



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:54 AM UTC

PDB ID : 5WEN / pdb_00005wen
EMDB ID : EMD-8822
Title : GluA2 bound to GSG1L in digitonin, state 2
Authors : Twomey, E.C.; Yelshanskaya, M.V.; Grassucci, R.A.; Frank, J.; Sobolevsky, A.I.
Deposited on : 2017-07-10
Resolution : 6.80 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:

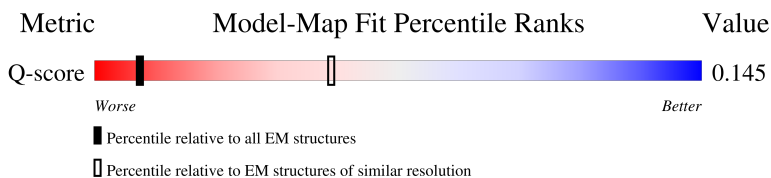
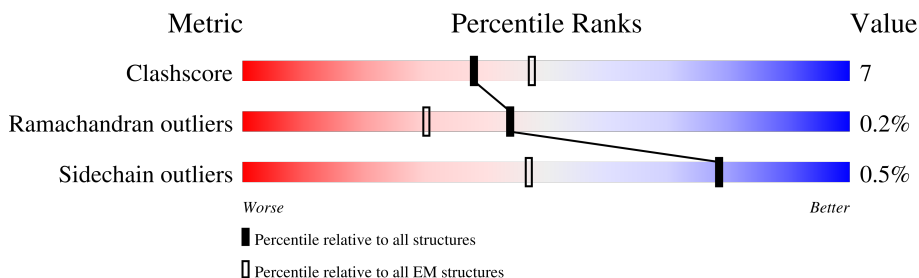
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 6.80 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	503 (6.30 - 7.30)

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	1057	28% 74% 17% 9%
1	B	1057	17% 62% 12% 26%
1	C	1057	27% 75% 16% 9%
1	D	1057	19% 62% 12% 26%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AJP	A	1301	X	-	X	-
2	AJP	C	1301	X	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27530 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, Germ cell-specific gene 1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	962	Total	C	N	O	S	0	0
			7555	4864	1248	1401	42		
1	B	780	Total	C	N	O	S	0	0
			6125	3932	1011	1152	30		
1	C	962	Total	C	N	O	S	0	0
			7555	4864	1248	1401	42		
1	D	780	Total	C	N	O	S	0	0
			6125	3932	1011	1152	30		

There are 60 discrepancies between the modelled and reference sequences:

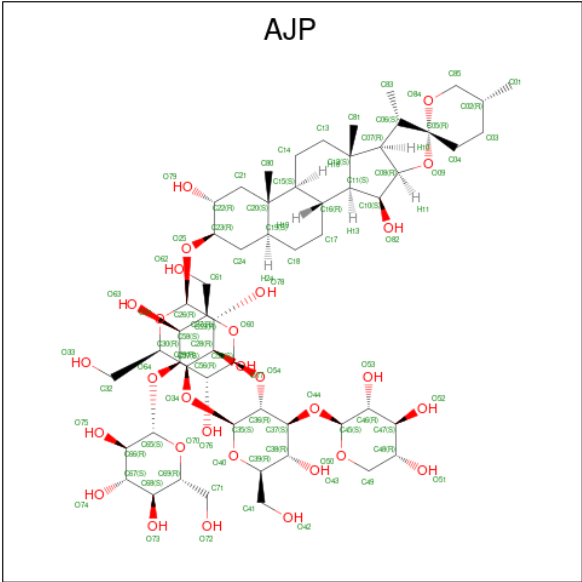
Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	382	LEU	VAL	engineered mutation	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	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	999	GLY	-	linker	UNP P19491
A	1000	THR	-	linker	UNP P19491
A	1001	GLY	-	linker	UNP P19491
A	1151	LEU	VAL	engineered mutation	UNP D3Z7H4
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	829	GLY	-	linker	UNP P19491
B	979	LEU	VAL	engineered mutation	UNP D3Z7H4
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	999	GLY	-	linker	UNP P19491
C	1000	THR	-	linker	UNP P19491
C	1001	GLY	-	linker	UNP P19491
C	1151	LEU	VAL	engineered mutation	UNP D3Z7H4
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	829	GLY	-	linker	UNP P19491
D	979	LEU	VAL	engineered mutation	UNP D3Z7H4

- Molecule 2 is Digitonin (CCD ID: AJP) (formula: C₅₆H₉₂O₂₉).

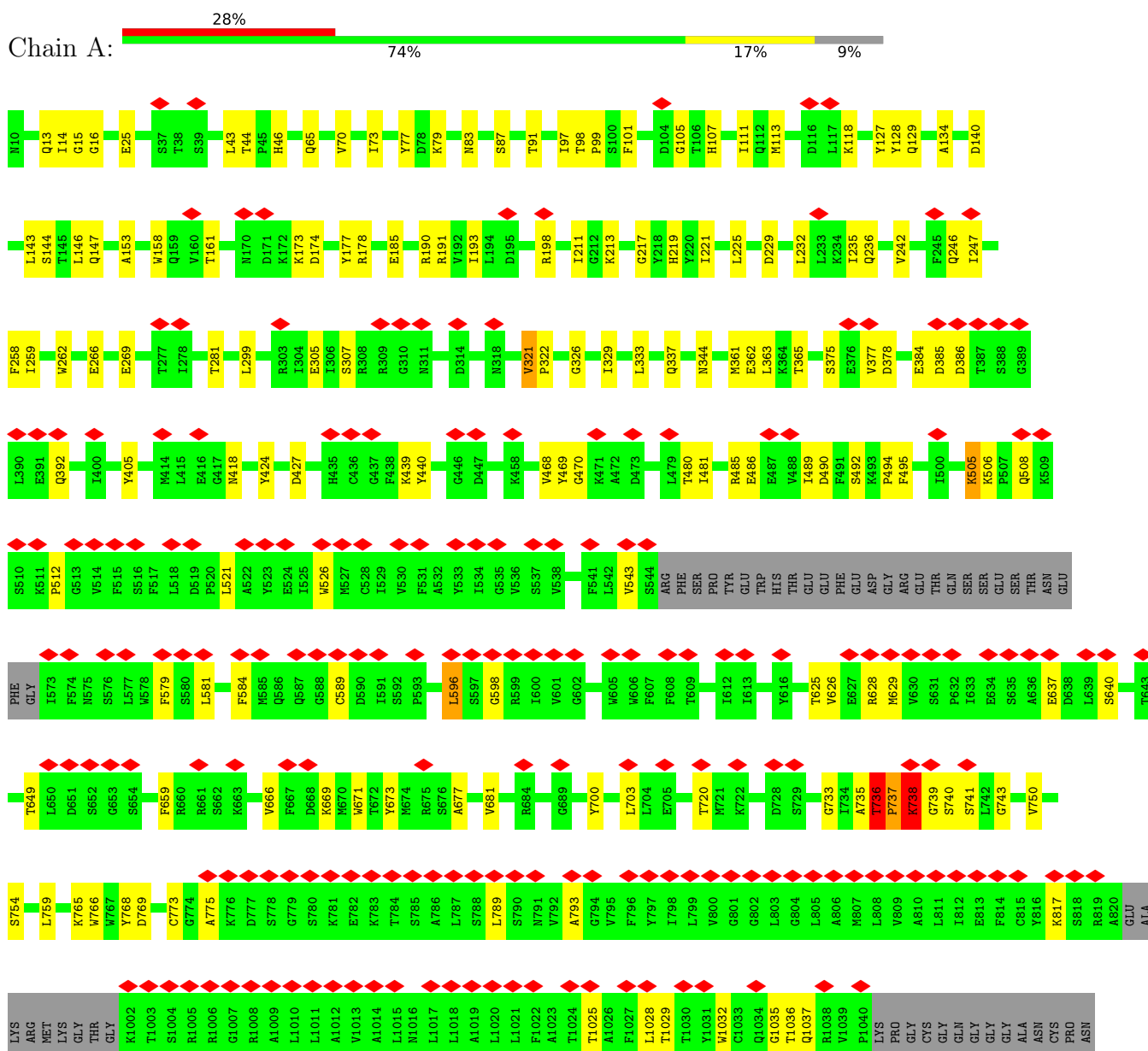


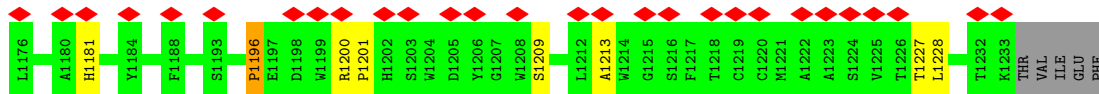
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			85	56	29	
2	C	1	Total	C	O	0
			85	56	29	

3 Residue-property plots

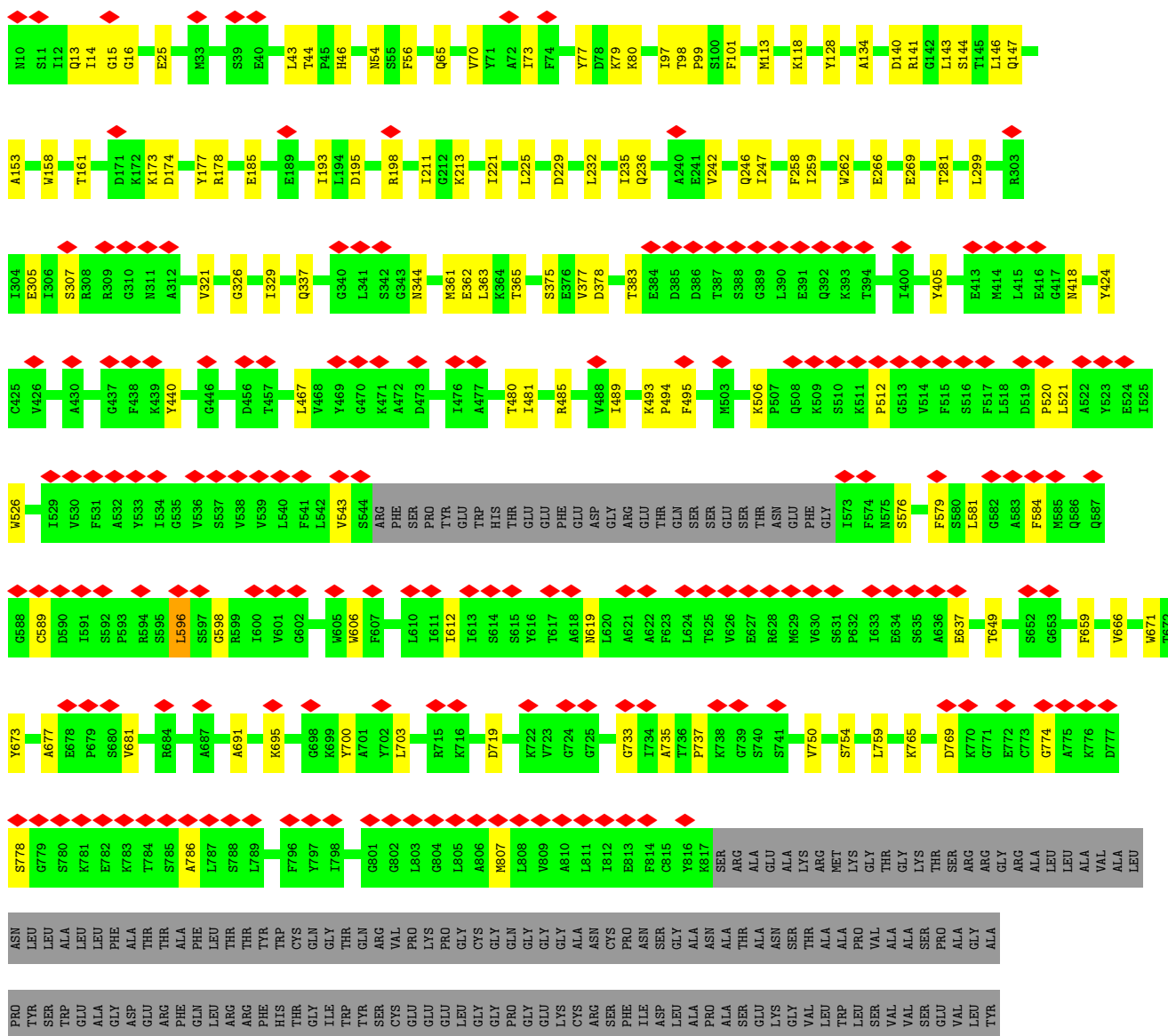
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutamate receptor 2, Germ cell-specific gene 1-like protein





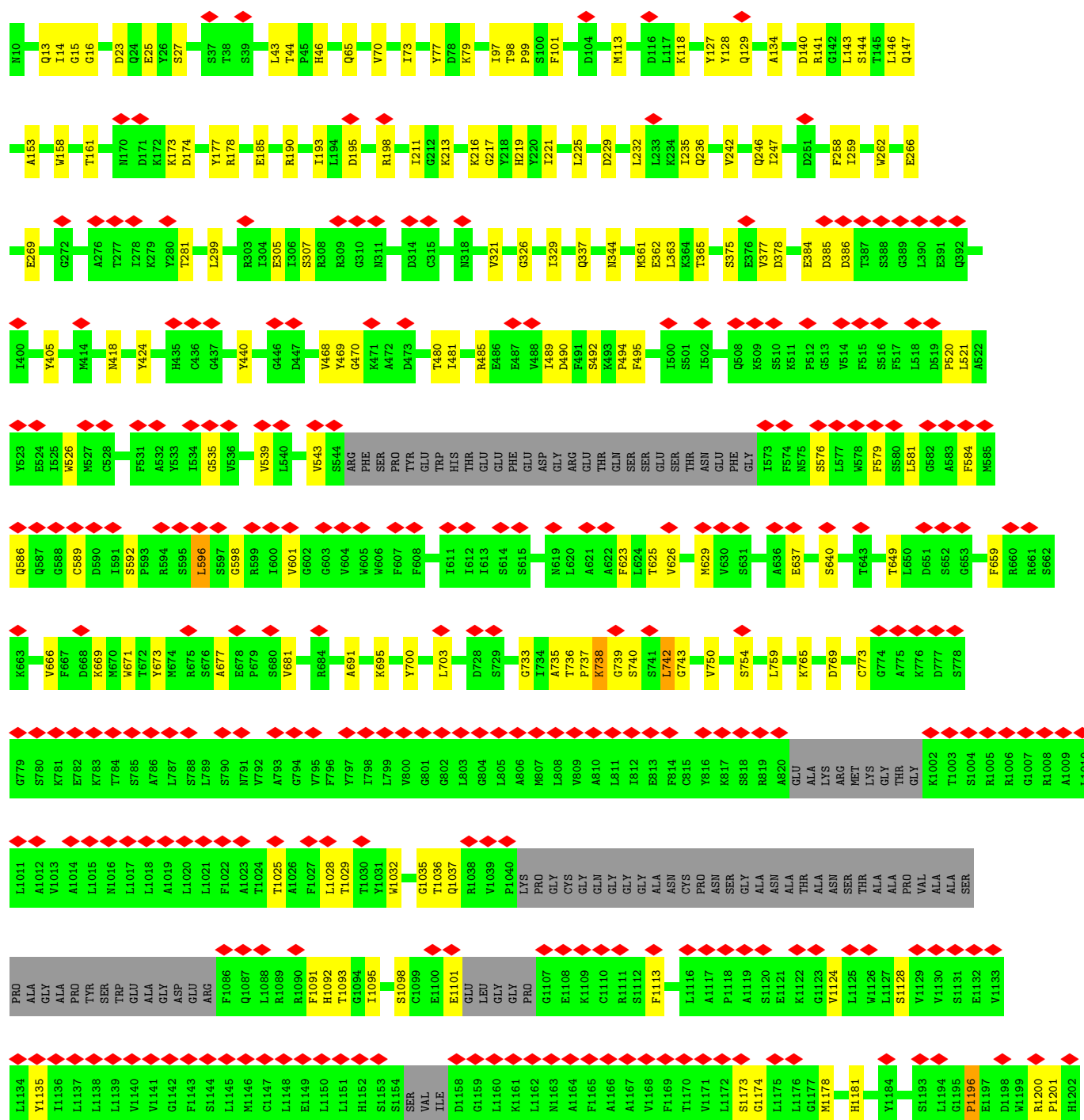
Chain B:

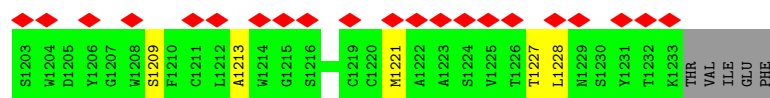


ILE	LEU	LEU	ASP	TRP	VAL	VAL	GLY	PHE	TRP	ASP	MET	CYS	LEU	GLU	LEU	LEU	HIS	SER	ALA	SER	TRP	GLY	SER	VAL	ASP	ILE	GLY	LEU	LYS	ASN	ALA	ASN	PHE	PHE	ALA	ALA	VAL	VAL	THR	THR	VAL	THR	LEU	SER	GLY	LEU	GLY	GLY	MET	VAL	ALA	HIS	MET	MET	THR	TVR	THR	GLN	VAL	PHE	GLN	VAL	THR	VAL	SER	LEU	GLY
PRO	GLU	ASP	TRP	ARG	PRO	HIS	SER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

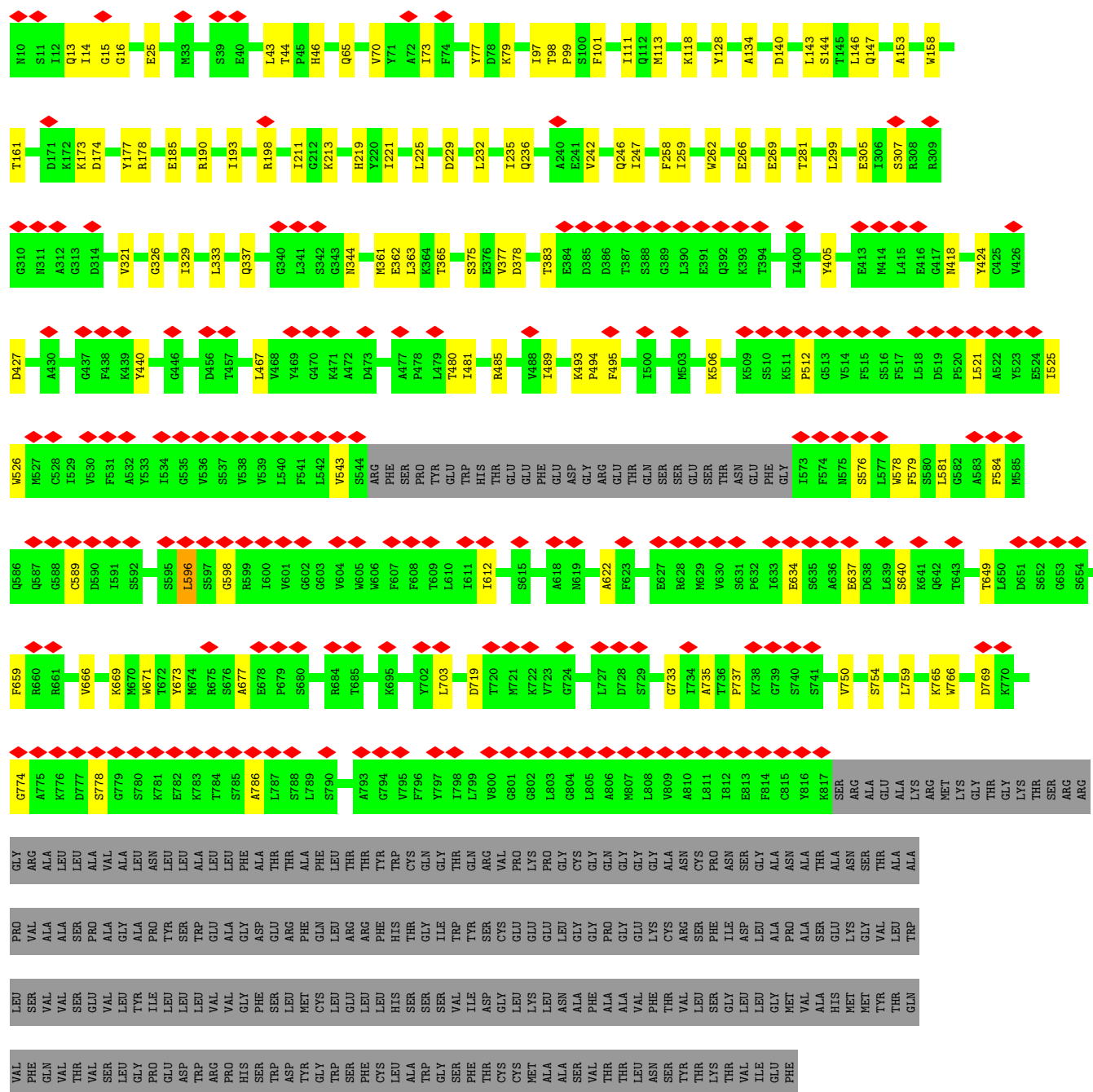
● Molecule 1: Glutamate receptor 2, Germ cell-specific gene 1-like protein

Chain C: 





● Molecule 1: Glutamate receptor 2, Germ cell-specific gene 1-like protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	18926	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	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	0.061	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	294.0, 294.0, 294.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98, 0.98, 0.98	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.19	0/7718	0.51	6/10438 (0.1%)
1	B	0.20	1/6253 (0.0%)	0.50	5/8450 (0.1%)
1	C	0.18	0/7718	0.48	3/10438 (0.0%)
1	D	0.22	2/6253 (0.0%)	0.49	5/8450 (0.1%)
All	All	0.20	3/27942 (0.0%)	0.49	19/37776 (0.1%)

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	5
1	C	0	3
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	612	ILE	C-N	8.88	1.43	1.34
1	B	612	ILE	C-N	-6.04	1.25	1.33
1	D	512	PRO	C-N	5.29	1.41	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	736	THR	C-N-CD	-12.60	73.33	125.00
1	B	512	PRO	O-C-N	6.26	131.09	122.64
1	D	383	THR	CA-C-N	5.88	130.06	121.31
1	D	383	THR	C-N-CA	5.88	130.06	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	383	THR	CA-C-N	5.73	129.85	121.31
1	B	383	THR	C-N-CA	5.73	129.85	121.31
1	C	377	VAL	N-CA-C	-5.48	108.16	113.53
1	D	377	VAL	N-CA-C	-5.47	108.17	113.53
1	B	377	VAL	N-CA-C	-5.47	108.17	113.53
1	A	377	VAL	N-CA-C	-5.46	108.18	113.53
1	D	786	ALA	N-CA-C	5.29	117.16	110.33
1	B	786	ALA	N-CA-C	5.27	117.12	110.33
1	A	512	PRO	CA-C-N	5.18	131.56	121.41
1	A	512	PRO	C-N-CA	5.18	131.56	121.41
1	D	634	GLU	O-C-N	5.10	128.36	122.09
1	A	1196	PRO	CA-C-N	5.02	128.35	120.82
1	A	1196	PRO	C-N-CA	5.02	128.35	120.82
1	C	1196	PRO	CA-C-N	5.01	128.33	120.82
1	C	1196	PRO	C-N-CA	5.01	128.33	120.82

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1196	PRO	Peptide
1	A	384	GLU	Peptide
1	A	505	LYS	Mainchain
1	A	773	CYS	Mainchain
1	A	817	LYS	Peptide
1	C	1196	PRO	Peptide
1	C	384	GLU	Peptide
1	C	773	CYS	Mainchain

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	7555	0	7536	137	0
1	B	6125	0	6110	71	0
1	C	7555	0	7536	129	0
1	D	6125	0	6110	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	85	0	0	36	0
2	C	85	0	0	37	0
All	All	27530	0	27292	406	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 (406) 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:490:ASP:CG	1:A:738:LYS:HA	1.17	1.60
1:C:469:TYR:C	2:C:1301:AJP:C80	1.86	1.48
1:C:469:TYR:CD1	2:C:1301:AJP:O82	1.74	1.40
1:A:470:GLY:N	2:A:1301:AJP:C80	1.88	1.35
1:C:217:GLY:N	2:C:1301:AJP:C01	1.91	1.31
1:A:490:ASP:OD2	1:A:739:GLY:N	1.66	1.28
1:A:469:TYR:C	2:A:1301:AJP:C80	2.05	1.27
1:C:470:GLY:N	2:C:1301:AJP:C80	1.94	1.26
1:A:741:SER:HB2	2:A:1301:AJP:O53	1.36	1.24
1:A:490:ASP:OD2	1:A:738:LYS:HA	1.37	1.23
1:A:490:ASP:CG	1:A:738:LYS:CA	2.12	1.22
1:C:217:GLY:CA	2:C:1301:AJP:C01	2.18	1.21
1:A:490:ASP:OD2	1:A:738:LYS:CA	1.96	1.13
1:A:490:ASP:OD1	1:A:738:LYS:HA	1.48	1.13
1:C:217:GLY:HA2	2:C:1301:AJP:C01	1.77	1.12
1:A:736:THR:OG1	1:A:737:PRO:HD2	1.31	1.11
1:C:217:GLY:H	2:C:1301:AJP:C01	1.58	1.09
1:A:217:GLY:N	2:A:1301:AJP:C01	2.16	1.08
1:C:490:ASP:CG	1:C:738:LYS:HA	1.81	1.05
1:C:469:TYR:CE1	2:C:1301:AJP:O82	2.10	1.04
1:A:217:GLY:HA2	2:A:1301:AJP:C01	1.89	1.03
1:A:217:GLY:CA	2:A:1301:AJP:C01	2.38	1.02
1:A:469:TYR:HA	2:A:1301:AJP:C16	1.90	1.00
1:A:490:ASP:OD2	1:A:738:LYS:C	2.07	0.97
1:A:736:THR:OG1	1:A:737:PRO:CD	2.15	0.94
1:C:469:TYR:CA	2:C:1301:AJP:C80	2.47	0.93
1:A:217:GLY:H	2:A:1301:AJP:C01	1.81	0.91
1:C:217:GLY:HA2	2:C:1301:AJP:C03	2.03	0.89
1:C:469:TYR:HD1	2:C:1301:AJP:O82	1.60	0.85
1:A:469:TYR:CG	2:A:1301:AJP:C08	2.59	0.85
1:C:490:ASP:OD2	1:C:738:LYS:HA	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:SER:CB	2:A:1301:AJP:O42	2.28	0.81
1:A:468:VAL:O	2:A:1301:AJP:C80	2.29	0.81
1:A:736:THR:HG1	1:A:737:PRO:HD2	1.45	0.80
1:A:740:SER:OG	2:A:1301:AJP:O42	2.00	0.79
1:C:736:THR:OG1	1:C:737:PRO:HD2	1.82	0.79
1:C:469:TYR:HA	2:C:1301:AJP:C16	2.12	0.78
1:A:469:TYR:CA	2:A:1301:AJP:C80	2.62	0.76
1:A:470:GLY:CA	2:A:1301:AJP:C80	2.63	0.75
1:A:741:SER:HB2	2:A:1301:AJP:C46	2.22	0.70
1:C:470:GLY:CA	2:C:1301:AJP:C80	2.70	0.69
1:C:127:TYR:HD1	2:C:1301:AJP:C71	2.06	0.69
1:A:217:GLY:HA2	2:A:1301:AJP:C03	2.24	0.68
1:D:596:LEU:HD22	1:D:598:GLY:H	1.60	0.66
1:C:736:THR:OG1	1:C:737:PRO:CD	2.43	0.66
1:C:469:TYR:HA	2:C:1301:AJP:C80	2.25	0.66
1:B:596:LEU:HD22	1:B:598:GLY:H	1.60	0.65
1:A:596:LEU:HD22	1:A:598:GLY:H	1.61	0.65
1:C:596:LEU:HD22	1:C:598:GLY:H	1.60	0.65
1:A:469:TYR:CA	2:A:1301:AJP:C16	2.71	0.65
1:A:736:THR:HG21	1:A:743:GLY:HA2	1.79	0.65
1:A:1037:GLN:HE21	1:A:1200:ARG:HG2	1.62	0.64
1:C:1037:GLN:HE21	1:C:1200:ARG:HG2	1.62	0.64
1:B:606:TRP:HZ2	1:C:586:GLN:HB2	1.61	0.64
1:B:337:GLN:HE21	1:B:344:ASN:HD21	1.46	0.64
1:A:470:GLY:HA3	2:A:1301:AJP:C21	2.29	0.63
1:B:493:LYS:NZ	1:C:492:SER:O	2.31	0.63
1:D:337:GLN:HE21	1:D:344:ASN:HD21	1.46	0.63
1:A:490:ASP:OD1	1:A:738:LYS:CA	2.31	0.63
1:A:470:GLY:H	2:A:1301:AJP:C80	2.06	0.62
1:C:217:GLY:HA2	2:C:1301:AJP:C02	2.29	0.62
1:A:337:GLN:HE21	1:A:344:ASN:HD21	1.46	0.61
1:C:337:GLN:HE21	1:C:344:ASN:HD21	1.46	0.61
1:B:16:GLY:H	1:B:65:GLN:HE22	1.49	0.60
1:A:737:PRO:HB2	1:A:740:SER:HB2	1.81	0.60
1:C:16:GLY:H	1:C:65:GLN:HE22	1.49	0.60
1:C:490:ASP:OD2	1:C:739:GLY:N	2.35	0.60
1:C:147:GLN:HE21	1:D:143:LEU:HD21	1.66	0.60
1:D:16:GLY:H	1:D:65:GLN:HE22	1.49	0.60
1:A:16:GLY:H	1:A:65:GLN:HE22	1.49	0.59
1:C:469:TYR:CD1	2:C:1301:AJP:C10	2.81	0.59
1:C:468:VAL:O	2:C:1301:AJP:C80	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1301:AJP:O33	2:A:1301:AJP:O76	2.21	0.59
2:C:1301:AJP:O76	2:C:1301:AJP:O33	2.21	0.59
1:C:469:TYR:CG	2:C:1301:AJP:C08	2.87	0.58
1:C:490:ASP:CG	1:C:738:LYS:CA	2.69	0.58
1:C:143:LEU:HD21	1:D:147:GLN:HE21	1.69	0.57
1:C:1032:TRP:N	1:C:1093:THR:O	2.37	0.57
1:B:153:ALA:HA	1:B:158:TRP:HB2	1.87	0.57
1:A:153:ALA:HA	1:A:158:TRP:HB2	1.87	0.57
1:C:490:ASP:OD2	1:C:738:LYS:CA	2.51	0.57
2:A:1301:AJP:O62	2:A:1301:AJP:O75	2.22	0.56
2:A:1301:AJP:O62	2:A:1301:AJP:O64	2.23	0.56
1:B:14:ILE:HG21	1:B:43:LEU:HD23	1.88	0.56
2:C:1301:AJP:O62	2:C:1301:AJP:O64	2.23	0.56
2:C:1301:AJP:O62	2:C:1301:AJP:O75	2.22	0.56
1:A:118:LYS:NZ	1:A:144:SER:OG	2.39	0.56
1:D:299:LEU:HD21	1:D:329:ILE:HG12	1.88	0.56
1:C:153:ALA:HA	1:C:158:TRP:HB2	1.87	0.56
1:C:299:LEU:HD21	1:C:329:ILE:HG12	1.88	0.56
1:D:118:LYS:NZ	1:D:144:SER:OG	2.39	0.56
1:B:506:LYS:HE3	1:B:719:ASP:HA	1.88	0.56
1:A:1032:TRP:N	1:A:1093:THR:O	2.37	0.56
1:C:14:ILE:HG21	1:C:43:LEU:HD23	1.88	0.56
1:C:118:LYS:NZ	1:C:144:SER:OG	2.39	0.56
1:A:505:LYS:NZ	1:A:508:GLN:OE1	2.37	0.55
1:A:789:LEU:HD13	1:D:525:ILE:HG12	1.87	0.55
1:D:14:ILE:HG21	1:D:43:LEU:HD23	1.88	0.55
1:D:153:ALA:HA	1:D:158:TRP:HB2	1.87	0.55
1:A:14:ILE:HG21	1:A:43:LEU:HD23	1.88	0.55
1:A:299:LEU:HD21	1:A:329:ILE:HG12	1.88	0.55
1:B:299:LEU:HD21	1:B:329:ILE:HG12	1.88	0.55
2:C:1301:AJP:C83	2:C:1301:AJP:C81	2.85	0.55
1:A:143:LEU:HD21	1:B:147:GLN:HE21	1.71	0.55
2:A:1301:AJP:C83	2:A:1301:AJP:C81	2.85	0.55
1:D:232:LEU:HD23	1:D:363:LEU:HD13	1.89	0.55
1:A:147:GLN:HE21	1:B:143:LEU:HD21	1.70	0.55
1:C:469:TYR:O	2:C:1301:AJP:C80	2.47	0.55
2:A:1301:AJP:C32	2:A:1301:AJP:C35	2.85	0.54
1:C:1098:SER:HB3	1:C:1113:PHE:HB2	1.89	0.54
1:A:628:ARG:HD3	1:D:622:ALA:HB1	1.89	0.54
1:B:118:LYS:NZ	1:B:144:SER:OG	2.39	0.54
2:C:1301:AJP:C32	2:C:1301:AJP:C35	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:ASP:OD2	1:D:178:ARG:NH1	2.40	0.54
1:A:232:LEU:HD23	1:A:363:LEU:HD13	1.89	0.54
1:A:77:TYR:HE1	1:A:98:THR:HG21	1.73	0.54
1:B:232:LEU:HD23	1:B:363:LEU:HD13	1.89	0.54
1:A:486:GLU:OE2	1:A:738:LYS:NZ	2.35	0.54
1:A:579:PHE:HD1	1:A:589:CYS:HB2	1.73	0.54
1:C:174:ASP:OD2	1:C:178:ARG:NH1	2.40	0.54
1:B:77:TYR:HE1	1:B:98:THR:HG21	1.73	0.54
1:B:174:ASP:OD2	1:B:178:ARG:NH1	2.40	0.54
1:D:77:TYR:HE1	1:D:98:THR:HG21	1.73	0.54
1:C:579:PHE:HD1	1:C:589:CYS:HB2	1.73	0.53
1:D:134:ALA:HA	1:D:161:THR:HB	1.90	0.53
1:C:77:TYR:HE1	1:C:98:THR:HG21	1.73	0.53
1:C:134:ALA:HA	1:C:161:THR:HB	1.90	0.53
1:A:236:GLN:NE2	1:A:365:THR:O	2.42	0.53
1:A:1098:SER:HB3	1:A:1113:PHE:HB2	1.89	0.53
1:A:134:ALA:HA	1:A:161:THR:HB	1.90	0.53
1:D:579:PHE:HD1	1:D:589:CYS:HB2	1.73	0.53
1:B:134:ALA:HA	1:B:161:THR:HB	1.90	0.53
1:C:232:LEU:HD23	1:C:363:LEU:HD13	1.89	0.52
1:C:236:GLN:NE2	1:C:365:THR:O	2.42	0.52
1:D:236:GLN:NE2	1:D:365:THR:O	2.42	0.52
1:B:480:THR:O	1:B:485:ARG:NH1	2.42	0.52
1:A:392:GLN:HG3	1:A:439:LYS:HD3	1.91	0.52
1:B:579:PHE:HD1	1:B:589:CYS:HB2	1.73	0.52
1:A:740:SER:CA	2:A:1301:AJP:O42	2.57	0.52
1:C:480:THR:O	1:C:485:ARG:NH1	2.42	0.52
1:A:1029:THR:H	1:A:1095:ILE:HG22	1.75	0.51
1:C:1029:THR:H	1:C:1095:ILE:HG22	1.75	0.51
2:C:1301:AJP:C02	2:C:1301:AJP:C06	2.85	0.51
1:A:1092:HIS:HD2	1:A:1101:GLU:HB3	1.76	0.51
2:A:1301:AJP:C06	2:A:1301:AJP:C02	2.86	0.51
1:B:236:GLN:NE2	1:B:365:THR:O	2.42	0.51
1:B:581:LEU:HA	1:B:584:PHE:HB2	1.93	0.51
2:A:1301:AJP:C56	2:A:1301:AJP:C30	2.89	0.51
1:A:174:ASP:OD2	1:A:178:ARG:NH1	2.40	0.50
1:C:469:TYR:O	2:C:1301:AJP:C81	2.54	0.50
1:C:1092:HIS:HD2	1:C:1101:GLU:HB3	1.76	0.50
1:A:13:GLN:HB3	1:A:70:VAL:HG12	1.93	0.50
1:C:99:PRO:HA	1:C:113:MET:HB2	1.94	0.50
1:C:217:GLY:CA	2:C:1301:AJP:C03	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:PRO:HA	1:A:113:MET:HB2	1.94	0.50
1:B:99:PRO:HA	1:B:113:MET:HB2	1.94	0.50
1:D:581:LEU:HA	1:D:584:PHE:HB2	1.93	0.50
1:A:480:THR:O	1:A:485:ARG:NH1	2.42	0.50
2:C:1301:AJP:C56	2:C:1301:AJP:C30	2.89	0.50
1:D:13:GLN:HB3	1:D:70:VAL:HG12	1.93	0.50
1:A:581:LEU:HA	1:A:584:PHE:HB2	1.93	0.50
1:B:520:PRO:O	1:B:619:ASN:ND2	2.44	0.50
1:C:1035:GLY:HA2	1:C:1201:PRO:HB3	1.94	0.50
1:D:480:THR:O	1:D:485:ARG:NH1	2.42	0.50
1:D:99:PRO:HA	1:D:113:MET:HB2	1.94	0.50
1:A:15:GLY:HA3	1:A:73:ILE:HA	1.94	0.49
1:B:15:GLY:HA3	1:B:73:ILE:HA	1.95	0.49
1:B:13:GLN:HB3	1:B:70:VAL:HG12	1.93	0.49
1:C:581:LEU:HA	1:C:584:PHE:HB2	1.93	0.49
1:C:13:GLN:HB3	1:C:70:VAL:HG12	1.93	0.49
1:C:193:ILE:HG12	1:C:221:ILE:HB	1.95	0.49
1:B:193:ILE:HG12	1:B:221:ILE:HB	1.95	0.49
1:A:77:TYR:OH	1:A:101:PHE:O	2.25	0.49
1:D:15:GLY:HA3	1:D:73:ILE:HA	1.95	0.49
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.95	0.49
2:A:1301:AJP:O72	2:A:1301:AJP:O73	2.31	0.49
1:C:128:TYR:OH	1:C:362:GLU:OE2	2.31	0.49
1:C:1035:GLY:O	1:C:1091:PHE:N	2.43	0.49
1:A:1035:GLY:HA2	1:A:1201:PRO:HB3	1.94	0.48
2:C:1301:AJP:O72	2:C:1301:AJP:O73	2.31	0.48
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.95	0.48
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.94	0.48
1:A:506:LYS:H	1:A:720:THR:HA	1.79	0.48
1:A:626:VAL:HA	1:A:629:MET:HB2	1.95	0.48
1:C:15:GLY:HA3	1:C:73:ILE:HA	1.95	0.48
1:A:193:ILE:HG12	1:A:221:ILE:HB	1.95	0.48
1:A:1036:THR:H	1:A:1201:PRO:HA	1.79	0.48
1:B:128:TYR:OH	1:B:362:GLU:OE2	2.31	0.48
1:C:217:GLY:O	2:C:1301:AJP:C03	2.62	0.48
1:C:626:VAL:HA	1:C:629:MET:HB2	1.95	0.48
1:B:521:LEU:O	1:B:526:TRP:NE1	2.47	0.48
1:A:521:LEU:O	1:A:526:TRP:NE1	2.47	0.48
1:D:521:LEU:O	1:D:526:TRP:NE1	2.47	0.48
1:A:242:VAL:HB	1:A:363:LEU:HB3	1.96	0.48
1:A:1035:GLY:N	1:A:1091:PHE:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1172:LEU:HD21	1:B:807:MET:HG3	1.94	0.48
1:B:242:VAL:HB	1:B:363:LEU:HB3	1.96	0.48
1:D:128:TYR:OH	1:D:362:GLU:OE2	2.31	0.48
1:D:305:GLU:OE2	1:D:307:SER:OG	2.32	0.48
1:C:242:VAL:HB	1:C:363:LEU:HB3	1.96	0.47
1:C:521:LEU:O	1:C:526:TRP:NE1	2.47	0.47
1:C:1035:GLY:N	1:C:1091:PHE:O	2.46	0.47
1:D:375:SER:HB3	1:D:378:ASP:HB2	1.96	0.47
1:A:128:TYR:OH	1:A:362:GLU:OE2	2.31	0.47
1:D:193:ILE:HG12	1:D:221:ILE:HB	1.95	0.47
1:A:191:ARG:NH2	1:A:469:TYR:OH	2.47	0.47
1:A:305:GLU:OE2	1:A:307:SER:OG	2.32	0.47
1:C:305:GLU:OE2	1:C:307:SER:OG	2.32	0.47
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.95	0.47
1:B:305:GLU:OE2	1:B:307:SER:OG	2.32	0.47
1:B:375:SER:HB3	1:B:378:ASP:HB2	1.96	0.47
1:C:375:SER:HB3	1:C:378:ASP:HB2	1.96	0.47
1:A:127:TYR:HD1	2:A:1301:AJP:C71	2.28	0.47
1:C:592:SER:HB2	1:D:578:TRP:HH2	1.79	0.47
1:C:1036:THR:H	1:C:1201:PRO:HA	1.79	0.47
1:B:246:GLN:HB3	1:B:361:MET:HG3	1.97	0.47
1:A:375:SER:HB3	1:A:378:ASP:HB2	1.96	0.46
1:A:736:THR:HG21	1:A:743:GLY:CA	2.44	0.46
1:C:127:TYR:CD1	2:C:1301:AJP:C71	2.93	0.46
1:D:242:VAL:HB	1:D:363:LEU:HB3	1.96	0.46
1:A:87:SER:OG	1:B:54:ASN:OD1	2.27	0.46
1:A:754:SER:HB3	1:A:759:LEU:HD12	1.97	0.46
1:A:1035:GLY:O	1:A:1091:PHE:N	2.43	0.46
1:C:470:GLY:HA3	2:C:1301:AJP:C21	2.45	0.46
1:D:754:SER:HB3	1:D:759:LEU:HD12	1.98	0.46
1:A:246:GLN:HB3	1:A:361:MET:HG3	1.97	0.46
1:A:13:GLN:HA	1:A:44:THR:HB	1.98	0.46
1:A:46:HIS:O	1:A:65:GLN:NE2	2.49	0.46
1:B:198:ARG:HE	1:B:229:ASP:HB3	1.81	0.46
1:C:211:ILE:HD12	1:C:213:LYS:HD2	1.98	0.46
1:D:467:LEU:HB3	1:D:737:PRO:HG3	1.98	0.46
1:A:469:TYR:HA	2:A:1301:AJP:C80	2.46	0.46
1:A:211:ILE:HD12	1:A:213:LYS:HD2	1.98	0.46
1:A:737:PRO:CB	1:A:740:SER:HB2	2.45	0.46
1:C:742:LEU:H	1:C:742:LEU:HG	1.49	0.46
1:D:198:ARG:HE	1:D:229:ASP:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:774:GLY:O	1:D:778:SER:N	2.45	0.46
1:A:198:ARG:HE	1:A:229:ASP:HB3	1.81	0.46
1:A:1135:TYR:O	1:A:1173:SER:OG	2.32	0.46
1:B:659:PHE:HB3	1:B:671:TRP:HB2	1.98	0.46
1:C:46:HIS:O	1:C:65:GLN:NE2	2.49	0.46
1:C:246:GLN:HB3	1:C:361:MET:HG3	1.97	0.46
1:D:13:GLN:HA	1:D:44:THR:HB	1.98	0.46
1:D:46:HIS:O	1:D:65:GLN:NE2	2.49	0.46
1:A:469:TYR:CD2	2:A:1301:AJP:C83	2.98	0.45
1:C:469:TYR:CA	2:C:1301:AJP:C16	2.91	0.45
1:C:13:GLN:HA	1:C:44:THR:HB	1.98	0.45
1:C:198:ARG:HE	1:C:229:ASP:HB3	1.81	0.45
1:C:489:ILE:C	1:C:738:LYS:HB2	2.41	0.45
1:D:246:GLN:HB3	1:D:361:MET:HG3	1.97	0.45
1:D:211:ILE:HD12	1:D:213:LYS:HD2	1.98	0.45
1:A:25:GLU:OE2	1:A:281:THR:OG1	2.32	0.45
1:B:46:HIS:O	1:B:65:GLN:NE2	2.49	0.45
1:B:211:ILE:HD12	1:B:213:LYS:HD2	1.98	0.45
1:A:659:PHE:HB3	1:A:671:TRP:HB2	1.98	0.45
1:C:754:SER:HB3	1:C:759:LEU:HD12	1.97	0.45
1:A:1025:THR:HG22	1:A:1209:SER:HB2	1.99	0.45
1:B:754:SER:HB3	1:B:759:LEU:HD12	1.97	0.45
1:C:659:PHE:HB3	1:C:671:TRP:HB2	1.98	0.45
1:A:469:TYR:CD2	2:A:1301:AJP:C08	2.98	0.45
1:A:740:SER:HA	2:A:1301:AJP:O42	2.17	0.45
1:D:659:PHE:HB3	1:D:671:TRP:HB2	1.98	0.45
1:C:737:PRO:HB2	1:C:740:SER:HB2	1.98	0.45
1:A:326:GLY:HA2	1:A:329:ILE:HD12	1.99	0.45
1:A:789:LEU:O	1:A:793:ALA:N	2.47	0.45
1:B:467:LEU:HB3	1:B:737:PRO:HG3	1.98	0.45
1:C:535:GLY:HA2	1:C:1221:MET:HE2	1.98	0.45
1:D:25:GLU:OE2	1:D:281:THR:OG1	2.32	0.45
1:A:266:GLU:HG2	1:A:269:GLU:H	1.82	0.45
1:A:495:PHE:HB3	1:A:750:VAL:HG13	1.99	0.44
1:B:258:PHE:O	1:B:262:TRP:N	2.48	0.44
1:C:1025:THR:HG22	1:C:1209:SER:HB2	1.99	0.44
1:C:1135:TYR:O	1:C:1173:SER:OG	2.32	0.44
1:B:326:GLY:HA2	1:B:329:ILE:HD12	1.99	0.44
1:C:520:PRO:HG3	1:C:623:PHE:HE2	1.82	0.44
1:D:97:ILE:HG23	1:D:113:MET:HE3	2.00	0.44
1:A:741:SER:N	2:A:1301:AJP:O43	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:GLN:HA	1:B:44:THR:HB	1.98	0.44
1:D:266:GLU:HG2	1:D:269:GLU:H	1.83	0.44
1:A:405:TYR:HA	1:A:424:TYR:HB3	2.00	0.44
1:B:774:GLY:O	1:B:778:SER:N	2.45	0.44
1:C:326:GLY:HA2	1:C:329:ILE:HD12	1.99	0.44
1:D:326:GLY:HA2	1:D:329:ILE:HD12	1.99	0.44
1:B:495:PHE:HB3	1:B:750:VAL:HG13	1.99	0.44
1:D:405:TYR:HA	1:D:424:TYR:HB3	2.00	0.44
1:A:97:ILE:HG23	1:A:113:MET:HE3	2.00	0.44
1:B:97:ILE:HG23	1:B:113:MET:HE3	2.00	0.44
1:C:736:THR:HG21	1:C:743:GLY:CA	2.47	0.44
1:A:129:GLN:NE2	2:A:1301:AJP:O78	2.51	0.44
1:A:173:LYS:HB2	1:A:177:TYR:HE2	1.83	0.44
1:B:143:LEU:HD23	1:B:146:LEU:HD23	2.00	0.44
1:C:266:GLU:HG2	1:C:269:GLU:H	1.83	0.44
1:D:258:PHE:O	1:D:262:TRP:N	2.48	0.44
1:D:495:PHE:HB3	1:D:750:VAL:HG13	1.99	0.44
1:A:1227:THR:HG23	1:A:1228:LEU:HD22	2.00	0.43
1:B:173:LYS:HB2	1:B:177:TYR:HE2	1.83	0.43
1:B:405:TYR:HA	1:B:424:TYR:HB3	2.00	0.43
1:C:129:GLN:NE2	2:C:1301:AJP:O78	2.50	0.43
1:C:216:LYS:HG2	2:C:1301:AJP:C01	2.48	0.43
1:C:405:TYR:HA	1:C:424:TYR:HB3	2.00	0.43
1:C:418:ASN:ND2	1:C:440:TYR:O	2.44	0.43
1:D:143:LEU:HD23	1:D:146:LEU:HD23	2.00	0.43
1:D:506:LYS:HE3	1:D:719:ASP:HA	1.99	0.43
1:B:543:VAL:HG22	1:B:596:LEU:HD21	2.01	0.43
1:C:495:PHE:HB3	1:C:750:VAL:HG13	1.99	0.43
1:A:543:VAL:HG22	1:A:596:LEU:HD21	2.01	0.43
1:B:266:GLU:HG2	1:B:269:GLU:H	1.83	0.43
1:C:225:LEU:HD22	1:C:247:ILE:HB	2.01	0.43
1:C:469:TYR:CD1	2:C:1301:AJP:C08	3.02	0.43
1:C:481:ILE:HD11	1:C:733:GLY:HA3	2.00	0.43
1:D:481:ILE:HD11	1:D:733:GLY:HA3	2.00	0.43
1:B:418:ASN:ND2	1:B:440:TYR:O	2.44	0.43
1:C:97:ILE:HG23	1:C:113:MET:HE3	2.00	0.43
1:C:143:LEU:HD23	1:C:146:LEU:HD23	2.00	0.43
1:C:173:LYS:HB2	1:C:177:TYR:HE2	1.83	0.43
1:A:427:ASP:OD2	1:A:766:TRP:NE1	2.43	0.43
1:A:469:TYR:HB3	2:A:1301:AJP:C83	2.44	0.43
1:B:185:GLU:HG3	1:B:213:LYS:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:ILE:HD11	1:B:733:GLY:HA3	2.00	0.43
1:B:681:VAL:O	1:B:700:TYR:OH	2.32	0.43
1:C:190:ARG:O	1:C:219:HIS:N	2.52	0.43
1:D:259:ILE:HA	1:D:262:TRP:HB3	2.01	0.43
1:A:185:GLU:HG3	1:A:213:LYS:HE3	2.01	0.43
1:A:190:ARG:O	1:A:219:HIS:N	2.52	0.43
1:A:481:ILE:HD11	1:A:733:GLY:HA3	2.00	0.43
1:B:691:ALA:O	1:B:695:LYS:N	2.47	0.43
1:C:543:VAL:HG22	1:C:596:LEU:HD21	2.01	0.43
1:C:625:THR:O	1:C:629:MET:N	2.52	0.43
1:C:691:ALA:O	1:C:695:LYS:N	2.47	0.43
1:D:225:LEU:HD22	1:D:247:ILE:HB	2.01	0.43
1:B:77:TYR:OH	1:B:101:PHE:O	2.25	0.43
1:C:490:ASP:CB	1:C:738:LYS:HA	2.45	0.43
1:D:543:VAL:HG22	1:D:596:LEU:HD21	2.01	0.43
1:A:143:LEU:HD23	1:A:146:LEU:HD23	2.00	0.42
1:A:1124:VAL:O	1:A:1128:SER:N	2.52	0.42
1:D:427:ASP:OD2	1:D:766:TRP:NE1	2.43	0.42
1:B:481:ILE:HD12	1:B:494:PRO:HG3	2.01	0.42
1:C:1227:THR:HG23	1:C:1228:LEU:HD22	2.00	0.42
1:D:79:LYS:HD3	1:D:140:ASP:HA	2.02	0.42
1:A:83:ASN:ND2	1:B:80:LYS:HA	2.35	0.42
1:A:258:PHE:O	1:A:262:TRP:N	2.48	0.42
1:A:481:ILE:HD12	1:A:494:PRO:HG3	2.02	0.42
1:C:79:LYS:HD3	1:C:140:ASP:HA	2.02	0.42
1:D:173:LYS:HB2	1:D:177:TYR:HE2	1.83	0.42
1:D:637:GLU:HG2	1:D:666:VAL:HG11	2.01	0.42
1:D:190:ARG:O	1:D:219:HIS:N	2.52	0.42
1:A:91:THR:HG21	1:B:56:PHE:CD2	2.54	0.42
1:A:259:ILE:HA	1:A:262:TRP:HB3	2.01	0.42
1:A:637:GLU:HG2	1:A:666:VAL:HG11	2.01	0.42
1:B:225:LEU:HD22	1:B:247:ILE:HB	2.01	0.42
1:D:481:ILE:HD12	1:D:494:PRO:HG3	2.01	0.42
1:B:141:ARG:NH2	1:B:195:ASP:OD1	2.45	0.42
1:C:1124:VAL:O	1:C:1128:SER:N	2.52	0.42
1:D:489:ILE:HD12	1:D:735:ALA:HB1	2.02	0.42
1:C:481:ILE:HD12	1:C:494:PRO:HG3	2.01	0.42
1:A:765:LYS:HA	1:A:769:ASP:HB2	2.02	0.42
1:B:673:TYR:O	1:B:677:ALA:N	2.53	0.42
1:C:25:GLU:OE2	1:C:281:THR:OG1	2.32	0.42
1:D:765:LYS:HA	1:D:769:ASP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:637:GLU:HG2	1:B:666:VAL:HG11	2.01	0.42
1:C:141:ARG:NH2	1:C:195:ASP:OD1	2.45	0.42
1:C:259:ILE:HA	1:C:262:TRP:HB3	2.01	0.42
1:C:673:TYR:O	1:C:677:ALA:N	2.53	0.42
1:A:225:LEU:HD22	1:A:247:ILE:HB	2.01	0.41
1:A:681:VAL:O	1:A:700:TYR:OH	2.32	0.41
1:D:185:GLU:HG3	1:D:213:LYS:HE3	2.01	0.41
1:D:418:ASN:ND2	1:D:440:TYR:O	2.44	0.41
1:C:23:ASP:O	1:C:27:SER:N	2.53	0.41
1:C:185:GLU:HG3	1:C:213:LYS:HE3	2.01	0.41
1:A:79:LYS:HD3	1:A:140:ASP:HA	2.02	0.41
1:A:1181:HIS:HE1	1:A:1213:ALA:HB1	1.86	0.41
1:A:1209:SER:O	1:A:1213:ALA:N	2.51	0.41
1:B:489:ILE:HD12	1:B:735:ALA:HB1	2.02	0.41
1:C:258:PHE:O	1:C:262:TRP:N	2.48	0.41
1:C:489:ILE:HD12	1:C:735:ALA:HB1	2.02	0.41
1:A:673:TYR:O	1:A:677:ALA:N	2.53	0.41
1:C:77:TYR:OH	1:C:101:PHE:O	2.25	0.41
1:C:681:VAL:O	1:C:700:TYR:OH	2.32	0.41
1:D:673:TYR:O	1:D:677:ALA:N	2.53	0.41
1:A:418:ASN:ND2	1:A:440:TYR:O	2.44	0.41
1:B:79:LYS:HD3	1:B:140:ASP:HA	2.01	0.41
1:B:606:TRP:CZ2	1:C:586:GLN:HB2	2.49	0.41
1:A:492:SER:O	1:D:493:LYS:NZ	2.54	0.41
1:C:637:GLU:HG2	1:C:666:VAL:HG11	2.01	0.41
1:A:489:ILE:HD12	1:A:735:ALA:HB1	2.02	0.41
1:B:259:ILE:HA	1:B:262:TRP:HB3	2.01	0.41
1:C:576:SER:HA	1:C:579:PHE:HB2	2.02	0.41
1:C:1174:GLY:O	1:C:1178:MET:N	2.48	0.41
1:D:640:SER:HB2	1:D:669:LYS:HD2	2.03	0.41
1:A:111:ILE:HG13	1:A:333:LEU:HD13	2.03	0.40
1:C:736:THR:HG21	1:C:743:GLY:HA3	2.02	0.40
1:A:105:GLY:O	1:A:107:HIS:ND1	2.55	0.40
1:B:576:SER:HA	1:B:579:PHE:HB2	2.03	0.40
1:B:765:LYS:HA	1:B:769:ASP:HB2	2.02	0.40
1:A:321:VAL:HA	1:A:322:PRO:HD3	1.87	0.40
1:A:625:THR:O	1:A:629:MET:N	2.52	0.40
1:A:768:TYR:HB3	1:A:775:ALA:HA	2.04	0.40
1:B:25:GLU:OE2	1:B:281:THR:OG1	2.32	0.40
1:C:640:SER:HB2	1:C:669:LYS:HD2	2.03	0.40
1:C:765:LYS:HA	1:C:769:ASP:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1181:HIS:HE1	1:C:1213:ALA:HB1	1.86	0.40
1:D:111:ILE:HG13	1:D:333:LEU:HD13	2.03	0.40
1:A:640:SER:HB2	1:A:669:LYS:HD2	2.03	0.40
1:C:539:VAL:HG11	1:C:601:VAL:HG21	2.04	0.40
1:D:77:TYR:OH	1:D:101:PHE:O	2.25	0.40
1:D:576:SER:HA	1:D:579:PHE:HB2	2.03	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	950/1057 (90%)	888 (94%)	57 (6%)	5 (0%)	24	63
1	B	776/1057 (73%)	724 (93%)	52 (7%)	0	100	100
1	C	950/1057 (90%)	888 (94%)	59 (6%)	3 (0%)	36	72
1	D	776/1057 (73%)	724 (93%)	52 (7%)	0	100	100
All	All	3452/4228 (82%)	3224 (93%)	220 (6%)	8 (0%)	44	78

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	736	THR
1	A	737	PRO
1	A	738	LYS
1	C	738	LYS
1	A	385	ASP
1	A	386	ASP
1	C	385	ASP
1	C	386	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	816/888 (92%)	811 (99%)	5 (1%)	78	83
1	B	662/888 (74%)	659 (100%)	3 (0%)	81	83
1	C	816/888 (92%)	811 (99%)	5 (1%)	78	83
1	D	662/888 (74%)	659 (100%)	3 (0%)	81	83
All	All	2956/3552 (83%)	2940 (100%)	16 (0%)	78	83

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	ILE
1	A	321	VAL
1	A	596	LEU
1	A	738	LYS
1	A	1028	LEU
1	B	235	ILE
1	B	321	VAL
1	B	596	LEU
1	C	235	ILE
1	C	321	VAL
1	C	596	LEU
1	C	742	LEU
1	C	1028	LEU
1	D	235	ILE
1	D	321	VAL
1	D	596	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	65	GLN
1	A	83	ASN

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Mol	Chain	Res	Type
1	A	147	GLN
1	A	337	GLN
1	A	355	ASN
1	A	412	HIS
1	A	586	GLN
1	A	619	ASN
1	A	714	GLN
1	A	1092	HIS
1	A	1181	HIS
1	A	1186	GLN
1	B	46	HIS
1	B	65	GLN
1	B	83	ASN
1	B	147	GLN
1	B	337	GLN
1	B	355	ASN
1	B	359	ASN
1	B	412	HIS
1	B	586	GLN
1	C	46	HIS
1	C	65	GLN
1	C	147	GLN
1	C	337	GLN
1	C	355	ASN
1	C	359	ASN
1	C	412	HIS
1	C	586	GLN
1	C	1092	HIS
1	C	1181	HIS
1	C	1186	GLN
1	D	46	HIS
1	D	65	GLN
1	D	83	ASN
1	D	147	GLN
1	D	214	HIS
1	D	337	GLN
1	D	355	ASN
1	D	392	GLN
1	D	412	HIS
1	D	586	GLN
1	D	619	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 ⓘ

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	$\# Z > 2$
2	AJP	C	1301	-	95,95,95	0.83	6 (6%)	144,149,149	1.45	20 (13%)
2	AJP	A	1301	-	95,95,95	0.84	6 (6%)	144,149,149	1.45	20 (13%)

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	AJP	C	1301	-	34/34/38/38	13/28/220/220	0/11/11/11
2	AJP	A	1301	-	34/34/38/38	13/28/220/220	0/11/11/11

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	AJP	C12-C11	-2.76	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1301	AJP	C12-C11	-2.73	1.51	1.56
2	C	1301	AJP	O09-C05	2.72	1.48	1.42
2	A	1301	AJP	O09-C05	2.69	1.48	1.42
2	A	1301	AJP	C16-C11	-2.66	1.50	1.54
2	A	1301	AJP	C07-C08	-2.65	1.49	1.53
2	C	1301	AJP	C07-C08	-2.64	1.49	1.53
2	C	1301	AJP	C16-C11	-2.60	1.50	1.54
2	A	1301	AJP	C12-C07	-2.21	1.51	1.56
2	C	1301	AJP	C20-C15	-2.21	1.52	1.56
2	A	1301	AJP	C20-C15	-2.18	1.52	1.56
2	C	1301	AJP	C12-C07	-2.12	1.52	1.56

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1301	AJP	C12-C11-C16	-5.39	106.39	113.90
2	A	1301	AJP	C12-C11-C16	-5.33	106.47	113.90
2	C	1301	AJP	C06-C07-C08	-3.66	98.40	104.28
2	A	1301	AJP	C06-C07-C08	-3.64	98.43	104.28
2	A	1301	AJP	C05-C06-C07	-3.62	98.03	103.37
2	A	1301	AJP	C65-O64-C57	-3.60	109.45	117.98
2	C	1301	AJP	C65-O64-C57	-3.59	109.46	117.98
2	C	1301	AJP	C05-C06-C07	-3.59	98.08	103.37
2	C	1301	AJP	C45-O44-C37	-3.56	109.53	117.98
2	A	1301	AJP	C45-O44-C37	-3.55	109.56	117.98
2	A	1301	AJP	C55-O54-C36	-3.52	109.63	117.98
2	C	1301	AJP	C26-O25-C23	-3.51	109.39	115.27
2	C	1301	AJP	C55-O54-C36	-3.51	109.66	117.98
2	A	1301	AJP	C26-O25-C23	-3.51	109.41	115.27
2	A	1301	AJP	C20-C15-C16	-3.42	108.95	112.43
2	C	1301	AJP	C20-C15-C16	-3.37	109.01	112.43
2	C	1301	AJP	C11-C12-C07	-3.36	95.09	100.16
2	A	1301	AJP	C11-C12-C07	-3.34	95.13	100.16
2	A	1301	AJP	C14-C13-C12	-3.33	107.13	112.74
2	C	1301	AJP	C14-C13-C12	-3.33	107.13	112.74
2	A	1301	AJP	C14-C15-C20	-3.32	110.17	113.91
2	C	1301	AJP	C14-C15-C20	-3.30	110.19	113.91
2	A	1301	AJP	C35-O34-C29	-3.17	110.46	117.98
2	C	1301	AJP	C35-O34-C29	-3.15	110.52	117.98
2	C	1301	AJP	O09-C08-C10	3.12	116.51	110.20
2	A	1301	AJP	O09-C08-C10	3.07	116.40	110.20
2	C	1301	AJP	C24-C19-C20	-3.00	109.47	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	AJP	C24-C19-C20	-2.97	109.50	112.66
2	A	1301	AJP	C83-C06-C05	-2.96	110.17	114.94
2	C	1301	AJP	C83-C06-C05	-2.94	110.19	114.94
2	A	1301	AJP	C20-C21-C22	-2.87	109.45	114.17
2	C	1301	AJP	C20-C21-C22	-2.84	109.50	114.17
2	A	1301	AJP	C04-C05-C06	-2.79	110.60	115.66
2	C	1301	AJP	C04-C05-C06	-2.75	110.69	115.66
2	A	1301	AJP	O09-C08-C07	-2.43	98.47	104.08
2	C	1301	AJP	O09-C08-C07	-2.42	98.50	104.08
2	C	1301	AJP	C21-C20-C19	2.39	109.52	107.23
2	A	1301	AJP	C21-C20-C19	2.38	109.50	107.23
2	A	1301	AJP	C65-O70-C69	-2.20	109.42	113.72
2	C	1301	AJP	C65-O70-C69	-2.14	109.55	113.72

All (68) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1301	AJP	C20
2	A	1301	AJP	C05
2	A	1301	AJP	C19
2	A	1301	AJP	C68
2	A	1301	AJP	C16
2	A	1301	AJP	C28
2	A	1301	AJP	C57
2	A	1301	AJP	C30
2	A	1301	AJP	C47
2	A	1301	AJP	C27
2	A	1301	AJP	C26
2	A	1301	AJP	C07
2	A	1301	AJP	C48
2	A	1301	AJP	C37
2	A	1301	AJP	C59
2	A	1301	AJP	C46
2	A	1301	AJP	C65
2	A	1301	AJP	C36
2	A	1301	AJP	C12
2	A	1301	AJP	C39
2	A	1301	AJP	C15
2	A	1301	AJP	C11
2	A	1301	AJP	C67
2	A	1301	AJP	C35
2	A	1301	AJP	C10

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Mol	Chain	Res	Type	Atom
2	A	1301	AJP	C55
2	A	1301	AJP	C02
2	A	1301	AJP	C66
2	A	1301	AJP	C45
2	A	1301	AJP	C56
2	A	1301	AJP	C69
2	A	1301	AJP	C23
2	A	1301	AJP	C38
2	A	1301	AJP	C22
2	C	1301	AJP	C20
2	C	1301	AJP	C05
2	C	1301	AJP	C19
2	C	1301	AJP	C68
2	C	1301	AJP	C16
2	C	1301	AJP	C28
2	C	1301	AJP	C57
2	C	1301	AJP	C30
2	C	1301	AJP	C47
2	C	1301	AJP	C27
2	C	1301	AJP	C26
2	C	1301	AJP	C07
2	C	1301	AJP	C48
2	C	1301	AJP	C37
2	C	1301	AJP	C59
2	C	1301	AJP	C46
2	C	1301	AJP	C65
2	C	1301	AJP	C36
2	C	1301	AJP	C12
2	C	1301	AJP	C39
2	C	1301	AJP	C15
2	C	1301	AJP	C11
2	C	1301	AJP	C67
2	C	1301	AJP	C35
2	C	1301	AJP	C10
2	C	1301	AJP	C55
2	C	1301	AJP	C02
2	C	1301	AJP	C66
2	C	1301	AJP	C45
2	C	1301	AJP	C56
2	C	1301	AJP	C69
2	C	1301	AJP	C23
2	C	1301	AJP	C38

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Mol	Chain	Res	Type	Atom
2	C	1301	AJP	C22

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	AJP	C46-C45-O44-C37
2	C	1301	AJP	C46-C45-O44-C37
2	A	1301	AJP	C56-C55-O54-C36
2	C	1301	AJP	C56-C55-O54-C36
2	A	1301	AJP	C66-C65-O64-C57
2	C	1301	AJP	C66-C65-O64-C57
2	A	1301	AJP	C30-C29-O34-C35
2	C	1301	AJP	C30-C29-O34-C35
2	A	1301	AJP	O40-C39-C41-O42
2	A	1301	AJP	O70-C69-C71-O72
2	C	1301	AJP	O40-C39-C41-O42
2	C	1301	AJP	O70-C69-C71-O72
2	A	1301	AJP	O70-C65-O64-C57
2	C	1301	AJP	O70-C65-O64-C57
2	C	1301	AJP	C38-C39-C41-O42
2	A	1301	AJP	C38-C39-C41-O42
2	C	1301	AJP	O31-C30-C32-O33
2	A	1301	AJP	O31-C30-C32-O33
2	A	1301	AJP	C28-C29-O34-C35
2	C	1301	AJP	C28-C29-O34-C35
2	C	1301	AJP	C68-C69-C71-O72
2	A	1301	AJP	C68-C69-C71-O72
2	A	1301	AJP	O60-C55-O54-C36
2	C	1301	AJP	O60-C55-O54-C36
2	A	1301	AJP	C22-C23-O25-C26
2	C	1301	AJP	C22-C23-O25-C26

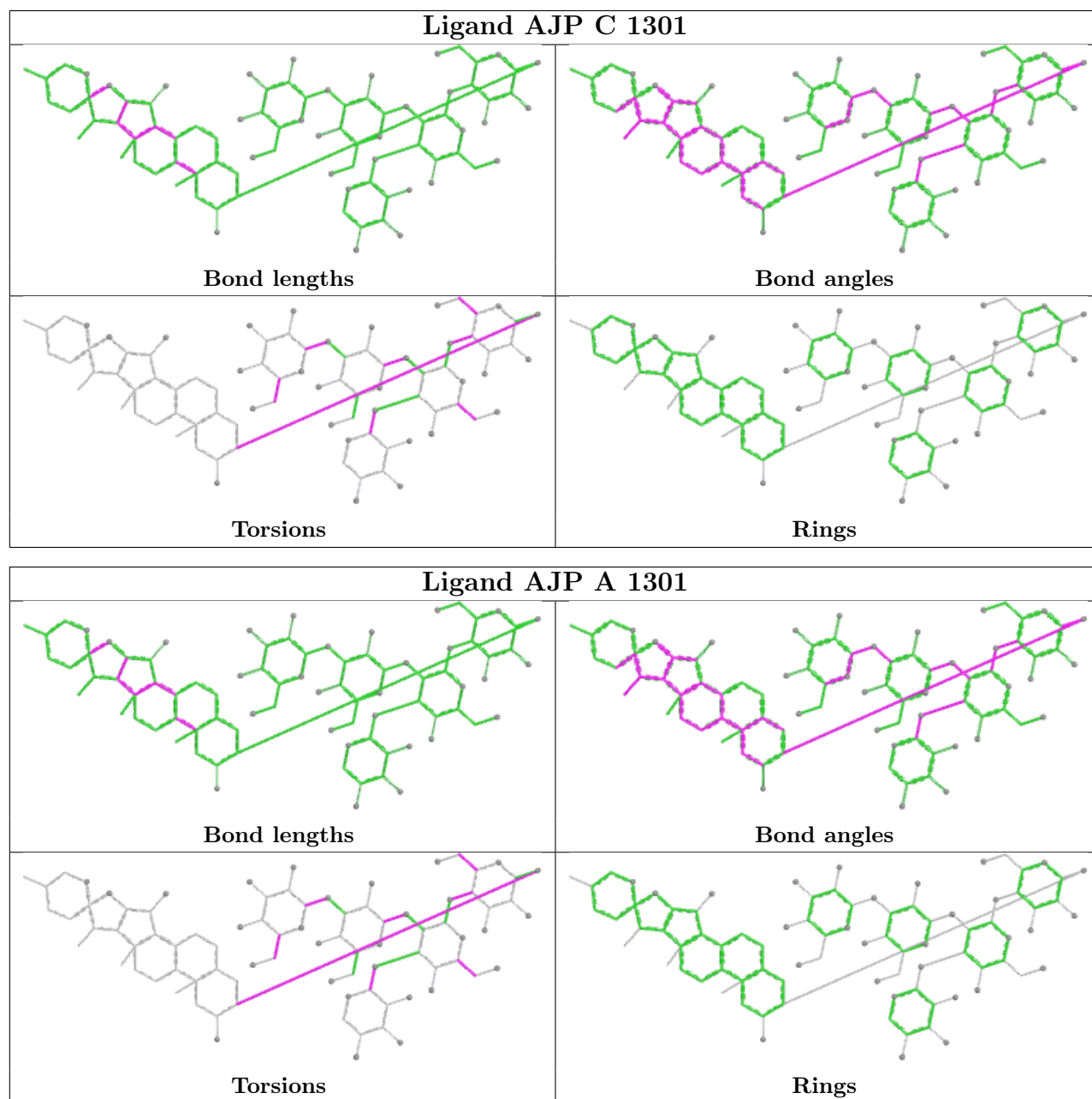
There are no ring outliers.

2 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1301	AJP	37	0
2	A	1301	AJP	36	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.

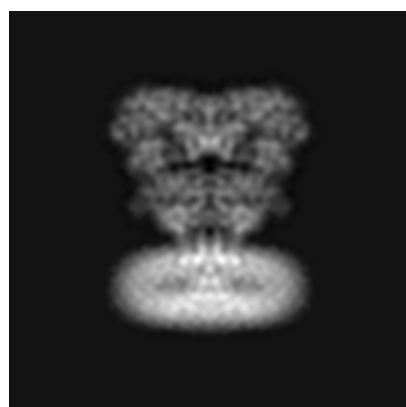
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8822. These allow visual inspection of the internal detail of the map and identification of artifacts.

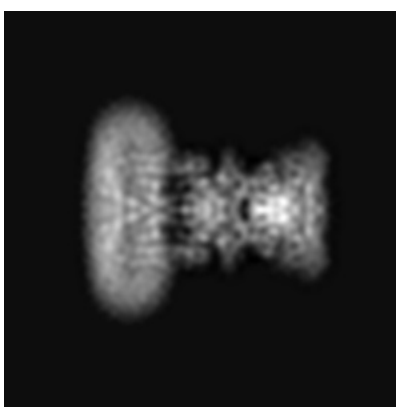
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

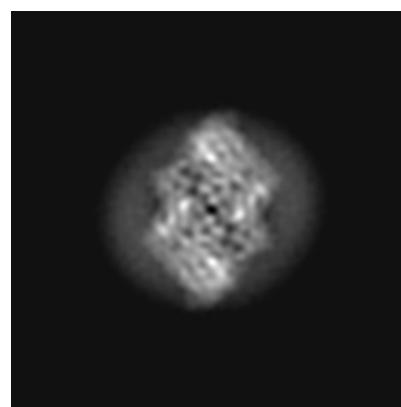
6.1.1 Primary map



X



Y



Z

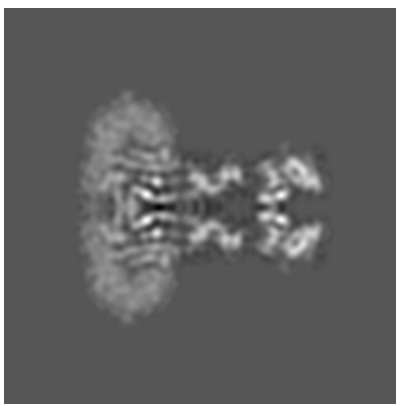
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

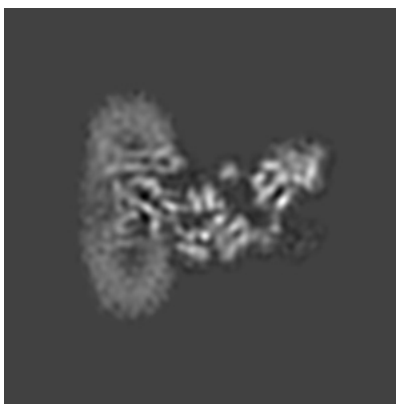
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 150



Y Index: 159

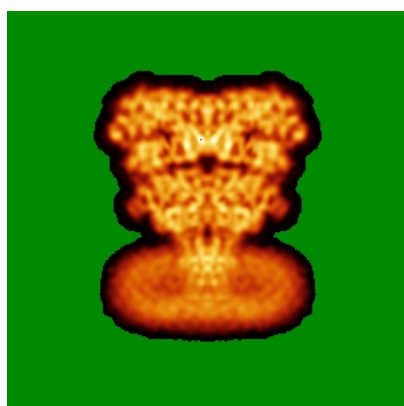


Z Index: 229

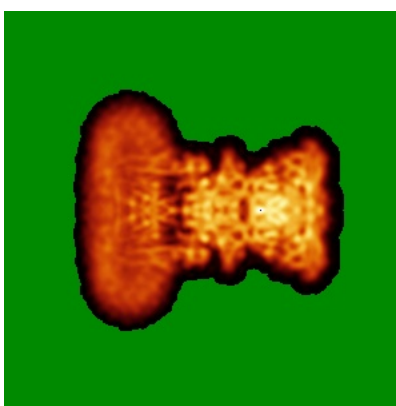
The images above show the largest variance slices of the map in three orthogonal directions.

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

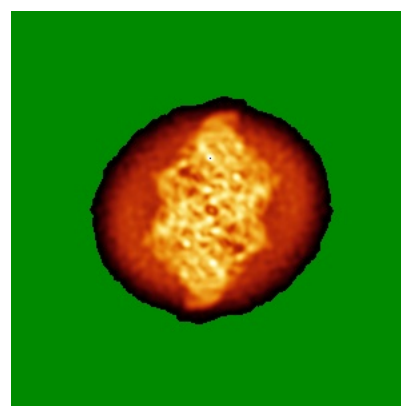
6.4.1 Primary map



X



Y

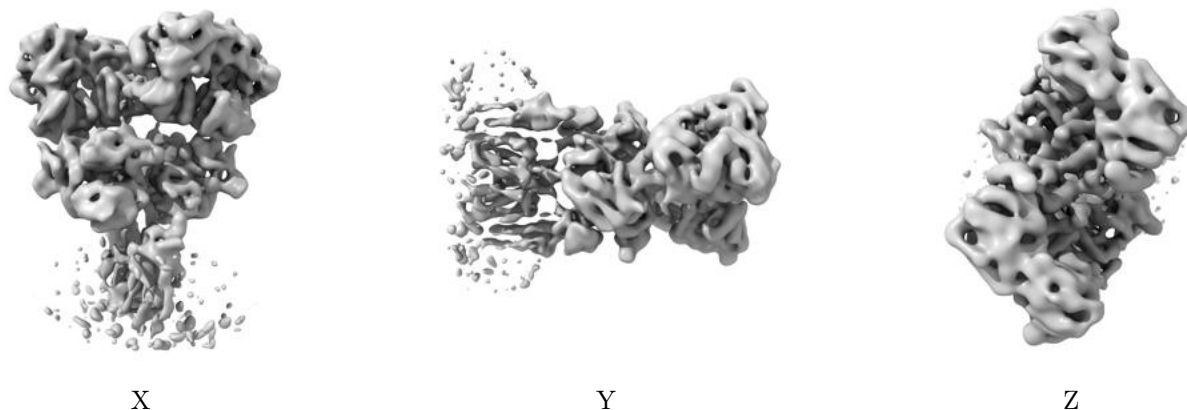


Z

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

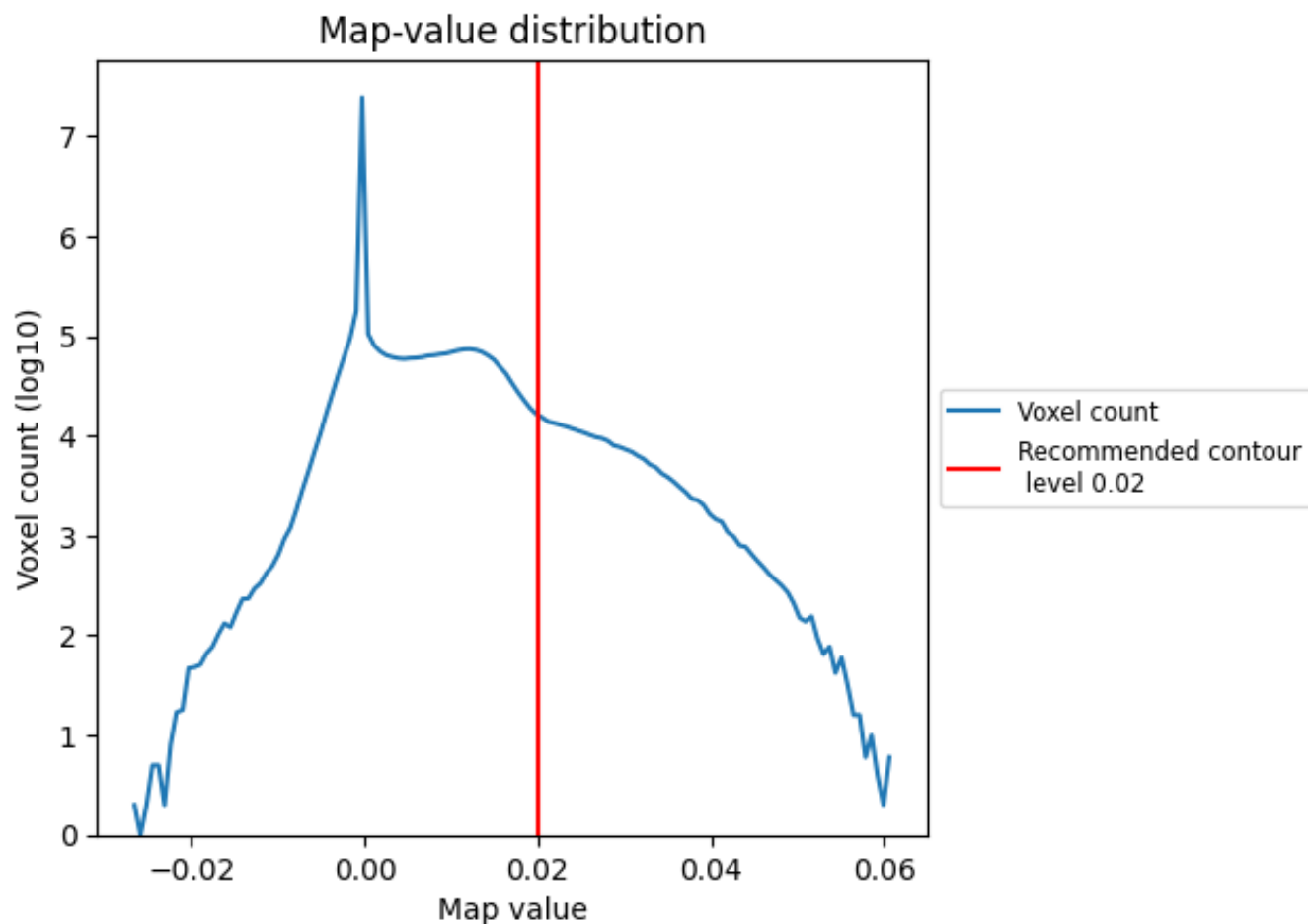
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

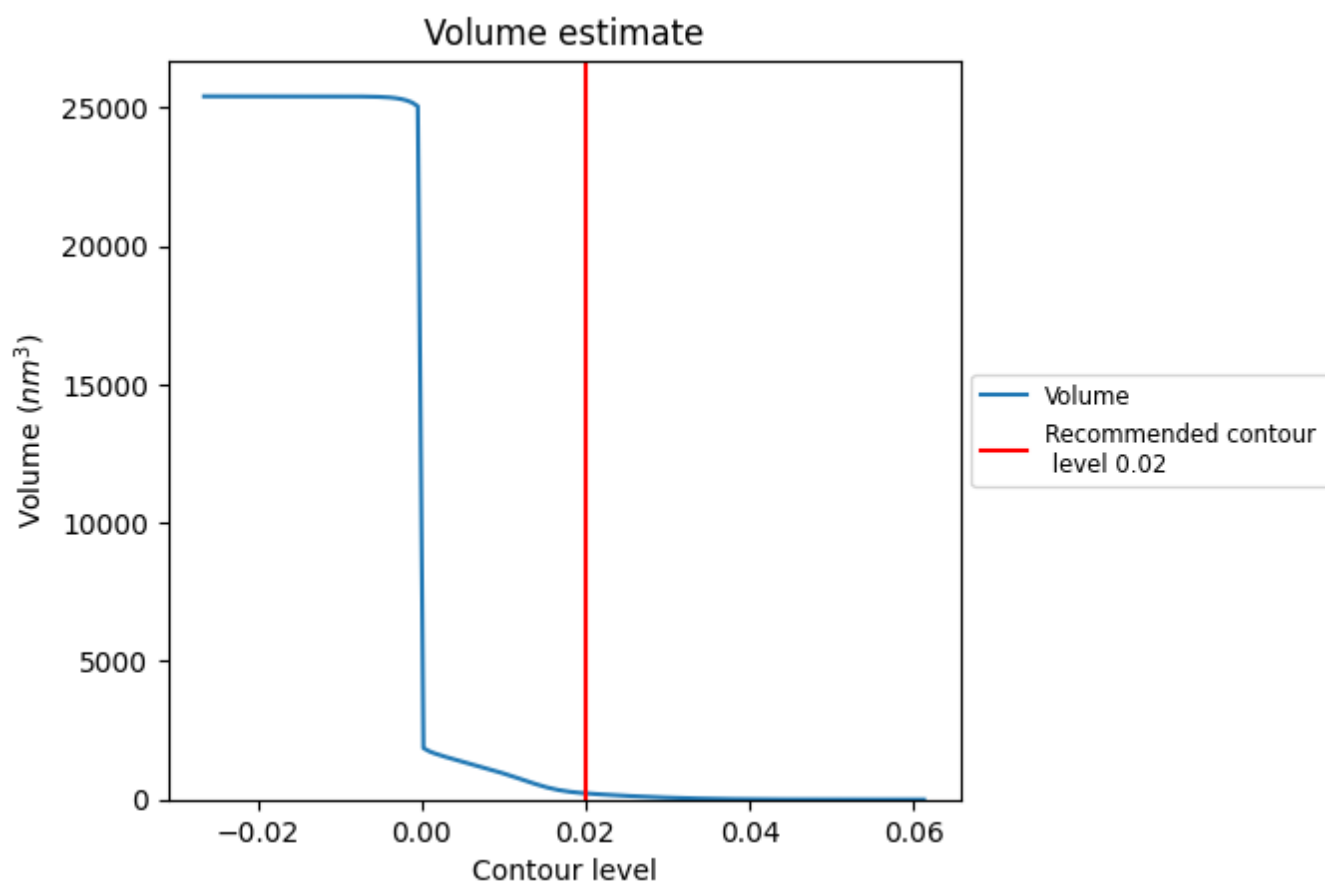
This section contains the results of statistical analysis of the map.

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.

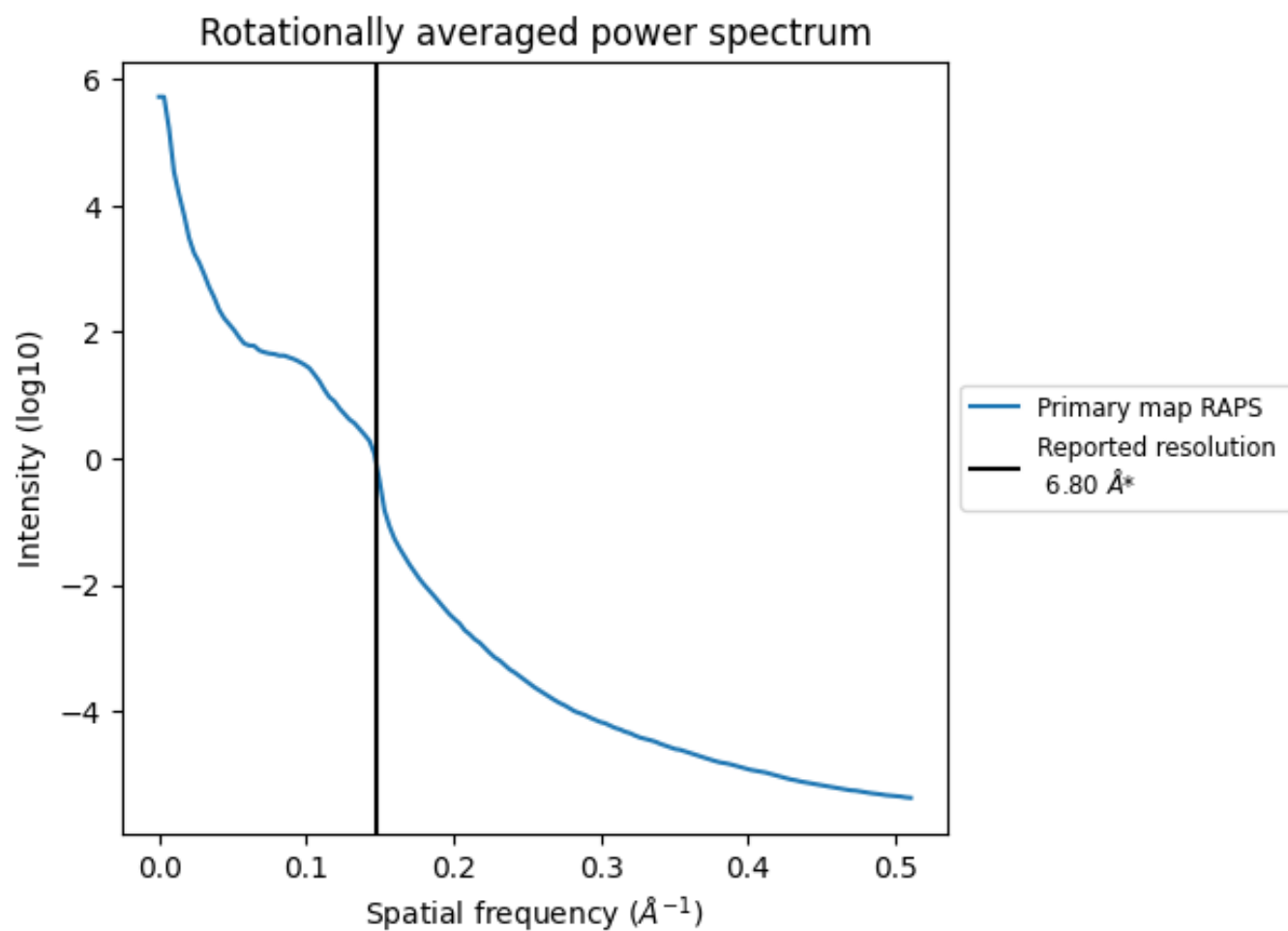
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 226 nm³; this corresponds to an approximate mass of 204 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 0.147 Å⁻¹

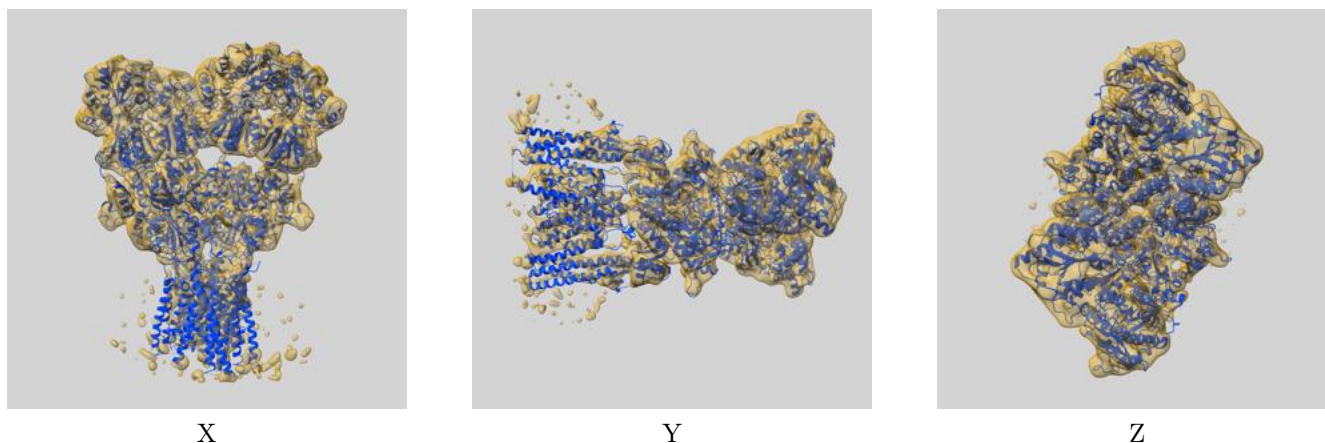
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

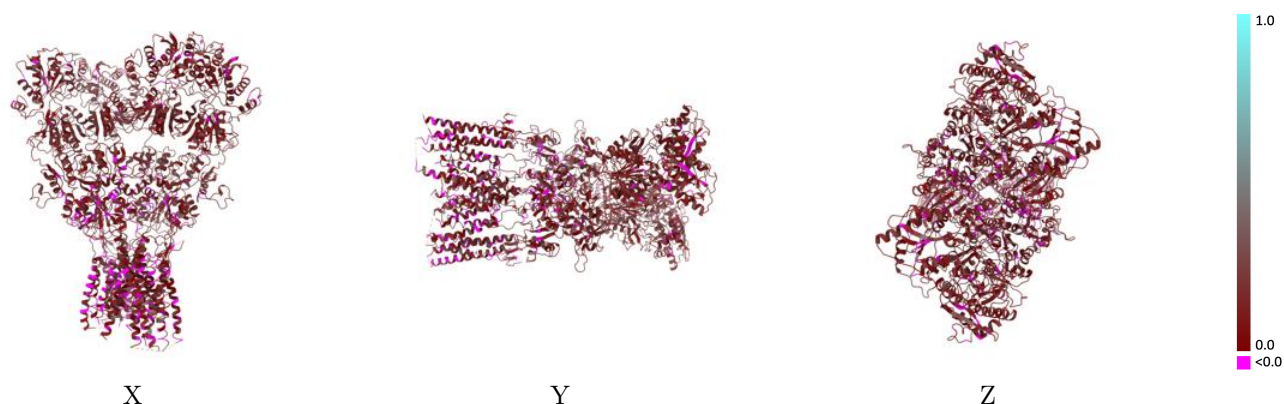
This section contains information regarding the fit between EMDB map EMD-8822 and PDB model 5WEN. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



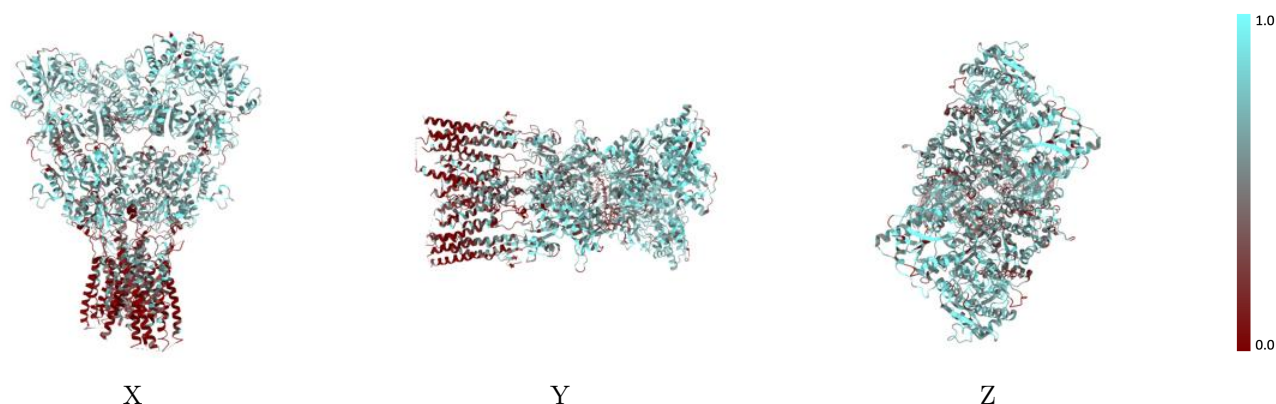
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



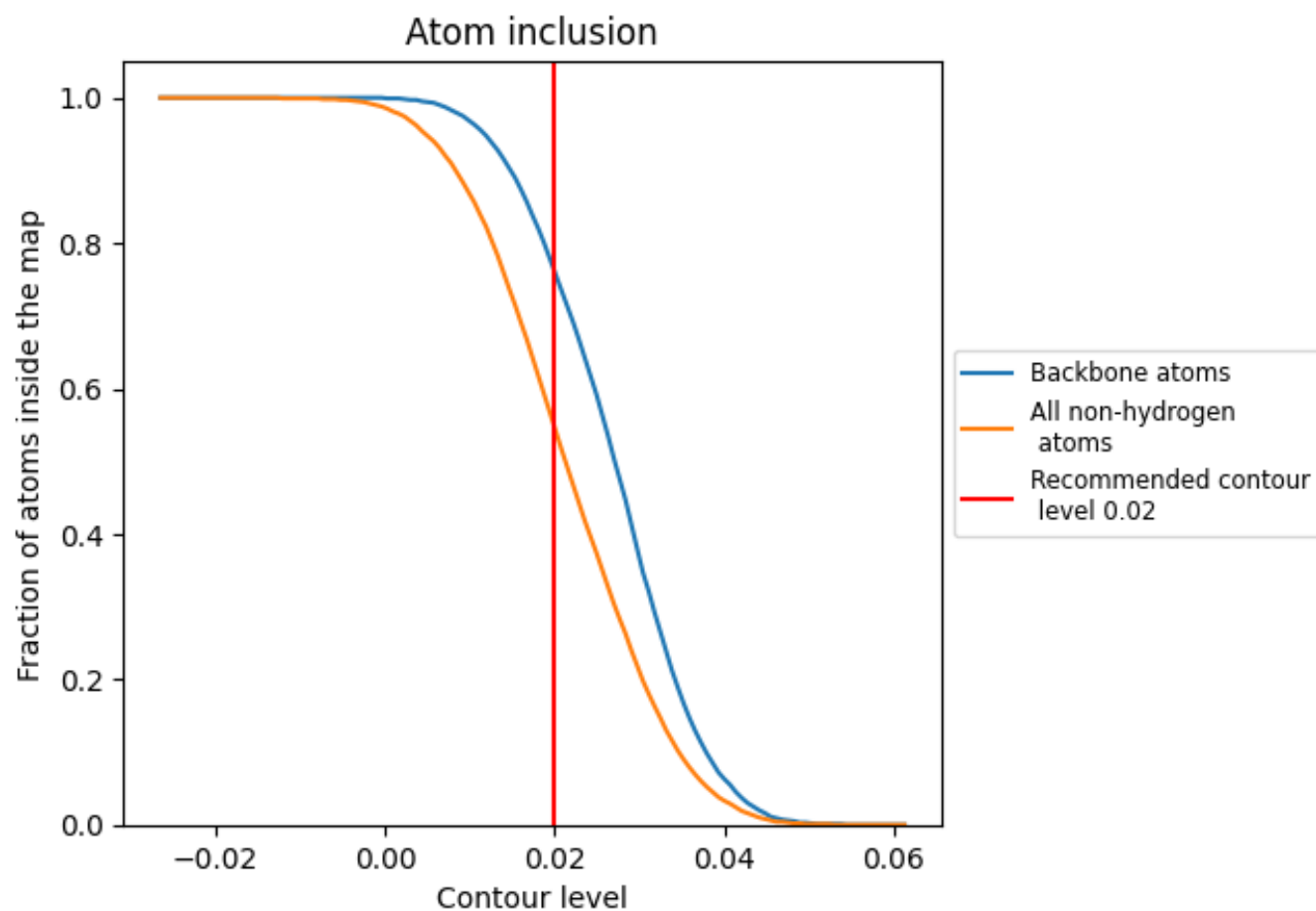
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 55% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5460	0.1450
A	0.5200	0.1380
B	0.5790	0.1530
C	0.5300	0.1450
D	0.5680	0.1470

