Full wwPDB EM Validation Report (i)

Nov 21, 2022 – 10:27 PM JST

PDB ID	:	7EB2
EMDB ID	:	EMD-31049
Title	:	Cryo-EM structure of human GABA(B) receptor-Gi protein complex
Authors	:	Shen, C.; Mao, C.; Xu, C.; Jin, N.; Zhang, H.; Shen, D.; Shen, Q.; Wang, X.; Hou, T.; Rondard, P.; Chen, Z.; Pin, J.; Zhang, Y.; Liu, J.
Deposited on	:	2021-03-08
Resolution	:	3.50 Å(reported)
Based on initial models	:	6PT0, 7C7Q

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 (i) 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 (1)) were used in the production of this report:

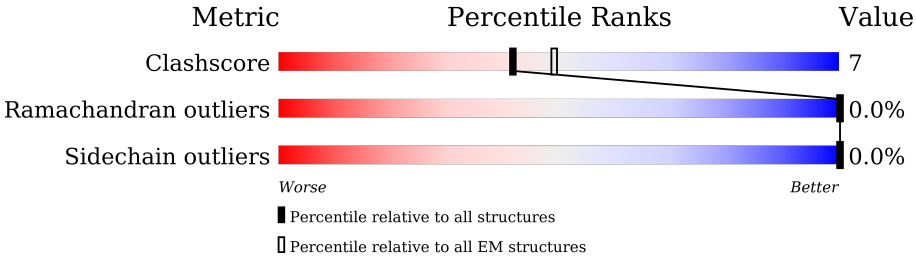
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	354	48%, 85%, 15%, •
2	B	358	7%, 94%, • 5%
3	Y	71	7%, 80%, 20%
4	N	269	10%, 84%, • 14%
5	C	937	•, 61%, 11%, 28%
6	D	808	8%, 68%, 16%, 16%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 18497 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 Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	352	2820	1782	480	540	18	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	engineered mutation	UNP P63096
A	203	ALA	GLY	engineered mutation	UNP P63096
A	245	ALA	GLU	engineered mutation	UNP P63096
A	326	SER	ALA	engineered mutation	UNP P63096

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	339	2607	1607	468	511	21	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	initiating methionine	UNP P62873
B	-16	HIS	-	expression tag	UNP P62873
B	-15	HIS	-	expression tag	UNP P62873
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	LEU	-	expression tag	UNP P62873
B	-9	GLU	-	expression tag	UNP P62873
B	-8	VAL	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873
B	-6	PHE	-	expression tag	UNP P62873

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLN	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Y	57	436	273	77	83	3	0	0

- Molecule 4 is a protein called ScFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	231	1777	1128	294	345	10	0	0

- Molecule 5 is a protein called Gamma-aminobutyric acid type B receptor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	678	5406	3503	897	981	25	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	expression tag	UNP Q9UBS5
C	0	LYS	-	expression tag	UNP Q9UBS5
C	1	THR	-	expression tag	UNP Q9UBS5
C	2	ILE	-	expression tag	UNP Q9UBS5
C	3	ILE	-	expression tag	UNP Q9UBS5
C	4	ALA	-	expression tag	UNP Q9UBS5
C	5	LEU	-	expression tag	UNP Q9UBS5
C	6	SER	-	expression tag	UNP Q9UBS5
C	7	TYR	-	expression tag	UNP Q9UBS5
C	8	ILE	-	expression tag	UNP Q9UBS5
C	9	PHE	-	expression tag	UNP Q9UBS5
C	10	CYS	-	expression tag	UNP Q9UBS5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	11	LEU	-	expression tag	UNP Q9UBS5
C	12	VAL	-	expression tag	UNP Q9UBS5
C	13	PHE	-	expression tag	UNP Q9UBS5
C	14	ALA	-	expression tag	UNP Q9UBS5
C	920	LEU	-	expression tag	UNP Q9UBS5
C	921	GLU	-	expression tag	UNP Q9UBS5
C	922	VAL	-	expression tag	UNP Q9UBS5
C	923	LEU	-	expression tag	UNP Q9UBS5
C	924	PHE	-	expression tag	UNP Q9UBS5
C	925	GLN	-	expression tag	UNP Q9UBS5
C	926	GLY	-	expression tag	UNP Q9UBS5
C	927	PRO	-	expression tag	UNP Q9UBS5
C	928	HIS	-	expression tag	UNP Q9UBS5
C	929	HIS	-	expression tag	UNP Q9UBS5
C	930	HIS	-	expression tag	UNP Q9UBS5
C	931	HIS	-	expression tag	UNP Q9UBS5
C	932	HIS	-	expression tag	UNP Q9UBS5
C	933	HIS	-	expression tag	UNP Q9UBS5
C	934	HIS	-	expression tag	UNP Q9UBS5
C	935	HIS	-	expression tag	UNP Q9UBS5

- Molecule 6 is a protein called Gamma-aminobutyric acid type B receptor subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	680	5414	3509	899	969	37	0	0

There are 29 discrepancies between the modelled and reference sequences:

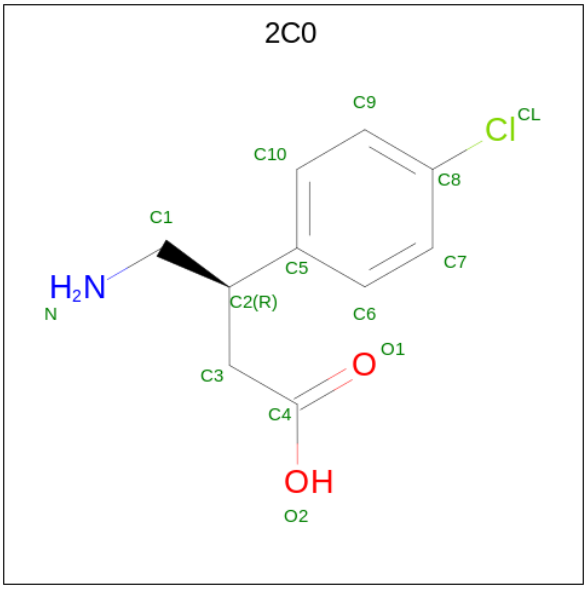
Chain	Residue	Modelled	Actual	Comment	Reference
D	12	MET	-	initiating methionine	UNP O75899
D	13	LYS	-	expression tag	UNP O75899
D	14	THR	-	expression tag	UNP O75899
D	15	ILE	-	expression tag	UNP O75899
D	16	ILE	-	expression tag	UNP O75899
D	17	ALA	-	expression tag	UNP O75899
D	18	LEU	-	expression tag	UNP O75899
D	19	SER	-	expression tag	UNP O75899
D	20	TYR	-	expression tag	UNP O75899
D	21	ILE	-	expression tag	UNP O75899
D	22	PHE	-	expression tag	UNP O75899
D	23	CYS	-	expression tag	UNP O75899

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	24	LEU	-	expression tag	UNP O75899
D	25	VAL	-	expression tag	UNP O75899
D	26	PHE	-	expression tag	UNP O75899
D	27	ALA	-	expression tag	UNP O75899
D	28	ASP	-	expression tag	UNP O75899
D	29	TYR	-	expression tag	UNP O75899
D	30	LYS	-	expression tag	UNP O75899
D	31	ASP	-	expression tag	UNP O75899
D	32	ASP	-	expression tag	UNP O75899
D	33	ASP	-	expression tag	UNP O75899
D	34	ASP	-	expression tag	UNP O75899
D	35	LYS	-	expression tag	UNP O75899
D	36	GLY	-	expression tag	UNP O75899
D	37	SER	-	expression tag	UNP O75899
D	38	GLY	-	expression tag	UNP O75899
D	39	GLY	-	expression tag	UNP O75899
D	40	SER	-	expression tag	UNP O75899

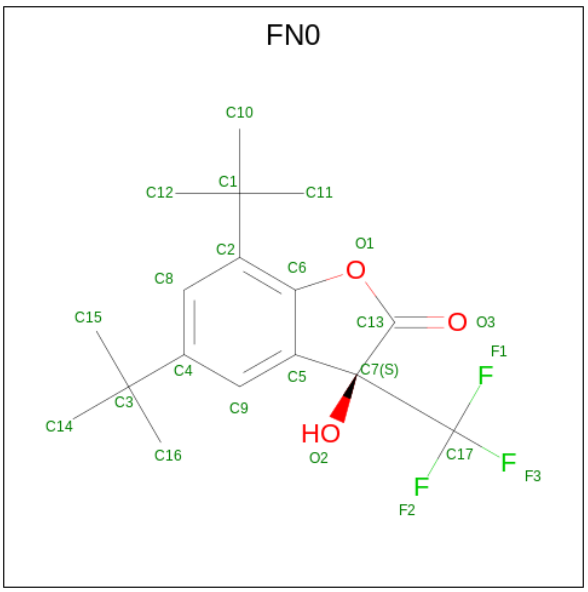
- Molecule 7 is baclofen (three-letter code: 2C0) (formula: $C_{10}H_{12}ClNO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
7	C	1	14	10	1	1	2	0

- Molecule 8 is (3S)-5,7-ditert-butyl-3-oxidanyl-3-(trifluoromethyl)-1-benzofuran-2-one (three-letter code: FN0) (formula: $C_{17}H_{21}F_3O_3$) (labeled as "Ligand of Interest" by

depositor).



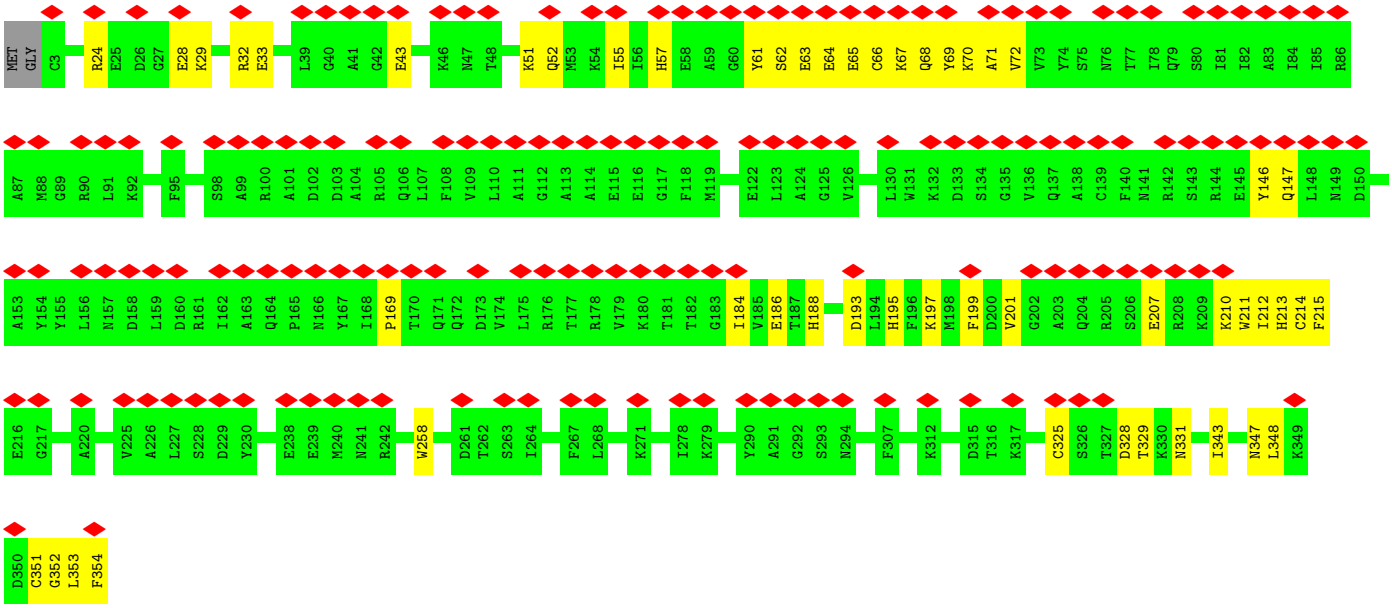
Mol	Chain	Residues	Atoms				AltConf
			Total	C	F	O	
8	D	1	23	17	3	3	0

3 Residue-property plots (i)

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.

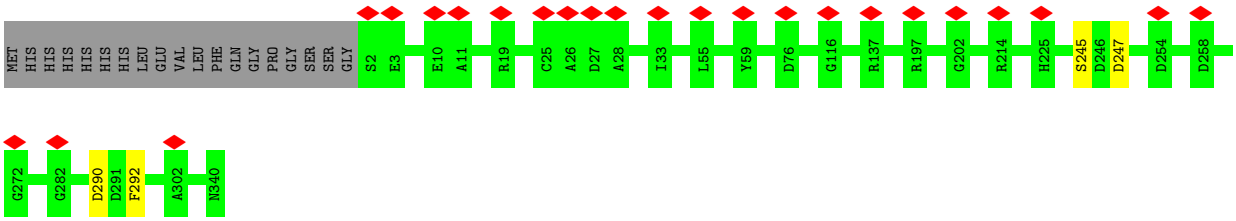
• Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain A: 48% 85% 15%



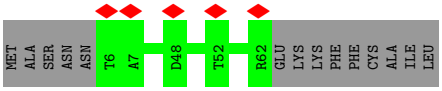
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B: 7% 94% 5%



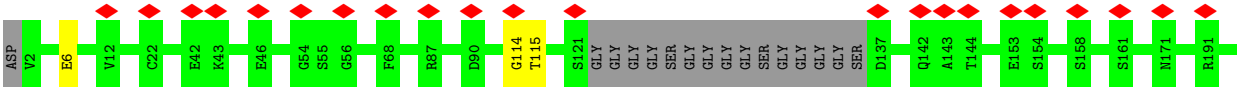
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

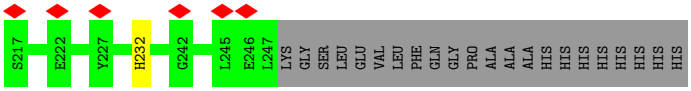
Chain Y: 7% 80% 20%



• Molecule 4: ScFv16

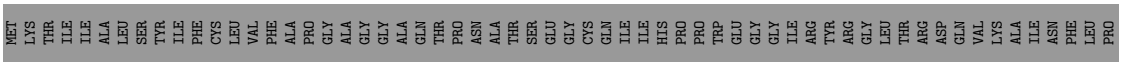
Chain N:

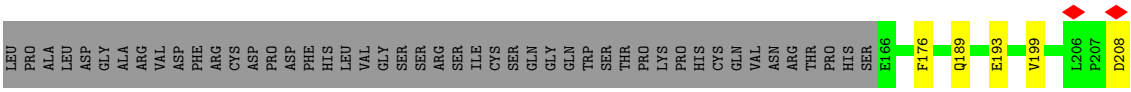


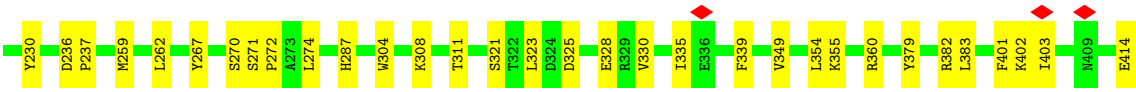


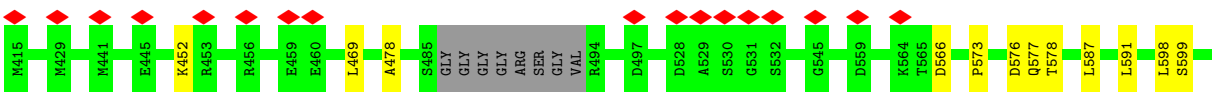
• Molecule 5: Gamma-aminobutyric acid type B receptor subunit 1

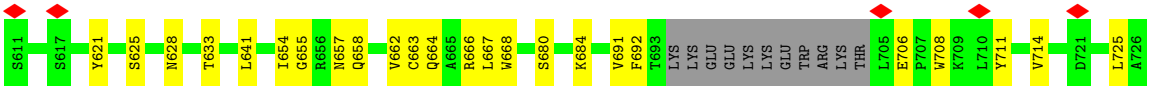
Chain C:

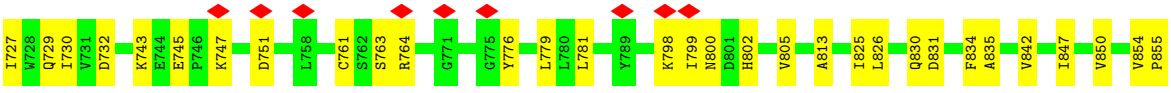


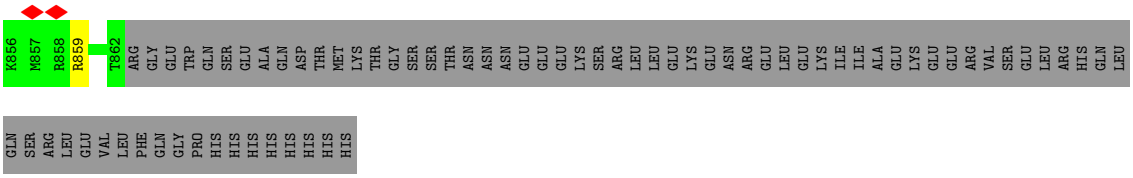








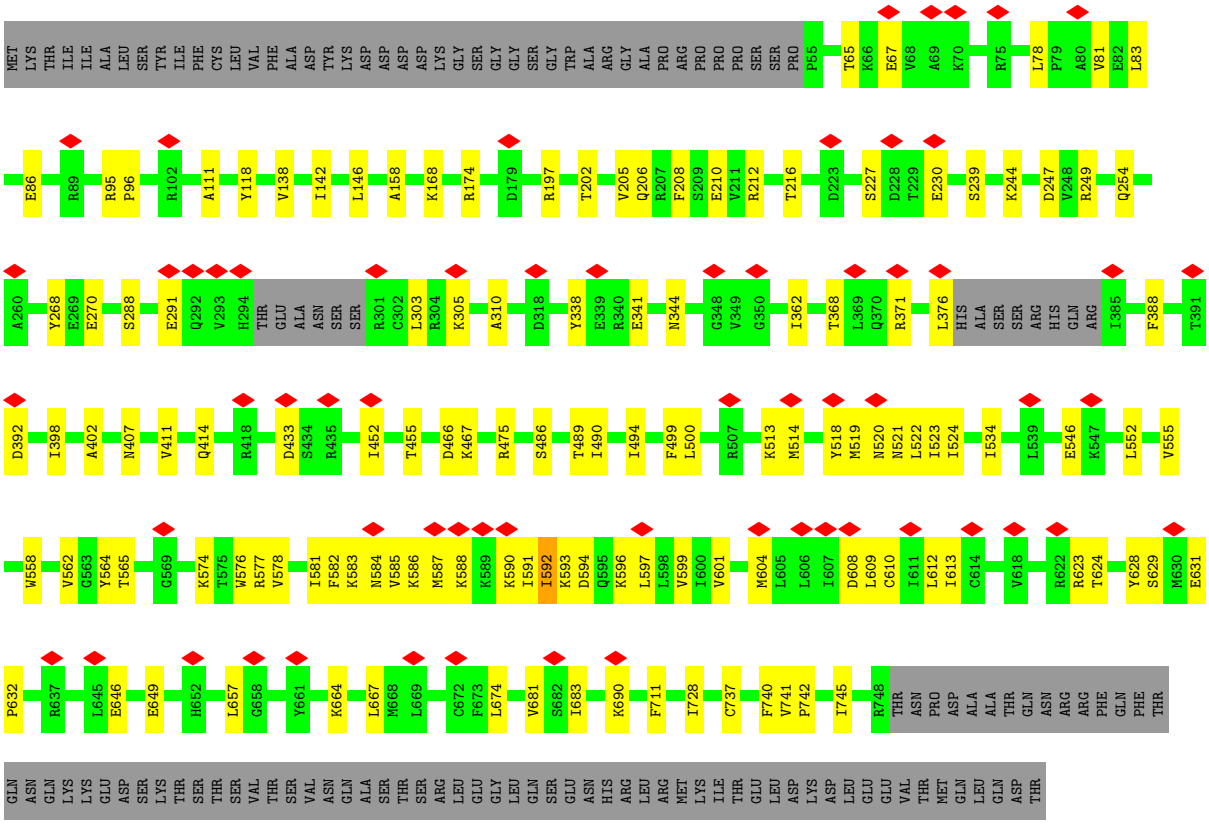




• Molecule 6: Gamma-aminobutyric acid type B receptor subunit 2

Chain D:

8%
68%
16%
16%


MET LYS THR ILE ILE ALA LEU SER TYR ILE PHE CYS LEU VAL PHE ALA ASP TYR LYS ASP ASP ASP ASP LYS GLY SER GLY GLY SER GLY TRP ALA ARG GLY ALA PRO ARG PRO PRO PRO SER SER PRO P55 T65 K66 E67 V68 A69 K70 R75 L78 F79 A80 V81 E82 L83
E86 R89 R95 P96 R102 A111 Y118 V138 I142 L146 A158 K168 R174 D179 R197 T202 V205 Q206 R207 F208 S209 E210 V211 R212 T216 D223 S227 D228 T229 E230 S239 K244 D247 V248 R249 Q254
A260 Y268 E269 E270 S288 E291 Q292 V293 H294 THR GLU ALA ASN SER SER R301 C302 L303 R304 K305 A310 D318 Y338 E339 R340 E341 N344 G348 V349 G350 I362 T368 L369 Q370 R371 L376 HIS ALA SER SER ARG HIS GLN ARG I385 F388 T391
D392 I398 A402 N407 V411 Q414 R418 D433 S434 R435 I452 T455 D466 K467 R475 S486 T489 I490 I494 F499 L500 R507 K513 M514 Y518 M519 N520 N521 L522 I523 I524 I534 L539 E546 K547 L552 V555
W558 V562 G563 Y564 T565 G569 K574 T575 W576 R577 V578 I581 F582 K583 N584 V585 K586 M587 K588 K589 K590 I591 I592 K593 D594 Q595 K596 L597 L598 V599 I600 V601 M604 L605 L606 I607 D608 L609 C610 I611 I612 I613 C614 V618 R622 R623 T624 Y628 S629 M630 E631
P632 R637 L645 E646 E649 H652 L657 G658 Y661 K664 L667 M668 L669 C672 F673 L674 V681 S682 I683 K690 F711 I728 C737 F740 V741 P742 I745 R748 THR ASN PRO ASP ALA ALA THR GLN ASN ARG ARG PHE GLN PHE THR
GLN ASN GLN LYS LYS GLU ASP SER LYS THR SER THR SER VAL THR SER VAL ASN GLN ALA SER THR SER ARG LEU GLU GLY LEU GLN SER GLU ASN HIS ARG LEU ARG MET LYS ILE THR GLU LEU ASP LYS ASP LEU GLU GLU VAL THR MET GLN LEU GLN ASP THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	275089	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 ($e^-/Å^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	49310	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.378	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	324.48, 324.48, 324.48	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	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: 2C0, FN0

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.60	0/2867	0.51	0/3857
2	B	0.58	0/2654	0.52	0/3597
3	Y	0.73	0/442	0.44	0/597
4	N	0.59	0/1821	0.56	0/2469
5	C	0.29	0/5541	0.43	0/7527
6	D	0.30	0/5533	0.46	0/7489
All	All	0.45	0/18858	0.48	0/25536

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	2820	0	2798	100	0
2	B	2607	0	2510	3	0
3	Y	436	0	448	0	0
4	N	1777	0	1714	4	0
5	C	5406	0	5411	72	0
6	D	5414	0	5515	118	0
7	C	14	0	11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	23	0	0	1	0
All	All	18497	0	18407	268	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 7.

All (268) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:CYS:SG	1:A:169:PRO:HG3	1.80	1.19
6:D:592:ILE:HG21	6:D:596:LYS:HB2	1.21	1.16
6:D:592:ILE:CG2	6:D:596:LYS:HB2	1.84	1.08
1:A:33:GLU:HG2	1:A:195:HIS:HB3	1.36	1.04
1:A:343:ILE:CG2	6:D:588:LYS:HB2	1.91	1.00
1:A:33:GLU:HG2	1:A:195:HIS:CB	1.93	0.98
1:A:65:GLU:OE1	1:A:188:HIS:HE1	1.50	0.95
1:A:66:CYS:SG	1:A:169:PRO:CG	2.54	0.95
6:D:578:VAL:HG13	6:D:582:PHE:CE1	2.05	0.92
1:A:353:LEU:O	6:D:513:LYS:C	2.09	0.91
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.35	0.90
1:A:61:TYR:HB2	1:A:69:TYR:HE2	1.38	0.89
1:A:184:ILE:HD12	1:A:201:VAL:HG22	1.56	0.86
1:A:343:ILE:HG21	6:D:588:LYS:CB	2.06	0.85
1:A:33:GLU:OE1	1:A:197:LYS:HE3	1.77	0.83
1:A:67:LYS:HA	1:A:70:LYS:HE2	1.60	0.83
1:A:343:ILE:CG2	6:D:588:LYS:CB	2.54	0.83
6:D:578:VAL:O	6:D:582:PHE:HD1	1.63	0.82
6:D:592:ILE:HG21	6:D:596:LYS:CB	2.08	0.81
1:A:343:ILE:HG21	6:D:588:LYS:HB3	1.62	0.79
1:A:353:LEU:HD21	6:D:577:ARG:HH12	1.47	0.79
1:A:63:GLU:OE1	1:A:63:GLU:N	2.17	0.77
1:A:65:GLU:OE1	1:A:188:HIS:CE1	2.36	0.77
1:A:61:TYR:HB2	1:A:69:TYR:CE2	2.20	0.76
1:A:51:LYS:O	1:A:55:ILE:HG13	1.85	0.76
6:D:578:VAL:HG13	6:D:582:PHE:HE1	1.50	0.75
1:A:29:LYS:O	1:A:29:LYS:HD3	1.86	0.75
1:A:343:ILE:HG23	6:D:588:LYS:HD2	1.68	0.74
1:A:32:ARG:H	1:A:32:ARG:HD2	1.53	0.74
1:A:210:LYS:O	1:A:213:HIS:ND1	2.21	0.74
1:A:353:LEU:HD21	6:D:577:ARG:NH1	2.04	0.72
5:C:308:LYS:HE2	5:C:577:GLN:HE22	1.54	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:CYS:SG	6:D:593:LYS:HA	2.30	0.72
6:D:81:VAL:HG23	6:D:362:ILE:HG13	1.71	0.71
1:A:32:ARG:HD2	1:A:32:ARG:N	2.06	0.71
5:C:360:ARG:HG3	5:C:576:ASP:HA	1.74	0.69
5:C:330:VAL:HG22	5:C:335:ILE:HB	1.73	0.69
1:A:213:HIS:HB2	1:A:258:TRP:CD2	2.28	0.69
5:C:308:LYS:CE	5:C:577:GLN:HE22	2.07	0.68
6:D:623:ARG:NH1	6:D:646:GLU:OE2	2.26	0.68
1:A:64:GLU:OE1	1:A:67:LYS:HD2	1.94	0.67
4:N:6:GLU:OE1	4:N:114:GLY:N	2.19	0.67
1:A:186:GLU:HB3	1:A:199:PHE:CD1	2.31	0.66
6:D:585:VAL:O	6:D:586:LYS:C	2.34	0.66
5:C:271:SER:HB3	5:C:274:LEU:HD12	1.76	0.65
5:C:308:LYS:HE2	5:C:577:GLN:NE2	2.12	0.65
1:A:52:GLN:HA	1:A:55:ILE:HG13	1.79	0.65
1:A:33:GLU:HG2	1:A:195:HIS:HB2	1.77	0.64
6:D:65:THR:HG22	6:D:67:GLU:H	1.62	0.64
1:A:66:CYS:HG	1:A:169:PRO:HG3	1.63	0.63
5:C:360:ARG:HB2	5:C:576:ASP:HB3	1.80	0.63
1:A:29:LYS:HD3	1:A:29:LYS:C	2.19	0.63
1:A:213:HIS:HB2	1:A:258:TRP:CE2	2.34	0.62
1:A:186:GLU:CB	1:A:199:PHE:CD1	2.83	0.62
1:A:347:ASN:OD1	1:A:348:LEU:N	2.33	0.61
1:A:353:LEU:O	6:D:513:LYS:CB	2.48	0.61
5:C:236:ASP:HB3	5:C:237:PRO:HD3	1.82	0.61
6:D:552:LEU:HA	6:D:555:VAL:HG12	1.80	0.61
1:A:186:GLU:CB	1:A:199:PHE:HD1	2.13	0.60
1:A:32:ARG:H	1:A:32:ARG:CD	2.12	0.60
6:D:585:VAL:O	6:D:585:VAL:HG22	2.01	0.60
1:A:353:LEU:O	6:D:513:LYS:HB3	2.01	0.60
1:A:24:ARG:HH11	1:A:24:ARG:CG	2.11	0.60
6:D:590:LYS:O	6:D:590:LYS:HG2	2.02	0.60
1:A:351:CYS:HA	6:D:593:LYS:HG3	1.84	0.60
1:A:61:TYR:CB	1:A:69:TYR:HE2	2.10	0.59
5:C:349:VAL:HG11	6:D:216:THR:HG21	1.84	0.59
6:D:158:ALA:O	6:D:174:ARG:HD3	2.01	0.59
1:A:211:TRP:HZ3	1:A:215:PHE:CE2	2.21	0.59
1:A:343:ILE:HG23	6:D:588:LYS:HB2	1.81	0.58
1:A:211:TRP:CZ3	1:A:215:PHE:CE2	2.91	0.58
1:A:52:GLN:HA	1:A:55:ILE:CD1	2.34	0.58
5:C:578:THR:HG21	5:C:751:ASP:O	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:303:LEU:HD11	6:D:305:LYS:HE3	1.85	0.58
1:A:353:LEU:O	6:D:513:LYS:O	2.21	0.57
1:A:24:ARG:HG2	1:A:24:ARG:NH1	2.12	0.57
1:A:52:GLN:HA	1:A:55:ILE:CG1	2.35	0.57
1:A:353:LEU:HD11	6:D:577:ARG:CZ	2.34	0.57
5:C:666:ARG:NH1	5:C:761:CYS:SG	2.78	0.57
1:A:193:ASP:OD1	1:A:193:ASP:O	2.24	0.56
1:A:146:TYR:CG	1:A:147:GLN:N	2.74	0.56
6:D:212:ARG:HH12	6:D:216:THR:HB	1.70	0.56
6:D:629:SER:O	6:D:632:PRO:HD2	2.06	0.56
6:D:268:TYR:HB2	6:D:310:ALA:HB2	1.88	0.56
5:C:628:ASN:ND2	5:C:711:TYR:OH	2.22	0.55
6:D:520:ASN:OD1	6:D:574:LYS:NZ	2.32	0.55
6:D:475:ARG:NE	6:D:628:TYR:OH	2.39	0.55
5:C:745:GLU:HB3	5:C:747:LYS:HE3	1.88	0.55
6:D:592:ILE:HG22	6:D:592:ILE:O	2.07	0.55
5:C:401:PHE:HE2	5:C:402:LYS:HE3	1.71	0.55
5:C:691:VAL:HG23	5:C:692:PHE:HD2	1.71	0.54
5:C:360:ARG:HB2	5:C:576:ASP:CB	2.36	0.54
6:D:452:ILE:O	6:D:455:THR:OG1	2.24	0.54
5:C:654:ILE:HG13	5:C:655:GLY:H	1.73	0.54
6:D:592:ILE:HG22	6:D:596:LYS:HB2	1.81	0.54
1:A:212:ILE:O	1:A:213:HIS:C	2.46	0.53
6:D:197:ARG:NH2	6:D:247:ASP:O	2.36	0.53
6:D:212:ARG:NH1	6:D:216:THR:HB	2.23	0.53
5:C:711:TYR:HA	5:C:714:VAL:HG12	1.91	0.53
1:A:33:GLU:CG	1:A:195:HIS:CB	2.80	0.53
6:D:592:ILE:CG2	6:D:596:LYS:CB	2.74	0.53
6:D:244:LYS:NZ	6:D:270:GLU:O	2.41	0.53
1:A:210:LYS:O	1:A:213:HIS:CE1	2.62	0.53
5:C:379:TYR:O	5:C:382:ARG:NH1	2.41	0.53
6:D:657:LEU:HD13	6:D:711:PHE:HZ	1.73	0.53
5:C:684:LYS:HD3	5:C:805:VAL:HG11	1.92	0.52
6:D:338:TYR:CD2	6:D:411:VAL:HG21	2.44	0.52
5:C:667:LEU:HG	5:C:725:LEU:HD21	1.90	0.52
4:N:6:GLU:HG2	4:N:115:THR:OG1	2.10	0.52
6:D:433:ASP:OD2	6:D:433:ASP:N	2.42	0.52
1:A:66:CYS:HA	1:A:69:TYR:HD2	1.75	0.52
1:A:68:GLN:O	1:A:71:ALA:HB3	2.10	0.52
5:C:401:PHE:CE2	5:C:402:LYS:HE3	2.45	0.51
5:C:798:LYS:HD2	5:C:799:ILE:HG13	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:PHE:CD1	2:B:292:PHE:N	2.78	0.51
5:C:825:ILE:HG22	5:C:826:LEU:HD22	1.92	0.51
1:A:186:GLU:HB2	1:A:199:PHE:HD1	1.74	0.51
1:A:354:PHE:OXT	6:D:513:LYS:HE3	2.11	0.51
6:D:499:PHE:HB3	6:D:740:PHE:HD2	1.75	0.51
1:A:352:GLY:O	6:D:513:LYS:HE3	2.11	0.51
5:C:599:SER:OG	5:C:641:LEU:O	2.29	0.50
5:C:633:THR:OG1	5:C:680:SER:OG	2.19	0.50
1:A:52:GLN:HA	1:A:55:ILE:HD12	1.93	0.50
1:A:186:GLU:HB2	1:A:199:PHE:CD1	2.47	0.50
5:C:621:TYR:OH	5:C:859:ARG:NE	2.45	0.50
6:D:519:MET:O	6:D:523:ILE:HG23	2.12	0.50
5:C:176:PHE:HD2	5:C:267:TYR:HH	1.58	0.49
6:D:486:SER:HA	6:D:489:THR:HG22	1.94	0.49
5:C:339:PHE:HD2	5:C:354:LEU:HD23	1.77	0.49
1:A:207:GLU:CB	1:A:210:LYS:HG2	2.43	0.49
5:C:230:TYR:HB2	6:D:118:TYR:CE1	2.48	0.49
6:D:591:ILE:O	6:D:592:ILE:HB	2.13	0.49
1:A:212:ILE:O	1:A:214:CYS:N	2.46	0.48
1:A:343:ILE:HG23	6:D:588:LYS:CD	2.40	0.48
6:D:741:VAL:N	6:D:742:PRO:HD2	2.29	0.48
1:A:66:CYS:SG	1:A:169:PRO:HG2	2.52	0.48
6:D:608:ASP:OD1	6:D:609:LEU:N	2.46	0.48
6:D:583:LYS:HG2	6:D:584:ASN:CG	2.35	0.48
1:A:328:ASP:OD1	1:A:329:THR:N	2.46	0.47
5:C:664:GLN:HE22	5:C:729:GLN:HE21	1.60	0.47
5:C:776:TYR:O	5:C:779:LEU:HG	2.14	0.47
6:D:202:THR:OG1	6:D:254:GLN:OE1	2.27	0.47
6:D:249:ARG:HG3	6:D:466:ASP:HA	1.96	0.47
5:C:664:GLN:HG3	5:C:668:TRP:HD1	1.78	0.47
1:A:33:GLU:CG	1:A:195:HIS:HB2	2.42	0.47
1:A:65:GLU:OE2	1:A:65:GLU:HA	2.15	0.47
6:D:288:SER:HB3	6:D:291:GLU:OE2	2.15	0.47
2:B:245:SER:OG	2:B:247:ASP:OD1	2.33	0.46
5:C:355:LYS:HD3	5:C:383:LEU:HD13	1.96	0.46
1:A:61:TYR:CB	1:A:69:TYR:CE2	2.92	0.46
1:A:28:GLU:HA	1:A:28:GLU:OE1	2.14	0.46
1:A:66:CYS:HA	1:A:69:TYR:CD2	2.50	0.46
6:D:466:ASP:N	6:D:466:ASP:OD1	2.42	0.46
5:C:625:SER:HB3	5:C:800:ASN:HB3	1.97	0.46
6:D:341:GLU:HA	6:D:344:ASN:ND2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLU:OE1	1:A:207:GLU:HA	2.16	0.46
6:D:737:CYS:O	6:D:741:VAL:HG12	2.16	0.46
1:A:51:LYS:O	1:A:55:ILE:N	2.49	0.46
5:C:287:HIS:HA	5:C:469:LEU:HD13	1.98	0.46
1:A:24:ARG:CG	1:A:24:ARG:NH1	2.72	0.45
6:D:624:THR:OG1	6:D:649:GLU:OE1	2.34	0.45
1:A:325:CYS:H	1:A:331:ASN:HD21	1.63	0.45
4:N:6:GLU:OE2	4:N:6:GLU:N	2.49	0.45
6:D:518:TYR:CD2	6:D:594:ASP:OD1	2.69	0.45
5:C:664:GLN:NE2	5:C:729:GLN:HE21	2.14	0.45
6:D:142:ILE:O	6:D:146:LEU:HG	2.16	0.45
6:D:690:LYS:HB3	8:D:901:FN0:F2	2.05	0.45
5:C:208:ASP:OD1	5:C:208:ASP:N	2.50	0.45
5:C:802:HIS:HA	5:C:805:VAL:HG22	1.98	0.45
6:D:562:VAL:HA	6:D:565:THR:HG22	1.98	0.45
6:D:576:TRP:HA	6:D:674:LEU:HD21	1.99	0.45
1:A:343:ILE:HG22	6:D:588:LYS:HB2	1.88	0.45
1:A:43:GLU:OE1	1:A:43:GLU:HA	2.17	0.45
1:A:214:CYS:SG	1:A:215:PHE:CE2	3.09	0.45
5:C:566:ASP:OD1	5:C:566:ASP:N	2.50	0.45
1:A:343:ILE:CG2	6:D:588:LYS:HD2	2.44	0.45
5:C:577:GLN:O	5:C:577:GLN:HG2	2.17	0.45
5:C:706:GLU:HG3	5:C:708:TRP:NE1	2.32	0.45
6:D:407:ASN:OD1	6:D:414:GLN:NE2	2.40	0.45
5:C:199:VAL:HG21	5:C:478:ALA:CB	2.47	0.44
5:C:654:ILE:HD13	5:C:662:VAL:HG21	1.98	0.44
6:D:230:GLU:HB3	6:D:239:SER:OG	2.17	0.44
6:D:596:LYS:O	6:D:599:VAL:HB	2.17	0.44
1:A:62:SER:H	1:A:65:GLU:HB2	1.83	0.44
1:A:62:SER:N	1:A:65:GLU:HB2	2.33	0.44
6:D:631:GLU:HG3	6:D:632:PRO:HD3	1.98	0.44
1:A:347:ASN:OD1	1:A:347:ASN:C	2.56	0.44
5:C:732:ASP:OD1	5:C:764:ARG:NH2	2.50	0.44
6:D:500:LEU:HD13	6:D:524:ILE:HG21	2.00	0.44
6:D:376:LEU:HD11	6:D:398:ILE:HD13	2.00	0.44
1:A:57:HIS:CG	1:A:57:HIS:O	2.70	0.44
1:A:62:SER:HB2	1:A:65:GLU:HB2	2.00	0.44
5:C:654:ILE:HG13	5:C:655:GLY:N	2.32	0.44
5:C:727:ILE:HA	5:C:730:ILE:HG12	2.00	0.44
1:A:343:ILE:CG2	6:D:588:LYS:CD	2.96	0.44
1:A:353:LEU:HA	6:D:513:LYS:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:83:LEU:O	6:D:86:GLU:HG3	2.17	0.44
5:C:189:GLN:O	5:C:193:GLU:HG2	2.17	0.43
6:D:578:VAL:O	6:D:582:PHE:CD1	2.55	0.43
5:C:763:SER:OG	5:C:764:ARG:N	2.51	0.43
5:C:379:TYR:CZ	5:C:414:GLU:HB3	2.54	0.43
6:D:197:ARG:HG3	6:D:227:SER:HB3	2.00	0.43
6:D:521:ASN:O	6:D:524:ILE:HG22	2.19	0.43
6:D:681:VAL:HG12	6:D:683:ILE:HG22	2.00	0.43
1:A:29:LYS:C	1:A:29:LYS:CD	2.86	0.43
6:D:522:LEU:HD23	6:D:522:LEU:HA	1.81	0.43
5:C:325:ASP:HA	5:C:328:GLU:OE2	2.19	0.43
5:C:452:LYS:HB2	5:C:452:LYS:HE3	1.79	0.43
4:N:6:GLU:O	4:N:115:THR:OG1	2.37	0.43
5:C:663:CYS:SG	5:C:664:GLN:N	2.91	0.43
5:C:591:LEU:HD21	5:C:835:ALA:HB2	2.01	0.43
5:C:349:VAL:CG1	6:D:216:THR:HG21	2.46	0.43
6:D:578:VAL:CG1	6:D:582:PHE:CE1	2.90	0.43
1:A:33:GLU:CD	1:A:197:LYS:HE3	2.39	0.42
5:C:641:LEU:HD21	5:C:842:VAL:HA	2.01	0.42
6:D:168:LYS:HB3	6:D:168:LYS:HE2	1.71	0.42
6:D:388:PHE:HA	6:D:392:ASP:OD1	2.19	0.42
6:D:303:LEU:HD23	6:D:303:LEU:H	1.83	0.42
6:D:610:CYS:HA	6:D:613:ILE:HG22	2.01	0.42
6:D:581:ILE:HD13	6:D:591:ILE:HD12	2.02	0.42
5:C:743:LYS:HE2	5:C:743:LYS:HB3	1.87	0.42
6:D:546:GLU:HB3	6:D:623:ARG:HH22	1.84	0.42
6:D:564:TYR:CD2	6:D:664:LYS:HD2	2.55	0.42
1:A:353:LEU:O	6:D:514:MET:N	2.50	0.42
5:C:270:SER:HB3	5:C:287:HIS:CE1	2.54	0.42
5:C:259:MET:HG2	6:D:111:ALA:HB1	2.00	0.42
6:D:206:GLN:O	6:D:210:GLU:HG2	2.20	0.42
1:A:68:GLN:O	1:A:72:VAL:N	2.51	0.42
6:D:138:VAL:O	6:D:142:ILE:HG12	2.19	0.42
6:D:597:LEU:C	6:D:599:VAL:N	2.72	0.42
5:C:850:VAL:O	5:C:854:VAL:HG12	2.20	0.41
6:D:558:TRP:HD1	6:D:612:LEU:HD21	1.85	0.41
1:A:32:ARG:HG3	6:D:586:LYS:O	2.19	0.41
1:A:214:CYS:SG	1:A:215:PHE:CD2	3.10	0.41
5:C:262:LEU:HD23	5:C:262:LEU:HA	1.86	0.41
5:C:311:THR:HG21	5:C:323:LEU:HD11	2.02	0.41
5:C:403:ILE:HD13	5:C:403:ILE:HA	1.96	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:585:VAL:C	6:D:587:MET:N	2.66	0.41
5:C:598:LEU:HD23	5:C:598:LEU:HA	1.89	0.41
5:C:781:LEU:HD22	5:C:813:ALA:HA	2.03	0.41
6:D:490:ILE:O	6:D:494:ILE:HG23	2.21	0.41
6:D:518:TYR:CE2	6:D:594:ASP:OD1	2.74	0.41
6:D:601:VAL:HA	6:D:604:MET:HE2	2.02	0.41
5:C:304:TRP:CD1	5:C:573:PRO:HG3	2.55	0.41
6:D:368:THR:HA	6:D:371:ARG:HG2	2.02	0.41
1:A:213:HIS:CB	1:A:258:TRP:CE2	3.01	0.41
5:C:272:PRO:HB2	5:C:321:SER:HB3	2.02	0.41
5:C:830:GLN:HG2	5:C:831:ASP:N	2.35	0.41
6:D:81:VAL:HG23	6:D:362:ILE:CG1	2.47	0.41
6:D:742:PRO:O	6:D:745:ILE:HG22	2.20	0.41
2:B:290:ASP:C	2:B:290:ASP:OD1	2.60	0.41
5:C:854:VAL:HG12	5:C:855:PRO:HD3	2.02	0.41
6:D:95:ARG:HB3	6:D:96:PRO:HD3	2.02	0.41
6:D:205:VAL:HG22	6:D:208:PHE:CD1	2.56	0.41
6:D:371:ARG:HG3	6:D:402:ALA:HB1	2.03	0.41
6:D:534:ILE:HD11	6:D:728:ILE:HB	2.03	0.41
1:A:63:GLU:O	1:A:66:CYS:HB3	2.21	0.40
1:A:64:GLU:O	1:A:67:LYS:HB2	2.21	0.40
5:C:847:ILE:HA	5:C:850:VAL:HG22	2.03	0.40
6:D:534:ILE:HD13	6:D:534:ILE:HA	1.90	0.40
1:A:68:GLN:HA	1:A:68:GLN:OE1	2.21	0.40
5:C:587:LEU:HD21	5:C:834:PHE:CD2	2.57	0.40
6:D:564:TYR:CE2	6:D:664:LYS:HD2	2.56	0.40
6:D:664:LYS:O	6:D:667:LEU:HG	2.21	0.40
5:C:657:ASN:OD1	5:C:658:GLN:HG3	2.22	0.40
6:D:78:LEU:HA	6:D:81:VAL:HG12	2.03	0.40
6:D:467:LYS:HD3	6:D:467:LYS:HA	1.81	0.40
1:A:354:PHE:OXT	6:D:513:LYS:CE	2.70	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	350/354 (99%)	342 (98%)	8 (2%)	0	100	100
2	B	337/358 (94%)	329 (98%)	8 (2%)	0	100	100
3	Y	55/71 (78%)	54 (98%)	1 (2%)	0	100	100
4	N	227/269 (84%)	217 (96%)	10 (4%)	0	100	100
5	C	672/937 (72%)	646 (96%)	26 (4%)	0	100	100
6	D	674/808 (83%)	643 (95%)	30 (4%)	1 (0%)	51	84
All	All	2315/2797 (83%)	2231 (96%)	83 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	592	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	304/305 (100%)	304 (100%)	0	100	100
2	B	282/298 (95%)	282 (100%)	0	100	100
3	Y	46/58 (79%)	46 (100%)	0	100	100
4	N	196/217 (90%)	195 (100%)	1 (0%)	88	94
5	C	590/814 (72%)	590 (100%)	0	100	100
6	D	595/708 (84%)	595 (100%)	0	100	100
All	All	2013/2400 (84%)	2012 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	N	232	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	HIS
1	A	331	ASN
5	C	577	GLN
5	C	628	ASN
5	C	729	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
7	2C0	C	1001	-	13,14,14	0.74	0	15,18,18	0.78	0
8	FN0	D	901	-	23,24,24	1.25	4 (17%)	35,42,42	1.67	5 (14%)

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
7	2C0	C	1001	-	-	0/10/10/10	0/1/1/1
8	FN0	D	901	-	-	8/21/37/37	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	901	FN0	C3-C4	-3.19	1.47	1.53
8	D	901	FN0	O3-C13	2.29	1.26	1.20
8	D	901	FN0	O1-C13	-2.18	1.35	1.38
8	D	901	FN0	C6-C2	-2.13	1.37	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	901	FN0	C5-C7-C13	-5.15	99.31	101.75
8	D	901	FN0	C17-C7-C5	5.02	120.90	112.72
8	D	901	FN0	C4-C9-C5	-3.23	118.78	123.80
8	D	901	FN0	C8-C2-C6	-2.51	113.53	117.11
8	D	901	FN0	C9-C4-C3	-2.24	117.20	121.38

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	901	FN0	F1-C17-C7-C5
8	D	901	FN0	F2-C17-C7-C5
8	D	901	FN0	F3-C17-C7-C5
8	D	901	FN0	C11-C1-C2-C6
8	D	901	FN0	C12-C1-C2-C6
8	D	901	FN0	C10-C1-C2-C6
8	D	901	FN0	C11-C1-C2-C8
8	D	901	FN0	C12-C1-C2-C8

There are no ring outliers.

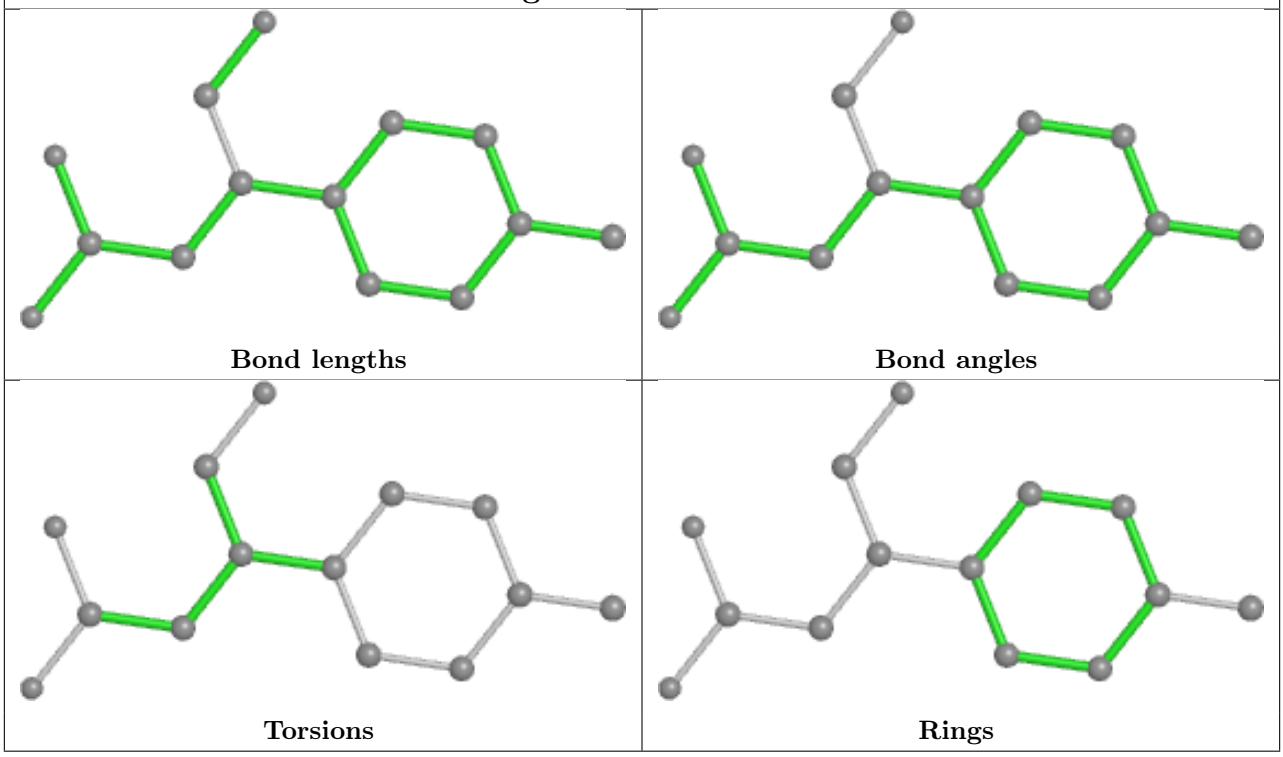
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	901	FN0	1	0

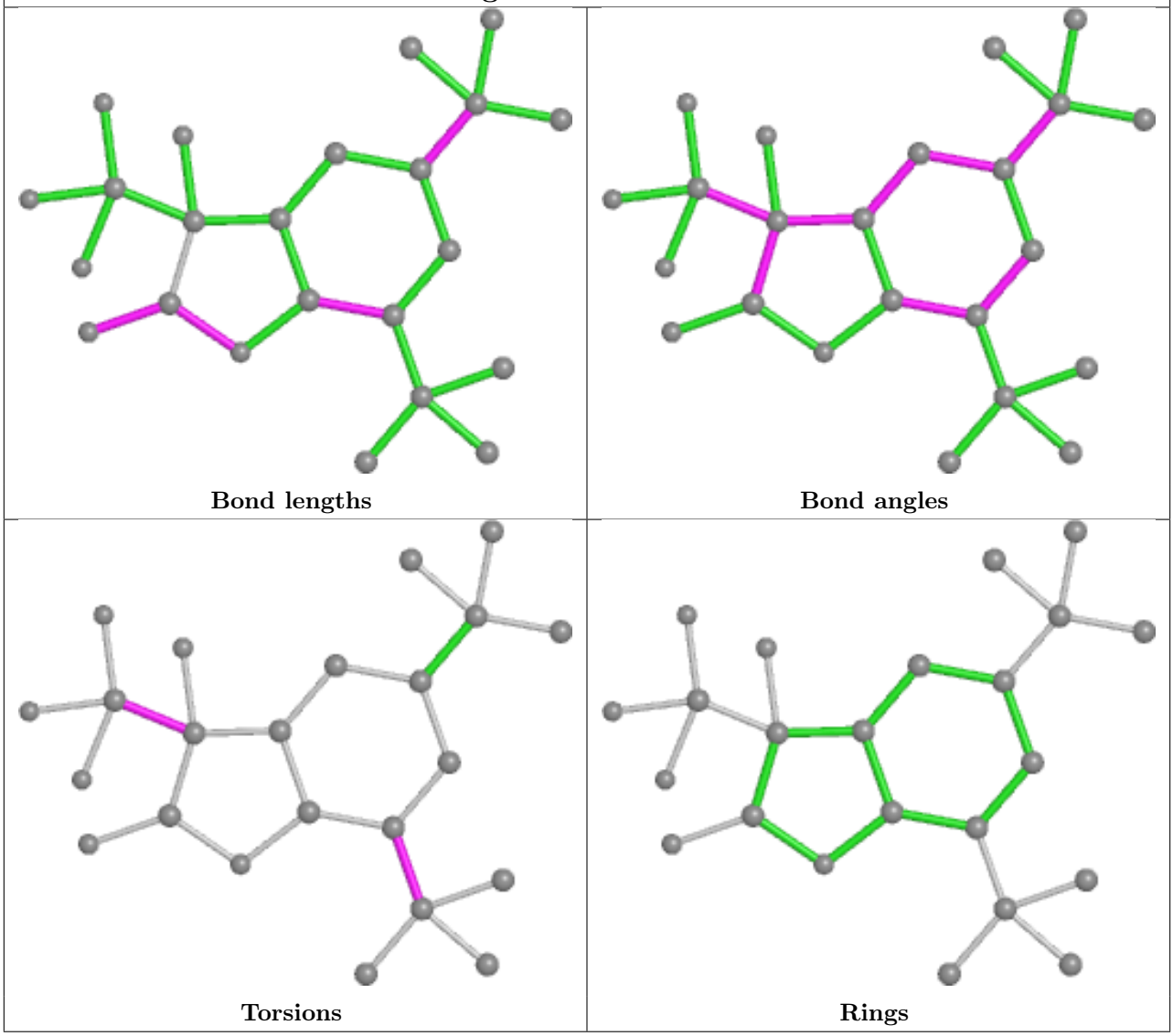
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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 2C0 C 1001



Ligand FN0 D 901



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.

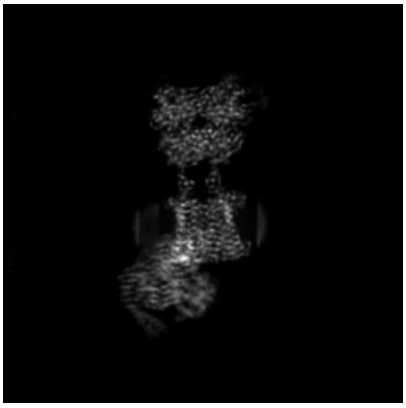
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-31049. These allow visual inspection of the internal detail of the map and identification of artifacts.

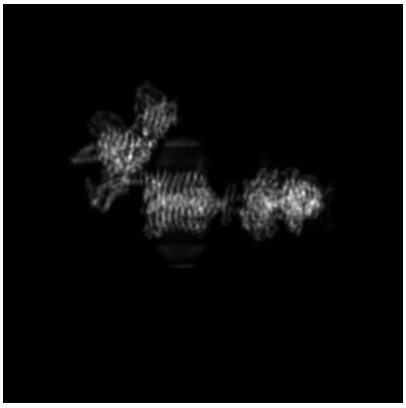
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

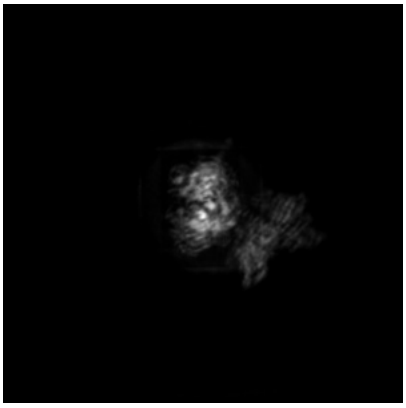
6.1.1 Primary map



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: 160

Y Index: 160

Z Index: 160

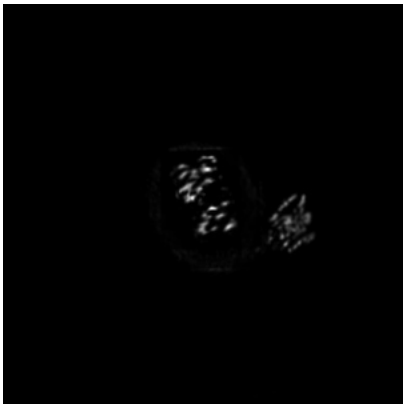
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 160

Y Index: 143



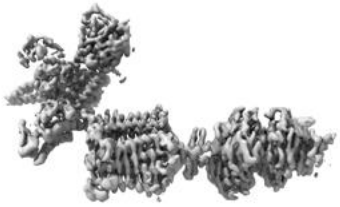
Z Index: 128

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

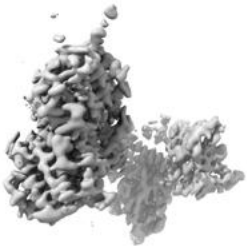
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

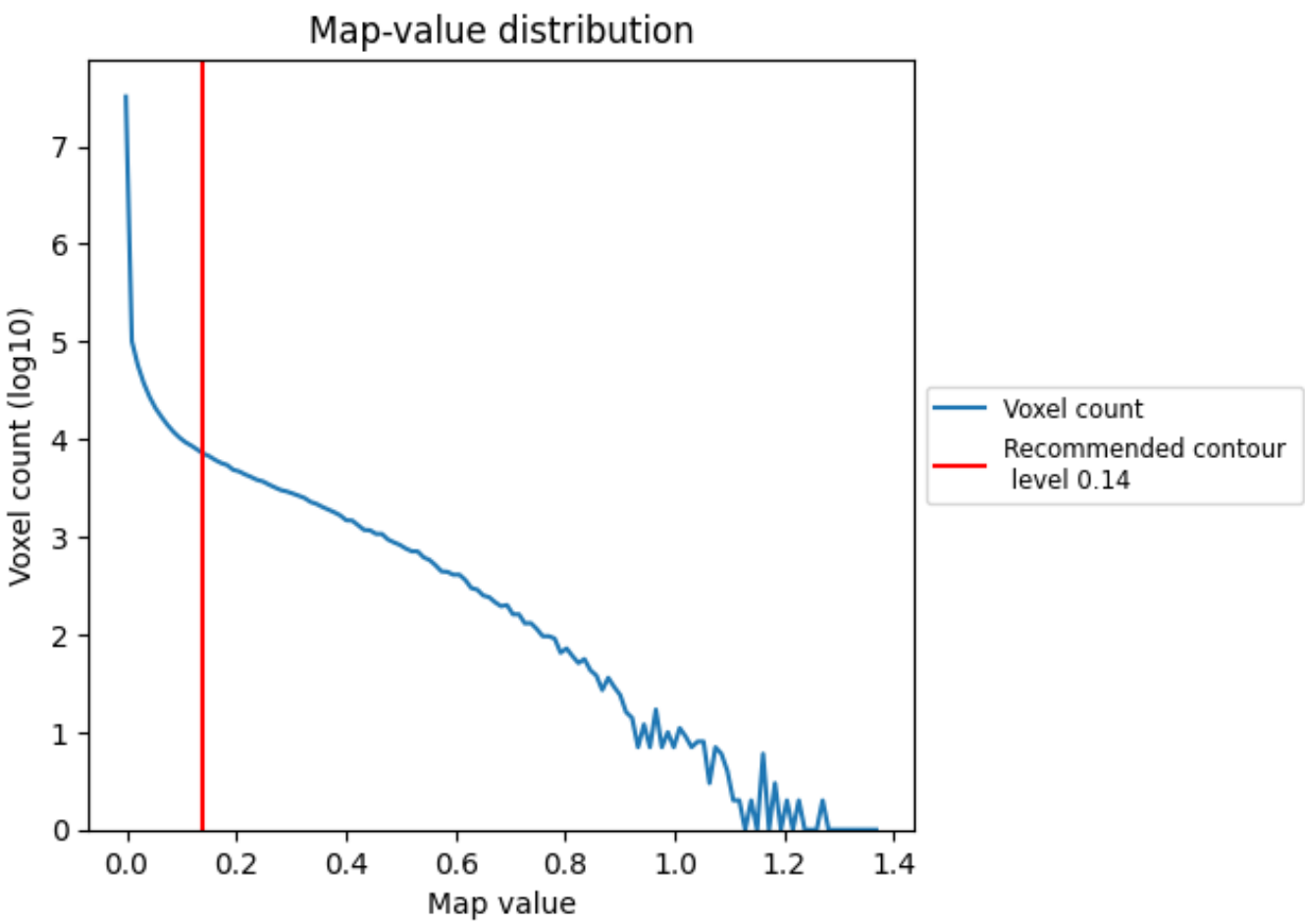
6.5 Mask visualisation (i)

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

7 Map analysis (i)

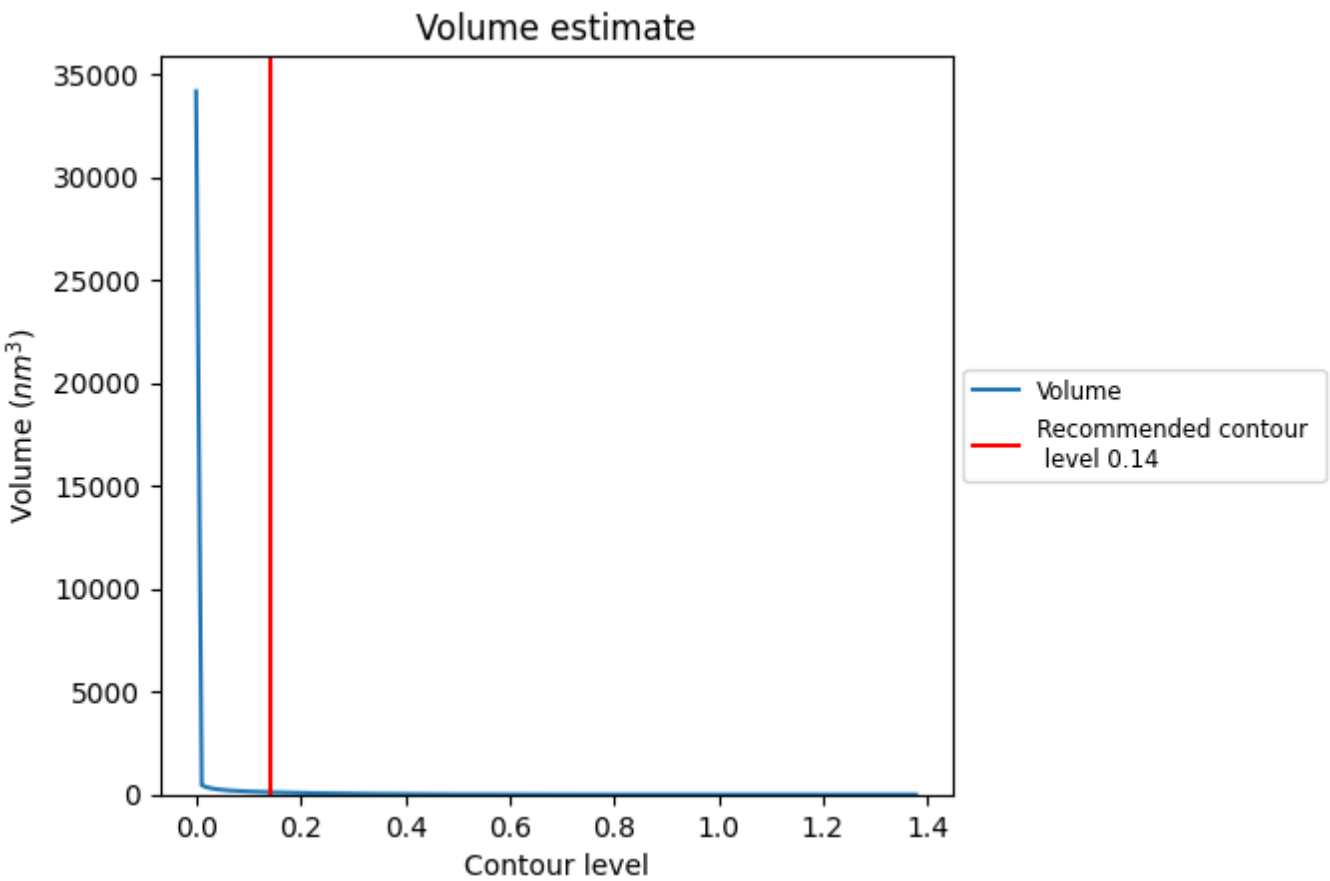
This section contains the results of statistical analysis of the map.

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.

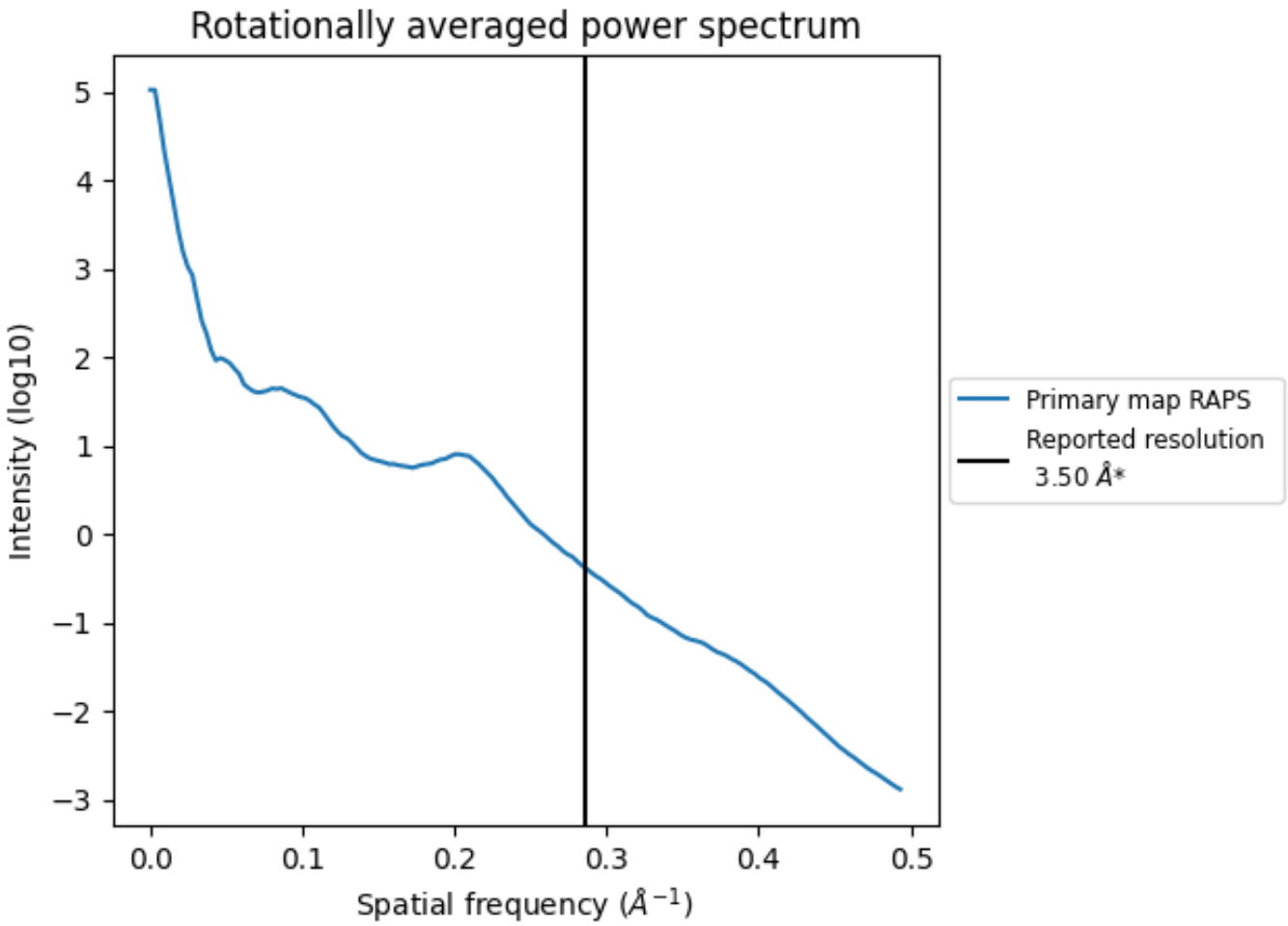
7.2 Volume estimate (i)



The volume at the recommended contour level is 114 nm^3; this corresponds to an approximate mass of 103 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 (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

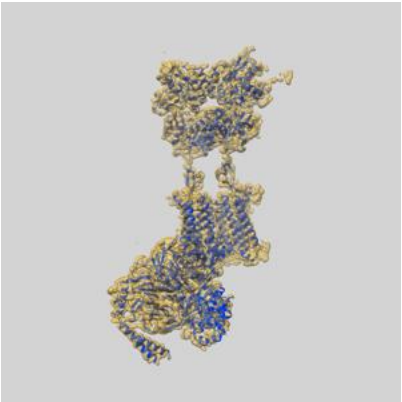
8 Fourier-Shell correlation (i)

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

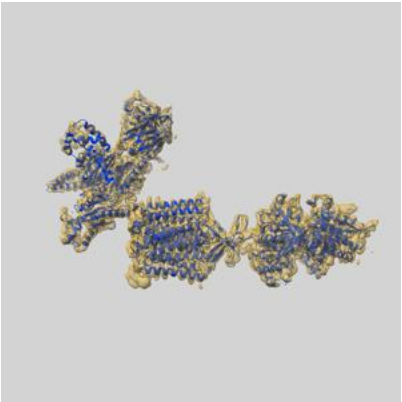
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31049 and PDB model 7EB2. Per-residue inclusion information can be found in section 3 on page 8.

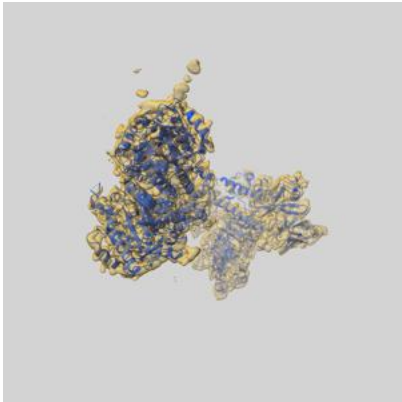
9.1 Map-model overlay (i)



X



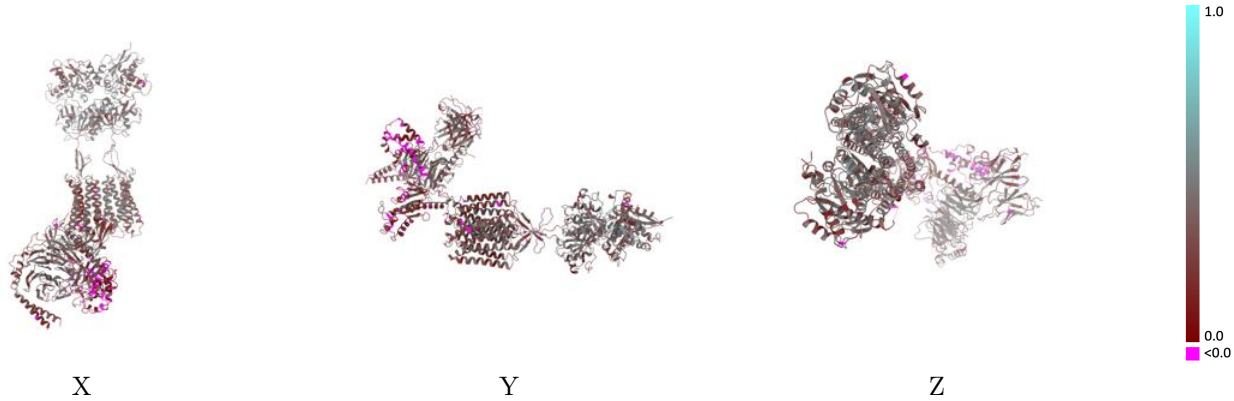
Y



Z

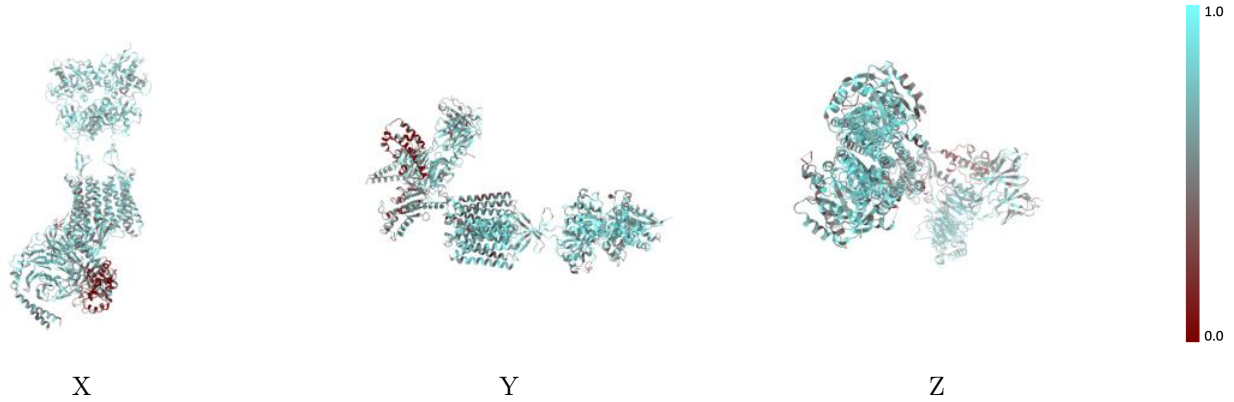
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



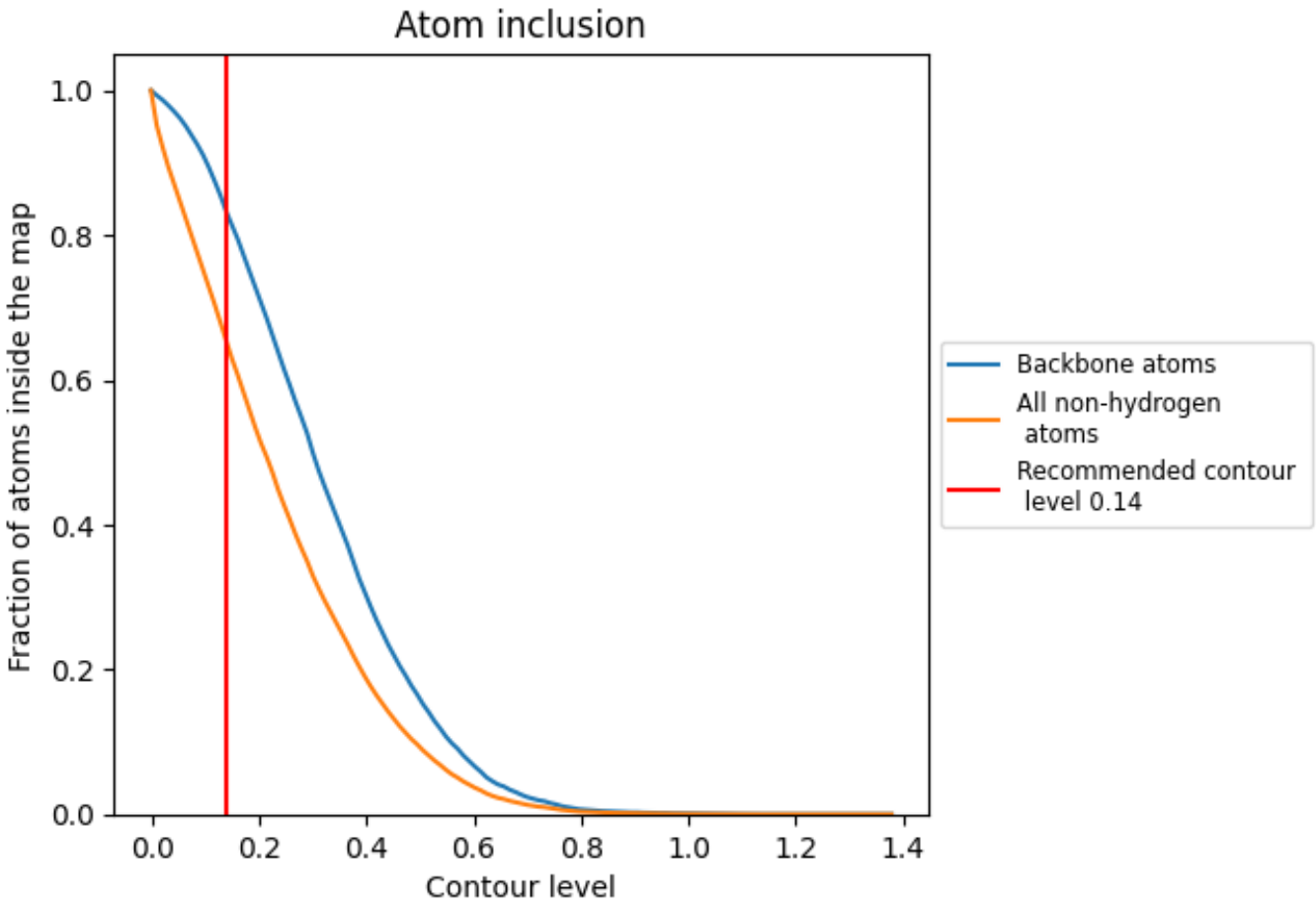
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.14).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6506	0.3230
A	0.3895	0.1340
B	0.7095	0.3590
C	0.7152	0.3740
D	0.6905	0.3470
N	0.6621	0.3500
Y	0.6434	0.2890