



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:51 PM UTC

PDB ID : 9ARH / pdb_00009arh
EMDB ID : EMD-43782
Title : Rat GluN1-GluN2B NMDA receptor channel in complex with glycine
Authors : Chou, T.-H.; Furukawa, H.
Deposited on : 2024-02-23
Resolution : 3.69 Å(reported)
Based on initial model : 6WHS

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

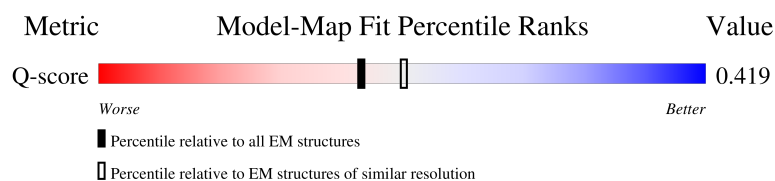
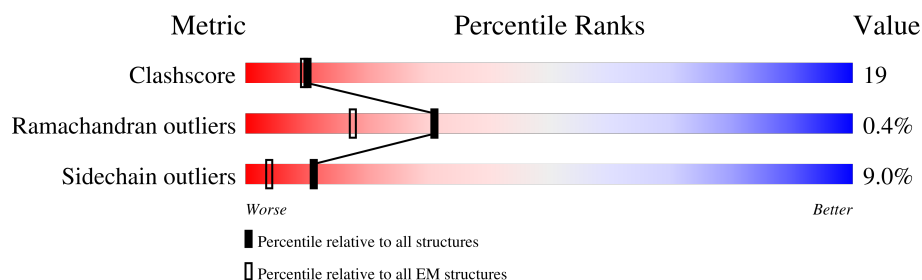
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.69 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	11284 (3.19 - 4.18)

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	959	5% 58% 17% 6% • 16%
1	C	959	5% 58% 17% 6% • 16%
2	B	883	7% 67% 19% •• 11%
2	D	883	7% 67% 18% •• 11%

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Mol	Chain	Length	Quality of chain
3	E	2	50% 100%
3	F	2	50% 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22792 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Isoform B of Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	802	Total	C	N	O	S	0	0
			5695	3665	949	1047	34		
1	C	802	Total	C	N	O	S	0	0
			5695	3665	949	1047	34		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	SER	CYS	conflict	UNP P35439
A	61	GLN	ASN	conflict	UNP P35439
A	260	ASP	ASN	conflict	UNP P35439
A	371	GLN	ASN	conflict	UNP P35439
A	492	GLN	ASN	conflict	UNP P35439
A	512	GLN	ASN	conflict	UNP P35439
A	615	GLN	GLU	conflict	UNP P35439
A	616	SER	GLU	conflict	UNP P35439
A	618	SER	GLU	conflict	UNP P35439
A	619	THR	GLU	conflict	UNP P35439
A	792	GLN	ASN	conflict	UNP P35439
A	831	CYS	PHE	conflict	UNP P35439
C	22	SER	CYS	conflict	UNP P35439
C	61	GLN	ASN	conflict	UNP P35439
C	260	ASP	ASN	conflict	UNP P35439
C	371	GLN	ASN	conflict	UNP P35439
C	492	GLN	ASN	conflict	UNP P35439
C	512	GLN	ASN	conflict	UNP P35439
C	615	GLN	GLU	conflict	UNP P35439
C	616	SER	GLU	conflict	UNP P35439
C	618	SER	GLU	conflict	UNP P35439
C	619	THR	GLU	conflict	UNP P35439
C	792	GLN	ASN	conflict	UNP P35439
C	831	CYS	PHE	conflict	UNP P35439

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	788	Total 5654	C 3654	N 909	O 1057	S 34	0	0
2	D	788	Total 5654	C 3654	N 909	O 1057	S 34	0	0

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-30	MET	-	initiating methionine	UNP Q00960
B	-29	GLY	-	expression tag	UNP Q00960
B	-28	THR	-	expression tag	UNP Q00960
B	-27	MET	-	expression tag	UNP Q00960
B	-26	ARG	-	expression tag	UNP Q00960
B	-25	LEU	-	expression tag	UNP Q00960
B	-24	PHE	-	expression tag	UNP Q00960
B	-23	LEU	-	expression tag	UNP Q00960
B	-22	LEU	-	expression tag	UNP Q00960
B	-21	ALA	-	expression tag	UNP Q00960
B	-20	VAL	-	expression tag	UNP Q00960
B	-19	LEU	-	expression tag	UNP Q00960
B	-18	PHE	-	expression tag	UNP Q00960
B	-17	LEU	-	expression tag	UNP Q00960
B	-16	PHE	-	expression tag	UNP Q00960
B	-15	SER	-	expression tag	UNP Q00960
B	-14	PHE	-	expression tag	UNP Q00960
B	-13	ALA	-	expression tag	UNP Q00960
B	-12	ARG	-	expression tag	UNP Q00960
B	-11	ALA	-	expression tag	UNP Q00960
B	-10	THR	-	expression tag	UNP Q00960
B	-9	GLY	-	expression tag	UNP Q00960
B	-8	TRP	-	expression tag	UNP Q00960
B	-7	SER	-	expression tag	UNP Q00960
B	-6	HIS	-	expression tag	UNP Q00960
B	-5	PRO	-	expression tag	UNP Q00960
B	-4	GLN	-	expression tag	UNP Q00960
B	-3	PHE	-	expression tag	UNP Q00960
B	-2	GLU	-	expression tag	UNP Q00960
B	-1	LYS	-	expression tag	UNP Q00960
B	0	GLY	-	expression tag	UNP Q00960
B	1	GLY	-	expression tag	UNP Q00960
B	2	GLY	-	expression tag	UNP Q00960
B	3	SER	-	expression tag	UNP Q00960
B	4	GLY	-	expression tag	UNP Q00960

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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	GLY	-	expression tag	UNP Q00960
B	6	GLY	-	expression tag	UNP Q00960
B	7	SER	-	expression tag	UNP Q00960
B	8	GLY	-	expression tag	UNP Q00960
B	9	GLY	-	expression tag	UNP Q00960
B	10	SER	-	expression tag	UNP Q00960
B	11	ALA	-	expression tag	UNP Q00960
B	12	TRP	-	expression tag	UNP Q00960
B	13	SER	-	expression tag	UNP Q00960
B	14	HIS	-	expression tag	UNP Q00960
B	15	PRO	-	expression tag	UNP Q00960
B	16	GLN	-	expression tag	UNP Q00960
B	17	PHE	-	expression tag	UNP Q00960
B	18	GLU	-	expression tag	UNP Q00960
B	19	LYS	-	expression tag	UNP Q00960
B	20	GLY	-	expression tag	UNP Q00960
B	21	ALA	-	expression tag	UNP Q00960
B	22	LEU	-	expression tag	UNP Q00960
B	23	VAL	-	expression tag	UNP Q00960
B	24	PRO	-	expression tag	UNP Q00960
B	25	ARG	-	expression tag	UNP Q00960
B	26	GLY	-	expression tag	UNP Q00960
B	348	ASP	ASN	conflict	UNP Q00960
B	557	CYS	ASP	conflict	UNP Q00960
B	588	SER	CYS	conflict	UNP Q00960
B	838	SER	CYS	conflict	UNP Q00960
B	849	SER	CYS	conflict	UNP Q00960
D	-30	MET	-	initiating methionine	UNP Q00960
D	-29	GLY	-	expression tag	UNP Q00960
D	-28	THR	-	expression tag	UNP Q00960
D	-27	MET	-	expression tag	UNP Q00960
D	-26	ARG	-	expression tag	UNP Q00960
D	-25	LEU	-	expression tag	UNP Q00960
D	-24	PHE	-	expression tag	UNP Q00960
D	-23	LEU	-	expression tag	UNP Q00960
D	-22	LEU	-	expression tag	UNP Q00960
D	-21	ALA	-	expression tag	UNP Q00960
D	-20	VAL	-	expression tag	UNP Q00960
D	-19	LEU	-	expression tag	UNP Q00960
D	-18	PHE	-	expression tag	UNP Q00960
D	-17	LEU	-	expression tag	UNP Q00960
D	-16	PHE	-	expression tag	UNP Q00960

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	SER	-	expression tag	UNP Q00960
D	-14	PHE	-	expression tag	UNP Q00960
D	-13	ALA	-	expression tag	UNP Q00960
D	-12	ARG	-	expression tag	UNP Q00960
D	-11	ALA	-	expression tag	UNP Q00960
D	-10	THR	-	expression tag	UNP Q00960
D	-9	GLY	-	expression tag	UNP Q00960
D	-8	TRP	-	expression tag	UNP Q00960
D	-7	SER	-	expression tag	UNP Q00960
D	-6	HIS	-	expression tag	UNP Q00960
D	-5	PRO	-	expression tag	UNP Q00960
D	-4	GLN	-	expression tag	UNP Q00960
D	-3	PHE	-	expression tag	UNP Q00960
D	-2	GLU	-	expression tag	UNP Q00960
D	-1	LYS	-	expression tag	UNP Q00960
D	0	GLY	-	expression tag	UNP Q00960
D	1	GLY	-	expression tag	UNP Q00960
D	2	GLY	-	expression tag	UNP Q00960
D	3	SER	-	expression tag	UNP Q00960
D	4	GLY	-	expression tag	UNP Q00960
D	5	GLY	-	expression tag	UNP Q00960
D	6	GLY	-	expression tag	UNP Q00960
D	7	SER	-	expression tag	UNP Q00960
D	8	GLY	-	expression tag	UNP Q00960
D	9	GLY	-	expression tag	UNP Q00960
D	10	SER	-	expression tag	UNP Q00960
D	11	ALA	-	expression tag	UNP Q00960
D	12	TRP	-	expression tag	UNP Q00960
D	13	SER	-	expression tag	UNP Q00960
D	14	HIS	-	expression tag	UNP Q00960
D	15	PRO	-	expression tag	UNP Q00960
D	16	GLN	-	expression tag	UNP Q00960
D	17	PHE	-	expression tag	UNP Q00960
D	18	GLU	-	expression tag	UNP Q00960
D	19	LYS	-	expression tag	UNP Q00960
D	20	GLY	-	expression tag	UNP Q00960
D	21	ALA	-	expression tag	UNP Q00960
D	22	LEU	-	expression tag	UNP Q00960
D	23	VAL	-	expression tag	UNP Q00960
D	24	PRO	-	expression tag	UNP Q00960
D	25	ARG	-	expression tag	UNP Q00960
D	26	GLY	-	expression tag	UNP Q00960

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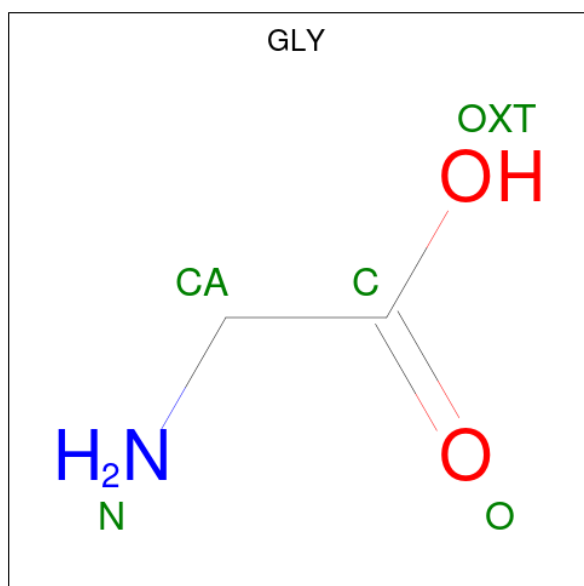
Chain	Residue	Modelled	Actual	Comment	Reference
D	348	ASP	ASN	conflict	UNP Q00960
D	557	CYS	ASP	conflict	UNP Q00960
D	588	SER	CYS	conflict	UNP Q00960
D	838	SER	CYS	conflict	UNP Q00960
D	849	SER	CYS	conflict	UNP Q00960

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂) (labeled as "Ligand of Interest" by depositor).



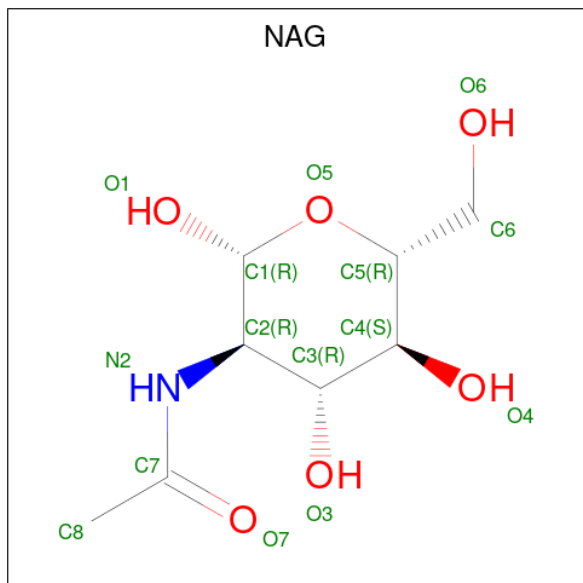
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			5	2	1	2	

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Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			5	2	1	2	

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

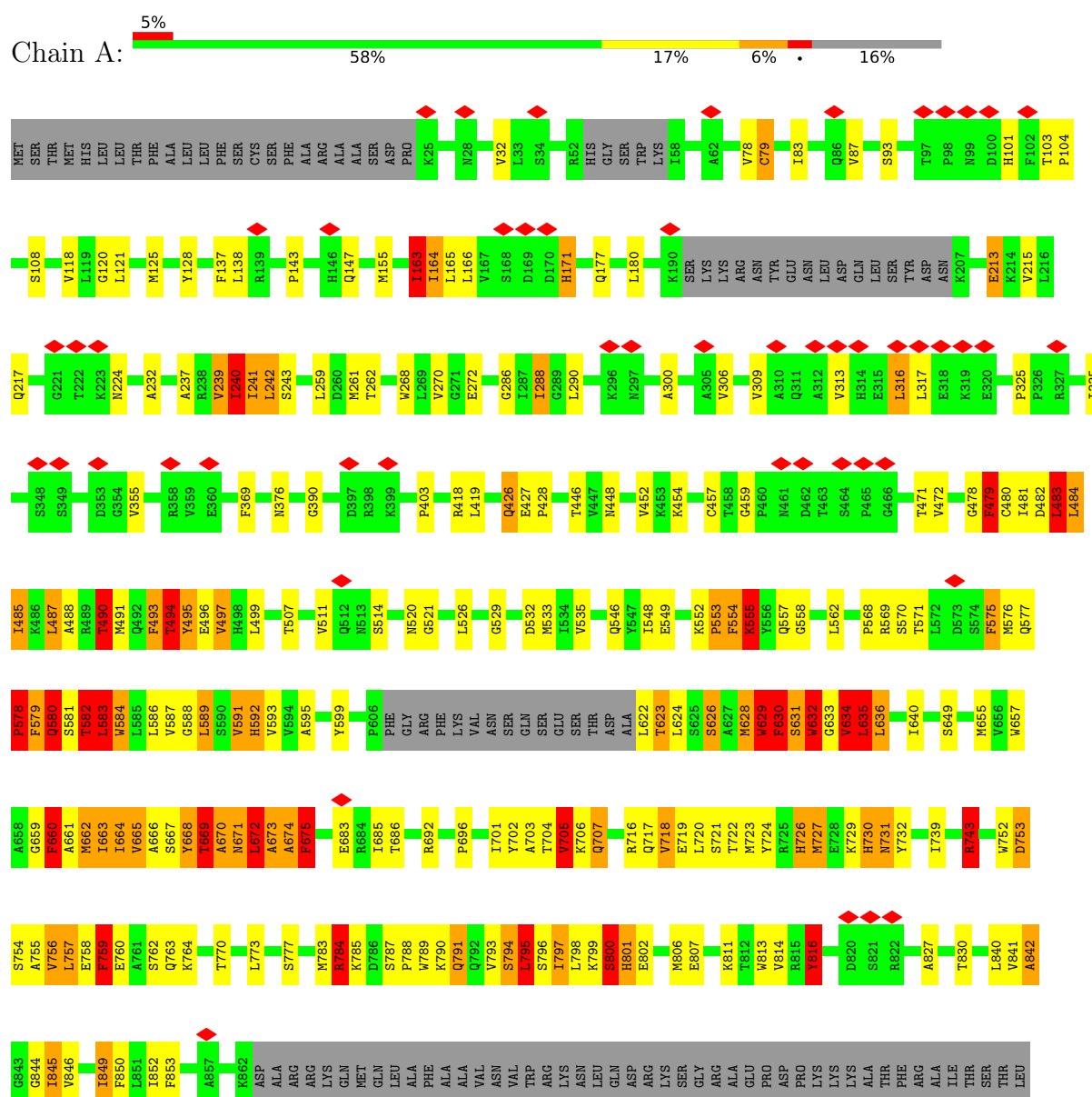


Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	

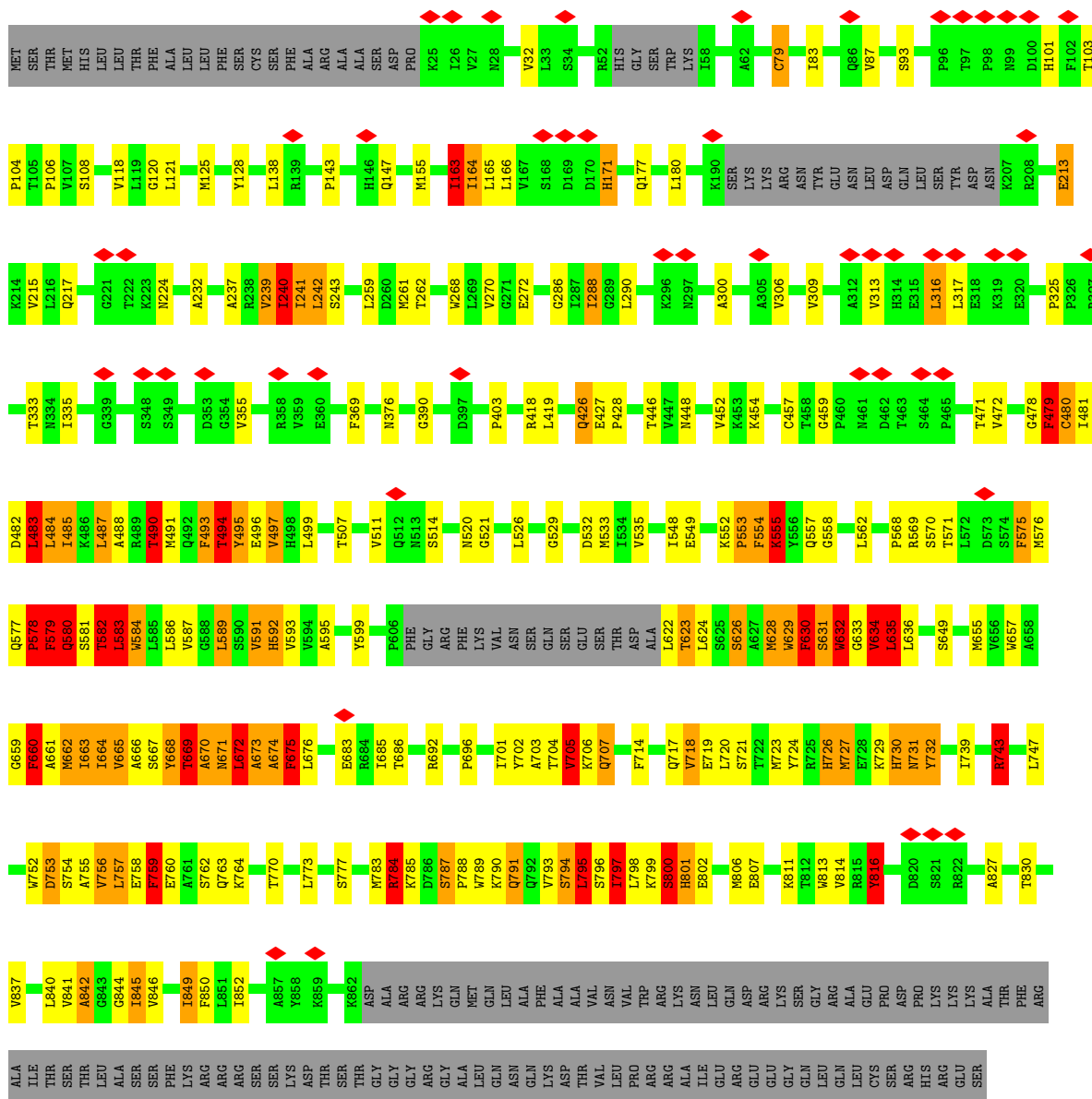
3 Residue-property plots

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.

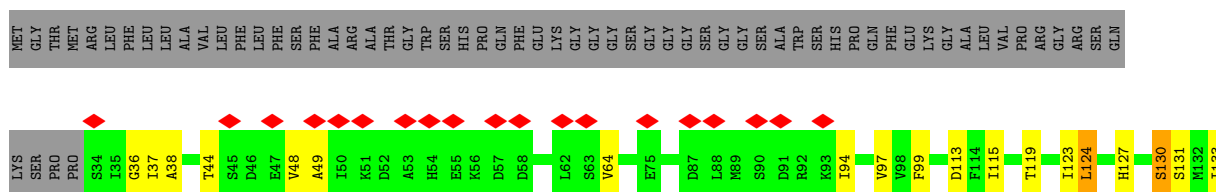
- Molecule 1: Isoform B of Glutamate receptor ionotropic, NMDA 1

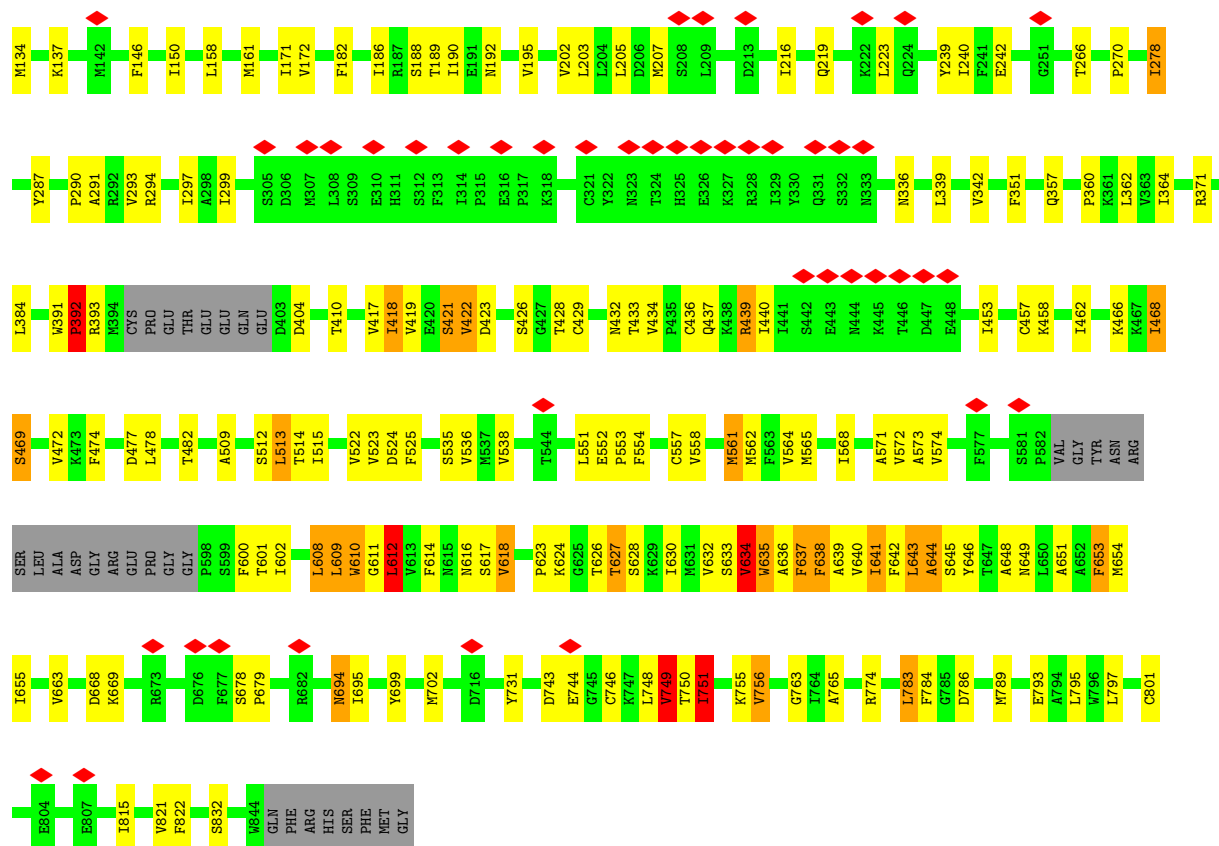


Chain C:

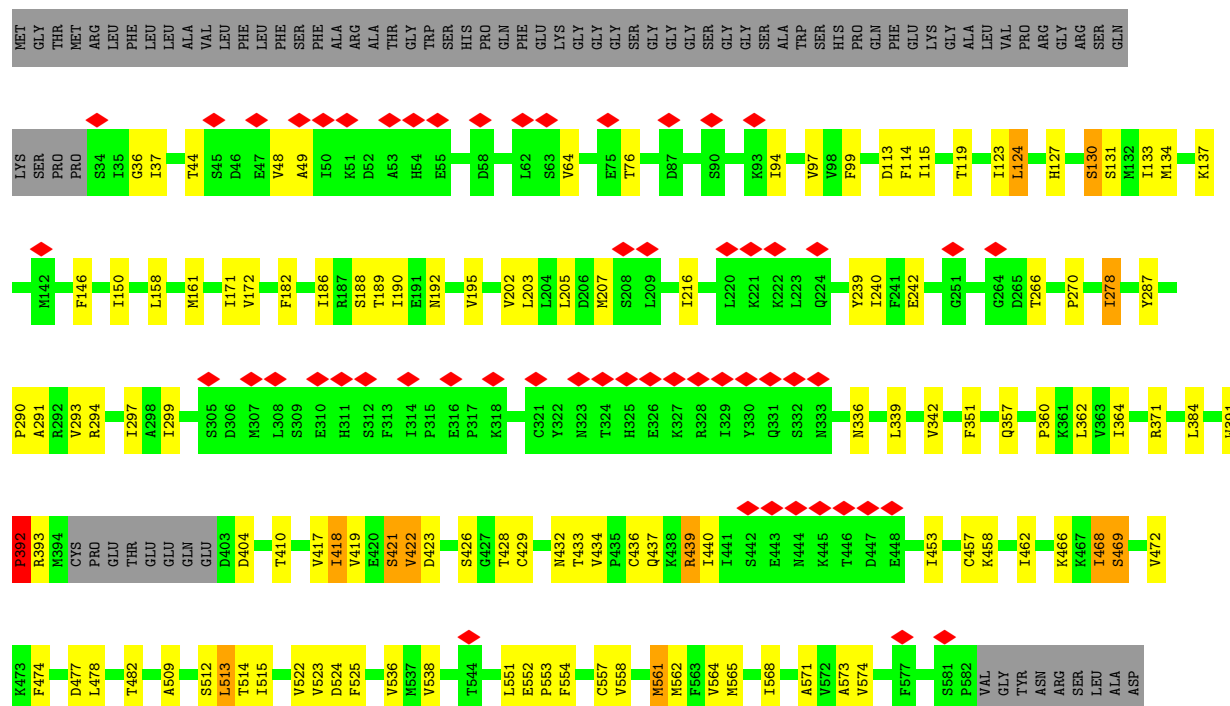


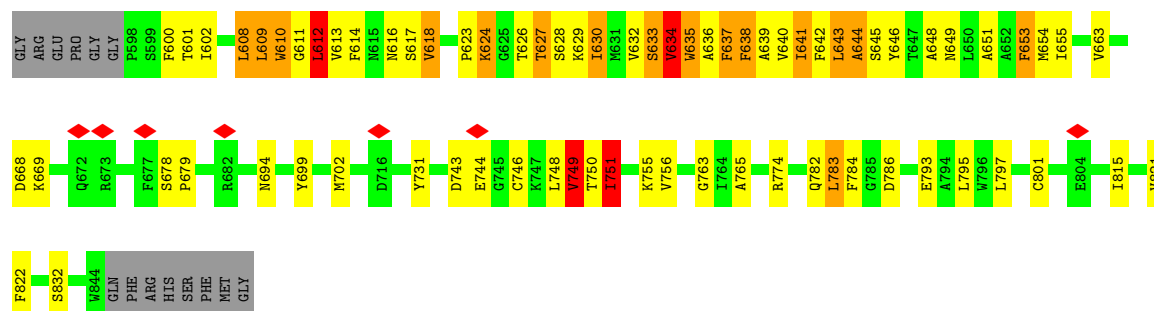
Chain B: 7% 67% 19% 11%





• Molecule 2: Glutamate receptor ionotropic, NMDA 2B





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	449208	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63.9	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.999	Depositor
Minimum map value	-1.185	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.138	Depositor
Map size ($\text{\AA}$)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.13	72/5816 (1.2%)	1.25	105/7959 (1.3%)
1	C	1.13	73/5816 (1.3%)	1.25	105/7959 (1.3%)
2	B	0.74	25/5778 (0.4%)	0.87	40/7911 (0.5%)
2	D	0.74	25/5778 (0.4%)	0.87	40/7911 (0.5%)
All	All	0.95	195/23188 (0.8%)	1.08	290/31740 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	4
All	All	0	8

All (195) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	553	PRO	C-O	-15.15	1.05	1.23
1	A	553	PRO	C-O	-15.05	1.05	1.23
1	C	555	LYS	C-O	-14.31	1.06	1.23
1	A	555	LYS	C-O	-14.30	1.06	1.23
2	D	636	ALA	C-O	-13.77	1.06	1.24
2	B	636	ALA	C-O	-13.72	1.06	1.24
2	B	610	TRP	C-O	-13.04	1.08	1.24
2	D	610	TRP	C-O	-12.94	1.08	1.24
1	C	668	TYR	C-O	-12.93	1.09	1.24
1	A	668	TYR	C-O	-12.88	1.09	1.24
1	A	672	LEU	C-O	-12.47	1.09	1.24
1	C	672	LEU	C-O	-12.38	1.09	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	666	ALA	C-O	-12.03	1.09	1.24
1	A	666	ALA	C-O	-11.99	1.09	1.24
2	D	643	LEU	C-O	-11.33	1.09	1.24
2	B	643	LEU	C-O	-11.27	1.09	1.24
1	A	240	ILE	C-O	-10.92	1.12	1.24
1	C	240	ILE	C-O	-10.91	1.12	1.24
1	C	665	VAL	C-O	-10.90	1.11	1.24
1	A	665	VAL	C-O	-10.89	1.11	1.24
1	C	669	THR	C-O	-10.78	1.11	1.24
1	A	669	THR	C-O	-10.68	1.11	1.24
2	B	645	SER	C-O	-10.51	1.10	1.24
2	D	645	SER	C-O	-10.44	1.10	1.24
1	A	241	ILE	C-O	-10.32	1.12	1.24
1	C	241	ILE	C-O	-10.30	1.12	1.24
2	B	644	ALA	C-O	-10.20	1.10	1.24
2	D	644	ALA	C-O	-10.14	1.10	1.24
2	B	635	TRP	C-O	-9.54	1.12	1.24
2	D	635	TRP	C-O	-9.49	1.12	1.24
1	A	661	ALA	C-O	-9.38	1.13	1.24
1	C	661	ALA	C-O	-9.28	1.13	1.24
1	A	756	VAL	C-O	-9.10	1.13	1.24
2	B	640	VAL	C-O	-9.08	1.13	1.24
1	C	763	GLN	C-O	9.07	1.35	1.24
1	A	763	GLN	C-O	9.07	1.35	1.24
1	C	756	VAL	C-O	-9.06	1.13	1.24
2	D	640	VAL	C-O	-9.03	1.13	1.24
1	C	757	LEU	C-O	-8.73	1.14	1.24
1	A	634	VAL	C-O	-8.68	1.12	1.24
1	A	495	TYR	C-O	-8.67	1.12	1.23
1	C	794	SER	CA-CB	-8.67	1.39	1.53
1	A	757	LEU	C-O	-8.66	1.14	1.24
1	A	794	SER	CA-CB	-8.66	1.39	1.53
1	C	495	TYR	C-O	-8.63	1.12	1.23
1	C	634	VAL	C-O	-8.63	1.13	1.24
2	B	638	PHE	C-O	-8.55	1.13	1.24
1	C	480	CYS	C-O	-8.55	1.12	1.24
2	D	638	PHE	C-O	-8.50	1.13	1.24
1	A	480	CYS	C-O	-8.45	1.12	1.24
1	A	487	LEU	C-O	-8.42	1.14	1.24
2	B	653	PHE	C-O	-8.42	1.14	1.24
2	D	653	PHE	C-O	-8.41	1.14	1.24
1	C	487	LEU	C-O	-8.40	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	705	VAL	C-O	-8.33	1.15	1.24
1	C	705	VAL	C-O	-8.33	1.15	1.24
1	A	629	TRP	C-O	-8.21	1.14	1.24
1	C	629	TRP	C-O	-8.17	1.14	1.24
2	D	611	GLY	C-O	-8.16	1.14	1.23
1	A	554	PHE	C-O	-8.13	1.14	1.24
2	B	611	GLY	C-O	-8.11	1.14	1.23
2	D	632	VAL	C-O	-8.08	1.14	1.24
1	C	754	SER	CA-CB	-8.08	1.41	1.54
1	C	554	PHE	C-O	-8.07	1.14	1.24
2	B	632	VAL	C-O	-8.05	1.14	1.24
1	A	754	SER	CA-CB	-8.03	1.41	1.54
1	A	675	PHE	C-O	-7.98	1.14	1.23
2	D	756	VAL	C-O	-7.95	1.15	1.24
1	C	675	PHE	C-O	-7.95	1.14	1.23
2	B	756	VAL	C-O	-7.92	1.15	1.24
1	C	800	SER	C-O	-7.86	1.13	1.24
1	A	633	GLY	C-O	-7.85	1.14	1.23
1	C	633	GLY	C-O	-7.84	1.14	1.23
2	D	633	SER	CA-CB	-7.81	1.41	1.53
1	A	800	SER	C-O	-7.80	1.13	1.24
2	B	633	SER	CA-CB	-7.79	1.41	1.53
1	C	667	SER	C-O	-7.79	1.14	1.24
1	A	667	SER	C-O	-7.71	1.15	1.24
2	B	639	ALA	C-O	-7.65	1.15	1.24
2	D	639	ALA	C-O	-7.65	1.15	1.24
1	A	789	TRP	C-O	-7.62	1.15	1.24
2	D	612	LEU	C-O	-7.61	1.14	1.24
2	B	612	LEU	C-O	-7.60	1.14	1.24
1	C	789	TRP	C-O	-7.59	1.15	1.24
1	A	479	PHE	C-O	-7.58	1.15	1.24
1	A	426	GLN	C-O	-7.58	1.14	1.23
1	C	426	GLN	C-O	-7.55	1.14	1.23
1	C	479	PHE	C-O	-7.54	1.15	1.24
2	B	645	SER	CA-CB	-7.52	1.41	1.53
1	A	578	PRO	C-O	-7.50	1.14	1.24
1	A	673	ALA	C-O	-7.50	1.14	1.24
2	D	645	SER	CA-CB	-7.49	1.41	1.53
1	C	673	ALA	C-O	-7.49	1.14	1.24
1	C	578	PRO	C-O	-7.45	1.14	1.24
1	C	631	SER	CA-CB	-7.38	1.41	1.53
1	A	631	SER	CA-CB	-7.35	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	794	SER	C-O	-7.31	1.15	1.24
1	C	794	SER	C-O	-7.31	1.15	1.24
2	B	646	TYR	C-O	-7.28	1.15	1.24
2	B	642	PHE	C-O	-7.27	1.15	1.24
2	D	646	TYR	C-O	-7.26	1.15	1.24
2	D	642	PHE	C-O	-7.23	1.15	1.24
1	A	707	GLN	C-O	-7.23	1.12	1.23
1	C	707	GLN	C-O	-7.16	1.12	1.23
2	D	646	TYR	C-N	7.14	1.43	1.33
1	C	630	PHE	C-O	-7.13	1.15	1.24
2	B	646	TYR	C-N	7.10	1.43	1.33
1	A	630	PHE	C-O	-7.07	1.15	1.24
1	A	636	LEU	C-O	-7.04	1.14	1.24
1	C	663	ILE	C-O	-7.01	1.16	1.24
1	A	664	ILE	C-O	-7.00	1.16	1.24
1	C	636	LEU	C-O	-7.00	1.14	1.24
1	A	663	ILE	C-O	-6.99	1.16	1.24
1	C	664	ILE	C-O	-6.97	1.16	1.24
1	C	583	LEU	C-O	-6.94	1.15	1.24
1	C	428	PRO	C-O	-6.93	1.15	1.24
1	A	583	LEU	C-O	-6.91	1.15	1.24
1	A	428	PRO	C-O	-6.90	1.15	1.24
1	A	163	ILE	C-O	-6.88	1.15	1.23
1	A	427	GLU	C-O	-6.84	1.18	1.24
1	C	427	GLU	C-O	-6.84	1.18	1.24
1	C	163	ILE	C-O	-6.81	1.16	1.23
2	B	608	LEU	C-O	-6.79	1.16	1.24
1	A	496	GLU	C-O	6.78	1.32	1.23
2	D	608	LEU	C-O	-6.77	1.16	1.24
1	C	496	GLU	C-O	6.76	1.32	1.23
1	C	799	LYS	C-O	-6.74	1.15	1.24
2	B	634	VAL	C-O	-6.73	1.15	1.24
1	A	799	LYS	C-O	-6.71	1.15	1.24
2	D	634	VAL	C-O	-6.65	1.15	1.24
1	A	667	SER	CA-CB	-6.54	1.42	1.53
1	C	667	SER	CA-CB	-6.49	1.43	1.53
1	C	755	ALA	C-O	-6.49	1.16	1.24
1	A	635	LEU	C-O	-6.48	1.15	1.24
1	C	484	LEU	C-O	-6.47	1.16	1.24
1	A	484	LEU	C-O	-6.45	1.16	1.24
1	A	755	ALA	C-O	-6.45	1.16	1.24
1	C	635	LEU	C-O	-6.40	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	706	LYS	C-O	-6.33	1.16	1.23
1	C	706	LYS	C-O	-6.28	1.16	1.23
1	A	553	PRO	N-CD	-6.21	1.39	1.47
1	A	483	LEU	C-O	-6.19	1.16	1.24
1	C	483	LEU	C-O	-6.14	1.17	1.24
1	C	553	PRO	N-CD	-6.10	1.39	1.47
1	C	662	MET	C-O	-6.06	1.17	1.24
1	A	762	SER	CA-CB	-6.05	1.45	1.53
1	A	662	MET	C-O	-6.01	1.17	1.24
1	C	762	SER	CA-CB	-6.00	1.45	1.53
2	D	609	LEU	C-O	-6.00	1.16	1.24
1	C	796	SER	CA-CB	-5.99	1.44	1.53
2	B	609	LEU	C-O	-5.97	1.16	1.24
1	A	796	SER	CA-CB	-5.96	1.44	1.53
2	D	641	ILE	C-O	-5.89	1.16	1.24
2	B	641	ILE	C-O	-5.79	1.16	1.24
1	A	662	MET	CG-SD	-5.78	1.66	1.80
1	C	662	MET	CG-SD	-5.76	1.66	1.80
1	A	732	TYR	C-O	-5.76	1.16	1.23
1	A	796	SER	C-O	5.73	1.30	1.24
1	C	670	ALA	C-O	-5.73	1.17	1.24
1	A	670	ALA	C-O	-5.71	1.17	1.24
1	C	732	TYR	C-O	-5.68	1.16	1.23
1	C	796	SER	C-O	5.67	1.30	1.24
1	A	485	ILE	C-O	-5.62	1.17	1.24
1	C	485	ILE	C-O	-5.58	1.17	1.24
1	A	428	PRO	N-CD	-5.57	1.40	1.47
1	C	428	PRO	N-CD	-5.57	1.40	1.47
2	B	783	LEU	C-O	-5.53	1.17	1.24
2	D	783	LEU	C-O	-5.52	1.17	1.24
1	C	801	HIS	CG-ND1	-5.51	1.32	1.38
1	A	801	HIS	C-O	-5.50	1.17	1.24
1	C	626	SER	C-O	-5.50	1.17	1.24
1	C	243	SER	CA-CB	-5.49	1.48	1.53
1	A	801	HIS	CG-ND1	-5.48	1.32	1.38
1	A	788	PRO	C-O	5.48	1.31	1.24
1	A	243	SER	CA-CB	-5.47	1.48	1.53
1	A	626	SER	C-O	-5.47	1.17	1.24
1	C	801	HIS	C-O	-5.47	1.17	1.24
1	C	788	PRO	C-O	5.46	1.31	1.24
1	A	239	VAL	C-O	-5.38	1.17	1.24
1	C	239	VAL	C-O	-5.35	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	674	ALA	C-O	-5.35	1.16	1.24
1	C	674	ALA	C-O	-5.31	1.16	1.24
1	C	632	TRP	C-O	-5.30	1.18	1.24
1	A	797	ILE	C-O	-5.29	1.18	1.24
1	A	731	ASN	C-O	-5.27	1.18	1.24
1	C	797	ILE	C-O	-5.26	1.18	1.24
2	D	469	SER	CA-CB	-5.24	1.45	1.53
1	C	584	TRP	C-O	-5.23	1.18	1.24
2	B	469	SER	CA-CB	-5.23	1.45	1.53
1	A	584	TRP	C-O	-5.22	1.18	1.24
1	A	632	TRP	C-O	-5.21	1.18	1.24
1	C	731	ASN	C-O	-5.15	1.18	1.24
1	A	494	THR	C-O	-5.12	1.18	1.24
1	C	494	THR	C-O	-5.10	1.18	1.24
1	C	787	SER	C-O	-5.07	1.18	1.24

All (290) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	653	PHE	CB-CA-C	-16.99	82.25	110.79
2	B	653	PHE	CB-CA-C	-16.97	82.27	110.79
1	A	668	TYR	CB-CA-C	-13.48	89.71	110.88
1	C	668	TYR	CB-CA-C	-13.48	89.72	110.88
1	A	630	PHE	CA-C-O	-12.99	106.78	120.55
1	C	630	PHE	CA-C-O	-12.99	106.78	120.55
1	C	759	PHE	CB-CA-C	12.74	131.94	110.79
1	A	759	PHE	CB-CA-C	12.73	131.92	110.79
1	A	669	THR	N-CA-CB	12.66	128.90	110.16
1	C	669	THR	N-CA-CB	12.66	128.90	110.16
2	B	626	THR	CB-CA-C	11.89	130.53	110.79
2	D	626	THR	CB-CA-C	11.88	130.52	110.79
2	B	642	PHE	CB-CA-C	-10.68	92.70	110.85
2	D	642	PHE	CB-CA-C	-10.68	92.70	110.85
1	A	669	THR	CA-C-O	-10.60	109.19	120.42
1	C	669	THR	CA-C-O	-10.55	109.24	120.42
1	C	753	ASP	CA-C-N	-10.09	106.22	122.26
1	C	753	ASP	C-N-CA	-10.09	106.22	122.26
1	A	753	ASP	CA-C-N	-10.08	106.24	122.26
1	A	753	ASP	C-N-CA	-10.08	106.24	122.26
1	A	662	MET	CA-C-O	-10.05	109.90	120.55
1	C	662	MET	CA-C-O	-9.96	109.99	120.55
1	A	554	PHE	CA-CB-CG	9.75	123.55	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	554	PHE	CA-CB-CG	9.75	123.55	113.80
2	B	694	ASN	CB-CA-C	-9.72	95.62	110.88
2	D	694	ASN	CB-CA-C	-9.71	95.63	110.88
1	C	758	GLU	CB-CA-C	9.34	126.29	110.79
1	A	758	GLU	CB-CA-C	9.34	126.29	110.79
1	A	631	SER	N-CA-CB	9.28	123.90	110.16
1	C	631	SER	N-CA-CB	9.26	123.86	110.16
2	D	756	VAL	CA-C-N	9.25	135.49	122.72
2	D	756	VAL	C-N-CA	9.25	135.49	122.72
2	B	756	VAL	CA-C-N	9.23	135.46	122.72
2	B	756	VAL	C-N-CA	9.23	135.46	122.72
1	C	495	TYR	CB-CA-C	-9.20	90.15	109.38
1	A	495	TYR	CB-CA-C	-9.20	90.16	109.38
1	C	789	TRP	CA-C-O	-9.18	110.72	120.63
1	A	479	PHE	CB-CA-C	-9.16	96.42	110.90
1	C	479	PHE	CB-CA-C	-9.16	96.42	110.90
1	A	789	TRP	CA-C-O	-9.15	110.75	120.63
1	C	427	GLU	CA-C-O	-8.98	109.93	118.73
1	A	427	GLU	CA-C-O	-8.96	109.95	118.73
1	A	668	TYR	CA-C-O	-8.80	111.58	120.82
1	C	763	GLN	N-CA-C	8.75	121.78	111.71
1	C	668	TYR	CA-C-O	-8.74	111.64	120.82
1	A	763	GLN	N-CA-C	8.71	121.73	111.71
1	A	663	ILE	N-CA-CB	8.31	121.84	110.54
1	C	790	LYS	CA-C-N	-8.30	109.15	120.44
1	C	790	LYS	C-N-CA	-8.30	109.15	120.44
1	C	663	ILE	N-CA-CB	8.29	121.81	110.54
1	A	790	LYS	CA-C-N	-8.28	109.17	120.44
1	A	790	LYS	C-N-CA	-8.28	109.17	120.44
1	A	662	MET	CB-CG-SD	-8.26	87.93	112.70
1	C	662	MET	CB-CG-SD	-8.25	87.95	112.70
1	A	490	THR	CA-CB-OG1	-8.24	97.25	109.60
1	C	490	THR	CA-CB-OG1	-8.23	97.26	109.60
1	A	706	LYS	CB-CA-C	-8.20	96.11	109.72
1	C	706	LYS	CB-CA-C	-8.15	96.18	109.72
1	A	479	PHE	CA-CB-CG	8.07	121.87	113.80
1	C	479	PHE	CA-CB-CG	8.05	121.85	113.80
1	A	675	PHE	N-CA-C	-8.01	103.72	113.97
1	C	675	PHE	N-CA-C	-8.00	103.73	113.97
1	C	661	ALA	N-CA-C	-7.96	102.54	111.14
1	A	660	PHE	CB-CA-C	7.92	123.71	109.29
1	C	660	PHE	CB-CA-C	7.92	123.71	109.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	582	THR	CA-CB-OG1	-7.92	97.72	109.60
1	A	661	ALA	N-CA-C	-7.91	102.59	111.14
1	A	582	THR	CA-CB-OG1	-7.90	97.74	109.60
1	C	629	TRP	CB-CA-C	-7.87	98.53	110.88
1	A	629	TRP	CB-CA-C	-7.83	98.58	110.88
1	C	758	GLU	CA-CB-CG	-7.81	98.47	114.10
1	A	758	GLU	CA-CB-CG	-7.81	98.48	114.10
1	C	801	HIS	CB-CA-C	-7.77	96.48	110.70
1	A	801	HIS	CB-CA-C	-7.76	96.50	110.70
2	B	640	VAL	CA-C-O	-7.72	112.67	120.85
2	D	640	VAL	CA-C-O	-7.68	112.71	120.85
2	D	608	LEU	CA-C-O	-7.64	112.80	120.82
2	B	608	LEU	CA-C-O	-7.59	112.85	120.82
1	A	579	PHE	CA-C-O	-7.52	110.05	118.69
1	C	579	PHE	CA-C-O	-7.50	110.06	118.69
2	B	392	PRO	N-CA-C	-7.37	97.28	112.47
2	D	392	PRO	N-CA-C	-7.37	97.29	112.47
2	D	646	TYR	CB-CA-C	-7.37	98.33	110.85
2	B	646	TYR	CB-CA-C	-7.35	98.35	110.85
2	B	783	LEU	N-CA-C	-7.28	103.27	111.14
1	A	480	CYS	CA-CB-SG	-7.28	97.65	114.40
1	C	480	CYS	CA-CB-SG	-7.28	97.66	114.40
2	D	783	LEU	N-CA-C	-7.26	103.30	111.14
2	D	639	ALA	CA-C-O	-7.16	112.83	120.42
1	A	664	ILE	CA-C-O	-7.16	113.58	121.17
2	B	639	ALA	CA-C-O	-7.15	112.85	120.42
1	C	664	ILE	CA-C-O	-7.13	113.61	121.17
1	C	163	ILE	CA-C-O	-7.11	114.28	120.96
1	A	553	PRO	CA-C-O	-7.10	113.63	121.23
1	C	241	ILE	CA-C-O	-7.10	112.97	120.57
1	A	163	ILE	CA-C-O	-7.09	114.29	120.96
1	C	553	PRO	CA-C-O	-7.08	113.66	121.23
1	A	241	ILE	CA-C-O	-7.07	113.01	120.57
1	A	241	ILE	N-CA-CB	-7.04	102.54	110.99
2	B	642	PHE	CA-CB-CG	7.04	120.84	113.80
1	C	241	ILE	N-CA-CB	-7.04	102.55	110.99
2	D	642	PHE	CA-CB-CG	6.99	120.79	113.80
1	A	758	GLU	CA-C-O	-6.95	113.18	120.55
1	C	589	LEU	N-CA-C	-6.93	103.74	111.71
1	C	758	GLU	CA-C-O	-6.93	113.20	120.55
1	A	589	LEU	N-CA-C	-6.93	103.74	111.71
1	C	630	PHE	CA-C-N	-6.87	110.54	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	630	PHE	C-N-CA	-6.87	110.54	120.29
1	C	428	PRO	CB-CA-C	-6.86	100.24	111.56
1	A	428	PRO	CB-CA-C	-6.82	100.30	111.56
1	A	630	PHE	CA-C-N	-6.82	110.60	120.29
1	A	630	PHE	C-N-CA	-6.82	110.60	120.29
1	A	479	PHE	CA-C-O	-6.82	113.68	120.70
1	C	672	LEU	CA-C-O	-6.82	113.20	120.42
1	C	670	ALA	N-CA-CB	6.81	120.24	110.16
1	A	493	PHE	CA-CB-CG	6.81	120.61	113.80
1	C	493	PHE	CA-CB-CG	6.81	120.61	113.80
1	A	670	ALA	N-CA-CB	6.80	120.22	110.16
1	C	479	PHE	CA-C-O	-6.79	113.71	120.70
1	C	578	PRO	N-CA-CB	-6.78	96.13	103.25
1	A	665	VAL	CA-C-O	-6.78	113.67	120.85
1	A	578	PRO	N-CA-CB	-6.76	96.15	103.25
1	C	665	VAL	CA-C-O	-6.75	113.70	120.85
1	A	672	LEU	CA-C-O	-6.73	113.29	120.42
1	A	554	PHE	CB-CA-C	6.65	122.16	110.85
1	C	795	LEU	CA-C-O	-6.64	113.51	120.55
1	A	795	LEU	CA-C-O	-6.64	113.51	120.55
1	A	634	VAL	CA-C-O	-6.63	113.31	120.47
1	C	634	VAL	CA-C-O	-6.62	113.32	120.47
1	C	554	PHE	CB-CA-C	6.61	122.09	110.85
1	A	427	GLU	CB-CA-C	-6.54	100.61	112.76
1	C	427	GLU	CB-CA-C	-6.54	100.60	112.76
1	C	662	MET	N-CA-CB	6.51	119.69	110.12
1	A	662	MET	N-CA-CB	6.47	119.63	110.12
1	C	663	ILE	CA-C-O	-6.43	114.26	120.95
1	A	663	ILE	CA-C-O	-6.40	114.29	120.95
2	D	626	THR	CA-C-O	-6.40	113.77	120.55
2	B	626	THR	CA-C-O	-6.38	113.79	120.55
1	A	591	VAL	CB-CA-C	-6.33	103.86	111.97
1	C	591	VAL	CB-CA-C	-6.29	103.93	111.97
1	C	796	SER	CA-C-O	-6.28	113.89	120.55
1	C	171	HIS	CA-CB-CG	-6.27	107.53	113.80
1	A	796	SER	CA-C-O	-6.26	113.92	120.55
1	C	842	ALA	N-CA-C	-6.25	104.47	111.28
1	A	171	HIS	CA-CB-CG	-6.24	107.56	113.80
1	A	842	ALA	N-CA-C	-6.21	104.51	111.28
2	B	643	LEU	CA-C-O	-6.15	112.90	119.97
2	D	643	LEU	CA-C-O	-6.13	112.92	119.97
1	C	239	VAL	N-CA-CB	-6.11	101.16	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	VAL	N-CA-CB	-6.09	101.18	111.23
1	C	626	SER	CA-C-O	-6.08	114.11	120.55
1	A	480	CYS	CA-C-O	-6.06	112.18	119.27
1	A	626	SER	CA-C-O	-6.06	114.13	120.55
1	C	480	CYS	CA-C-O	-6.05	112.19	119.27
1	C	662	MET	CA-C-N	-6.03	112.20	120.46
1	C	662	MET	C-N-CA	-6.03	112.20	120.46
1	C	592	HIS	CA-C-N	-6.02	112.04	120.53
1	C	592	HIS	C-N-CA	-6.02	112.04	120.53
2	D	644	ALA	N-CA-C	-6.02	105.90	113.18
1	A	662	MET	CA-C-N	-6.01	112.22	120.46
1	A	662	MET	C-N-CA	-6.01	112.22	120.46
1	C	553	PRO	N-CA-CB	-6.01	97.86	103.27
1	A	592	HIS	CA-C-N	-6.00	112.07	120.53
1	A	592	HIS	C-N-CA	-6.00	112.07	120.53
1	A	487	LEU	CA-C-O	-6.00	114.19	120.55
1	A	669	THR	CA-CB-CG2	6.00	120.70	110.50
1	C	487	LEU	CA-C-O	-5.99	114.20	120.55
1	C	669	THR	CA-CB-CG2	5.99	120.68	110.50
2	B	644	ALA	N-CA-C	-5.97	105.95	113.18
1	A	636	LEU	N-CA-C	-5.97	105.58	112.92
1	C	636	LEU	N-CA-C	-5.97	105.58	112.92
1	A	554	PHE	CA-C-O	-5.96	114.11	120.42
2	D	633	SER	CA-C-O	-5.95	114.24	120.55
1	A	553	PRO	N-CA-CB	-5.95	97.92	103.27
2	B	633	SER	CA-C-O	-5.94	114.25	120.55
1	C	801	HIS	N-CA-C	-5.94	104.39	111.69
1	C	554	PHE	CA-C-O	-5.92	114.14	120.42
1	C	628	MET	CB-CG-SD	-5.91	94.96	112.70
1	A	801	HIS	N-CA-C	-5.91	104.42	111.69
1	A	628	MET	CB-CG-SD	-5.91	94.97	112.70
1	C	743	ARG	CB-CG-CD	-5.90	97.72	111.30
2	D	632	VAL	CA-C-O	-5.90	114.59	120.85
1	A	743	ARG	CB-CG-CD	-5.89	97.75	111.30
1	C	796	SER	O-C-N	5.89	128.36	122.12
2	B	632	VAL	CA-C-O	-5.88	114.62	120.85
1	A	796	SER	O-C-N	5.85	128.32	122.12
2	B	513	LEU	N-CA-CB	-5.81	102.59	110.67
2	D	645	SER	CA-C-O	-5.80	112.94	119.79
2	B	645	SER	CA-C-O	-5.80	112.95	119.79
2	D	646	TYR	N-CA-CB	-5.78	101.61	110.16
2	D	513	LEU	N-CA-CB	-5.78	102.64	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	814	VAL	N-CA-C	5.77	115.96	110.42
1	A	757	LEU	CA-C-O	-5.76	114.44	120.55
2	B	646	TYR	N-CA-CB	-5.75	101.66	110.16
1	C	757	LEU	CA-C-O	-5.73	114.47	120.55
1	C	814	VAL	N-CA-C	5.73	115.92	110.42
2	D	421	SER	CA-C-N	-5.67	111.77	121.97
2	D	421	SER	C-N-CA	-5.67	111.77	121.97
1	C	784	ARG	CA-C-O	-5.65	115.55	121.99
2	B	421	SER	CA-C-N	-5.63	111.84	121.97
2	B	421	SER	C-N-CA	-5.63	111.84	121.97
1	A	793	VAL	CA-C-O	-5.62	114.89	120.85
1	A	784	ARG	CA-C-O	-5.61	115.60	121.99
1	C	793	VAL	CA-C-O	-5.60	114.91	120.85
1	A	242	LEU	CA-C-O	-5.60	115.07	121.68
1	C	844	GLY	CA-C-O	-5.60	114.98	120.75
2	B	614	PHE	CA-C-N	5.60	132.23	121.54
2	B	614	PHE	C-N-CA	5.60	132.23	121.54
2	B	612	LEU	CA-C-O	-5.60	111.78	119.05
2	D	131	SER	N-CA-C	-5.59	105.10	111.14
1	C	242	LEU	CA-C-O	-5.58	115.09	121.68
2	D	612	LEU	CA-C-O	-5.57	111.80	119.05
2	D	614	PHE	CA-C-N	5.57	132.19	121.54
2	D	614	PHE	C-N-CA	5.57	132.19	121.54
1	A	844	GLY	CA-C-O	-5.57	115.01	120.75
2	B	131	SER	N-CA-C	-5.57	105.12	111.14
1	A	555	LYS	CA-C-O	-5.56	114.76	120.99
1	C	816	TYR	CB-CA-C	5.56	119.02	110.62
2	B	392	PRO	N-CA-CB	-5.55	97.42	103.25
1	A	816	TYR	CB-CA-C	5.54	118.98	110.62
2	D	392	PRO	N-CA-CB	-5.52	97.45	103.25
1	C	555	LYS	CA-C-O	-5.51	114.82	120.99
1	A	802	GLU	CB-CA-C	-5.48	101.53	110.85
1	C	802	GLU	CB-CA-C	-5.48	101.54	110.85
1	A	669	THR	CA-C-N	-5.45	112.55	120.29
1	A	669	THR	C-N-CA	-5.45	112.55	120.29
2	B	755	LYS	CA-C-O	-5.42	115.64	122.63
1	C	669	THR	CA-C-N	-5.42	112.60	120.29
1	C	669	THR	C-N-CA	-5.42	112.60	120.29
1	A	483	LEU	CA-C-O	-5.41	114.81	120.55
1	C	763	GLN	CA-C-O	5.41	126.21	120.10
2	D	755	LYS	CA-C-O	-5.40	115.67	122.63
1	C	483	LEU	CA-C-O	-5.38	114.85	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	485	ILE	N-CA-CB	5.38	118.65	110.58
1	C	800	SER	CA-C-O	-5.37	112.78	119.28
1	A	485	ILE	N-CA-CB	5.37	118.64	110.58
2	D	641	ILE	CA-CB-CG1	-5.36	101.28	110.40
1	C	490	THR	CA-C-O	-5.35	114.88	120.55
1	A	628	MET	N-CA-CB	5.35	118.57	110.28
1	A	800	SER	CA-C-O	-5.35	112.81	119.28
1	A	763	GLN	CA-C-O	5.34	126.14	120.10
2	B	641	ILE	CA-CB-CG1	-5.34	101.32	110.40
1	A	490	THR	CA-C-O	-5.33	114.90	120.55
1	C	628	MET	N-CA-CB	5.33	118.54	110.28
2	B	751	ILE	CA-C-O	-5.31	115.75	121.27
2	D	635	TRP	CA-C-O	-5.30	114.80	120.42
1	C	758	GLU	CA-C-N	-5.30	113.18	120.28
1	C	758	GLU	C-N-CA	-5.30	113.18	120.28
2	B	635	TRP	CA-C-O	-5.28	114.82	120.42
1	C	791	GLN	N-CA-CB	5.28	117.73	110.07
1	A	758	GLU	CA-C-N	-5.27	113.22	120.28
1	A	758	GLU	C-N-CA	-5.27	113.22	120.28
1	A	791	GLN	N-CA-CB	5.27	117.71	110.07
2	D	640	VAL	N-CA-CB	5.26	118.47	110.58
1	C	790	LYS	CB-CA-C	-5.26	102.06	110.79
2	B	640	VAL	N-CA-CB	5.25	118.46	110.58
1	A	790	LYS	CB-CA-C	-5.25	102.08	110.79
2	D	751	ILE	CA-C-O	-5.23	115.83	121.27
1	A	575	PHE	CA-C-N	-5.23	111.56	121.54
1	A	575	PHE	C-N-CA	-5.23	111.56	121.54
1	C	575	PHE	CA-C-N	-5.22	111.57	121.54
1	C	575	PHE	C-N-CA	-5.22	111.57	121.54
2	B	749	VAL	N-CA-C	5.19	120.14	109.34
2	D	749	VAL	N-CA-C	5.19	120.14	109.34
2	D	623	PRO	CA-C-N	5.18	131.44	121.54
2	D	623	PRO	C-N-CA	5.18	131.44	121.54
2	B	623	PRO	CA-C-N	5.18	131.43	121.54
2	B	623	PRO	C-N-CA	5.18	131.43	121.54
2	B	611	GLY	CA-C-O	-5.17	115.42	120.75
2	D	611	GLY	CA-C-O	-5.15	115.45	120.75
2	D	640	VAL	N-CA-C	-5.14	105.53	110.72
1	A	743	ARG	CG-CD-NE	-5.13	100.71	112.00
2	B	640	VAL	N-CA-C	-5.13	105.54	110.72
1	C	743	ARG	CG-CD-NE	-5.13	100.72	112.00
1	C	553	PRO	N-CD-CG	-5.12	95.52	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	665	VAL	N-CA-CB	5.12	118.26	110.58
2	B	637	PHE	CA-CB-CG	-5.12	108.68	113.80
1	A	665	VAL	N-CA-CB	5.10	118.23	110.58
1	A	794	SER	N-CA-CB	5.09	117.69	110.16
2	D	637	PHE	CA-CB-CG	-5.09	108.71	113.80
1	A	553	PRO	N-CD-CG	-5.08	95.58	103.20
1	C	794	SER	N-CA-CB	5.08	117.67	110.16
1	C	794	SER	CA-C-O	-5.07	115.04	120.42
2	D	627	THR	CA-CB-OG1	-5.07	102.00	109.60
2	B	627	THR	CA-CB-OG1	-5.06	102.00	109.60
1	A	659	GLY	CA-C-N	-5.06	113.17	121.92
1	A	659	GLY	C-N-CA	-5.06	113.17	121.92
1	C	659	GLY	CA-C-N	-5.04	113.19	121.92
1	C	659	GLY	C-N-CA	-5.04	113.19	121.92
1	A	794	SER	CA-C-O	-5.02	115.10	120.42

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	555	LYS	Mainchain
1	A	580	GLN	Mainchain
1	A	800	SER	Mainchain
1	A	813	TRP	Mainchain
1	C	555	LYS	Mainchain
1	C	580	GLN	Mainchain
1	C	800	SER	Mainchain
1	C	813	TRP	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	5695	0	5285	274	0
1	C	5695	0	5285	283	0
2	B	5654	0	5220	187	0
2	D	5654	0	5220	189	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	28	0	25	0	0
3	F	28	0	25	0	0
4	A	5	0	2	0	0
4	C	5	0	2	0	0
5	B	14	0	13	0	0
5	D	14	0	13	0	0
All	All	22792	0	21090	843	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 19.

All (843) 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)
2:D:278:ILE:HD11	2:D:391:TRP:CH2	1.36	1.60
2:B:278:ILE:HD11	2:B:391:TRP:CH2	1.36	1.56
1:C:599:TYR:CB	1:C:624:LEU:HD12	1.45	1.46
1:A:599:TYR:CB	1:A:624:LEU:HD12	1.45	1.46
1:A:582:THR:CG2	2:B:815:ILE:HD13	1.55	1.37
1:C:582:THR:CG2	2:D:815:ILE:HD13	1.55	1.36
1:A:591:VAL:HG21	1:A:632:TRP:CZ3	1.63	1.34
2:D:746:CYS:SG	2:D:801:CYS:SG	1.33	1.33
1:C:591:VAL:HG21	1:C:632:TRP:CZ3	1.63	1.33
2:B:538:VAL:O	2:B:749:VAL:CG1	1.74	1.33
2:D:538:VAL:O	2:D:749:VAL:CG1	1.74	1.33
1:A:578:PRO:HB2	1:A:671:ASN:ND2	1.44	1.33
2:B:746:CYS:SG	2:B:801:CYS:SG	1.33	1.32
1:C:578:PRO:HB2	1:C:671:ASN:ND2	1.44	1.30
2:B:538:VAL:O	2:B:749:VAL:HG12	1.18	1.29
2:B:644:ALA:HB1	1:C:669:THR:CG2	1.63	1.28
2:B:746:CYS:SG	2:B:801:CYS:CB	2.21	1.27
2:D:746:CYS:SG	2:D:801:CYS:CB	2.21	1.27
2:B:743:ASP:OD2	2:B:748:LEU:CD1	1.84	1.25
2:D:743:ASP:OD2	2:D:748:LEU:CD1	1.84	1.25
2:D:743:ASP:OD2	2:D:748:LEU:HD12	1.08	1.24
2:B:743:ASP:OD2	2:B:748:LEU:HD12	1.08	1.23
2:B:635:TRP:CH2	2:B:638:PHE:HE2	1.57	1.23
2:D:538:VAL:O	2:D:749:VAL:HG12	1.18	1.23
2:D:635:TRP:CH2	2:D:638:PHE:HE2	1.57	1.22
2:B:278:ILE:CD1	2:B:391:TRP:HH2	1.52	1.22
2:D:278:ILE:CD1	2:D:391:TRP:HH2	1.52	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:THR:CG2	2:D:644:ALA:HB1	1.70	1.21
1:C:163:ILE:HG22	1:C:239:VAL:HG12	1.28	1.16
2:B:391:TRP:O	2:B:393:ARG:N	1.83	1.12
2:D:391:TRP:O	2:D:393:ARG:N	1.83	1.11
1:A:582:THR:HG22	2:B:815:ILE:HD13	1.24	1.10
2:D:635:TRP:CH2	2:D:638:PHE:CE2	2.40	1.10
1:A:163:ILE:HG22	1:A:239:VAL:HG12	1.28	1.09
1:A:507:THR:HG22	1:A:707:GLN:HG2	1.30	1.09
2:B:635:TRP:CH2	2:B:638:PHE:CE2	2.40	1.09
2:B:644:ALA:CB	1:C:669:THR:HG22	1.80	1.09
1:C:507:THR:HG22	1:C:707:GLN:HG2	1.30	1.08
1:C:582:THR:HG22	2:D:815:ILE:HD13	1.32	1.08
1:A:669:THR:HG22	2:D:644:ALA:HB1	1.10	1.08
2:B:134:MET:HE3	2:B:137:LYS:HG2	1.28	1.08
2:D:134:MET:HE3	2:D:137:LYS:HG2	1.27	1.07
2:B:278:ILE:CD1	2:B:391:TRP:CH2	2.32	1.07
1:C:655:MET:HG3	2:D:610:TRP:CD1	1.90	1.06
2:D:469:SER:O	2:D:472:VAL:O	1.74	1.06
2:D:635:TRP:CZ3	2:D:638:PHE:CD2	2.44	1.06
2:B:635:TRP:CZ3	2:B:638:PHE:CD2	2.44	1.05
2:B:469:SER:O	2:B:472:VAL:O	1.74	1.05
2:D:635:TRP:CZ3	2:D:638:PHE:CE2	2.46	1.04
1:C:582:THR:HG23	2:D:815:ILE:HD13	1.39	1.03
2:B:635:TRP:CZ3	2:B:638:PHE:CE2	2.46	1.02
1:C:599:TYR:CB	1:C:624:LEU:CD1	2.38	1.02
1:A:582:THR:HG23	2:B:815:ILE:HD13	1.43	1.01
2:B:648:ALA:CB	1:C:673:ALA:HB2	1.91	1.01
1:A:599:TYR:CB	1:A:624:LEU:CD1	2.38	1.01
2:D:278:ILE:CD1	2:D:391:TRP:CH2	2.33	0.99
1:A:163:ILE:HG22	1:A:239:VAL:CG1	1.92	0.99
1:C:163:ILE:HG22	1:C:239:VAL:CG1	1.92	0.99
1:A:578:PRO:HB2	1:A:671:ASN:HD21	1.24	0.99
1:A:582:THR:CG2	2:B:815:ILE:CD1	2.41	0.99
1:A:655:MET:HG3	2:B:610:TRP:CD1	1.99	0.98
1:C:582:THR:CG2	2:D:815:ILE:CD1	2.43	0.96
2:B:648:ALA:HB1	1:C:673:ALA:HB2	1.48	0.95
2:B:644:ALA:HB1	1:C:669:THR:HG22	0.95	0.95
1:C:591:VAL:HG21	1:C:632:TRP:HZ3	1.12	0.95
1:C:595:ALA:HB1	1:C:628:MET:HB2	1.49	0.95
1:A:632:TRP:HE3	1:A:632:TRP:HA	1.33	0.94
1:A:155:MET:HE1	1:A:163:ILE:HD13	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:ALA:HB1	1:A:628:MET:HB2	1.49	0.92
1:A:632:TRP:HA	1:A:632:TRP:CE3	2.03	0.92
1:C:632:TRP:HE3	1:C:632:TRP:HA	1.33	0.92
1:C:578:PRO:HB2	1:C:671:ASN:HD21	1.24	0.92
1:A:669:THR:HG22	2:D:644:ALA:CB	2.00	0.91
1:A:578:PRO:CB	1:A:671:ASN:ND2	2.35	0.90
1:C:155:MET:HE1	1:C:163:ILE:HD13	1.50	0.89
1:A:673:ALA:HB2	2:D:648:ALA:HB1	1.52	0.89
1:C:632:TRP:HA	1:C:632:TRP:CE3	2.03	0.89
1:A:591:VAL:HG21	1:A:632:TRP:HZ3	1.12	0.89
2:B:643:LEU:O	2:B:643:LEU:HD23	1.73	0.89
2:D:643:LEU:HD23	2:D:643:LEU:O	1.73	0.88
1:C:578:PRO:CB	1:C:671:ASN:ND2	2.35	0.88
2:B:746:CYS:SG	2:B:801:CYS:HB3	2.13	0.87
2:D:746:CYS:CB	2:D:801:CYS:HG	1.87	0.87
2:D:746:CYS:SG	2:D:801:CYS:HB3	2.13	0.87
1:C:507:THR:CG2	1:C:707:GLN:HG2	2.06	0.86
1:A:507:THR:CG2	1:A:707:GLN:HG2	2.06	0.86
1:A:529:GLY:HA2	1:A:784:ARG:HH22	1.41	0.85
1:C:655:MET:HG3	2:D:610:TRP:NE1	1.91	0.85
1:C:578:PRO:CB	1:C:671:ASN:HD21	1.90	0.84
1:C:703:ALA:CB	1:C:730:HIS:O	2.25	0.84
1:A:703:ALA:CB	1:A:730:HIS:O	2.25	0.84
1:C:155:MET:CE	1:C:163:ILE:HD13	2.07	0.84
1:C:529:GLY:HA2	1:C:784:ARG:HH22	1.42	0.84
1:A:483:LEU:HD12	1:A:483:LEU:O	1.78	0.84
1:A:155:MET:CE	1:A:163:ILE:HD13	2.07	0.83
1:A:791:GLN:NE2	1:A:791:GLN:O	2.12	0.83
1:A:622:LEU:C	1:A:623:THR:HG22	2.04	0.83
2:B:644:ALA:CB	1:C:669:THR:CG2	2.46	0.82
1:C:622:LEU:C	1:C:623:THR:HG22	2.04	0.82
1:C:622:LEU:O	1:C:623:THR:HG22	1.80	0.82
2:B:635:TRP:CZ3	2:B:638:PHE:HD2	1.96	0.82
1:C:483:LEU:HD12	1:C:483:LEU:O	1.78	0.82
1:C:649:SER:HG	2:D:832:SER:HG	1.21	0.82
1:A:673:ALA:HB2	2:D:648:ALA:CB	2.09	0.81
1:A:578:PRO:CB	1:A:671:ASN:HD21	1.90	0.81
1:A:622:LEU:O	1:A:623:THR:HG22	1.79	0.81
1:C:791:GLN:O	1:C:791:GLN:NE2	2.12	0.81
2:D:635:TRP:CZ3	2:D:638:PHE:HD2	1.96	0.81
2:B:609:LEU:HG	2:B:635:TRP:CD1	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:278:ILE:HD11	2:D:391:TRP:CZ3	2.15	0.81
2:B:278:ILE:HD11	2:B:391:TRP:CZ3	2.15	0.80
1:C:576:MET:HB2	1:C:584:TRP:NE1	1.97	0.80
2:D:609:LEU:HG	2:D:635:TRP:CD1	2.15	0.80
2:B:643:LEU:HD23	2:B:643:LEU:C	2.06	0.80
2:B:648:ALA:CA	1:C:673:ALA:HB2	2.11	0.80
1:C:583:LEU:O	1:C:583:LEU:HD12	1.83	0.79
2:D:643:LEU:HD23	2:D:643:LEU:C	2.06	0.79
1:A:576:MET:HB2	1:A:584:TRP:NE1	1.97	0.79
1:A:583:LEU:HD12	1:A:583:LEU:O	1.83	0.78
1:C:655:MET:O	2:D:610:TRP:NE1	2.13	0.78
1:C:575:PHE:C	1:C:577:GLN:H	1.92	0.77
1:A:155:MET:HE1	1:A:163:ILE:CD1	2.14	0.77
2:D:635:TRP:HH2	2:D:638:PHE:HE2	1.32	0.77
1:C:562:LEU:HB2	1:C:757:LEU:HD13	1.66	0.77
2:D:391:TRP:O	2:D:392:PRO:C	2.28	0.77
1:C:155:MET:HE1	1:C:163:ILE:CD1	2.14	0.77
1:A:575:PHE:C	1:A:577:GLN:H	1.92	0.77
2:B:746:CYS:CB	2:B:801:CYS:HG	1.95	0.77
1:C:760:GLU:HA	1:C:760:GLU:OE1	1.85	0.77
1:C:670:ALA:HB1	2:D:651:ALA:HA	1.66	0.77
2:B:391:TRP:O	2:B:392:PRO:C	2.28	0.77
1:A:562:LEU:HB2	1:A:757:LEU:HD13	1.66	0.75
1:A:760:GLU:HA	1:A:760:GLU:OE1	1.85	0.75
1:A:791:GLN:HE21	1:A:791:GLN:C	1.95	0.74
1:C:164:ILE:HD11	1:C:232:ALA:HB1	1.69	0.74
1:A:669:THR:CG2	2:D:644:ALA:CB	2.59	0.74
2:B:635:TRP:HH2	2:B:638:PHE:HE2	1.32	0.74
1:C:582:THR:HG21	2:D:815:ILE:HB	1.69	0.74
1:A:622:LEU:O	1:A:623:THR:CG2	2.35	0.74
1:C:622:LEU:O	1:C:623:THR:CG2	2.35	0.74
2:B:552:GLU:CB	2:B:653:PHE:HE2	2.02	0.73
2:D:538:VAL:O	2:D:749:VAL:HG13	1.87	0.73
1:C:791:GLN:HE21	1:C:791:GLN:C	1.95	0.73
1:A:703:ALA:HB2	1:A:730:HIS:O	1.88	0.73
1:A:164:ILE:HD11	1:A:232:ALA:HB1	1.69	0.72
1:C:703:ALA:HB2	1:C:730:HIS:O	1.88	0.72
1:C:484:LEU:HB2	1:C:535:VAL:HG11	1.72	0.72
1:A:582:THR:HG21	2:B:815:ILE:HB	1.70	0.72
2:B:437:GLN:O	2:B:439:ARG:HG3	1.90	0.72
1:A:484:LEU:HB2	1:A:535:VAL:HG11	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:SER:OG	2:B:130:SER:O	2.05	0.72
2:D:552:GLU:CB	2:D:653:PHE:HE2	2.02	0.71
1:A:655:MET:HG3	2:B:610:TRP:NE1	2.04	0.71
1:A:582:THR:HG22	2:B:815:ILE:CD1	2.10	0.71
2:D:299:ILE:HG23	2:D:342:VAL:HG11	1.73	0.71
2:D:437:GLN:O	2:D:439:ARG:HG3	1.90	0.70
2:B:648:ALA:HA	1:C:673:ALA:HB2	1.73	0.70
1:A:552:LYS:HG2	1:A:794:SER:OG	1.92	0.70
1:A:785:LYS:NZ	2:D:774:ARG:HH21	1.90	0.70
1:A:578:PRO:HG3	1:A:668:TYR:HE1	1.57	0.69
2:B:299:ILE:HG23	2:B:342:VAL:HG11	1.73	0.69
1:A:240:ILE:HG12	1:A:240:ILE:O	1.91	0.69
1:A:426:GLN:OE1	1:A:426:GLN:HA	1.91	0.69
1:C:240:ILE:HG12	1:C:240:ILE:O	1.91	0.69
1:C:552:LYS:HG2	1:C:794:SER:OG	1.92	0.69
1:A:669:THR:HG21	2:D:644:ALA:HB1	1.68	0.69
2:B:644:ALA:HB1	1:C:669:THR:HG21	1.72	0.69
1:C:426:GLN:HA	1:C:426:GLN:OE1	1.91	0.69
1:A:640:ILE:CD1	2:D:633:SER:HB2	2.23	0.68
1:C:163:ILE:CG2	1:C:239:VAL:CG1	2.71	0.68
1:C:578:PRO:HG3	1:C:668:TYR:HE1	1.57	0.68
1:C:655:MET:CG	2:D:610:TRP:NE1	2.56	0.68
1:C:286:GLY:HA3	1:C:403:PRO:HD3	1.76	0.68
2:D:130:SER:O	2:D:130:SER:OG	2.05	0.67
1:A:286:GLY:HA3	1:A:403:PRO:HD3	1.76	0.67
2:B:774:ARG:HH21	1:C:785:LYS:NZ	1.93	0.67
2:D:750:THR:O	2:D:750:THR:OG1	2.07	0.67
2:B:538:VAL:O	2:B:749:VAL:HG13	1.87	0.67
2:B:750:THR:O	2:B:750:THR:OG1	2.07	0.67
2:B:699:TYR:HB3	2:B:702:MET:HB2	1.77	0.67
1:C:529:GLY:HA2	1:C:784:ARG:NH2	2.11	0.66
1:A:163:ILE:CG2	1:A:239:VAL:CG1	2.71	0.66
1:A:784:ARG:NH1	1:A:784:ARG:HG2	2.09	0.66
1:A:419:LEU:HD11	1:A:493:PHE:HE2	1.60	0.66
1:C:419:LEU:HD11	1:C:493:PHE:HE2	1.60	0.66
1:C:591:VAL:CG2	1:C:632:TRP:HZ3	2.00	0.66
1:A:87:VAL:HG22	1:A:325:PRO:HD2	1.77	0.66
1:C:784:ARG:NH1	1:C:784:ARG:HG2	2.09	0.66
1:C:87:VAL:HG22	1:C:325:PRO:HD2	1.77	0.66
1:C:703:ALA:HA	1:C:727:MET:HG2	1.78	0.66
2:B:423:ASP:HB3	2:B:428:THR:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:576:MET:HB2	1:C:584:TRP:HE1	1.61	0.65
2:D:699:TYR:HB3	2:D:702:MET:HB2	1.77	0.65
1:A:164:ILE:CD1	1:A:232:ALA:HB1	2.26	0.65
1:A:628:MET:HG2	1:A:628:MET:O	1.97	0.65
1:C:800:SER:O	1:C:800:SER:OG	2.11	0.65
1:A:529:GLY:HA2	1:A:784:ARG:NH2	2.11	0.65
1:A:703:ALA:HA	1:A:727:MET:HG2	1.78	0.65
1:A:488:ALA:HA	1:A:493:PHE:CE1	2.33	0.64
1:C:488:ALA:HA	1:C:493:PHE:CE1	2.33	0.64
2:D:635:TRP:CE3	2:D:638:PHE:HD2	2.15	0.64
2:D:793:GLU:HG2	2:D:797:LEU:HD12	1.79	0.64
1:C:300:ALA:HB1	1:C:355:VAL:HG21	1.78	0.64
2:D:423:ASP:HB3	2:D:428:THR:O	1.96	0.64
1:A:576:MET:HB2	1:A:584:TRP:HE1	1.61	0.64
1:A:622:LEU:C	1:A:623:THR:CG2	2.70	0.64
1:A:634:VAL:HG11	1:A:657:TRP:HD1	1.62	0.64
2:B:608:LEU:HD12	2:B:608:LEU:C	2.22	0.64
1:C:164:ILE:CD1	1:C:232:ALA:HB1	2.26	0.64
2:B:793:GLU:HG2	2:B:797:LEU:HD12	1.80	0.64
1:A:784:ARG:HG2	1:A:784:ARG:HH11	1.63	0.64
1:A:300:ALA:HB1	1:A:355:VAL:HG21	1.78	0.64
1:A:575:PHE:C	1:A:577:GLN:N	2.53	0.64
1:A:685:ILE:HG12	1:A:692:ARG:HD2	1.80	0.64
1:C:628:MET:O	1:C:628:MET:HG2	1.97	0.64
1:C:164:ILE:O	1:C:164:ILE:HG12	1.98	0.64
1:C:622:LEU:C	1:C:623:THR:CG2	2.70	0.64
1:C:685:ILE:HG12	1:C:692:ARG:HD2	1.80	0.64
1:A:164:ILE:HG12	1:A:164:ILE:O	1.98	0.63
2:B:635:TRP:CE3	2:B:638:PHE:HD2	2.15	0.63
1:C:419:LEU:HD21	1:C:493:PHE:CD2	2.33	0.63
1:A:670:ALA:HB1	2:B:651:ALA:HA	1.81	0.63
2:D:617:SER:O	2:D:618:VAL:HG13	1.99	0.63
1:C:634:VAL:HG11	1:C:657:TRP:HD1	1.62	0.63
2:D:133:ILE:HG23	2:D:133:ILE:O	1.99	0.63
2:D:608:LEU:C	2:D:608:LEU:HD12	2.23	0.62
1:C:578:PRO:HB2	1:C:671:ASN:HD22	1.59	0.62
1:C:592:HIS:O	1:C:593:VAL:C	2.42	0.62
1:C:635:LEU:HD12	1:C:635:LEU:O	2.00	0.62
2:D:469:SER:HA	2:D:474:PHE:CE2	2.34	0.62
1:C:784:ARG:HG2	1:C:784:ARG:HH11	1.63	0.62
1:A:419:LEU:HD21	1:A:493:PHE:CD2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:ALA:HB1	1:A:628:MET:CB	2.26	0.62
2:B:133:ILE:HG23	2:B:133:ILE:O	1.98	0.62
2:B:469:SER:HA	2:B:474:PHE:CE2	2.34	0.62
1:A:635:LEU:O	1:A:635:LEU:HD12	2.00	0.62
2:B:134:MET:HG3	2:B:134:MET:O	2.00	0.62
1:C:213:GLU:OE1	1:C:213:GLU:HA	1.99	0.62
1:A:213:GLU:OE1	1:A:213:GLU:HA	1.99	0.62
1:A:591:VAL:CG2	1:A:632:TRP:HZ3	2.00	0.62
2:B:617:SER:O	2:B:618:VAL:HG13	1.99	0.62
1:A:592:HIS:O	1:A:593:VAL:C	2.42	0.62
1:A:623:THR:HG23	1:A:626:SER:HB3	1.82	0.62
1:A:634:VAL:HG11	1:A:657:TRP:CD1	2.35	0.62
1:A:704:THR:O	1:A:731:ASN:OD1	2.18	0.62
1:A:578:PRO:HG3	1:A:668:TYR:CE1	2.35	0.61
1:C:623:THR:HG23	1:C:626:SER:HB3	1.82	0.61
2:D:663:VAL:O	2:D:751:ILE:HG21	2.00	0.61
1:A:816:TYR:HD1	1:A:816:TYR:O	1.83	0.61
1:A:479:PHE:O	1:A:479:PHE:HD1	1.84	0.61
1:C:591:VAL:CG2	1:C:632:TRP:CZ3	2.60	0.61
2:B:663:VAL:O	2:B:751:ILE:HG21	2.01	0.61
1:C:634:VAL:HG11	1:C:657:TRP:CD1	2.35	0.61
1:A:655:MET:O	2:B:610:TRP:NE1	2.26	0.61
1:C:704:THR:O	1:C:731:ASN:OD1	2.18	0.61
2:D:513:LEU:O	2:D:514:THR:CG2	2.49	0.61
1:C:578:PRO:HG3	1:C:668:TYR:CE1	2.35	0.61
1:C:816:TYR:HD1	1:C:816:TYR:O	1.83	0.61
1:A:586:LEU:HD23	1:A:586:LEU:C	2.25	0.61
2:B:513:LEU:O	2:B:514:THR:CG2	2.49	0.60
1:C:582:THR:HG22	2:D:815:ILE:CD1	2.18	0.60
1:A:568:PRO:HB2	1:A:827:ALA:HB2	1.82	0.60
1:C:575:PHE:C	1:C:577:GLN:N	2.53	0.60
2:D:653:PHE:O	2:D:654:MET:C	2.42	0.60
1:C:586:LEU:C	1:C:586:LEU:HD23	2.25	0.60
1:A:419:LEU:HD21	1:A:493:PHE:HD2	1.67	0.60
1:A:479:PHE:CD1	1:A:479:PHE:C	2.80	0.60
1:C:479:PHE:HD1	1:C:479:PHE:O	1.84	0.60
2:D:134:MET:HE3	2:D:137:LYS:CG	2.19	0.60
1:A:591:VAL:CG2	1:A:632:TRP:CZ3	2.60	0.60
1:A:640:ILE:HD11	2:D:633:SER:HB2	1.84	0.60
1:C:595:ALA:CB	1:C:628:MET:HB2	2.29	0.59
1:C:674:ALA:HB1	2:D:655:ILE:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:PRO:HB2	1:C:827:ALA:HB2	1.82	0.59
2:D:134:MET:O	2:D:134:MET:HG3	2.00	0.59
1:A:800:SER:O	1:A:800:SER:OG	2.11	0.59
1:C:791:GLN:HE21	1:C:791:GLN:CA	2.14	0.59
1:A:239:VAL:HG12	1:A:239:VAL:O	2.02	0.59
1:A:791:GLN:HE21	1:A:791:GLN:CA	2.14	0.59
2:B:134:MET:CE	2:B:137:LYS:HG2	2.19	0.59
1:C:631:SER:OG	1:C:657:TRP:NE1	2.36	0.59
1:A:631:SER:OG	1:A:657:TRP:NE1	2.36	0.59
2:B:609:LEU:N	2:B:609:LEU:HD12	2.18	0.59
1:A:705:VAL:HG12	1:A:705:VAL:O	2.02	0.59
1:C:479:PHE:CD1	1:C:479:PHE:C	2.80	0.59
1:C:705:VAL:HG12	1:C:705:VAL:O	2.02	0.59
1:A:582:THR:CG2	2:B:815:ILE:CG1	2.80	0.59
1:A:582:THR:HG23	2:B:815:ILE:CD1	2.21	0.59
1:C:239:VAL:HG12	1:C:239:VAL:O	2.02	0.59
1:C:675:PHE:C	1:C:675:PHE:CD2	2.81	0.59
2:B:422:VAL:HG23	2:B:429:CYS:SG	2.43	0.58
2:D:422:VAL:HG23	2:D:429:CYS:SG	2.43	0.58
2:D:36:GLY:HA3	2:D:94:ILE:HA	1.84	0.58
2:D:609:LEU:HD12	2:D:609:LEU:N	2.18	0.58
1:A:634:VAL:CG1	1:A:657:TRP:CD1	2.86	0.58
2:B:36:GLY:HA3	2:B:94:ILE:HA	1.84	0.58
1:C:665:VAL:HG12	1:C:665:VAL:O	2.03	0.58
2:B:509:ALA:HB3	2:B:765:ALA:HB3	1.85	0.58
2:D:134:MET:CE	2:D:137:LYS:HG2	2.19	0.58
1:C:589:LEU:C	1:C:589:LEU:HD12	2.28	0.58
1:A:675:PHE:C	1:A:675:PHE:CD2	2.81	0.58
1:A:791:GLN:NE2	1:A:791:GLN:HA	2.18	0.58
1:C:662:MET:SD	1:C:662:MET:C	2.87	0.58
1:A:495:TYR:N	1:A:495:TYR:CD1	2.72	0.58
1:A:582:THR:CG2	2:B:815:ILE:HB	2.34	0.58
1:A:701:ILE:HG23	1:A:730:HIS:CE1	2.39	0.58
1:C:419:LEU:HD21	1:C:493:PHE:HD2	1.67	0.58
1:C:701:ILE:HG23	1:C:730:HIS:CE1	2.39	0.58
2:D:609:LEU:CG	2:D:635:TRP:CD1	2.86	0.58
1:C:683:GLU:O	1:C:692:ARG:NH1	2.37	0.58
1:A:791:GLN:NE2	1:A:791:GLN:CA	2.66	0.57
1:C:630:PHE:CD1	1:C:630:PHE:C	2.82	0.57
1:A:595:ALA:CB	1:A:628:MET:HB2	2.29	0.57
1:A:662:MET:SD	1:A:662:MET:C	2.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:VAL:CG1	1:C:657:TRP:CD1	2.86	0.57
2:D:270:PRO:O	2:D:371:ARG:NH2	2.37	0.57
2:B:391:TRP:O	2:B:393:ARG:CA	2.52	0.57
1:C:791:GLN:NE2	1:C:791:GLN:HA	2.18	0.57
1:A:630:PHE:CD1	1:A:630:PHE:C	2.82	0.57
1:C:483:LEU:HD12	1:C:483:LEU:C	2.26	0.57
1:A:683:GLU:O	1:A:692:ARG:NH1	2.37	0.57
1:C:595:ALA:HB1	1:C:628:MET:CB	2.26	0.57
2:B:553:PRO:O	2:B:649:ASN:ND2	2.38	0.57
2:B:609:LEU:CG	2:B:635:TRP:CD1	2.86	0.57
1:C:147:GLN:HE21	1:C:290:LEU:HB2	1.69	0.57
1:C:495:TYR:CD1	1:C:495:TYR:N	2.72	0.57
1:C:120:GLY:N	1:C:138:LEU:O	2.37	0.57
1:A:783:MET:SD	1:A:783:MET:N	2.77	0.57
1:C:586:LEU:CD2	2:D:822:PHE:CE1	2.88	0.57
1:C:791:GLN:NE2	1:C:791:GLN:CA	2.66	0.57
1:A:589:LEU:C	1:A:589:LEU:HD12	2.28	0.57
1:A:665:VAL:HG12	1:A:665:VAL:O	2.03	0.56
1:C:783:MET:SD	1:C:783:MET:N	2.77	0.56
2:D:609:LEU:CD2	2:D:635:TRP:CD1	2.88	0.56
1:A:582:THR:HG21	2:B:815:ILE:CG1	2.35	0.56
2:B:418:ILE:HG12	2:B:458:LYS:O	2.06	0.56
1:C:717:GLN:HB3	1:C:720:LEU:HB2	1.87	0.56
1:C:759:PHE:CD1	1:C:759:PHE:C	2.83	0.56
2:D:509:ALA:HB3	2:D:765:ALA:HB3	1.85	0.56
1:A:586:LEU:HD23	1:A:586:LEU:O	2.06	0.56
1:A:673:ALA:HB2	2:D:648:ALA:CA	2.35	0.56
1:C:582:THR:HG23	2:D:815:ILE:CD1	2.22	0.56
1:A:120:GLY:N	1:A:138:LEU:O	2.37	0.56
1:C:696:PRO:HG2	1:C:726:HIS:CD2	2.41	0.56
2:D:391:TRP:O	2:D:393:ARG:CA	2.52	0.56
2:D:418:ILE:HG12	2:D:458:LYS:O	2.06	0.56
2:D:538:VAL:HG23	2:D:749:VAL:HG11	1.87	0.56
1:C:507:THR:CG2	1:C:707:GLN:CG	2.83	0.56
1:C:702:TYR:OH	1:C:723:MET:SD	2.62	0.56
2:D:205:LEU:HD11	2:D:216:ILE:HD13	1.87	0.56
1:A:553:PRO:O	1:A:553:PRO:HG2	2.05	0.56
1:A:582:THR:HG21	2:B:815:ILE:CB	2.35	0.56
1:A:655:MET:CG	2:B:610:TRP:NE1	2.69	0.56
2:D:432:ASN:O	2:D:466:LYS:NZ	2.39	0.56
2:B:270:PRO:O	2:B:371:ARG:NH2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:GLN:HB3	1:A:720:LEU:HB2	1.87	0.56
2:B:609:LEU:CD2	2:B:635:TRP:CD1	2.88	0.56
1:C:705:VAL:HB	1:C:752:TRP:CZ3	2.41	0.56
2:B:538:VAL:HG23	2:B:749:VAL:HG11	1.87	0.55
1:C:286:GLY:HA3	1:C:403:PRO:CD	2.36	0.55
1:C:570:SER:HB3	1:C:827:ALA:HB3	1.89	0.55
2:D:188:SER:O	2:D:192:ASN:ND2	2.39	0.55
1:A:147:GLN:HE21	1:A:290:LEU:HB2	1.69	0.55
1:A:717:GLN:HG2	1:A:720:LEU:HD23	1.88	0.55
2:B:653:PHE:O	2:B:654:MET:C	2.42	0.55
1:C:660:PHE:HD1	2:D:821:VAL:CG1	2.19	0.55
2:D:553:PRO:O	2:D:649:ASN:ND2	2.38	0.55
2:B:205:LEU:HD11	2:B:216:ILE:HD13	1.87	0.55
2:D:608:LEU:HG	2:D:609:LEU:HD12	1.89	0.55
1:A:507:THR:HG22	1:A:707:GLN:CG	2.21	0.55
2:B:188:SER:O	2:B:192:ASN:ND2	2.39	0.55
2:B:561:MET:HA	2:B:564:VAL:HG12	1.88	0.55
1:C:586:LEU:HD23	1:C:586:LEU:O	2.06	0.55
1:A:286:GLY:HA3	1:A:403:PRO:CD	2.37	0.55
1:A:570:SER:HB3	1:A:827:ALA:HB3	1.88	0.55
1:A:705:VAL:HB	1:A:752:TRP:CZ3	2.41	0.55
2:B:432:ASN:O	2:B:466:LYS:NZ	2.39	0.55
1:A:483:LEU:HD12	1:A:483:LEU:C	2.26	0.55
1:C:717:GLN:HG2	1:C:720:LEU:HD23	1.88	0.55
2:D:48:VAL:HG22	2:D:49:ALA:H	1.71	0.55
2:D:668:ASP:OD1	2:D:669:LYS:N	2.40	0.55
2:D:417:VAL:HG12	2:D:462:ILE:HG12	1.89	0.55
2:D:561:MET:HA	2:D:564:VAL:HG12	1.88	0.55
1:A:696:PRO:HG2	1:A:726:HIS:CD2	2.41	0.55
2:B:48:VAL:HG22	2:B:49:ALA:H	1.71	0.55
1:C:624:LEU:O	1:C:624:LEU:HG	2.07	0.55
1:A:759:PHE:C	1:A:759:PHE:CD1	2.83	0.54
2:B:743:ASP:CG	2:B:748:LEU:HD12	2.15	0.54
1:C:553:PRO:HG2	1:C:553:PRO:O	2.05	0.54
1:C:478:GLY:O	1:C:482:ASP:HB2	2.08	0.54
2:B:572:VAL:HG21	1:C:845:ILE:CG2	2.37	0.54
1:C:557:GLN:NE2	1:C:777:SER:O	2.41	0.54
1:C:696:PRO:HG2	1:C:726:HIS:HD2	1.73	0.54
1:C:286:GLY:CA	1:C:403:PRO:HD3	2.37	0.54
1:A:557:GLN:NE2	1:A:777:SER:O	2.41	0.54
2:B:150:ILE:HD11	2:B:182:PHE:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:417:VAL:HG12	2:B:462:ILE:HG12	1.89	0.54
2:B:522:VAL:HG13	2:B:523:VAL:HG23	1.90	0.54
2:B:608:LEU:HG	2:B:609:LEU:HD12	1.89	0.54
2:D:522:VAL:HG13	2:D:523:VAL:HG23	1.90	0.54
1:A:488:ALA:HA	1:A:493:PHE:HE1	1.72	0.54
2:B:648:ALA:HB1	1:C:673:ALA:CB	2.31	0.54
1:C:555:LYS:O	1:C:555:LYS:HG2	2.07	0.54
1:A:286:GLY:CA	1:A:403:PRO:HD3	2.37	0.53
1:C:632:TRP:CE3	1:C:632:TRP:CA	2.87	0.53
1:A:478:GLY:O	1:A:482:ASP:HB2	2.08	0.53
1:A:696:PRO:HG2	1:A:726:HIS:HD2	1.73	0.53
1:C:586:LEU:HD21	2:D:822:PHE:CE1	2.43	0.53
2:D:436:CYS:SG	2:D:457:CYS:N	2.82	0.53
1:A:93:SER:HB2	1:A:121:LEU:HD12	1.90	0.53
2:B:436:CYS:SG	2:B:457:CYS:N	2.82	0.53
2:B:668:ASP:OD1	2:B:669:LYS:N	2.40	0.53
1:C:488:ALA:HA	1:C:493:PHE:HE1	1.72	0.53
1:C:784:ARG:HH11	1:C:784:ARG:CG	2.20	0.53
2:D:574:VAL:HB	2:D:602:ILE:HD11	1.91	0.53
1:A:624:LEU:O	1:A:624:LEU:HG	2.07	0.53
1:C:93:SER:HB2	1:C:121:LEU:HD12	1.91	0.53
1:C:163:ILE:CG2	1:C:239:VAL:HG12	2.19	0.53
2:B:158:LEU:HA	2:B:161:MET:HE3	1.91	0.53
1:A:668:TYR:CD1	1:A:668:TYR:C	2.85	0.52
2:B:574:VAL:HB	2:B:602:ILE:HD11	1.91	0.52
1:C:583:LEU:HD12	1:C:583:LEU:C	2.34	0.52
1:A:555:LYS:O	1:A:555:LYS:HG2	2.07	0.52
1:A:743:ARG:NH1	1:A:764:LYS:HD3	2.24	0.52
2:B:513:LEU:C	2:B:514:THR:HG22	2.34	0.52
1:C:582:THR:CG2	2:D:815:ILE:HB	2.38	0.52
2:B:513:LEU:O	2:B:514:THR:HG22	2.09	0.52
1:C:668:TYR:CD1	1:C:668:TYR:C	2.85	0.52
2:D:513:LEU:C	2:D:514:THR:HG22	2.34	0.52
2:B:134:MET:HE3	2:B:137:LYS:CG	2.19	0.52
1:C:106:PRO:HB3	2:D:114:PHE:CZ	2.44	0.52
1:C:628:MET:SD	1:C:628:MET:C	2.92	0.52
2:D:513:LEU:O	2:D:514:THR:HG22	2.09	0.52
1:A:696:PRO:CG	1:A:726:HIS:HD2	2.23	0.52
1:C:743:ARG:NH1	1:C:764:LYS:HD3	2.24	0.52
2:D:609:LEU:HD23	2:D:635:TRP:CD1	2.45	0.52
2:D:158:LEU:HA	2:D:161:MET:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LEU:HD13	1:A:180:LEU:HD23	1.92	0.52
2:B:513:LEU:N	2:B:513:LEU:CD2	2.72	0.52
1:C:586:LEU:HD22	2:D:822:PHE:CZ	2.45	0.52
2:D:150:ILE:HD11	2:D:182:PHE:HB2	1.90	0.52
1:A:163:ILE:CG2	1:A:239:VAL:HG12	2.19	0.52
1:C:171:HIS:C	1:C:171:HIS:CD2	2.88	0.52
1:C:177:GLN:OE1	1:C:217:GLN:NE2	2.42	0.52
1:C:582:THR:HG21	2:D:815:ILE:CB	2.38	0.52
2:D:513:LEU:N	2:D:513:LEU:CD2	2.72	0.52
1:A:177:GLN:OE1	1:A:217:GLN:NE2	2.42	0.52
2:B:336:ASN:HA	2:B:339:LEU:HB3	1.92	0.52
1:A:640:ILE:HD13	2:D:633:SER:HB2	1.92	0.51
2:B:648:ALA:HA	1:C:673:ALA:CB	2.40	0.51
1:C:259:LEU:HD23	1:C:261:MET:HE3	1.92	0.51
1:A:578:PRO:HB2	1:A:671:ASN:HD22	1.59	0.51
1:A:628:MET:SD	1:A:628:MET:C	2.92	0.51
2:B:644:ALA:CB	1:C:669:THR:HG21	2.35	0.51
1:A:419:LEU:HD11	1:A:493:PHE:CE2	2.43	0.51
1:A:724:TYR:HD1	1:A:727:MET:CE	2.24	0.51
1:A:164:ILE:CG2	1:A:237:ALA:HB3	2.41	0.51
2:B:172:VAL:HG22	2:B:203:LEU:HD12	1.92	0.51
1:C:724:TYR:HD1	1:C:727:MET:CE	2.24	0.51
2:D:172:VAL:HG22	2:D:203:LEU:HD12	1.91	0.51
1:C:582:THR:CG2	2:D:815:ILE:CG1	2.89	0.51
1:C:674:ALA:CB	2:D:655:ILE:HG12	2.41	0.51
1:A:578:PRO:CA	1:A:671:ASN:HD21	2.24	0.51
2:B:609:LEU:HD23	2:B:635:TRP:CD1	2.45	0.51
1:C:569:ARG:HG3	1:C:571:THR:HG23	1.92	0.51
1:C:655:MET:HG3	2:D:610:TRP:CE2	2.46	0.51
2:D:524:ASP:OD1	2:D:525:PHE:N	2.43	0.51
1:A:171:HIS:C	1:A:171:HIS:CD2	2.88	0.50
2:B:609:LEU:HG	2:B:635:TRP:HD1	1.71	0.50
1:C:578:PRO:CA	1:C:671:ASN:HD21	2.24	0.50
1:C:582:THR:HG21	2:D:815:ILE:CG1	2.41	0.50
1:C:696:PRO:CG	1:C:726:HIS:HD2	2.23	0.50
1:A:595:ALA:HB1	1:A:628:MET:HA	1.93	0.50
1:C:576:MET:CB	1:C:584:TRP:NE1	2.72	0.50
1:C:595:ALA:HB1	1:C:628:MET:HA	1.93	0.50
2:D:336:ASN:HA	2:D:339:LEU:HB3	1.92	0.50
1:A:578:PRO:O	1:A:671:ASN:ND2	2.44	0.50
2:D:171:ILE:HD11	2:D:186:ILE:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:ARG:HG3	1:A:571:THR:HG23	1.92	0.50
1:A:849:ILE:HG22	1:A:850:PHE:CD1	2.47	0.50
1:C:165:LEU:HD13	1:C:180:LEU:HD23	1.92	0.50
1:C:849:ILE:HG22	1:C:850:PHE:CD1	2.47	0.50
1:A:103:THR:HB	1:A:104:PRO:HD3	1.93	0.50
1:A:730:HIS:H	1:A:730:HIS:CD2	2.30	0.50
1:C:419:LEU:HD11	1:C:493:PHE:CE2	2.44	0.50
2:D:608:LEU:HD12	2:D:608:LEU:O	2.10	0.50
1:A:586:LEU:CD2	2:B:822:PHE:CE1	2.94	0.50
2:D:743:ASP:OD1	2:D:744:GLU:N	2.45	0.50
1:A:491:MET:HE1	1:A:533:MET:HE1	1.94	0.50
1:A:507:THR:CG2	1:A:707:GLN:CG	2.83	0.50
1:A:576:MET:CB	1:A:584:TRP:NE1	2.72	0.50
2:B:608:LEU:HD12	2:B:608:LEU:O	2.10	0.50
1:C:578:PRO:O	1:C:671:ASN:ND2	2.44	0.50
2:D:538:VAL:C	2:D:749:VAL:CG1	2.74	0.50
1:A:259:LEU:HD23	1:A:261:MET:HE3	1.92	0.50
1:A:784:ARG:HH11	1:A:784:ARG:CG	2.20	0.50
2:B:643:LEU:C	2:B:643:LEU:CD2	2.80	0.50
1:C:662:MET:O	1:C:662:MET:HG2	2.12	0.50
2:B:515:ILE:HD11	2:B:763:GLY:HA3	1.93	0.49
1:C:103:THR:HB	1:C:104:PRO:HD3	1.94	0.49
1:A:807:GLU:OE2	1:A:811:LYS:NZ	2.43	0.49
1:C:491:MET:HE1	1:C:533:MET:HE1	1.94	0.49
2:D:515:ILE:HD11	2:D:763:GLY:HA3	1.93	0.49
1:C:507:THR:HG22	1:C:707:GLN:CG	2.21	0.49
1:A:634:VAL:HG13	1:A:634:VAL:O	2.12	0.49
1:C:655:MET:HG3	2:D:610:TRP:CG	2.44	0.49
1:A:662:MET:O	1:A:662:MET:HG2	2.12	0.49
1:A:841:VAL:O	1:A:845:ILE:HG13	2.13	0.49
2:B:743:ASP:OD1	2:B:744:GLU:N	2.45	0.49
2:D:609:LEU:HG	2:D:635:TRP:HD1	1.71	0.49
1:C:164:ILE:CG2	1:C:237:ALA:HB3	2.41	0.49
1:A:241:ILE:O	1:A:241:ILE:HG22	2.13	0.49
1:C:147:GLN:HE22	1:C:272:GLU:H	1.61	0.49
1:C:578:PRO:O	1:C:578:PRO:HG2	2.12	0.49
1:C:675:PHE:O	1:C:675:PHE:CG	2.65	0.49
2:D:561:MET:O	2:D:562:MET:C	2.54	0.49
2:D:743:ASP:CG	2:D:748:LEU:HD12	2.15	0.49
1:A:636:LEU:CD2	2:D:637:PHE:HD1	2.26	0.49
1:A:674:ALA:HB1	2:B:655:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:ILE:HD11	2:B:186:ILE:HG21	1.93	0.48
2:D:643:LEU:C	2:D:643:LEU:CD2	2.80	0.48
1:A:660:PHE:HD1	2:B:821:VAL:CG1	2.26	0.48
1:A:795:LEU:HD12	1:A:795:LEU:HA	1.57	0.48
1:A:773:LEU:HD23	1:A:773:LEU:H	1.77	0.48
2:B:653:PHE:O	2:B:655:ILE:N	2.46	0.48
2:B:561:MET:O	2:B:562:MET:C	2.54	0.48
1:C:634:VAL:O	1:C:634:VAL:HG13	2.12	0.48
1:C:773:LEU:HD23	1:C:773:LEU:H	1.77	0.48
1:C:730:HIS:H	1:C:730:HIS:CD2	2.30	0.48
1:A:418:ARG:NH1	1:A:494:THR:OG1	2.46	0.48
1:C:841:VAL:O	1:C:845:ILE:HG13	2.13	0.48
1:A:484:LEU:HD12	1:A:484:LEU:O	2.14	0.48
2:B:538:VAL:C	2:B:749:VAL:CG1	2.74	0.48
1:C:791:GLN:HE21	1:C:791:GLN:HA	1.78	0.48
1:A:675:PHE:O	1:A:675:PHE:CG	2.65	0.48
2:B:294:ARG:HA	2:B:297:ILE:HG22	1.96	0.48
2:B:751:ILE:H	2:B:751:ILE:HG12	1.55	0.48
2:D:437:GLN:C	2:D:439:ARG:HG3	2.39	0.48
1:A:147:GLN:HE22	1:A:272:GLU:H	1.61	0.48
1:A:850:PHE:CD1	1:A:850:PHE:N	2.82	0.48
1:C:807:GLU:OE2	1:C:811:LYS:NZ	2.43	0.48
2:D:557:CYS:SG	2:D:558:VAL:N	2.87	0.48
2:D:565:MET:HA	2:D:568:ILE:HG12	1.96	0.47
2:D:653:PHE:O	2:D:655:ILE:N	2.46	0.47
1:A:664:ILE:HA	1:A:664:ILE:HD13	1.54	0.47
1:A:739:ILE:HG21	1:A:760:GLU:HG3	1.96	0.47
2:D:477:ASP:N	2:D:477:ASP:OD1	2.47	0.47
1:A:704:THR:N	1:A:731:ASN:OD1	2.45	0.47
1:A:495:TYR:O	1:A:495:TYR:CD2	2.67	0.47
2:B:557:CYS:SG	2:B:558:VAL:N	2.87	0.47
1:C:163:ILE:CG2	1:C:239:VAL:HG11	2.45	0.47
1:C:726:HIS:ND1	1:C:726:HIS:C	2.72	0.47
1:C:795:LEU:HD12	1:C:795:LEU:HA	1.57	0.47
1:A:125:MET:HB3	1:A:143:PRO:HB3	1.97	0.47
1:A:791:GLN:HE21	1:A:791:GLN:HA	1.78	0.47
2:B:158:LEU:HD23	2:B:161:MET:HE3	1.97	0.47
1:C:664:ILE:HA	1:C:664:ILE:HD13	1.53	0.47
2:B:37:ILE:HD13	2:B:297:ILE:HG13	1.97	0.47
1:C:164:ILE:O	1:C:164:ILE:CG1	2.63	0.47
1:C:418:ARG:NH1	1:C:494:THR:OG1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:LEU:HD12	1:C:484:LEU:O	2.14	0.47
1:A:798:LEU:HA	1:A:798:LEU:HD23	1.49	0.47
2:B:207:MET:HE1	2:B:240:ILE:HD11	1.97	0.47
1:C:479:PHE:HD1	1:C:479:PHE:C	2.22	0.47
1:C:495:TYR:O	1:C:495:TYR:CD2	2.67	0.47
2:D:294:ARG:HA	2:D:297:ILE:HG22	1.96	0.47
2:B:291:ALA:HA	2:B:294:ARG:HG2	1.97	0.47
2:B:437:GLN:C	2:B:439:ARG:HG3	2.39	0.47
1:A:313:VAL:HA	1:A:316:LEU:HD23	1.98	0.46
1:A:757:LEU:N	1:A:757:LEU:HD23	2.30	0.46
2:B:774:ARG:HH21	1:C:785:LYS:HZ3	1.60	0.46
1:C:125:MET:HB3	1:C:143:PRO:HB3	1.97	0.46
2:D:158:LEU:HD23	2:D:161:MET:HE3	1.97	0.46
2:B:634:VAL:HG22	2:B:634:VAL:O	2.15	0.46
1:C:701:ILE:HG12	1:C:730:HIS:HE1	1.80	0.46
1:C:800:SER:O	1:C:806:MET:HG2	2.15	0.46
2:B:422:VAL:CG2	2:B:429:CYS:SG	3.04	0.46
2:B:468:ILE:HA	2:B:468:ILE:HD13	1.35	0.46
1:C:739:ILE:HG21	1:C:760:GLU:HG3	1.97	0.46
1:A:163:ILE:CG2	1:A:239:VAL:HG11	2.45	0.46
1:A:426:GLN:HE21	1:A:756:VAL:HG21	1.81	0.46
1:A:701:ILE:HG12	1:A:730:HIS:HE1	1.80	0.46
1:A:726:HIS:ND1	1:A:726:HIS:C	2.73	0.46
2:B:468:ILE:HD12	2:B:468:ILE:HG23	1.66	0.46
2:B:565:MET:HA	2:B:568:ILE:HG12	1.96	0.46
1:C:313:VAL:HA	1:C:316:LEU:HD23	1.97	0.46
1:C:752:TRP:CG	1:C:753:ASP:H	2.33	0.46
1:C:622:LEU:O	1:C:623:THR:HG23	2.16	0.46
2:D:186:ILE:O	2:D:190:ILE:HB	2.16	0.46
1:A:164:ILE:O	1:A:164:ILE:CG1	2.62	0.46
1:C:757:LEU:N	1:C:757:LEU:HD23	2.30	0.46
1:C:842:ALA:HA	1:C:845:ILE:CD1	2.45	0.46
1:C:241:ILE:O	1:C:241:ILE:HG22	2.13	0.46
2:D:207:MET:HE1	2:D:240:ILE:HD11	1.97	0.46
1:A:452:VAL:HG13	1:A:454:LYS:HG3	1.98	0.46
1:A:845:ILE:HG13	1:A:845:ILE:H	1.51	0.46
2:B:239:TYR:O	2:B:242:GLU:HG3	2.16	0.46
1:C:426:GLN:HE21	1:C:756:VAL:HG21	1.81	0.46
2:D:291:ALA:HA	2:D:294:ARG:HG2	1.97	0.46
1:A:306:VAL:HA	1:A:309:VAL:HG12	1.98	0.46
1:A:672:LEU:HA	1:A:672:LEU:HD23	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:SER:O	2:B:422:VAL:CB	2.62	0.46
2:B:561:MET:HB3	2:B:561:MET:HE2	1.54	0.46
1:C:452:VAL:HG13	1:C:454:LYS:HG3	1.98	0.46
2:D:573:ALA:HB1	2:D:600:PHE:HE2	1.80	0.46
1:A:672:LEU:C	1:A:672:LEU:CD2	2.87	0.45
1:A:791:GLN:NE2	1:A:791:GLN:C	2.71	0.45
2:B:524:ASP:OD1	2:B:525:PHE:N	2.43	0.45
1:C:164:ILE:HG22	1:C:237:ALA:HB3	1.97	0.45
1:C:660:PHE:HD1	2:D:821:VAL:HG12	1.80	0.45
1:C:816:TYR:O	1:C:816:TYR:CD1	2.67	0.45
2:D:37:ILE:HD13	2:D:297:ILE:HG13	1.97	0.45
2:D:290:PRO:HA	2:D:293:VAL:HG12	1.98	0.45
2:D:404:ASP:OD1	2:D:404:ASP:N	2.49	0.45
1:A:164:ILE:HG22	1:A:237:ALA:HB3	1.97	0.45
1:A:583:LEU:HD12	1:A:583:LEU:C	2.34	0.45
1:A:800:SER:O	1:A:806:MET:HG2	2.15	0.45
2:B:477:ASP:OD1	2:B:477:ASP:N	2.47	0.45
2:B:783:LEU:O	2:B:786:ASP:OD1	2.35	0.45
1:A:660:PHE:HD1	2:B:821:VAL:HG12	1.81	0.45
2:B:186:ILE:O	2:B:190:ILE:HB	2.16	0.45
2:B:512:SER:O	2:B:513:LEU:HD22	2.17	0.45
2:D:195:VAL:HG22	2:D:426:SER:HB2	1.97	0.45
2:D:634:VAL:HG22	2:D:634:VAL:O	2.15	0.45
1:A:842:ALA:HA	1:A:845:ILE:CD1	2.45	0.45
2:B:573:ALA:HB1	2:B:600:PHE:HE2	1.80	0.45
1:C:583:LEU:HD13	1:C:583:LEU:HA	1.76	0.45
2:D:422:VAL:CG2	2:D:429:CYS:SG	3.04	0.45
2:D:783:LEU:O	2:D:786:ASP:OD1	2.35	0.45
1:A:580:GLN:O	1:A:582:THR:N	2.49	0.45
1:A:752:TRP:CG	1:A:753:ASP:H	2.34	0.45
2:B:637:PHE:O	2:B:637:PHE:CG	2.69	0.45
1:C:670:ALA:HB1	2:D:651:ALA:CA	2.44	0.45
2:D:146:PHE:HA	2:D:357:GLN:HE21	1.81	0.45
1:A:488:ALA:HA	1:A:493:PHE:CD1	2.52	0.45
2:B:127:HIS:HE1	2:B:287:TYR:HB3	1.81	0.45
2:B:351:PHE:HE1	2:B:357:GLN:HG2	1.82	0.45
2:B:404:ASP:OD1	2:B:404:ASP:N	2.49	0.45
1:C:147:GLN:HE22	1:C:272:GLU:N	2.15	0.45
1:C:511:VAL:HG21	1:C:514:SER:HB2	1.98	0.45
1:A:511:VAL:HG21	1:A:514:SER:HB2	1.98	0.45
1:A:649:SER:OG	2:B:832:SER:OG	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:436:CYS:HB3	2:B:478:LEU:HD22	1.99	0.45
1:C:580:GLN:O	1:C:582:THR:N	2.49	0.45
2:D:239:TYR:O	2:D:242:GLU:HG3	2.16	0.45
1:A:101:HIS:O	1:A:128:TYR:OH	2.34	0.45
1:C:369:PHE:HD1	1:C:390:GLY:HA2	1.82	0.45
1:C:579:PHE:HD1	1:C:579:PHE:HA	1.60	0.45
1:C:592:HIS:O	1:C:595:ALA:N	2.50	0.45
2:D:641:ILE:O	2:D:641:ILE:HG22	2.16	0.45
1:A:586:LEU:HD22	2:B:822:PHE:CZ	2.52	0.45
2:B:290:PRO:HA	2:B:293:VAL:HG12	1.99	0.45
2:D:637:PHE:O	2:D:637:PHE:CD2	2.70	0.45
1:A:147:GLN:HE22	1:A:272:GLU:N	2.15	0.45
2:B:99:PHE:N	2:B:124:LEU:O	2.50	0.45
2:B:146:PHE:HA	2:B:357:GLN:HE21	1.81	0.45
2:B:195:VAL:HG22	2:B:426:SER:HB2	1.97	0.45
2:B:637:PHE:O	2:B:637:PHE:CD2	2.70	0.45
1:C:165:LEU:H	1:C:165:LEU:HD23	1.82	0.45
1:C:306:VAL:HA	1:C:309:VAL:HG12	1.98	0.45
2:D:351:PHE:HE1	2:D:357:GLN:HG2	1.82	0.45
2:D:637:PHE:O	2:D:637:PHE:CG	2.69	0.45
2:B:458:LYS:HA	2:B:462:ILE:HG21	1.99	0.44
2:B:572:VAL:HG21	1:C:845:ILE:HG21	1.99	0.44
1:C:459:GLY:HA3	1:C:499:LEU:H	1.82	0.44
2:D:421:SER:O	2:D:422:VAL:CB	2.62	0.44
1:A:578:PRO:O	1:A:578:PRO:HG2	2.12	0.44
1:A:629:TRP:HH2	2:D:630:ILE:HD13	1.83	0.44
2:D:99:PHE:N	2:D:124:LEU:O	2.50	0.44
2:D:561:MET:HB3	2:D:561:MET:HE2	1.54	0.44
1:A:730:HIS:O	1:A:730:HIS:CD2	2.70	0.44
1:C:101:HIS:O	1:C:128:TYR:OH	2.34	0.44
1:C:488:ALA:HA	1:C:493:PHE:CD1	2.51	0.44
1:C:634:VAL:CG1	1:C:634:VAL:O	2.63	0.44
2:D:458:LYS:HA	2:D:462:ILE:HG21	2.00	0.44
2:D:512:SER:C	2:D:513:LEU:HD22	2.43	0.44
1:A:369:PHE:HD1	1:A:390:GLY:HA2	1.82	0.44
1:C:672:LEU:C	1:C:672:LEU:CD2	2.87	0.44
1:A:426:GLN:NE2	1:A:752:TRP:HE1	2.16	0.44
1:A:583:LEU:HD12	1:A:587:VAL:HG23	1.98	0.44
1:A:634:VAL:HG12	1:A:657:TRP:CD1	2.52	0.44
1:A:668:TYR:CD1	1:A:668:TYR:O	2.70	0.44
1:C:481:ILE:N	1:C:481:ILE:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:VAL:HG12	1:C:657:TRP:CD1	2.52	0.44
1:C:704:THR:N	1:C:731:ASN:OD1	2.45	0.44
1:C:730:HIS:O	1:C:730:HIS:CD2	2.70	0.44
2:B:638:PHE:HB2	1:C:837:VAL:HG22	1.99	0.44
2:D:512:SER:O	2:D:513:LEU:HD22	2.17	0.44
1:A:165:LEU:H	1:A:165:LEU:HD23	1.82	0.44
1:A:495:TYR:O	1:A:495:TYR:CG	2.69	0.44
1:A:669:THR:HG21	2:D:644:ALA:CB	2.41	0.44
1:A:721:SER:HA	1:A:724:TYR:HB3	2.00	0.44
1:C:672:LEU:HA	1:C:672:LEU:HD23	1.74	0.44
2:D:127:HIS:HE1	2:D:287:TYR:HB3	1.81	0.44
2:D:436:CYS:HB3	2:D:478:LEU:HD22	1.99	0.44
2:D:612:LEU:HA	2:D:612:LEU:HD12	1.46	0.44
1:A:552:LYS:CG	1:A:794:SER:OG	2.64	0.44
1:A:592:HIS:O	1:A:595:ALA:N	2.50	0.44
2:B:512:SER:C	2:B:513:LEU:HD22	2.43	0.44
1:C:495:TYR:O	1:C:495:TYR:CG	2.69	0.44
1:C:583:LEU:HD12	1:C:587:VAL:HG23	1.98	0.44
1:C:850:PHE:CD1	1:C:850:PHE:N	2.82	0.44
1:C:672:LEU:O	1:C:672:LEU:HD22	2.18	0.44
1:C:730:HIS:CD2	1:C:730:HIS:N	2.86	0.44
1:C:333:THR:HG21	2:D:76:THR:H	1.83	0.43
1:C:721:SER:HA	1:C:724:TYR:HB3	2.00	0.43
1:C:446:THR:HG23	1:C:448:ASN:H	1.83	0.43
2:D:630:ILE:HD13	2:D:630:ILE:HA	1.72	0.43
1:C:798:LEU:HD23	1:C:798:LEU:HA	1.49	0.43
2:D:513:LEU:C	2:D:514:THR:CG2	2.91	0.43
1:A:165:LEU:HD21	1:A:215:VAL:HG22	2.01	0.43
1:A:459:GLY:HA3	1:A:499:LEU:H	1.82	0.43
1:A:816:TYR:O	1:A:816:TYR:CD1	2.67	0.43
1:C:520:ASN:OD1	1:C:521:GLY:N	2.52	0.43
2:D:536:VAL:O	2:D:750:THR:HA	2.19	0.43
1:A:672:LEU:O	1:A:672:LEU:HD22	2.18	0.43
1:A:730:HIS:CD2	1:A:730:HIS:N	2.86	0.43
1:A:487:LEU:HD23	1:A:487:LEU:HA	1.75	0.43
2:B:127:HIS:CE1	2:B:287:TYR:HB3	2.54	0.43
1:C:165:LEU:HD21	1:C:215:VAL:HG22	2.01	0.43
1:C:240:ILE:HD11	1:C:268:TRP:CZ3	2.53	0.43
1:C:668:TYR:CD1	1:C:668:TYR:O	2.71	0.43
1:A:108:SER:HA	1:A:118:VAL:HG21	2.00	0.43
1:A:240:ILE:HD11	1:A:268:TRP:CZ3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:LEU:HD21	2:B:822:PHE:CE1	2.54	0.43
2:B:513:LEU:C	2:B:514:THR:CG2	2.91	0.43
1:C:108:SER:HA	1:C:118:VAL:HG21	1.99	0.43
1:A:446:THR:HG23	1:A:448:ASN:H	1.83	0.43
1:A:673:ALA:HB2	2:D:648:ALA:HA	1.99	0.43
1:C:457:CYS:SG	1:C:497:VAL:HG22	2.59	0.43
1:C:759:PHE:C	1:C:759:PHE:HD1	2.26	0.43
2:B:789:MET:HE3	2:B:789:MET:HB2	1.96	0.43
2:D:278:ILE:CD1	2:D:391:TRP:CZ3	2.90	0.43
2:D:678:SER:O	2:D:679:PRO:C	2.62	0.43
1:A:520:ASN:OD1	1:A:521:GLY:N	2.52	0.42
1:C:426:GLN:NE2	1:C:752:TRP:HE1	2.16	0.42
1:A:457:CYS:SG	1:A:497:VAL:HG22	2.59	0.42
1:A:526:LEU:HD23	1:A:548:ILE:HD12	2.01	0.42
2:B:421:SER:O	2:B:422:VAL:HB	2.19	0.42
2:B:536:VAL:O	2:B:750:THR:HA	2.19	0.42
1:C:419:LEU:HB2	1:C:532:ASP:HB2	2.02	0.42
1:C:526:LEU:HD23	1:C:548:ILE:HD12	2.01	0.42
1:C:672:LEU:CD2	1:C:672:LEU:O	2.67	0.42
1:A:622:LEU:O	1:A:623:THR:HG23	2.16	0.42
1:A:662:MET:O	1:A:662:MET:CG	2.67	0.42
1:C:479:PHE:O	1:C:479:PHE:CD1	2.68	0.42
2:D:127:HIS:CE1	2:D:287:TYR:HB3	2.54	0.42
1:A:636:LEU:HD23	1:A:636:LEU:HA	1.85	0.42
1:A:672:LEU:CD2	1:A:672:LEU:O	2.67	0.42
1:C:552:LYS:CG	1:C:794:SER:OG	2.64	0.42
1:C:703:ALA:HB1	1:C:730:HIS:O	2.14	0.42
1:A:419:LEU:HB2	1:A:532:ASP:HB2	2.02	0.42
2:B:571:ALA:O	2:B:574:VAL:HG12	2.20	0.42
2:D:468:ILE:HD12	2:D:468:ILE:HG23	1.66	0.42
1:A:457:CYS:SG	1:A:497:VAL:CG2	3.08	0.42
2:B:278:ILE:CD1	2:B:391:TRP:CZ3	2.90	0.42
1:C:662:MET:O	1:C:662:MET:CG	2.67	0.42
2:D:115:ILE:O	2:D:119:THR:HG22	2.20	0.42
1:A:481:ILE:N	1:A:481:ILE:CD1	2.81	0.42
1:A:785:LYS:HZ3	2:D:774:ARG:HH21	1.64	0.42
2:B:115:ILE:O	2:B:119:THR:HG22	2.20	0.42
2:B:612:LEU:HD12	2:B:612:LEU:HA	1.46	0.42
2:D:571:ALA:O	2:D:574:VAL:HG12	2.20	0.42
1:A:79:CYS:HA	1:A:83:ILE:HD11	2.02	0.42
1:A:718:VAL:O	1:A:721:SER:OG	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:133:ILE:O	2:D:133:ILE:CG2	2.68	0.42
2:D:360:PRO:HG2	2:D:362:LEU:HG	2.01	0.42
1:A:586:LEU:O	1:A:586:LEU:CG	2.68	0.41
1:A:634:VAL:CG1	1:A:634:VAL:O	2.63	0.41
2:B:512:SER:C	2:B:513:LEU:CD2	2.92	0.41
2:B:678:SER:O	2:B:679:PRO:C	2.62	0.41
2:B:678:SER:HB2	2:B:679:PRO:HD2	2.02	0.41
2:B:641:ILE:O	2:B:641:ILE:HG22	2.16	0.41
2:B:38:ALA:HB2	2:B:94:ILE:HD13	2.02	0.41
2:B:364:ILE:HD11	2:B:384:LEU:HD11	2.02	0.41
1:A:759:PHE:C	1:A:759:PHE:HD1	2.26	0.41
2:D:512:SER:C	2:D:513:LEU:CD2	2.92	0.41
1:C:660:PHE:HD1	2:D:821:VAL:HG11	1.84	0.41
1:C:664:ILE:HD12	1:C:664:ILE:HG23	1.71	0.41
1:C:718:VAL:O	1:C:721:SER:OG	2.37	0.41
2:B:433:THR:OG1	2:B:434:VAL:N	2.54	0.41
1:C:655:MET:CG	2:D:610:TRP:CE2	3.04	0.41
1:A:288:ILE:HG12	1:A:376:ASN:HD22	1.86	0.41
1:A:588:GLY:O	1:A:589:LEU:C	2.61	0.41
1:A:853:PHE:HD1	1:A:853:PHE:HA	1.76	0.41
2:B:649:ASN:HA	1:C:676:LEU:HD23	2.02	0.41
1:C:241:ILE:HG21	1:C:241:ILE:HD13	1.79	0.41
1:C:586:LEU:O	1:C:586:LEU:CG	2.68	0.41
2:D:364:ILE:HD11	2:D:384:LEU:HD11	2.02	0.41
2:D:601:THR:OG1	2:D:602:ILE:N	2.54	0.41
1:C:845:ILE:HG13	1:C:845:ILE:H	1.51	0.41
2:D:678:SER:HB2	2:D:679:PRO:HD2	2.03	0.41
1:A:213:GLU:OE1	1:A:213:GLU:CA	2.68	0.41
1:A:481:ILE:N	1:A:481:ILE:HD12	2.32	0.41
1:A:546:GLN:O	1:A:785:LYS:NZ	2.52	0.41
1:A:696:PRO:CG	1:A:726:HIS:CD2	3.02	0.41
1:A:704:THR:C	1:A:731:ASN:OD1	2.63	0.41
2:B:97:VAL:HB	2:B:123:ILE:HG22	2.02	0.41
2:B:360:PRO:HG2	2:B:362:LEU:HG	2.01	0.41
2:B:694:ASN:O	2:B:695:ILE:C	2.64	0.41
1:C:481:ILE:O	1:C:481:ILE:CG2	2.67	0.41
1:C:558:GLY:HA3	1:C:773:LEU:HB2	2.03	0.41
2:D:421:SER:O	2:D:422:VAL:HB	2.19	0.41
1:A:558:GLY:HA3	1:A:773:LEU:HB2	2.03	0.41
1:A:586:LEU:O	1:A:586:LEU:HG	2.20	0.41
1:A:716:ARG:HH22	2:D:782:GLN:NE2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:418:ILE:HG12	2:B:418:ILE:H	1.73	0.41
2:B:601:THR:OG1	2:B:602:ILE:N	2.54	0.41
1:C:480:CYS:SG	1:C:481:ILE:N	2.90	0.41
2:D:433:THR:OG1	2:D:434:VAL:N	2.54	0.41
2:D:552:GLU:CB	2:D:653:PHE:CE2	2.93	0.41
1:A:702:TYR:OH	1:A:723:MET:SD	2.62	0.40
1:A:719:GLU:O	1:A:722:THR:OG1	2.26	0.40
1:C:288:ILE:HG12	1:C:376:ASN:HD22	1.86	0.40
1:C:487:LEU:HD23	1:C:487:LEU:HA	1.75	0.40
2:D:613:VAL:O	2:D:613:VAL:HG12	2.22	0.40
1:A:78:VAL:O	1:A:83:ILE:HG12	2.22	0.40
1:A:125:MET:HE1	1:A:137:PHE:CD2	2.56	0.40
1:A:718:VAL:HG23	1:A:719:GLU:H	1.86	0.40
2:B:219:GLN:O	2:B:223:LEU:HG	2.21	0.40
2:B:535:SER:OG	2:B:756:VAL:HG12	2.21	0.40
1:C:457:CYS:SG	1:C:497:VAL:CG2	3.08	0.40
1:C:490:THR:O	1:C:490:THR:HG23	2.21	0.40
1:C:704:THR:C	1:C:731:ASN:OD1	2.63	0.40
1:C:717:GLN:CB	1:C:720:LEU:HB2	2.51	0.40
1:A:632:TRP:CE3	1:A:632:TRP:CA	2.87	0.40
2:B:133:ILE:O	2:B:133:ILE:CG2	2.68	0.40
1:C:714:PHE:HD2	1:C:727:MET:HE1	1.87	0.40
1:C:797:ILE:O	1:C:797:ILE:HG22	2.20	0.40
2:D:469:SER:C	2:D:472:VAL:O	2.58	0.40
2:D:624:LYS:HA	2:D:629:LYS:HE3	2.04	0.40
1:A:490:THR:O	1:A:490:THR:HG23	2.21	0.40
1:A:623:THR:CG2	1:A:626:SER:HB3	2.51	0.40
1:A:717:GLN:CB	1:A:720:LEU:HB2	2.51	0.40
2:B:351:PHE:CE1	2:B:357:GLN:HG2	2.57	0.40
2:B:608:LEU:C	2:B:608:LEU:CD1	2.86	0.40
2:B:663:VAL:O	2:B:751:ILE:HD12	2.22	0.40
1:C:79:CYS:HA	1:C:83:ILE:HD11	2.02	0.40
1:C:635:LEU:O	1:C:635:LEU:CG	2.69	0.40
2:D:97:VAL:HB	2:D:123:ILE:HG22	2.02	0.40
1:C:586:LEU:O	1:C:586:LEU:HG	2.20	0.40
1:C:718:VAL:HG23	1:C:719:GLU:H	1.86	0.40
1:C:732:TYR:HE1	1:C:747:LEU:HD13	1.87	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	794/959 (83%)	743 (94%)	48 (6%)	3 (0%)	30	60
1	C	794/959 (83%)	743 (94%)	48 (6%)	3 (0%)	30	60
2	B	782/883 (89%)	711 (91%)	68 (9%)	3 (0%)	30	60
2	D	782/883 (89%)	711 (91%)	68 (9%)	3 (0%)	30	60
All	All	3152/3684 (86%)	2908 (92%)	232 (7%)	12 (0%)	31	60

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	392	PRO
2	B	624	LYS
2	D	392	PRO
2	D	624	LYS
1	A	578	PRO
1	A	580	GLN
2	B	616	ASN
1	C	578	PRO
1	C	580	GLN
2	D	616	ASN
1	A	623	THR
1	C	623	THR

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	539/826 (65%)	474 (88%)	65 (12%)	5	22
1	C	539/826 (65%)	474 (88%)	65 (12%)	5	22
2	B	552/762 (72%)	519 (94%)	33 (6%)	17	44
2	D	552/762 (72%)	519 (94%)	33 (6%)	17	44
All	All	2182/3176 (69%)	1986 (91%)	196 (9%)	11	33

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	79	CYS
1	A	163	ILE
1	A	164	ILE
1	A	166	LEU
1	A	213	GLU
1	A	224	ASN
1	A	240	ILE
1	A	242	LEU
1	A	262	THR
1	A	270	VAL
1	A	288	ILE
1	A	316	LEU
1	A	317	LEU
1	A	335	ILE
1	A	471	THR
1	A	472	VAL
1	A	479	PHE
1	A	483	LEU
1	A	485	ILE
1	A	490	THR
1	A	494	THR
1	A	497	VAL
1	A	549	GLU
1	A	554	PHE
1	A	555	LYS
1	A	578	PRO
1	A	579	PHE
1	A	581	SER
1	A	582	THR
1	A	583	LEU
1	A	629	TRP
1	A	630	PHE

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Mol	Chain	Res	Type
1	A	632	TRP
1	A	634	VAL
1	A	635	LEU
1	A	660	PHE
1	A	663	ILE
1	A	669	THR
1	A	671	ASN
1	A	672	LEU
1	A	675	PHE
1	A	686	THR
1	A	705	VAL
1	A	718	VAL
1	A	726	HIS
1	A	727	MET
1	A	729	LYS
1	A	730	HIS
1	A	743	ARG
1	A	759	PHE
1	A	770	THR
1	A	784	ARG
1	A	787	SER
1	A	795	LEU
1	A	797	ILE
1	A	800	SER
1	A	801	HIS
1	A	816	TYR
1	A	830	THR
1	A	840	LEU
1	A	845	ILE
1	A	846	VAL
1	A	849	ILE
1	A	852	ILE
2	B	44	THR
2	B	64	VAL
2	B	113	ASP
2	B	124	LEU
2	B	130	SER
2	B	189	THR
2	B	202	VAL
2	B	266	THR
2	B	278	ILE
2	B	392	PRO

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Mol	Chain	Res	Type
2	B	410	THR
2	B	418	ILE
2	B	419	VAL
2	B	422	VAL
2	B	439	ARG
2	B	440	ILE
2	B	453	ILE
2	B	468	ILE
2	B	482	THR
2	B	551	LEU
2	B	554	PHE
2	B	561	MET
2	B	612	LEU
2	B	618	VAL
2	B	627	THR
2	B	628	SER
2	B	630	ILE
2	B	634	VAL
2	B	731	TYR
2	B	749	VAL
2	B	751	ILE
2	B	784	PHE
2	B	795	LEU
1	C	32	VAL
1	C	79	CYS
1	C	163	ILE
1	C	164	ILE
1	C	166	LEU
1	C	213	GLU
1	C	224	ASN
1	C	240	ILE
1	C	242	LEU
1	C	262	THR
1	C	270	VAL
1	C	288	ILE
1	C	316	LEU
1	C	317	LEU
1	C	335	ILE
1	C	471	THR
1	C	472	VAL
1	C	479	PHE
1	C	483	LEU

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Mol	Chain	Res	Type
1	C	485	ILE
1	C	490	THR
1	C	494	THR
1	C	497	VAL
1	C	549	GLU
1	C	554	PHE
1	C	555	LYS
1	C	578	PRO
1	C	579	PHE
1	C	581	SER
1	C	582	THR
1	C	583	LEU
1	C	629	TRP
1	C	630	PHE
1	C	632	TRP
1	C	634	VAL
1	C	635	LEU
1	C	660	PHE
1	C	663	ILE
1	C	669	THR
1	C	671	ASN
1	C	672	LEU
1	C	675	PHE
1	C	686	THR
1	C	705	VAL
1	C	718	VAL
1	C	726	HIS
1	C	727	MET
1	C	729	LYS
1	C	730	HIS
1	C	743	ARG
1	C	759	PHE
1	C	770	THR
1	C	784	ARG
1	C	787	SER
1	C	795	LEU
1	C	797	ILE
1	C	800	SER
1	C	801	HIS
1	C	816	TYR
1	C	830	THR
1	C	840	LEU

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Mol	Chain	Res	Type
1	C	845	ILE
1	C	846	VAL
1	C	849	ILE
1	C	852	ILE
2	D	44	THR
2	D	64	VAL
2	D	113	ASP
2	D	124	LEU
2	D	130	SER
2	D	189	THR
2	D	202	VAL
2	D	266	THR
2	D	278	ILE
2	D	392	PRO
2	D	410	THR
2	D	418	ILE
2	D	419	VAL
2	D	422	VAL
2	D	439	ARG
2	D	440	ILE
2	D	453	ILE
2	D	468	ILE
2	D	482	THR
2	D	551	LEU
2	D	554	PHE
2	D	561	MET
2	D	612	LEU
2	D	618	VAL
2	D	627	THR
2	D	628	SER
2	D	630	ILE
2	D	634	VAL
2	D	731	TYR
2	D	749	VAL
2	D	751	ILE
2	D	784	PHE
2	D	795	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN

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Mol	Chain	Res	Type
1	A	161	ASN
1	A	171	HIS
1	A	177	GLN
1	A	217	GLN
1	A	376	ASN
1	A	414	GLN
1	A	470	HIS
1	A	474	GLN
1	A	492	GLN
1	A	637	ASN
1	A	671	ASN
1	A	695	ASN
1	A	730	HIS
1	A	791	GLN
1	A	792	GLN
1	A	801	HIS
2	B	357	GLN
2	B	615	ASN
2	B	675	ASN
1	C	147	GLN
1	C	161	ASN
1	C	171	HIS
1	C	177	GLN
1	C	217	GLN
1	C	376	ASN
1	C	414	GLN
1	C	470	HIS
1	C	474	GLN
1	C	492	GLN
1	C	637	ASN
1	C	671	ASN
1	C	695	ASN
1	C	730	HIS
1	C	791	GLN
1	C	801	HIS
2	D	357	GLN
2	D	615	ASN
2	D	675	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

4 monosaccharides 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	$\# Z > 2$
3	NAG	E	1	3,1	14,14,15	0.30	0	17,19,21	0.57	0
3	NAG	E	2	3	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	F	1	3,1	14,14,15	0.29	0	17,19,21	0.57	0
3	NAG	F	2	3	14,14,15	0.20	0	17,19,21	0.43	0

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
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6

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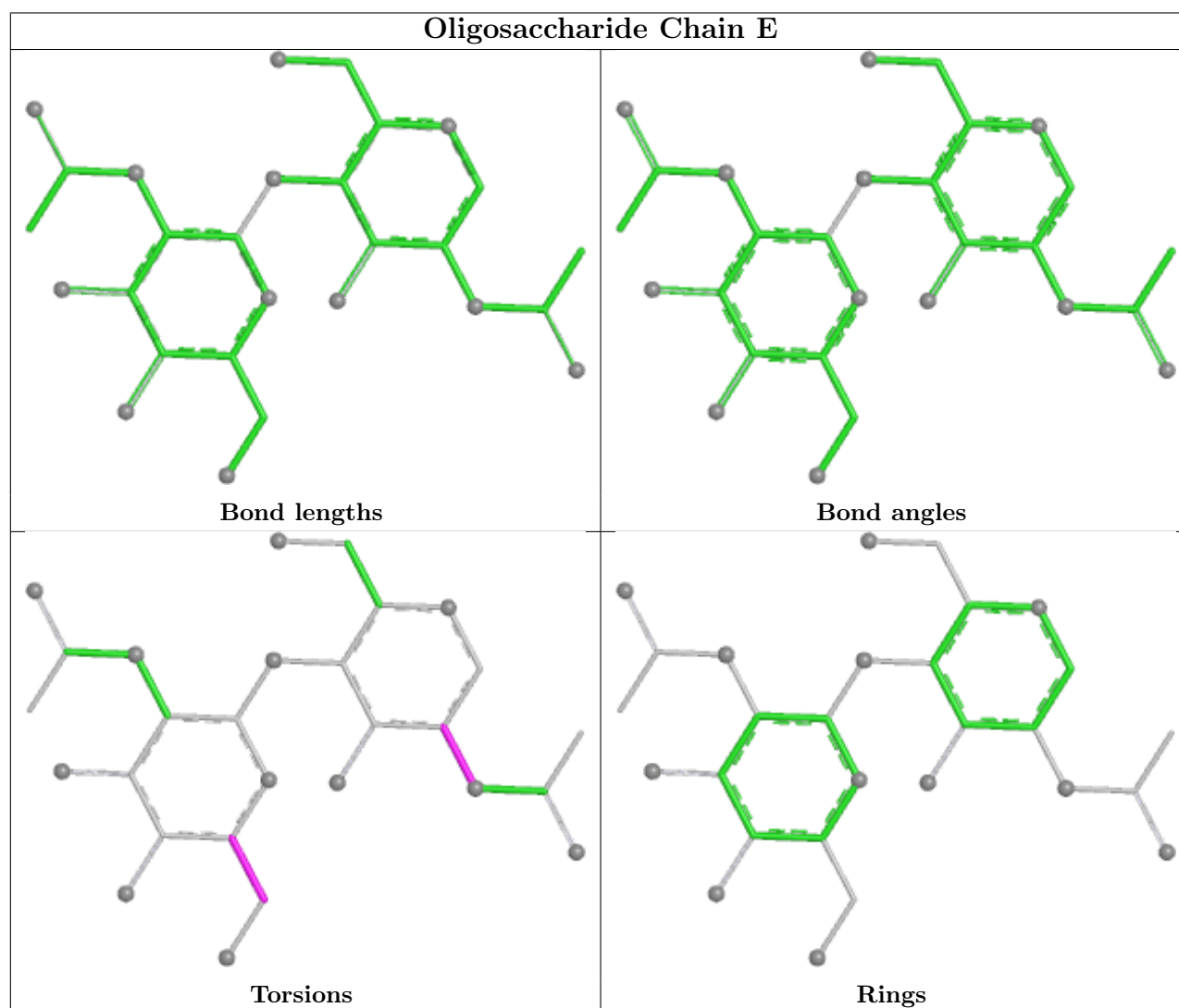
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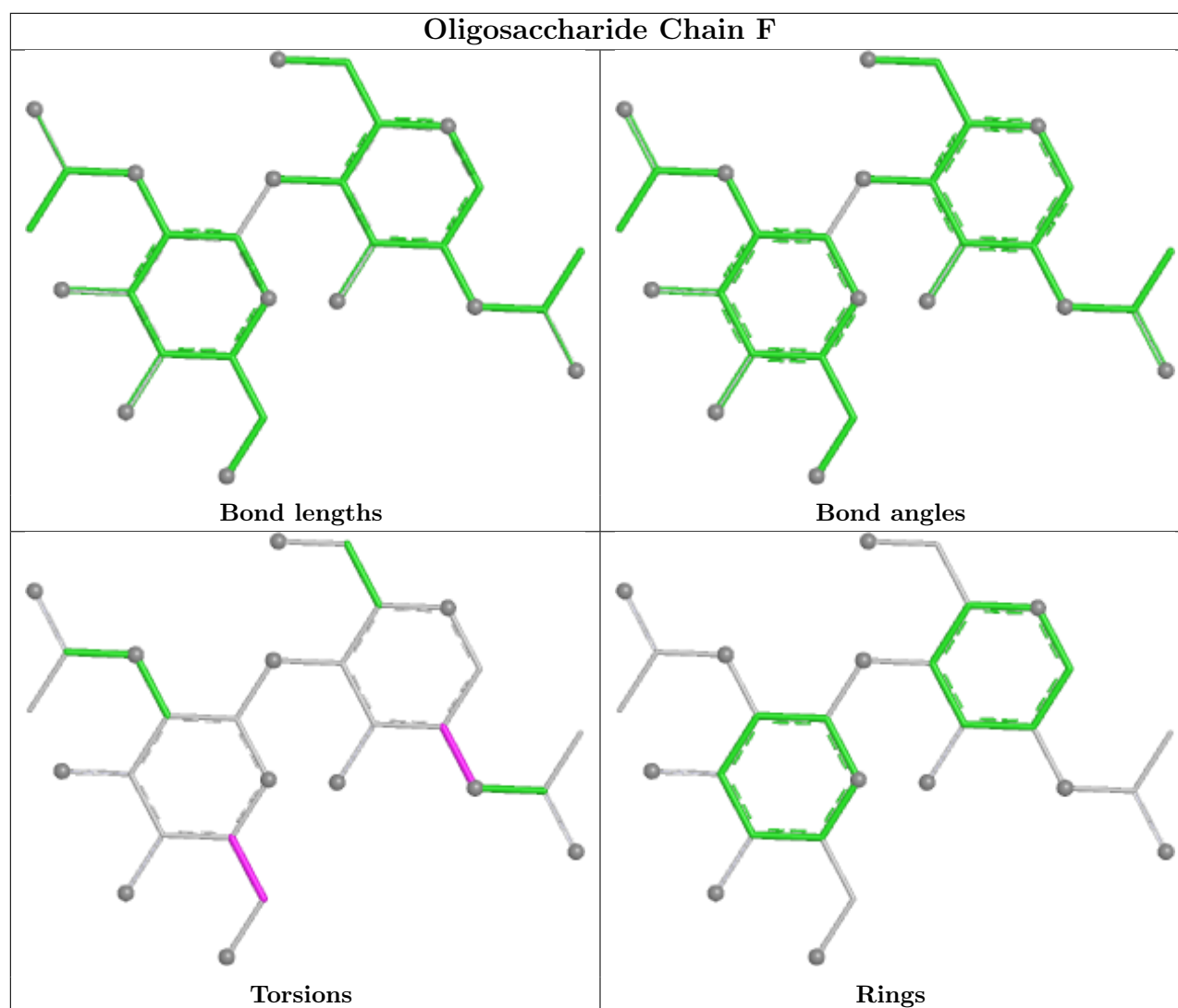
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C1-C2-N2-C7
3	F	1	NAG	C1-C2-N2-C7
3	E	1	NAG	C3-C2-N2-C7
3	F	1	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
5	NAG	D	901	2	14,14,15	0.25	0	17,19,21	0.45	0
5	NAG	B	901	2	14,14,15	0.25	0	17,19,21	0.45	0
4	GLY	A	1001	-	4,4,4	1.16	1 (25%)	3,4,4	1.65	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GLY	C	1001	-	4,4,4	1.16	1 (25%)	3,4,4	1.64	1 (33%)

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
5	NAG	D	901	2	-	1/6/23/26	0/1/1/1
5	NAG	B	901	2	-	1/6/23/26	0/1/1/1
4	GLY	A	1001	-	-	0/2/2/2	-
4	GLY	C	1001	-	-	0/2/2/2	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	GLY	OXT-C	-2.20	1.23	1.30
4	C	1001	GLY	OXT-C	-2.19	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	GLY	OXT-C-O	-2.09	117.95	123.33
4	C	1001	GLY	OXT-C-O	-2.08	117.97	123.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

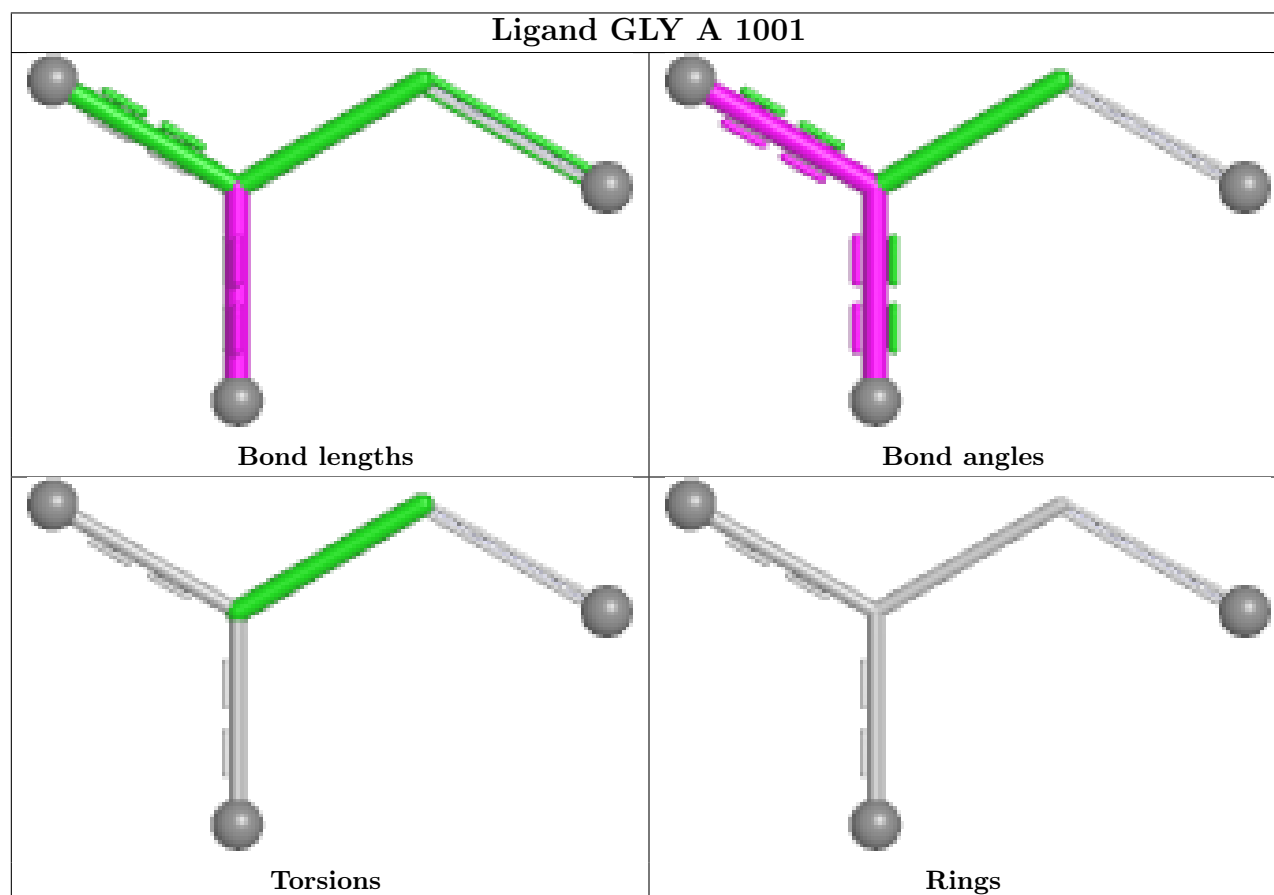
Mol	Chain	Res	Type	Atoms
5	B	901	NAG	O5-C5-C6-O6
5	D	901	NAG	O5-C5-C6-O6

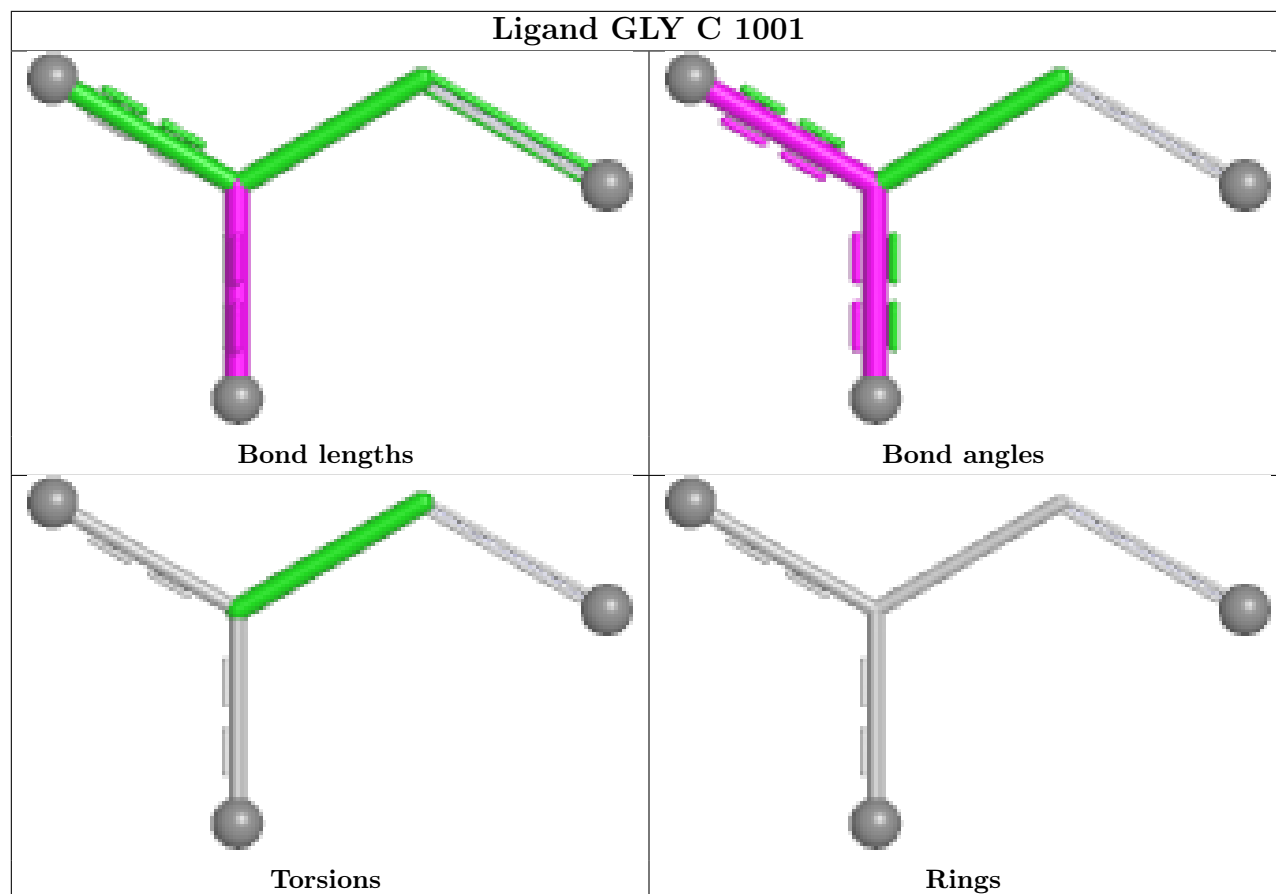
There are no ring outliers.

No monomer is involved in short contacts.

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.

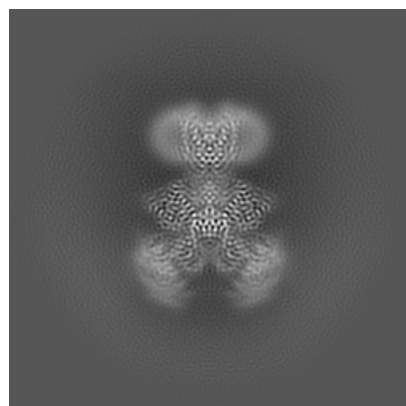
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43782. These allow visual inspection of the internal detail of the map and identification of artifacts.

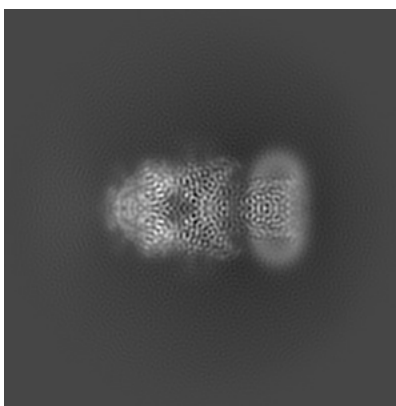
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

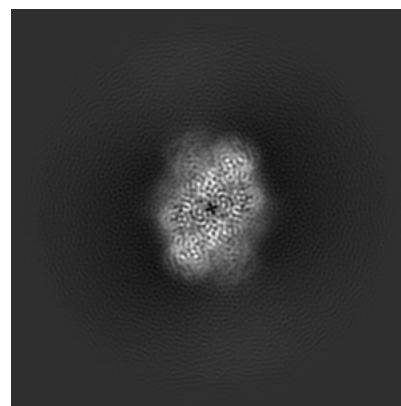
6.1.1 Primary map



X

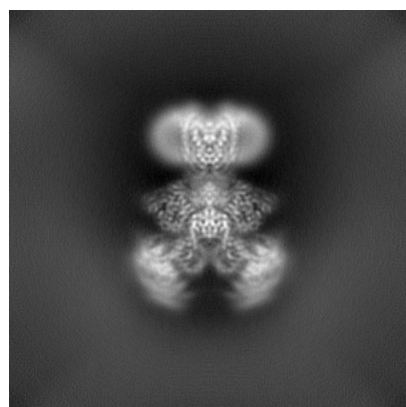


Y

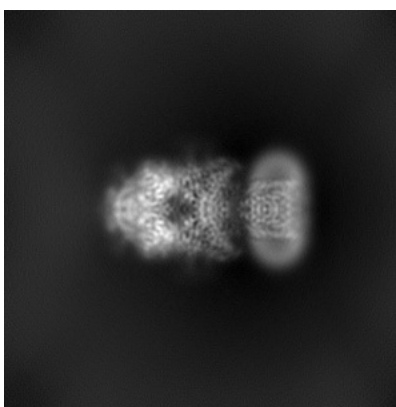


Z

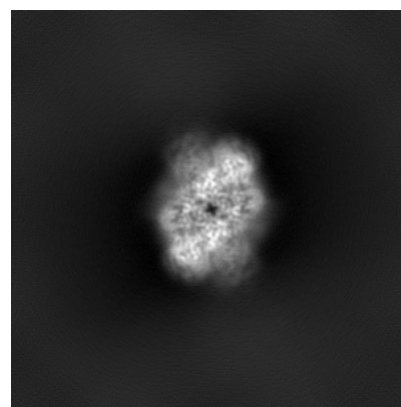
6.1.2 Raw map



X



Y

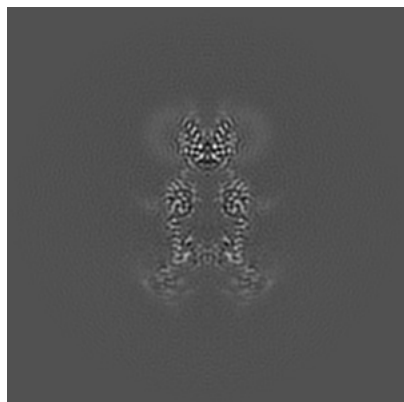


Z

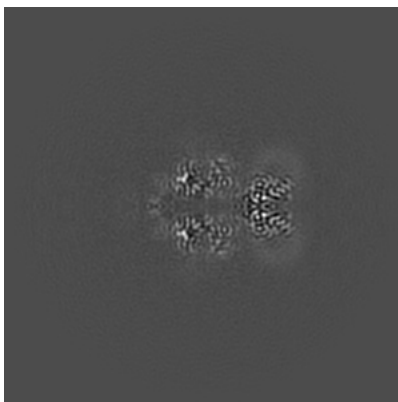
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

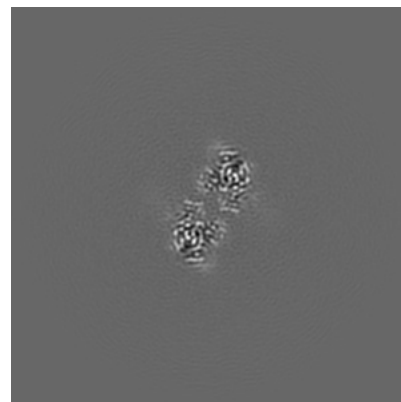
6.2.1 Primary map



X Index: 160

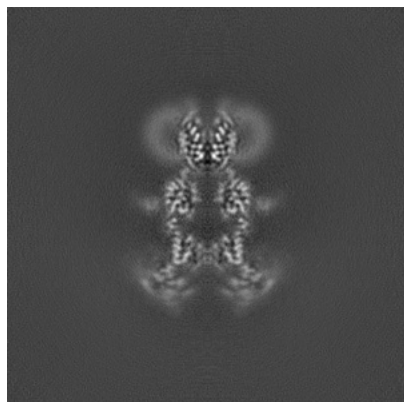


Y Index: 160

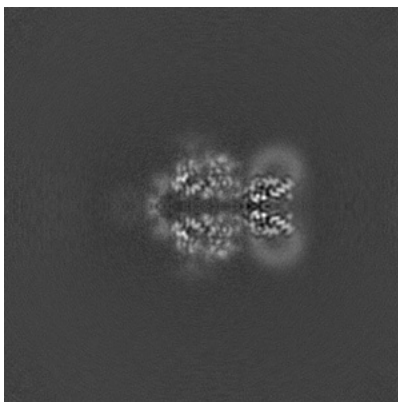


Z Index: 160

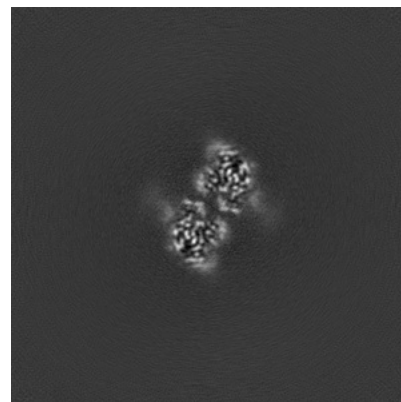
6.2.2 Raw map



X Index: 160



Y Index: 160

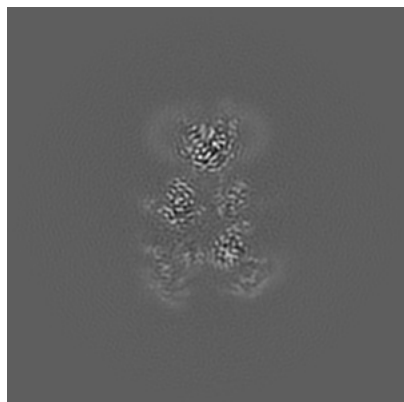


Z Index: 160

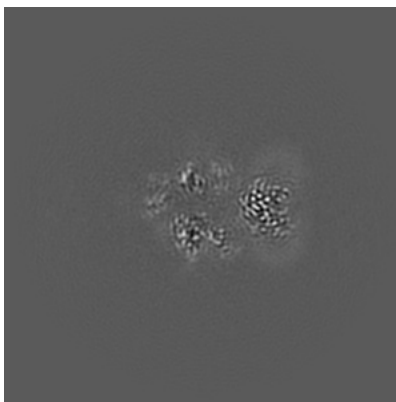
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

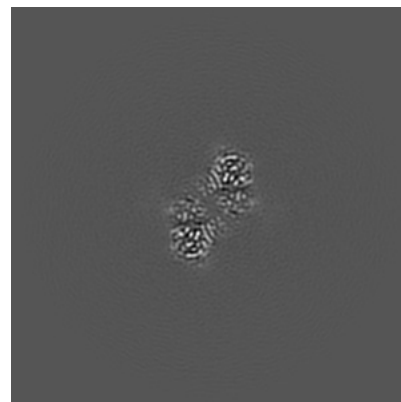
6.3.1 Primary map



X Index: 155

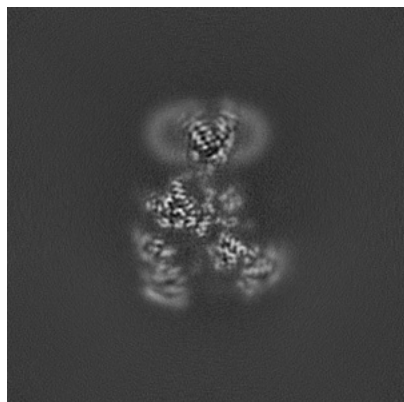


Y Index: 155

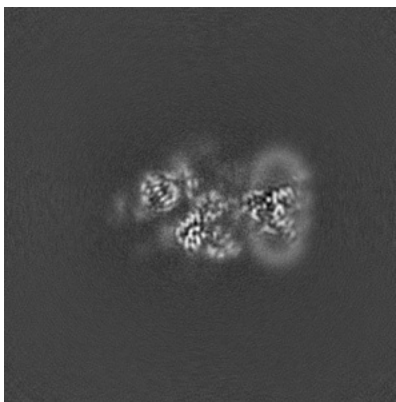


Z Index: 157

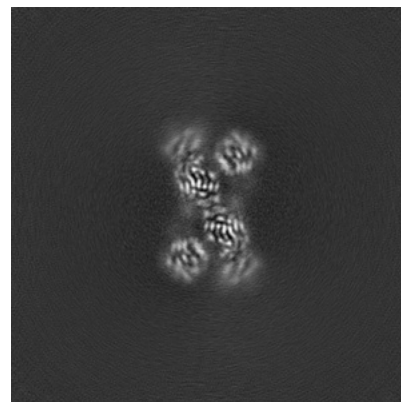
6.3.2 Raw map



X Index: 149



Y Index: 148

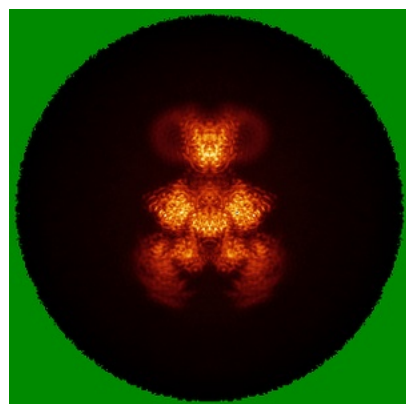


Z Index: 122

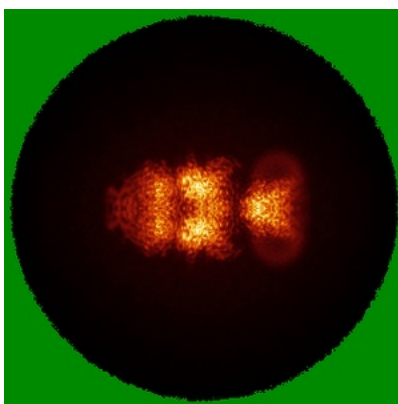
The images above show the largest variance slices of the map in three orthogonal directions.

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

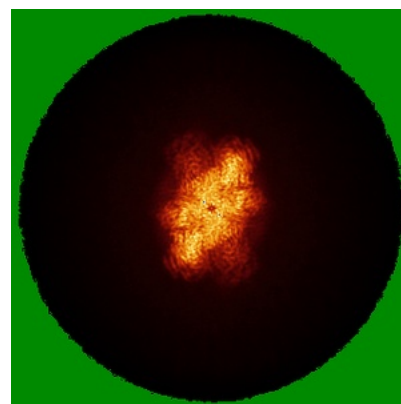
6.4.1 Primary map



X

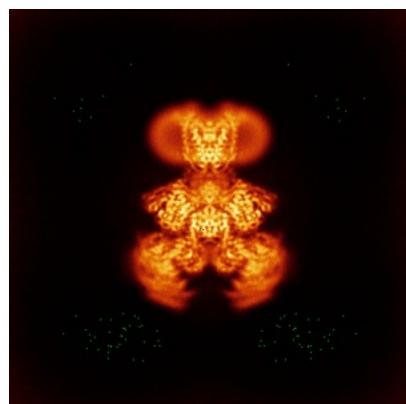


Y

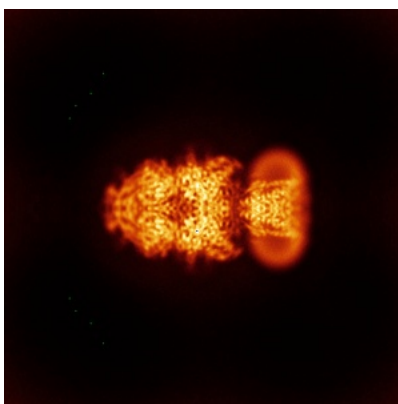


Z

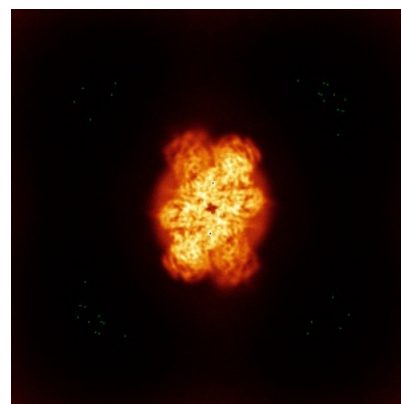
6.4.2 Raw map



X



Y

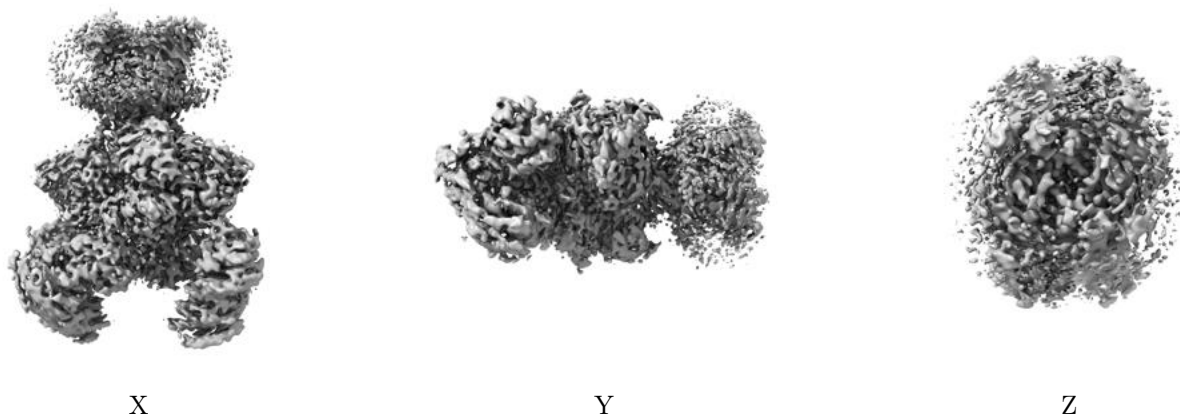


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

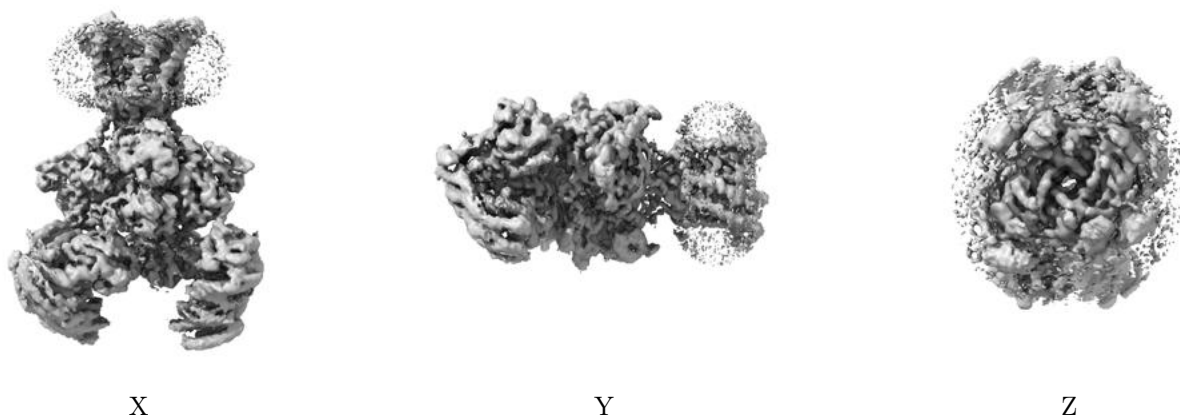
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.138. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

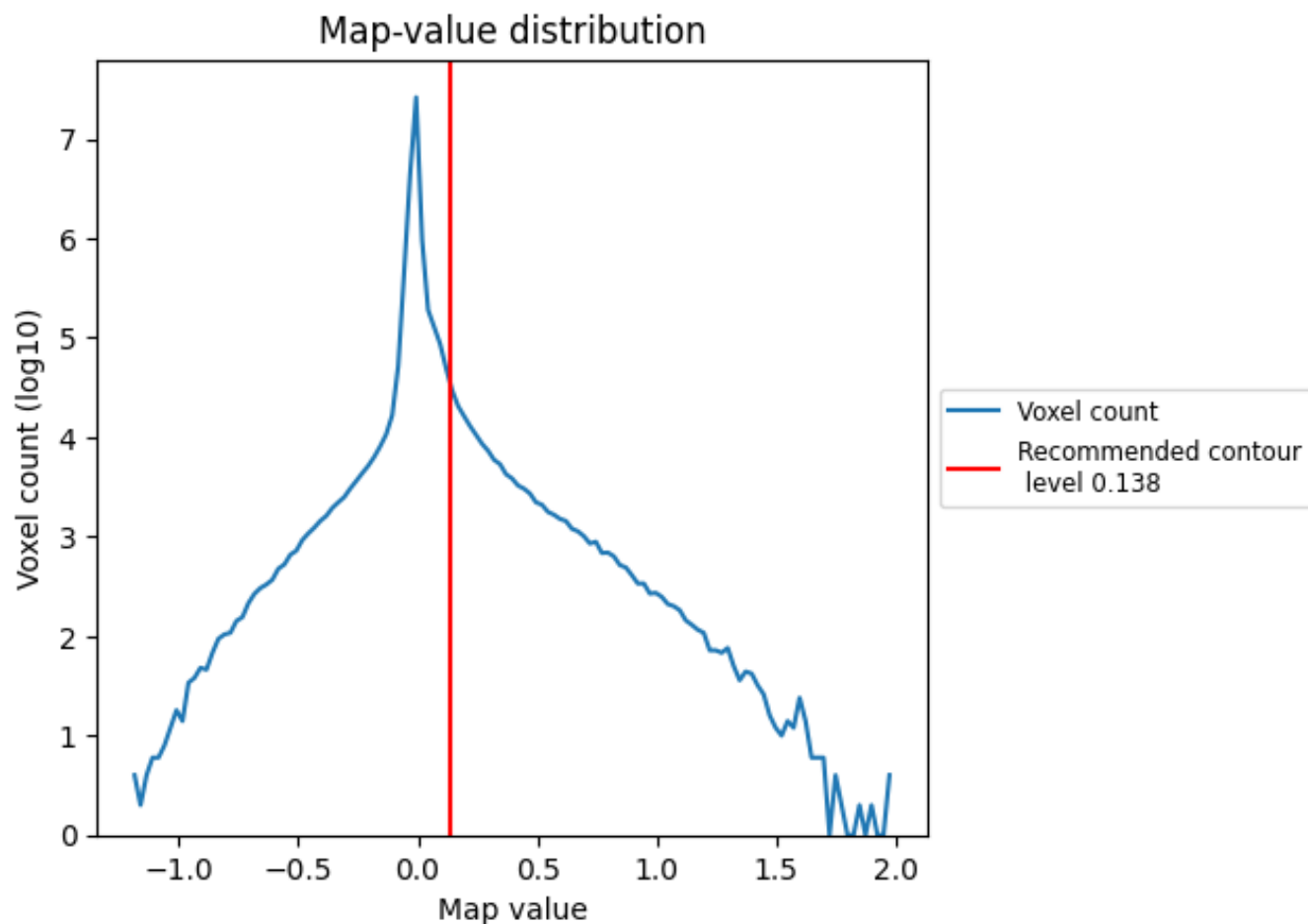
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

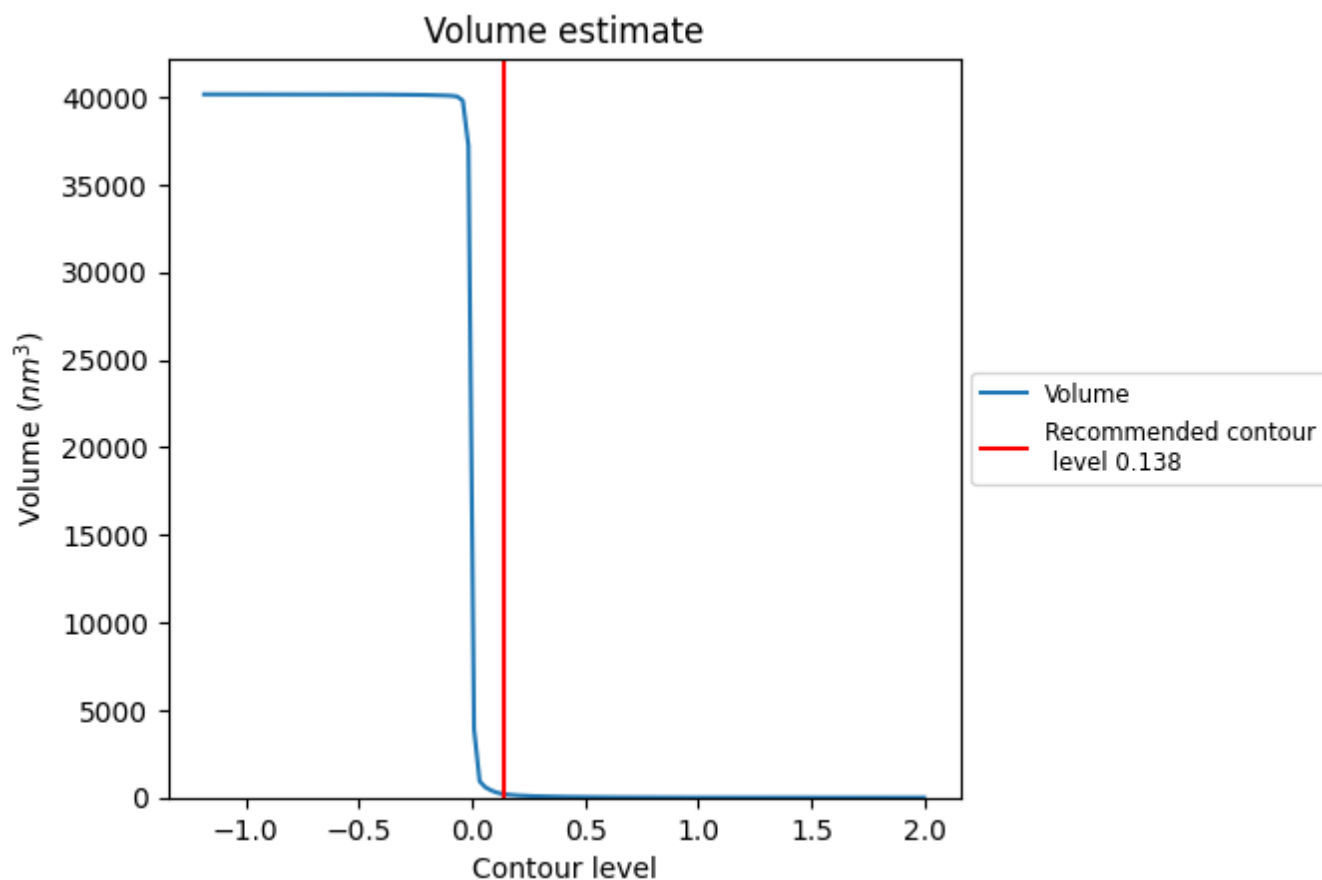
This section contains the results of statistical analysis of the map.

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.

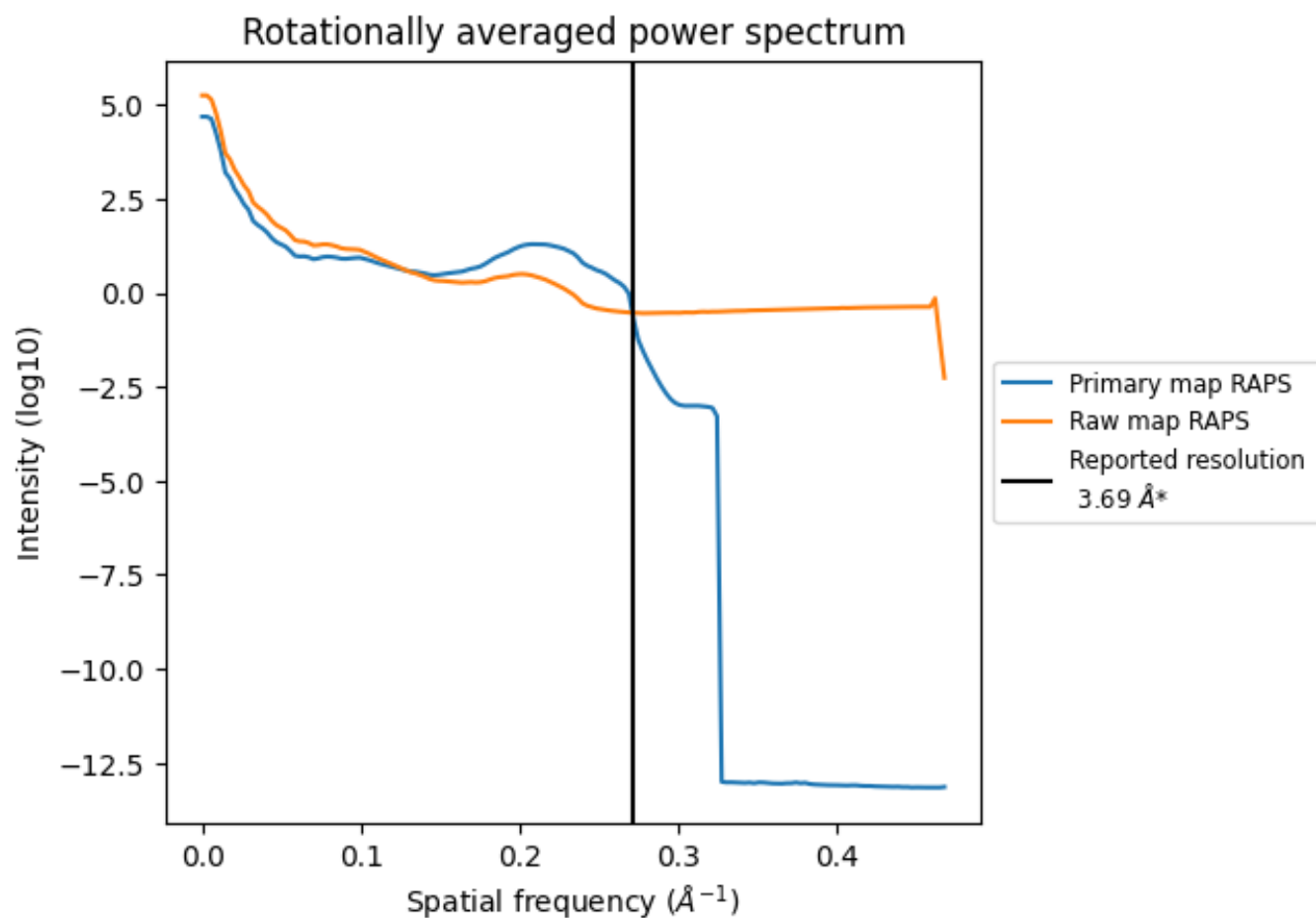
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 205 nm^3 ; this corresponds to an approximate mass of 185 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 ⓘ

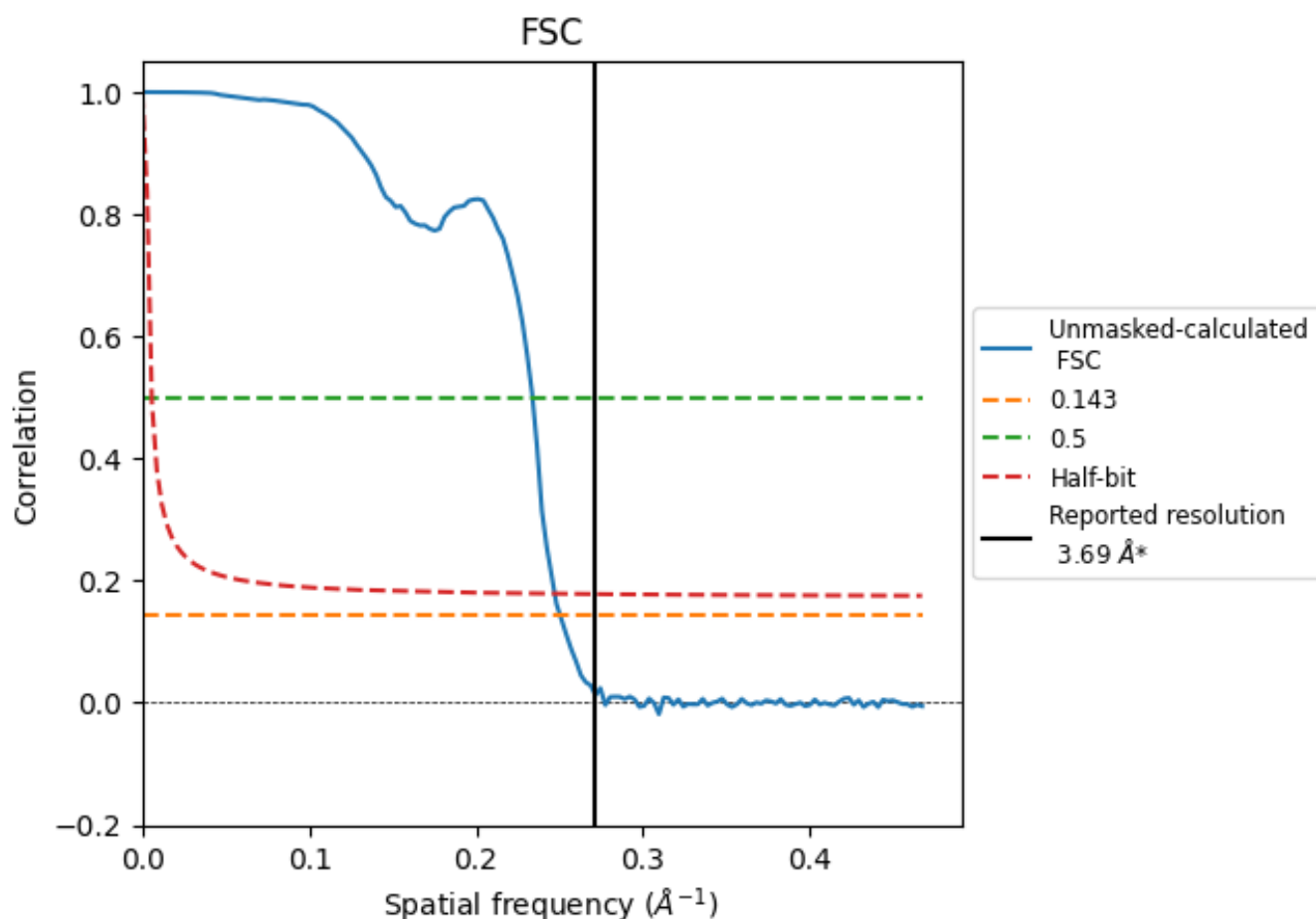


*Reported resolution corresponds to spatial frequency of 0.271 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.271 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

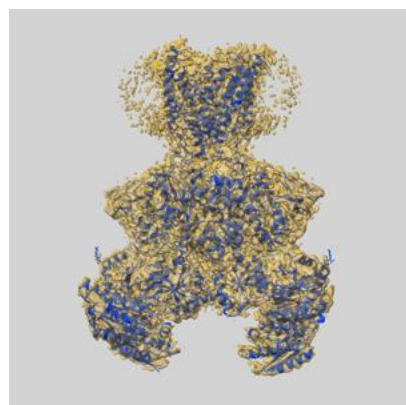
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.69	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.99	4.28	4.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

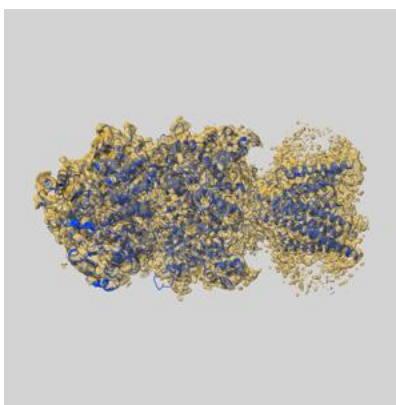
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43782 and PDB model 9ARH. Per-residue inclusion information can be found in section [3](#) on page [10](#).

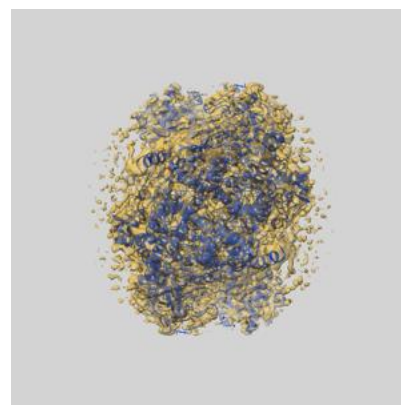
9.1 Map-model overlay [i](#)



X



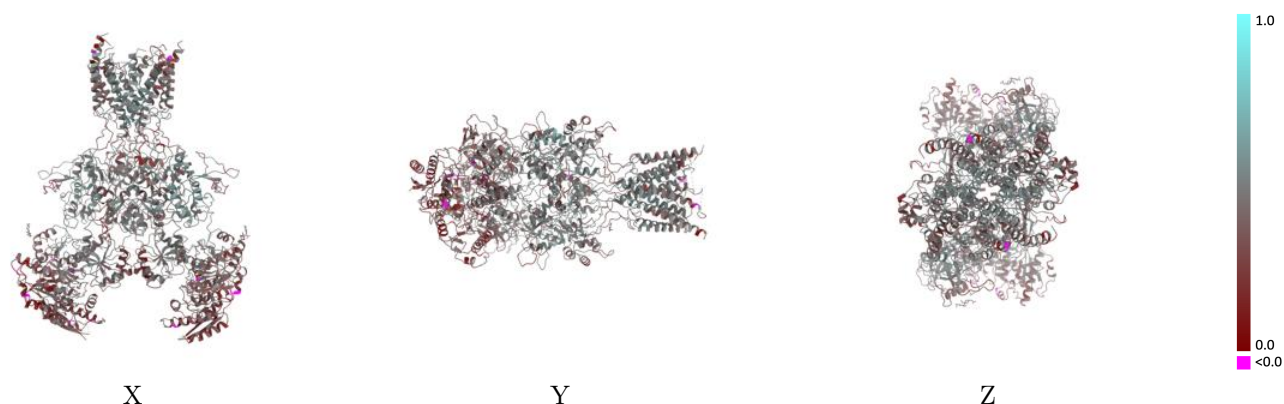
Y



Z

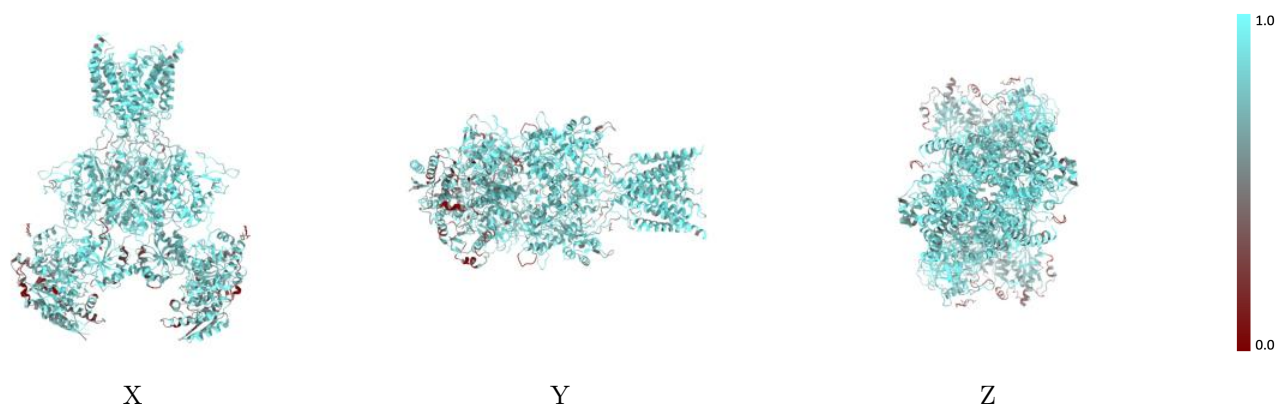
The images above show the 3D surface view of the map at the recommended contour level 0.138 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



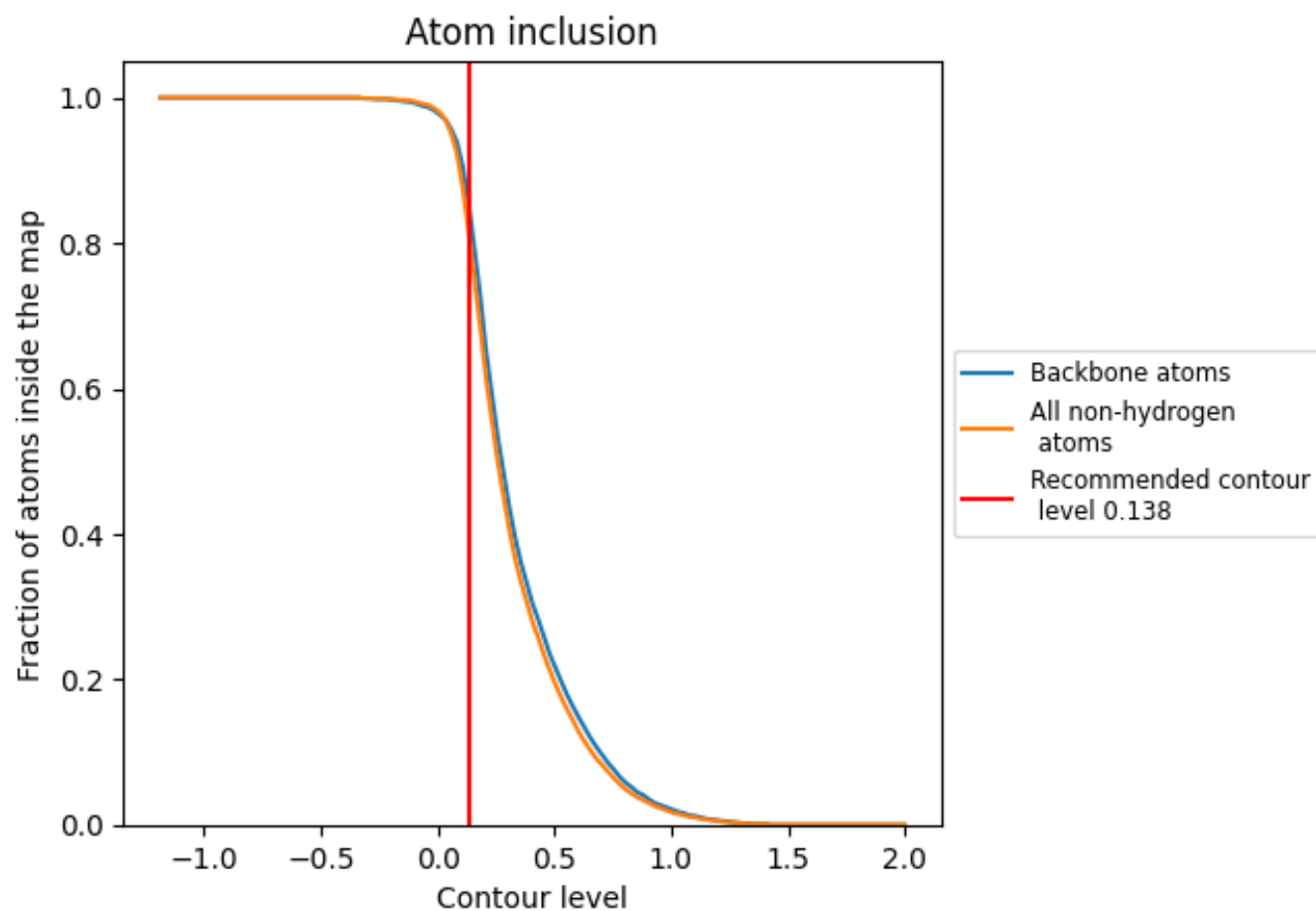
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.138).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 80% 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 (0.138) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8050	0.4190
A	0.8220	0.4270
B	0.7870	0.4130
C	0.8250	0.4270
D	0.7900	0.4100
E	0.2140	0.4020
F	0.2140	0.4030

1.0

0.0

<0.0