



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:35 AM UTC

PDB ID : 7TNO / pdb_00007tno
EMDB ID : EMD-26016
Title : Complex GGGN of AMPA-subtype iGluR GluA2 in complex with auxiliary subunit gamma2 (Stargazin) at low glutamate concentration (20 uM) in the presence of cyclothiazide (100 uM)
Authors : Yelshanskaya, M.V.; Sobolevsky, A.I.
Deposited on : 2022-01-21
Resolution : 4.02 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 : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

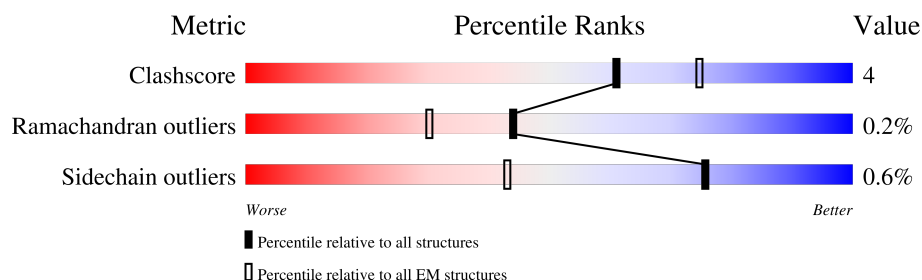
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.02 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1033	52% 6% 42%
1	B	1033	52% 6% 42%
1	C	1033	52% 6% 42%
1	D	1033	51% 6% 42%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18810 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Isoform Flip of Glutamate receptor 2, Voltage-dependent calcium channel gamma-3 subunit chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	601	Total	C	N	O	S	0	0
			4673	3033	757	851	32		
1	B	600	Total	C	N	O	S	0	0
			4667	3029	757	849	32		
1	C	601	Total	C	N	O	S	0	0
			4673	3033	757	851	32		
1	D	600	Total	C	N	O	S	0	0
			4671	3032	758	849	32		

There are 52 discrepancies between the modelled and reference sequences:

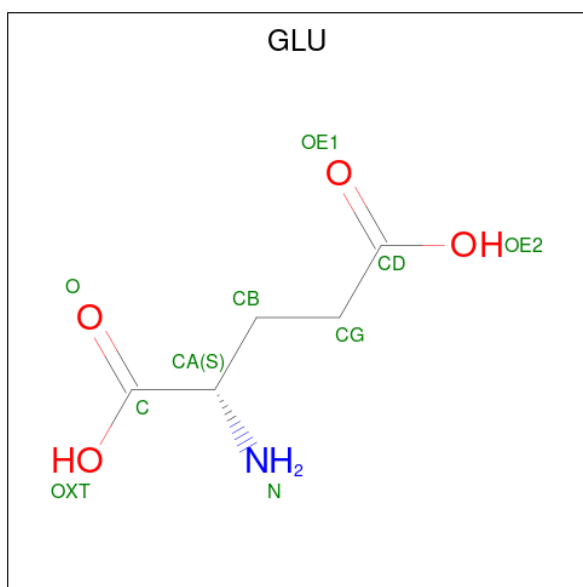
Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	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
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
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

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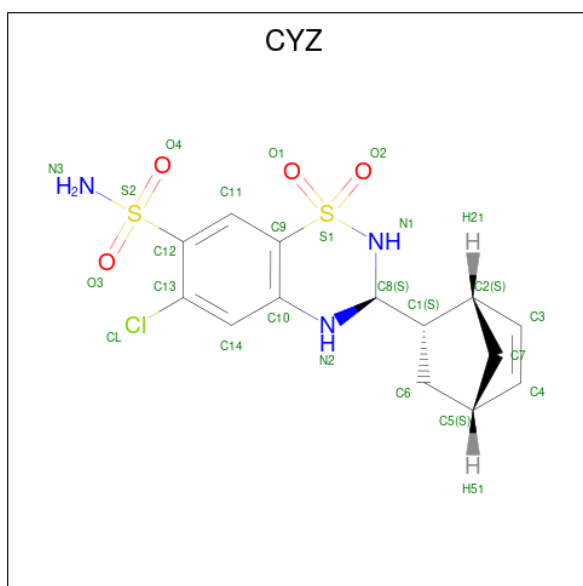
Chain	Residue	Modelled	Actual	Comment	Reference
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	999	GLY	-	linker	UNP P19491
B	1000	THR	-	linker	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP 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
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
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

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$) (labeled as "Ligand of Interest" by depositor).



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	

- Molecule 3 is CYCLOTHIAZIDE (CCD ID: CYZ) (formula: $C_{14}H_{16}ClN_3O_4S_2$) (labeled as "Ligand of Interest" by depositor).

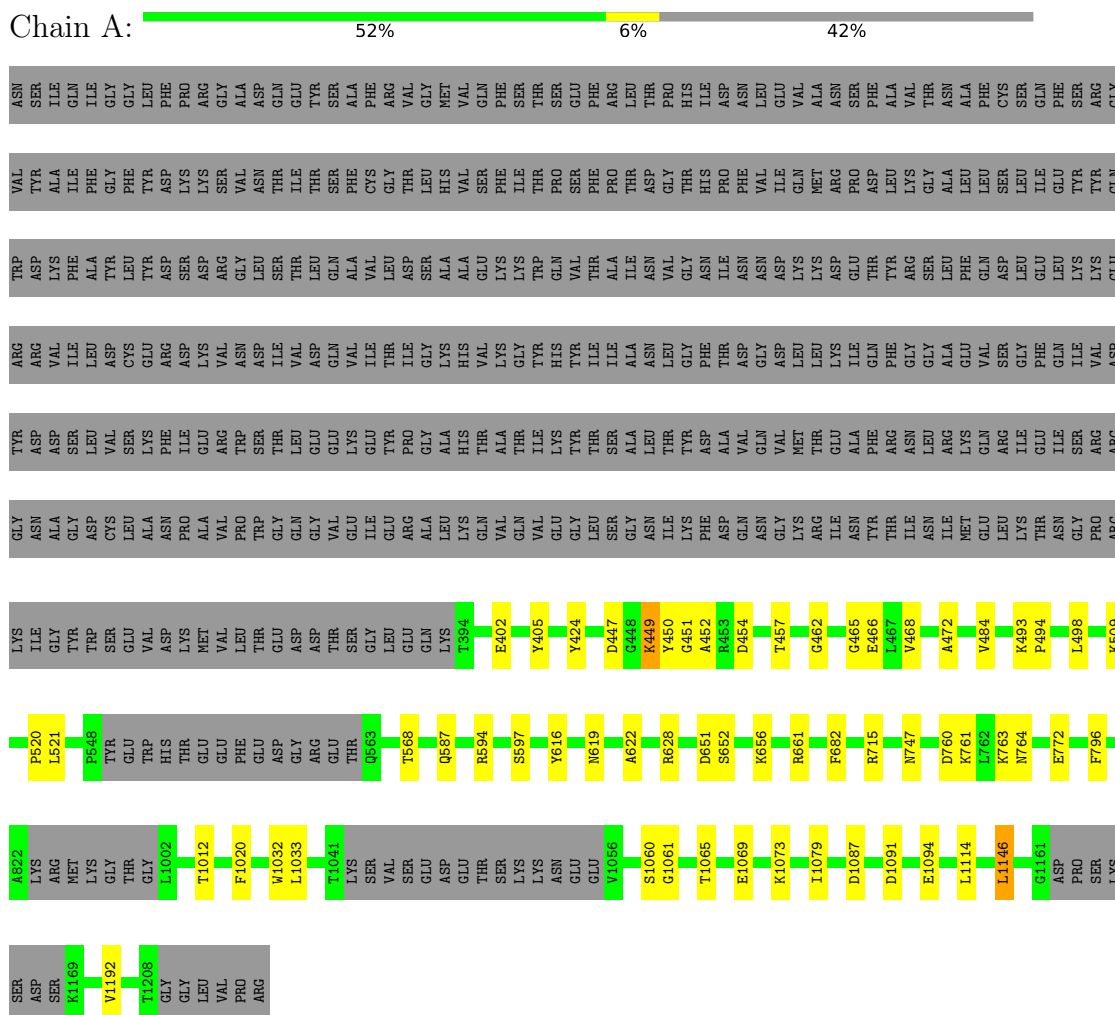


Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	0
3	B	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	0
3	C	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	0
3	D	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	0

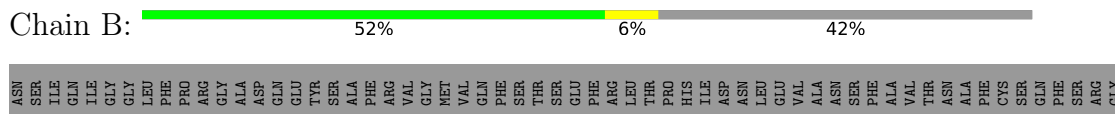
3 Residue-property plots

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. 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. 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.

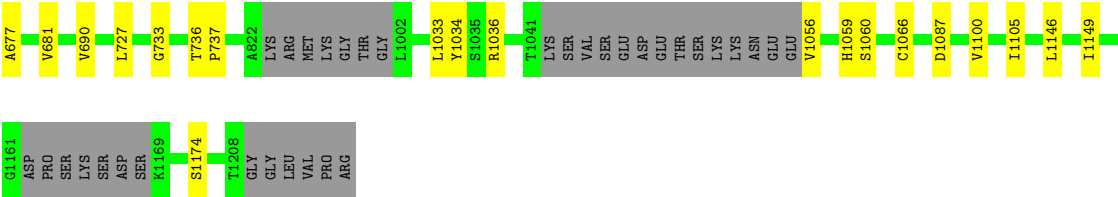
- Molecule 1: Isoform Flip of Glutamate receptor 2, Voltage-dependent calcium channel gamma-3 subunit chimera



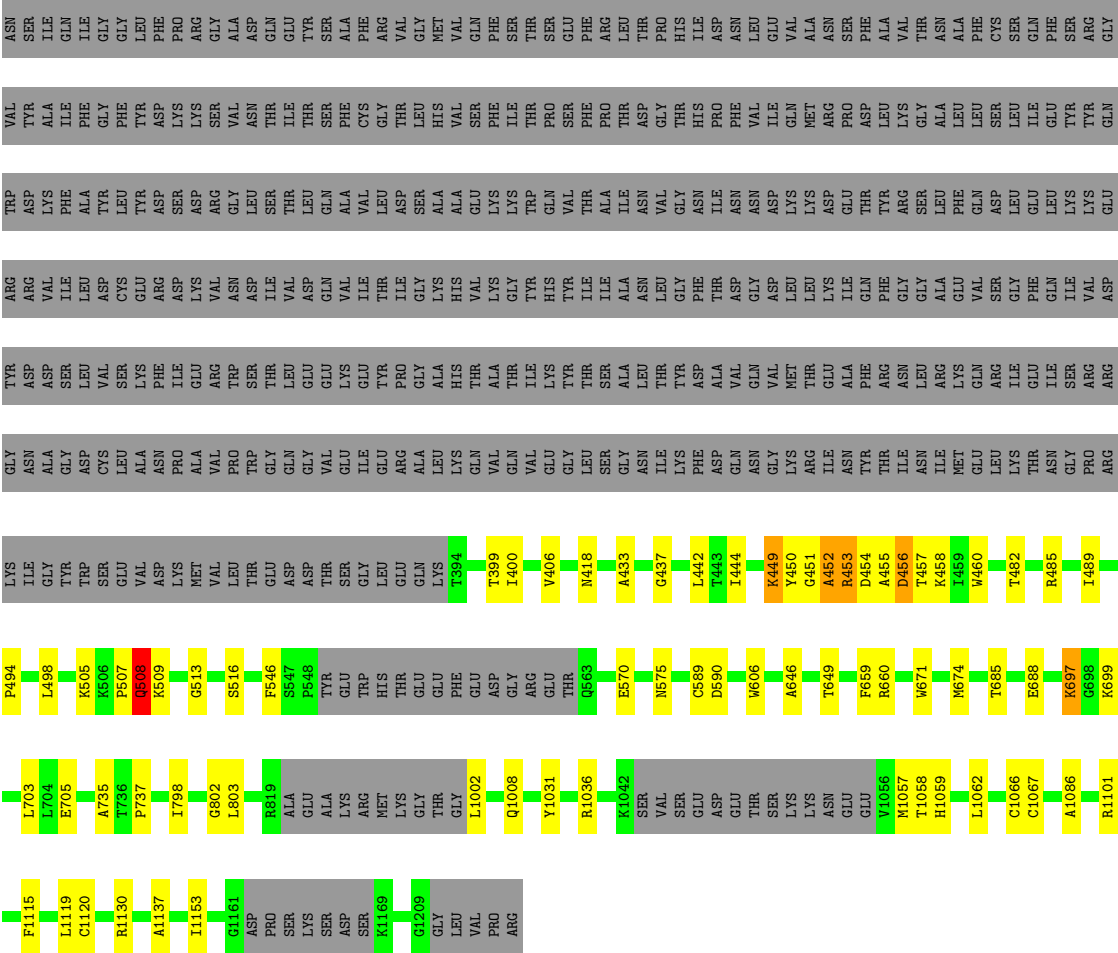
- Molecule 1: Isoform Flip of Glutamate receptor 2, Voltage-dependent calcium channel gamma-3 subunit chimera







● Molecule 1: Isoform Flip of Glutamate receptor 2,Voltage-dependent calcium channel gamma-3 subunit chimera



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51538	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	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: CYZ

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	0.21	0/4775	0.53	0/6445
1	B	0.20	0/4769	0.54	0/6436
1	C	0.24	0/4775	0.55	0/6445
1	D	0.23	0/4773	0.59	8/6440 (0.1%)
All	All	0.22	0/19092	0.55	8/25766 (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	D	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	507	PRO	CA-C-N	6.36	133.70	121.54
1	D	507	PRO	C-N-CA	6.36	133.70	121.54
1	D	508	GLN	CA-C-N	5.96	132.92	121.54
1	D	508	GLN	C-N-CA	5.96	132.92	121.54
1	D	1086	ALA	CA-C-N	5.38	131.82	121.54
1	D	1086	ALA	C-N-CA	5.38	131.82	121.54
1	D	1130	ARG	CA-C-N	5.01	129.44	122.08
1	D	1130	ARG	C-N-CA	5.01	129.44	122.08

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	508	GLN	Peptide

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	4673	0	4699	37	0
1	B	4667	0	4697	37	0
1	C	4673	0	4699	48	0
1	D	4671	0	4705	46	0
2	A	10	0	5	1	0
2	B	10	0	5	0	0
2	C	10	0	5	2	0
3	A	24	0	16	6	0
3	B	24	0	16	2	0
3	C	24	0	16	1	0
3	D	24	0	16	2	0
All	All	18810	0	18879	167	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 (167) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:760:ASP:OD1	3:B:1302:CYZ:CL	2.02	1.13
1:B:686:THR:HG21	1:B:708:MET:SD	2.06	0.95
1:D:453:ARG:HB2	1:D:460:TRP:CD2	2.05	0.92
1:A:447:ASP:OD2	1:A:449:LYS:HB2	1.72	0.88
1:C:460:TRP:HH2	1:C:484:VAL:HB	1.51	0.73
1:C:451:GLY:CA	1:C:462:GLY:HA3	2.22	0.69
1:C:454:ASP:HB3	1:C:458:LYS:H	1.59	0.68
1:A:494:PRO:O	3:A:1302:CYZ:H31A	1.94	0.67
1:C:454:ASP:OD2	1:C:457:THR:HB	1.95	0.66
1:C:453:ARG:HE	1:C:454:ASP:H	1.45	0.66
1:A:493:LYS:HG2	1:A:747:ASN:HD21	1.61	0.65
1:C:451:GLY:HA2	1:C:462:GLY:HA3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:TYR:CG	2:C:1301:GLU:HB3	2.32	0.64
1:D:453:ARG:HB2	1:D:460:TRP:CE3	2.33	0.64
1:C:1059:HIS:HB2	1:C:1066:CYS:HB2	1.78	0.64
1:C:450:TYR:CD2	2:C:1301:GLU:HB3	2.33	0.63
1:C:451:GLY:HA2	1:C:461:ASN:O	1.99	0.63
1:C:454:ASP:HB3	1:C:458:LYS:N	2.14	0.63
1:C:459:ILE:O	1:C:460:TRP:C	2.43	0.62
1:C:503:MET:HE1	1:C:690:VAL:HG22	1.82	0.62
1:D:455:ALA:O	1:D:456:ASP:C	2.43	0.61
1:C:661:ARG:HH12	1:C:663:LYS:HE2	1.64	0.61
1:D:453:ARG:HB3	1:D:453:ARG:HH11	1.65	0.61
1:D:453:ARG:HB2	1:D:460:TRP:CE2	2.36	0.61
3:D:1301:CYZ:CL	3:D:1301:CYZ:N3	2.69	0.60
1:C:1033:LEU:HB3	1:C:1060:SER:HB3	1.82	0.60
1:A:1087:ASP:H	1:B:697:LYS:HE2	1.65	0.60
1:D:1062:LEU:HA	1:D:1101:ARG:HH22	1.66	0.60
3:B:1302:CYZ:CL	3:B:1302:CYZ:N3	2.72	0.60
1:C:449:LYS:HD2	1:C:652:SER:HB3	1.84	0.60
3:A:1302:CYZ:N3	3:A:1302:CYZ:CL	2.72	0.60
1:C:1034:TYR:HB2	1:C:1174:SER:HB3	1.83	0.59
1:D:589:CYS:SG	1:D:590:ASP:N	2.76	0.59
1:D:451:GLY:O	1:D:452:ALA:HB2	2.03	0.59
1:D:659:PHE:HB3	1:D:671:TRP:HB2	1.85	0.59
1:C:445:VAL:HG22	1:C:447:ASP:H	1.69	0.58
1:C:460:TRP:H	1:C:460:TRP:CD1	2.21	0.57
1:D:1002:LEU:N	1:D:1008:GLN:OE1	2.37	0.57
1:A:715:ARG:NH2	1:A:772:GLU:OE1	2.38	0.56
1:C:474:ILE:HG22	1:C:736:THR:HG22	1.87	0.56
3:C:1302:CYZ:CL	3:C:1302:CYZ:O4	2.60	0.56
1:C:457:THR:O	1:C:458:LYS:HB2	2.05	0.55
1:A:509:LYS:HE2	1:A:628:ARG:HA	1.89	0.55
1:A:484:VAL:HG21	1:A:661:ARG:HH22	1.73	0.54
1:C:459:ILE:HG21	1:C:469:TYR:CE1	2.43	0.54
1:D:494:PRO:O	3:D:1301:CYZ:N1	2.41	0.54
1:B:475:ALA:HB3	1:B:735:ALA:HB3	1.89	0.54
1:B:1008:GLN:HB2	1:B:1195:LEU:HD21	1.90	0.53
1:A:1069:GLU:HA	1:A:1073:LYS:HE2	1.90	0.52
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.90	0.52
1:C:460:TRP:CH2	1:C:484:VAL:HB	2.40	0.52
1:D:570:GLU:O	1:D:575:ASN:ND2	2.41	0.52
1:A:763:LYS:HD3	3:A:1302:CYZ:H32	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:LYS:HG3	1:B:451:GLY:H	1.74	0.51
1:B:686:THR:CG2	1:B:708:MET:SD	2.89	0.51
1:D:798:ILE:O	1:D:802:GLY:N	2.43	0.51
1:B:788:SER:H	1:B:791:ASN:HD22	1.59	0.51
1:C:405:TYR:HE1	1:C:496:MET:HE1	1.74	0.51
1:A:520:PRO:HB3	1:A:619:ASN:HB3	1.91	0.51
1:C:453:ARG:HA	1:C:460:TRP:CE3	2.45	0.51
1:A:651:ASP:HB3	1:A:682:PHE:HB3	1.93	0.51
1:C:651:ASP:OD1	1:C:656:LYS:NZ	2.40	0.51
1:A:760:ASP:OD2	1:A:764:ASN:ND2	2.44	0.50
3:A:1302:CYZ:HN1	3:A:1302:CYZ:C3	2.23	0.50
1:B:401:LEU:HD23	1:B:444:ILE:HG21	1.92	0.50
1:C:500:ILE:HB	1:C:727:LEU:HB2	1.93	0.50
1:B:521:LEU:HD23	1:B:616:TYR:HD1	1.77	0.50
1:C:450:TYR:HE1	1:C:478:PRO:HG2	1.76	0.50
1:A:449:LYS:HG3	1:A:652:SER:HB2	1.94	0.49
1:A:465:GLY:HA2	1:A:468:VAL:HG12	1.93	0.49
1:A:1020:PHE:HD1	1:A:1114:LEU:HB3	1.75	0.49
1:D:1036:ARG:HH11	1:D:1057:MET:HB2	1.77	0.49
1:D:649:THR:HG23	1:D:674:MET:HE1	1.94	0.49
1:B:480:THR:HA	1:B:732:TYR:HA	1.94	0.49
1:C:1087:ASP:HB2	1:D:508:GLN:HE22	1.78	0.48
1:C:458:LYS:HA	1:C:458:LYS:HD2	1.63	0.48
1:D:406:VAL:HG11	1:D:444:ILE:HD11	1.96	0.48
1:C:536:VAL:HG22	1:D:803:LEU:HD21	1.94	0.48
1:B:714:GLN:O	1:B:773:CYS:N	2.43	0.48
1:A:761:LYS:HA	1:A:764:ASN:HB2	1.96	0.48
1:A:450:TYR:CD1	2:A:1301:GLU:HB3	2.50	0.47
1:B:1026:ALA:O	1:B:1032:TRP:NE1	2.45	0.47
1:A:451:GLY:HA2	1:A:462:GLY:HA3	1.96	0.47
1:A:597:SER:OG	1:B:806:ALA:O	2.31	0.47
1:A:451:GLY:O	1:A:452:ALA:HB2	2.14	0.47
1:B:498:LEU:HD12	1:B:705:GLU:HB3	1.95	0.47
1:B:639:LEU:O	1:B:647:TYR:OH	2.33	0.47
1:A:1146:LEU:HD12	1:B:800:VAL:HG13	1.96	0.47
1:C:619:ASN:HD22	1:C:622:ALA:HB3	1.80	0.47
1:A:1032:TRP:HB2	1:A:1061:GLY:HA2	1.96	0.47
1:C:455:ALA:C	1:C:457:THR:H	2.22	0.47
1:C:460:TRP:HB2	1:C:464:VAL:HB	1.97	0.47
1:B:569:ASN:HD22	1:B:570:GLU:H	1.63	0.46
1:D:449:LYS:HB3	1:D:449:LYS:HE2	1.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:489:ILE:HD12	1:D:735:ALA:HB1	1.98	0.46
1:B:1084:GLU:HG2	1:B:1088:TYR:HD1	1.79	0.46
1:C:520:PRO:HB3	1:C:619:ASN:HB3	1.96	0.46
1:D:1058:THR:HG22	1:D:1067:CYS:HA	1.96	0.46
1:D:660:ARG:HH21	1:D:671:TRP:HZ2	1.64	0.46
1:D:482:THR:OG1	1:D:485:ARG:NH1	2.47	0.46
1:D:1120:CYS:HB3	1:D:1137:ALA:HB2	1.98	0.46
1:A:568:THR:O	1:A:594:ARG:NH2	2.48	0.46
1:B:395:VAL:HG21	1:B:438:PHE:HB3	1.97	0.46
1:A:760:ASP:HA	3:A:1302:CYZ:CL	2.53	0.45
1:A:1065:THR:HB	1:A:1079:ILE:HD12	1.99	0.45
1:B:636:ALA:HA	1:B:639:LEU:HB2	1.98	0.45
1:B:1187:ILE:HG22	1:B:1191:MET:HE2	1.98	0.45
1:D:498:LEU:HD12	1:D:705:GLU:HB3	1.99	0.45
1:C:408:MET:HE2	1:C:412:HIS:HB2	1.98	0.44
1:C:459:ILE:H	1:C:459:ILE:HG13	1.48	0.44
1:B:452:ALA:H	1:B:461:ASN:H	1.62	0.44
1:B:489:ILE:HD12	1:B:735:ALA:HB1	1.99	0.44
1:B:1068:LEU:HA	1:B:1073:LYS:HG2	1.99	0.44
1:D:455:ALA:O	1:D:458:LYS:N	2.48	0.44
1:A:619:ASN:HD22	1:A:622:ALA:HB3	1.83	0.44
1:A:1033:LEU:HB3	1:A:1060:SER:HB3	2.00	0.44
1:B:1031:TYR:HA	1:B:1059:HIS:HB2	1.98	0.44
1:A:405:TYR:HA	1:A:424:TYR:HB3	2.00	0.43
1:B:542:LEU:HD21	1:B:1139:ILE:HG12	2.00	0.43
1:B:1109:LEU:HA	1:B:1112:ILE:HG12	1.99	0.43
1:C:481:ILE:HD11	1:C:733:GLY:HA3	2.00	0.43
1:B:399:THR:HB	1:B:406:VAL:HG21	2.00	0.43
1:D:399:THR:HG23	1:D:444:ILE:HD13	2.01	0.43
1:D:454:ASP:O	1:D:455:ALA:C	2.62	0.43
1:D:513:GLY:N	1:D:516:SER:OG	2.51	0.43
1:A:454:ASP:HB3	1:A:457:THR:HB	1.99	0.43
1:A:796:PHE:HB3	1:D:1153:ILE:HD13	1.99	0.43
1:A:587:GLN:HG3	1:D:606:TRP:CD1	2.54	0.43
3:A:1302:CYZ:C3	3:A:1302:CYZ:N1	2.81	0.43
1:B:706:SER:OG	1:B:726:ASN:OD1	2.36	0.43
1:B:418:ASN:HD22	1:B:441:LYS:HA	1.83	0.43
1:C:1100:VAL:HG13	1:C:1105:ILE:HG22	2.00	0.43
1:D:685:THR:HG23	1:D:688:GLU:H	1.83	0.43
1:D:453:ARG:HB3	1:D:453:ARG:NH1	2.33	0.43
1:A:651:ASP:HA	1:A:656:LYS:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:GLU:HG2	1:A:472:ALA:HB2	2.02	0.42
1:C:449:LYS:HD2	1:C:652:SER:CB	2.50	0.42
1:D:546:PHE:HD1	1:D:546:PHE:HA	1.79	0.42
1:D:646:ALA:N	1:D:699:LYS:O	2.47	0.42
1:B:645:ILE:HG22	1:B:699:LYS:HA	2.02	0.42
1:A:521:LEU:HD13	1:A:616:TYR:HD1	1.84	0.42
1:C:521:LEU:HD12	1:C:525:ILE:HG21	2.01	0.42
1:D:418:ASN:OD1	1:D:442:LEU:N	2.51	0.42
1:D:1059:HIS:CE1	1:D:1066:CYS:HB2	2.54	0.42
1:B:533:TYR:OH	1:B:577:LEU:O	2.37	0.41
1:B:1032:TRP:HA	1:B:1178:SER:HB3	2.01	0.41
1:D:433:ALA:O	1:D:437:GLY:N	2.51	0.41
1:A:1012:THR:HG23	1:A:1192:VAL:HG13	2.01	0.41
1:B:474:ILE:HG13	1:B:736:THR:HG22	2.01	0.41
1:C:637:GLU:HG2	1:C:666:VAL:HG21	2.02	0.41
1:C:1146:LEU:HA	1:C:1149:ILE:HG22	2.02	0.41
1:D:1115:PHE:O	1:D:1119:LEU:N	2.48	0.41
1:D:489:ILE:HG22	1:D:737:PRO:HA	2.02	0.41
1:A:402:GLU:HG2	1:A:450:TYR:OH	2.20	0.41
1:C:677:ALA:HB1	1:C:681:VAL:HG13	2.02	0.41
1:C:1036:ARG:HH21	1:C:1056:VAL:HB	1.86	0.41
1:D:400:ILE:HD12	1:D:449:LYS:O	2.21	0.41
1:A:1091:ASP:HB2	1:A:1094:GLU:HB3	2.03	0.41
1:B:1088:TYR:HB2	1:B:1091:ASP:HB2	2.02	0.41
1:D:455:ALA:O	1:D:457:THR:N	2.54	0.41
1:C:492:SER:OG	1:C:493:LYS:N	2.54	0.40
1:B:681:VAL:HA	1:B:692:ARG:HH12	1.85	0.40
1:D:453:ARG:HA	1:D:460:TRP:HA	2.03	0.40
1:D:1031:TYR:HA	1:D:1059:HIS:HB2	2.02	0.40
1:C:489:ILE:HG22	1:C:737:PRO:HA	2.03	0.40
1:C:406:VAL:HG22	1:C:426:VAL:HG23	2.04	0.40
1:D:505:LYS:HE2	1:D:697:LYS:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	591/1033 (57%)	570 (96%)	21 (4%)	0	100	100
1	B	590/1033 (57%)	576 (98%)	14 (2%)	0	100	100
1	C	591/1033 (57%)	564 (95%)	26 (4%)	1 (0%)	43	75
1	D	590/1033 (57%)	561 (95%)	26 (4%)	3 (0%)	24	60
All	All	2362/4132 (57%)	2271 (96%)	87 (4%)	4 (0%)	44	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	452	ALA
1	D	509	LYS
1	C	460	TRP
1	D	456	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	500/876 (57%)	497 (99%)	3 (1%)	78	81
1	B	500/876 (57%)	499 (100%)	1 (0%)	87	87
1	C	500/876 (57%)	495 (99%)	5 (1%)	68	76
1	D	501/876 (57%)	497 (99%)	4 (1%)	73	78
All	All	2001/3504 (57%)	1988 (99%)	13 (1%)	76	81

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	449	LYS
1	A	498	LEU

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Mol	Chain	Res	Type
1	A	1146	LEU
1	B	569	ASN
1	C	453	ARG
1	C	457	THR
1	C	458	LYS
1	C	459	ILE
1	C	626	VAL
1	D	449	LYS
1	D	450	TYR
1	D	453	ARG
1	D	697	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	435	HIS
1	A	587	GLN
1	A	619	ASN
1	A	747	ASN
1	A	1132	ASN
1	A	1204	HIS
1	B	508	GLN
1	B	569	ASN
1	B	587	GLN
1	B	791	ASN
1	B	1131	HIS
1	B	1132	ASN
1	C	619	ASN
1	C	1078	GLN
1	D	508	GLN
1	D	791	ASN
1	D	1008	GLN
1	D	1132	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	A	1301	-	8,9,9	1.11	1 (12%)	8,11,11	1.23	1 (12%)
2	GLU	B	1301	-	8,9,9	1.09	1 (12%)	8,11,11	1.23	1 (12%)
3	CYZ	B	1302	-	26,27,27	0.48	0	38,44,44	0.51	0
3	CYZ	A	1302	-	26,27,27	0.52	0	38,44,44	0.61	1 (2%)
3	CYZ	D	1301	-	26,27,27	0.50	0	38,44,44	0.57	0
3	CYZ	C	1302	-	26,27,27	0.48	0	38,44,44	0.52	1 (2%)
2	GLU	C	1301	-	8,9,9	1.09	1 (12%)	8,11,11	1.21	1 (12%)

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	A	1301	-	-	2/9/9/9	-
2	GLU	B	1301	-	-	2/9/9/9	-
3	CYZ	B	1302	-	-	7/7/42/42	0/5/4/4
3	CYZ	A	1302	-	-	6/7/42/42	0/5/4/4
3	CYZ	D	1301	-	-	6/7/42/42	0/5/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYZ	C	1302	-	-	7/7/42/42	0/5/4/4
2	GLU	C	1301	-	-	2/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	GLU	OXT-C	-2.30	1.23	1.30
2	C	1301	GLU	OXT-C	-2.27	1.23	1.30
2	B	1301	GLU	OXT-C	-2.23	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	GLU	OXT-C-O	-2.86	117.59	124.08
2	B	1301	GLU	OXT-C-O	-2.77	117.79	124.08
2	C	1301	GLU	OXT-C-O	-2.70	117.95	124.08
3	A	1302	CYZ	C2-C1-C8	2.57	118.57	114.88
3	C	1302	CYZ	C2-C1-C8	2.00	117.75	114.88

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1301	GLU	O-C-CA-N
3	A	1302	CYZ	C11-C12-S2-N3
3	A	1302	CYZ	C13-C12-S2-O3
3	A	1302	CYZ	C13-C12-S2-N3
3	B	1302	CYZ	C6-C1-C8-N2
3	B	1302	CYZ	C11-C12-S2-N3
3	B	1302	CYZ	C13-C12-S2-O3
3	B	1302	CYZ	C13-C12-S2-N3
3	C	1302	CYZ	C6-C1-C8-N2
3	C	1302	CYZ	C11-C12-S2-O3
3	C	1302	CYZ	C11-C12-S2-O4
3	C	1302	CYZ	C11-C12-S2-N3
3	C	1302	CYZ	C13-C12-S2-O3
3	C	1302	CYZ	C13-C12-S2-O4
3	C	1302	CYZ	C13-C12-S2-N3
3	D	1301	CYZ	C11-C12-S2-O3
3	D	1301	CYZ	C11-C12-S2-O4
3	D	1301	CYZ	C11-C12-S2-N3

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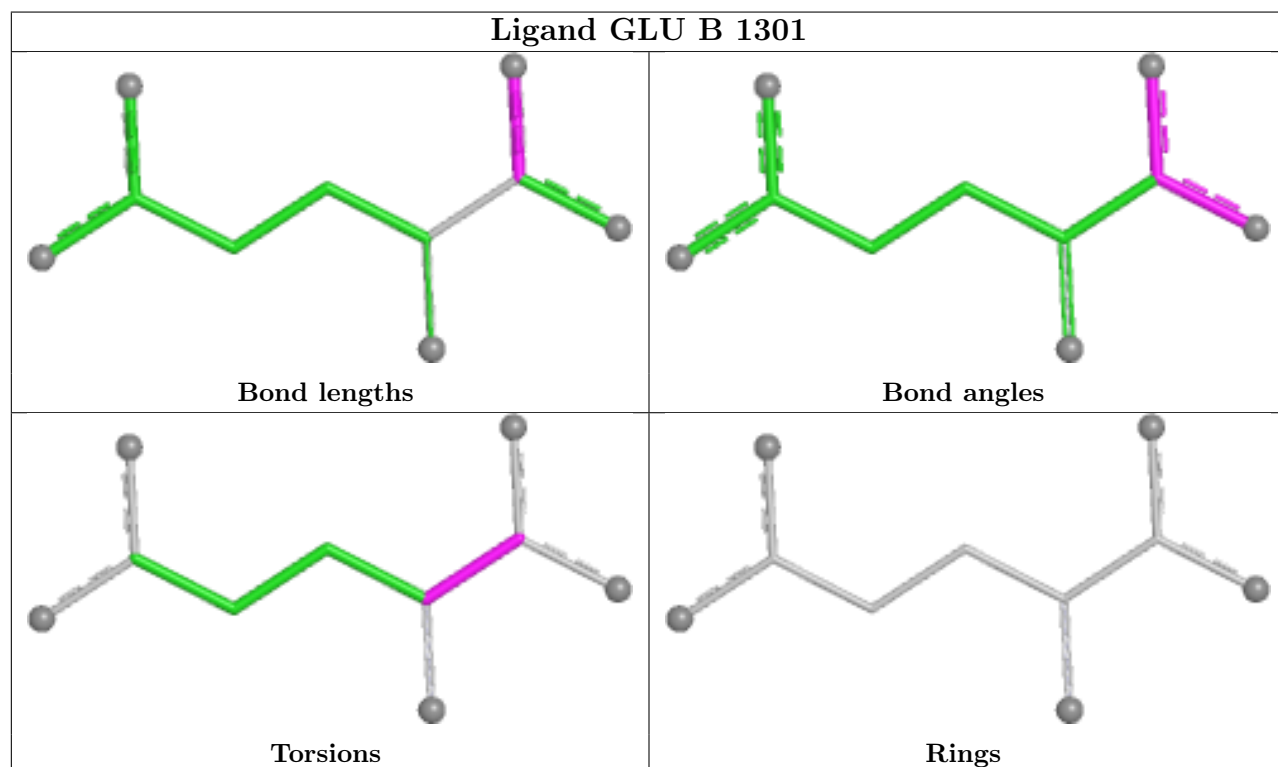
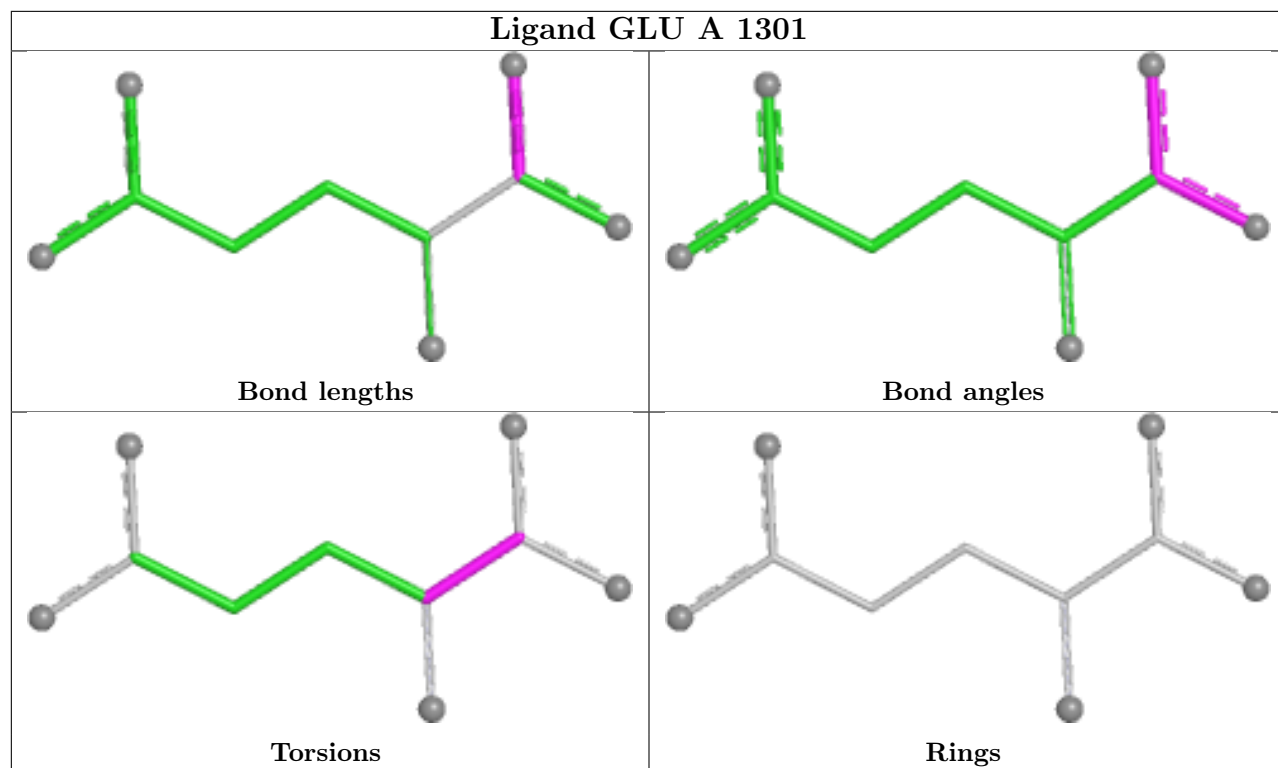
Mol	Chain	Res	Type	Atoms
3	D	1301	CYZ	C13-C12-S2-O3
3	D	1301	CYZ	C13-C12-S2-O4
3	D	1301	CYZ	C13-C12-S2-N3
3	A	1302	CYZ	C11-C12-S2-O3
3	B	1302	CYZ	C11-C12-S2-O3
2	B	1301	GLU	OXT-C-CA-N
3	A	1302	CYZ	C11-C12-S2-O4
3	B	1302	CYZ	C11-C12-S2-O4
3	A	1302	CYZ	C13-C12-S2-O4
3	B	1302	CYZ	C13-C12-S2-O4
2	C	1301	GLU	OXT-C-CA-N
2	C	1301	GLU	O-C-CA-N
2	A	1301	GLU	OXT-C-CA-N
2	A	1301	GLU	O-C-CA-N

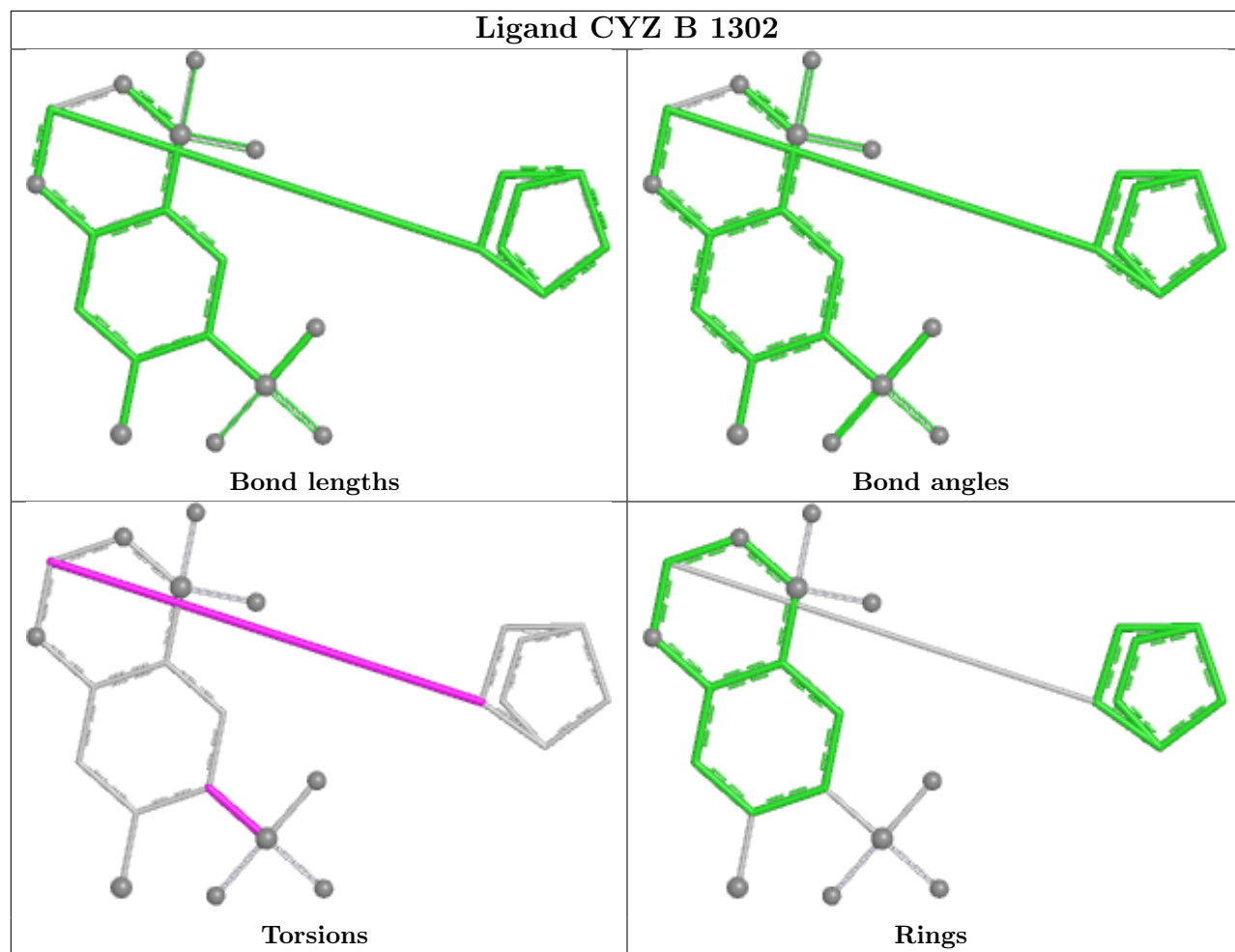
There are no ring outliers.

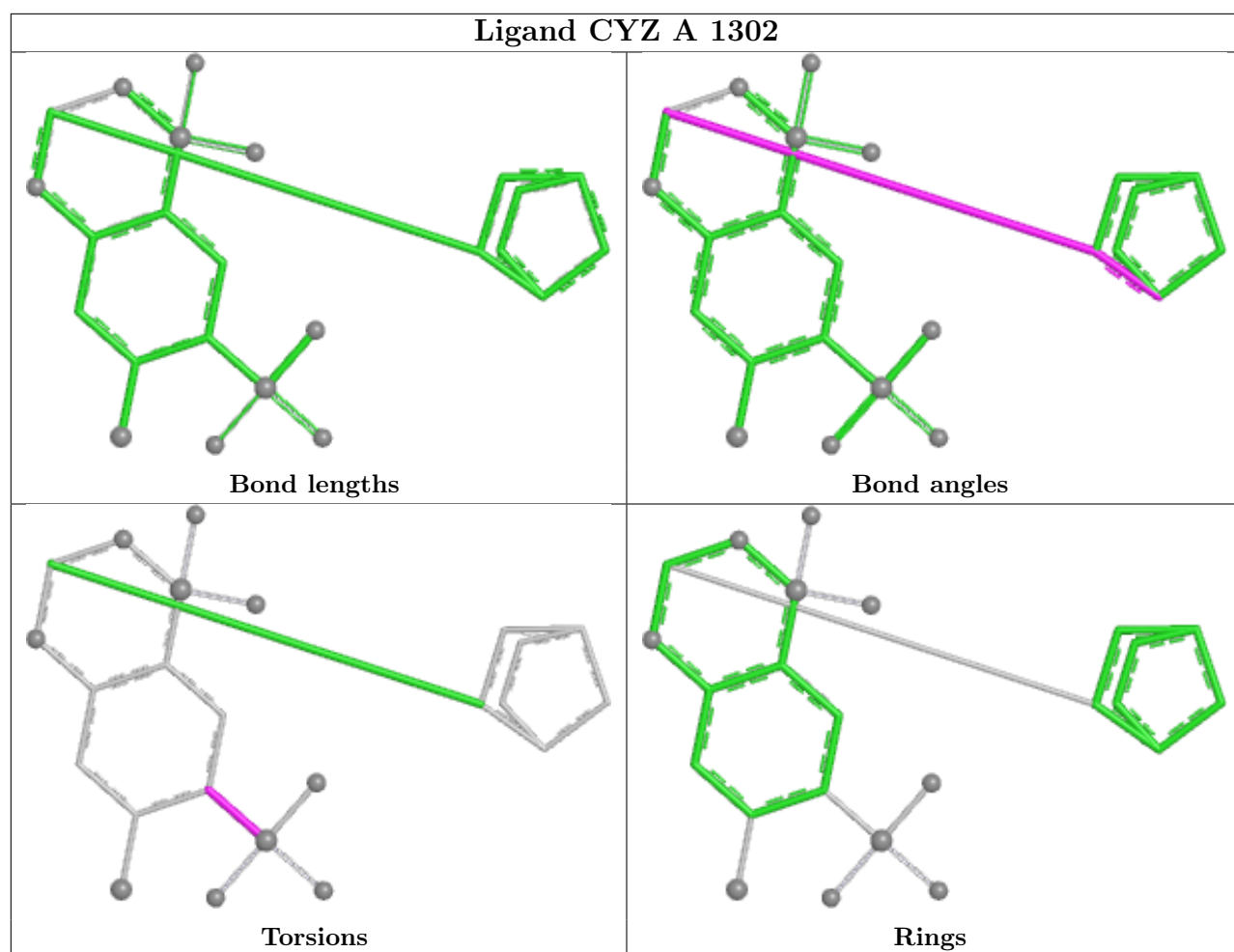
6 monomers are involved in 14 short contacts:

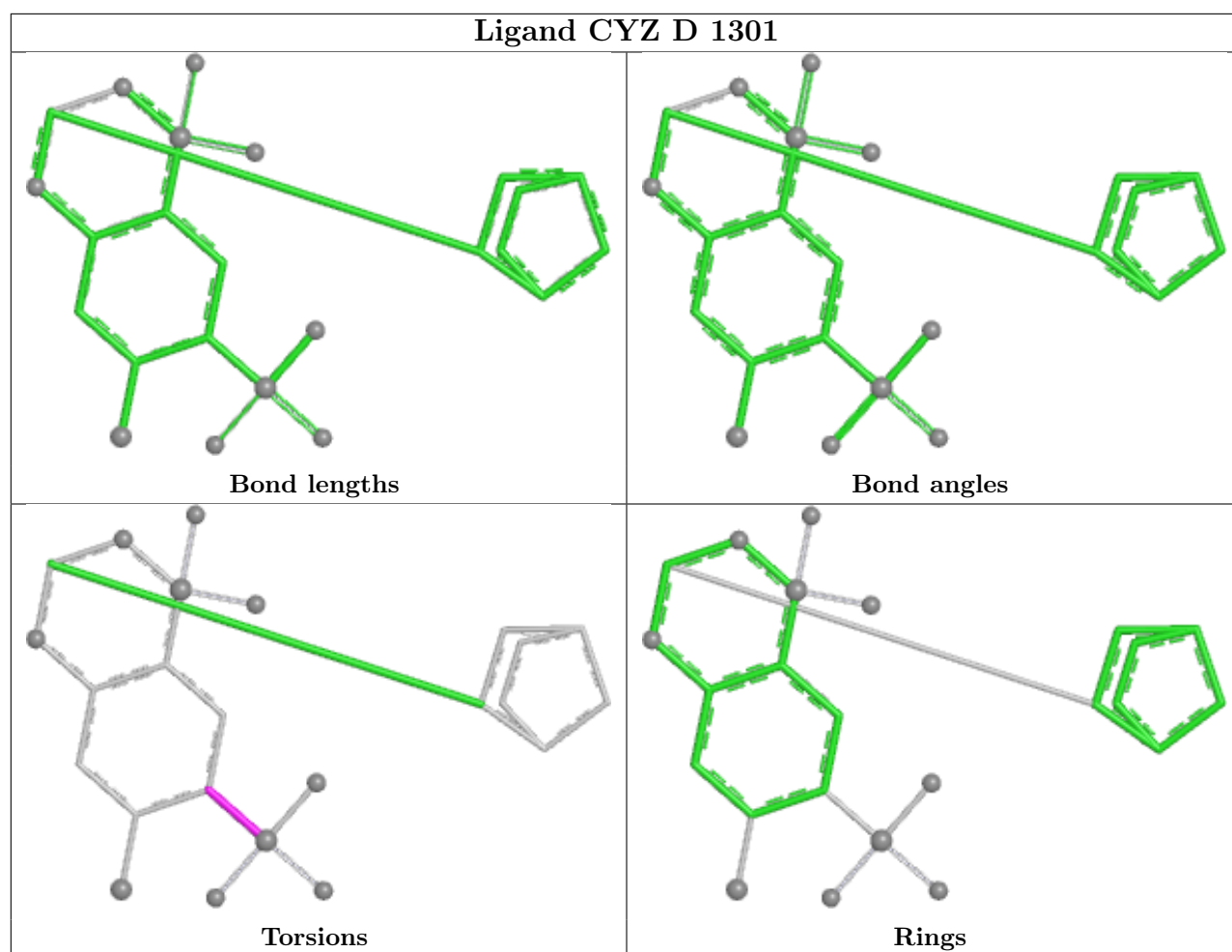
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	GLU	1	0
3	B	1302	CYZ	2	0
3	A	1302	CYZ	6	0
3	D	1301	CYZ	2	0
3	C	1302	CYZ	1	0
2	C	1301	GLU	2	0

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

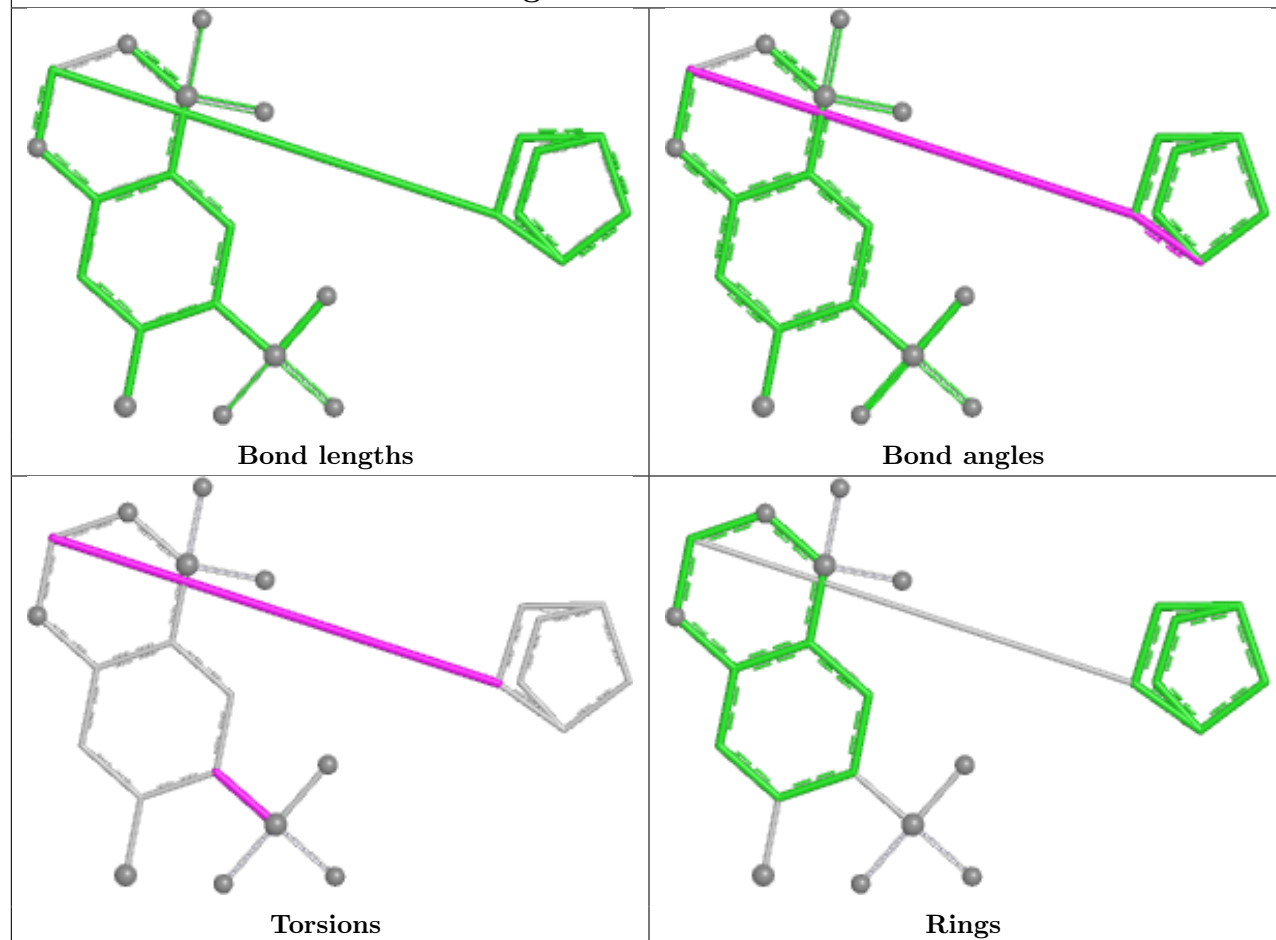




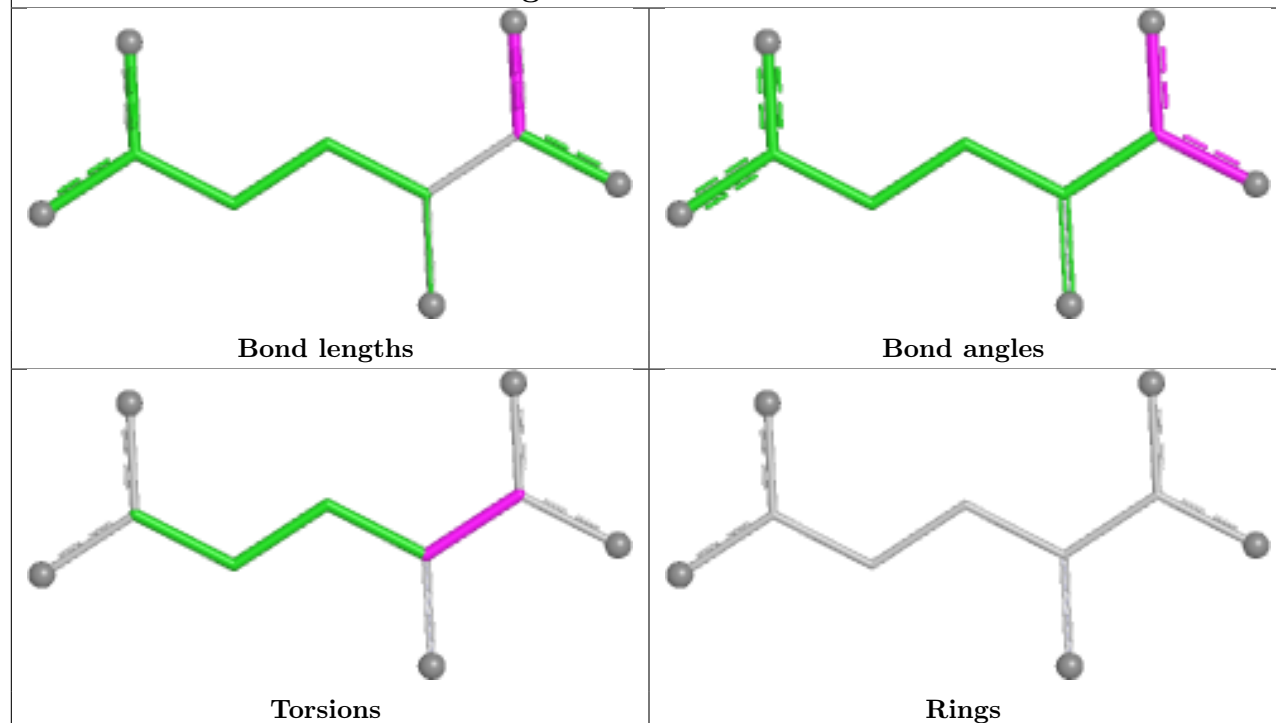




Ligand CYZ C 1302



Ligand GLU C 1301



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26016. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.