



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:58 AM UTC

PDB ID : 5WEO / pdb_00005weo
EMDB ID : EMD-8823
Title : Activated GluA2 complex bound to glutamate, cyclothiazide, and STZ in digi-
tonin
Authors : Twomey, E.C.; Yelshanskaya, M.V.; Grassucci, R.A.; Frank, J.; Sobolevsky,
A.I.
Deposited on : 2017-07-10
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

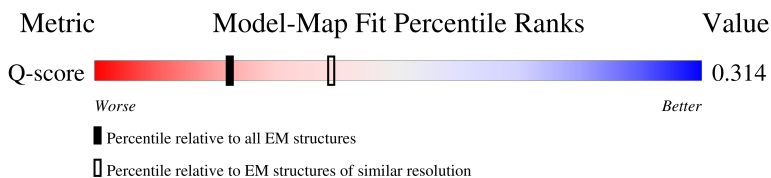
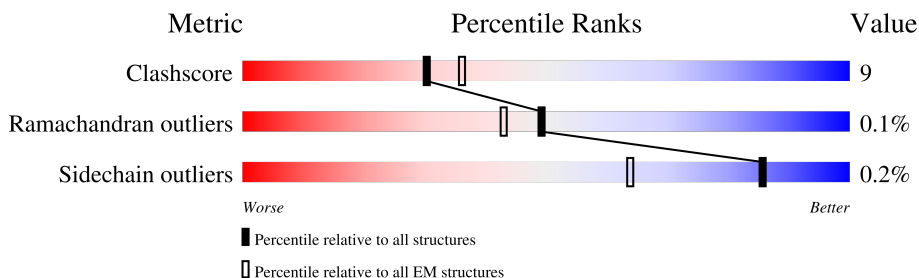
1 Overall quality at a glance

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	1034	15% 73% 22% .
1	B	1034	17% 72% 23% 5%
1	C	1034	15% 72% 23% .
1	D	1034	16% 73% 22% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31168 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, Voltage-dependent calcium channel gamma-2 subunit chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	988	Total	C	N	O	S	0	0
			7765	4997	1283	1444	41		
1	B	987	Total	C	N	O	S	0	0
			7753	4991	1279	1442	41		
1	C	988	Total	C	N	O	S	0	0
			7765	4997	1283	1444	41		
1	D	987	Total	C	N	O	S	0	0
			7749	4988	1278	1442	41		

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	382	LEU	VAL	engineered mutation	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	engineered mutation	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	engineered mutation	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	1047	ASP	ASN	conflict	UNP O88602
A	1208	THR	-	expression tag	UNP O88602
A	1209	GLY	-	expression tag	UNP O88602
A	1210	GLY	-	expression tag	UNP O88602
A	1211	LEU	-	expression tag	UNP O88602
A	1212	VAL	-	expression tag	UNP O88602
A	1213	PRO	-	expression tag	UNP O88602
A	1214	ARG	-	expression tag	UNP O88602

Continued on next page...

Continued from previous page...

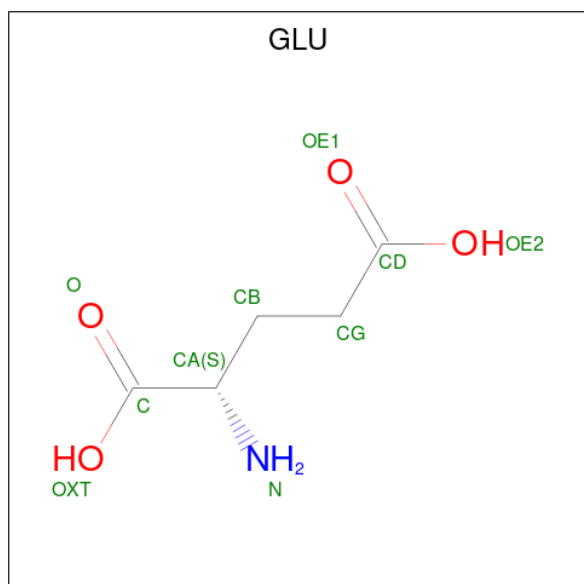
Chain	Residue	Modelled	Actual	Comment	Reference
A	1215	GLY	-	expression tag	UNP O88602
B	241	GLU	ASN	engineered mutation	UNP P19491
B	382	LEU	VAL	engineered mutation	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	engineered mutation	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	1047	ASP	ASN	conflict	UNP O88602
B	1208	THR	-	expression tag	UNP O88602
B	1209	GLY	-	expression tag	UNP O88602
B	1210	GLY	-	expression tag	UNP O88602
B	1211	LEU	-	expression tag	UNP O88602
B	1212	VAL	-	expression tag	UNP O88602
B	1213	PRO	-	expression tag	UNP O88602
B	1214	ARG	-	expression tag	UNP O88602
B	1215	GLY	-	expression tag	UNP O88602
C	241	GLU	ASN	engineered mutation	UNP P19491
C	382	LEU	VAL	engineered mutation	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	engineered mutation	UNP P19491
C	385	ASP	ASN	engineered mutation	UNP P19491
C	392	GLN	ASN	engineered mutation	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	1047	ASP	ASN	conflict	UNP O88602
C	1208	THR	-	expression tag	UNP O88602
C	1209	GLY	-	expression tag	UNP O88602
C	1210	GLY	-	expression tag	UNP O88602
C	1211	LEU	-	expression tag	UNP O88602
C	1212	VAL	-	expression tag	UNP O88602

Continued on next page...

Continued from previous page...

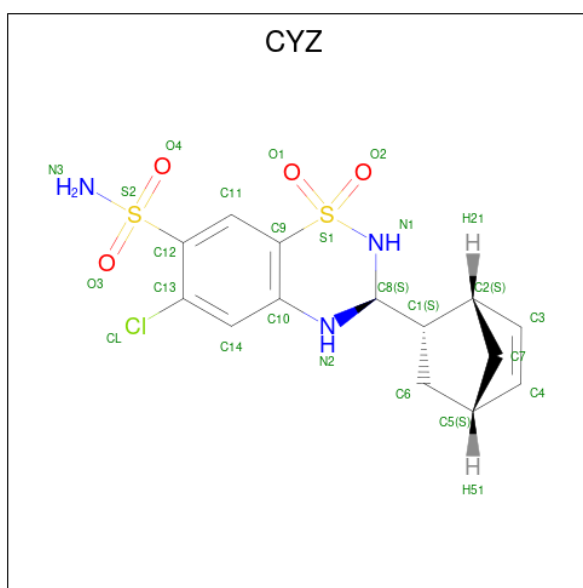
Chain	Residue	Modelled	Actual	Comment	Reference
C	1213	PRO	-	expression tag	UNP O88602
C	1214	ARG	-	expression tag	UNP O88602
C	1215	GLY	-	expression tag	UNP O88602
D	241	GLU	ASN	engineered mutation	UNP P19491
D	382	LEU	VAL	engineered mutation	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	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	engineered mutation	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	engineered mutation	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	1047	ASP	ASN	conflict	UNP O88602
D	1208	THR	-	expression tag	UNP O88602
D	1209	GLY	-	expression tag	UNP O88602
D	1210	GLY	-	expression tag	UNP O88602
D	1211	LEU	-	expression tag	UNP O88602
D	1212	VAL	-	expression tag	UNP O88602
D	1213	PRO	-	expression tag	UNP O88602
D	1214	ARG	-	expression tag	UNP O88602
D	1215	GLY	-	expression tag	UNP O88602

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

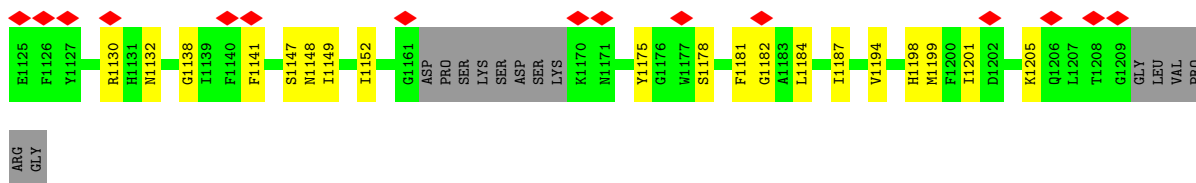


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			10	5	1	4	
2	B	1	Total	C	N	O	0
			10	5	1	4	
2	C	1	Total	C	N	O	0
			10	5	1	4	
2	D	1	Total	C	N	O	0
			10	5	1	4	

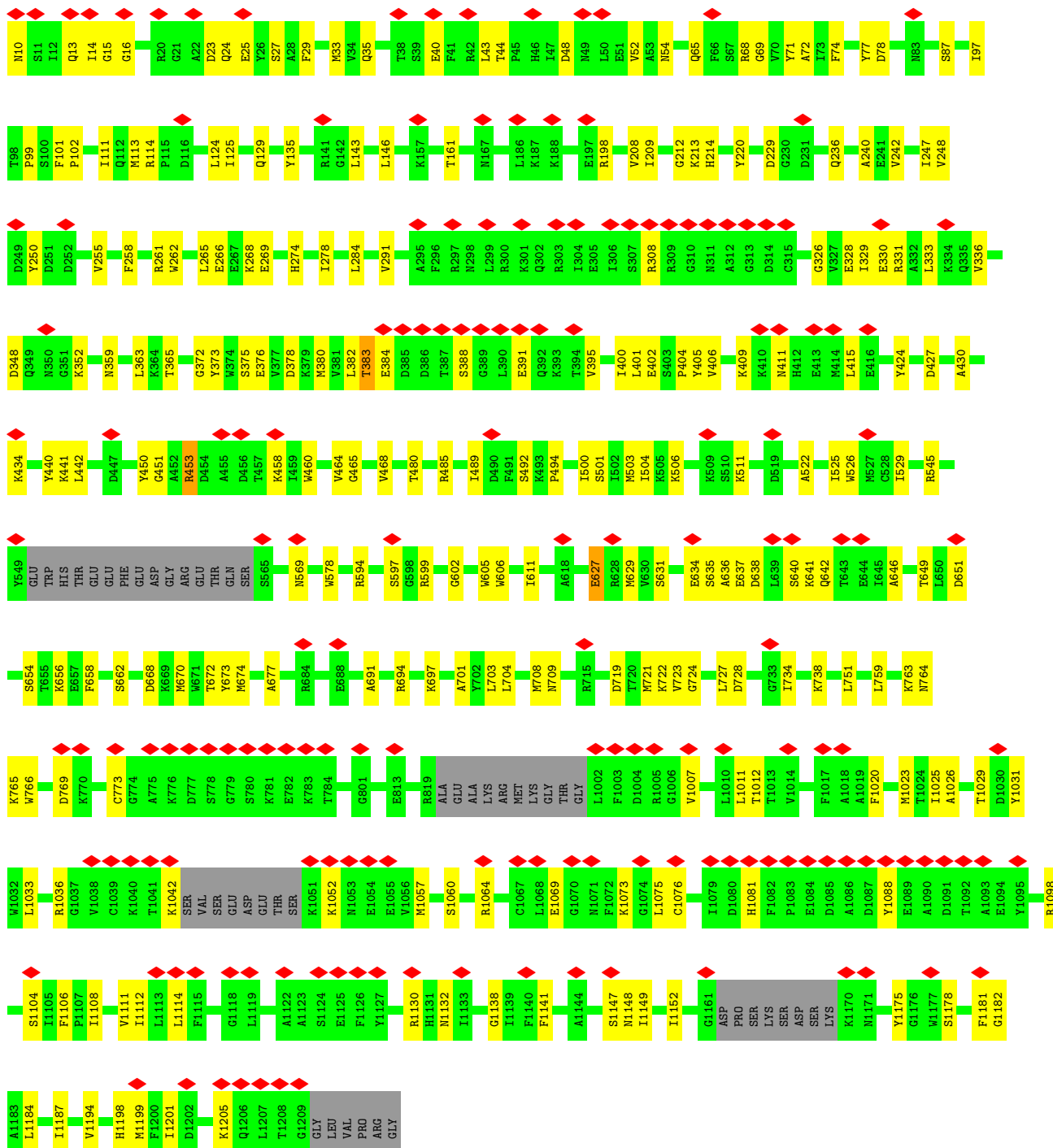
- Molecule 3 is CYCLOTHIAZIDE (CCD ID: CYZ) (formula: $C_{14}H_{16}ClN_3O_4S_2$).

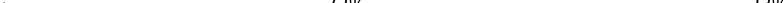


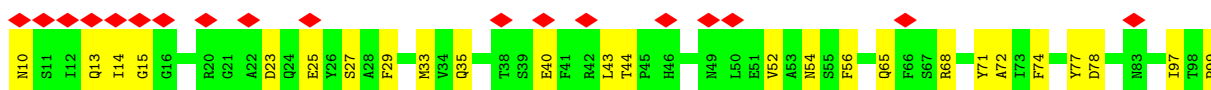
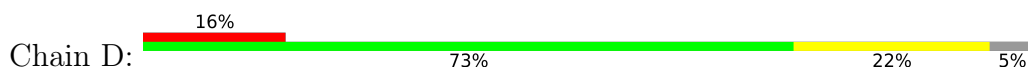
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	
3	B	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	
3	C	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	
3	D	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	

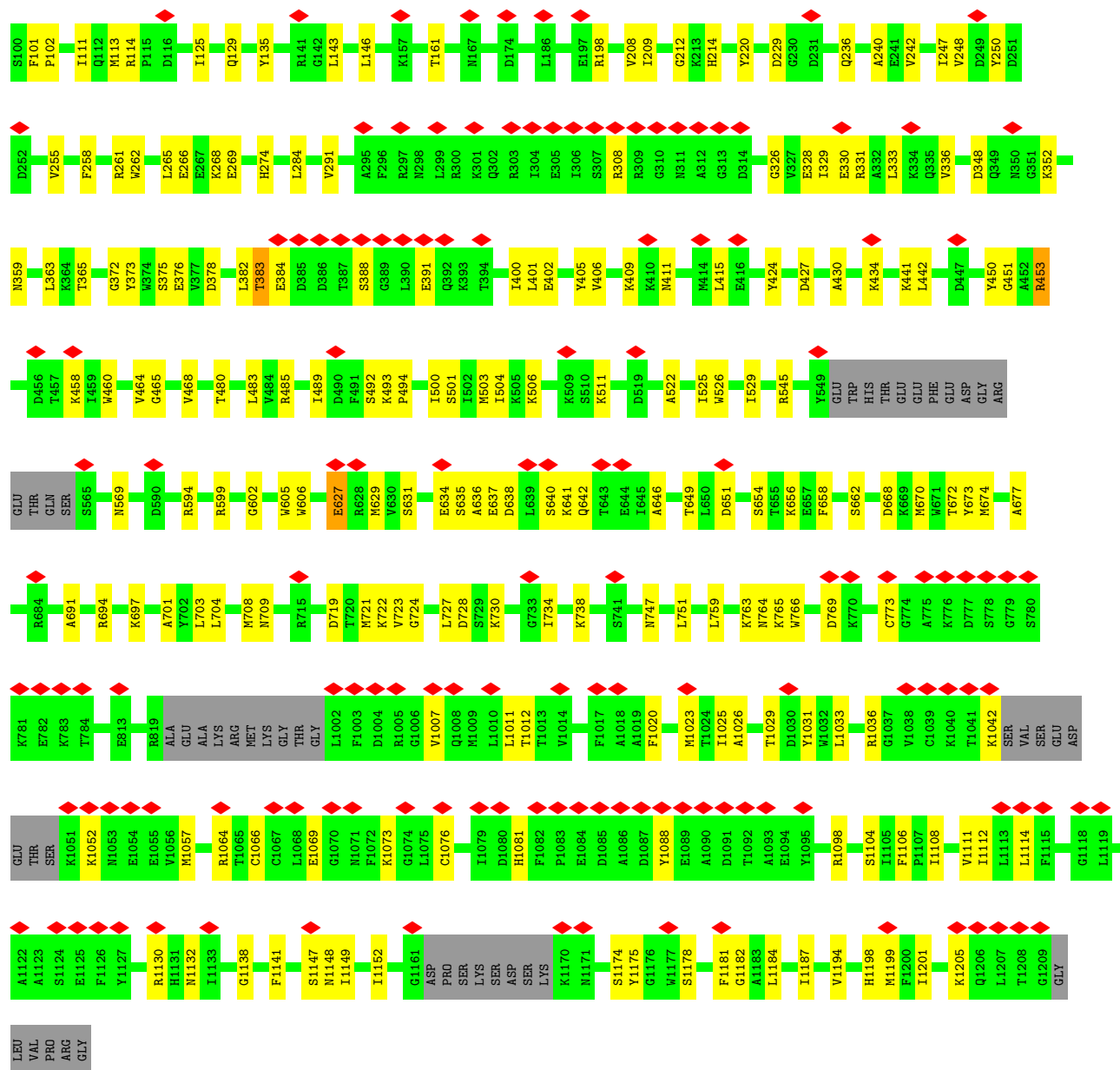


- Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-2 subunit chimera



- Chain C:  15% 72% 23%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	69207	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	0.164	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	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

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	0.40	1/7931 (0.0%)	0.61	0/10712
1	B	0.39	0/7919	0.61	1/10697 (0.0%)
1	C	0.40	1/7931 (0.0%)	0.61	0/10712
1	D	0.39	0/7915	0.61	1/10693 (0.0%)
All	All	0.39	2/31696 (0.0%)	0.61	2/42814 (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	4
1	B	0	4
1	C	0	4
1	D	0	4
All	All	0	16

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	383	THR	C-N	8.31	1.45	1.33
1	C	383	THR	C-N	-6.84	1.23	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	GLU	N-CA-C	8.15	120.45	110.91
1	D	384	GLU	N-CA-C	8.14	120.44	110.91

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	383	THR	Peptide
1	A	507	PRO	Peptide
1	A	632	PRO	Peptide
1	A	635	SER	Peptide
1	B	383	THR	Peptide
1	B	627	GLU	Peptide
1	B	635	SER	Peptide
1	B	773	CYS	Peptide
1	C	383	THR	Peptide
1	C	507	PRO	Peptide
1	C	632	PRO	Peptide
1	C	635	SER	Peptide
1	D	383	THR	Peptide
1	D	627	GLU	Peptide
1	D	635	SER	Peptide
1	D	773	CYS	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	7765	0	7733	138	0
1	B	7753	0	7714	146	0
1	C	7765	0	7733	142	0
1	D	7749	0	7703	137	0
2	A	10	0	5	2	0
2	B	10	0	5	2	0
2	C	10	0	5	2	0
2	D	10	0	5	2	0
3	A	24	0	16	4	0
3	B	24	0	16	3	0
3	C	24	0	16	3	0
3	D	24	0	16	3	0
All	All	31168	0	30967	559	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 9.

All (559) 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)
3:C:1302:CYZ:C6	3:C:1302:CYZ:C1	1.75	1.47
3:A:1302:CYZ:C1	3:A:1302:CYZ:C6	1.75	1.42
3:D:1302:CYZ:C6	3:D:1302:CYZ:C1	1.75	1.34
3:B:1302:CYZ:C6	3:B:1302:CYZ:C1	1.75	1.31
1:B:480:THR:HG1	2:B:1301:GLU:N	1.83	0.76
1:D:480:THR:HG1	2:D:1301:GLU:N	1.84	0.75
1:A:480:THR:HG1	2:A:1301:GLU:N	1.83	0.75
3:B:1302:CYZ:C6	3:B:1302:CYZ:C8	2.64	0.75
1:C:480:THR:HG1	2:C:1301:GLU:N	1.86	0.72
3:D:1302:CYZ:C6	3:D:1302:CYZ:C8	2.65	0.72
1:B:14:ILE:HD13	1:B:43:LEU:HD23	1.73	0.70
1:A:14:ILE:HD13	1:A:43:LEU:HD23	1.73	0.70
1:D:14:ILE:HD13	1:D:43:LEU:HD23	1.73	0.70
1:C:14:ILE:HD13	1:C:43:LEU:HD23	1.73	0.70
3:C:1302:CYZ:C6	3:C:1302:CYZ:C8	2.66	0.70
3:A:1302:CYZ:C6	3:A:1302:CYZ:C8	2.66	0.69
1:C:409:LYS:HG3	1:C:411:ASN:H	1.61	0.66
1:A:409:LYS:HG3	1:A:411:ASN:H	1.61	0.66
1:A:586:GLN:HE22	1:A:613:ILE:HD11	1.62	0.65
1:D:409:LYS:HG3	1:D:411:ASN:H	1.61	0.65
1:B:409:LYS:HG3	1:B:411:ASN:H	1.61	0.65
1:C:586:GLN:HE22	1:C:613:ILE:HD11	1.62	0.64
1:B:99:PRO:HA	1:B:113:MET:HB2	1.81	0.63
1:A:99:PRO:HA	1:A:113:MET:HB2	1.81	0.62
1:C:99:PRO:HA	1:C:113:MET:HB2	1.81	0.62
1:D:99:PRO:HA	1:D:113:MET:HB2	1.81	0.62
1:B:522:ALA:H	1:B:525:ILE:HD12	1.65	0.62
1:D:522:ALA:H	1:D:525:ILE:HD12	1.65	0.62
1:A:1081:HIS:NE2	1:A:1098:ARG:O	2.33	0.62
1:B:1081:HIS:NE2	1:B:1098:ARG:O	2.33	0.61
1:C:1081:HIS:NE2	1:C:1098:ARG:O	2.33	0.61
1:D:594:ARG:HA	1:D:599:ARG:HH21	1.65	0.61
1:A:395:VAL:H	1:A:440:TYR:HA	1.65	0.61
1:D:1081:HIS:NE2	1:D:1098:ARG:O	2.33	0.61
1:B:594:ARG:HA	1:B:599:ARG:HH21	1.65	0.60
1:B:427:ASP:OD2	1:B:766:TRP:NE1	2.34	0.60
1:C:427:ASP:OD2	1:C:766:TRP:NE1	2.34	0.60
1:B:634:GLU:HA	1:B:723:VAL:HB	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:ASP:OD2	1:D:766:TRP:NE1	2.34	0.60
1:D:634:GLU:HA	1:D:723:VAL:HB	1.84	0.59
1:B:220:TYR:HB2	1:B:242:VAL:HG22	1.85	0.59
1:A:401:LEU:HD23	1:A:406:VAL:HG12	1.85	0.59
1:A:1085:ASP:OD1	1:B:697:LYS:NZ	2.35	0.59
1:A:220:TYR:HB2	1:A:242:VAL:HG22	1.85	0.59
1:C:401:LEU:HD23	1:C:406:VAL:HG12	1.85	0.59
1:A:1064:ARG:HB3	1:A:1076:CYS:HB3	1.85	0.58
1:C:369:ARG:HH12	1:C:386:ASP:HB2	1.68	0.58
1:A:87:SER:OG	1:B:54:ASN:OD1	2.19	0.58
1:B:1042:LYS:H	1:B:1052:LYS:HE3	1.69	0.58
1:D:220:TYR:HB2	1:D:242:VAL:HG22	1.85	0.58
1:D:494:PRO:O	3:D:1302:CYZ:N1	2.33	0.58
1:B:1031:TYR:O	1:B:1178:SER:OG	2.22	0.58
1:C:220:TYR:HB2	1:C:242:VAL:HG22	1.85	0.58
1:C:1042:LYS:H	1:C:1052:LYS:HE3	1.69	0.58
1:D:1042:LYS:H	1:D:1052:LYS:HE3	1.69	0.58
1:D:359:ASN:HA	1:D:373:TYR:HA	1.86	0.58
1:B:359:ASN:HA	1:B:373:TYR:HA	1.86	0.58
1:D:401:LEU:HD23	1:D:406:VAL:HG12	1.84	0.58
1:D:465:GLY:HA2	1:D:468:VAL:HB	1.86	0.58
1:D:1064:ARG:HB3	1:D:1076:CYS:HB3	1.85	0.58
1:A:1042:LYS:H	1:A:1052:LYS:HE3	1.69	0.57
1:C:1069:GLU:H	1:C:1073:LYS:HE3	1.68	0.57
1:D:638:ASP:O	1:D:642:GLN:N	2.35	0.57
1:B:401:LEU:HD23	1:B:406:VAL:HG12	1.84	0.57
1:C:1064:ARG:HB3	1:C:1076:CYS:HB3	1.85	0.57
1:A:427:ASP:OD2	1:A:766:TRP:NE1	2.34	0.57
1:B:465:GLY:HA2	1:B:468:VAL:HB	1.86	0.57
1:A:1031:TYR:O	1:A:1178:SER:OG	2.22	0.57
1:C:722:LYS:NZ	1:C:724:GLY:O	2.38	0.57
1:D:722:LYS:NZ	1:D:724:GLY:O	2.37	0.57
1:A:722:LYS:NZ	1:A:724:GLY:O	2.38	0.57
1:A:1069:GLU:H	1:A:1073:LYS:HE3	1.68	0.57
1:B:1064:ARG:HB3	1:B:1076:CYS:HB3	1.85	0.57
1:C:359:ASN:HA	1:C:373:TYR:HA	1.86	0.57
1:D:1031:TYR:O	1:D:1178:SER:OG	2.22	0.57
1:A:465:GLY:HA2	1:A:468:VAL:HB	1.86	0.57
1:D:1069:GLU:H	1:D:1073:LYS:HE3	1.68	0.57
1:B:1069:GLU:H	1:B:1073:LYS:HE3	1.68	0.57
1:C:33:MET:HE1	1:C:43:LEU:HB2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:LYS:NZ	1:B:724:GLY:O	2.37	0.56
1:B:265:LEU:O	1:B:274:HIS:ND1	2.36	0.56
1:C:247:ILE:HG23	1:C:248:VAL:HG23	1.88	0.56
1:B:638:ASP:O	1:B:642:GLN:N	2.35	0.56
1:C:638:ASP:O	1:C:642:GLN:N	2.35	0.56
1:A:359:ASN:HA	1:A:373:TYR:HA	1.86	0.56
1:C:35:GLN:OE1	1:C:261:ARG:NH2	2.39	0.56
1:C:465:GLY:HA2	1:C:468:VAL:HB	1.86	0.56
1:A:1149:ILE:HA	1:A:1152:ILE:HD12	1.87	0.56
1:B:33:MET:HE1	1:B:43:LEU:HB2	1.87	0.56
1:C:1149:ILE:HA	1:C:1152:ILE:HD12	1.87	0.56
1:D:328:GLU:OE2	1:D:331:ARG:NH2	2.39	0.56
1:A:35:GLN:OE1	1:A:261:ARG:NH2	2.39	0.56
1:B:328:GLU:OE2	1:B:331:ARG:NH2	2.39	0.56
1:A:1138:GLY:HA2	1:A:1141:PHE:HD2	1.71	0.56
1:D:35:GLN:OE1	1:D:261:ARG:NH2	2.39	0.56
1:C:1031:TYR:O	1:C:1178:SER:OG	2.22	0.56
1:A:638:ASP:O	1:A:642:GLN:N	2.35	0.55
1:D:247:ILE:HG23	1:D:248:VAL:HG23	1.87	0.55
1:B:405:TYR:HA	1:B:424:TYR:HB3	1.88	0.55
1:B:1149:ILE:HA	1:B:1152:ILE:HD12	1.87	0.55
1:C:497:SER:N	3:C:1302:CYZ:O3	2.39	0.55
1:D:33:MET:HE1	1:D:43:LEU:HB2	1.87	0.55
1:D:405:TYR:HA	1:D:424:TYR:HB3	1.88	0.55
1:D:1149:ILE:HA	1:D:1152:ILE:HD12	1.87	0.55
1:A:247:ILE:HG23	1:A:248:VAL:HG23	1.88	0.55
1:A:328:GLU:OE2	1:A:331:ARG:NH2	2.39	0.55
1:A:33:MET:HE1	1:A:43:LEU:HB2	1.87	0.55
1:B:35:GLN:OE1	1:B:261:ARG:NH2	2.39	0.55
1:B:506:LYS:HD2	1:B:719:ASP:HA	1.89	0.55
1:D:1138:GLY:HA2	1:D:1141:PHE:HD2	1.71	0.55
1:C:1138:GLY:HA2	1:C:1141:PHE:HD2	1.71	0.55
1:B:1138:GLY:HA2	1:B:1141:PHE:HD2	1.71	0.54
1:B:13:GLN:HA	1:B:44:THR:HB	1.90	0.54
1:C:328:GLU:OE2	1:C:331:ARG:NH2	2.39	0.54
1:A:265:LEU:O	1:A:274:HIS:ND1	2.36	0.54
1:A:494:PRO:O	3:A:1302:CYZ:N1	2.37	0.54
1:A:651:ASP:OD1	1:A:656:LYS:NZ	2.40	0.54
1:A:1025:ILE:O	1:A:1029:THR:OG1	2.25	0.54
1:B:247:ILE:HG23	1:B:248:VAL:HG23	1.87	0.54
1:B:526:TRP:HA	1:B:529:ILE:HD12	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:526:TRP:HA	1:D:529:ILE:HD12	1.90	0.54
1:C:405:TYR:HA	1:C:424:TYR:HB3	1.88	0.54
1:D:658:PHE:O	1:D:662:SER:N	2.41	0.54
1:A:405:TYR:HA	1:A:424:TYR:HB3	1.88	0.54
1:C:1026:ALA:HB2	1:C:1181:PHE:HB2	1.90	0.54
1:C:1025:ILE:O	1:C:1029:THR:OG1	2.25	0.53
1:A:497:SER:N	3:A:1302:CYZ:O3	2.38	0.53
1:A:15:GLY:N	1:A:72:ALA:O	2.41	0.53
1:B:1026:ALA:HB2	1:B:1181:PHE:HB2	1.90	0.53
1:C:15:GLY:N	1:C:72:ALA:O	2.41	0.53
1:A:658:PHE:O	1:A:662:SER:N	2.41	0.53
1:C:395:VAL:H	1:C:440:TYR:HA	1.73	0.53
1:D:265:LEU:O	1:D:274:HIS:ND1	2.36	0.53
1:A:10:ASN:N	1:A:40:GLU:O	2.42	0.53
1:C:658:PHE:O	1:C:662:SER:N	2.41	0.53
1:D:13:GLN:HA	1:D:44:THR:HB	1.90	0.53
1:B:658:PHE:O	1:B:662:SER:N	2.41	0.53
1:D:1025:ILE:O	1:D:1029:THR:OG1	2.25	0.53
1:A:1026:ALA:HB2	1:A:1181:PHE:HB2	1.90	0.53
1:B:236:GLN:NE2	1:B:365:THR:O	2.42	0.53
1:C:10:ASN:N	1:C:40:GLU:O	2.42	0.53
1:A:236:GLN:NE2	1:A:365:THR:O	2.42	0.53
1:B:1025:ILE:O	1:B:1029:THR:OG1	2.25	0.53
1:D:236:GLN:NE2	1:D:365:THR:O	2.42	0.53
1:A:250:TYR:HA	1:A:255:VAL:HG11	1.91	0.53
1:C:13:GLN:HA	1:C:44:THR:HB	1.90	0.53
1:D:15:GLY:N	1:D:72:ALA:O	2.41	0.53
1:A:764:ASN:O	1:A:769:ASP:N	2.38	0.53
1:A:77:TYR:OH	1:A:101:PHE:O	2.22	0.52
1:B:10:ASN:N	1:B:40:GLU:O	2.42	0.52
1:B:250:TYR:HA	1:B:255:VAL:HG11	1.91	0.52
1:A:71:TYR:OH	1:A:308:ARG:O	2.25	0.52
1:D:1026:ALA:HB2	1:D:1181:PHE:HB2	1.90	0.52
1:C:545:ARG:NH1	1:C:569:ASN:O	2.41	0.52
1:B:651:ASP:OD1	1:B:656:LYS:NZ	2.40	0.52
1:A:13:GLN:HA	1:A:44:THR:HB	1.90	0.52
1:A:545:ARG:NH1	1:A:569:ASN:O	2.41	0.52
1:D:1012:THR:HG21	1:D:1199:MET:HE1	1.92	0.52
1:C:637:GLU:O	1:C:640:SER:OG	2.28	0.52
1:D:10:ASN:N	1:D:40:GLU:O	2.42	0.52
1:D:102:PRO:HD3	1:D:114:ARG:HD2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:651:ASP:OD1	1:D:656:LYS:NZ	2.40	0.52
1:C:236:GLN:NE2	1:C:365:THR:O	2.42	0.52
1:A:213:LYS:O	1:A:220:TYR:OH	2.23	0.51
1:A:102:PRO:HD3	1:A:114:ARG:HD2	1.92	0.51
1:B:15:GLY:N	1:B:72:ALA:O	2.41	0.51
1:C:348:ASP:OD1	1:C:352:LYS:N	2.43	0.51
1:D:480:THR:O	1:D:485:ARG:NH1	2.42	0.51
1:D:1148:ASN:ND2	1:D:1182:GLY:O	2.42	0.51
1:A:1088:TYR:OH	1:A:1098:ARG:NH2	2.44	0.51
1:C:250:TYR:HA	1:C:255:VAL:HG11	1.91	0.51
1:C:265:LEU:O	1:C:274:HIS:ND1	2.36	0.51
1:D:1088:TYR:OH	1:D:1098:ARG:NH2	2.44	0.51
1:A:125:ILE:O	1:A:129:GLN:N	2.44	0.51
1:C:102:PRO:HD3	1:C:114:ARG:HD2	1.92	0.51
1:C:572:GLY:H	1:C:575:ASN:HB3	1.76	0.51
1:C:382:LEU:HB2	1:C:384:GLU:HG3	1.92	0.51
1:A:143:LEU:HD23	1:A:146:LEU:HD23	1.93	0.51
1:A:1012:THR:HG21	1:A:1199:MET:HE1	1.92	0.51
1:D:250:TYR:HA	1:D:255:VAL:HG11	1.91	0.51
1:A:25:GLU:O	1:A:29:PHE:N	2.40	0.51
1:B:494:PRO:O	3:B:1302:CYZ:N1	2.39	0.51
1:A:646:ALA:O	1:A:701:ALA:N	2.38	0.50
1:B:402:GLU:N	1:B:406:VAL:O	2.43	0.50
1:C:125:ILE:O	1:C:129:GLN:N	2.44	0.50
1:C:143:LEU:HD23	1:C:146:LEU:HD23	1.93	0.50
1:C:1012:THR:HG21	1:C:1199:MET:HE1	1.92	0.50
1:D:125:ILE:O	1:D:129:GLN:N	2.44	0.50
1:B:125:ILE:O	1:B:129:GLN:N	2.44	0.50
1:B:1012:THR:HG21	1:B:1199:MET:HE1	1.92	0.50
1:D:143:LEU:HD23	1:D:146:LEU:HD23	1.93	0.50
1:A:198:ARG:NH2	1:A:229:ASP:O	2.45	0.50
1:A:572:GLY:H	1:A:575:ASN:HB3	1.76	0.50
1:B:198:ARG:NH2	1:B:229:ASP:O	2.45	0.50
1:B:1088:TYR:OH	1:B:1098:ARG:NH2	2.44	0.50
1:B:102:PRO:HD3	1:B:114:ARG:HD2	1.92	0.50
1:D:430:ALA:O	1:D:434:LYS:N	2.41	0.50
1:D:654:SER:O	1:D:658:PHE:N	2.45	0.50
1:B:348:ASP:OD1	1:B:352:LYS:N	2.43	0.50
1:C:198:ARG:NH2	1:C:229:ASP:O	2.45	0.50
1:C:1088:TYR:OH	1:C:1098:ARG:NH2	2.44	0.50
1:D:637:GLU:O	1:D:640:SER:OG	2.28	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:654:SER:O	1:C:658:PHE:N	2.45	0.50
1:D:101:PHE:HA	1:D:114:ARG:HD2	1.94	0.50
1:C:402:GLU:O	1:C:406:VAL:N	2.43	0.50
1:C:1184:LEU:HD12	1:C:1187:ILE:HD12	1.94	0.50
1:D:1130:ARG:HH12	1:D:1132:ASN:HD22	1.60	0.50
1:A:101:PHE:HA	1:A:114:ARG:HD2	1.94	0.49
1:B:506:LYS:N	1:B:719:ASP:O	2.43	0.49
1:B:764:ASN:O	1:B:769:ASP:N	2.38	0.49
1:C:668:ASP:O	1:C:672:THR:N	2.40	0.49
1:A:538:VAL:O	1:A:542:LEU:N	2.43	0.49
1:B:25:GLU:O	1:B:29:PHE:N	2.40	0.49
1:B:1184:LEU:HD12	1:B:1187:ILE:HD12	1.94	0.49
1:B:1148:ASN:ND2	1:B:1182:GLY:O	2.42	0.49
1:A:509:LYS:HG2	1:A:629:MET:HG3	1.95	0.49
1:D:198:ARG:NH2	1:D:229:ASP:O	2.45	0.49
1:C:25:GLU:O	1:C:29:PHE:N	2.40	0.49
1:C:509:LYS:HG2	1:C:629:MET:HG3	1.94	0.49
1:D:25:GLU:O	1:D:29:PHE:N	2.40	0.49
1:D:77:TYR:OH	1:D:101:PHE:O	2.22	0.49
1:D:764:ASN:O	1:D:769:ASP:N	2.38	0.49
1:B:441:LYS:NZ	1:B:442:LEU:O	2.46	0.49
1:D:1029:THR:HG22	1:D:1031:TYR:H	1.78	0.49
1:A:1130:ARG:HH12	1:A:1132:ASN:HD22	1.60	0.49
1:B:143:LEU:HD23	1:B:146:LEU:HD23	1.93	0.49
1:D:402:GLU:N	1:D:406:VAL:O	2.43	0.49
1:B:101:PHE:HA	1:B:114:ARG:HD2	1.94	0.48
1:C:480:THR:O	1:C:485:ARG:NH1	2.42	0.48
1:C:651:ASP:OD1	1:C:656:LYS:NZ	2.40	0.48
1:D:1007:VAL:O	1:D:1011:LEU:N	2.46	0.48
1:B:1007:VAL:O	1:B:1011:LEU:N	2.46	0.48
1:C:1130:ARG:HH12	1:C:1132:ASN:HD22	1.61	0.48
1:A:266:GLU:HG2	1:A:268:LYS:H	1.78	0.48
1:A:441:LYS:NZ	1:A:442:LEU:O	2.46	0.48
1:A:480:THR:O	1:A:485:ARG:NH1	2.42	0.48
1:A:654:SER:O	1:A:658:PHE:N	2.45	0.48
1:B:71:TYR:OH	1:B:308:ARG:O	2.25	0.48
1:B:77:TYR:OH	1:B:101:PHE:O	2.22	0.48
1:B:480:THR:O	1:B:485:ARG:NH1	2.42	0.48
1:A:788:SER:OG	1:A:791:ASN:N	2.44	0.48
1:A:1029:THR:HG22	1:A:1031:TYR:H	1.78	0.48
1:B:266:GLU:HG2	1:B:268:LYS:H	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1130:ARG:HH12	1:B:1132:ASN:HD22	1.61	0.48
1:C:402:GLU:N	1:C:406:VAL:O	2.43	0.48
1:C:1007:VAL:O	1:C:1011:LEU:N	2.46	0.48
1:C:1029:THR:HG22	1:C:1031:TYR:H	1.78	0.48
1:A:1184:LEU:HD12	1:A:1187:ILE:HD12	1.94	0.48
1:B:35:GLN:HB2	1:B:261:ARG:HH22	1.79	0.48
1:B:214:HIS:O	1:B:240:ALA:N	2.43	0.48
1:B:654:SER:O	1:B:658:PHE:N	2.45	0.48
1:B:668:ASP:O	1:B:672:THR:N	2.40	0.48
1:A:348:ASP:OD1	1:A:352:LYS:N	2.43	0.48
1:A:599:ARG:HD3	1:B:578:TRP:CD2	2.48	0.48
1:A:1007:VAL:O	1:A:1011:LEU:N	2.46	0.48
1:B:1029:THR:HG22	1:B:1031:TYR:H	1.78	0.48
1:D:506:LYS:HD2	1:D:719:ASP:HA	1.95	0.48
1:D:1184:LEU:HD12	1:D:1187:ILE:HD12	1.94	0.48
1:C:35:GLN:HB2	1:C:261:ARG:HH22	1.79	0.48
1:C:266:GLU:HG2	1:C:268:LYS:H	1.78	0.48
1:C:788:SER:OG	1:C:791:ASN:N	2.44	0.48
1:A:637:GLU:O	1:A:640:SER:OG	2.28	0.48
1:C:1033:LEU:HA	1:C:1175:TYR:HA	1.96	0.48
1:D:348:ASP:OD1	1:D:352:LYS:N	2.43	0.48
1:D:441:LYS:NZ	1:D:442:LEU:O	2.46	0.48
1:A:35:GLN:HB2	1:A:261:ARG:HH22	1.79	0.48
1:B:637:GLU:O	1:B:640:SER:OG	2.28	0.48
1:B:629:MET:HE3	1:B:631:SER:HB2	1.96	0.47
1:C:258:PHE:O	1:C:262:TRP:N	2.43	0.47
1:D:629:MET:HE3	1:D:631:SER:HB2	1.96	0.47
1:D:1033:LEU:HA	1:D:1175:TYR:HA	1.96	0.47
1:A:402:GLU:N	1:A:406:VAL:O	2.43	0.47
1:A:430:ALA:O	1:A:434:LYS:N	2.41	0.47
1:B:258:PHE:O	1:B:262:TRP:N	2.43	0.47
1:C:101:PHE:HA	1:C:114:ARG:HD2	1.94	0.47
1:D:266:GLU:HG2	1:D:268:LYS:H	1.79	0.47
1:A:266:GLU:HB3	1:A:269:GLU:HB3	1.96	0.47
1:B:402:GLU:O	1:B:406:VAL:N	2.43	0.47
1:C:71:TYR:OH	1:C:308:ARG:O	2.25	0.47
1:C:372:GLY:HA3	1:C:382:LEU:HA	1.96	0.47
1:D:372:GLY:HA3	1:D:382:LEU:HA	1.96	0.47
1:A:402:GLU:O	1:A:406:VAL:N	2.43	0.47
1:A:1033:LEU:HA	1:A:1175:TYR:HA	1.96	0.47
1:C:441:LYS:NZ	1:C:442:LEU:O	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1201:ILE:O	1:C:1205:LYS:N	2.46	0.47
1:D:668:ASP:O	1:D:672:THR:N	2.40	0.47
1:C:646:ALA:O	1:C:701:ALA:N	2.38	0.47
1:B:266:GLU:HB3	1:B:269:GLU:HB3	1.96	0.47
1:D:35:GLN:HB2	1:D:261:ARG:HH22	1.79	0.47
1:D:266:GLU:HB3	1:D:269:GLU:HB3	1.96	0.47
1:D:489:ILE:HA	1:D:738:LYS:HB2	1.97	0.47
1:D:602:GLY:O	1:D:606:TRP:N	2.37	0.47
1:C:538:VAL:O	1:C:542:LEU:N	2.43	0.47
1:A:489:ILE:HA	1:A:738:LYS:HB2	1.97	0.47
1:B:1033:LEU:HA	1:B:1175:TYR:HA	1.96	0.47
1:C:65:GLN:HA	1:C:68:ARG:HB2	1.97	0.47
1:C:1020:PHE:HD1	1:C:1114:LEU:HG	1.80	0.47
1:A:1020:PHE:HD1	1:A:1114:LEU:HG	1.80	0.47
1:B:372:GLY:HA3	1:B:382:LEU:HA	1.96	0.47
1:C:1194:VAL:HG22	1:C:1198:HIS:HE1	1.80	0.47
1:D:375:SER:HB3	1:D:378:ASP:HB2	1.97	0.47
1:B:375:SER:HB3	1:B:378:ASP:HB2	1.97	0.46
1:B:395:VAL:H	1:B:440:TYR:HA	1.81	0.46
1:B:1020:PHE:HD1	1:B:1114:LEU:HG	1.80	0.46
1:C:1148:ASN:ND2	1:C:1182:GLY:O	2.42	0.46
1:D:691:ALA:HA	1:D:694:ARG:HB2	1.98	0.46
1:D:1020:PHE:HD1	1:D:1114:LEU:HG	1.80	0.46
1:B:430:ALA:O	1:B:434:LYS:N	2.41	0.46
1:B:489:ILE:HA	1:B:738:LYS:HB2	1.97	0.46
1:A:375:SER:HB3	1:A:378:ASP:HB2	1.97	0.46
1:B:751:LEU:HB2	1:C:483:LEU:HD13	1.98	0.46
1:D:1036:ARG:HG2	1:D:1057:MET:HG2	1.97	0.46
1:B:1036:ARG:HG2	1:B:1057:MET:HG2	1.98	0.46
1:C:489:ILE:HA	1:C:738:LYS:HB2	1.97	0.46
1:A:65:GLN:HA	1:A:68:ARG:HB2	1.97	0.46
1:B:691:ALA:HA	1:B:694:ARG:HB2	1.98	0.46
1:C:430:ALA:O	1:C:434:LYS:N	2.41	0.46
1:A:504:ILE:O	1:A:721:MET:N	2.49	0.46
1:A:691:ALA:HA	1:A:694:ARG:HB2	1.98	0.46
1:B:65:GLN:HA	1:B:68:ARG:HB2	1.97	0.46
1:B:1194:VAL:HG22	1:B:1198:HIS:HE1	1.80	0.46
1:C:375:SER:HB3	1:C:378:ASP:HB2	1.97	0.46
1:C:504:ILE:O	1:C:721:MET:N	2.49	0.46
1:D:1201:ILE:O	1:D:1205:LYS:N	2.46	0.46
1:A:483:LEU:HD13	1:D:751:LEU:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ILE:O	1:B:721:MET:N	2.49	0.46
1:D:71:TYR:OH	1:D:308:ARG:O	2.25	0.46
1:B:409:LYS:HG2	1:B:415:LEU:HD12	1.98	0.46
1:A:372:GLY:HA3	1:A:382:LEU:HA	1.96	0.45
1:A:1194:VAL:HG22	1:A:1198:HIS:HE1	1.80	0.45
1:B:375:SER:OG	1:B:376:GLU:OE1	2.34	0.45
1:B:1033:LEU:O	1:B:1060:SER:OG	2.32	0.45
1:C:525:ILE:HA	1:C:528:CYS:HB2	1.98	0.45
1:D:759:LEU:O	1:D:763:LYS:N	2.48	0.45
1:B:602:GLY:O	1:B:606:TRP:N	2.37	0.45
1:C:375:SER:OG	1:C:376:GLU:OE1	2.34	0.45
1:C:409:LYS:HG2	1:C:415:LEU:HD12	1.98	0.45
1:C:1036:ARG:HG2	1:C:1057:MET:HG2	1.97	0.45
1:A:628:ARG:NH2	1:A:780:SER:O	2.49	0.45
1:C:691:ALA:HA	1:C:694:ARG:HB2	1.98	0.45
1:C:1085:ASP:OD1	1:D:697:LYS:NZ	2.40	0.45
1:A:525:ILE:HA	1:A:528:CYS:HB2	1.98	0.45
1:C:673:TYR:O	1:C:677:ALA:N	2.50	0.45
1:D:402:GLU:O	1:D:406:VAL:N	2.43	0.45
1:D:1194:VAL:HG22	1:D:1198:HIS:HE1	1.80	0.45
1:A:375:SER:OG	1:A:376:GLU:OE1	2.34	0.45
1:C:266:GLU:HB3	1:C:269:GLU:HB3	1.97	0.45
1:C:628:ARG:NH2	1:C:780:SER:O	2.49	0.45
1:D:65:GLN:HA	1:D:68:ARG:HB2	1.97	0.45
1:D:511:LYS:HA	1:D:627:GLU:HA	1.98	0.45
1:A:1036:ARG:HG2	1:A:1057:MET:HG2	1.97	0.45
1:A:1201:ILE:O	1:A:1205:LYS:N	2.46	0.45
1:D:375:SER:OG	1:D:376:GLU:OE1	2.34	0.45
1:D:504:ILE:O	1:D:721:MET:N	2.49	0.45
1:C:764:ASN:O	1:C:769:ASP:N	2.38	0.45
1:D:209:ILE:HA	1:D:214:HIS:HD2	1.82	0.45
1:B:638:ASP:HA	1:B:641:LYS:HB2	1.99	0.45
1:C:638:ASP:HA	1:C:641:LYS:HB2	1.99	0.45
1:D:506:LYS:N	1:D:719:ASP:O	2.50	0.45
1:D:1106:PHE:O	1:D:1147:SER:OG	2.34	0.45
1:A:517:PHE:O	1:A:616:TYR:OH	2.35	0.45
1:A:673:TYR:O	1:A:677:ALA:N	2.50	0.45
1:A:1148:ASN:ND2	1:A:1182:GLY:O	2.42	0.45
1:C:1033:LEU:O	1:C:1060:SER:OG	2.32	0.45
1:A:492:SER:N	1:A:734:ILE:O	2.50	0.44
1:B:135:TYR:N	1:B:161:THR:O	2.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ILE:HA	1:B:214:HIS:HD2	1.82	0.44
1:B:1106:PHE:O	1:B:1147:SER:OG	2.34	0.44
1:C:135:TYR:N	1:C:161:THR:O	2.49	0.44
1:C:492:SER:N	1:C:734:ILE:O	2.50	0.44
1:A:1104:SER:O	1:A:1108:ILE:N	2.33	0.44
1:C:113:MET:HB3	1:C:284:LEU:HD22	2.00	0.44
1:C:209:ILE:HA	1:C:214:HIS:HD2	1.82	0.44
1:D:646:ALA:O	1:D:701:ALA:N	2.38	0.44
1:A:209:ILE:HA	1:A:214:HIS:HD2	1.82	0.44
1:A:668:ASP:O	1:A:672:THR:N	2.40	0.44
1:A:409:LYS:HG2	1:A:415:LEU:HD12	1.98	0.44
1:B:113:MET:HB3	1:B:284:LEU:HD22	2.00	0.44
1:D:409:LYS:HG2	1:D:415:LEU:HD12	1.98	0.44
1:D:673:TYR:O	1:D:677:ALA:N	2.50	0.44
1:A:54:ASN:OD1	1:B:87:SER:OG	2.33	0.44
1:B:511:LYS:HA	1:B:627:GLU:HA	1.99	0.44
1:B:673:TYR:O	1:B:677:ALA:N	2.50	0.44
1:C:190:ARG:HE	1:C:469:TYR:HB3	1.83	0.44
1:C:371:ILE:O	1:C:383:THR:N	2.42	0.44
1:A:214:HIS:O	1:A:240:ALA:N	2.43	0.44
1:A:638:ASP:HA	1:A:641:LYS:HB2	1.99	0.44
1:C:87:SER:OG	1:D:56:PHE:N	2.46	0.44
1:C:1174:SER:OG	1:C:1175:TYR:N	2.51	0.44
1:D:492:SER:N	1:D:734:ILE:O	2.50	0.43
1:A:369:ARG:HH12	1:A:386:ASP:HB2	1.84	0.43
1:B:23:ASP:O	1:B:27:SER:N	2.41	0.43
1:C:506:LYS:N	1:C:719:ASP:O	2.51	0.43
1:D:135:TYR:N	1:D:161:THR:O	2.49	0.43
1:A:113:MET:HB3	1:A:284:LEU:HD22	2.00	0.43
1:B:16:GLY:O	1:B:48:ASP:N	2.50	0.43
1:B:646:ALA:O	1:B:701:ALA:N	2.38	0.43
1:C:16:GLY:O	1:C:48:ASP:N	2.50	0.43
1:C:97:ILE:HG13	1:C:111:ILE:HB	2.01	0.43
1:A:15:GLY:O	1:A:74:PHE:N	2.52	0.43
1:A:326:GLY:HA2	1:A:329:ILE:HD12	2.01	0.43
1:A:1106:PHE:O	1:A:1147:SER:OG	2.34	0.43
1:D:638:ASP:HA	1:D:641:LYS:HB2	1.99	0.43
1:A:692:ARG:O	1:A:696:SER:OG	2.29	0.43
1:B:492:SER:N	1:B:734:ILE:O	2.50	0.43
1:B:545:ARG:H	1:B:569:ASN:ND2	2.17	0.43
1:B:97:ILE:HG13	1:B:111:ILE:HB	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:TYR:N	1:A:161:THR:O	2.49	0.43
1:B:602:GLY:HA2	1:B:605:TRP:HB3	2.00	0.43
1:B:1023:MET:HG3	1:B:1111:VAL:HG22	2.01	0.43
1:B:1201:ILE:O	1:B:1205:LYS:N	2.46	0.43
1:D:326:GLY:HA2	1:D:329:ILE:HD12	2.01	0.43
1:D:1174:SER:OG	1:D:1175:TYR:N	2.51	0.43
1:A:16:GLY:O	1:A:48:ASP:N	2.50	0.43
1:B:404:PRO:O	1:B:424:TYR:N	2.49	0.43
1:C:1106:PHE:O	1:C:1147:SER:OG	2.34	0.43
1:D:23:ASP:O	1:D:27:SER:N	2.41	0.43
1:D:388:SER:OG	1:D:391:GLU:OE2	2.37	0.43
1:A:452:ALA:N	1:A:461:ASN:OD1	2.43	0.43
1:C:209:ILE:HG13	1:C:214:HIS:CD2	2.54	0.43
1:C:670:MET:HB3	1:C:674:MET:HE2	2.01	0.43
1:D:97:ILE:HG13	1:D:111:ILE:HB	2.01	0.43
1:B:15:GLY:O	1:B:74:PHE:N	2.52	0.42
1:B:501:SER:HB2	1:B:709:ASN:HD22	1.84	0.42
1:D:113:MET:HB3	1:D:284:LEU:HD22	2.00	0.42
1:D:258:PHE:O	1:D:262:TRP:N	2.43	0.42
1:D:415:LEU:HD23	1:D:415:LEU:HA	1.87	0.42
1:D:501:SER:HB2	1:D:709:ASN:HD22	1.84	0.42
1:B:209:ILE:HG13	1:B:214:HIS:CD2	2.54	0.42
1:B:500:ILE:HB	1:B:727:LEU:HB2	2.01	0.42
1:C:517:PHE:O	1:C:616:TYR:OH	2.36	0.42
1:D:214:HIS:O	1:D:240:ALA:N	2.43	0.42
1:A:599:ARG:HB3	1:B:578:TRP:CZ3	2.54	0.42
1:A:759:LEU:O	1:A:763:LYS:N	2.48	0.42
1:A:1023:MET:HG3	1:A:1111:VAL:HG22	2.01	0.42
1:C:1023:MET:HG3	1:C:1111:VAL:HG22	2.01	0.42
1:D:209:ILE:HG13	1:D:214:HIS:CD2	2.54	0.42
1:D:602:GLY:HA2	1:D:605:TRP:HB3	2.00	0.42
1:D:1104:SER:O	1:D:1108:ILE:N	2.33	0.42
1:D:15:GLY:O	1:D:74:PHE:N	2.52	0.42
1:D:670:MET:HB3	1:D:674:MET:HE2	2.01	0.42
1:B:451:GLY:HA3	1:B:464:VAL:HG23	2.02	0.42
1:C:214:HIS:O	1:C:240:ALA:N	2.43	0.42
1:C:728:ASP:N	1:C:728:ASP:OD1	2.52	0.42
1:D:500:ILE:HB	1:D:727:LEU:HB2	2.01	0.42
1:D:545:ARG:H	1:D:569:ASN:ND2	2.17	0.42
1:D:1023:MET:HG3	1:D:1111:VAL:HG22	2.01	0.42
1:A:500:ILE:HB	1:A:727:LEU:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:SER:OG	1:D:54:ASN:OD1	2.25	0.42
1:C:1075:LEU:HD13	1:C:1075:LEU:HA	1.92	0.42
1:B:759:LEU:O	1:B:763:LYS:N	2.48	0.42
1:C:15:GLY:O	1:C:74:PHE:N	2.52	0.42
1:C:451:GLY:HA3	1:C:464:VAL:HG23	2.02	0.42
1:C:549:TYR:HE1	1:C:1204:HIS:CE1	2.38	0.42
1:D:451:GLY:HA3	1:D:464:VAL:HG23	2.02	0.42
1:A:501:SER:HB2	1:A:709:ASN:HD22	1.84	0.42
1:A:728:ASP:OD1	1:A:728:ASP:N	2.52	0.42
1:B:213:LYS:O	1:B:220:TYR:OH	2.23	0.42
1:A:97:ILE:HG13	1:A:111:ILE:HB	2.01	0.42
1:C:77:TYR:OH	1:C:101:PHE:O	2.22	0.42
1:D:522:ALA:HB3	1:D:525:ILE:HG13	2.01	0.42
1:A:209:ILE:HG13	1:A:214:HIS:CD2	2.54	0.42
1:A:451:GLY:HA3	1:A:464:VAL:HG23	2.02	0.42
1:B:326:GLY:HA2	1:B:329:ILE:HD12	2.01	0.42
1:C:326:GLY:HA2	1:C:329:ILE:HD12	2.01	0.42
1:C:501:SER:HB2	1:C:709:ASN:HD22	1.84	0.42
1:D:208:VAL:O	1:D:212:GLY:N	2.53	0.42
1:D:728:ASP:N	1:D:728:ASP:OD1	2.52	0.42
1:A:52:VAL:HG22	1:A:78:ASP:HB2	2.02	0.41
1:A:751:LEU:HB2	1:D:483:LEU:HD13	2.00	0.41
1:A:765:LYS:HE3	1:A:766:TRP:CZ2	2.55	0.41
1:B:503:MET:HE3	1:B:704:LEU:HD11	2.02	0.41
1:C:208:VAL:O	1:C:212:GLY:N	2.53	0.41
1:C:404:PRO:O	1:C:424:TYR:N	2.49	0.41
1:C:704:LEU:HD13	1:C:708:MET:HB2	2.02	0.41
1:D:704:LEU:HD13	1:D:708:MET:HB2	2.02	0.41
1:B:52:VAL:HG22	1:B:78:ASP:HB2	2.02	0.41
1:B:388:SER:OG	1:B:391:GLU:OE2	2.37	0.41
1:B:611:ILE:HD12	1:B:611:ILE:HA	1.92	0.41
1:B:1104:SER:O	1:B:1108:ILE:N	2.33	0.41
1:A:670:MET:HB3	1:A:674:MET:HE2	2.01	0.41
1:B:208:VAL:O	1:B:212:GLY:N	2.53	0.41
1:B:291:VAL:HG13	1:B:336:VAL:HG11	2.03	0.41
1:B:453:ARG:HG3	1:B:458:LYS:HD2	2.02	0.41
1:C:52:VAL:HG22	1:C:78:ASP:HB2	2.02	0.41
1:C:213:LYS:O	1:C:220:TYR:OH	2.23	0.41
1:C:500:ILE:HB	1:C:727:LEU:HB2	2.01	0.41
1:C:765:LYS:HE3	1:C:766:TRP:CZ2	2.56	0.41
1:D:236:GLN:HA	1:D:363:LEU:HD21	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:654:SER:N	2:D:1301:GLU:OE2	2.54	0.41
1:A:208:VAL:O	1:A:212:GLY:N	2.53	0.41
1:A:503:MET:HE3	1:A:704:LEU:HD11	2.02	0.41
1:A:654:SER:N	2:A:1301:GLU:OE2	2.54	0.41
1:B:670:MET:HB3	1:B:674:MET:HE2	2.01	0.41
1:B:1201:ILE:HD12	1:B:1201:ILE:HA	1.95	0.41
1:A:400:ILE:HG21	1:A:450:TYR:HE1	1.86	0.41
1:B:522:ALA:HB3	1:B:525:ILE:HG13	2.01	0.41
1:B:728:ASP:OD1	1:B:728:ASP:N	2.52	0.41
1:D:52:VAL:HG22	1:D:78:ASP:HB2	2.02	0.41
1:A:236:GLN:HA	1:A:363:LEU:HD21	2.03	0.41
1:A:318:ASN:HA	1:A:319:PRO:HA	1.91	0.41
1:B:330:GLU:HA	1:B:333:LEU:HD12	2.03	0.41
1:C:330:GLU:HA	1:C:333:LEU:HD12	2.03	0.41
1:D:291:VAL:HG13	1:D:336:VAL:HG11	2.03	0.41
1:B:654:SER:N	2:B:1301:GLU:OE2	2.54	0.41
1:B:704:LEU:HD13	1:B:708:MET:HB2	2.02	0.41
1:B:1075:LEU:HD13	1:B:1075:LEU:HA	1.92	0.41
1:C:372:GLY:HA2	1:C:383:THR:HG23	2.03	0.41
1:C:569:ASN:OD1	1:C:570:GLU:N	2.54	0.41
1:C:759:LEU:O	1:C:763:LYS:N	2.48	0.41
1:D:765:LYS:HE3	1:D:766:TRP:CZ2	2.56	0.41
1:A:23:ASP:O	1:A:27:SER:N	2.41	0.41
1:A:1075:LEU:HD13	1:A:1075:LEU:HA	1.92	0.41
1:B:597:SER:OG	1:C:806:ALA:O	2.39	0.41
1:D:372:GLY:HA2	1:D:383:THR:HG23	2.03	0.41
1:A:330:GLU:HA	1:A:333:LEU:HD12	2.03	0.41
1:A:372:GLY:HA2	1:A:383:THR:HG23	2.03	0.41
1:A:636:ALA:C	1:A:638:ASP:H	2.29	0.41
1:A:704:LEU:HD13	1:A:708:MET:HB2	2.02	0.41
1:B:372:GLY:HA2	1:B:383:THR:HG23	2.03	0.41
1:B:395:VAL:N	1:B:440:TYR:HA	2.35	0.41
1:B:636:ALA:C	1:B:638:ASP:H	2.29	0.41
1:B:649:THR:HG22	1:B:703:LEU:HB2	2.02	0.41
1:C:403:SER:HA	1:C:404:PRO:HA	1.87	0.41
1:C:453:ARG:HG3	1:C:458:LYS:HD2	2.02	0.41
1:B:236:GLN:HA	1:B:363:LEU:HD21	2.03	0.41
1:B:453:ARG:HA	1:B:460:TRP:HA	2.03	0.41
1:D:400:ILE:HG21	1:D:450:TYR:HE1	1.86	0.41
1:B:400:ILE:HG21	1:B:450:TYR:HE1	1.86	0.40
1:D:636:ALA:C	1:D:638:ASP:H	2.29	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:649:THR:HG22	1:D:703:LEU:HB2	2.02	0.40
1:C:480:THR:HG21	1:C:730:LYS:HD2	2.04	0.40
1:C:1066:CYS:HA	1:C:1076:CYS:HA	2.04	0.40
1:D:330:GLU:HA	1:D:333:LEU:HD12	2.03	0.40
1:D:453:ARG:HG3	1:D:458:LYS:HD2	2.02	0.40
1:D:503:MET:HE3	1:D:704:LEU:HD11	2.02	0.40
1:D:1066:CYS:HA	1:D:1076:CYS:HA	2.04	0.40
1:A:209:ILE:HA	1:A:214:HIS:CD2	2.57	0.40
1:A:453:ARG:HG3	1:A:458:LYS:HD2	2.02	0.40
1:A:1066:CYS:HA	1:A:1076:CYS:HA	2.04	0.40
1:C:452:ALA:N	1:C:461:ASN:OD1	2.43	0.40
1:D:480:THR:HG21	1:D:730:LYS:HD2	2.04	0.40
1:D:1108:ILE:O	1:D:1112:ILE:HG12	2.22	0.40
1:B:24:GLN:HE21	1:B:278:ILE:HG13	1.87	0.40
1:B:124:LEU:HB2	1:B:380:MET:HE1	2.04	0.40
1:B:765:LYS:HE3	1:B:766:TRP:CZ2	2.56	0.40
1:C:453:ARG:HA	1:C:460:TRP:HA	2.03	0.40
1:C:525:ILE:O	1:C:529:ILE:N	2.52	0.40
1:D:453:ARG:HA	1:D:460:TRP:HA	2.03	0.40
1:A:569:ASN:OD1	1:A:570:GLU:N	2.54	0.40
1:A:649:THR:HG22	1:A:703:LEU:HB2	2.02	0.40
1:B:65:GLN:O	1:B:69:GLY:N	2.55	0.40
1:B:1108:ILE:O	1:B:1112:ILE:HG12	2.22	0.40
1:C:291:VAL:HG13	1:C:336:VAL:HG11	2.03	0.40
1:C:346:LYS:HD3	1:C:355:ASN:HD22	1.87	0.40
1:C:463:MET:HE2	1:C:463:MET:HB3	1.90	0.40
1:C:577:LEU:O	1:C:580:SER:OG	2.35	0.40
1:C:654:SER:N	2:C:1301:GLU:OE2	2.54	0.40
1:D:493:LYS:HG2	1:D:747:ASN:HD21	1.87	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	978/1034 (95%)	910 (93%)	67 (7%)	1 (0%)	48	82
1	B	977/1034 (94%)	903 (92%)	74 (8%)	0	100	100
1	C	978/1034 (95%)	908 (93%)	69 (7%)	1 (0%)	48	82
1	D	977/1034 (94%)	903 (92%)	74 (8%)	0	100	100
All	All	3910/4136 (94%)	3624 (93%)	284 (7%)	2 (0%)	49	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	632	PRO
1	C	632	PRO

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	835/876 (95%)	832 (100%)	3 (0%)	84	82
1	B	833/876 (95%)	832 (100%)	1 (0%)	88	88
1	C	835/876 (95%)	832 (100%)	3 (0%)	84	82
1	D	832/876 (95%)	831 (100%)	1 (0%)	88	88
All	All	3335/3504 (95%)	3327 (100%)	8 (0%)	85	85

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	453	ARG
1	A	591	ILE
1	A	792	VAL
1	B	453	ARG
1	C	453	ARG
1	C	591	ILE
1	C	792	VAL
1	D	453	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	170	ASN
1	A	214	HIS
1	A	298	ASN
1	A	337	GLN
1	A	412	HIS
1	A	508	GLN
1	A	587	GLN
1	A	709	ASN
1	A	764	ASN
1	A	1132	ASN
1	B	24	GLN
1	B	214	HIS
1	B	298	ASN
1	B	337	GLN
1	B	412	HIS
1	B	569	ASN
1	B	709	ASN
1	B	764	ASN
1	B	791	ASN
1	B	1132	ASN
1	C	24	GLN
1	C	170	ASN
1	C	214	HIS
1	C	298	ASN
1	C	337	GLN
1	C	412	HIS
1	C	508	GLN
1	C	709	ASN
1	C	764	ASN
1	C	1132	ASN
1	D	24	GLN
1	D	214	HIS
1	D	298	ASN
1	D	337	GLN
1	D	412	HIS
1	D	569	ASN
1	D	709	ASN
1	D	764	ASN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLU	A	1301	-	8,9,9	1.10	1 (12%)	8,11,11	1.19	1 (12%)
2	GLU	C	1301	-	8,9,9	1.10	1 (12%)	8,11,11	1.19	1 (12%)
2	GLU	D	1301	-	8,9,9	1.12	1 (12%)	8,11,11	1.19	1 (12%)
3	CYZ	C	1302	-	26,27,27	4.47	10 (38%)	38,44,44	2.95	15 (39%)
3	CYZ	D	1302	-	26,27,27	4.46	10 (38%)	38,44,44	2.95	18 (47%)
3	CYZ	B	1302	-	26,27,27	4.47	10 (38%)	38,44,44	2.94	17 (44%)
3	CYZ	A	1302	-	26,27,27	4.46	10 (38%)	38,44,44	2.81	14 (36%)
2	GLU	B	1301	-	8,9,9	1.12	1 (12%)	8,11,11	1.19	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	-	-	0/9/9/9	-
2	GLU	C	1301	-	-	0/9/9/9	-
2	GLU	D	1301	-	-	1/9/9/9	-
3	CYZ	C	1302	-	-	1/7/42/42	0/5/4/4
3	CYZ	D	1302	-	-	0/7/42/42	0/5/4/4
3	CYZ	B	1302	-	-	0/7/42/42	0/5/4/4
3	CYZ	A	1302	-	-	0/7/42/42	0/5/4/4
2	GLU	B	1301	-	-	1/9/9/9	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1302	CYZ	C1-C8	-14.86	1.40	1.53
3	D	1302	CYZ	C1-C8	-14.78	1.40	1.53
3	C	1302	CYZ	C1-C8	-14.75	1.40	1.53
3	A	1302	CYZ	C1-C8	-14.67	1.40	1.53
3	A	1302	CYZ	C6-C1	8.49	1.75	1.53
3	B	1302	CYZ	C6-C1	8.48	1.75	1.53
3	D	1302	CYZ	C6-C1	8.47	1.75	1.53
3	C	1302	CYZ	C6-C1	8.46	1.75	1.53
3	A	1302	CYZ	C4-C3	-6.69	1.13	1.32
3	B	1302	CYZ	C4-C3	-6.69	1.13	1.32
3	C	1302	CYZ	C4-C3	-6.68	1.13	1.32
3	D	1302	CYZ	C4-C3	-6.65	1.13	1.32
3	A	1302	CYZ	O1-S1	6.62	1.51	1.43
3	C	1302	CYZ	O1-S1	6.60	1.51	1.43
3	C	1302	CYZ	O2-S1	6.49	1.51	1.43
3	A	1302	CYZ	O2-S1	6.47	1.51	1.43
3	B	1302	CYZ	O2-S1	6.41	1.51	1.43
3	C	1302	CYZ	C2-C1	-6.38	1.42	1.55
3	D	1302	CYZ	O2-S1	6.37	1.50	1.43
3	B	1302	CYZ	O1-S1	6.36	1.50	1.43
3	D	1302	CYZ	O1-S1	6.35	1.50	1.43
3	B	1302	CYZ	C2-C1	-6.30	1.42	1.55
3	A	1302	CYZ	C2-C1	-6.29	1.42	1.55
3	D	1302	CYZ	C2-C1	-6.29	1.42	1.55
3	D	1302	CYZ	C7-C2	-4.74	1.43	1.54
3	C	1302	CYZ	C7-C2	-4.72	1.43	1.54
3	B	1302	CYZ	C7-C2	-4.71	1.43	1.54
3	A	1302	CYZ	C7-C2	-4.69	1.43	1.54
3	D	1302	CYZ	S2-N3	2.97	1.66	1.60
3	B	1302	CYZ	S2-N3	2.87	1.66	1.60
3	C	1302	CYZ	S2-N3	2.84	1.66	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1302	CYZ	S2-N3	2.80	1.65	1.60
3	A	1302	CYZ	C2-C3	-2.63	1.44	1.51
3	B	1302	CYZ	C2-C3	-2.58	1.44	1.51
3	C	1302	CYZ	C2-C3	-2.55	1.44	1.51
3	D	1302	CYZ	C2-C3	-2.51	1.44	1.51
3	B	1302	CYZ	C7-C5	-2.29	1.39	1.52
3	C	1302	CYZ	C7-C5	-2.29	1.39	1.52
3	D	1302	CYZ	C7-C5	-2.28	1.39	1.52
3	A	1302	CYZ	C7-C5	-2.28	1.39	1.52
2	B	1301	GLU	OXT-C	-2.27	1.23	1.30
2	D	1301	GLU	OXT-C	-2.27	1.23	1.30
2	C	1301	GLU	OXT-C	-2.23	1.23	1.30
2	A	1301	GLU	OXT-C	-2.22	1.23	1.30

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1302	CYZ	O4-S2-O3	-12.00	100.33	118.80
3	A	1302	CYZ	O4-S2-O3	-11.42	101.23	118.80
3	B	1302	CYZ	O4-S2-O3	-11.37	101.31	118.80
3	D	1302	CYZ	O4-S2-O3	-11.18	101.61	118.80
3	D	1302	CYZ	C11-C9-S1	-5.26	115.63	119.82
3	C	1302	CYZ	C11-C9-S1	-5.07	115.78	119.82
3	A	1302	CYZ	C11-C9-S1	-5.04	115.80	119.82
3	B	1302	CYZ	C11-C9-S1	-4.98	115.86	119.82
3	C	1302	CYZ	O2-S1-O1	-4.94	113.42	118.44
3	A	1302	CYZ	O2-S1-O1	-4.79	113.56	118.44
3	B	1302	CYZ	O2-S1-O1	-4.65	113.70	118.44
3	D	1302	CYZ	O2-S1-O1	-4.64	113.72	118.44
3	B	1302	CYZ	O3-S2-N3	3.96	113.06	107.35
3	B	1302	CYZ	C11-C9-C10	3.89	124.73	120.85
3	C	1302	CYZ	O2-S1-N1	3.88	111.86	108.00
3	D	1302	CYZ	C11-C9-C10	3.86	124.71	120.85
3	D	1302	CYZ	O3-S2-N3	3.73	112.73	107.35
3	D	1302	CYZ	C1-C2-C3	3.70	112.57	106.86
3	C	1302	CYZ	C1-C2-C3	3.70	112.56	106.86
3	B	1302	CYZ	C1-C2-C3	3.68	112.54	106.86
3	C	1302	CYZ	C11-C9-C10	3.67	124.51	120.85
3	B	1302	CYZ	O1-S1-N1	3.59	111.57	108.00
3	D	1302	CYZ	C12-C13-CL	-3.54	118.95	121.52
3	A	1302	CYZ	C1-C2-C3	3.54	112.31	106.86
3	B	1302	CYZ	C12-C11-C9	-3.50	117.33	120.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1302	CYZ	C11-C9-C10	3.46	124.31	120.85
3	D	1302	CYZ	C12-C11-C9	-3.46	117.37	120.89
3	C	1302	CYZ	O4-S2-N3	3.46	112.34	107.35
3	C	1302	CYZ	O4-S2-C12	3.34	112.12	107.26
3	D	1302	CYZ	O1-S1-N1	3.28	111.26	108.00
3	D	1302	CYZ	O2-S1-N1	3.27	111.25	108.00
3	A	1302	CYZ	O4-S2-N3	3.26	112.06	107.35
3	B	1302	CYZ	O2-S1-N1	3.23	111.21	108.00
3	D	1302	CYZ	C6-C1-C2	-3.10	98.98	104.04
3	D	1302	CYZ	O4-S2-N3	3.05	111.76	107.35
3	B	1302	CYZ	C6-C1-C2	-3.05	99.07	104.04
3	B	1302	CYZ	O4-S2-N3	3.05	111.75	107.35
3	B	1302	CYZ	C12-C13-CL	-3.00	119.35	121.52
3	C	1302	CYZ	C9-S1-N1	-3.00	99.78	103.42
3	C	1302	CYZ	C5-C6-C1	-2.99	93.12	103.97
3	A	1302	CYZ	O3-S2-C12	2.99	111.61	107.26
3	A	1302	CYZ	O1-S1-N1	2.99	110.97	108.00
3	A	1302	CYZ	C5-C6-C1	-2.97	93.20	103.97
3	A	1302	CYZ	C6-C1-C2	-2.94	99.24	104.04
3	B	1302	CYZ	C5-C6-C1	-2.91	93.41	103.97
3	C	1302	CYZ	C6-C1-C2	-2.90	99.30	104.04
3	D	1302	CYZ	C5-C6-C1	-2.90	93.45	103.97
3	C	1302	CYZ	O1-S1-N1	2.90	110.88	108.00
3	A	1302	CYZ	O4-S2-C12	2.82	111.36	107.26
3	A	1302	CYZ	O2-S1-N1	2.72	110.70	108.00
3	D	1302	CYZ	C13-C12-S2	-2.60	120.35	123.47
3	C	1302	CYZ	C12-C11-C9	-2.59	118.26	120.89
3	C	1302	CYZ	O3-S2-C12	2.57	110.99	107.26
3	A	1302	CYZ	C12-C11-C9	-2.55	118.30	120.89
2	A	1301	GLU	OXT-C-O	-2.51	118.39	124.08
2	D	1301	GLU	OXT-C-O	-2.51	118.39	124.08
2	B	1301	GLU	OXT-C-O	-2.50	118.40	124.08
2	C	1301	GLU	OXT-C-O	-2.49	118.43	124.08
3	B	1302	CYZ	O4-S2-C12	2.45	110.82	107.26
3	B	1302	CYZ	C13-C12-S2	-2.38	120.61	123.47
3	D	1302	CYZ	C11-C12-C13	2.35	120.80	118.33
3	B	1302	CYZ	C9-S1-N1	-2.34	100.58	103.42
3	D	1302	CYZ	O4-S2-C12	2.32	110.64	107.26
3	B	1302	CYZ	C11-C12-C13	2.27	120.71	118.33
3	D	1302	CYZ	C9-S1-N1	-2.26	100.68	103.42
3	D	1302	CYZ	O3-S2-C12	2.20	110.45	107.26
3	C	1302	CYZ	O3-S2-N3	2.17	110.48	107.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1302	CYZ	C9-S1-N1	-2.03	100.95	103.42

There are no chirality outliers.

All (3) torsion outliers are listed below:

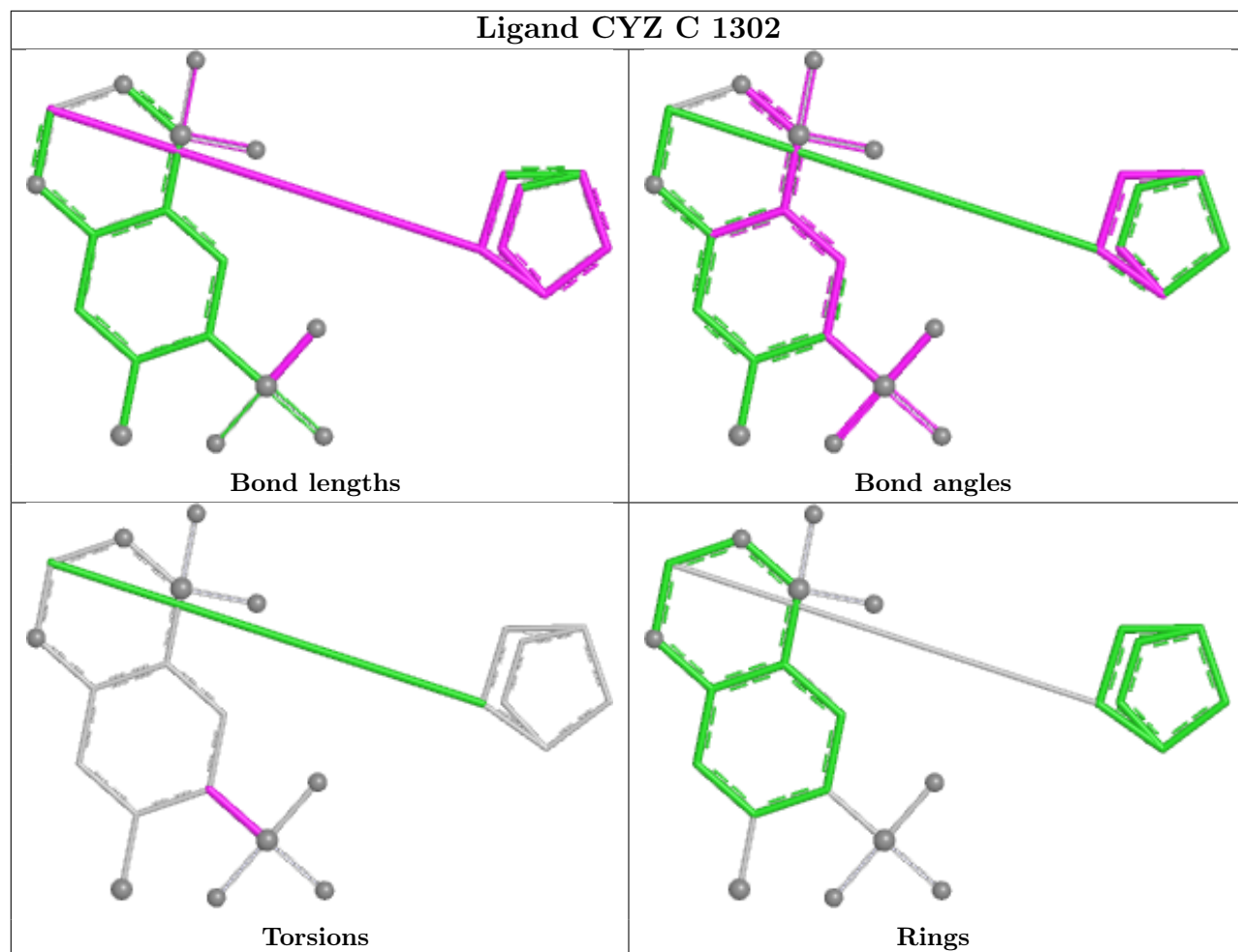
Mol	Chain	Res	Type	Atoms
3	C	1302	CYZ	C13-C12-S2-O3
2	B	1301	GLU	OXT-C-CA-N
2	D	1301	GLU	OXT-C-CA-N

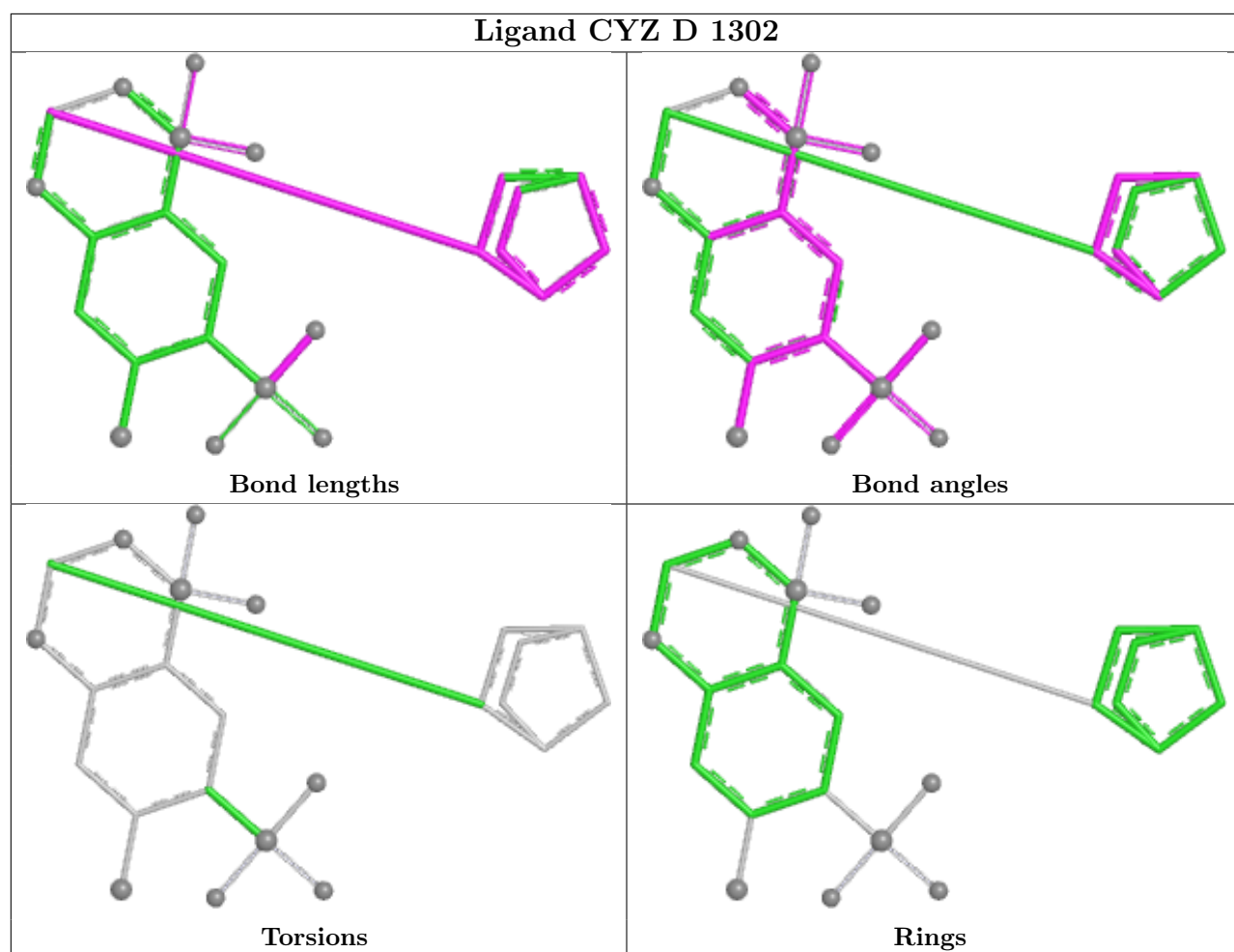
There are no ring outliers.

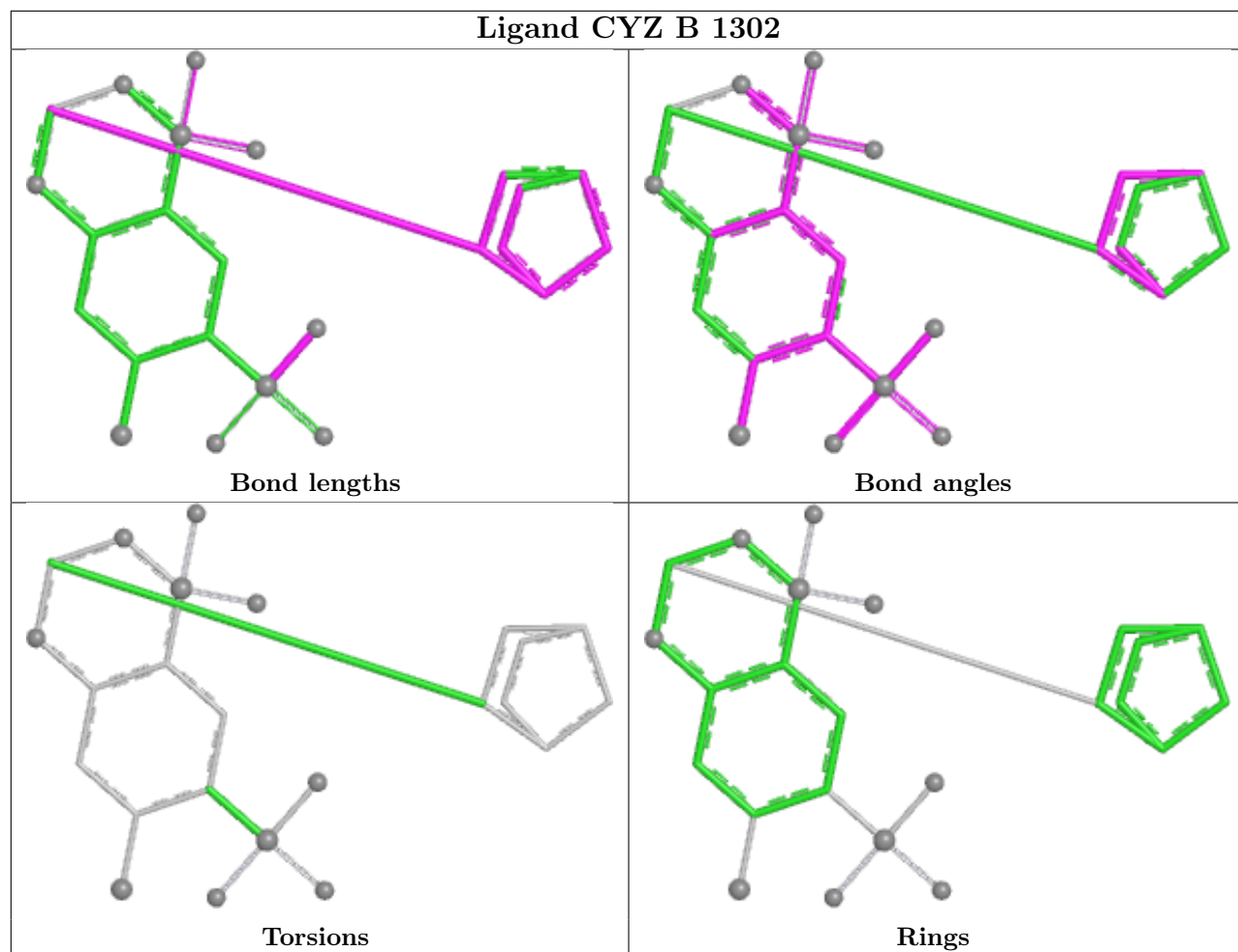
8 monomers are involved in 21 short contacts:

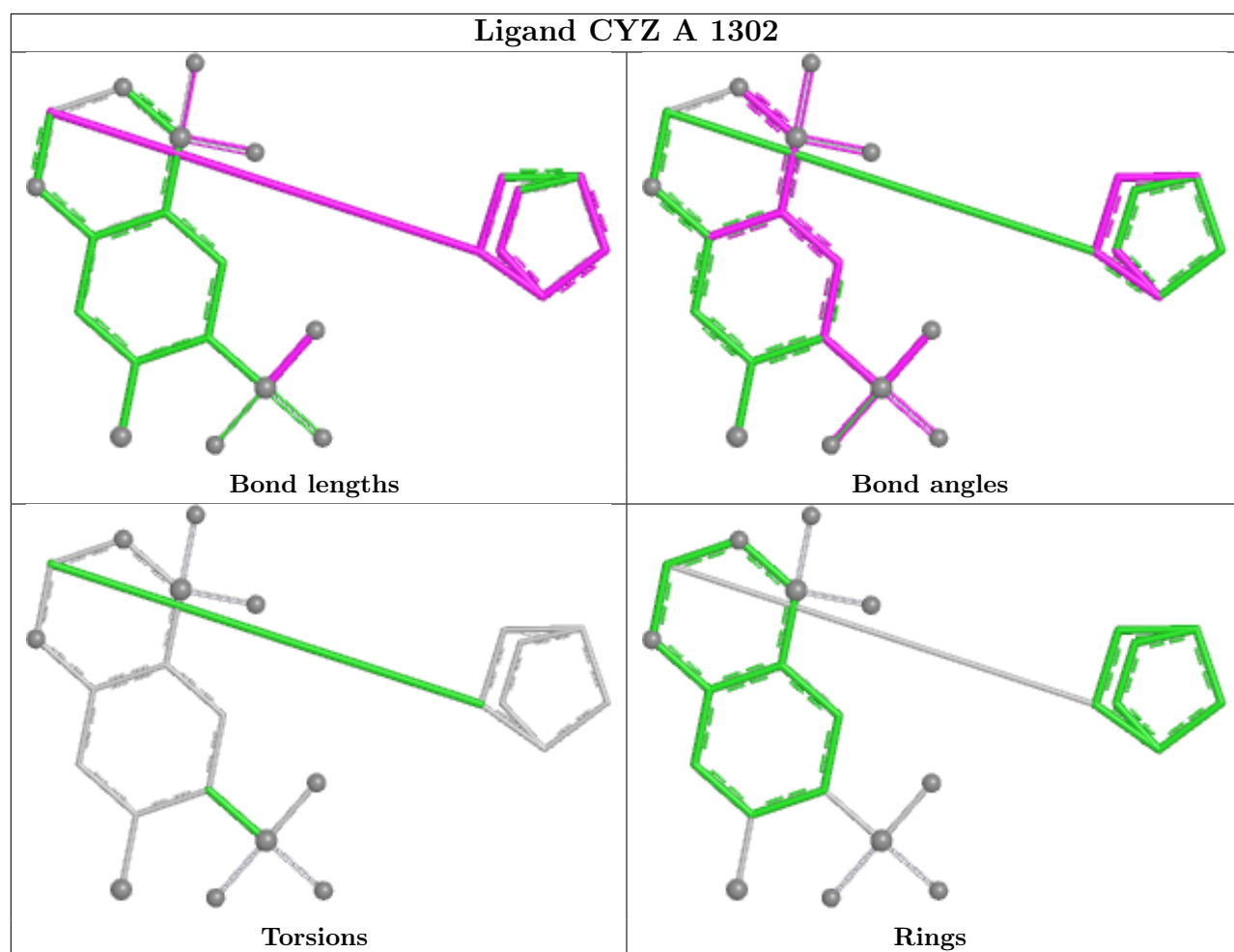
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	GLU	2	0
2	C	1301	GLU	2	0
2	D	1301	GLU	2	0
3	C	1302	CYZ	3	0
3	D	1302	CYZ	3	0
3	B	1302	CYZ	3	0
3	A	1302	CYZ	4	0
2	B	1301	GLU	2	0

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.









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.

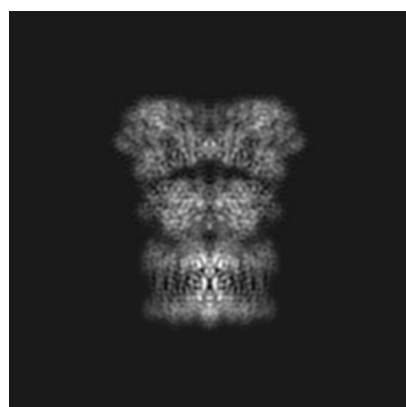
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8823. These allow visual inspection of the internal detail of the map and identification of artifacts.

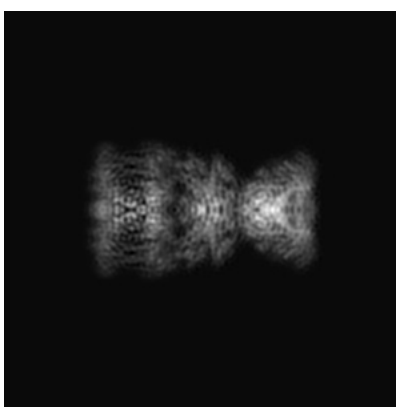
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

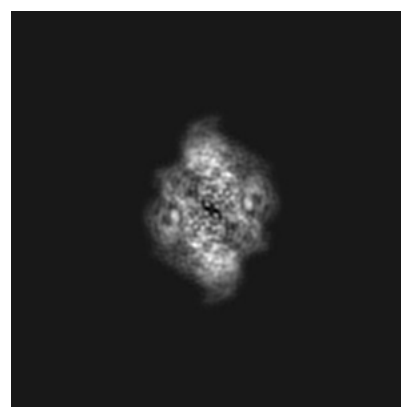
6.1.1 Primary map



X



Y



Z

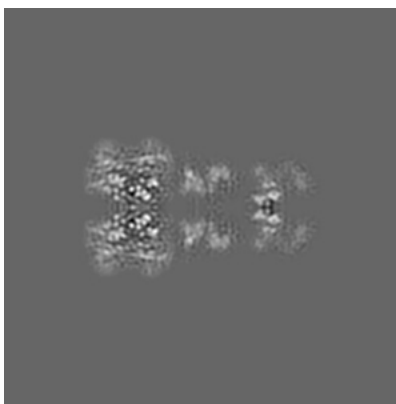
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

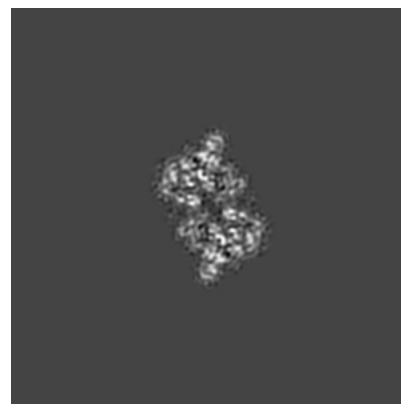
6.2.1 Primary map



X Index: 150



Y Index: 150

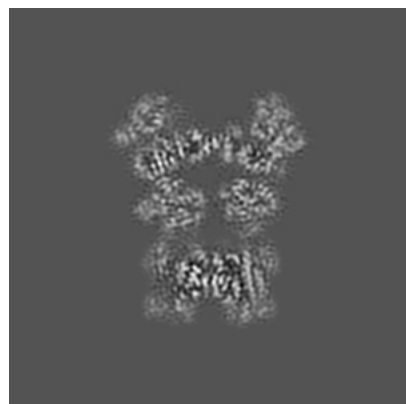


Z Index: 150

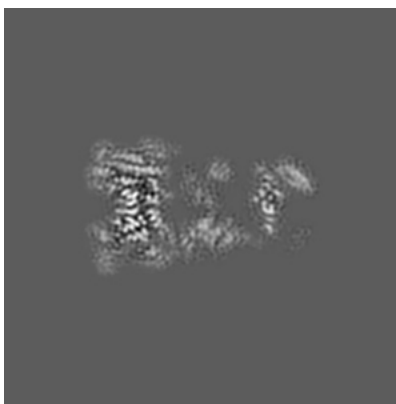
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

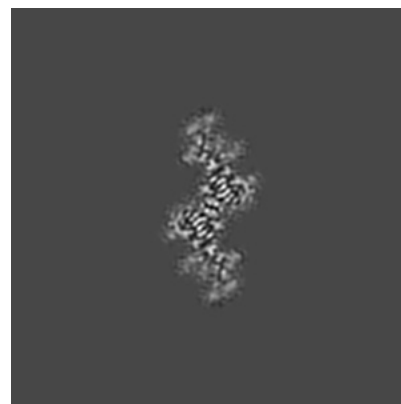
6.3.1 Primary map



X Index: 147



Y Index: 154

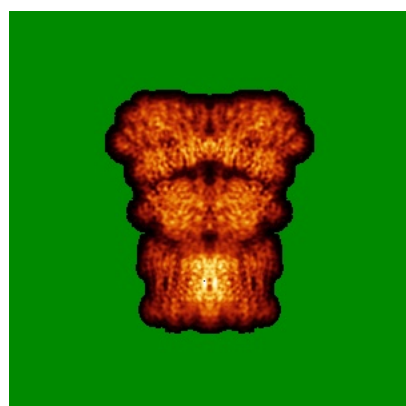


Z Index: 195

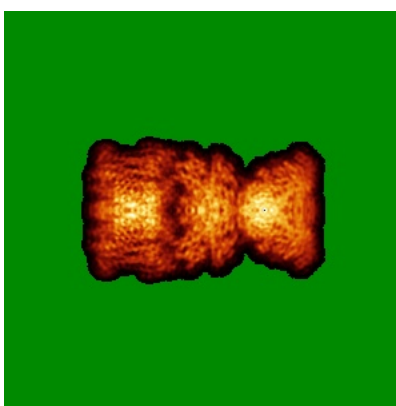
The images above show the largest variance slices of the map in three orthogonal directions.

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

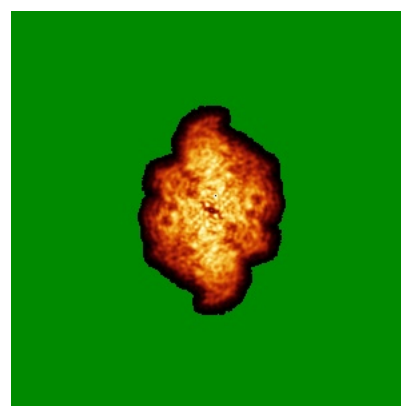
6.4.1 Primary map



X



Y

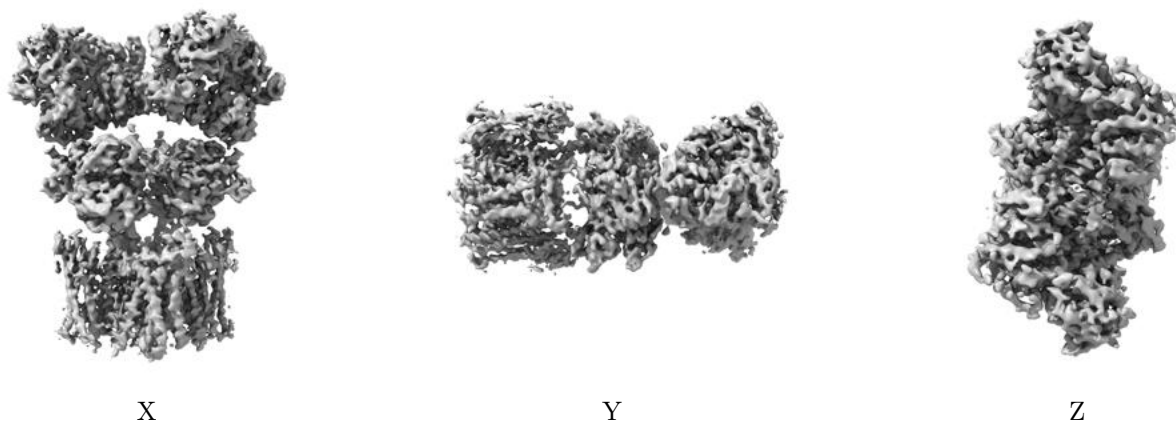


Z

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 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

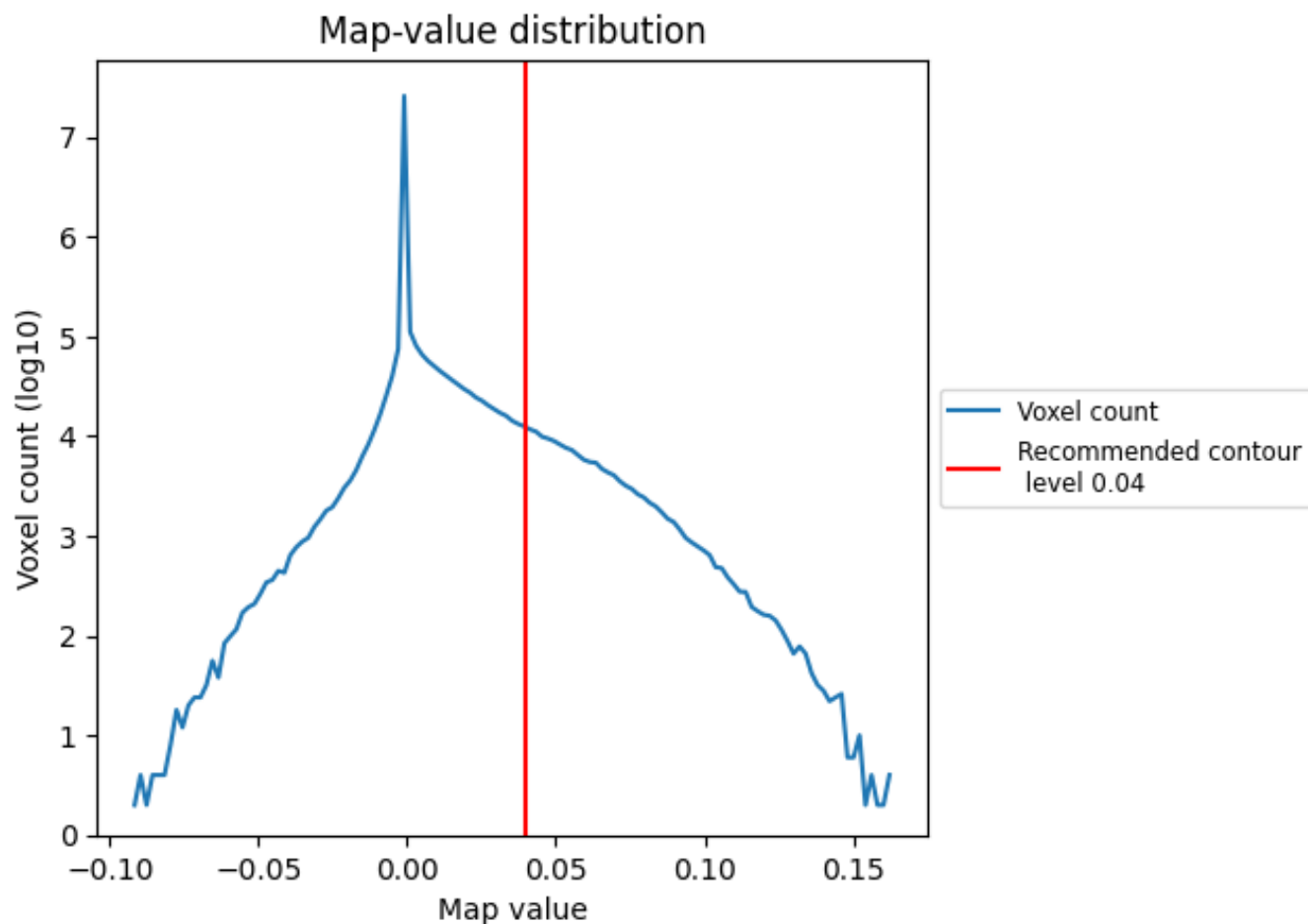
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

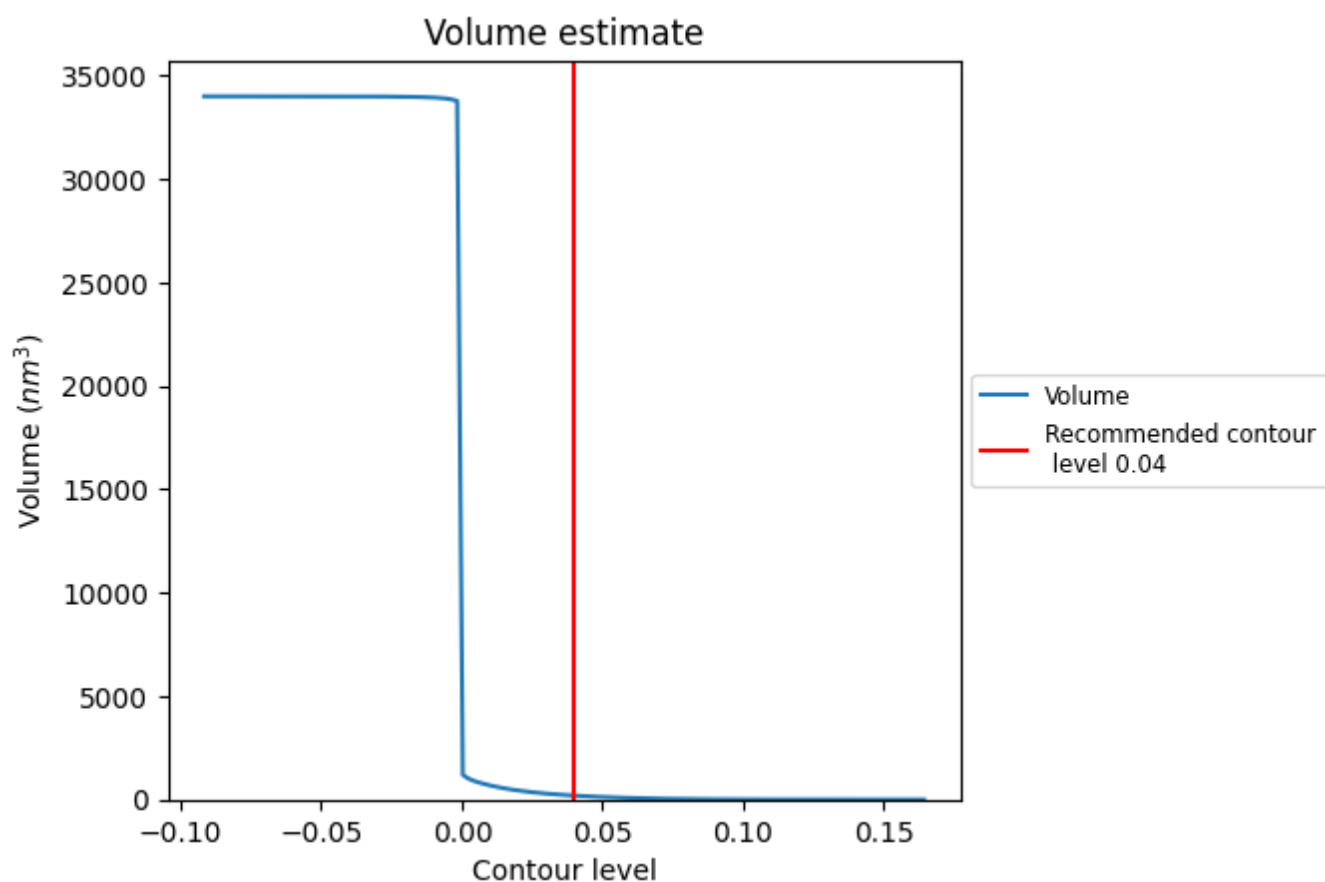
This section contains the results of statistical analysis of the map.

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.

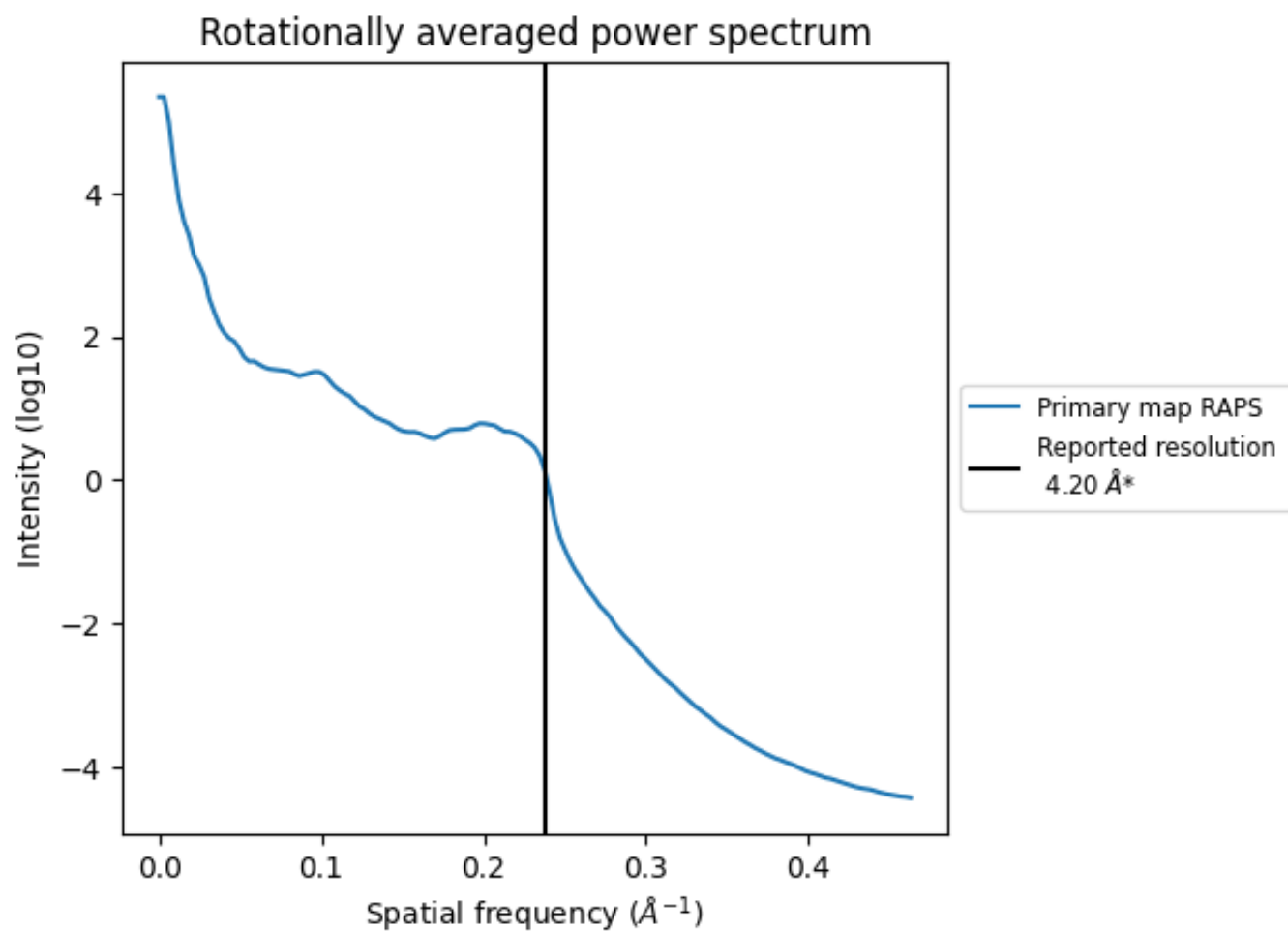
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm³; this corresponds to an approximate mass of 172 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 $\text{\AA}^{-1}$

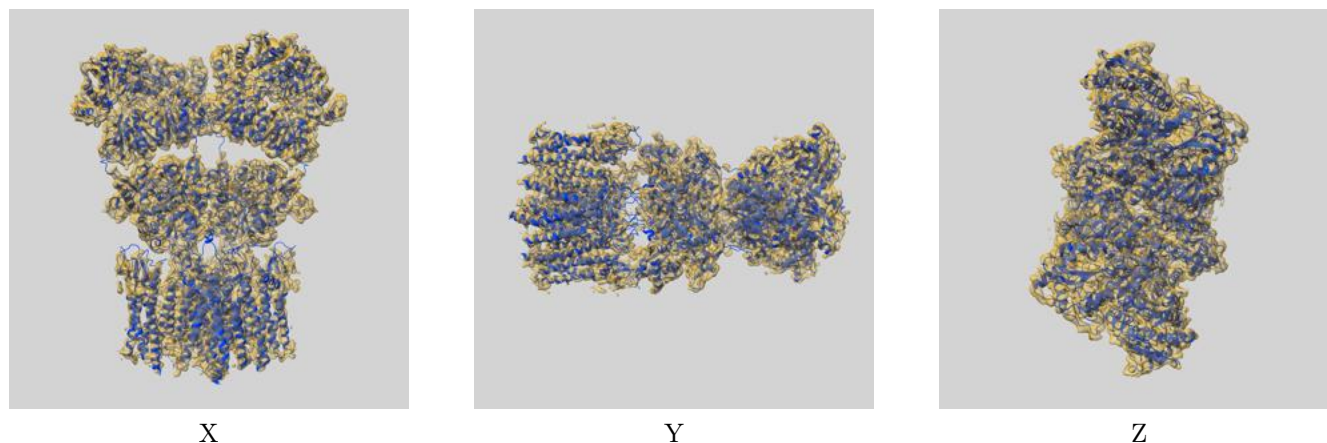
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

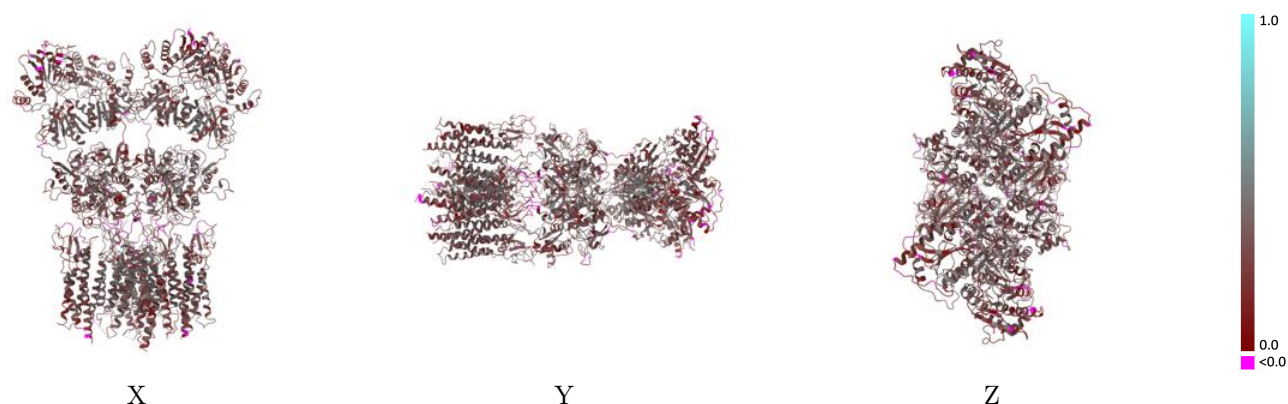
This section contains information regarding the fit between EMDB map EMD-8823 and PDB model 5WEO. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.04 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](#)

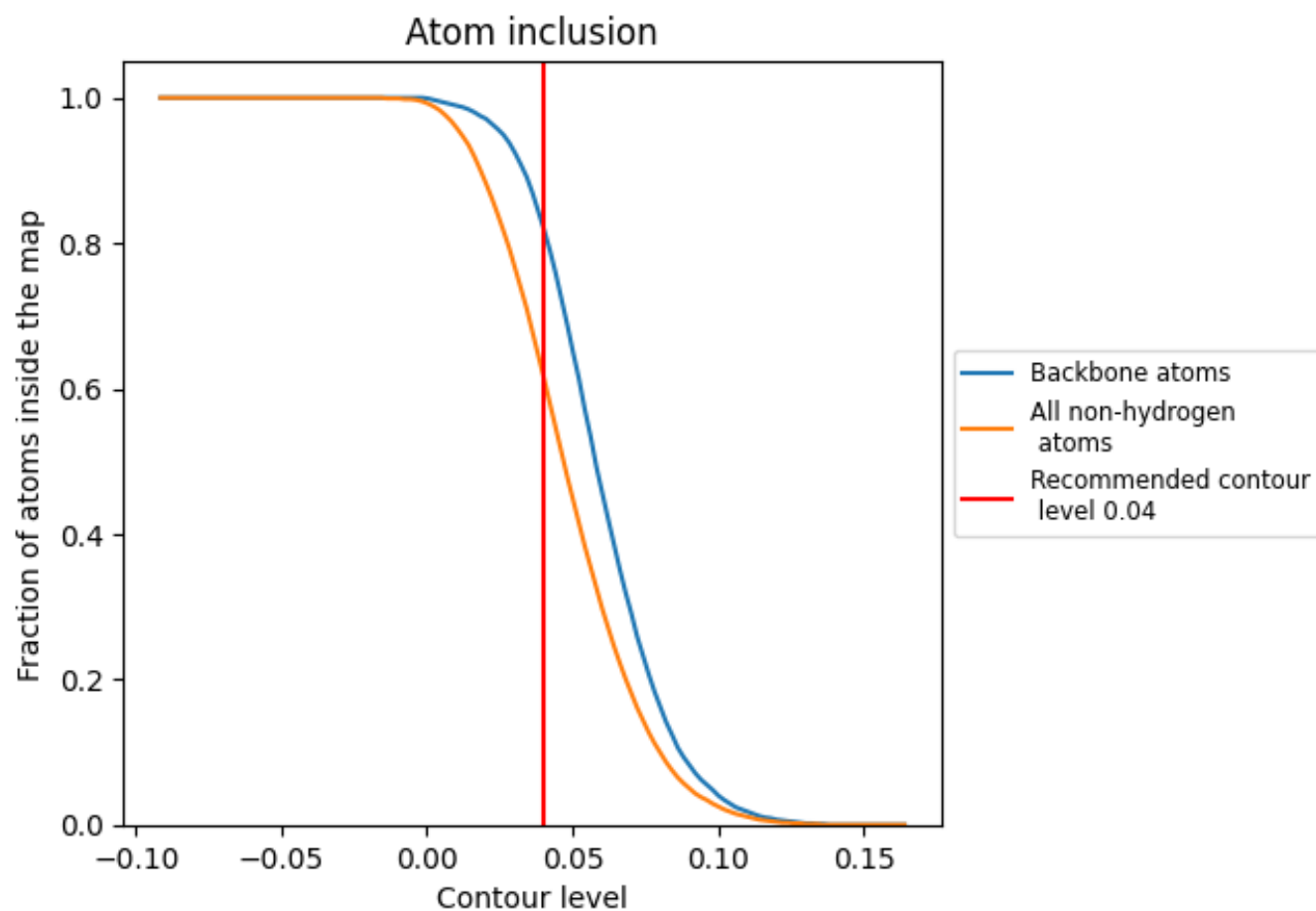


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 62% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6180	0.3140
A	0.6210	0.3170
B	0.6150	0.3090
C	0.6220	0.3200
D	0.6150	0.3090

