TYR:HD2	1:D:1091:ASP:HB2	1.73	0.53
1:C:113:MET:HB3	1:C:284:LEU:HD22	1.91	0.53
1:D:235:ILE:HD13	1:D:242:VAL:HG21	1.91	0.53
1:A:113:MET:HB3	1:A:284:LEU:HD22	1.91	0.53
1:C:13:GLN:HA	1:C:44:THR:HB	1.91	0.53
1:C:16:GLY:HA2	1:C:74:PHE:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:GLN:HE21	1:D:352:LYS:HG2	1.73	0.53
1:A:13:GLN:HA	1:A:44:THR:HB	1.91	0.52
1:C:249:ASP:OD1	1:C:359:ASN:ND2	2.42	0.52
1:A:10:ASN:N	1:A:40:GLU:O	2.42	0.52
1:D:337:GLN:HE21	1:D:344:ASN:HD21	1.57	0.52
1:B:235:ILE:HD13	1:B:242:VAL:HG21	1.91	0.52
1:B:294:GLU:HG2	1:B:336:VAL:HG13	1.92	0.52
1:B:516:SER:O	1:B:519:ASP:HB2	2.09	0.52
1:C:628:ARG:NH2	1:C:780:SER:O	2.43	0.52
1:D:48:ASP:OD2	1:D:65:GLN:NE2	2.43	0.52
1:B:112:GLN:HE21	1:B:352:LYS:HG2	1.73	0.52
1:A:628:ARG:NH2	1:A:780:SER:O	2.43	0.52
1:B:48:ASP:OD2	1:B:65:GLN:NE2	2.43	0.52
1:D:516:SER:O	1:D:519:ASP:HB2	2.10	0.52
1:A:1138:GLY:HA2	1:A:1141:PHE:HD2	1.75	0.52
1:B:1025:ILE:O	1:B:1029:THR:OG1	2.24	0.52
1:D:348:ASP:OD1	1:D:351:GLY:N	2.43	0.52
1:D:637:GLU:O	1:D:640:SER:OG	2.24	0.52
1:B:638:ASP:HA	1:B:641:LYS:HB2	1.91	0.51
1:A:16:GLY:HA2	1:A:74:PHE:O	2.10	0.51
1:D:196:CYS:HB3	1:D:200:LYS:HB2	1.92	0.51
1:D:13:GLN:HB3	1:D:70:VAL:HG12	1.91	0.51
1:A:87:SER:OG	1:B:54:ASN:OD1	2.26	0.51
1:A:647:TYR:HB3	1:A:701:ALA:HB3	1.92	0.51
1:C:1138:GLY:HA2	1:C:1141:PHE:HD2	1.75	0.51
1:C:10:ASN:N	1:C:40:GLU:O	2.43	0.51
1:C:647:TYR:HB3	1:C:701:ALA:HB3	1.92	0.51
1:D:294:GLU:HG2	1:D:336:VAL:HG13	1.91	0.51
1:B:13:GLN:HB3	1:B:70:VAL:HG12	1.91	0.51
1:B:196:CYS:HB3	1:B:200:LYS:HB2	1.92	0.51
1:C:657:GLU:OE2	1:C:661:ARG:NH2	2.44	0.51
1:D:1025:ILE:O	1:D:1029:THR:OG1	2.24	0.51
1:A:586:GLN:HE22	1:A:613:ILE:HD13	1.76	0.50
1:B:348:ASP:OD1	1:B:351:GLY:N	2.44	0.50
1:D:1125:GLU:HA	1:D:1128:LYS:HB3	1.93	0.50
1:D:1029:THR:HG22	1:D:1031:TYR:H	1.75	0.50
1:A:657:GLU:OE2	1:A:661:ARG:NH2	2.45	0.50
1:C:33:MET:HE1	1:C:43:LEU:HB2	1.94	0.50
1:B:1029:THR:HG22	1:B:1031:TYR:H	1.76	0.50
1:B:494:PRO:O	3:B:1302:CYZ:N1	2.45	0.50
1:C:586:GLN:HE22	1:C:613:ILE:HD13	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:PHE:HZ	1:D:327:VAL:HG22	1.77	0.49
1:D:265:LEU:O	1:D:274:HIS:ND1	2.34	0.49
1:A:190:ARG:HE	1:A:469:TYR:HB3	1.77	0.49
1:A:33:MET:HE1	1:A:43:LEU:HB2	1.93	0.49
1:C:87:SER:OG	1:D:54:ASN:OD1	2.26	0.49
1:B:109:PHE:HZ	1:B:327:VAL:HG22	1.77	0.49
1:C:190:ARG:HE	1:C:469:TYR:HB3	1.77	0.49
1:C:348:ASP:OD1	1:C:352:LYS:N	2.46	0.49
1:D:494:PRO:O	3:D:1302:CYZ:N1	2.45	0.49
1:D:640:SER:HB2	1:D:669:LYS:HD3	1.95	0.49
1:C:638:ASP:HA	1:C:641:LYS:HB2	1.94	0.49
1:D:174:ASP:O	1:D:178:ARG:NH1	2.46	0.49
1:D:1068:LEU:HA	1:D:1073:LYS:HG3	1.94	0.49
1:B:1125:GLU:HA	1:B:1128:LYS:HB3	1.93	0.49
1:D:99:PRO:HA	1:D:113:MET:HB2	1.95	0.49
1:B:181:PHE:HB3	1:B:213:LYS:HE3	1.95	0.48
1:C:231:ASP:O	1:C:234:LYS:NZ	2.44	0.48
1:A:638:ASP:HA	1:A:641:LYS:HB2	1.95	0.48
1:D:163:ILE:HD13	1:D:180:LEU:HD11	1.94	0.48
1:B:232:LEU:HD23	1:B:363:LEU:HD22	1.96	0.48
1:A:147:GLN:HE21	1:B:143:LEU:HD21	1.78	0.48
1:D:1036:ARG:HA	1:D:1056:VAL:O	2.14	0.48
1:B:375:SER:OG	1:B:376:GLU:OE1	2.32	0.48
1:B:492:SER:O	1:C:493:LYS:NZ	2.45	0.48
1:B:1036:ARG:HA	1:B:1056:VAL:O	2.13	0.48
1:C:494:PRO:O	3:C:1302:CYZ:N1	2.46	0.48
1:A:494:PRO:O	3:A:1302:CYZ:N1	2.46	0.48
1:A:1110:SER:O	1:A:1114:LEU:HB2	2.13	0.48
1:C:488:VAL:HG23	1:C:489:ILE:HG13	1.96	0.48
1:D:181:PHE:HB3	1:D:213:LYS:HE3	1.95	0.48
1:A:348:ASP:OD1	1:A:352:LYS:N	2.45	0.48
1:B:99:PRO:HA	1:B:113:MET:HB2	1.96	0.47
1:B:118:LYS:NZ	1:B:144:SER:OG	2.40	0.47
1:C:143:LEU:HD21	1:D:147:GLN:HE21	1.79	0.47
1:A:1025:ILE:O	1:A:1029:THR:OG1	2.21	0.47
1:B:516:SER:O	1:B:519:ASP:CB	2.62	0.47
1:D:506:LYS:N	1:D:719:ASP:O	2.48	0.47
1:D:516:SER:O	1:D:519:ASP:CB	2.62	0.47
1:A:143:LEU:HD21	1:B:147:GLN:HE21	1.79	0.47
1:A:231:ASP:O	1:A:234:LYS:NZ	2.43	0.47
1:B:163:ILE:HD13	1:B:180:LEU:HD11	1.94	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:LYS:N	1:B:719:ASP:O	2.47	0.47
1:A:488:VAL:HG23	1:A:489:ILE:HG13	1.96	0.47
1:B:174:ASP:O	1:B:178:ARG:NH1	2.46	0.47
1:B:784:THR:OG1	1:B:785:SER:N	2.47	0.47
1:D:375:SER:OG	1:D:376:GLU:OE1	2.32	0.47
1:A:69:GLY:HA2	1:A:309:ARG:HH12	1.80	0.47
1:A:427:ASP:OD2	1:A:766:TRP:NE1	2.47	0.47
1:B:640:SER:HB2	1:B:669:LYS:HD3	1.96	0.47
1:D:232:LEU:HD23	1:D:363:LEU:HD22	1.97	0.47
1:C:1110:SER:O	1:C:1114:LEU:HB2	2.15	0.47
1:C:147:GLN:HE21	1:D:143:LEU:HD21	1.79	0.47
1:A:545:ARG:NH1	1:A:569:ASN:O	2.48	0.47
1:D:11:SER:HG	1:D:44:THR:HG1	1.59	0.47
1:A:793:ALA:HA	1:A:796:PHE:HD2	1.81	0.46
1:B:1068:LEU:HA	1:B:1073:LYS:HG3	1.96	0.46
1:C:427:ASP:OD2	1:C:766:TRP:NE1	2.47	0.46
1:D:297:ARG:HG3	1:D:301:LYS:HE2	1.96	0.46
1:C:1133:ILE:O	1:C:1136:SER:OG	2.32	0.46
1:A:800:VAL:HG21	1:D:1150:ILE:HD13	1.98	0.46
1:B:510:SER:OG	1:B:628:ARG:O	2.33	0.46
1:C:793:ALA:HA	1:C:796:PHE:HD2	1.80	0.46
1:C:545:ARG:NH1	1:C:569:ASN:O	2.48	0.46
1:D:722:LYS:NZ	1:D:724:GLY:O	2.49	0.46
1:B:334:LYS:HA	1:B:347:PHE:HD2	1.81	0.46
1:A:597:SER:HA	1:A:600:ILE:HG22	1.97	0.46
1:C:326:GLY:HA2	1:C:329:ILE:HD12	1.98	0.45
1:C:597:SER:HA	1:C:600:ILE:HG22	1.97	0.45
1:C:69:GLY:HA2	1:C:309:ARG:HH12	1.81	0.45
1:B:77:TYR:HE1	1:B:98:THR:HG21	1.81	0.45
1:B:722:LYS:NZ	1:B:724:GLY:O	2.49	0.45
1:D:77:TYR:HE1	1:D:98:THR:HG21	1.80	0.45
1:D:143:LEU:HD23	1:D:146:LEU:HD23	1.98	0.45
1:A:1133:ILE:O	1:A:1136:SER:OG	2.32	0.45
1:D:401:LEU:HD23	1:D:406:VAL:HG12	1.98	0.45
1:D:510:SER:OG	1:D:628:ARG:O	2.33	0.45
1:D:266:GLU:HG2	1:D:268:LYS:H	1.82	0.45
1:D:1031:TYR:CE2	1:D:1177:TRP:HB2	2.52	0.45
1:B:297:ARG:HG3	1:B:301:LYS:HE2	1.97	0.44
1:A:130:TRP:CD2	1:A:191:ARG:HD3	2.53	0.44
1:A:1069:GLU:H	1:A:1073:LYS:HG2	1.83	0.44
1:D:334:LYS:HA	1:D:347:PHE:HD2	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:GLY:HA2	1:A:329:ILE:HD12	1.98	0.44
1:B:1150:ILE:HD13	1:C:800:VAL:HG21	1.98	0.44
1:C:1069:GLU:H	1:C:1073:LYS:HG2	1.83	0.44
1:B:375:SER:HG	1:B:376:GLU:H	1.66	0.44
1:C:109:PHE:HZ	1:C:327:VAL:HG22	1.83	0.44
1:C:130:TRP:CD2	1:C:191:ARG:HD3	2.52	0.44
1:C:1031:TYR:HB3	1:C:1059:HIS:NE2	2.33	0.44
1:A:109:PHE:HZ	1:A:327:VAL:HG22	1.83	0.43
1:B:209:ILE:HG13	1:B:214:HIS:CD2	2.53	0.43
1:B:401:LEU:HD23	1:B:406:VAL:HG12	1.99	0.43
1:B:510:SER:OG	1:B:628:ARG:NH1	2.51	0.43
1:C:132:LYS:HA	1:C:159:GLN:O	2.18	0.43
1:D:209:ILE:HG13	1:D:214:HIS:CD2	2.53	0.43
1:D:1059:HIS:HB2	1:D:1068:LEU:HD23	2.00	0.43
1:B:637:GLU:O	1:B:640:SER:OG	2.24	0.43
1:C:334:LYS:HA	1:C:347:PHE:HD2	1.83	0.43
1:A:334:LYS:HA	1:A:347:PHE:HD2	1.83	0.43
1:A:493:LYS:NZ	1:D:492:SER:O	2.45	0.43
1:D:105:GLY:O	1:D:107:HIS:ND1	2.52	0.43
1:B:143:LEU:HD23	1:B:146:LEU:HD23	1.99	0.43
1:C:633:ILE:H	1:C:633:ILE:HG12	1.49	0.43
1:D:348:ASP:OD1	1:D:352:LYS:N	2.48	0.43
1:D:510:SER:OG	1:D:628:ARG:NH1	2.52	0.43
1:A:132:LYS:HA	1:A:159:GLN:O	2.19	0.42
1:B:105:GLY:O	1:B:107:HIS:ND1	2.52	0.42
1:B:1068:LEU:HD12	1:B:1069:GLU:HB2	2.01	0.42
1:D:1068:LEU:HD12	1:D:1069:GLU:HB2	2.01	0.42
1:C:1106:PHE:O	1:C:1147:SER:OG	2.34	0.42
1:D:1081:HIS:HB3	1:D:1098:ARG:HD2	2.01	0.42
1:A:83:ASN:HA	1:A:86:THR:HG22	2.01	0.42
1:D:1031:TYR:HB3	1:D:1059:HIS:NE2	2.35	0.42
1:C:1002:LEU:HB3	1:C:1003:PHE:H	1.66	0.42
1:C:306:ILE:H	1:C:306:ILE:HG13	1.77	0.42
1:D:77:TYR:OH	1:D:101:PHE:O	2.26	0.42
1:A:1106:PHE:O	1:A:1147:SER:OG	2.35	0.42
1:C:141:ARG:NH2	1:C:195:ASP:OD1	2.51	0.42
1:D:467:LEU:HD22	1:D:737:PRO:HD3	2.02	0.42
1:A:1002:LEU:HB3	1:A:1003:PHE:H	1.67	0.41
1:B:348:ASP:OD1	1:B:352:LYS:N	2.47	0.41
1:B:642:GLN:HE22	1:B:645:ILE:HD12	1.85	0.41
1:B:266:GLU:HG2	1:B:268:LYS:H	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:GLU:HG2	1:C:269:GLU:H	1.86	0.41
1:A:141:ARG:NH2	1:A:195:ASP:OD1	2.53	0.41
1:B:624:LEU:HD23	1:B:624:LEU:HA	1.89	0.41
1:B:1032:TRP:HB2	1:B:1061:GLY:HA2	2.02	0.41
1:C:83:ASN:HA	1:C:86:THR:HG22	2.01	0.41
1:A:266:GLU:HG2	1:A:269:GLU:H	1.84	0.41
1:B:474:ILE:HG13	1:B:736:THR:HG22	2.02	0.41
1:D:642:GLN:HE22	1:D:645:ILE:HD12	1.85	0.41
1:A:633:ILE:H	1:A:633:ILE:HG12	1.49	0.41
1:B:611:ILE:HD11	1:C:517:PHE:HB2	2.02	0.41
1:A:517:PHE:HB2	1:D:611:ILE:HD11	2.02	0.41
1:D:98:THR:HA	1:D:99:PRO:HD3	1.86	0.41
1:B:163:ILE:HG21	1:B:180:LEU:HD11	2.03	0.41
1:B:658:PHE:O	1:B:662:SER:HB2	2.21	0.41
1:B:1031:TYR:CE2	1:B:1177:TRP:HB2	2.55	0.41
1:C:348:ASP:OD1	1:C:351:GLY:N	2.54	0.41
1:C:637:GLU:O	1:C:640:SER:OG	2.36	0.41
1:A:348:ASP:OD1	1:A:351:GLY:N	2.54	0.41
1:B:14:ILE:HD13	1:B:43:LEU:HD23	2.03	0.41
1:B:16:GLY:HA2	1:B:74:PHE:O	2.21	0.41
1:B:48:ASP:HB3	1:B:50:LEU:HD13	2.02	0.41
1:B:467:LEU:HD22	1:B:737:PRO:HD3	2.03	0.41
1:B:596:LEU:HD22	1:B:597:SER:H	1.86	0.41
1:C:116:ASP:OD1	1:C:117:LEU:N	2.53	0.41
1:C:1012:THR:HG21	1:C:1199:MET:HE1	2.03	0.41
1:D:596:LEU:HD22	1:D:597:SER:H	1.86	0.41
1:D:658:PHE:O	1:D:662:SER:HB2	2.21	0.41
1:A:309:ARG:H	1:A:309:ARG:HD3	1.87	0.40
1:B:647:TYR:HB3	1:B:701:ALA:HB3	2.02	0.40
1:C:97:ILE:HD13	1:C:292:MET:HE1	2.04	0.40
1:C:1205:LYS:O	1:C:1208:THR:OG1	2.34	0.40
1:D:118:LYS:NZ	1:D:144:SER:OG	2.41	0.40
1:B:596:LEU:HD13	1:B:597:SER:HB3	2.04	0.40
1:B:1059:HIS:HB2	1:B:1068:LEU:HD23	2.03	0.40
1:B:1081:HIS:HB3	1:B:1098:ARG:HD2	2.02	0.40
1:D:48:ASP:HB3	1:D:50:LEU:HD13	2.02	0.40
1:D:647:TYR:HB3	1:D:701:ALA:HB3	2.03	0.40
1:D:402:GLU:HG2	1:D:708:MET:HE2	2.04	0.40
1:D:474:ILE:HG13	1:D:736:THR:HG22	2.04	0.40
1:A:375:SER:OG	1:A:376:GLU:N	2.53	0.40
1:A:705:GLU:OE1	1:A:732:TYR:OH	2.28	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:GLU:HG2	1:B:708:MET:HE2	2.03	0.40
1:D:16:GLY:HA2	1:D:74:PHE:O	2.21	0.40
1:D:101:PHE:HA	1:D:102:PRO:HD3	1.96	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	973/1031 (94%)	884 (91%)	84 (9%)	5 (0%)	24	62
1	B	975/1031 (95%)	892 (92%)	80 (8%)	3 (0%)	36	71
1	C	974/1031 (94%)	888 (91%)	81 (8%)	5 (0%)	24	62
1	D	975/1031 (95%)	889 (91%)	83 (8%)	3 (0%)	36	71
All	All	3897/4124 (94%)	3553 (91%)	328 (8%)	16 (0%)	31	66

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	633	ILE
1	A	1178	SER
1	B	1171	ASN
1	C	633	ILE
1	C	1178	SER
1	D	1171	ASN
1	A	632	PRO
1	B	636	ALA
1	B	637	GLU
1	C	632	PRO
1	D	636	ALA
1	D	637	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	634	GLU
1	C	634	GLU
1	A	314	ASP
1	C	314	ASP

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	832/873 (95%)	825 (99%)	7 (1%)	73	77
1	B	831/873 (95%)	828 (100%)	3 (0%)	84	82
1	C	832/873 (95%)	825 (99%)	7 (1%)	73	77
1	D	831/873 (95%)	828 (100%)	3 (0%)	84	82
All	All	3326/3492 (95%)	3306 (99%)	20 (1%)	76	80

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	489	ILE
1	A	500	ILE
1	A	504	ILE
1	A	521	LEU
1	A	577	LEU
1	A	591	ILE
1	A	798	ILE
1	B	235	ILE
1	B	504	ILE
1	B	577	LEU
1	C	489	ILE
1	C	500	ILE
1	C	504	ILE
1	C	521	LEU
1	C	577	LEU
1	C	591	ILE
1	C	798	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	235	ILE
1	D	504	ILE
1	D	577	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	147	GLN
1	A	214	HIS
1	A	302	GLN
1	A	355	ASN
1	A	418	ASN
1	A	508	GLN
1	A	586	GLN
1	B	24	GLN
1	B	147	GLN
1	B	224	ASN
1	B	337	GLN
1	B	412	HIS
1	B	508	GLN
1	B	586	GLN
1	B	642	GLN
1	B	747	ASN
1	B	764	ASN
1	B	1198	HIS
1	C	13	GLN
1	C	147	GLN
1	C	302	GLN
1	C	355	ASN
1	C	418	ASN
1	C	508	GLN
1	C	586	GLN
1	D	24	GLN
1	D	147	GLN
1	D	224	ASN
1	D	302	GLN
1	D	337	GLN
1	D	412	HIS
1	D	508	GLN
1	D	586	GLN
1	D	642	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	747	ASN
1	D	764	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLU	D	1301	-	8,9,9	1.16	1 (12%)	8,11,11	1.15	1 (12%)
3	CYZ	A	1302	-	26,27,27	8.13	19 (73%)	38,44,44	4.75	17 (44%)
2	GLU	B	1301	-	8,9,9	1.15	1 (12%)	8,11,11	1.14	1 (12%)
2	GLU	A	1301	-	8,9,9	1.07	1 (12%)	8,11,11	1.19	1 (12%)
3	CYZ	C	1302	-	26,27,27	8.14	19 (73%)	38,44,44	4.76	17 (44%)
3	CYZ	B	1302	-	26,27,27	8.17	19 (73%)	38,44,44	4.82	16 (42%)
3	CYZ	D	1302	-	26,27,27	8.15	19 (73%)	38,44,44	4.82	16 (42%)
2	GLU	C	1301	-	8,9,9	1.08	1 (12%)	8,11,11	1.19	1 (12%)
4	GYG	C	1303	-	28,28,28	1.38	3 (10%)	32,33,33	1.32	3 (9%)

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	GLU	D	1301	-	-	0/9/9/9	-
3	CYZ	A	1302	-	-	0/7/42/42	0/5/4/4
2	GLU	B	1301	-	-	0/9/9/9	-
2	GLU	A	1301	-	-	0/9/9/9	-
3	CYZ	C	1302	-	-	0/7/42/42	0/5/4/4
3	CYZ	B	1302	-	-	0/7/42/42	0/5/4/4
3	CYZ	D	1302	-	-	0/7/42/42	0/5/4/4
2	GLU	C	1301	-	-	0/9/9/9	-
4	GYG	C	1303	-	-	5/18/18/18	0/2/2/2

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1302	CYZ	C1-C8	20.45	1.72	1.53
3	D	1302	CYZ	C1-C8	20.36	1.72	1.53
3	C	1302	CYZ	C1-C8	20.13	1.72	1.53
3	A	1302	CYZ	C1-C8	20.11	1.72	1.53
3	C	1302	CYZ	C2-C1	-19.88	1.13	1.55
3	A	1302	CYZ	C2-C1	-19.85	1.13	1.55
3	B	1302	CYZ	C2-C1	-19.80	1.13	1.55
3	D	1302	CYZ	C2-C1	-19.78	1.13	1.55
3	C	1302	CYZ	C2-C3	-14.29	1.13	1.51
3	D	1302	CYZ	C2-C3	-14.25	1.13	1.51
3	A	1302	CYZ	C2-C3	-14.22	1.13	1.51
3	B	1302	CYZ	C2-C3	-14.20	1.13	1.51
3	B	1302	CYZ	C9-S1	-13.66	1.63	1.75
3	D	1302	CYZ	C9-S1	-13.46	1.63	1.75
3	C	1302	CYZ	C9-S1	-13.43	1.63	1.75
3	A	1302	CYZ	C9-S1	-13.42	1.63	1.75
3	D	1302	CYZ	C10-N2	9.74	1.57	1.39
3	B	1302	CYZ	C10-N2	9.74	1.57	1.39
3	C	1302	CYZ	C10-N2	9.67	1.56	1.39
3	A	1302	CYZ	C10-N2	9.66	1.56	1.39
3	A	1302	CYZ	C4-C3	9.46	1.59	1.32
3	C	1302	CYZ	C4-C3	9.43	1.59	1.32
3	B	1302	CYZ	C4-C3	9.42	1.59	1.32
3	D	1302	CYZ	C4-C3	9.39	1.59	1.32
3	B	1302	CYZ	C5-C4	-9.15	1.08	1.51
3	D	1302	CYZ	C5-C4	-9.13	1.08	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1302	CYZ	C5-C4	-9.12	1.08	1.51
3	A	1302	CYZ	C5-C4	-9.11	1.08	1.51
3	C	1302	CYZ	S2-N3	7.63	1.75	1.60
3	D	1302	CYZ	S2-N3	7.61	1.75	1.60
3	A	1302	CYZ	S2-N3	7.61	1.75	1.60
3	B	1302	CYZ	S2-N3	7.58	1.75	1.60
3	C	1302	CYZ	C6-C5	-7.06	1.12	1.52
3	A	1302	CYZ	C6-C5	-7.06	1.12	1.52
3	B	1302	CYZ	C6-C5	-7.06	1.12	1.52
3	D	1302	CYZ	C6-C5	-7.05	1.12	1.52
4	C	1303	GYG	CAG-NAH	5.26	1.45	1.33
3	D	1302	CYZ	C12-S2	5.23	1.84	1.77
3	B	1302	CYZ	C12-S2	5.17	1.84	1.77
3	B	1302	CYZ	C6-C1	-5.04	1.39	1.53
3	D	1302	CYZ	C6-C1	-5.04	1.39	1.53
3	A	1302	CYZ	C6-C1	-4.92	1.39	1.53
3	C	1302	CYZ	C12-S2	4.89	1.83	1.77
3	C	1302	CYZ	C6-C1	-4.89	1.40	1.53
3	A	1302	CYZ	C12-S2	4.87	1.83	1.77
3	C	1302	CYZ	C10-C9	-4.58	1.34	1.40
3	A	1302	CYZ	C10-C9	-4.54	1.34	1.40
3	B	1302	CYZ	C10-C9	-4.53	1.34	1.40
3	D	1302	CYZ	C10-C9	-4.52	1.34	1.40
3	D	1302	CYZ	O2-S1	4.44	1.48	1.43
3	B	1302	CYZ	O2-S1	4.44	1.48	1.43
3	C	1302	CYZ	O2-S1	4.41	1.48	1.43
3	A	1302	CYZ	O2-S1	4.35	1.48	1.43
3	A	1302	CYZ	O3-S2	4.18	1.51	1.43
3	C	1302	CYZ	O3-S2	4.16	1.51	1.43
3	C	1302	CYZ	C8-N2	4.10	1.51	1.46
3	B	1302	CYZ	O3-S2	4.05	1.50	1.43
3	A	1302	CYZ	C8-N2	4.03	1.51	1.46
3	D	1302	CYZ	O3-S2	4.02	1.50	1.43
3	B	1302	CYZ	C8-N2	3.79	1.51	1.46
3	D	1302	CYZ	C7-C5	-3.75	1.31	1.52
3	B	1302	CYZ	C7-C5	-3.75	1.31	1.52
3	C	1302	CYZ	C7-C5	-3.74	1.31	1.52
3	A	1302	CYZ	C7-C5	-3.72	1.31	1.52
3	D	1302	CYZ	C8-N2	3.71	1.50	1.46
4	C	1303	GYG	CAW-CAV	-3.33	1.36	1.43
3	D	1302	CYZ	C13-CL	2.91	1.80	1.73
3	B	1302	CYZ	C13-CL	2.90	1.80	1.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1302	CYZ	C13-CL	2.89	1.80	1.73
3	C	1302	CYZ	C13-CL	2.83	1.80	1.73
4	C	1303	GYG	OAC-CAG	-2.41	1.18	1.23
3	C	1302	CYZ	S1-N1	-2.33	1.59	1.62
2	D	1301	GLU	OXT-C	-2.30	1.23	1.30
3	A	1302	CYZ	S1-N1	-2.30	1.59	1.62
3	D	1302	CYZ	O4-S2	2.29	1.47	1.43
3	C	1302	CYZ	O4-S2	2.29	1.47	1.43
3	B	1302	CYZ	O4-S2	2.29	1.47	1.43
2	B	1301	GLU	OXT-C	-2.27	1.23	1.30
3	A	1302	CYZ	O4-S2	2.25	1.47	1.43
3	D	1302	CYZ	S1-N1	-2.25	1.59	1.62
3	B	1302	CYZ	S1-N1	-2.23	1.59	1.62
2	C	1301	GLU	OXT-C	-2.20	1.23	1.30
2	A	1301	GLU	OXT-C	-2.19	1.23	1.30

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1302	CYZ	C1-C2-C3	20.08	137.85	106.86
3	B	1302	CYZ	C1-C2-C3	20.03	137.77	106.86
3	C	1302	CYZ	C1-C2-C3	19.99	137.71	106.86
3	A	1302	CYZ	C1-C2-C3	19.96	137.66	106.86
3	D	1302	CYZ	O4-S2-O3	-11.99	100.36	118.80
3	B	1302	CYZ	O4-S2-O3	-11.94	100.43	118.80
3	A	1302	CYZ	C9-S1-N1	11.11	116.91	103.42
3	C	1302	CYZ	C9-S1-N1	11.09	116.89	103.42
3	C	1302	CYZ	O4-S2-O3	-11.01	101.86	118.80
3	A	1302	CYZ	O4-S2-O3	-11.00	101.88	118.80
3	B	1302	CYZ	C9-S1-N1	10.90	116.66	103.42
3	D	1302	CYZ	C9-S1-N1	10.89	116.65	103.42
3	B	1302	CYZ	O2-S1-O1	-6.64	111.68	118.44
3	D	1302	CYZ	O2-S1-O1	-6.58	111.74	118.44
3	C	1302	CYZ	C7-C2-C1	-6.38	87.27	101.21
3	A	1302	CYZ	C7-C2-C1	-6.37	87.29	101.21
3	C	1302	CYZ	O2-S1-O1	-6.19	112.14	118.44
3	A	1302	CYZ	O2-S1-O1	-6.18	112.15	118.44
3	D	1302	CYZ	C7-C2-C1	-5.92	88.26	101.21
3	B	1302	CYZ	C7-C2-C1	-5.92	88.27	101.21
4	C	1303	GYG	CAF-CAG-NAH	5.11	123.15	116.06
3	C	1302	CYZ	C2-C1-C8	-4.85	107.92	114.88
3	A	1302	CYZ	C2-C1-C8	-4.84	107.94	114.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1302	CYZ	C2-C1-C8	-4.61	108.26	114.88
3	D	1302	CYZ	C7-C2-C3	-4.50	87.75	99.72
3	D	1302	CYZ	C2-C1-C8	-4.50	108.42	114.88
3	B	1302	CYZ	C7-C2-C3	-4.49	87.78	99.72
3	C	1302	CYZ	C7-C2-C3	-3.96	89.21	99.72
3	A	1302	CYZ	C7-C2-C3	-3.93	89.27	99.72
3	C	1302	CYZ	C6-C5-C4	3.93	132.25	101.77
3	A	1302	CYZ	C6-C5-C4	3.93	132.23	101.77
3	B	1302	CYZ	C6-C5-C4	3.92	132.19	101.77
3	D	1302	CYZ	C6-C5-C4	3.90	132.06	101.77
3	B	1302	CYZ	O4-S2-N3	3.38	112.22	107.35
3	D	1302	CYZ	O4-S2-N3	3.33	112.15	107.35
3	A	1302	CYZ	O3-S2-N3	3.25	112.04	107.35
3	C	1302	CYZ	O3-S2-N3	3.25	112.04	107.35
3	D	1302	CYZ	O3-S2-N3	3.16	111.92	107.35
3	B	1302	CYZ	O3-S2-N3	3.11	111.84	107.35
3	C	1302	CYZ	O4-S2-N3	3.08	111.79	107.35
3	A	1302	CYZ	O4-S2-N3	3.03	111.72	107.35
4	C	1303	GYV	OAC-CAG-NAH	-2.99	117.16	123.03
3	B	1302	CYZ	O2-S1-C9	-2.93	105.64	109.30
3	D	1302	CYZ	O2-S1-C9	-2.81	105.79	109.30
3	D	1302	CYZ	O4-S2-C12	2.76	111.27	107.26
3	B	1302	CYZ	O4-S2-C12	2.74	111.23	107.26
2	D	1301	GLU	OXT-C-O	-2.68	117.99	124.08
2	B	1301	GLU	OXT-C-O	-2.65	118.07	124.08
3	C	1302	CYZ	O2-S1-C9	-2.62	106.02	109.30
3	A	1302	CYZ	C2-C3-C4	-2.61	101.53	107.97
3	C	1302	CYZ	C2-C3-C4	-2.59	101.58	107.97
3	B	1302	CYZ	C12-C13-CL	-2.58	119.65	121.52
3	A	1302	CYZ	O2-S1-C9	-2.56	106.10	109.30
2	C	1301	GLU	OXT-C-O	-2.53	118.33	124.08
3	D	1302	CYZ	C12-C13-CL	-2.53	119.69	121.52
3	B	1302	CYZ	C2-C3-C4	-2.52	101.75	107.97
2	A	1301	GLU	OXT-C-O	-2.50	118.42	124.08
3	D	1302	CYZ	C2-C3-C4	-2.48	101.85	107.97
3	C	1302	CYZ	C12-C13-CL	-2.45	119.74	121.52
3	A	1302	CYZ	C12-C13-CL	-2.43	119.76	121.52
3	A	1302	CYZ	O4-S2-C12	2.32	110.63	107.26
3	D	1302	CYZ	C13-C12-S2	-2.31	120.70	123.47
3	A	1302	CYZ	C11-C12-C13	2.29	120.73	118.33
3	C	1302	CYZ	C11-C12-C13	2.29	120.73	118.33
3	A	1302	CYZ	O1-S1-C9	-2.28	106.45	109.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1302	CYZ	O3-S2-C12	2.26	110.55	107.26
3	C	1302	CYZ	O1-S1-C9	-2.25	106.49	109.30
3	B	1302	CYZ	C13-C12-S2	-2.23	120.80	123.47
3	C	1302	CYZ	O4-S2-C12	2.21	110.47	107.26
3	B	1302	CYZ	O3-S2-C12	2.21	110.47	107.26
3	C	1302	CYZ	C12-C11-C9	-2.19	118.66	120.89
3	A	1302	CYZ	C12-C11-C9	-2.16	118.69	120.89
4	C	1303	GYG	CAJ-CAK-NAL	-2.07	106.51	112.07

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1303	GYG	CAF-CAG-NAH-CAI
4	C	1303	GYG	OAC-CAG-NAH-CAI
4	C	1303	GYG	CAJ-CAK-NAL-CAM
4	C	1303	GYG	CAI-CAJ-CAK-NAL
4	C	1303	GYG	NAL-CAM-CAN-CAO

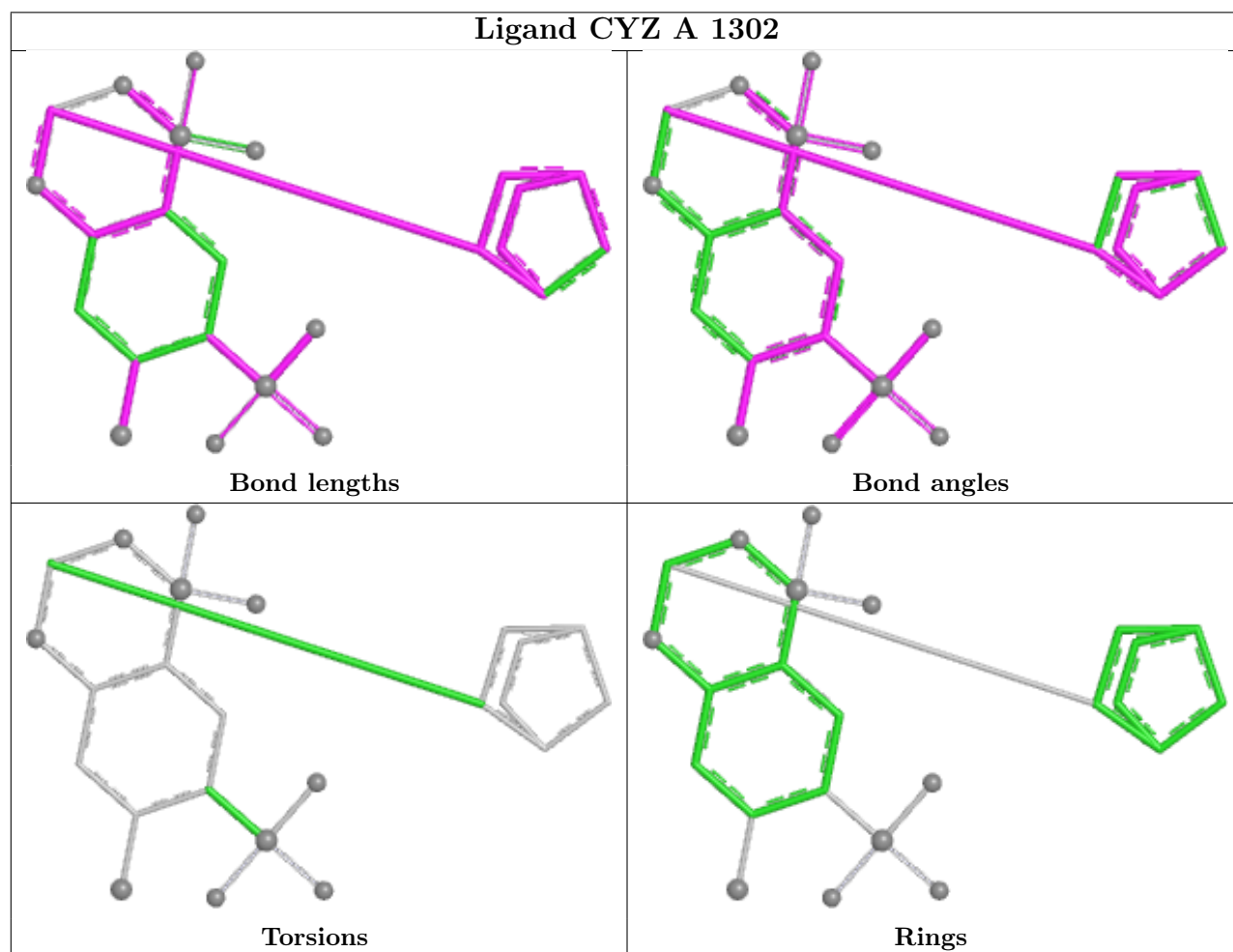
There are no ring outliers.

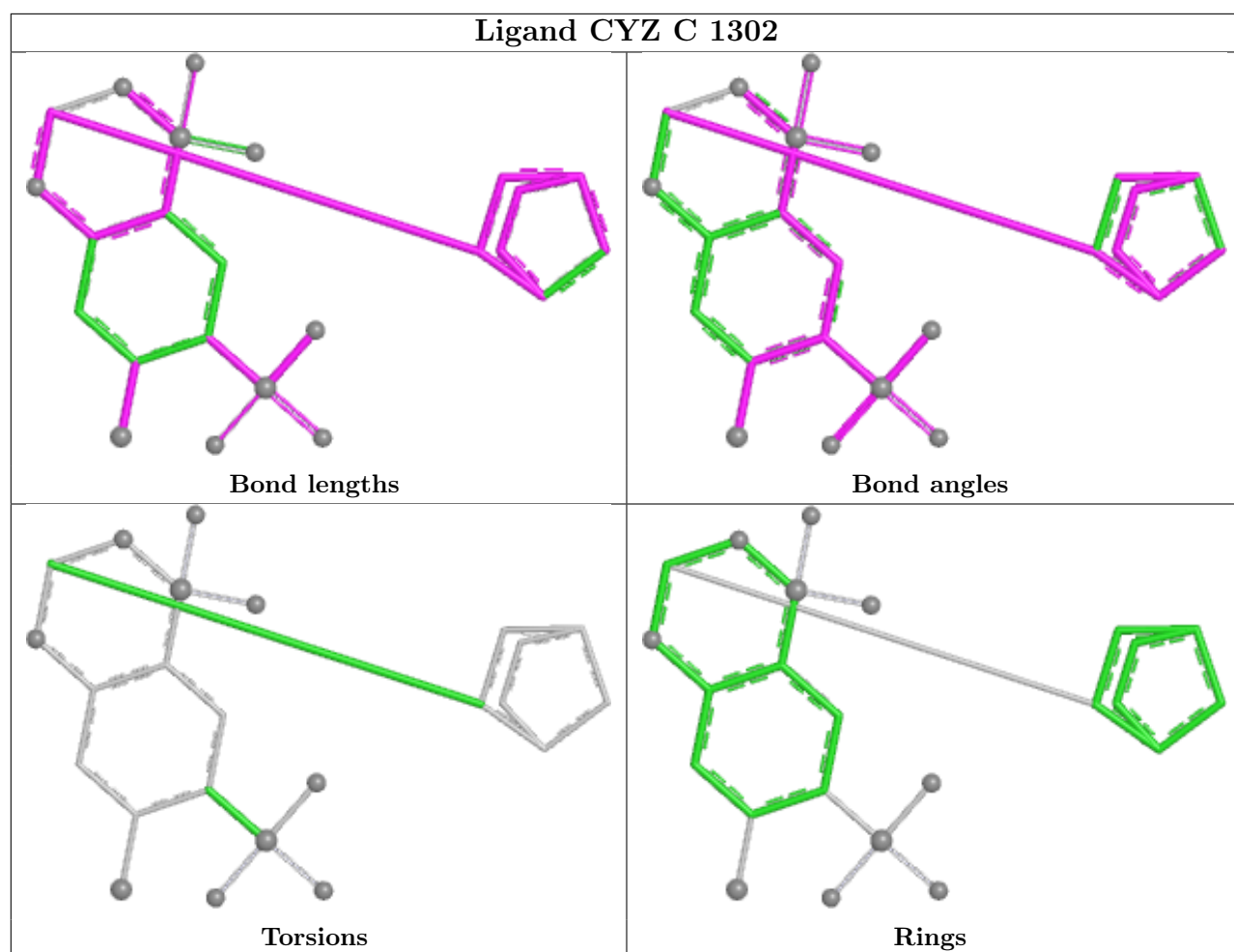
8 monomers are involved in 8 short contacts:

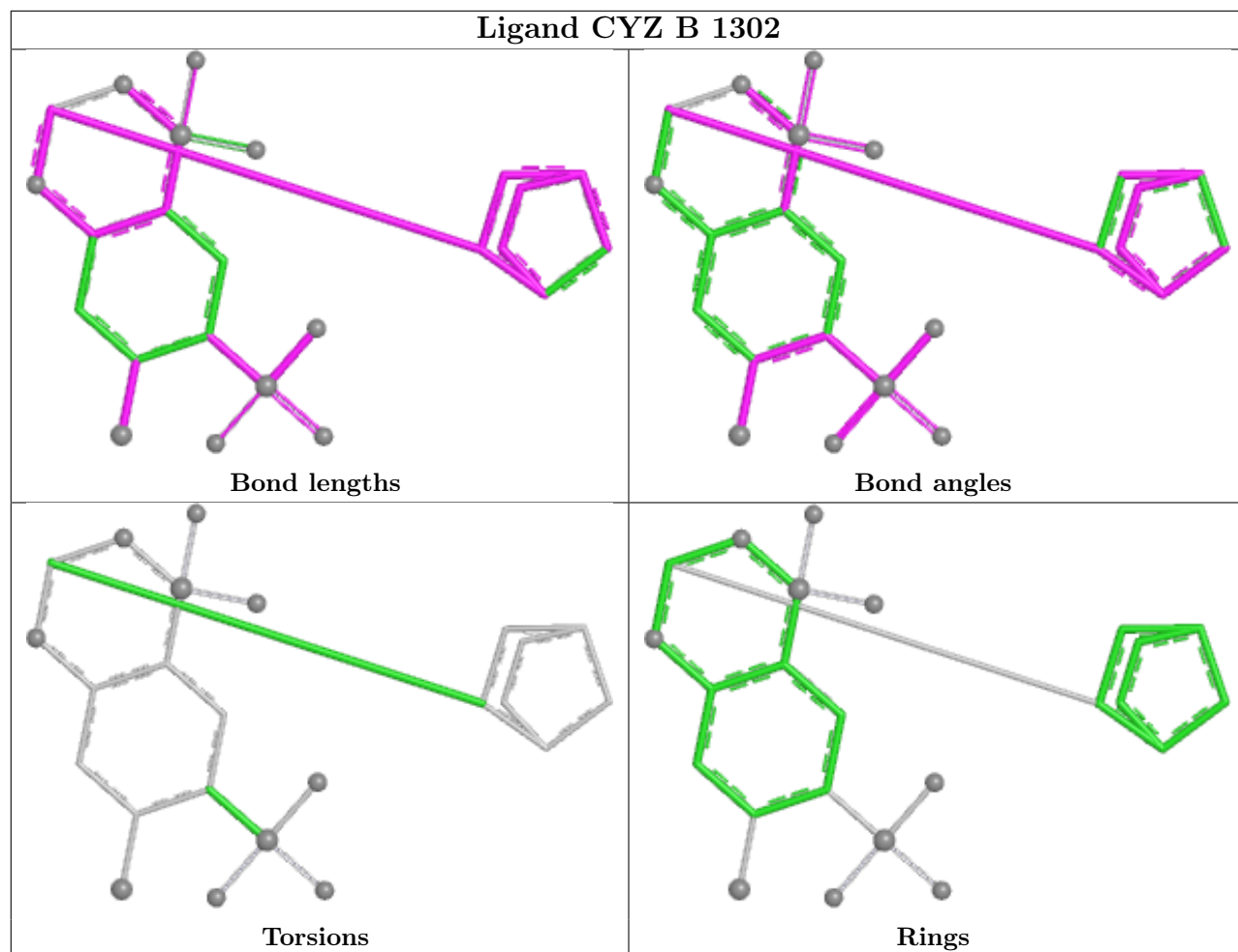
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1301	GLU	1	0
3	A	1302	CYZ	1	0
2	B	1301	GLU	1	0
2	A	1301	GLU	1	0
3	C	1302	CYZ	1	0
3	B	1302	CYZ	1	0
3	D	1302	CYZ	1	0
2	C	1301	GLU	1	0

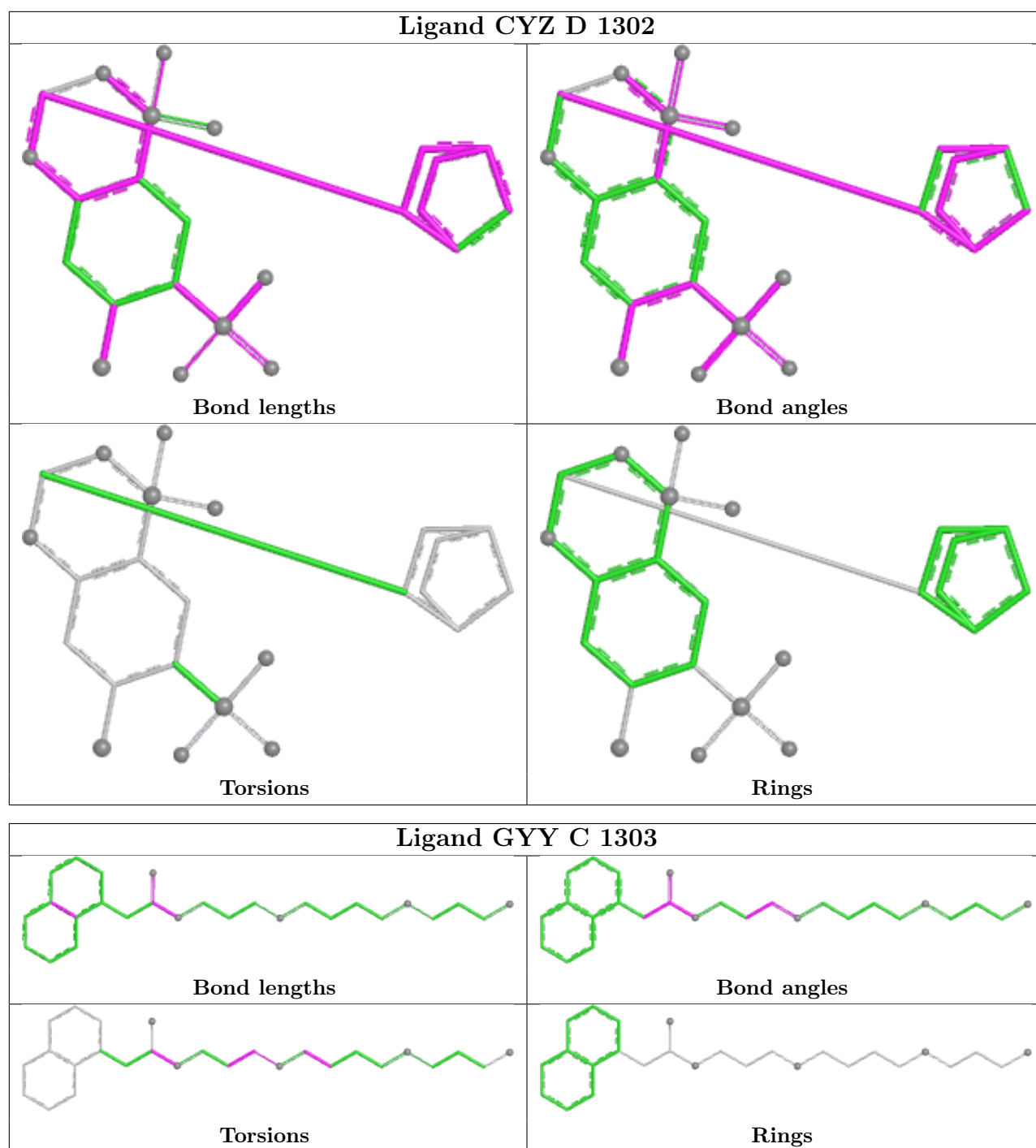
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

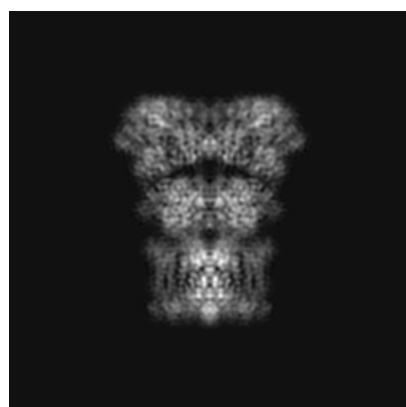
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7961. These allow visual inspection of the internal detail of the map and identification of artifacts.

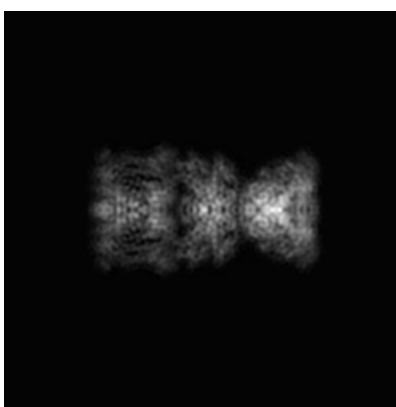
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

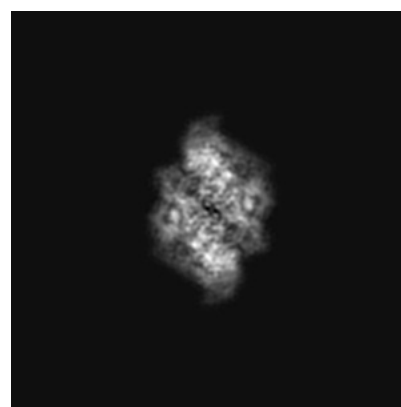
6.1.1 Primary map



X



Y



Z

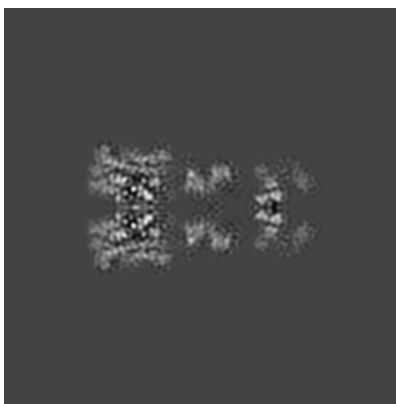
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

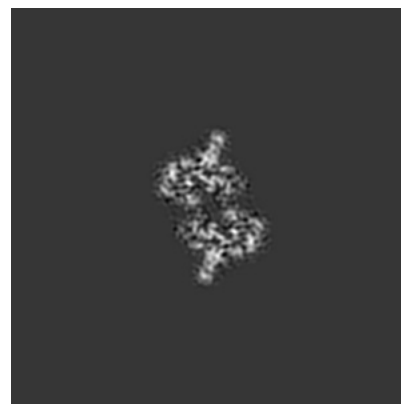
6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

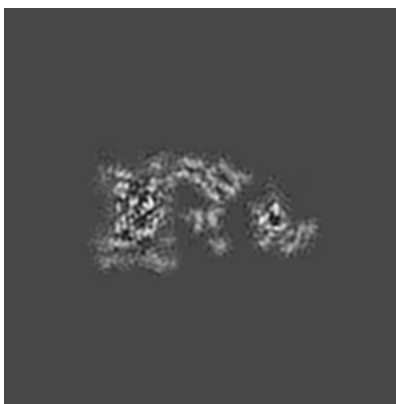
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

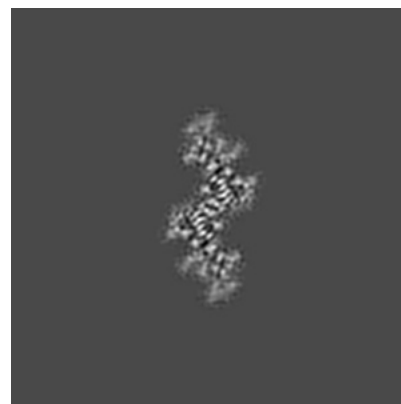
6.3.1 Primary map



X Index: 153



Y Index: 142

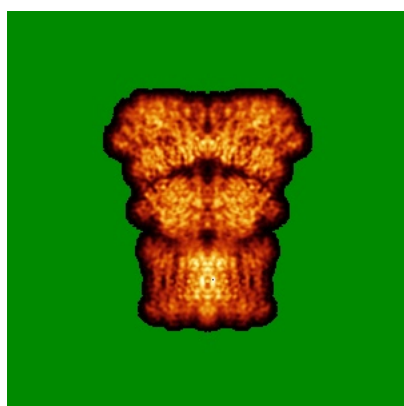


Z Index: 196

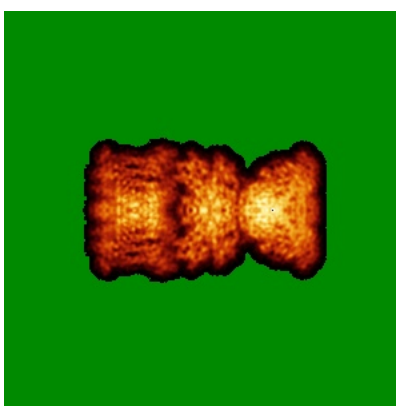
The images above show the largest variance slices of the map in three orthogonal directions.

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

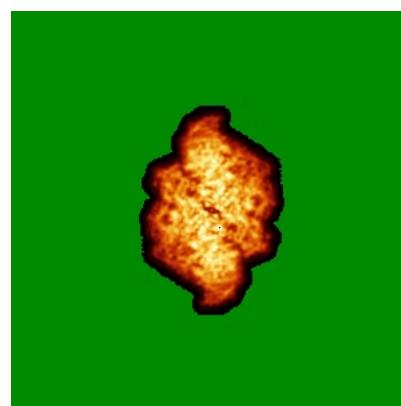
6.4.1 Primary map



X



Y

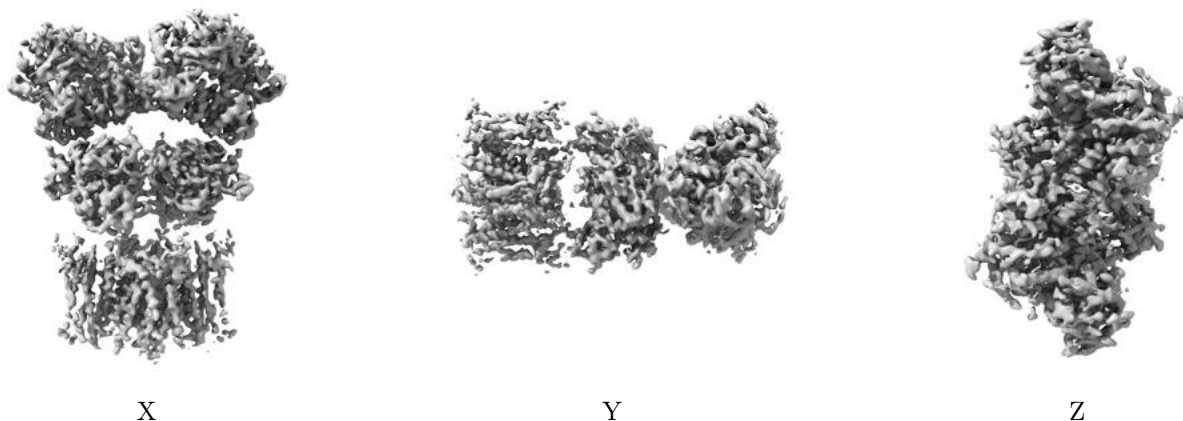


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

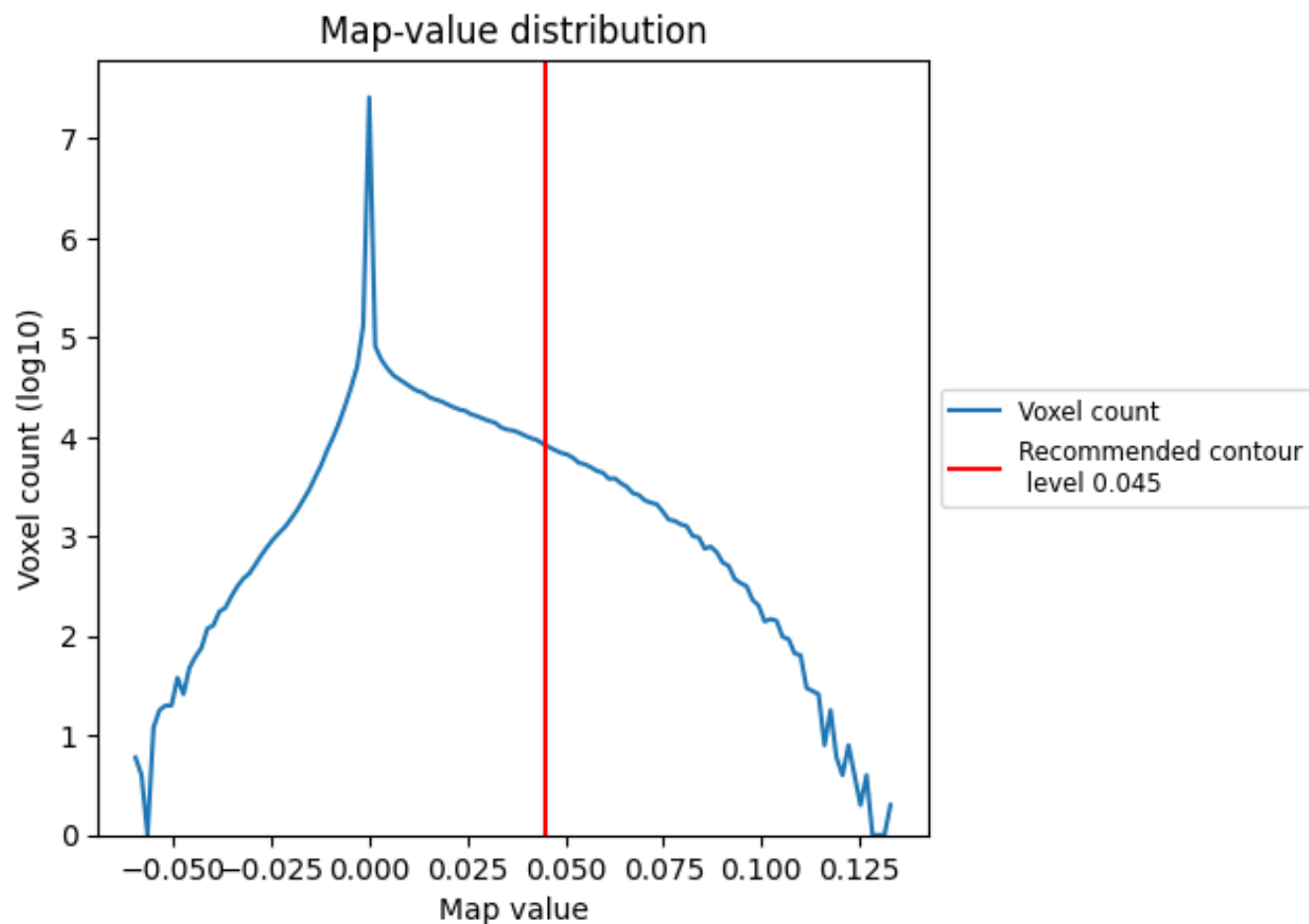
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

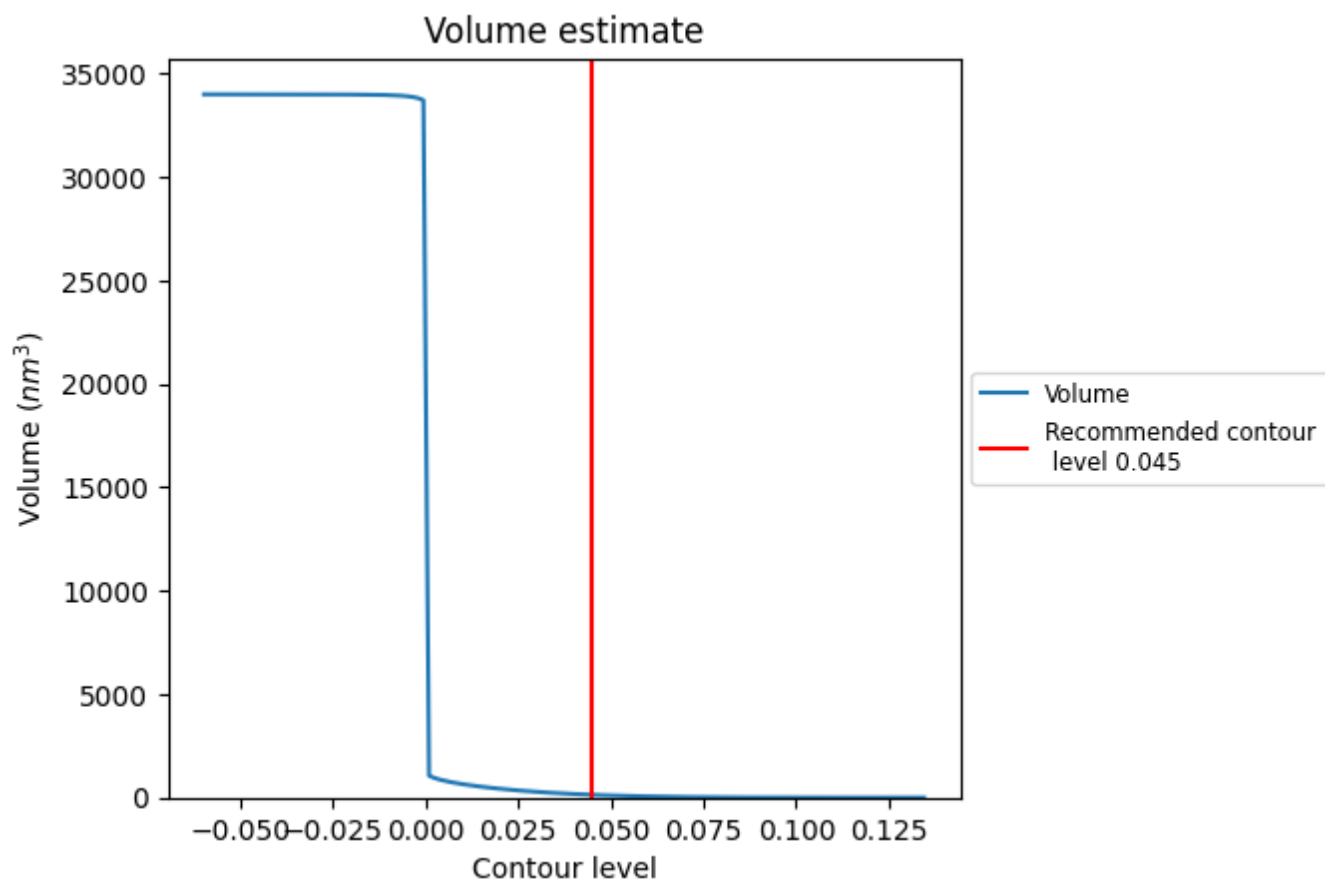
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

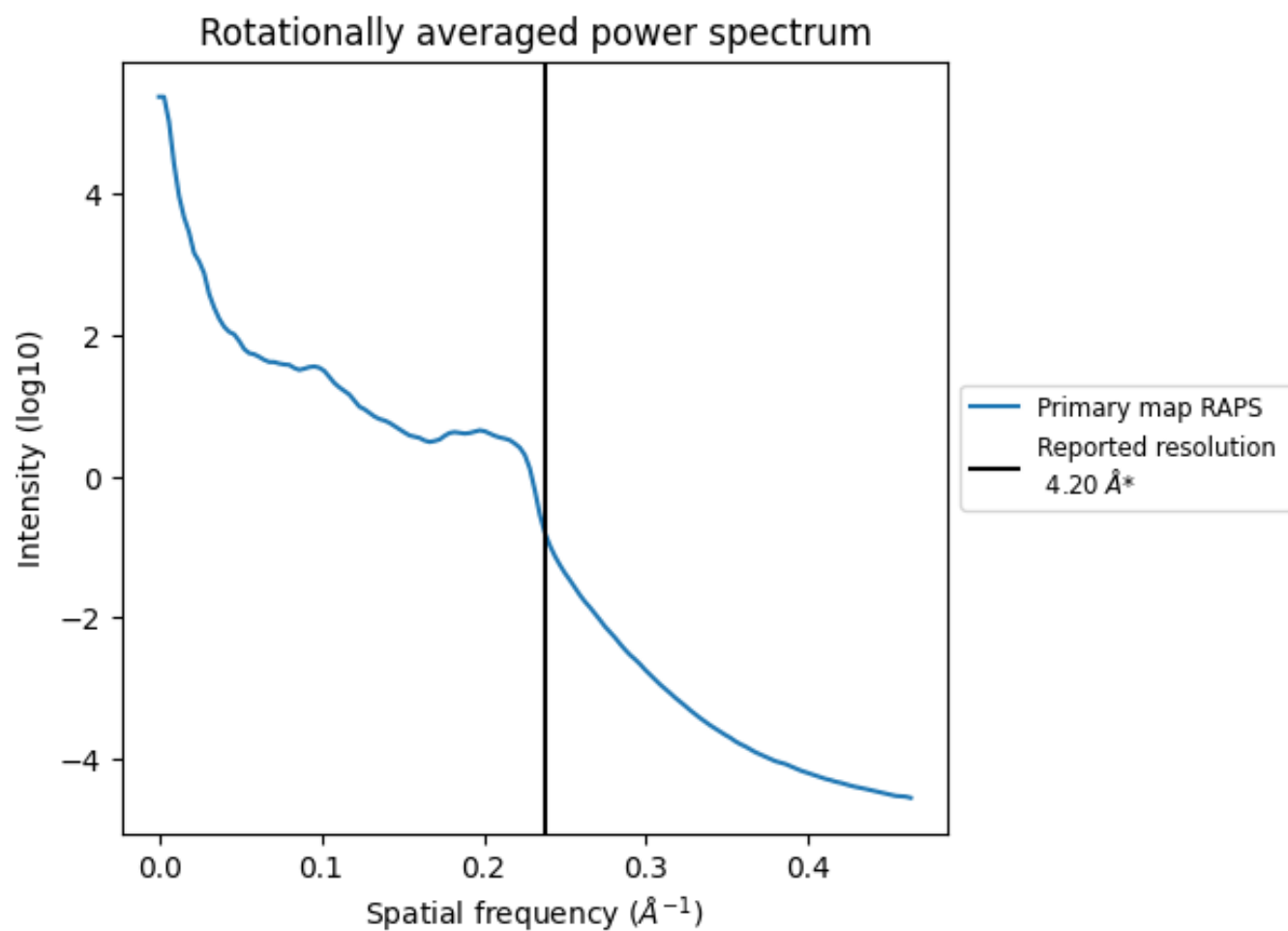
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 133 nm³; this corresponds to an approximate mass of 120 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 0.238 Å⁻¹

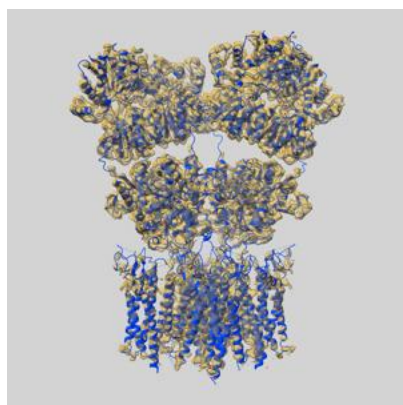
8 Fourier-Shell correlation

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

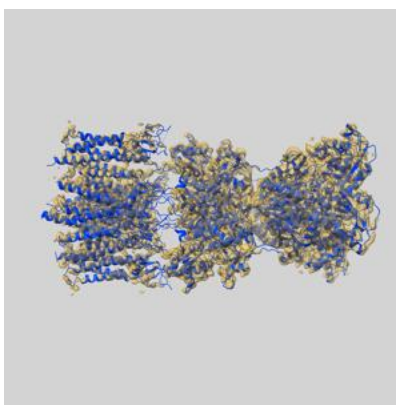
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7961 and PDB model 6DM1. Per-residue inclusion information can be found in section 3 on page 8.

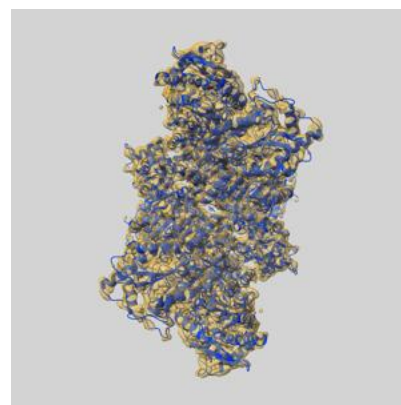
9.1 Map-model overlay [i](#)



X



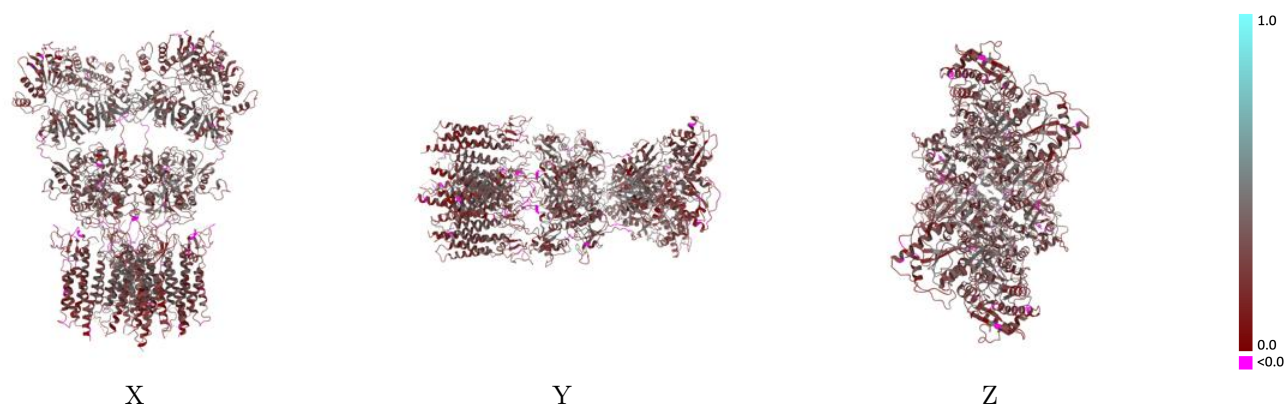
Y



Z

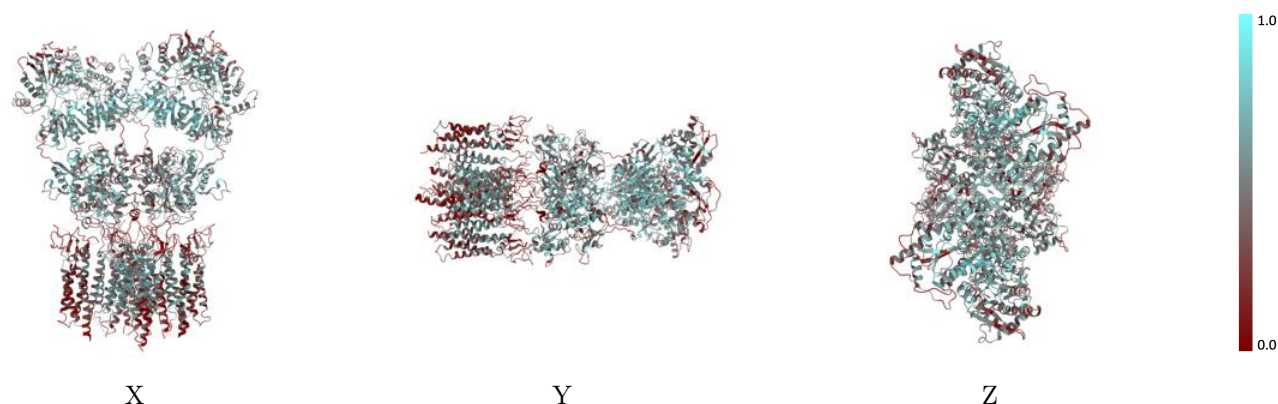
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



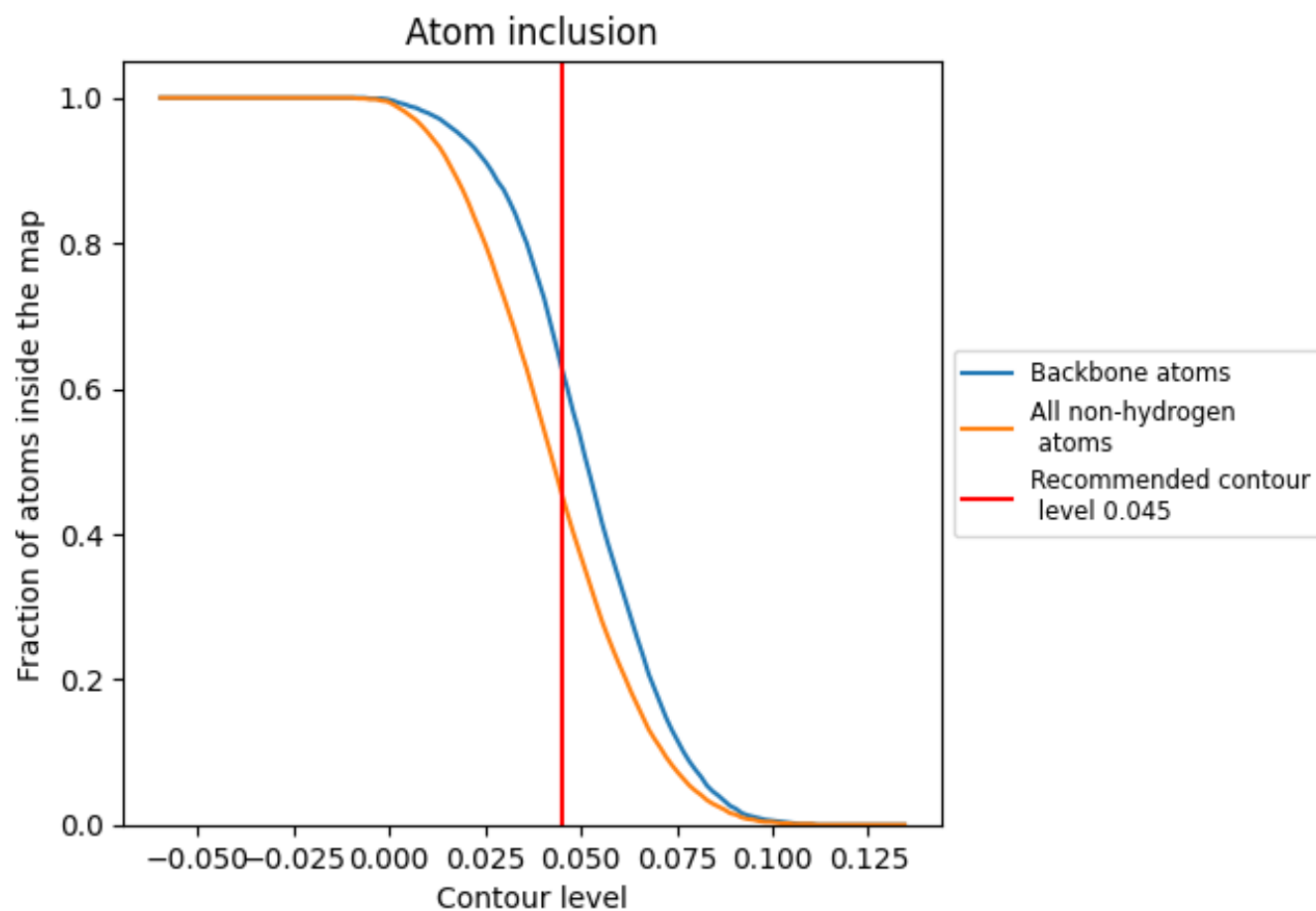
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 46% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4550	0.2970
A	0.4580	0.2980
B	0.4540	0.2950
C	0.4570	0.2990
D	0.4550	0.2960

