



## Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 09:04 PM EDT

PDB ID : 8FQG  
EMDB ID : EMD-29387  
Title : LBD conformation 1 (LBDconf1) of GluA2 flip Q isoform of AMPA receptor in complex with gain-of-function TARP gamma-2, with 150mM NaCl, 330uM CTZ, and 100mM glutamate (Open-Na260)  
Authors : Nakagawa, T.  
Deposited on : 2023-01-06  
Resolution : 3.01 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

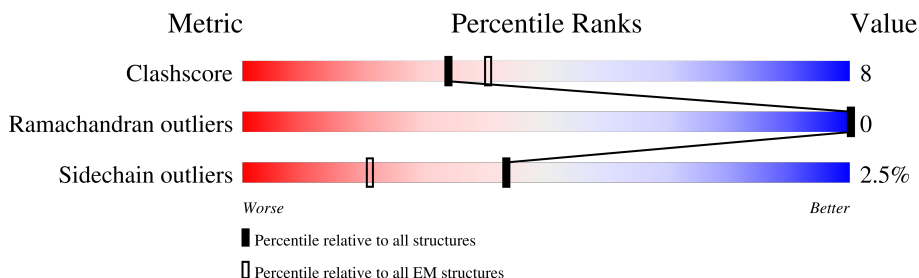
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.01 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	889	
1	B	889	
1	C	889	
1	D	889	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8392 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	260	Total 2012	C 1282	N 333	O 384	S 13	0	0
1	B	270	Total 2111	C 1346	N 351	O 399	S 15	0	0
1	C	260	Total 2012	C 1282	N 333	O 384	S 13	0	0
1	D	270	Total 2111	C 1346	N 351	O 399	S 15	0	0

There are 28 discrepancies between the modelled and reference sequences:

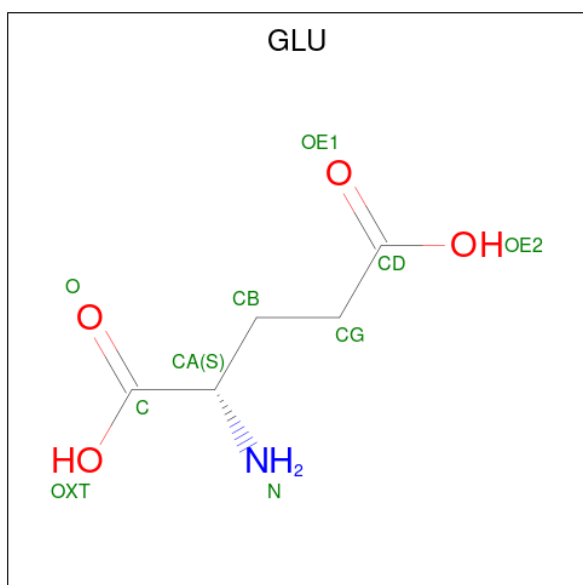
Chain	Residue	Modelled	Actual	Comment	Reference
A	848	ASP	TYR	engineered mutation	UNP P19491
A	849	TYR	-	insertion	UNP P19491
A	850	LYS	-	insertion	UNP P19491
A	851	ASP	-	insertion	UNP P19491
A	852	ASP	-	insertion	UNP P19491
A	853	ASP	-	insertion	UNP P19491
A	854	ASP	-	insertion	UNP P19491
B	848	ASP	TYR	engineered mutation	UNP P19491
B	849	TYR	-	insertion	UNP P19491
B	850	LYS	-	insertion	UNP P19491
B	851	ASP	-	insertion	UNP P19491
B	852	ASP	-	insertion	UNP P19491
B	853	ASP	-	insertion	UNP P19491
B	854	ASP	-	insertion	UNP P19491
C	848	ASP	TYR	engineered mutation	UNP P19491
C	849	TYR	-	insertion	UNP P19491
C	850	LYS	-	insertion	UNP P19491
C	851	ASP	-	insertion	UNP P19491
C	852	ASP	-	insertion	UNP P19491
C	853	ASP	-	insertion	UNP P19491
C	854	ASP	-	insertion	UNP P19491
D	848	ASP	TYR	engineered mutation	UNP P19491

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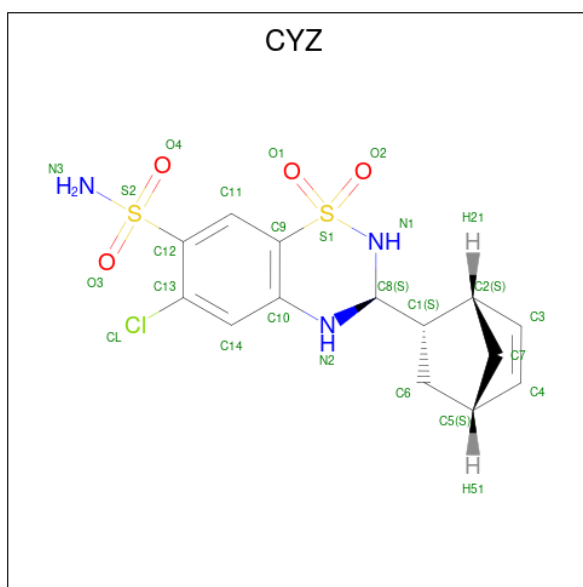
Chain	Residue	Modelled	Actual	Comment	Reference
D	849	TYR	-	insertion	UNP P19491
D	850	LYS	-	insertion	UNP P19491
D	851	ASP	-	insertion	UNP P19491
D	852	ASP	-	insertion	UNP P19491
D	853	ASP	-	insertion	UNP P19491
D	854	ASP	-	insertion	UNP P19491

- Molecule 2 is GLUTAMIC ACID (three-letter code: 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	
2	D	1	Total	C	N	O	0
			10	5	1	4	

- Molecule 3 is CYCLOTHIAZIDE (three-letter code: 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

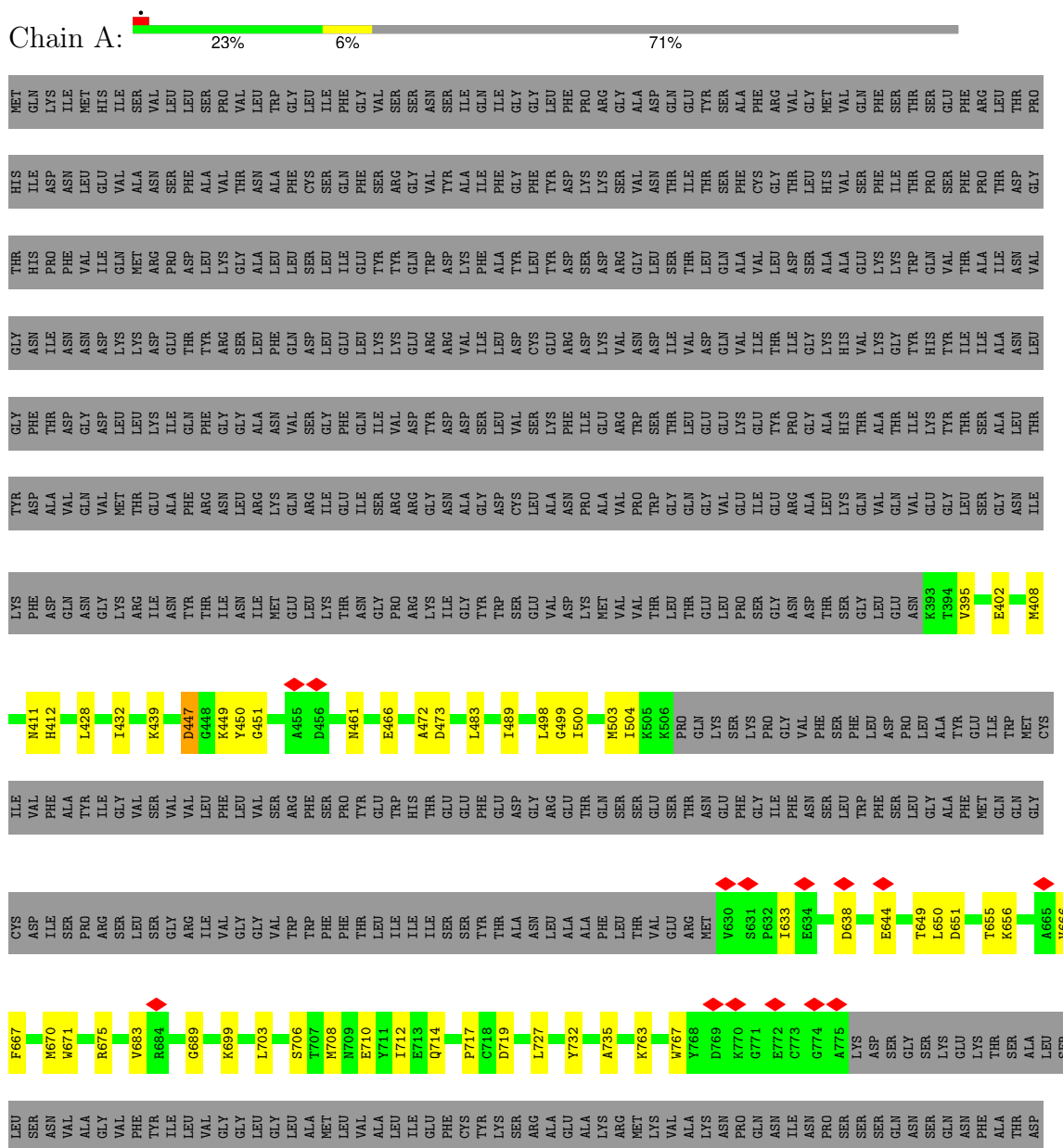
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	O	0
			1	1	
4	B	3	Total	O	0
			3	3	
4	C	2	Total	O	0
			2	2	
4	D	4	Total	O	0
			4	4	

### 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: Glutamate receptor 2



TYR  
LYS  
ASP  
ASP  
ASP  
ASP  
LYS  
GLU  
GLY  
TYR  
TYR  
VAL  
VAL  
GLY  
ILE  
SER  
SER  
VAL  
LYS  
ILE

● Molecule 1: Glutamate receptor 2



MET	GLN	LYS	ASP	ASP	ASP	ASP	LYS	GLU	GLY	TYR	TYR	VAL	VAL	GLY	ILE	SER	SER	VAL	LYS	ILE
HIS	ILE	ASP	ASN	ASN	ASP	LEU	MET	ILE	TLE	SER	VAL	ALA	ASN	LEU	LEU	LEU	LEU	VAL	PRO	VAL
THR	HIS	PRO	PHE	ASP	ASN	GLN	VAL	ILE	GLN	MET	GLN	VAL	LEU	TYR	GLY	THR	ALA	ASN	LEU	ALA
GLY	ASN	ILE	ASN	ASN	ASP	ASP	LYS	LYS	ASP	ASP	THR	ARG	THR	TYR	ARG	THR	GLN	LEU	LEU	GLY
GLY	PHE	THR	THR	GLY	ASP	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	THR
TYR	ASP	ALA	VAL	GLN	GLN	VAL	MET	THR	THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
LYS	PHE	ASP	GLN	GLN	GLY	ASP	LYS	ARG	ILE	ARG	ILE	THR	ASN	ILE	ILE	ILE	ILE	ILE	ILE	ILE
Y405	Y406	K409	T410	M411	H412	F413	M414	L415	F416	E422	C425	Y426	F438	K439	Y440	F441	L442	D447	D454	A455
Y456	W460	M463	V464	C465	D473	T474	A475	T476	A477	P478	E486	T489	D490	F491	L498	G499	I500	S501	I502	K505
Q508	P512																			
GLY	VAL	PHE	SER	PHE	ASP	PRO	ASP	LEU	LEU	TRP	ILE	TRP	ALA	TYR	GLN	MET	CYS	VAL	VAL	PHE
ILE	PHE	ASN	SER	TRP	PHE	SER	LEU	GLY	ALA	GLY	GLN	GLN	GLN	GLN	GLN	GLN	CYS	VAL	PHE	ALA
D638	L639	S640	K641	Q642	T643	E644	I645	T655	V683	G689	V690	K695	L703	S706	E710	Y711	I712	R715	D719	L727
K730	G731	Y732	A735	L751	K763	N764	K765	W766	W767	Y768	D769	K770	C773	GLY	ALA	PRO	LYS	ASP	GLY	GLY
THR	SER	ALA	LEU	SER	LEU	SER	ASN	VAL	GLY	TYR	ILE	ASN	ASN	ILE	ASN	ALA	GLN	ASN	ILE	ASN
ASN	PHE	ALA	THR	TYR	LYS	ASP	ASP	ASP	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY

● Molecule 1: Glutamate receptor 2



MET	GLN	LYS	ASP	ASP	ASP	ASP	LYS	GLU	GLY	TYR	TYR	VAL	VAL	GLY	ILE	SER	SER	VAL	PRO	VAL
HIS	ILE	ASN	ASN	LEU	LEU	VAL	VAL	VAL	VAL	THR	ASN	ASN	PHE	PHE	GLN	PHE	GLY	ARG	THR	PRO
THR	HIS	PRO	PHE	ASP	ASP	GLN	VAL	ILE	GLN	MET	GLN	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
GLY	ASN	ILE	ASN	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
THR	HIS	PRO	PHE	ASP	ASP	GLN	VAL	ILE	GLN	MET	GLN	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	314443	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 ( $e^-/\text{\AA}^2$ )	51	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.110	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0155	Depositor
Map size (Å)	295.2, 295.2, 295.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82000005, 0.82000005, 0.82000005	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	0.25	0/2048	0.47	0/2759
1	B	0.26	0/2149	0.48	0/2891
1	C	0.25	0/2048	0.46	0/2759
1	D	0.27	0/2149	0.48	0/2891
All	All	0.26	0/8394	0.47	0/11300

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2012	0	2021	29	0
1	B	2111	0	2150	43	0
1	C	2012	0	2021	35	0
1	D	2111	0	2150	30	0
2	A	10	0	5	1	0
2	B	10	0	5	0	0
2	C	10	0	5	0	0
2	D	10	0	5	0	0
3	A	24	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	16	0	0
3	C	24	0	16	1	0
3	D	24	0	16	0	0
4	A	1	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	4	0	0	0	0
All	All	8392	0	8426	134	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 8.

All (134) 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:638:ASP:HA	1:B:641:LYS:HE2	1.72	0.71
1:B:454:ASP:OD2	1:B:455:ALA:N	2.23	0.71
1:C:711:TYR:HA	1:C:714:GLN:HE21	1.55	0.70
1:D:475:ALA:HB3	1:D:735:ALA:HB3	1.74	0.69
1:A:650:LEU:HD23	2:A:1301:GLU:HG2	1.76	0.68
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.74	0.68
1:D:399:THR:HG21	1:D:406:VAL:HG21	1.77	0.66
1:B:475:ALA:HB3	1:B:735:ALA:HB3	1.77	0.66
1:D:638:ASP:HA	1:D:641:LYS:HE2	1.78	0.65
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.79	0.63
1:C:449:LYS:HD2	1:C:652:SER:HB3	1.81	0.62
1:C:485:ARG:HH12	1:C:654:SER:HB2	1.64	0.61
1:C:681:VAL:HA	1:C:692:ARG:HH22	1.66	0.61
1:C:763:LYS:O	1:C:767:TRP:HB2	2.01	0.60
1:A:763:LYS:O	1:A:767:TRP:HB2	2.02	0.59
1:A:651:ASP:HA	1:A:656:LYS:HE3	1.85	0.59
1:D:763:LYS:O	1:D:767:TRP:HB2	2.03	0.58
1:A:644:GLU:OE2	1:A:699:LYS:NZ	2.31	0.58
1:A:671:TRP:O	1:A:675:ARG:HG2	2.03	0.57
1:B:642:GLN:OE1	1:B:644:GLU:N	2.37	0.57
1:B:399:THR:HG23	1:B:477:ALA:HB2	1.87	0.56
1:B:633:ILE:HD11	1:B:642:GLN:HG2	1.87	0.56
1:B:395:VAL:HG23	1:B:473:ASP:HB2	1.88	0.56
1:C:500:ILE:HB	1:C:727:LEU:HB2	1.87	0.55
1:D:657:GLU:OE1	1:D:661:ARG:NH2	2.39	0.55
1:C:500:ILE:HD12	1:C:655:THR:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:763:LYS:O	1:B:767:TRP:HB2	2.07	0.54
1:A:708:MET:O	1:A:712:ILE:HG12	2.07	0.54
1:D:642:GLN:OE1	1:D:644:GLU:N	2.41	0.54
1:C:467:LEU:HD22	1:C:737:PRO:HD3	1.89	0.54
1:D:419:GLU:N	1:D:419:GLU:OE1	2.41	0.54
1:B:422:GLU:HA	1:B:426:VAL:HG21	1.90	0.54
1:D:422:GLU:HA	1:D:426:VAL:HG21	1.90	0.53
1:C:412:HIS:HA	1:C:415:LEU:HB2	1.89	0.53
1:A:466:GLU:HG2	1:A:472:ALA:HB2	1.90	0.53
1:D:657:GLU:OE2	1:D:660:ARG:NH2	2.39	0.53
1:D:669:LYS:HB3	1:D:669:LYS:NZ	2.24	0.53
1:C:640:SER:HB2	1:C:669:LYS:HD2	1.92	0.53
1:A:667:PHE:CE2	1:A:727:LEU:HD23	2.44	0.52
1:A:667:PHE:HE2	1:A:727:LEU:HD23	1.73	0.52
1:C:671:TRP:O	1:C:675:ARG:HG2	2.10	0.52
1:A:402:GLU:OE2	1:A:450:TYR:OH	2.24	0.52
1:B:500:ILE:HD13	1:B:655:THR:HG23	1.90	0.52
1:A:408:MET:O	1:A:412:HIS:ND1	2.44	0.51
1:B:405:TYR:HH	1:B:732:TYR:HE2	1.59	0.50
1:B:642:GLN:NE2	1:B:645:ILE:O	2.42	0.50
1:B:690:VAL:HG21	1:B:712:ILE:HD13	1.94	0.50
1:C:399:THR:HG23	1:C:444:ILE:HD13	1.94	0.49
1:C:404:PRO:HA	1:C:407:MET:SD	2.52	0.49
1:C:691:ALA:O	1:C:695:LYS:HG3	2.12	0.49
1:C:710:GLU:O	1:C:714:GLN:HG3	2.12	0.49
1:D:486:GLU:HG2	1:D:491:PHE:HD2	1.77	0.49
1:B:460:TRP:HB3	1:B:465:GLY:HA2	1.94	0.49
1:C:714:GLN:OE1	1:C:715:ARG:NH1	2.46	0.48
1:A:666:VAL:O	1:A:670:MET:HG3	2.13	0.48
1:B:399:THR:HA	1:B:463:MET:HE3	1.96	0.48
1:A:489:ILE:HD12	1:A:735:ALA:HB1	1.95	0.48
1:B:438:PHE:HE1	1:B:440:TYR:HB3	1.79	0.48
1:D:399:THR:CG2	1:D:406:VAL:HG21	2.43	0.48
1:C:412:HIS:HB2	1:C:420:ARG:HB2	1.95	0.48
1:D:463:MET:HE3	1:D:479:LEU:HD13	1.96	0.47
1:A:483:LEU:HD21	1:D:752:LYS:HG2	1.96	0.47
1:C:466:GLU:HG2	1:C:472:ALA:HB2	1.97	0.47
1:A:717:PRO:HG2	1:A:719:ASP:OD2	2.14	0.47
1:B:412:HIS:HA	1:B:415:LEU:HB2	1.97	0.47
1:A:504:ILE:HG21	1:A:633:ILE:HD11	1.96	0.46
1:A:447:ASP:OD1	1:A:449:LYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:GLU:O	1:A:714:GLN:HG2	2.15	0.46
1:B:765:LYS:HE3	1:B:766:TRP:NE1	2.30	0.46
1:A:499:GLY:O	1:A:706:SER:N	2.49	0.46
1:D:749:ALA:HA	1:D:752:LYS:HE3	1.98	0.46
1:B:505:LYS:NZ	1:B:719:ASP:OD2	2.39	0.46
1:B:399:THR:HG21	1:B:406:VAL:HG21	1.97	0.45
1:C:498:LEU:HD22	1:C:732:TYR:CZ	2.52	0.45
1:B:489:ILE:HD12	1:B:735:ALA:HB1	1.98	0.45
1:D:681:VAL:O	1:D:700:TYR:OH	2.29	0.45
1:C:485:ARG:HB3	1:C:491:PHE:HE2	1.82	0.45
1:C:409:LYS:HE2	1:C:422:GLU:HB3	1.99	0.44
1:D:489:ILE:HD12	1:D:735:ALA:HB1	1.99	0.44
1:A:500:ILE:HG12	1:A:655:THR:HG22	1.98	0.44
1:D:458:LYS:HA	1:D:458:LYS:HD3	1.79	0.44
1:C:485:ARG:NH1	1:C:654:SER:HB2	2.32	0.44
1:C:402:GLU:O	1:C:406:VAL:N	2.43	0.44
1:B:625:THR:O	1:B:625:THR:HG23	2.18	0.44
1:A:395:VAL:HG13	1:A:473:ASP:HB3	2.00	0.43
1:B:405:TYR:HB3	1:B:425:CYS:SG	2.58	0.43
1:B:498:LEU:HD22	1:B:732:TYR:CZ	2.52	0.43
1:B:751:LEU:HB2	1:C:483:LEU:HD13	2.00	0.43
1:C:490:ASP:OD1	1:C:738:LYS:HA	2.18	0.43
1:D:670:MET:O	1:D:674:MET:HG3	2.18	0.43
1:B:409:LYS:HG2	1:B:422:GLU:HG2	1.99	0.43
1:B:415:LEU:HD23	1:B:415:LEU:HA	1.85	0.43
1:D:498:LEU:HD22	1:D:732:TYR:CZ	2.53	0.43
1:D:633:ILE:HD11	1:D:642:GLN:HG2	2.00	0.43
1:D:433:ALA:HA	1:D:438:PHE:CE1	2.53	0.43
1:D:642:GLN:NE2	1:D:645:ILE:O	2.44	0.43
1:B:706:SER:O	1:B:710:GLU:HG3	2.19	0.43
1:C:464:VAL:HG21	1:C:485:ARG:HE	1.84	0.43
1:B:502:ILE:HG12	1:B:703:LEU:HD23	2.01	0.43
1:D:428:LEU:O	1:D:432:ILE:HG12	2.19	0.43
1:B:715:ARG:NH1	1:B:767:TRP:O	2.27	0.42
1:C:683:VAL:HG11	1:C:689:GLY:HA2	2.01	0.42
1:B:683:VAL:HG11	1:B:689:GLY:HA2	2.00	0.42
1:A:498:LEU:HD22	1:A:732:TYR:CZ	2.54	0.42
1:B:414:MET:H	1:B:414:MET:HG2	1.68	0.42
1:B:477:ALA:HB1	1:B:478:PRO:HD2	2.02	0.42
1:D:403:SER:HB3	1:D:711:TYR:CE2	2.55	0.42
1:C:765:LYS:HA	1:C:769:ASP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:MET:HE1	1:C:690:VAL:HG22	2.02	0.42
1:B:508:GLN:HA	1:B:508:GLN:OE1	2.20	0.42
1:B:502:ILE:HD13	1:B:639:LEU:HD22	2.01	0.41
1:D:427:ASP:OD1	1:D:427:ASP:N	2.54	0.41
1:A:683:VAL:HG11	1:A:689:GLY:HA2	2.01	0.41
1:C:647:TYR:HB3	1:C:701:ALA:HB3	2.02	0.41
1:A:633:ILE:O	1:A:638:ASP:HB2	2.21	0.41
1:B:486:GLU:HG2	1:B:491:PHE:HD2	1.85	0.41
1:D:462:GLY:O	1:D:466:GLU:HG3	2.20	0.41
1:B:486:GLU:OE2	1:C:493:LYS:NZ	2.45	0.41
1:D:412:HIS:HA	1:D:415:LEU:HB2	2.01	0.41
1:D:460:TRP:HB3	1:D:465:GLY:HA2	2.01	0.41
1:A:428:LEU:O	1:A:432:ILE:HG12	2.21	0.41
1:B:498:LEU:HD11	1:B:730:LYS:HB2	2.02	0.41
1:B:438:PHE:CE1	1:B:440:TYR:HB3	2.56	0.41
1:A:451:GLY:HA2	1:A:461:ASN:O	2.21	0.41
1:D:405:TYR:HB3	1:D:425:CYS:SG	2.61	0.41
1:A:500:ILE:HB	1:A:727:LEU:HB2	2.03	0.41
1:B:426:VAL:HG12	1:B:442:LEU:HD21	2.03	0.40
1:B:425:CYS:SG	1:B:477:ALA:HA	2.62	0.40
1:A:411:ASN:N	1:A:411:ASN:OD1	2.53	0.40
1:B:464:VAL:HG13	1:B:489:ILE:HD13	2.03	0.40
1:B:636:ALA:HB2	1:B:727:LEU:HD21	2.03	0.40
1:C:494:PRO:O	3:C:1302:CYZ:N1	2.55	0.40
1:C:395:VAL:HG13	1:C:473:ASP:HB3	2.04	0.40
1:C:742:LEU:HD23	1:C:742:LEU:HA	1.92	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	256/889 (29%)	251 (98%)	5 (2%)	0	100	100
1	B	266/889 (30%)	260 (98%)	6 (2%)	0	100	100
1	C	256/889 (29%)	248 (97%)	8 (3%)	0	100	100
1	D	266/889 (30%)	261 (98%)	5 (2%)	0	100	100
All	All	1044/3556 (29%)	1020 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	215/763 (28%)	212 (99%)	3 (1%)	62	83
1	B	230/763 (30%)	223 (97%)	7 (3%)	36	68
1	C	215/763 (28%)	213 (99%)	2 (1%)	75	89
1	D	230/763 (30%)	220 (96%)	10 (4%)	25	57
All	All	890/3052 (29%)	868 (98%)	22 (2%)	43	72

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	439	LYS
1	A	447	ASP
1	A	503	MET
1	B	401	LEU
1	B	447	ASP
1	B	629	MET
1	B	695	LYS
1	B	765	LYS
1	B	767	TRP
1	B	768	TYR
1	C	447	ASP
1	C	673	TYR
1	D	414	MET

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Mol	Chain	Res	Type
1	D	628	ARG
1	D	651	ASP
1	D	654	SER
1	D	696	SER
1	D	718	CYS
1	D	719	ASP
1	D	765	LYS
1	D	767	TRP
1	D	773	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

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](#)

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	$\# Z  > 2$
2	GLU	C	1301	-	8,9,9	1.12	1 (12%)	8,11,11	1.19	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CYZ	B	1302	-	26,27,27	7.84	20 (76%)	38,44,44	2.47	9 (23%)
2	GLU	D	1301	-	8,9,9	1.11	1 (12%)	8,11,11	1.16	1 (12%)
3	CYZ	C	1302	-	26,27,27	7.81	20 (76%)	38,44,44	2.45	9 (23%)
3	CYZ	D	1302	-	26,27,27	7.84	20 (76%)	38,44,44	2.46	9 (23%)
3	CYZ	A	1302	-	26,27,27	7.82	20 (76%)	38,44,44	2.44	9 (23%)
2	GLU	A	1301	-	8,9,9	1.11	1 (12%)	8,11,11	1.20	1 (12%)
2	GLU	B	1301	-	8,9,9	1.10	1 (12%)	8,11,11	1.17	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	C	1301	-	-	0/9/9/9	-
3	CYZ	B	1302	-	-	0/7/42/42	0/5/4/4
2	GLU	D	1301	-	-	3/9/9/9	-
3	CYZ	C	1302	-	-	0/7/42/42	0/5/4/4
3	CYZ	D	1302	-	-	0/7/42/42	0/5/4/4
3	CYZ	A	1302	-	-	0/7/42/42	0/5/4/4
2	GLU	A	1301	-	-	2/9/9/9	-
2	GLU	B	1301	-	-	3/9/9/9	-

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1302	CYZ	O2-S1	20.06	1.66	1.43
3	A	1302	CYZ	O2-S1	20.06	1.66	1.43
3	D	1302	CYZ	O2-S1	19.99	1.66	1.43
3	B	1302	CYZ	O2-S1	19.98	1.66	1.43
3	D	1302	CYZ	O1-S1	19.10	1.65	1.43
3	B	1302	CYZ	O1-S1	19.07	1.65	1.43
3	A	1302	CYZ	O1-S1	18.94	1.65	1.43
3	C	1302	CYZ	O1-S1	18.90	1.65	1.43
3	B	1302	CYZ	O3-S2	11.38	1.63	1.43
3	D	1302	CYZ	O3-S2	11.31	1.63	1.43
3	C	1302	CYZ	O3-S2	11.29	1.63	1.43
3	A	1302	CYZ	O3-S2	11.29	1.63	1.43
3	D	1302	CYZ	O4-S2	10.58	1.62	1.43
3	B	1302	CYZ	O4-S2	10.54	1.62	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1302	CYZ	O4-S2	10.48	1.62	1.43
3	C	1302	CYZ	O4-S2	10.48	1.62	1.43
3	D	1302	CYZ	C1-C8	10.33	1.63	1.53
3	A	1302	CYZ	C1-C8	10.29	1.63	1.53
3	B	1302	CYZ	C1-C8	10.27	1.63	1.53
3	C	1302	CYZ	C1-C8	10.23	1.63	1.53
3	B	1302	CYZ	C10-N2	9.09	1.55	1.39
3	A	1302	CYZ	C10-N2	8.98	1.55	1.39
3	B	1302	CYZ	C4-C3	8.97	1.58	1.32
3	D	1302	CYZ	C10-N2	8.96	1.55	1.39
3	D	1302	CYZ	C4-C3	8.96	1.58	1.32
3	C	1302	CYZ	C4-C3	8.93	1.58	1.32
3	A	1302	CYZ	C4-C3	8.93	1.58	1.32
3	C	1302	CYZ	C10-N2	8.91	1.55	1.39
3	D	1302	CYZ	C2-C1	-8.90	1.36	1.55
3	C	1302	CYZ	C2-C1	-8.85	1.36	1.55
3	B	1302	CYZ	C2-C1	-8.85	1.36	1.55
3	A	1302	CYZ	C2-C1	-8.85	1.36	1.55
3	B	1302	CYZ	C12-S2	6.19	1.85	1.77
3	D	1302	CYZ	C12-S2	6.17	1.85	1.77
3	A	1302	CYZ	C12-S2	6.14	1.85	1.77
3	C	1302	CYZ	C12-S2	6.13	1.85	1.77
3	B	1302	CYZ	C9-S1	-6.10	1.70	1.75
3	D	1302	CYZ	C9-S1	-6.10	1.70	1.75
3	C	1302	CYZ	C9-S1	-5.97	1.70	1.75
3	A	1302	CYZ	C9-S1	-5.93	1.70	1.75
3	A	1302	CYZ	S2-N3	5.51	1.71	1.60
3	D	1302	CYZ	S2-N3	5.50	1.71	1.60
3	C	1302	CYZ	S2-N3	5.48	1.71	1.60
3	B	1302	CYZ	S2-N3	5.47	1.71	1.60
3	A	1302	CYZ	C10-C9	-5.19	1.33	1.40
3	C	1302	CYZ	C10-C9	-5.15	1.33	1.40
3	D	1302	CYZ	C10-C9	-5.14	1.33	1.40
3	B	1302	CYZ	C10-C9	-5.13	1.33	1.40
3	B	1302	CYZ	C8-N2	5.09	1.52	1.46
3	C	1302	CYZ	C8-N2	5.07	1.52	1.46
3	D	1302	CYZ	C8-N2	4.98	1.52	1.46
3	A	1302	CYZ	C8-N2	4.97	1.52	1.46
3	B	1302	CYZ	C6-C1	-4.19	1.41	1.53
3	D	1302	CYZ	C6-C1	-4.19	1.41	1.53
3	C	1302	CYZ	C6-C1	-4.19	1.41	1.53
3	A	1302	CYZ	C6-C1	-4.17	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1302	CYZ	C11-C9	4.00	1.45	1.39
3	C	1302	CYZ	C11-C9	3.97	1.45	1.39
3	A	1302	CYZ	C7-C2	3.93	1.63	1.54
3	C	1302	CYZ	C7-C2	3.93	1.63	1.54
3	D	1302	CYZ	C11-C9	3.91	1.45	1.39
3	B	1302	CYZ	C11-C9	3.90	1.45	1.39
3	D	1302	CYZ	C7-C2	3.87	1.63	1.54
3	B	1302	CYZ	C7-C2	3.84	1.63	1.54
3	C	1302	CYZ	C6-C5	-3.35	1.33	1.52
3	D	1302	CYZ	C6-C5	-3.34	1.33	1.52
3	A	1302	CYZ	C6-C5	-3.34	1.33	1.52
3	B	1302	CYZ	C6-C5	-3.33	1.33	1.52
3	D	1302	CYZ	C2-C3	-2.93	1.43	1.51
3	B	1302	CYZ	C2-C3	-2.92	1.43	1.51
3	C	1302	CYZ	C2-C3	-2.92	1.43	1.51
3	A	1302	CYZ	C2-C3	-2.91	1.43	1.51
3	D	1302	CYZ	C7-C5	2.61	1.66	1.52
3	C	1302	CYZ	C7-C5	2.60	1.66	1.52
3	A	1302	CYZ	C7-C5	2.59	1.66	1.52
3	B	1302	CYZ	C7-C5	2.59	1.66	1.52
3	C	1302	CYZ	C13-CL	2.44	1.79	1.73
3	A	1302	CYZ	C13-CL	2.43	1.79	1.73
3	B	1302	CYZ	C13-CL	2.36	1.79	1.73
3	D	1302	CYZ	C13-CL	2.35	1.79	1.73
2	A	1301	GLU	OXT-C	-2.29	1.23	1.30
2	C	1301	GLU	OXT-C	-2.28	1.23	1.30
2	D	1301	GLU	OXT-C	-2.27	1.23	1.30
2	B	1301	GLU	OXT-C	-2.27	1.23	1.30

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1302	CYZ	O2-S1-O1	-6.48	111.84	118.44
3	A	1302	CYZ	O2-S1-O1	-6.43	111.90	118.44
3	D	1302	CYZ	C9-S1-N1	6.35	111.13	103.42
3	D	1302	CYZ	O2-S1-O1	-6.31	112.02	118.44
3	B	1302	CYZ	C9-S1-N1	6.28	111.05	103.42
3	C	1302	CYZ	C9-S1-N1	6.23	110.99	103.42
3	B	1302	CYZ	O2-S1-O1	-6.23	112.10	118.44
3	A	1302	CYZ	C9-S1-N1	6.20	110.96	103.42
3	C	1302	CYZ	O4-S2-O3	-6.09	109.44	118.80
3	A	1302	CYZ	O4-S2-O3	-6.05	109.49	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1302	CYZ	O4-S2-O3	-6.04	109.50	118.80
3	B	1302	CYZ	O4-S2-O3	-5.97	109.61	118.80
3	B	1302	CYZ	C2-C1-C8	-4.67	108.18	114.88
3	D	1302	CYZ	C2-C1-C8	-4.44	108.50	114.88
3	A	1302	CYZ	C2-C1-C8	-4.03	109.10	114.88
3	C	1302	CYZ	C2-C1-C8	-3.98	109.17	114.88
3	B	1302	CYZ	C6-C1-C2	3.91	110.41	104.04
3	D	1302	CYZ	C6-C1-C2	3.88	110.37	104.04
3	C	1302	CYZ	C6-C1-C2	3.88	110.37	104.04
3	A	1302	CYZ	C6-C1-C2	3.87	110.36	104.04
3	A	1302	CYZ	C1-C2-C3	3.86	112.82	106.86
3	C	1302	CYZ	C1-C2-C3	3.86	112.81	106.86
3	B	1302	CYZ	C1-C2-C3	3.82	112.75	106.86
3	D	1302	CYZ	C1-C2-C3	3.75	112.65	106.86
3	C	1302	CYZ	C7-C2-C1	-3.41	93.75	101.21
3	A	1302	CYZ	C7-C2-C1	-3.41	93.75	101.21
3	C	1302	CYZ	C13-C12-S2	-3.41	119.38	123.47
3	A	1302	CYZ	C13-C12-S2	-3.38	119.42	123.47
3	D	1302	CYZ	C7-C2-C1	-3.33	93.93	101.21
3	B	1302	CYZ	C7-C2-C1	-3.31	93.98	101.21
3	B	1302	CYZ	C12-C13-CL	-3.27	119.15	121.52
3	B	1302	CYZ	C13-C12-S2	-3.23	119.59	123.47
3	D	1302	CYZ	C13-C12-S2	-3.18	119.66	123.47
3	D	1302	CYZ	C12-C13-CL	-2.92	119.41	121.52
2	A	1301	GLU	OXT-C-O	-2.71	117.93	124.08
2	C	1301	GLU	OXT-C-O	-2.67	118.03	124.08
2	B	1301	GLU	OXT-C-O	-2.58	118.22	124.08
2	D	1301	GLU	OXT-C-O	-2.54	118.33	124.08
3	A	1302	CYZ	C12-C13-CL	-2.31	119.85	121.52
3	C	1302	CYZ	C12-C13-CL	-2.28	119.87	121.52

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1301	GLU	O-C-CA-CB
2	D	1301	GLU	O-C-CA-CB
2	B	1301	GLU	OXT-C-CA-CB
2	D	1301	GLU	OXT-C-CA-CB
2	A	1301	GLU	OE2-CD-CG-CB
2	B	1301	GLU	CA-CB-CG-CD
2	D	1301	GLU	CA-CB-CG-CD

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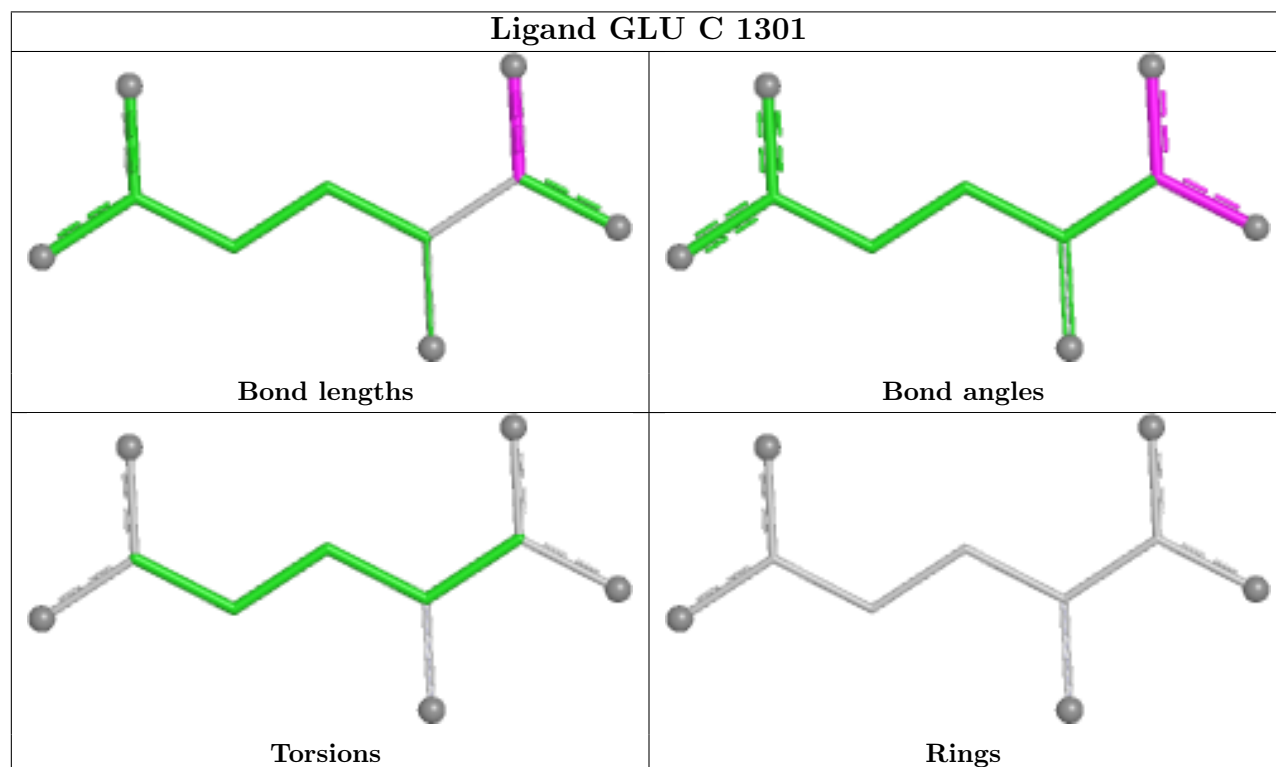
Mol	Chain	Res	Type	Atoms
2	A	1301	GLU	OE1-CD-CG-CB

There are no ring outliers.

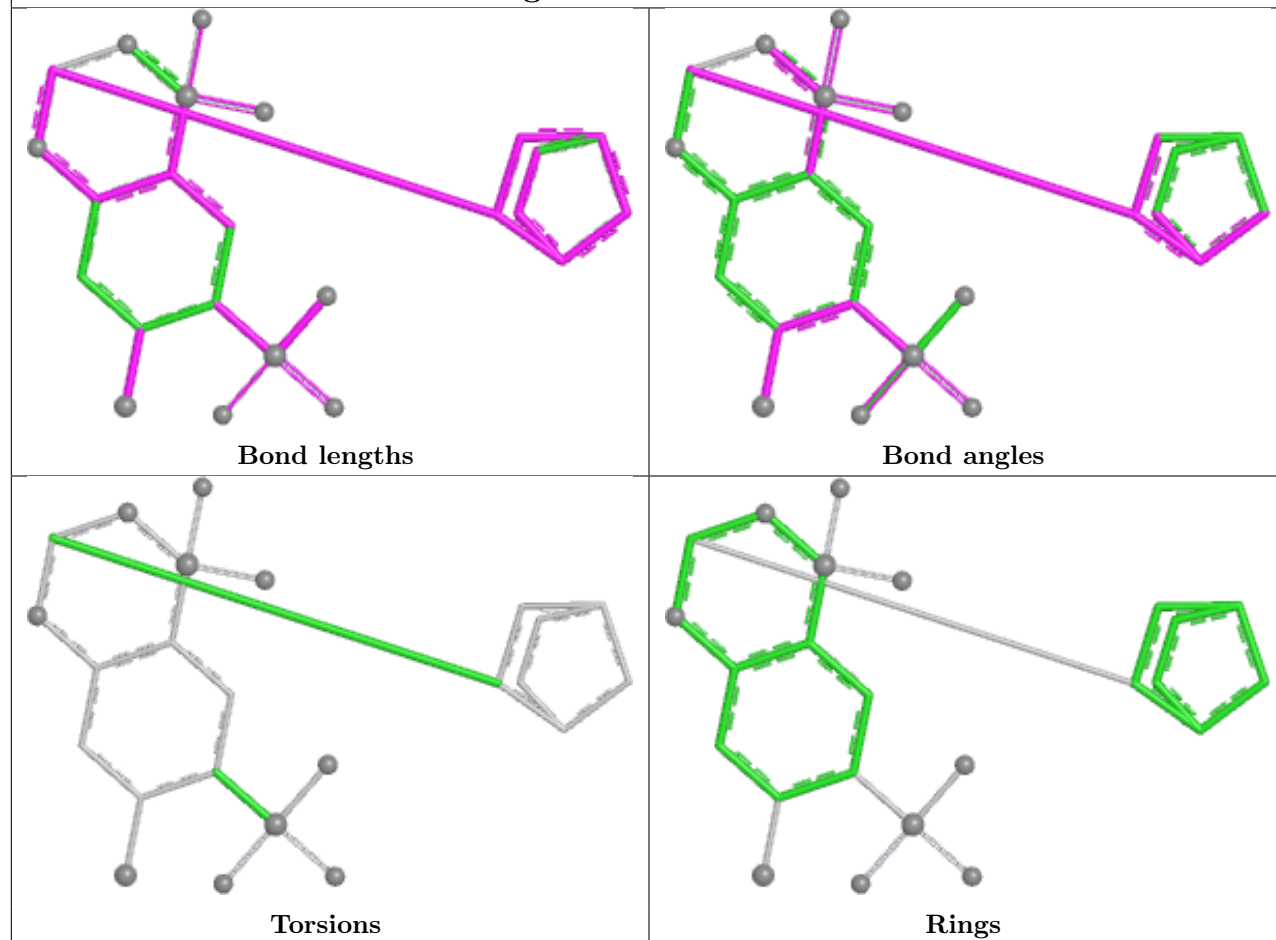
2 monomers are involved in 2 short contacts:

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

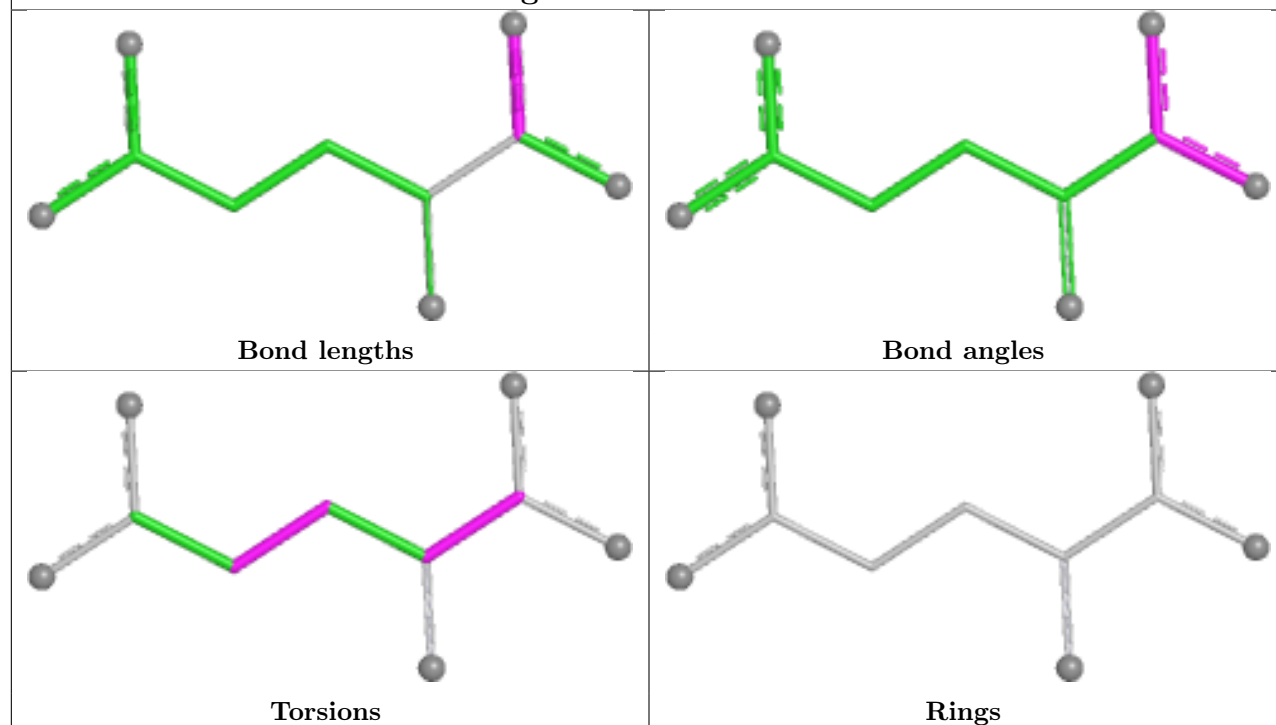
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

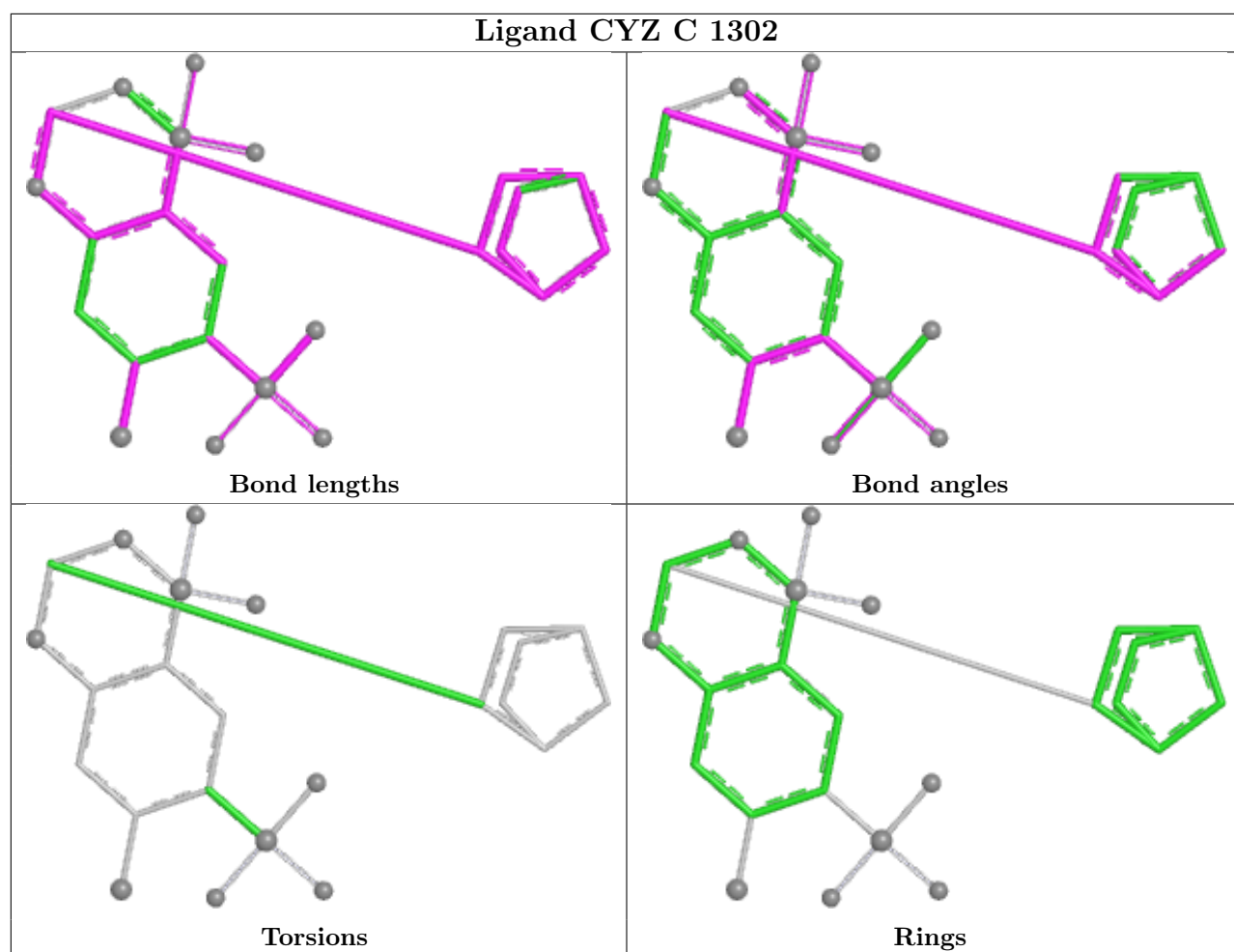


## Ligand CYZ B 1302

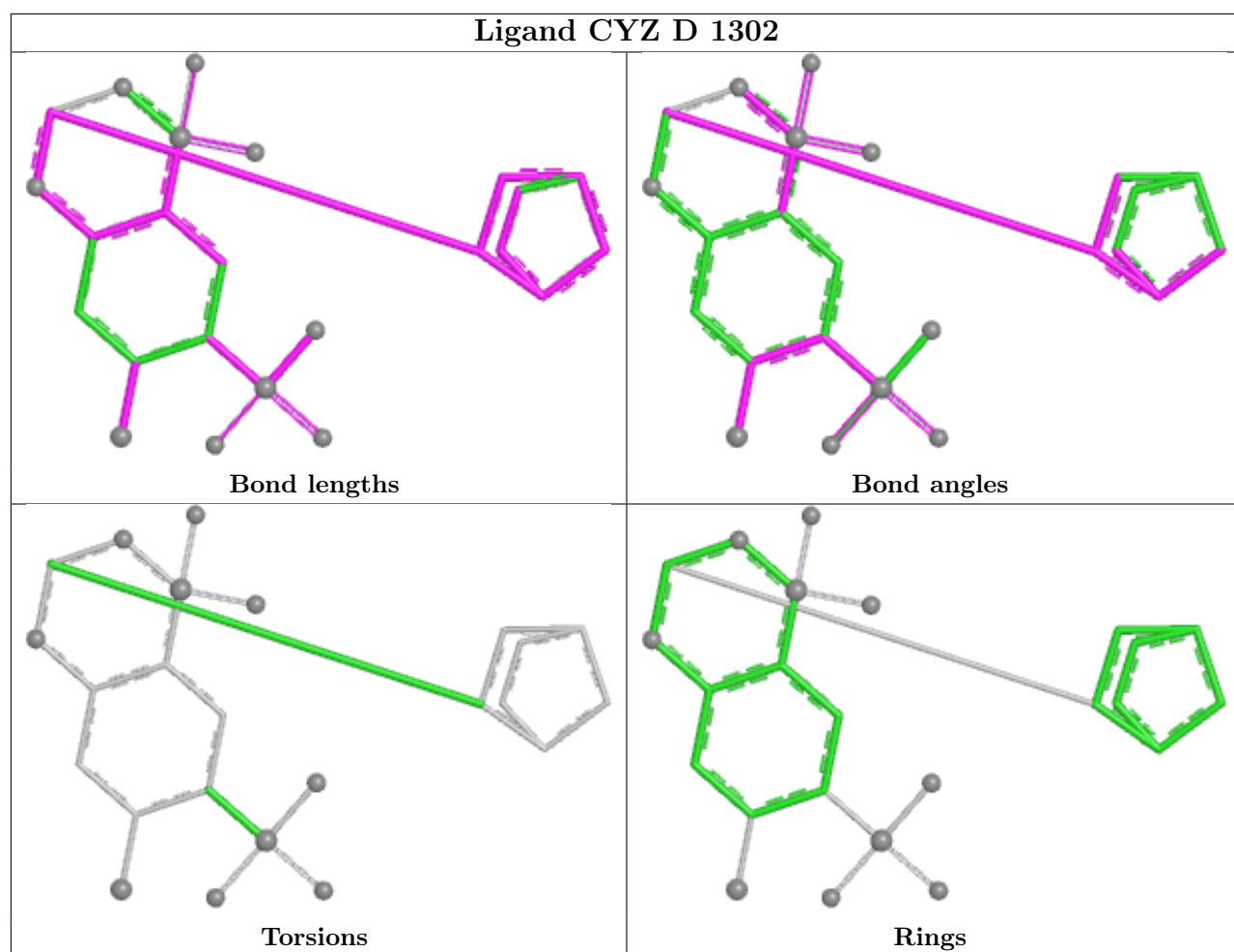


## Ligand GLU D 1301

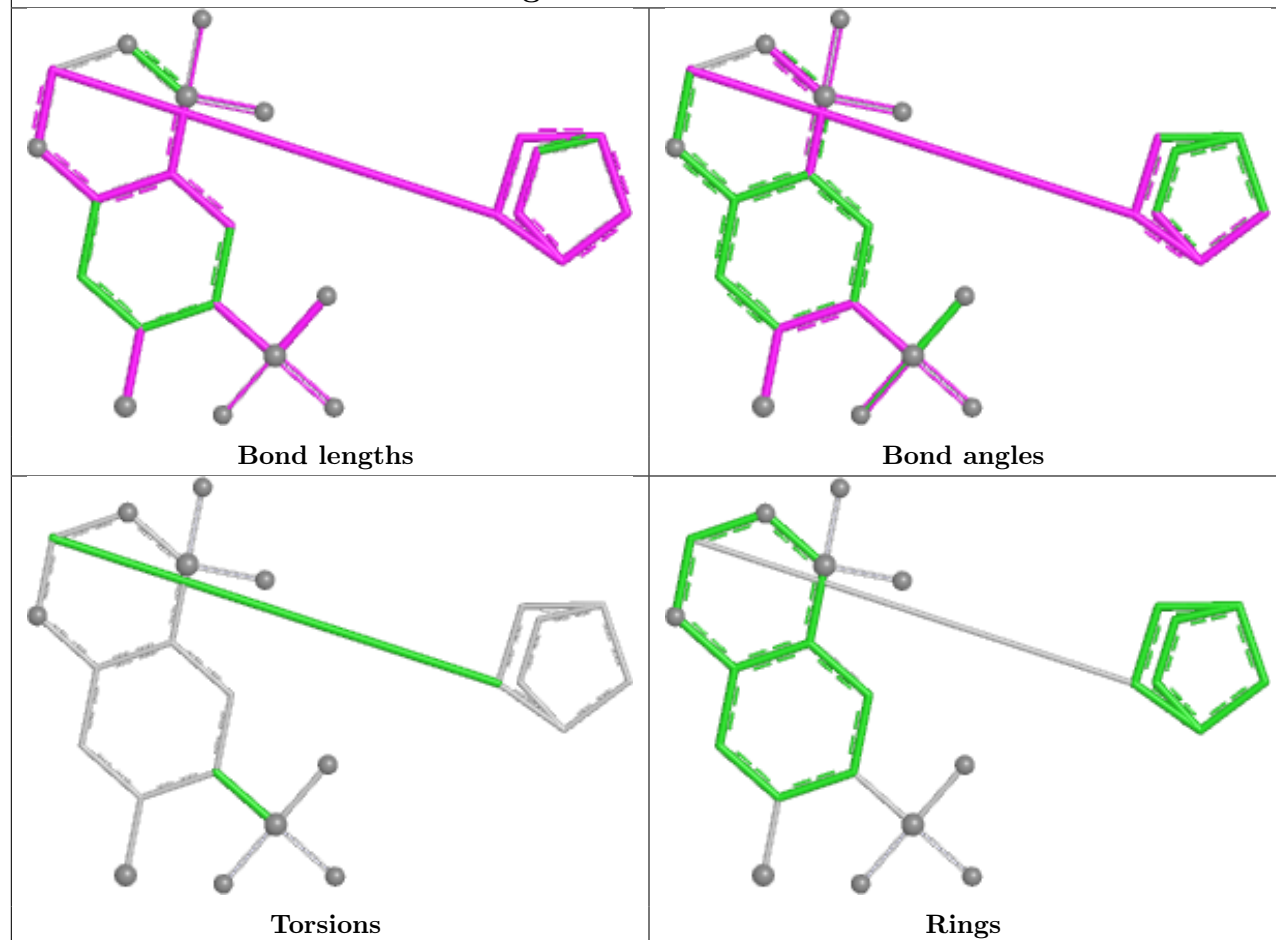




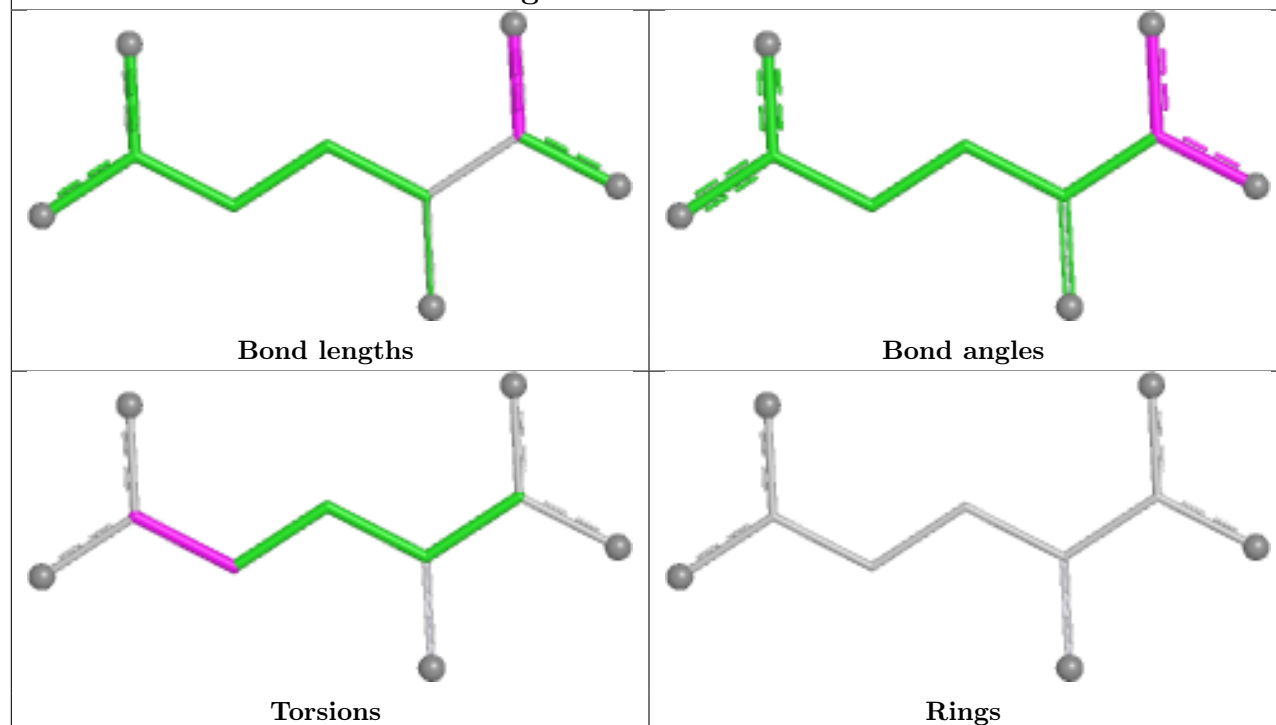


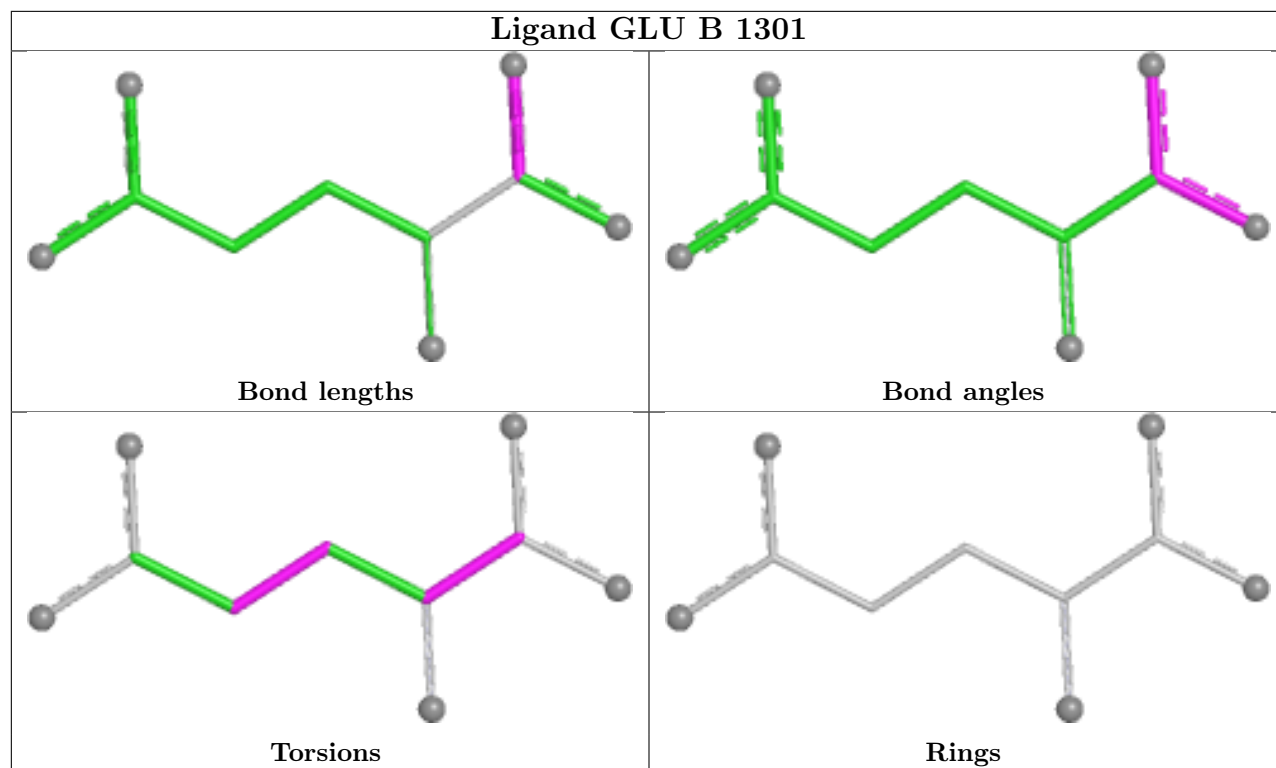


## Ligand CYZ A 1302



## Ligand GLU A 1301





## 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.

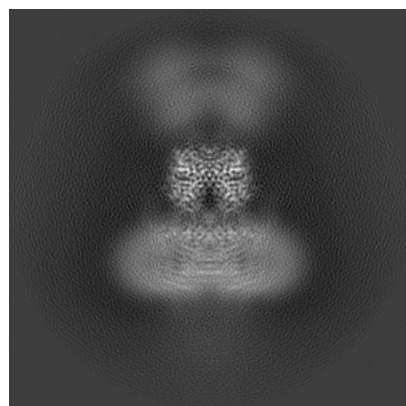
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29387. These allow visual inspection of the internal detail of the map and identification of artifacts.

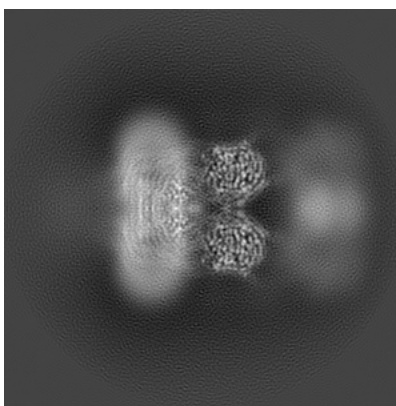
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

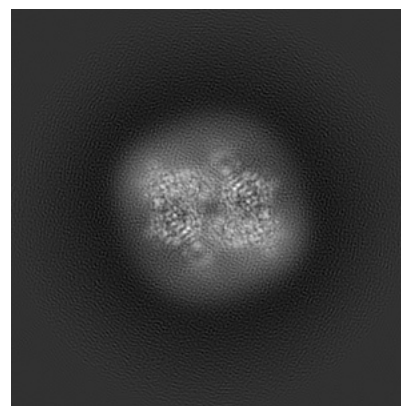
#### 6.1.1 Primary map



X

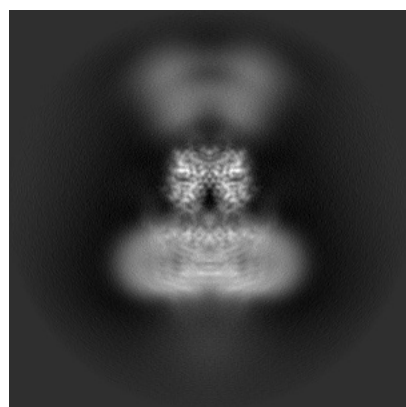


Y

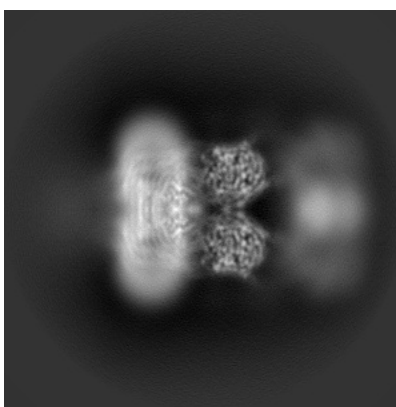


Z

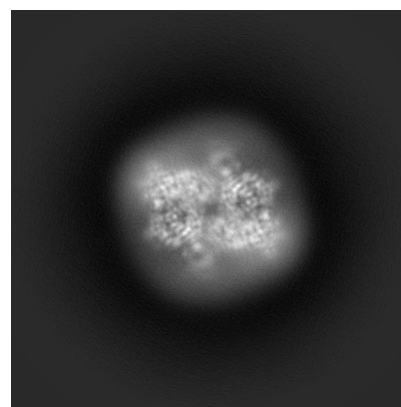
#### 6.1.2 Raw map



X



Y

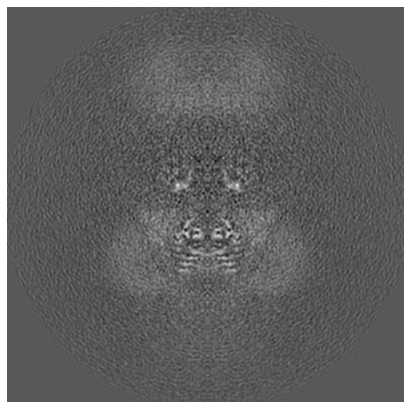


Z

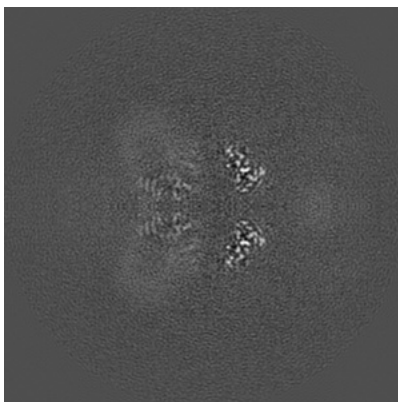
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

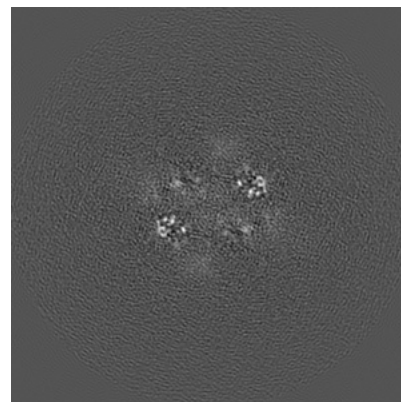
### 6.2.1 Primary map



X Index: 180

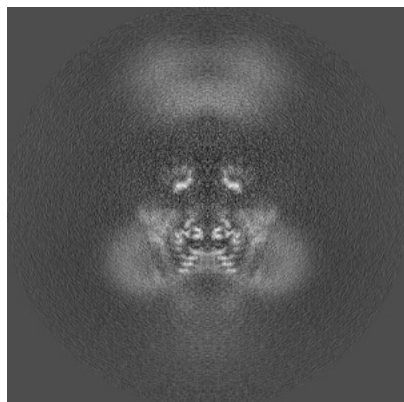


Y Index: 180

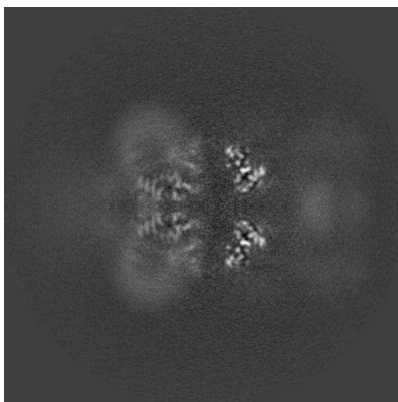


Z Index: 180

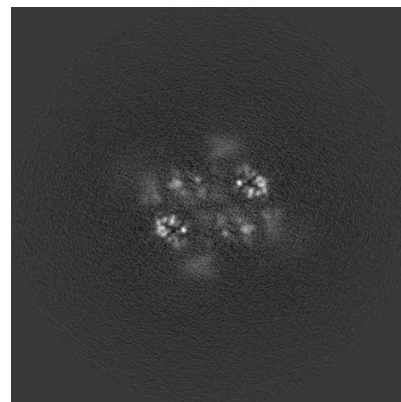
### 6.2.2 Raw map



X Index: 180



Y Index: 180

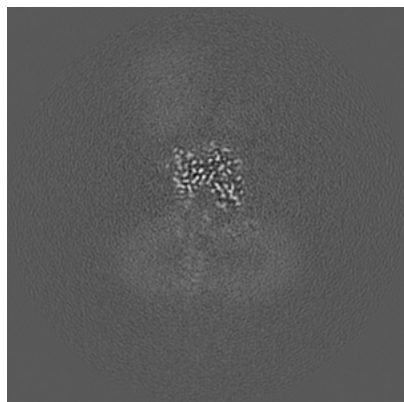


Z Index: 180

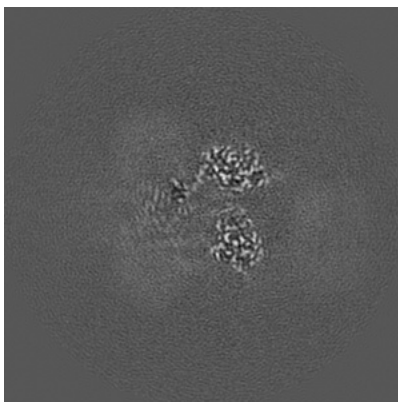
The images above show central slices of the map in three orthogonal directions.

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

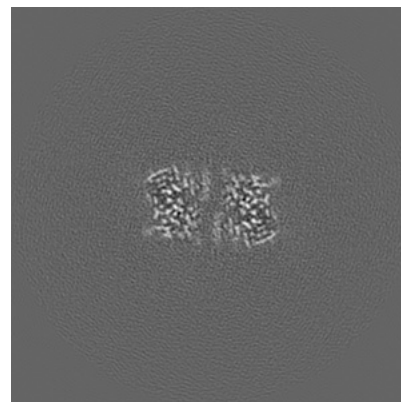
### 6.3.1 Primary map



X Index: 216

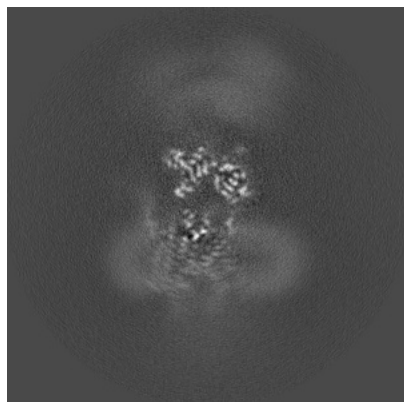


Y Index: 195

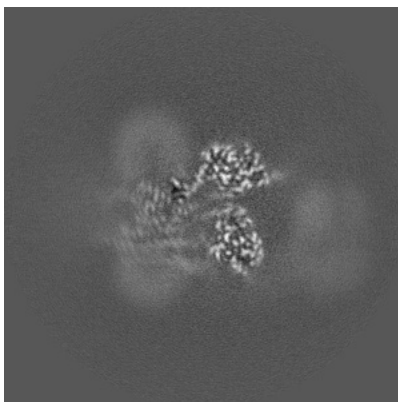


Z Index: 214

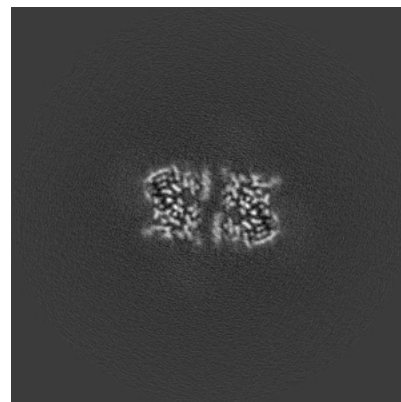
### 6.3.2 Raw map



X Index: 163



Y Index: 195



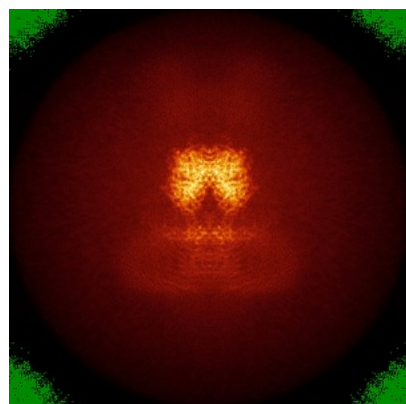
Z Index: 214

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

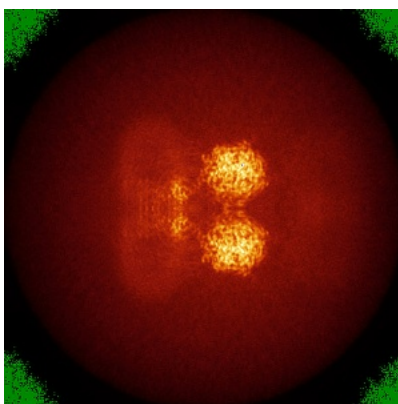


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

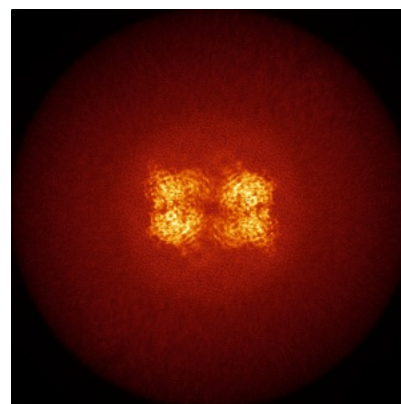
### 6.4.1 Primary map



X

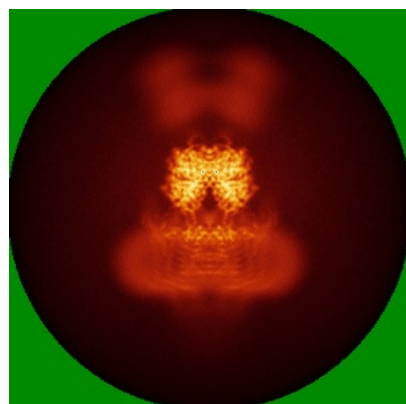


Y

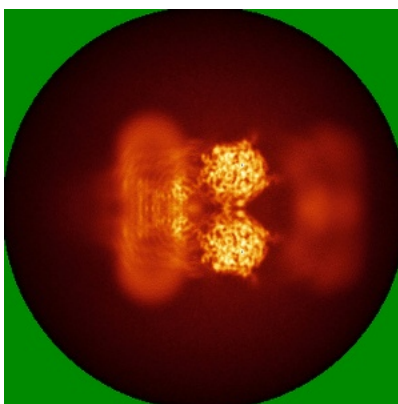


Z

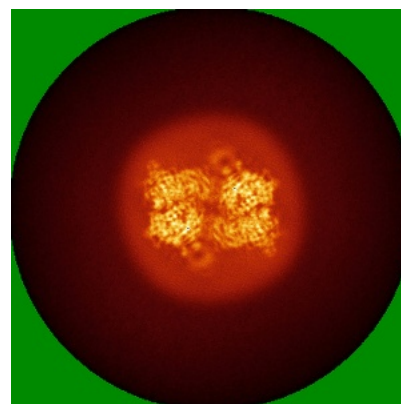
### 6.4.2 Raw map



X



Y

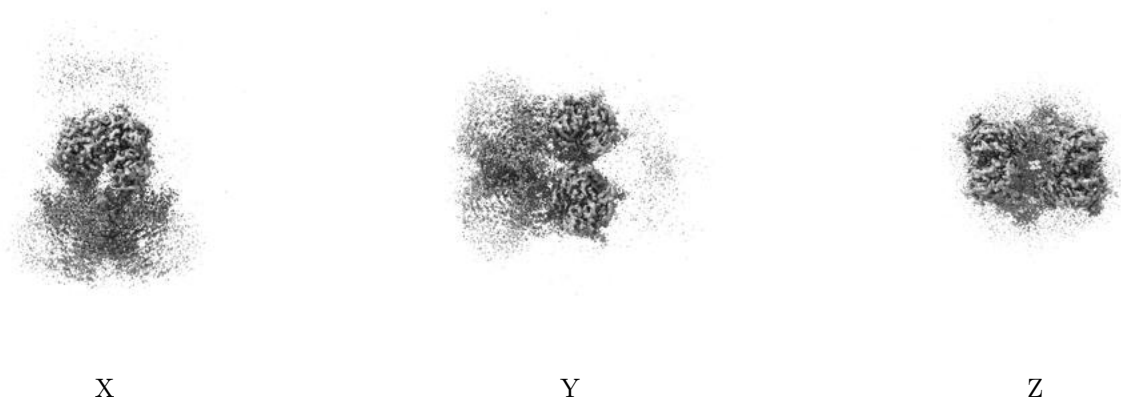


Z

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.

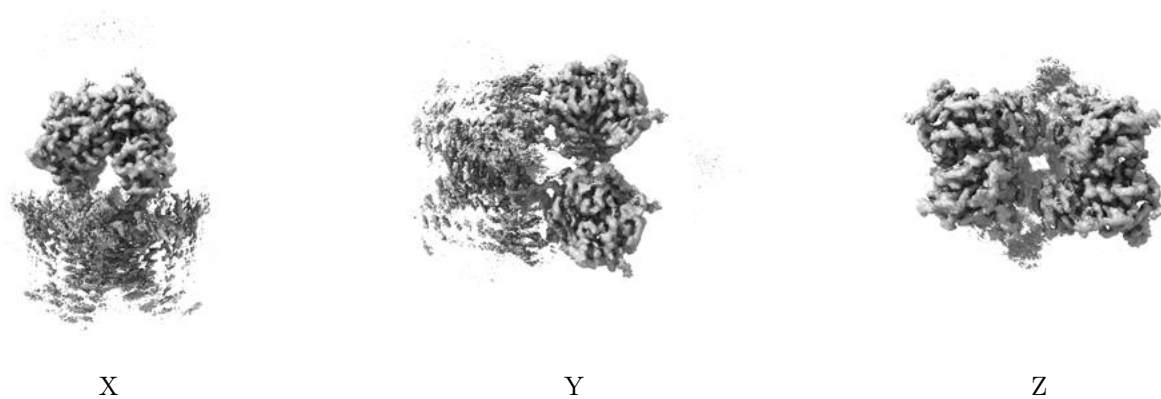
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0155. 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.



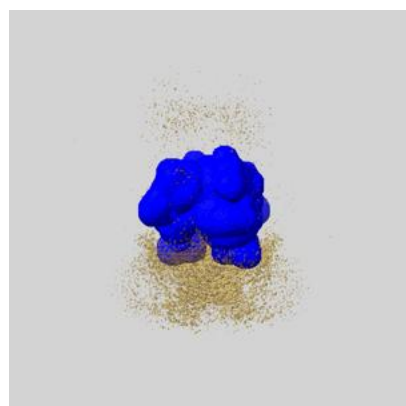
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

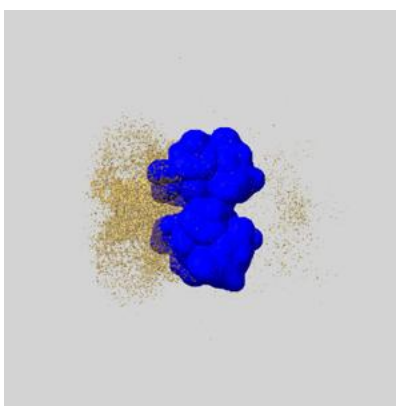
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

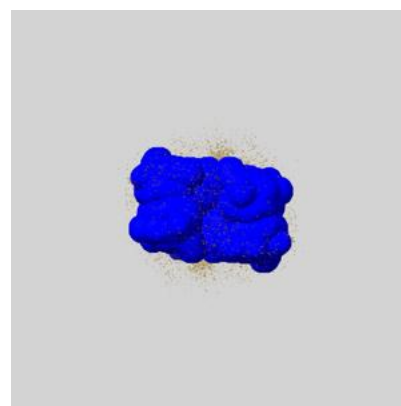
### 6.6.1 emd\_29387\_msk\_1.map [i](#)



X



Y

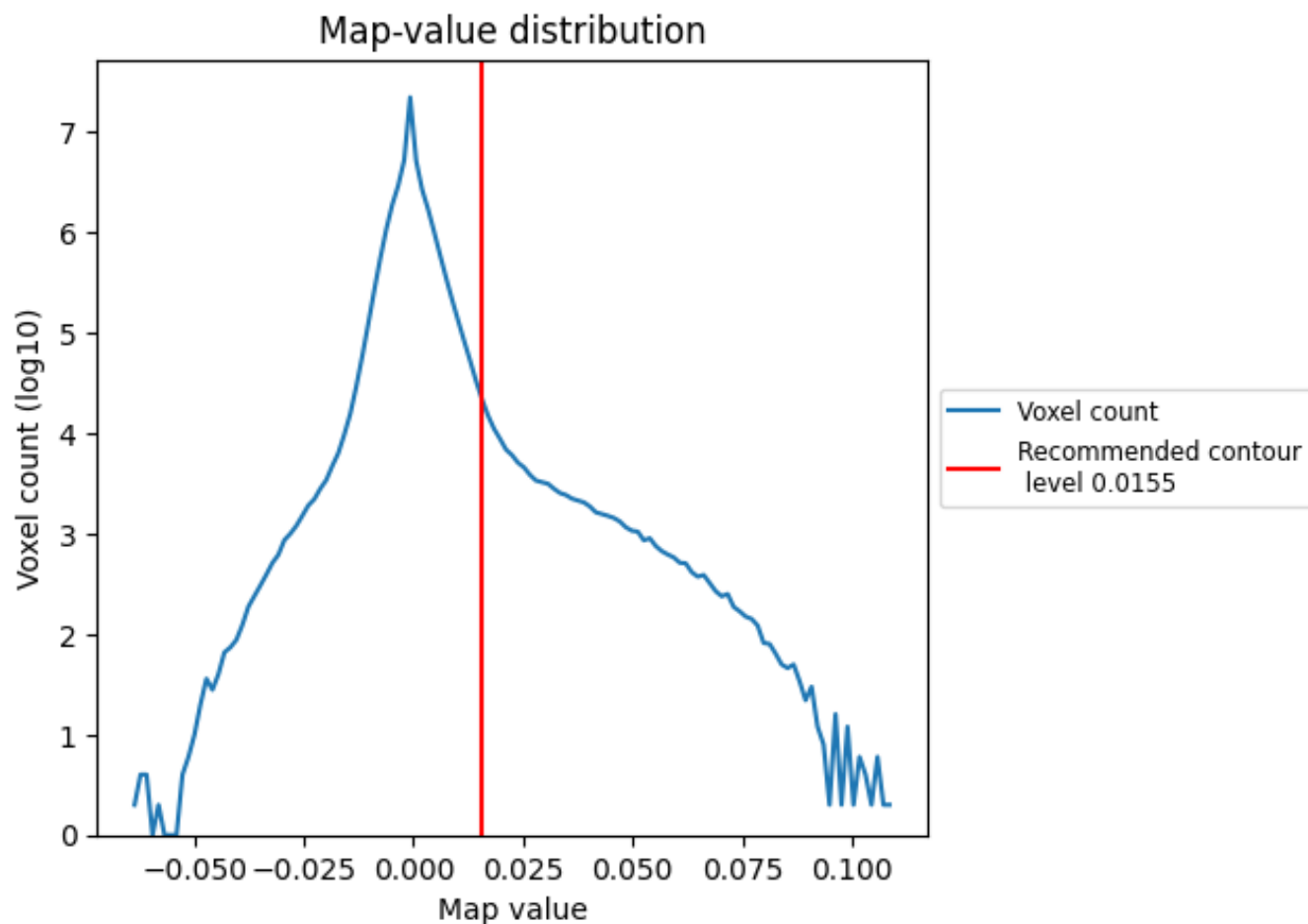


Z

## 7 Map analysis [i](#)

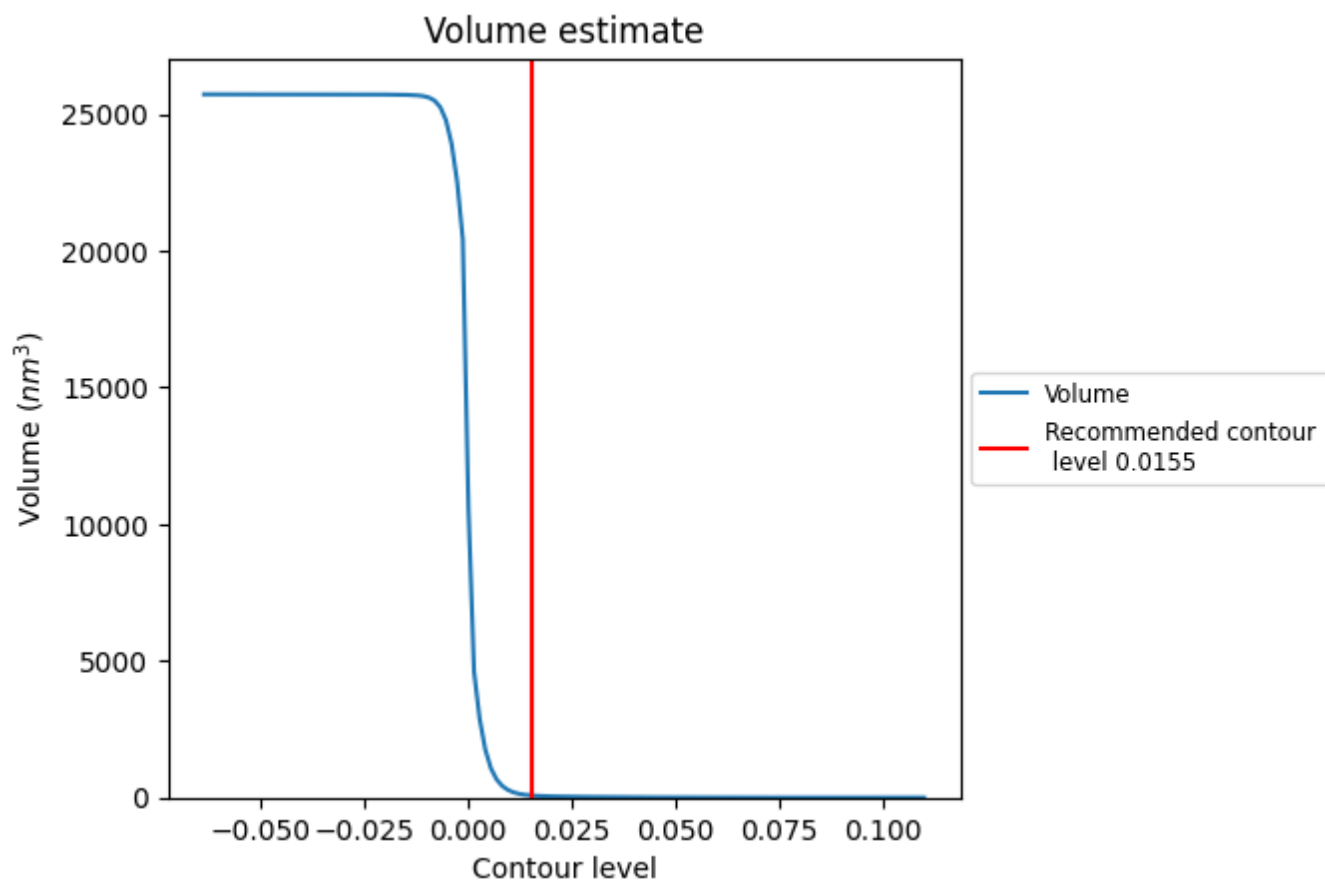
This section contains the results of statistical analysis of the map.

### 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.

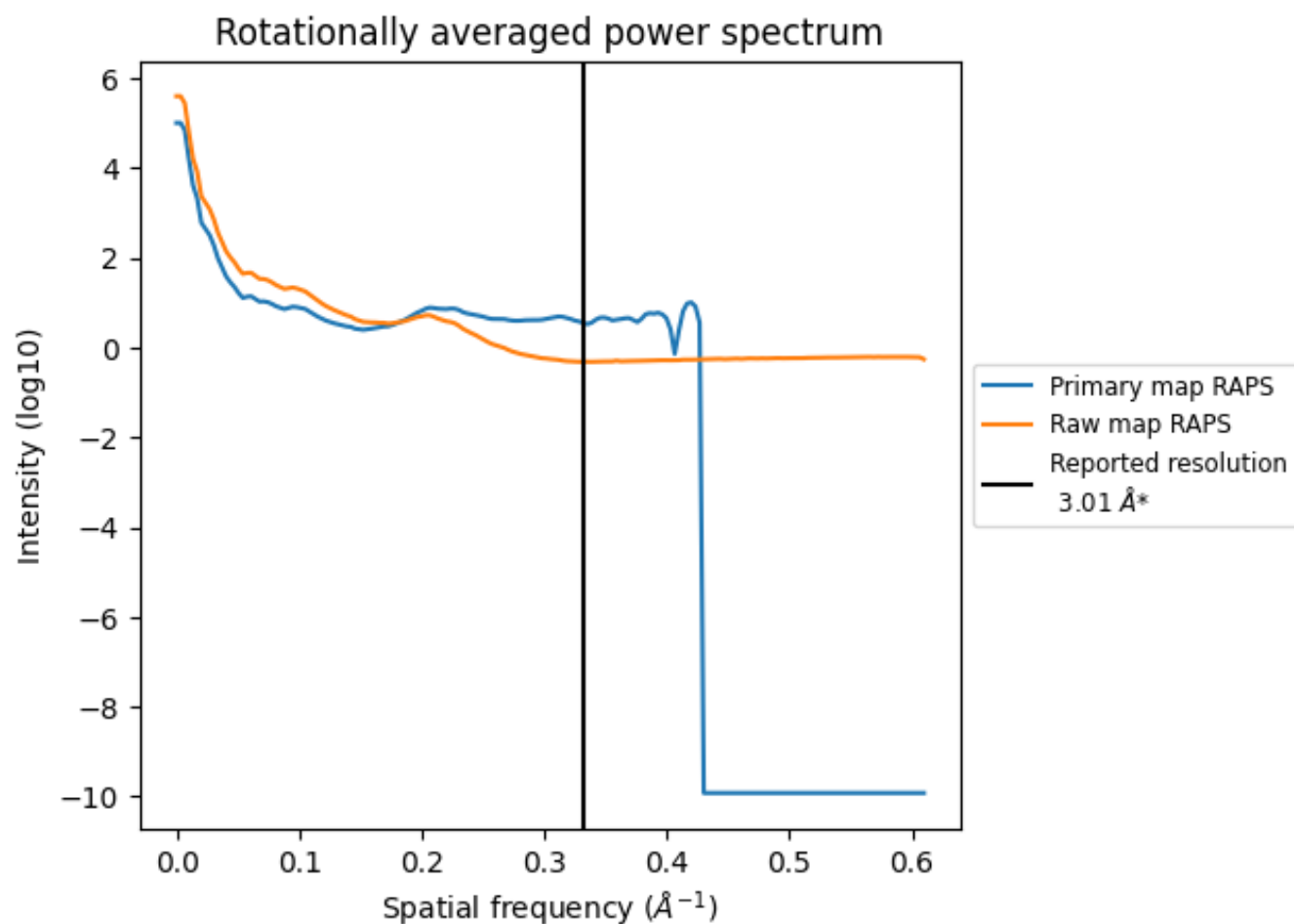
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $73 \text{ nm}^3$ ; this corresponds to an approximate mass of 66 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 ⓘ

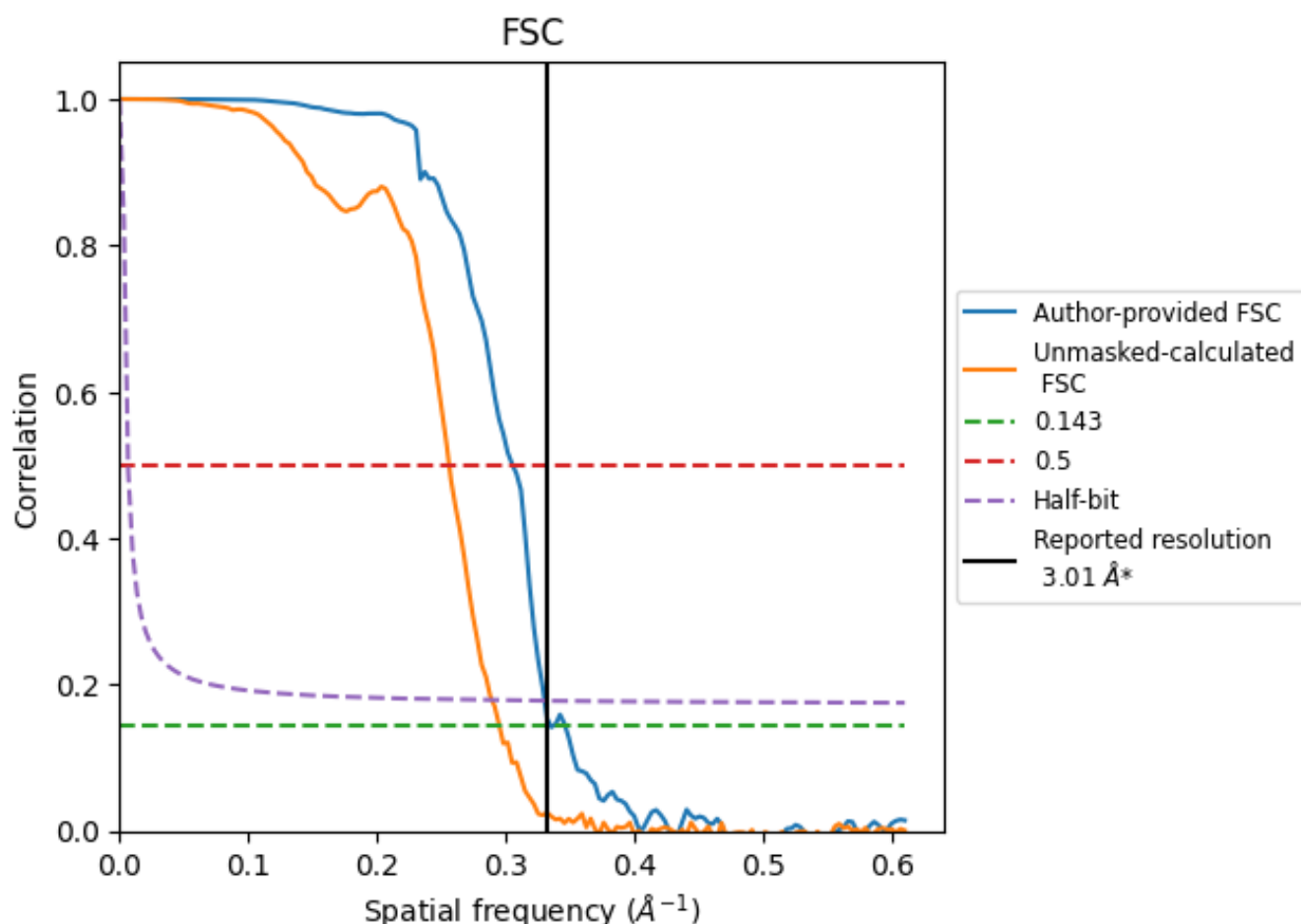


\*Reported resolution corresponds to spatial frequency of 0.332  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.332 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

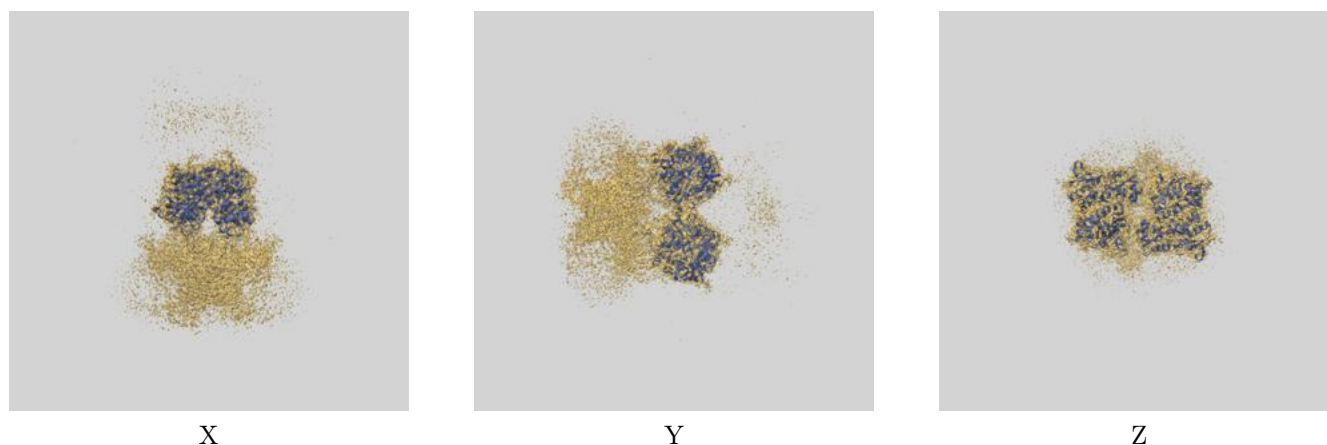
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	2.99	3.28	3.03
Unmasked-calculated*	3.39	3.91	3.46

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.39 differs from the reported value 3.01 by more than 10 %

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

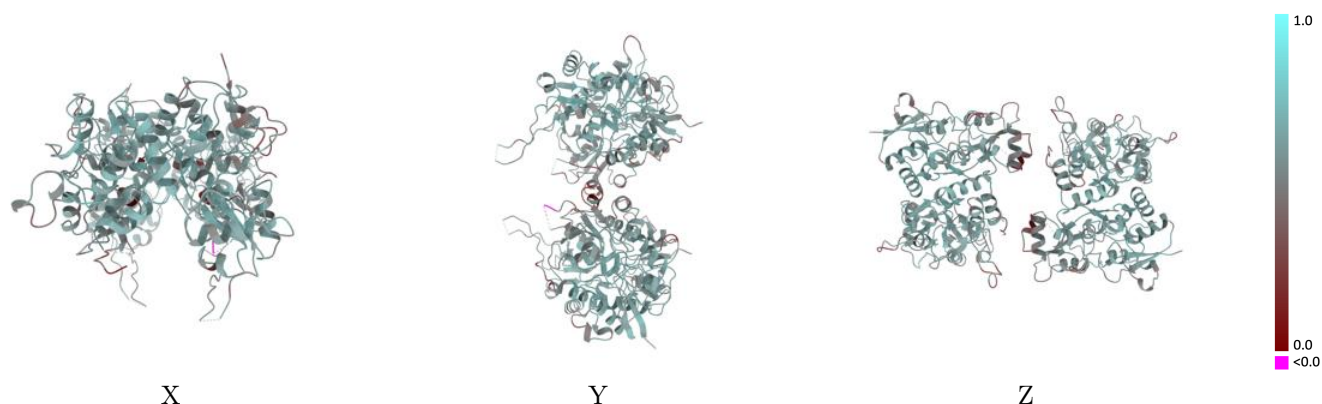
This section contains information regarding the fit between EMDB map EMD-29387 and PDB model 8FQG. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

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



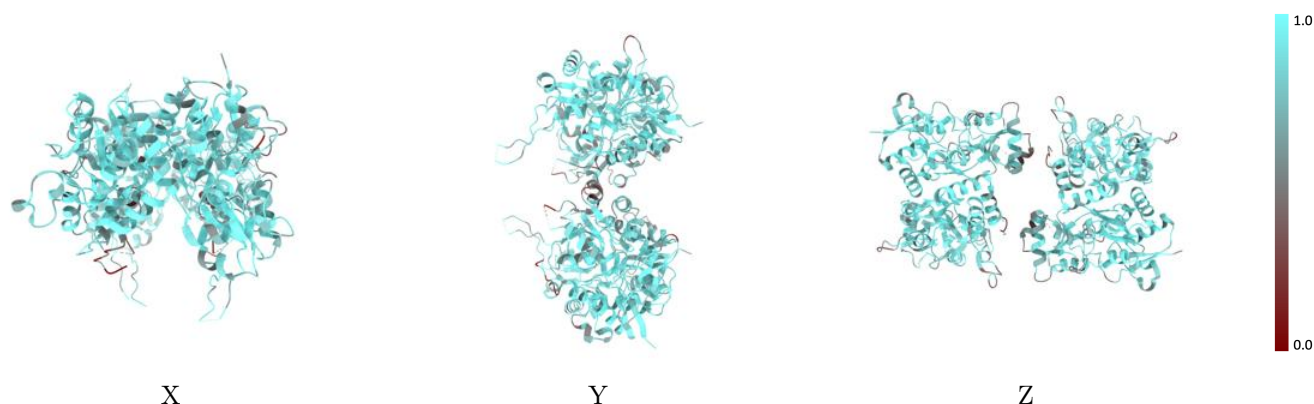
The images above show the 3D surface view of the map at the recommended contour level 0.0155 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

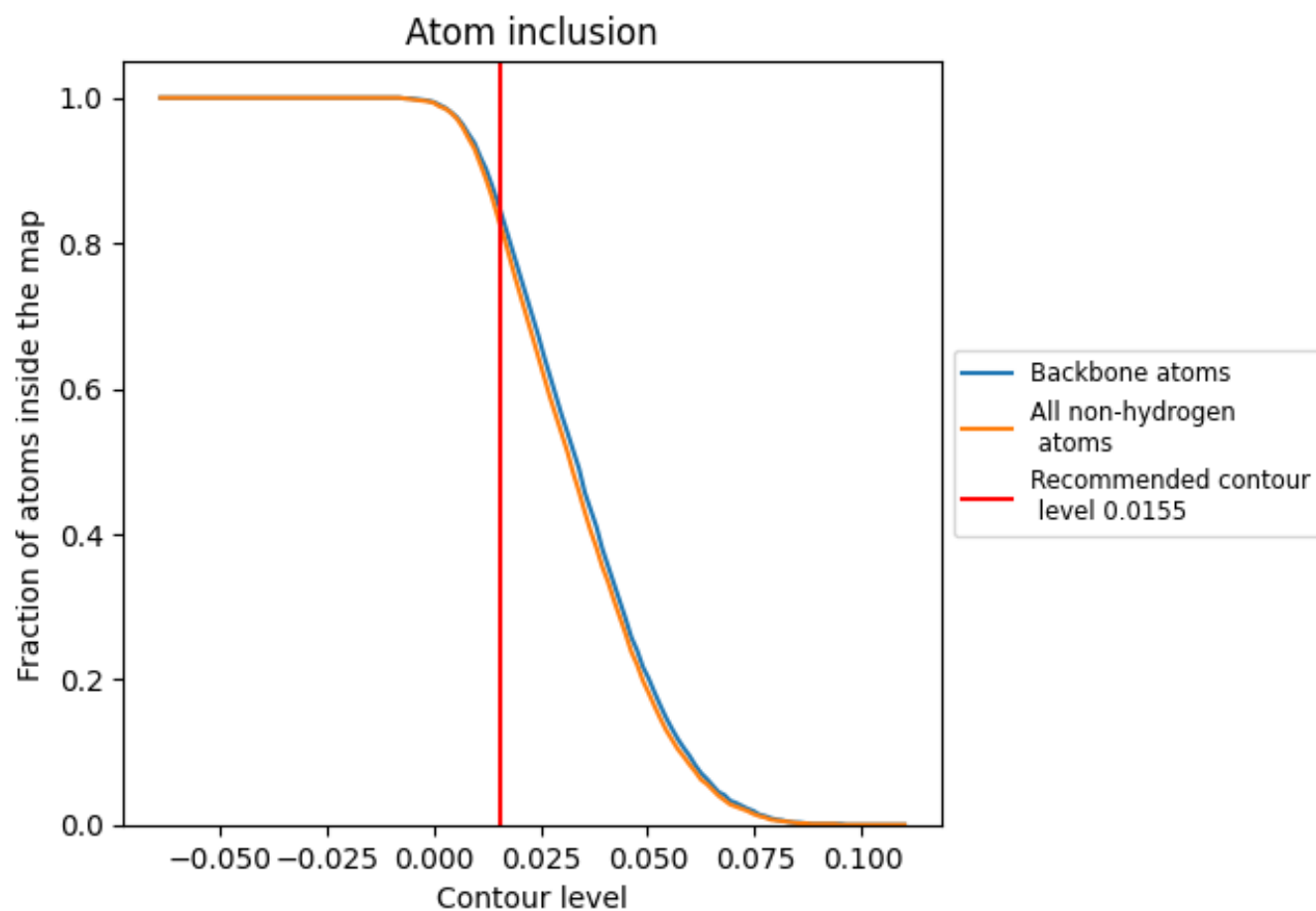
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0155).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 83% 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 (0.0155) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8270	<div></div> 0.5620
A	<div></div> 0.8220	<div></div> 0.5560
B	<div></div> 0.8400	<div></div> 0.5690
C	<div></div> 0.8200	<div></div> 0.5540
D	<div></div> 0.8400	<div></div> 0.5680

