



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:47 PM UTC

PDB ID : 6WHS / pdb_00006whs
EMDB ID : EMD-21674
Title : GluN1b-GluN2B NMDA receptor in non-active 1 conformation at 3.95 angstrom resolution
Authors : Chou, T.; Tajima, N.; Furukawa, H.
Deposited on : 2020-04-08
Resolution : 4.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
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

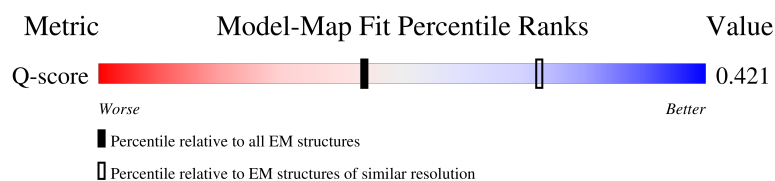
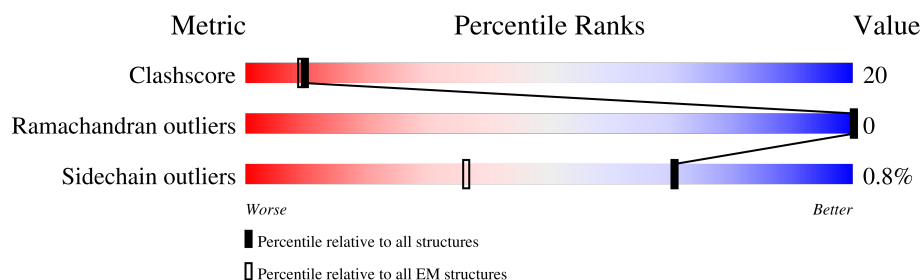
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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.



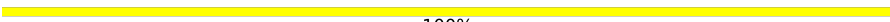
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	 51% 31% 17%
1	C	959	 51% 32% 17%
2	B	883	 57% 31% 11%
2	D	883	 59% 30% 11%

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22866 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	799	Total	C	N	O	S	0	0
			5705	3659	948	1074	24		
1	C	799	Total	C	N	O	S	0	0
			5705	3659	948	1074	24		

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	787	Total	C	N	O	S	0	0
			5644	3640	911	1062	31		
2	D	787	Total	C	N	O	S	0	0
			5644	3640	911	1062	31		

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-30	MET	-	expression tag	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	-	expression tag	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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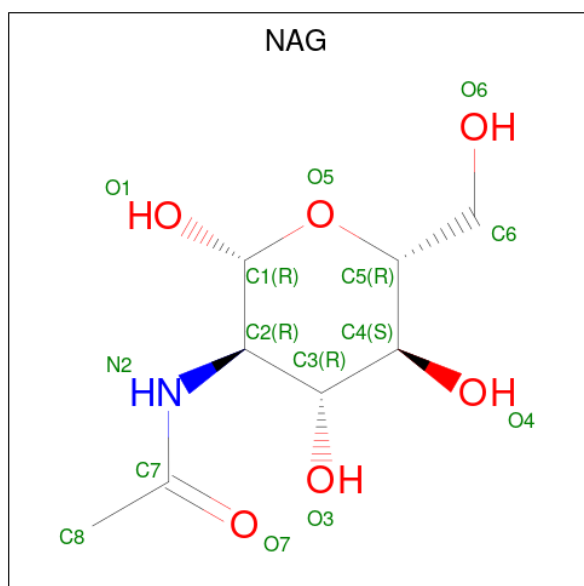
Chain	Residue	Modelled	Actual	Comment	Reference
D	348	ASP	ASN	conflict	UNP Q00960
D	557	CYS	ASP	conflict	UNP Q00960
D	588	SER	CYS	conflict	UNP Q00960
D	838	SER	CYS	conflict	UNP Q00960
D	849	SER	CYS	conflict	UNP Q00960

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



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	

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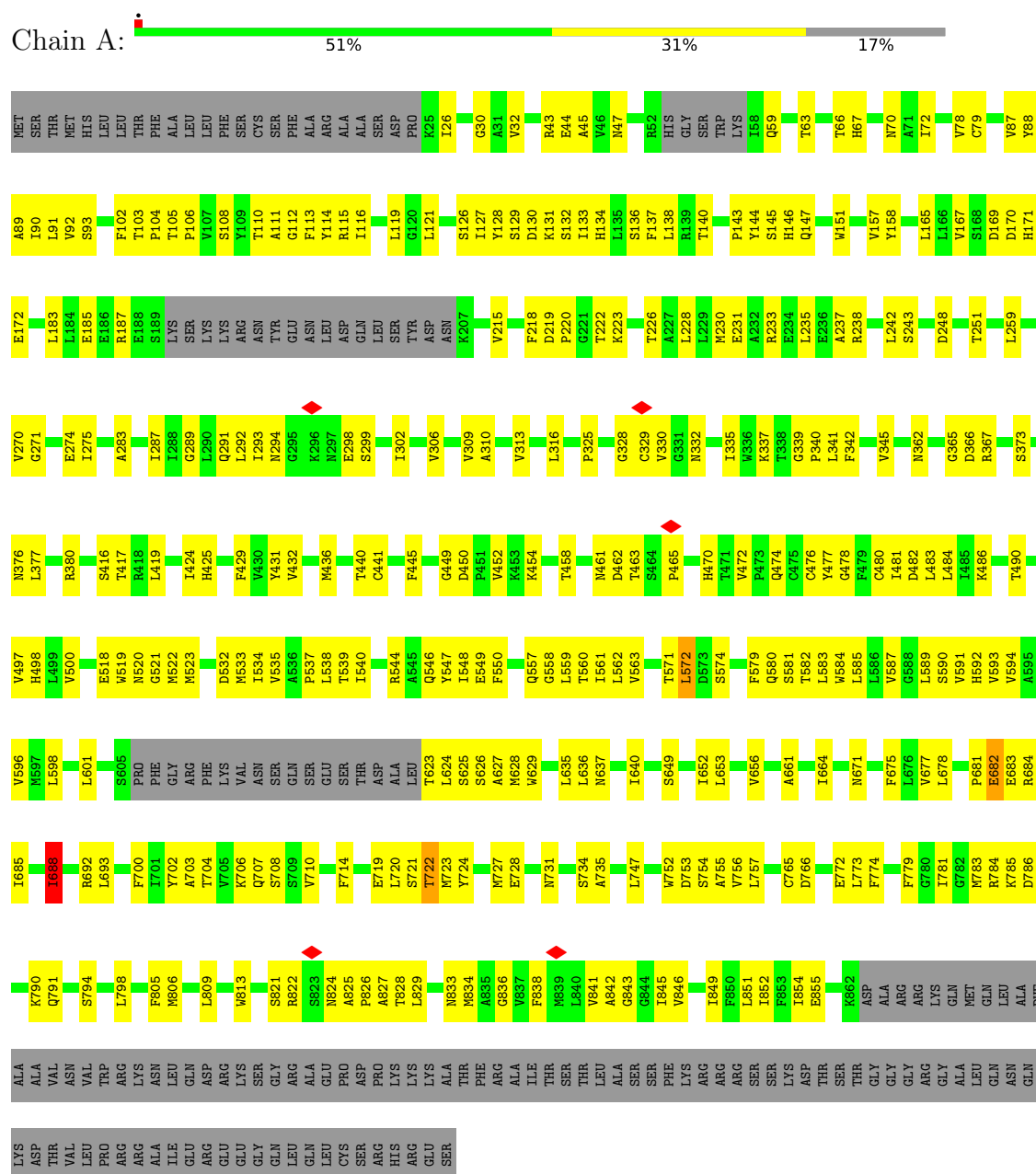
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Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C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

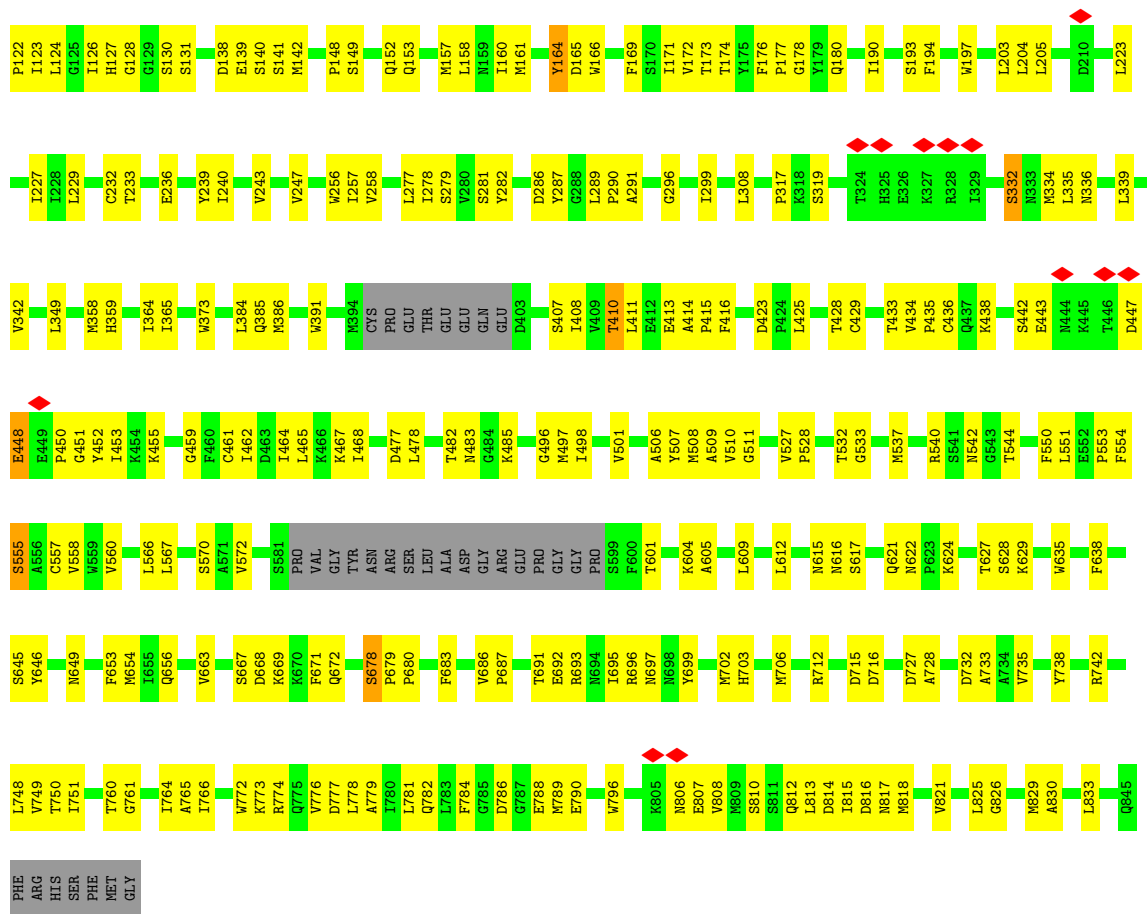
- Molecule 1: Glutamate receptor ionotropic, NMDA 1



[illegible]

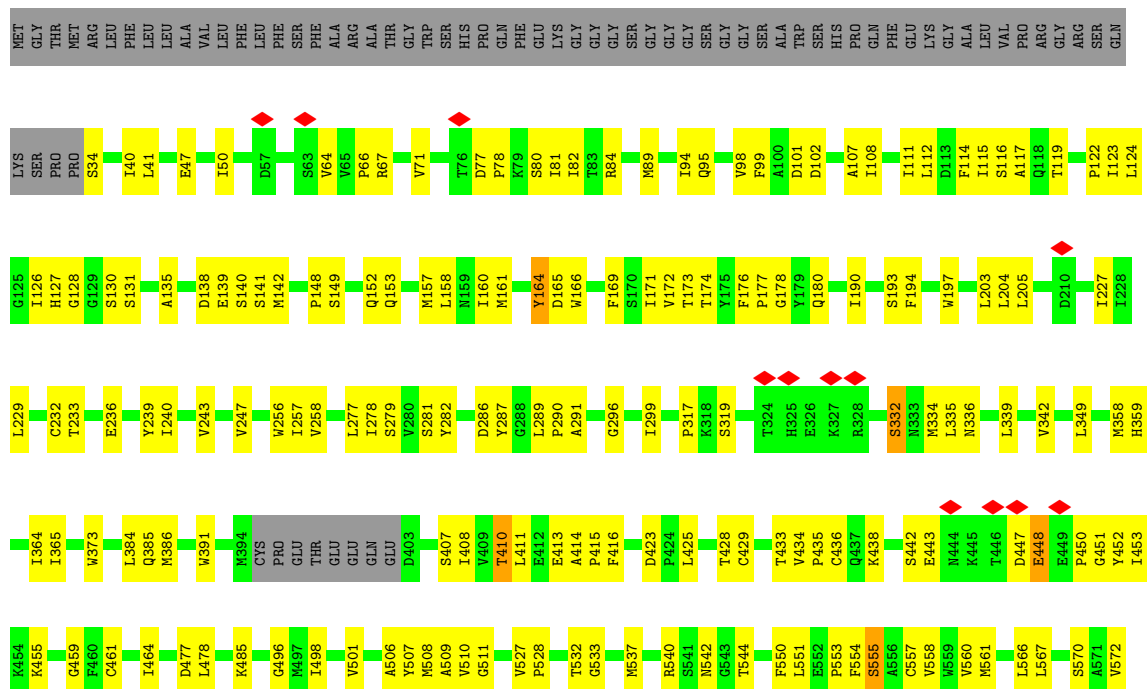
Chain B:

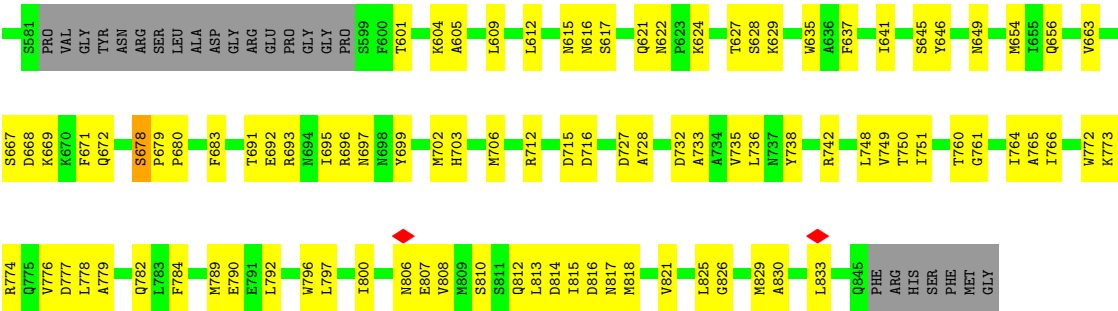
MET	GLY	THR	MET	ARG	LEU	PHE	LEU	ALA	VAL	PHE	LEU	PHE	SER	PHE	ALA	ARG	ALA	THR	GLY	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	GLY	GLY	GLY	GLY	ALA	TRP	HIS	PRO	GLN	PHE	GLU	LYS	GLY	ALA	LEU	VAL	PRO	ARG	GLY	ARG	SER	GLN
LYS	SER	PRO	PRO	S34	I40	L41	E47	I50	D57	S63	V64	V65	P66	R67	V71	T76	D77	P78	K79	S80	I81	I82	T83	R84	T85	C86	M89	S90	I94	Q95	V98	F99	A100	D101	D102	A107	I108	I111	L112	D113	F114	I115	S116	A117	G118	T119				



• Molecule 2: Glutamate receptor ionotropic, NMDA 2B

Chain D: 59% 30% 11%





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

Chain E: 100%



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

Chain F: 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	105348	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	18.665	Depositor
Minimum map value	-10.421	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.725	Depositor
Recommended contour level	3.15	Depositor
Map size (Å)	350.72, 350.72, 350.72	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	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	0.46	0/5830	0.57	2/7998 (0.0%)
1	C	0.46	0/5830	0.57	2/7998 (0.0%)
2	B	0.44	0/5764	0.53	0/7899
2	D	0.44	0/5764	0.53	0/7899
All	All	0.45	0/23188	0.55	4/31794 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
2	B	0	4
2	D	0	4
All	All	0	12

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	682	GLU	N-CA-C	6.15	118.78	111.71
1	A	682	GLU	N-CA-C	6.11	118.74	111.71
1	C	688	ILE	CB-CA-C	-5.53	102.22	111.29
1	A	688	ILE	CB-CA-C	-5.48	102.31	111.29

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	681	PRO	Peptide
1	A	682	GLU	Peptide
2	B	164	TYR	Peptide
2	B	448	GLU	Peptide
2	B	555	SER	Peptide
2	B	678	SER	Peptide
1	C	681	PRO	Peptide
1	C	682	GLU	Peptide
2	D	164	TYR	Peptide
2	D	448	GLU	Peptide
2	D	555	SER	Peptide
2	D	678	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5705	0	5225	232	0
1	C	5705	0	5225	237	0
2	B	5644	0	5192	220	0
2	D	5644	0	5192	214	0
3	E	28	0	25	0	0
3	F	28	0	25	1	0
4	A	28	0	26	0	0
4	B	28	0	26	0	0
4	C	28	0	26	0	0
4	D	28	0	26	0	0
All	All	22866	0	20988	864	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 20.

All (864) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:TYR:HB2	1:C:477:TYR:O	1.74	0.88
1:A:431:TYR:HB2	1:A:477:TYR:O	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:SER:HA	1:A:584:TRP:HD1	1.43	0.83
1:C:783:MET:HE1	1:C:790:LYS:HA	1.61	0.81
1:C:581:SER:HA	1:C:584:TRP:HD1	1.44	0.81
1:A:783:MET:HE1	1:A:790:LYS:HA	1.61	0.80
1:A:477:TYR:HA	1:A:481:ILE:HD11	1.64	0.80
1:C:477:TYR:HA	1:C:481:ILE:HD11	1.64	0.78
1:A:337:LYS:O	1:A:341:LEU:HB2	1.84	0.77
2:B:693:ARG:O	2:B:693:ARG:NH1	2.17	0.77
1:C:337:LYS:O	1:C:341:LEU:HB2	1.84	0.77
2:D:693:ARG:NH1	2:D:693:ARG:O	2.17	0.77
2:B:410:THR:OG1	2:B:411:LEU:N	2.13	0.76
2:B:621:GLN:NE2	2:B:622:ASN:O	2.18	0.76
1:C:132:SER:HB3	2:D:177:PRO:HG2	1.67	0.76
2:D:621:GLN:NE2	2:D:622:ASN:O	2.18	0.76
1:C:112:GLY:O	1:C:115:ARG:NH1	2.19	0.75
1:C:519:TRP:NE1	1:C:547:TYR:OH	2.20	0.75
2:D:410:THR:OG1	2:D:411:LEU:N	2.13	0.75
1:A:112:GLY:O	1:A:115:ARG:NH1	2.19	0.75
1:A:692:ARG:HB3	1:A:700:PHE:HE2	1.51	0.75
1:C:93:SER:HB3	1:C:121:LEU:HD12	1.69	0.75
2:D:289:LEU:HD12	2:D:291:ALA:H	1.52	0.75
2:D:160:ILE:HD12	2:D:364:ILE:HD13	1.70	0.74
2:B:790:GLU:N	2:B:790:GLU:OE1	2.21	0.74
2:B:289:LEU:HD12	2:B:291:ALA:H	1.52	0.74
1:C:330:VAL:HA	2:D:77:ASP:HB3	1.70	0.73
2:D:89:MET:HE2	2:D:319:SER:HB3	1.70	0.73
2:D:566:LEU:HD11	2:D:609:LEU:HB3	1.69	0.73
1:C:692:ARG:HB3	1:C:700:PHE:HE2	1.51	0.73
1:A:93:SER:HB3	1:A:121:LEU:HD12	1.69	0.73
1:A:111:ALA:HB1	1:A:116:ILE:HB	1.70	0.73
2:B:160:ILE:HD12	2:B:364:ILE:HD13	1.70	0.73
2:D:790:GLU:OE1	2:D:790:GLU:N	2.21	0.73
2:B:566:LEU:HD11	2:B:609:LEU:HB3	1.69	0.73
2:B:89:MET:HE2	2:B:319:SER:HB3	1.70	0.72
1:A:519:TRP:NE1	1:A:547:TYR:OH	2.20	0.72
1:C:111:ALA:HB1	1:C:116:ILE:HB	1.70	0.72
1:C:520:ASN:ND2	1:C:707:GLN:OE1	2.23	0.72
1:C:535:VAL:HG22	1:C:781:ILE:HD12	1.72	0.72
1:A:535:VAL:HG22	1:A:781:ILE:HD12	1.72	0.71
1:C:233:ARG:NH2	1:C:259:LEU:O	2.22	0.71
1:A:520:ASN:ND2	1:A:707:GLN:OE1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:ASN:OD1	1:C:377:LEU:N	2.24	0.70
2:B:567:LEU:O	2:B:570:SER:OG	2.09	0.70
1:A:376:ASN:OD1	1:A:377:LEU:N	2.24	0.70
2:D:138:ASP:OD1	2:D:140:SER:N	2.24	0.70
1:A:233:ARG:NH2	1:A:259:LEU:O	2.22	0.70
2:D:567:LEU:O	2:D:570:SER:OG	2.09	0.70
2:B:358:MET:SD	2:B:359:HIS:N	2.65	0.69
1:A:330:VAL:HA	2:B:77:ASP:HB3	1.73	0.69
2:B:232:CYS:SG	2:B:233:THR:N	2.65	0.69
1:A:520:ASN:OD1	1:A:521:GLY:N	2.25	0.69
1:C:520:ASN:OD1	1:C:521:GLY:N	2.25	0.69
1:C:688:ILE:HG23	1:C:774:PHE:CZ	2.28	0.69
1:C:547:TYR:O	1:C:548:ILE:HG13	1.93	0.69
2:D:358:MET:SD	2:D:359:HIS:N	2.65	0.69
2:B:627:THR:HB	1:C:852:ILE:HG12	1.74	0.69
1:A:547:TYR:O	1:A:548:ILE:HG13	1.93	0.68
1:A:78:VAL:HG11	1:A:110:THR:HG21	1.76	0.68
1:A:688:ILE:HG23	1:A:774:PHE:CZ	2.28	0.68
1:A:237:ALA:O	1:A:238:ARG:NH1	2.26	0.68
1:C:78:VAL:HG11	1:C:110:THR:HG21	1.76	0.68
1:A:362:ASN:OD1	1:A:365:GLY:N	2.27	0.68
2:B:138:ASP:OD1	2:B:140:SER:N	2.24	0.68
1:C:237:ALA:O	1:C:238:ARG:NH1	2.26	0.68
1:C:362:ASN:OD1	1:C:365:GLY:N	2.27	0.67
1:A:132:SER:HB3	2:B:177:PRO:HG2	1.76	0.67
2:B:668:ASP:OD1	2:B:669:LYS:N	2.28	0.67
2:B:34:SER:N	2:B:64:VAL:O	2.28	0.67
2:B:385:GLN:NE2	2:B:386:MET:O	2.27	0.67
2:B:816:ASP:OD1	2:B:817:ASN:N	2.28	0.67
2:D:668:ASP:OD1	2:D:669:LYS:N	2.28	0.67
2:D:816:ASP:OD1	2:D:817:ASN:N	2.28	0.67
1:C:26:ILE:HG12	1:C:59:GLN:HB2	1.77	0.67
2:D:385:GLN:NE2	2:D:386:MET:O	2.27	0.67
1:A:26:ILE:HG12	1:A:59:GLN:HB2	1.77	0.67
1:C:752:TRP:CG	1:C:753:ASP:H	2.13	0.67
1:A:283:ALA:HB1	1:A:287:ILE:HD12	1.77	0.67
1:A:752:TRP:CG	1:A:753:ASP:H	2.13	0.66
2:D:172:VAL:HG12	2:D:203:LEU:HB2	1.77	0.66
2:D:413:GLU:OE2	2:D:414:ALA:N	2.28	0.66
2:D:71:VAL:HG11	2:D:84:ARG:HD2	1.77	0.66
2:D:34:SER:N	2:D:64:VAL:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:VAL:HG11	2:B:84:ARG:HD2	1.77	0.66
2:B:413:GLU:OE2	2:B:414:ALA:N	2.28	0.66
1:C:140:THR:O	1:C:367:ARG:NH1	2.26	0.65
1:C:532:ASP:OD1	1:C:784:ARG:NH2	2.29	0.65
1:C:283:ALA:HB1	1:C:287:ILE:HD12	1.77	0.65
1:A:549:GLU:N	1:A:549:GLU:OE1	2.30	0.64
2:B:172:VAL:HG12	2:B:203:LEU:HB2	1.77	0.64
1:A:532:ASP:OD1	1:A:784:ARG:NH2	2.29	0.64
1:A:140:THR:O	1:A:367:ARG:NH1	2.26	0.64
1:A:130:ASP:OD2	1:A:133:ILE:N	2.24	0.64
1:C:523:MET:HE1	1:C:544:ARG:HA	1.80	0.64
2:B:554:PHE:HA	1:C:829:LEU:HG	1.79	0.64
1:C:562:LEU:HD22	1:C:757:LEU:HD11	1.80	0.64
1:C:587:VAL:O	1:C:591:VAL:HG23	1.98	0.64
2:B:601:THR:HG23	2:B:604:LYS:H	1.63	0.63
2:B:616:ASN:ND2	1:C:637:ASN:O	2.31	0.63
1:C:292:LEU:HG	1:C:294:ASN:H	1.64	0.63
1:C:549:GLU:N	1:C:549:GLU:OE1	2.30	0.63
2:D:601:THR:HG23	2:D:604:LYS:H	1.63	0.63
1:A:144:TYR:O	1:A:147:GLN:HG3	1.98	0.63
1:A:523:MET:HE1	1:A:544:ARG:HA	1.80	0.63
1:A:292:LEU:HG	1:A:294:ASN:H	1.64	0.63
1:A:587:VAL:O	1:A:591:VAL:HG23	1.99	0.63
1:A:562:LEU:HD22	1:A:757:LEU:HD11	1.80	0.63
1:C:130:ASP:OD2	1:C:133:ILE:N	2.24	0.63
1:C:144:TYR:O	1:C:147:GLN:HG3	1.98	0.62
2:D:232:CYS:SG	2:D:233:THR:N	2.65	0.62
2:D:715:ASP:N	2:D:715:ASP:OD1	2.32	0.62
1:C:549:GLU:OE1	1:C:785:LYS:HA	2.00	0.62
1:C:30:GLY:O	1:C:90:ILE:HA	2.00	0.62
2:B:166:TRP:HB3	2:B:227:ILE:HG13	1.81	0.62
1:A:549:GLU:OE1	1:A:785:LYS:HA	2.00	0.61
2:D:166:TRP:HB3	2:D:227:ILE:HG13	1.81	0.61
1:A:30:GLY:O	1:A:90:ILE:HA	2.00	0.61
2:D:112:LEU:HD11	2:D:123:ILE:HG21	1.82	0.61
1:A:461:ASN:OD1	1:A:462:ASP:N	2.34	0.61
2:D:64:VAL:HG23	2:D:66:PRO:HD3	1.83	0.61
2:B:177:PRO:O	2:B:180:GLN:NE2	2.34	0.61
2:B:615:ASN:O	2:B:617:SER:N	2.31	0.61
1:A:539:THR:HG22	1:A:540:ILE:H	1.66	0.61
2:B:814:ASP:OD1	2:B:815:ILE:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:PHE:O	1:C:105:THR:OG1	2.12	0.60
2:D:78:PRO:HA	2:D:81:ILE:HD12	1.83	0.60
2:D:177:PRO:O	2:D:180:GLN:NE2	2.34	0.60
1:C:461:ASN:OD1	1:C:462:ASP:N	2.34	0.60
2:B:112:LEU:HD11	2:B:123:ILE:HG21	1.82	0.60
1:A:559:LEU:HB2	1:A:774:PHE:HB2	1.82	0.60
1:C:539:THR:HG22	1:C:540:ILE:H	1.66	0.60
1:C:559:LEU:HB2	1:C:774:PHE:HB2	1.82	0.60
2:D:507:TYR:HH	2:D:772:TRP:CD1	2.20	0.59
2:B:78:PRO:HA	2:B:81:ILE:HD12	1.83	0.59
2:B:555:SER:HB2	2:B:558:VAL:HG22	1.85	0.59
1:A:671:ASN:HD22	2:B:813:LEU:HD11	1.67	0.59
2:B:34:SER:O	2:B:67:ARG:NH1	2.35	0.59
1:A:784:ARG:HG2	1:A:785:LYS:H	1.68	0.59
1:C:791:GLN:OE1	1:C:791:GLN:N	2.35	0.59
1:A:791:GLN:OE1	1:A:791:GLN:N	2.35	0.59
1:C:766:ASP:OD1	1:C:766:ASP:N	2.36	0.59
2:D:281:SER:OG	2:D:282:TYR:N	2.36	0.59
1:A:126:SER:O	1:A:129:SER:OG	2.14	0.59
1:A:147:GLN:HE22	1:A:271:GLY:HA3	1.68	0.59
2:B:715:ASP:N	2:B:715:ASP:OD1	2.32	0.59
1:C:833:ASN:OD1	1:C:834:MET:N	2.36	0.59
2:D:34:SER:O	2:D:67:ARG:NH1	2.35	0.59
1:A:671:ASN:ND2	2:B:813:LEU:HD11	2.18	0.59
2:D:77:ASP:O	2:D:80:SER:OG	2.20	0.59
1:A:248:ASP:O	1:A:251:THR:OG1	2.20	0.59
1:A:480:CYS:SG	1:A:481:ILE:N	2.76	0.59
1:A:833:ASN:OD1	1:A:834:MET:N	2.36	0.59
2:B:64:VAL:HG23	2:B:66:PRO:HD3	1.83	0.58
1:A:766:ASP:N	1:A:766:ASP:OD1	2.36	0.58
1:A:722:THR:OG1	1:A:723:MET:N	2.37	0.58
1:C:719:GLU:N	1:C:719:GLU:OE1	2.36	0.58
2:B:77:ASP:O	2:B:80:SER:OG	2.20	0.58
2:D:277:LEU:HD12	2:D:278:ILE:H	1.69	0.58
2:B:784:PHE:CE1	2:B:789:MET:HG3	2.38	0.58
1:C:784:ARG:HG2	1:C:785:LYS:H	1.68	0.58
2:D:555:SER:HB2	2:D:558:VAL:HG22	1.84	0.58
1:A:829:LEU:HG	2:D:554:PHE:HA	1.85	0.58
1:C:299:SER:HA	1:C:302:ILE:HD12	1.86	0.58
1:C:842:ALA:HA	1:C:845:ILE:HD12	1.85	0.57
1:A:105:THR:O	1:A:108:SER:OG	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:GLN:HE22	1:C:271:GLY:HA3	1.68	0.57
1:C:105:THR:O	1:C:108:SER:OG	2.20	0.57
2:D:332:SER:O	2:D:334:MET:N	2.37	0.57
1:A:299:SER:HA	1:A:302:ILE:HD12	1.86	0.57
1:A:842:ALA:HA	1:A:845:ILE:HD12	1.85	0.57
1:C:480:CYS:SG	1:C:481:ILE:N	2.76	0.57
1:A:721:SER:O	1:A:724:TYR:HB3	2.04	0.57
2:B:102:ASP:OD1	2:B:102:ASP:N	2.37	0.57
2:B:277:LEU:HD12	2:B:278:ILE:H	1.69	0.57
2:B:332:SER:O	2:B:334:MET:N	2.37	0.57
2:B:116:SER:HG	2:B:142:MET:H	1.51	0.57
2:D:257:ILE:HD13	2:D:278:ILE:HB	1.87	0.57
2:B:107:ALA:O	2:B:111:ILE:HG13	2.05	0.57
1:C:721:SER:O	1:C:724:TYR:HB3	2.04	0.57
2:D:784:PHE:CE1	2:D:789:MET:HG3	2.38	0.57
2:B:257:ILE:HD13	2:B:278:ILE:HB	1.87	0.57
1:A:275:ILE:HD11	1:A:289:GLY:HA3	1.87	0.57
2:B:507:TYR:HH	2:B:772:TRP:CD1	2.22	0.57
1:A:623:THR:O	1:A:626:SER:OG	2.16	0.57
2:B:281:SER:OG	2:B:282:TYR:N	2.36	0.56
2:B:461:CYS:O	2:B:464:ILE:HG22	2.05	0.56
2:B:742:ARG:HA	2:B:742:ARG:HH21	1.71	0.56
1:C:722:THR:OG1	1:C:723:MET:N	2.37	0.56
2:D:461:CYS:O	2:D:464:ILE:HG22	2.05	0.56
2:D:742:ARG:HA	2:D:742:ARG:HH21	1.71	0.56
2:B:148:PRO:HG2	2:B:153:GLN:HE21	1.71	0.56
2:D:107:ALA:O	2:D:111:ILE:HG13	2.05	0.56
2:D:776:VAL:O	2:D:779:ALA:HB3	2.06	0.56
1:A:102:PHE:O	1:A:105:THR:OG1	2.12	0.56
1:A:115:ARG:HG2	1:A:335:ILE:HD12	1.88	0.56
2:D:138:ASP:OD1	2:D:139:GLU:N	2.39	0.56
2:D:669:LYS:HA	2:D:672:GLN:HB2	1.88	0.56
2:B:669:LYS:HA	2:B:672:GLN:HB2	1.88	0.56
1:C:583:LEU:HD11	2:D:818:MET:HG3	1.88	0.56
2:D:814:ASP:OD1	2:D:815:ILE:N	2.33	0.56
1:C:623:THR:O	1:C:626:SER:OG	2.16	0.56
2:B:256:TRP:HB2	2:B:277:LEU:HD13	1.88	0.56
1:C:275:ILE:HD11	1:C:289:GLY:HA3	1.87	0.56
2:D:615:ASN:O	2:D:617:SER:N	2.31	0.56
2:D:89:MET:HA	2:D:94:ILE:HB	1.88	0.55
1:C:115:ARG:HG2	1:C:335:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:537:MET:HE3	2:D:748:LEU:HB3	1.88	0.55
1:A:87:VAL:HG11	1:A:90:ILE:HG13	1.88	0.55
2:D:258:VAL:O	2:D:279:SER:OG	2.18	0.55
2:D:825:LEU:O	2:D:829:MET:HG3	2.07	0.55
2:B:537:MET:HE3	2:B:748:LEU:HB3	1.88	0.55
1:C:291:GLN:HB2	1:C:373:SER:OG	2.06	0.55
1:C:671:ASN:HD22	2:D:813:LEU:HD11	1.70	0.55
1:A:719:GLU:N	1:A:719:GLU:OE1	2.36	0.55
2:B:138:ASP:OD1	2:B:139:GLU:N	2.39	0.55
2:B:825:LEU:O	2:B:829:MET:HG3	2.07	0.55
1:C:734:SER:OG	1:C:735:ALA:N	2.39	0.55
2:B:193:SER:OG	2:B:194:PHE:N	2.39	0.55
2:B:776:VAL:O	2:B:779:ALA:HB3	2.06	0.55
1:C:445:PHE:HB3	1:C:449:GLY:HA2	1.89	0.55
1:C:522:MET:HE1	1:C:534:ILE:HG23	1.89	0.55
1:A:560:THR:OG1	1:A:561:ILE:N	2.38	0.55
1:C:127:ILE:HD13	1:C:171:HIS:HD2	1.72	0.55
2:D:193:SER:OG	2:D:194:PHE:N	2.39	0.55
1:A:114:TYR:OH	1:A:329:CYS:HB2	2.07	0.55
1:C:688:ILE:HG23	1:C:774:PHE:CE1	2.42	0.55
1:C:32:VAL:HG12	1:C:67:HIS:CE1	2.42	0.55
2:D:148:PRO:HG2	2:D:153:GLN:HE21	1.71	0.55
1:A:127:ILE:HD13	1:A:171:HIS:HD2	1.72	0.54
2:B:258:VAL:O	2:B:279:SER:OG	2.18	0.54
1:A:32:VAL:HG12	1:A:67:HIS:CE1	2.42	0.54
1:A:274:GLU:H	1:A:274:GLU:CD	2.14	0.54
1:A:806:MET:HA	1:A:809:LEU:HD12	1.89	0.54
2:B:47:GLU:HA	2:B:50:ILE:HD12	1.89	0.54
1:C:114:TYR:OH	1:C:329:CYS:HB2	2.07	0.54
1:A:291:GLN:HB2	1:A:373:SER:OG	2.07	0.54
1:A:688:ILE:HG23	1:A:774:PHE:CE1	2.42	0.54
1:A:841:VAL:O	1:A:845:ILE:HG13	2.08	0.54
2:B:89:MET:HA	2:B:94:ILE:HB	1.88	0.54
1:A:522:MET:HE1	1:A:534:ILE:HG23	1.89	0.54
1:A:734:SER:OG	1:A:735:ALA:N	2.39	0.54
1:C:313:VAL:HA	1:C:316:LEU:HB3	1.89	0.54
1:A:130:ASP:OD1	1:A:131:LYS:N	2.41	0.54
1:C:237:ALA:C	1:C:238:ARG:HH11	2.16	0.54
1:A:445:PHE:HB3	1:A:449:GLY:HA2	1.89	0.54
2:B:624:LYS:O	2:B:629:LYS:NZ	2.41	0.54
1:C:130:ASP:OD1	1:C:131:LYS:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:GLU:H	1:C:274:GLU:CD	2.14	0.54
2:D:256:TRP:HB2	2:D:277:LEU:HD13	1.88	0.54
1:A:429:PHE:HD2	1:A:537:PRO:HB3	1.73	0.53
1:A:693:LEU:HD22	1:A:702:TYR:CE1	2.43	0.53
1:C:806:MET:HA	1:C:809:LEU:HD12	1.89	0.53
1:C:841:VAL:O	1:C:845:ILE:HG13	2.08	0.53
2:D:157:MET:O	2:D:160:ILE:HG22	2.08	0.53
1:A:313:VAL:HA	1:A:316:LEU:HB3	1.89	0.53
2:B:99:PHE:O	2:B:126:ILE:HG12	2.09	0.53
2:B:286:ASP:OD1	2:B:286:ASP:N	2.41	0.53
1:C:424:ILE:HD11	1:C:522:MET:HG2	1.90	0.53
1:C:571:THR:OG1	1:C:572:LEU:N	2.42	0.53
1:A:132:SER:OG	1:A:133:ILE:N	2.42	0.53
1:A:838:PHE:HA	1:A:841:VAL:HG12	1.89	0.53
1:C:87:VAL:HG11	1:C:90:ILE:HG13	1.88	0.53
1:C:248:ASP:O	1:C:251:THR:OG1	2.20	0.53
2:D:99:PHE:O	2:D:126:ILE:HG12	2.09	0.53
2:D:102:ASP:OD1	2:D:102:ASP:N	2.37	0.53
2:D:624:LYS:O	2:D:629:LYS:NZ	2.41	0.53
1:C:429:PHE:HD2	1:C:537:PRO:HB3	1.73	0.53
1:C:693:LEU:HD22	1:C:702:TYR:CE1	2.43	0.53
1:A:563:VAL:HG11	1:A:685:ILE:HD12	1.91	0.53
2:D:566:LEU:HD13	2:D:635:TRP:CZ2	2.44	0.53
1:C:560:THR:OG1	1:C:561:ILE:N	2.38	0.52
1:C:752:TRP:CD1	1:C:753:ASP:H	2.27	0.52
2:D:47:GLU:HA	2:D:50:ILE:HD12	1.90	0.52
1:A:424:ILE:HD11	1:A:522:MET:HG2	1.90	0.52
2:B:164:TYR:HB2	2:B:166:TRP:CZ3	2.44	0.52
2:D:101:ASP:CG	2:D:102:ASP:H	2.16	0.52
2:B:566:LEU:HD13	2:B:635:TRP:CZ2	2.44	0.52
1:C:563:VAL:HG11	1:C:685:ILE:HD12	1.91	0.52
1:C:838:PHE:HA	1:C:841:VAL:HG12	1.89	0.52
2:B:101:ASP:CG	2:B:102:ASP:H	2.16	0.52
2:B:732:ASP:OD1	2:B:732:ASP:N	2.43	0.52
1:C:128:TYR:HA	1:C:134:HIS:HD2	1.75	0.52
1:C:549:GLU:CD	1:C:786:ASP:H	2.17	0.52
2:B:138:ASP:HB3	2:B:141:SER:H	1.75	0.52
1:C:416:SER:OG	1:C:417:THR:N	2.43	0.52
1:A:549:GLU:OE2	1:A:786:ASP:N	2.43	0.52
2:B:157:MET:O	2:B:160:ILE:HG22	2.08	0.52
2:D:299:ILE:HD12	2:D:349:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:GLU:CD	1:A:786:ASP:H	2.17	0.52
2:B:336:ASN:N	2:B:336:ASN:OD1	2.43	0.52
2:B:544:THR:HG22	2:B:808:VAL:HG21	1.92	0.52
2:B:236:GLU:O	2:B:240:ILE:HG12	2.10	0.52
2:D:696:ARG:HG3	2:D:703:HIS:CG	2.45	0.52
1:C:549:GLU:OE2	1:C:786:ASP:N	2.43	0.51
2:D:164:TYR:HB2	2:D:166:TRP:CZ3	2.44	0.51
2:B:696:ARG:HG3	2:B:703:HIS:CG	2.45	0.51
1:C:132:SER:OG	1:C:133:ILE:N	2.42	0.51
2:D:138:ASP:HB3	2:D:141:SER:H	1.75	0.51
2:B:299:ILE:HD12	2:B:349:LEU:HD23	1.92	0.51
2:B:727:ASP:OD1	2:B:727:ASP:N	2.42	0.51
2:D:157:MET:O	2:D:161:MET:HG2	2.11	0.51
1:A:752:TRP:CD1	1:A:753:ASP:H	2.27	0.51
2:D:236:GLU:O	2:D:240:ILE:HG12	2.10	0.51
2:D:727:ASP:OD1	2:D:727:ASP:N	2.42	0.51
1:A:581:SER:O	1:A:585:LEU:HG	2.11	0.51
1:C:649:SER:HA	1:C:652:ILE:HD12	1.92	0.51
2:D:544:THR:HG22	2:D:808:VAL:HG21	1.92	0.51
2:D:477:ASP:N	2:D:477:ASP:OD1	2.42	0.51
1:C:482:ASP:OD1	1:C:482:ASP:N	2.41	0.51
2:D:115:ILE:O	2:D:119:THR:OG1	2.25	0.51
1:A:640:ILE:HD11	2:D:629:LYS:HG2	1.93	0.51
1:C:291:GLN:HB2	1:C:373:SER:HG	1.76	0.51
1:C:474:GLN:N	1:C:474:GLN:OE1	2.43	0.51
1:A:328:GLY:O	1:A:332:ASN:N	2.44	0.51
2:B:112:LEU:HA	2:B:115:ILE:HD12	1.93	0.51
2:B:450:PRO:O	2:B:452:TYR:N	2.42	0.51
1:C:306:VAL:HA	1:C:309:VAL:HG12	1.92	0.51
1:C:574:SER:HB3	1:C:836:GLY:HA3	1.93	0.51
1:A:474:GLN:N	1:A:474:GLN:OE1	2.43	0.51
1:A:534:ILE:HG21	1:A:538:LEU:HD22	1.93	0.51
1:A:851:LEU:O	1:A:855:GLU:HG2	2.11	0.51
2:B:239:TYR:O	2:B:243:VAL:HG23	2.11	0.51
2:B:299:ILE:HG13	2:B:342:VAL:HG21	1.94	0.51
1:C:328:GLY:O	1:C:332:ASN:N	2.44	0.51
1:A:237:ALA:C	1:A:238:ARG:HH11	2.16	0.50
1:A:580:GLN:HG3	1:A:582:THR:HG23	1.93	0.50
1:A:703:ALA:HB2	1:A:747:LEU:HD11	1.93	0.50
1:C:482:ASP:OD1	1:C:483:LEU:N	2.43	0.50
2:B:157:MET:O	2:B:161:MET:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:LEU:O	2:B:339:LEU:N	2.45	0.50
2:D:239:TYR:O	2:D:243:VAL:HG23	2.11	0.50
2:D:336:ASN:OD1	2:D:336:ASN:N	2.43	0.50
1:A:429:PHE:CD2	1:A:537:PRO:HB3	2.46	0.50
1:C:126:SER:O	1:C:126:SER:OG	2.25	0.50
1:C:429:PHE:CD2	1:C:537:PRO:HB3	2.46	0.50
1:C:580:GLN:HG3	1:C:582:THR:HG23	1.93	0.50
1:C:581:SER:O	1:C:585:LEU:HG	2.11	0.50
1:A:482:ASP:OD1	1:A:483:LEU:N	2.43	0.50
1:A:838:PHE:CE2	2:D:561:MET:HG2	2.46	0.50
2:B:508:MET:HE2	2:B:766:ILE:HG22	1.92	0.50
1:C:30:GLY:HA2	1:C:63:THR:O	2.11	0.50
2:D:510:VAL:HG23	2:D:764:ILE:HD12	1.94	0.50
2:B:95:GLN:HE22	2:B:317:PRO:HD2	1.76	0.50
2:B:415:PRO:HB3	2:B:738:TYR:CD2	2.47	0.50
2:B:784:PHE:CD1	2:B:789:MET:HG3	2.47	0.50
1:A:714:PHE:HB3	1:A:724:TYR:HD2	1.76	0.50
1:A:852:ILE:HG12	2:D:627:THR:HB	1.94	0.50
2:D:299:ILE:HG13	2:D:342:VAL:HG21	1.94	0.50
2:D:335:LEU:O	2:D:339:LEU:N	2.45	0.50
2:D:508:MET:HE2	2:D:766:ILE:HG22	1.92	0.50
1:A:128:TYR:HA	1:A:134:HIS:HD2	1.75	0.50
1:A:440:THR:OG1	1:A:441:CYS:N	2.45	0.50
1:A:752:TRP:CG	1:A:753:ASP:N	2.79	0.50
1:C:534:ILE:HG21	1:C:538:LEU:HD22	1.93	0.50
2:D:95:GLN:HE22	2:D:317:PRO:HD2	1.77	0.50
2:D:286:ASP:N	2:D:286:ASP:OD1	2.41	0.50
2:D:332:SER:C	2:D:334:MET:H	2.20	0.50
1:A:306:VAL:HA	1:A:309:VAL:HG12	1.92	0.50
2:B:332:SER:C	2:B:334:MET:H	2.19	0.50
2:B:678:SER:O	2:B:679:PRO:C	2.55	0.50
1:A:30:GLY:HA2	1:A:63:THR:O	2.11	0.50
1:A:649:SER:HA	1:A:652:ILE:HD12	1.92	0.50
2:B:656:GLN:HE21	1:C:826:PRO:HB3	1.77	0.50
1:C:703:ALA:HB2	1:C:747:LEU:HD11	1.93	0.50
2:D:243:VAL:O	2:D:247:VAL:HG23	2.12	0.50
2:D:732:ASP:N	2:D:732:ASP:OD1	2.43	0.50
1:A:66:THR:OG1	1:A:67:HIS:N	2.45	0.49
1:A:416:SER:OG	1:A:417:THR:N	2.43	0.49
1:A:518:GLU:OE1	1:A:519:TRP:N	2.45	0.49
1:A:574:SER:HB3	1:A:836:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:MET:N	1:C:440:THR:O	2.40	0.49
1:A:292:LEU:HD12	1:A:293:ILE:H	1.77	0.49
1:A:580:GLN:OE1	1:A:581:SER:N	2.38	0.49
1:C:44:GLU:HA	1:C:47:ASN:HD22	1.77	0.49
2:D:112:LEU:HA	2:D:115:ILE:HD12	1.93	0.49
2:D:173:THR:OG1	2:D:174:THR:N	2.45	0.49
2:D:415:PRO:HB3	2:D:738:TYR:CD2	2.47	0.49
1:A:482:ASP:OD1	1:A:482:ASP:N	2.41	0.49
2:B:243:VAL:O	2:B:247:VAL:HG23	2.12	0.49
1:C:518:GLU:OE1	1:C:519:TRP:N	2.45	0.49
1:C:851:LEU:O	1:C:855:GLU:HG2	2.11	0.49
1:A:44:GLU:HA	1:A:47:ASN:HD22	1.77	0.49
1:A:470:HIS:O	1:A:472:VAL:HG13	2.13	0.49
2:B:407:SER:OG	2:B:506:ALA:O	2.29	0.49
2:B:477:ASP:OD1	2:B:477:ASP:N	2.42	0.49
1:C:424:ILE:HG22	1:C:425:HIS:H	1.77	0.49
1:A:113:PHE:HE2	2:B:78:PRO:HD3	1.77	0.49
1:A:424:ILE:HG22	1:A:425:HIS:H	1.77	0.49
2:D:784:PHE:CD1	2:D:789:MET:HG3	2.47	0.49
1:A:337:LYS:C	1:A:339:GLY:H	2.21	0.49
1:A:341:LEU:O	1:A:345:VAL:HG13	2.13	0.49
1:C:714:PHE:HB3	1:C:724:TYR:HD2	1.77	0.49
2:B:806:ASN:OD1	2:B:806:ASN:N	2.46	0.49
1:C:66:THR:OG1	1:C:67:HIS:N	2.45	0.49
1:C:292:LEU:HD12	1:C:293:ILE:H	1.77	0.49
2:D:605:ALA:O	2:D:609:LEU:HD23	2.13	0.49
2:B:173:THR:OG1	2:B:174:THR:N	2.45	0.49
1:C:440:THR:OG1	1:C:441:CYS:N	2.45	0.49
1:C:671:ASN:ND2	2:D:813:LEU:HD11	2.28	0.49
2:D:111:ILE:O	2:D:115:ILE:HG13	2.13	0.49
2:B:111:ILE:O	2:B:115:ILE:HG13	2.13	0.48
2:B:510:VAL:HG23	2:B:764:ILE:HD12	1.94	0.48
2:B:774:ARG:NH2	1:C:546:GLN:O	2.46	0.48
1:A:167:VAL:O	1:A:218:PHE:HB3	2.14	0.48
1:C:91:LEU:HD12	1:C:121:LEU:HD21	1.94	0.48
1:C:310:ALA:HA	1:C:313:VAL:HG12	1.95	0.48
1:C:470:HIS:O	1:C:472:VAL:HG13	2.13	0.48
1:C:580:GLN:N	2:D:812:GLN:O	2.46	0.48
2:D:678:SER:O	2:D:679:PRO:C	2.55	0.48
1:A:91:LEU:HD12	1:A:121:LEU:HD21	1.94	0.48
1:A:310:ALA:HA	1:A:313:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:ILE:O	2:B:119:THR:OG1	2.25	0.48
1:C:523:MET:SD	1:C:544:ARG:HG2	2.54	0.48
2:D:407:SER:OG	2:D:506:ALA:O	2.29	0.48
2:D:683:PHE:HD1	2:D:706:MET:HE3	1.79	0.48
1:A:821:SER:OG	1:A:822:ARG:N	2.46	0.48
1:C:341:LEU:O	1:C:345:VAL:HG13	2.13	0.48
1:C:821:SER:OG	1:C:822:ARG:N	2.46	0.48
2:D:692:GLU:O	2:D:695:ILE:N	2.46	0.48
2:B:692:GLU:O	2:B:695:ILE:N	2.46	0.48
1:C:337:LYS:C	1:C:339:GLY:H	2.21	0.48
1:C:582:THR:HB	2:D:815:ILE:HD11	1.96	0.48
1:A:436:MET:N	1:A:440:THR:O	2.40	0.48
1:A:523:MET:SD	1:A:544:ARG:HG2	2.54	0.48
2:D:669:LYS:O	2:D:672:GLN:N	2.46	0.48
1:A:754:SER:OG	1:A:755:ALA:N	2.47	0.48
2:B:671:PHE:HB3	2:B:702:MET:HE1	1.96	0.48
1:C:683:GLU:CD	1:C:684:ARG:H	2.22	0.48
2:D:507:TYR:HH	2:D:772:TRP:HD1	1.60	0.48
1:C:167:VAL:O	1:C:218:PHE:HB3	2.14	0.48
2:D:671:PHE:HB3	2:D:702:MET:HE1	1.96	0.48
2:B:605:ALA:O	2:B:609:LEU:HD23	2.13	0.47
2:D:498:ILE:HA	2:D:501:VAL:HG12	1.95	0.47
1:C:580:GLN:OE1	1:C:581:SER:N	2.38	0.47
2:B:498:ILE:HA	2:B:501:VAL:HG12	1.95	0.47
2:B:669:LYS:O	2:B:672:GLN:N	2.46	0.47
2:B:786:ASP:HA	1:C:717:GLN:HE22	1.77	0.47
1:C:625:SER:HA	1:C:628:MET:HE3	1.97	0.47
2:D:830:ALA:O	2:D:833:LEU:HG	2.14	0.47
1:A:572:LEU:HD21	1:A:675:PHE:CE1	2.50	0.47
1:C:43:ARG:O	1:C:47:ASN:ND2	2.47	0.47
2:D:693:ARG:HH22	2:D:697:ASN:HD21	1.62	0.47
1:A:546:GLN:O	2:D:774:ARG:NH2	2.48	0.47
1:A:571:THR:OG1	1:A:572:LEU:N	2.42	0.47
1:A:706:LYS:O	1:A:708:SER:OG	2.32	0.47
2:B:165:ASP:OD2	2:B:435:PRO:HG2	2.14	0.47
2:B:683:PHE:HD1	2:B:706:MET:HE3	1.79	0.47
1:C:165:LEU:HB3	1:C:215:VAL:HG12	1.97	0.47
2:D:78:PRO:O	2:D:82:ILE:HG12	2.15	0.47
2:D:108:ILE:HA	2:D:111:ILE:HD12	1.95	0.47
2:D:391:TRP:HA	2:D:391:TRP:CE3	2.49	0.47
2:B:108:ILE:HA	2:B:111:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:391:TRP:CE3	2:B:391:TRP:HA	2.49	0.47
1:C:843:GLY:HA2	1:C:846:VAL:HG22	1.97	0.47
2:D:158:LEU:HD23	2:D:158:LEU:HA	1.67	0.47
2:D:384:LEU:HD12	2:D:385:GLN:H	1.80	0.47
2:B:384:LEU:HD12	2:B:385:GLN:H	1.80	0.47
2:D:442:SER:OG	2:D:443:GLU:N	2.47	0.47
1:A:637:ASN:O	2:D:616:ASN:ND2	2.47	0.47
1:A:165:LEU:HB3	1:A:215:VAL:HG12	1.97	0.47
2:B:174:THR:HG23	2:B:176:PHE:H	1.80	0.47
2:B:693:ARG:HH22	2:B:697:ASN:HD21	1.62	0.47
1:C:222:THR:OG1	1:C:223:LYS:N	2.48	0.47
1:C:523:MET:HE3	1:C:548:ILE:HD12	1.97	0.47
1:A:43:ARG:O	1:A:47:ASN:ND2	2.47	0.46
1:A:625:SER:HA	1:A:628:MET:HE3	1.96	0.46
1:A:754:SER:O	1:A:756:VAL:N	2.48	0.46
1:A:851:LEU:HA	1:A:854:ILE:HD12	1.97	0.46
1:C:106:PRO:O	1:C:110:THR:OG1	2.21	0.46
1:C:754:SER:O	1:C:757:LEU:N	2.48	0.46
2:D:174:THR:HG23	2:D:176:PHE:H	1.80	0.46
1:A:106:PRO:O	1:A:110:THR:OG1	2.22	0.46
1:A:532:ASP:O	1:A:533:MET:HG3	2.15	0.46
1:A:754:SER:O	1:A:757:LEU:N	2.48	0.46
2:B:78:PRO:O	2:B:82:ILE:HG12	2.15	0.46
2:B:461:CYS:SG	2:B:510:VAL:HG22	2.55	0.46
2:B:830:ALA:O	2:B:833:LEU:HG	2.15	0.46
1:C:706:LYS:O	1:C:708:SER:OG	2.32	0.46
2:D:806:ASN:N	2:D:806:ASN:OD1	2.46	0.46
1:A:102:PHE:O	1:A:106:PRO:HD3	2.16	0.46
1:A:683:GLU:CD	1:A:684:ARG:H	2.22	0.46
2:B:410:THR:HG21	2:B:478:LEU:HD21	1.97	0.46
2:B:442:SER:OG	2:B:443:GLU:N	2.47	0.46
1:C:583:LEU:O	1:C:587:VAL:HG22	2.16	0.46
2:D:410:THR:HG21	2:D:478:LEU:HD21	1.97	0.46
1:A:222:THR:OG1	1:A:223:LYS:N	2.48	0.46
1:A:849:ILE:HA	1:A:852:ILE:HD12	1.98	0.46
2:D:165:ASP:OD2	2:D:435:PRO:HG2	2.14	0.46
2:D:461:CYS:SG	2:D:510:VAL:HG22	2.55	0.46
2:D:527:VAL:HG13	2:D:528:PRO:HD2	1.98	0.46
2:B:296:GLY:O	2:B:299:ILE:HG22	2.16	0.46
2:B:699:TYR:O	2:B:702:MET:N	2.49	0.46
1:C:754:SER:O	1:C:756:VAL:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:851:LEU:HA	1:C:854:ILE:HD12	1.97	0.46
1:A:219:ASP:OD1	1:A:220:PRO:HD2	2.16	0.46
2:B:176:PHE:HD1	2:B:178:GLY:H	1.63	0.46
2:D:438:LYS:HA	2:D:451:GLY:C	2.41	0.46
2:B:148:PRO:CG	2:B:153:GLN:HE21	2.29	0.46
2:B:438:LYS:HA	2:B:451:GLY:C	2.41	0.46
1:C:157:VAL:HG23	1:C:158:TYR:CD1	2.51	0.46
1:C:425:HIS:HD2	1:C:432:VAL:HB	1.80	0.46
1:C:452:VAL:O	1:C:454:LYS:HG2	2.16	0.46
1:A:92:VAL:O	1:A:121:LEU:HG	2.16	0.46
1:A:425:HIS:HD2	1:A:432:VAL:HB	1.81	0.46
2:D:508:MET:HE3	2:D:508:MET:HB2	1.79	0.46
1:A:157:VAL:HG23	1:A:158:TYR:CD1	2.51	0.46
1:A:523:MET:HE3	1:A:548:ILE:HD12	1.97	0.46
1:A:843:GLY:HA2	1:A:846:VAL:HG22	1.97	0.46
2:B:123:ILE:C	2:B:124:LEU:HD22	2.41	0.46
1:C:92:VAL:O	1:C:121:LEU:HG	2.16	0.46
1:C:572:LEU:HD21	1:C:675:PHE:CE1	2.50	0.46
2:D:176:PHE:HD1	2:D:178:GLY:H	1.63	0.46
1:A:88:TYR:CZ	1:A:325:PRO:HD2	2.51	0.45
1:C:78:VAL:HG13	1:C:79:CYS:H	1.80	0.45
1:C:88:TYR:CZ	1:C:325:PRO:HD2	2.51	0.45
1:C:754:SER:OG	1:C:755:ALA:N	2.47	0.45
1:A:452:VAL:O	1:A:454:LYS:HG2	2.16	0.45
1:A:805:PHE:CZ	1:A:809:LEU:HD11	2.51	0.45
1:C:102:PHE:O	1:C:106:PRO:HD3	2.16	0.45
2:D:414:ALA:HB3	2:D:415:PRO:HD3	1.98	0.45
1:A:274:GLU:CD	1:A:274:GLU:N	2.74	0.45
1:C:532:ASP:O	1:C:533:MET:HG3	2.15	0.45
1:A:583:LEU:O	1:A:587:VAL:HG22	2.16	0.45
2:B:447:ASP:OD1	2:B:448:GLU:N	2.40	0.45
1:C:629:TRP:HA	1:C:629:TRP:CE3	2.52	0.45
1:C:752:TRP:CG	1:C:753:ASP:N	2.79	0.45
2:D:557:CYS:O	2:D:560:VAL:HG22	2.17	0.45
2:D:683:PHE:CD1	2:D:706:MET:HE3	2.51	0.45
2:D:760:THR:OG1	2:D:761:GLY:N	2.47	0.45
1:A:589:LEU:O	1:A:593:VAL:HG23	2.17	0.45
1:A:677:VAL:HG13	1:A:678:LEU:HD12	1.98	0.45
2:B:190:ILE:HD13	2:B:190:ILE:HA	1.81	0.45
2:B:509:ALA:HB3	2:B:765:ALA:HB3	1.99	0.45
2:B:557:CYS:O	2:B:560:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:849:ILE:HA	1:C:852:ILE:HD12	1.98	0.45
2:D:123:ILE:C	2:D:124:LEU:HD22	2.41	0.45
1:A:78:VAL:HG13	1:A:79:CYS:H	1.80	0.45
1:A:845:ILE:HG23	2:D:572:VAL:HG21	1.97	0.45
2:B:365:ILE:HD12	2:B:373:TRP:CG	2.52	0.45
1:C:133:ILE:HD11	2:D:135:ALA:HB3	1.99	0.45
1:C:145:SER:OG	1:C:146:HIS:N	2.49	0.45
1:C:671:ASN:OD1	2:D:654:MET:HG2	2.16	0.45
1:C:677:VAL:HG13	1:C:678:LEU:HD12	1.98	0.45
2:D:627:THR:OG1	2:D:628:SER:N	2.49	0.45
2:D:692:GLU:OE2	2:D:693:ARG:N	2.50	0.45
2:B:171:ILE:HG22	2:B:229:LEU:HB3	1.99	0.45
2:B:532:THR:HG22	2:B:761:GLY:HA2	1.99	0.45
2:B:760:THR:OG1	2:B:761:GLY:N	2.47	0.45
2:D:365:ILE:HD12	2:D:373:TRP:HB3	1.97	0.45
2:B:527:VAL:HG13	2:B:528:PRO:HD2	1.98	0.45
1:C:151:TRP:HZ2	1:C:270:VAL:C	2.25	0.45
2:D:50:ILE:HG12	2:D:290:PRO:HG3	1.99	0.45
2:D:164:TYR:CE2	2:D:386:MET:HE2	2.52	0.45
2:D:693:ARG:HH12	2:D:697:ASN:ND2	2.15	0.45
1:A:377:LEU:HD11	1:A:380:ARG:HA	1.99	0.45
2:B:365:ILE:HD12	2:B:373:TRP:HB3	1.97	0.45
2:B:508:MET:HE3	2:B:508:MET:HB2	1.79	0.45
1:C:589:LEU:O	1:C:593:VAL:HG23	2.17	0.45
1:C:728:GLU:HA	1:C:731:ASN:HD21	1.82	0.45
2:D:130:SER:OG	2:D:131:SER:N	2.50	0.45
2:B:50:ILE:HG12	2:B:290:PRO:HG3	1.99	0.45
2:B:149:SER:OG	2:B:152:GLN:HG2	2.17	0.45
2:B:164:TYR:CE2	2:B:386:MET:HE2	2.52	0.45
2:B:683:PHE:CD1	2:B:706:MET:HE3	2.51	0.45
1:C:477:TYR:HA	1:C:481:ILE:CD1	2.43	0.45
2:D:296:GLY:O	2:D:299:ILE:HG22	2.16	0.45
2:D:408:ILE:HG12	2:D:508:MET:HB3	1.99	0.45
2:D:450:PRO:O	2:D:452:TYR:N	2.42	0.45
1:A:151:TRP:HZ2	1:A:270:VAL:C	2.25	0.44
1:C:274:GLU:CD	1:C:274:GLU:N	2.74	0.44
1:C:534:ILE:HD13	1:C:534:ILE:HA	1.78	0.44
2:D:149:SER:OG	2:D:152:GLN:HG2	2.17	0.44
2:B:693:ARG:HH12	2:B:697:ASN:ND2	2.15	0.44
1:C:219:ASP:OD1	1:C:220:PRO:HD2	2.16	0.44
1:C:458:THR:HG23	1:C:498:HIS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:805:PHE:CZ	1:C:809:LEU:HD11	2.51	0.44
2:D:365:ILE:HD12	2:D:373:TRP:CG	2.52	0.44
1:A:500:VAL:HG21	1:A:522:MET:HB3	1.99	0.44
1:A:557:GLN:OE1	1:A:558:GLY:N	2.51	0.44
2:B:414:ALA:HB3	2:B:415:PRO:HD3	1.98	0.44
2:B:555:SER:CB	2:B:558:VAL:HG22	2.47	0.44
2:B:686:VAL:HA	2:B:687:PRO:HD3	1.88	0.44
1:C:127:ILE:HD13	1:C:171:HIS:CD2	2.51	0.44
1:C:231:GLU:O	1:C:235:LEU:HG	2.17	0.44
1:A:601:LEU:HD23	1:A:601:LEU:HA	1.80	0.44
1:A:629:TRP:CE3	1:A:629:TRP:HA	2.52	0.44
2:B:415:PRO:HG2	2:B:416:PHE:CD1	2.52	0.44
2:B:692:GLU:OE2	2:B:693:ARG:N	2.50	0.44
2:D:148:PRO:CG	2:D:153:GLN:HE21	2.29	0.44
2:D:277:LEU:HD12	2:D:278:ILE:N	2.33	0.44
2:D:736:LEU:HD23	2:D:736:LEU:HA	1.60	0.44
1:A:342:PHE:O	1:A:345:VAL:HG22	2.18	0.44
2:B:40:ILE:C	2:B:41:LEU:HD22	2.42	0.44
1:C:362:ASN:OD1	1:C:366:ASP:N	2.40	0.44
1:A:458:THR:HG23	1:A:498:HIS:HB2	1.99	0.44
2:B:540:ARG:O	2:B:542:ASN:N	2.51	0.44
2:B:663:VAL:HG13	2:B:751:ILE:CD1	2.47	0.44
1:C:581:SER:HA	1:C:584:TRP:CD1	2.36	0.44
1:C:702:TYR:HD2	1:C:727:MET:HE3	1.83	0.44
2:D:40:ILE:C	2:D:41:LEU:HD22	2.42	0.44
2:D:679:PRO:HA	2:D:680:PRO:HD3	1.87	0.44
1:A:702:TYR:HD2	1:A:727:MET:HE3	1.83	0.44
2:B:408:ILE:HG12	2:B:508:MET:HB3	1.99	0.44
2:B:462:ILE:HD13	2:B:462:ILE:HA	1.72	0.44
2:B:497:MET:HE2	2:B:497:MET:HB3	1.82	0.44
2:B:627:THR:OG1	2:B:628:SER:N	2.49	0.44
1:C:132:SER:CB	2:D:177:PRO:HG2	2.44	0.44
1:C:134:HIS:C	1:C:136:SER:H	2.26	0.44
1:C:377:LEU:HD11	1:C:380:ARG:HA	1.99	0.44
2:D:415:PRO:HG2	2:D:416:PHE:CD1	2.52	0.44
2:D:532:THR:HG22	2:D:761:GLY:HA2	1.99	0.44
1:A:145:SER:OG	1:A:146:HIS:N	2.49	0.44
1:C:103:THR:OG1	1:C:104:PRO:HD3	2.18	0.44
1:C:728:GLU:O	1:C:731:ASN:ND2	2.51	0.44
1:C:797:ILE:HD13	1:C:797:ILE:HA	1.86	0.44
2:D:540:ARG:O	2:D:542:ASN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:826:GLY:HA2	2:D:829:MET:SD	2.58	0.44
1:A:134:HIS:C	1:A:136:SER:H	2.26	0.44
1:A:728:GLU:HA	1:A:731:ASN:HD21	1.81	0.44
2:B:554:PHE:CD1	1:C:829:LEU:HD11	2.52	0.44
2:B:695:ILE:HG22	2:B:703:HIS:HB2	1.99	0.44
1:C:772:GLU:O	1:C:773:LEU:HD23	2.18	0.44
2:D:171:ILE:HG22	2:D:229:LEU:HB3	1.99	0.44
2:D:190:ILE:HD12	2:D:197:TRP:CG	2.53	0.44
1:A:231:GLU:O	1:A:235:LEU:HG	2.17	0.43
2:B:223:LEU:HD23	2:B:223:LEU:HA	1.81	0.43
2:B:609:LEU:HD13	2:B:635:TRP:CE3	2.52	0.43
2:B:826:GLY:HA2	2:B:829:MET:SD	2.58	0.43
1:C:342:PHE:O	1:C:345:VAL:HG22	2.18	0.43
1:C:557:GLN:OE1	1:C:558:GLY:N	2.51	0.43
2:D:699:TYR:O	2:D:702:MET:N	2.49	0.43
1:A:581:SER:HA	1:A:584:TRP:CD1	2.35	0.43
2:B:277:LEU:HD12	2:B:278:ILE:N	2.33	0.43
1:C:500:VAL:HG21	1:C:522:MET:HB3	1.99	0.43
2:D:127:HIS:CG	2:D:128:GLY:N	2.86	0.43
2:D:451:GLY:O	2:D:453:ILE:HG12	2.18	0.43
1:A:103:THR:OG1	1:A:104:PRO:HD3	2.18	0.43
1:A:127:ILE:HD13	1:A:171:HIS:CD2	2.51	0.43
2:B:507:TYR:HH	2:B:772:TRP:HD1	1.63	0.43
2:D:555:SER:CB	2:D:558:VAL:HG22	2.47	0.43
2:D:663:VAL:HG13	2:D:751:ILE:CD1	2.47	0.43
2:D:779:ALA:O	2:D:782:GLN:HB3	2.18	0.43
1:A:165:LEU:HA	1:A:165:LEU:HD12	1.61	0.43
1:A:226:THR:O	1:A:230:MET:HG2	2.18	0.43
1:A:271:GLY:H	1:A:274:GLU:CD	2.26	0.43
2:B:127:HIS:CG	2:B:128:GLY:N	2.86	0.43
2:B:158:LEU:HD23	2:B:158:LEU:HA	1.67	0.43
1:C:226:THR:O	1:C:230:MET:HG2	2.18	0.43
1:C:271:GLY:H	1:C:274:GLU:CD	2.27	0.43
2:D:609:LEU:HD13	2:D:635:TRP:CE3	2.52	0.43
1:A:362:ASN:OD1	1:A:366:ASP:N	2.40	0.43
2:B:157:MET:HE3	2:B:157:MET:HB2	1.68	0.43
2:B:451:GLY:O	2:B:453:ILE:HG12	2.18	0.43
1:C:653:LEU:O	1:C:656:VAL:HG12	2.19	0.43
2:D:447:ASP:OD1	2:D:448:GLU:N	2.40	0.43
2:D:509:ALA:HB3	2:D:765:ALA:HB3	1.99	0.43
2:D:555:SER:OG	2:D:557:CYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:695:ILE:HG22	2:D:703:HIS:HB2	1.99	0.43
1:A:183:LEU:HD12	1:A:183:LEU:HA	1.78	0.43
1:A:298:GLU:O	1:A:302:ILE:HG13	2.18	0.43
1:A:653:LEU:O	1:A:656:VAL:HG12	2.19	0.43
1:A:772:GLU:O	1:A:773:LEU:HD23	2.18	0.43
2:B:122:PRO:O	2:B:123:ILE:HD13	2.18	0.43
2:B:645:SER:OG	2:B:646:TYR:N	2.52	0.43
2:D:287:TYR:O	2:D:289:LEU:N	2.51	0.43
2:B:190:ILE:HD12	2:B:197:TRP:CG	2.53	0.43
2:B:485:LYS:O	2:B:496:GLY:HA3	2.19	0.43
2:B:679:PRO:HA	2:B:680:PRO:HD3	1.87	0.43
1:C:151:TRP:HZ2	1:C:270:VAL:O	2.02	0.43
2:D:386:MET:HE3	2:D:386:MET:HB3	1.88	0.43
2:D:433:THR:OG1	2:D:434:VAL:N	2.52	0.43
2:B:542:ASN:N	2:B:542:ASN:OD1	2.52	0.43
1:C:45:ALA:HB1	1:C:306:VAL:HG21	2.01	0.43
2:D:114:PHE:O	2:D:117:ALA:HB3	2.19	0.43
2:B:386:MET:HE3	2:B:386:MET:HB3	1.88	0.43
2:B:555:SER:OG	2:B:557:CYS:N	2.51	0.43
1:C:478:GLY:HA2	1:C:813:TRP:CZ3	2.54	0.43
2:D:691:THR:OG1	2:D:692:GLU:N	2.52	0.43
1:A:728:GLU:O	1:A:731:ASN:ND2	2.51	0.43
2:B:779:ALA:O	2:B:782:GLN:HB3	2.18	0.43
1:C:540:ILE:HG12	1:C:550:PHE:CE2	2.54	0.43
2:D:98:VAL:HB	2:D:126:ILE:HD13	2.01	0.43
1:A:540:ILE:HG12	1:A:550:PHE:CE2	2.54	0.42
2:B:130:SER:OG	2:B:131:SER:N	2.50	0.42
2:B:287:TYR:O	2:B:289:LEU:N	2.51	0.42
2:B:459:GLY:HA2	2:B:796:TRP:CH2	2.54	0.42
2:B:553:PRO:HB2	2:B:649:ASN:HD22	1.84	0.42
2:B:691:THR:OG1	2:B:692:GLU:N	2.52	0.42
1:C:298:GLU:O	1:C:302:ILE:HG13	2.18	0.42
1:C:471:THR:O	1:C:471:THR:OG1	2.34	0.42
1:A:143:PRO:HD2	1:A:146:HIS:CE1	2.54	0.42
1:A:594:VAL:O	1:A:598:LEU:HD23	2.19	0.42
1:A:827:ALA:HB3	1:A:828:THR:HG23	2.02	0.42
1:C:388:TYR:OH	1:C:390:GLY:O	2.21	0.42
2:D:459:GLY:HA2	2:D:796:TRP:CH2	2.54	0.42
2:D:507:TYR:OH	2:D:772:TRP:HD1	2.03	0.42
1:A:45:ALA:HB1	1:A:306:VAL:HG21	2.01	0.42
1:A:784:ARG:HG2	1:A:785:LYS:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:LEU:HD12	1:C:228:LEU:H	1.85	0.42
1:C:590:SER:O	1:C:594:VAL:HG23	2.19	0.42
2:D:122:PRO:O	2:D:123:ILE:HD13	2.18	0.42
2:D:551:LEU:HD23	2:D:551:LEU:HA	1.86	0.42
1:A:185:GLU:O	1:A:187:ARG:N	2.51	0.42
1:A:594:VAL:HG12	1:A:598:LEU:HD23	2.02	0.42
2:B:98:VAL:HB	2:B:126:ILE:HD13	2.01	0.42
2:B:612:LEU:HB3	2:B:635:TRP:HZ3	1.84	0.42
2:D:485:LYS:O	2:D:496:GLY:HA3	2.19	0.42
2:D:510:VAL:HG22	2:D:511:GLY:H	1.84	0.42
1:A:70:ASN:OD1	1:A:72:ILE:HG12	2.20	0.42
1:A:478:GLY:HA2	1:A:813:TRP:CZ3	2.54	0.42
1:A:486:LYS:O	1:A:490:THR:OG1	2.32	0.42
2:B:86:CYS:O	2:B:90:SER:OG	2.35	0.42
2:B:114:PHE:O	2:B:117:ALA:HB3	2.19	0.42
1:C:70:ASN:OD1	1:C:72:ILE:HG12	2.20	0.42
1:C:552:LYS:HD3	1:C:552:LYS:HA	1.86	0.42
2:D:157:MET:HE1	2:D:229:LEU:HD13	2.02	0.42
2:D:553:PRO:HB2	2:D:649:ASN:HD22	1.84	0.42
1:A:538:LEU:HD12	1:A:538:LEU:HA	1.79	0.42
1:A:636:LEU:HD13	1:A:636:LEU:HA	1.81	0.42
1:A:826:PRO:HG3	2:D:656:GLN:HE21	1.84	0.42
2:B:433:THR:OG1	2:B:434:VAL:N	2.52	0.42
2:B:572:VAL:HG21	1:C:845:ILE:HG23	2.02	0.42
2:B:656:GLN:HE21	1:C:826:PRO:HG3	1.84	0.42
1:C:479:PHE:O	1:C:479:PHE:CG	2.72	0.42
1:A:151:TRP:HZ2	1:A:270:VAL:O	2.02	0.42
2:B:289:LEU:CD1	2:B:291:ALA:H	2.28	0.42
2:B:683:PHE:HB3	2:B:728:ALA:HB3	2.01	0.42
2:D:792:LEU:HA	2:D:792:LEU:HD23	1.76	0.42
1:A:228:LEU:HD12	1:A:228:LEU:H	1.85	0.42
1:A:445:PHE:HA	1:A:450:ASP:O	2.20	0.42
1:A:590:SER:O	1:A:594:VAL:HG23	2.19	0.42
2:B:467:LYS:NZ	2:B:788:GLU:OE1	2.26	0.42
1:A:87:VAL:HG12	1:A:89:ALA:H	1.85	0.42
1:A:419:LEU:H	1:A:419:LEU:HG	1.59	0.42
1:C:87:VAL:HG12	1:C:89:ALA:H	1.85	0.42
1:C:419:LEU:H	1:C:419:LEU:HG	1.58	0.42
1:C:445:PHE:HA	1:C:450:ASP:O	2.20	0.42
1:C:692:ARG:HD2	2:D:800:ILE:HD13	2.01	0.42
2:D:204:LEU:C	2:D:205:LEU:HD22	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ALA:O	1:A:664:ILE:HG22	2.20	0.42
2:B:507:TYR:OH	2:B:772:TRP:HD1	2.03	0.42
2:B:510:VAL:HG22	2:B:511:GLY:H	1.84	0.42
1:C:486:LYS:O	1:C:490:THR:OG1	2.32	0.42
2:D:544:THR:HG21	2:D:810:SER:HB2	2.02	0.42
2:B:157:MET:HE1	2:B:229:LEU:HD13	2.02	0.41
2:B:164:TYR:HE2	2:B:386:MET:HE2	1.85	0.41
2:B:781:LEU:HD21	1:C:540:ILE:HG22	2.02	0.41
1:C:143:PRO:HD2	1:C:146:HIS:CE1	2.55	0.41
1:C:169:ASP:N	1:C:218:PHE:O	2.53	0.41
1:C:827:ALA:HB3	1:C:828:THR:HG23	2.02	0.41
2:D:612:LEU:HB3	2:D:635:TRP:HZ3	1.84	0.41
2:D:645:SER:OG	2:D:646:TYR:N	2.52	0.41
2:D:683:PHE:HB3	2:D:728:ALA:HB3	2.01	0.41
2:D:712:ARG:O	2:D:716:ASP:HB2	2.20	0.41
1:A:557:GLN:HG2	1:A:779:PHE:HE1	1.85	0.41
2:B:778:LEU:HA	2:B:778:LEU:HD23	1.80	0.41
1:C:594:VAL:O	1:C:598:LEU:HD23	2.19	0.41
1:A:242:LEU:HD12	1:A:243:SER:N	2.36	0.41
1:A:463:THR:O	1:A:465:PRO:HD3	2.20	0.41
2:B:653:PHE:HD1	1:C:827:ALA:HB2	1.85	0.41
2:B:712:ARG:O	2:B:716:ASP:HB2	2.20	0.41
2:B:818:MET:O	2:B:821:VAL:HG22	2.20	0.41
1:C:692:ARG:O	1:C:693:LEU:HD23	2.20	0.41
1:A:170:ASP:OD1	1:A:172:GLU:N	2.40	0.41
2:B:772:TRP:O	2:B:773:LYS:C	2.63	0.41
2:B:806:ASN:O	2:B:807:GLU:HB2	2.20	0.41
1:C:238:ARG:N	1:C:412:GLY:O	2.54	0.41
1:C:557:GLN:HG2	1:C:779:PHE:HE1	1.84	0.41
2:D:116:SER:HG	2:D:142:MET:H	1.64	0.41
2:D:161:MET:HE2	2:D:169:PHE:CD2	2.55	0.41
2:B:436:CYS:N	2:B:455:LYS:O	2.29	0.41
1:C:183:LEU:HD12	1:C:183:LEU:HA	1.78	0.41
1:C:431:TYR:O	1:C:476:CYS:HA	2.21	0.41
1:C:624:LEU:O	1:C:627:ALA:N	2.53	0.41
1:C:661:ALA:O	1:C:664:ILE:HG22	2.20	0.41
1:A:635:LEU:HA	1:A:635:LEU:HD12	1.81	0.41
1:A:636:LEU:HD11	2:D:637:PHE:HD2	1.86	0.41
1:A:671:ASN:OD1	2:B:654:MET:HG2	2.21	0.41
1:A:798:LEU:HD23	1:A:798:LEU:HA	1.71	0.41
2:B:161:MET:HE2	2:B:169:PHE:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:544:THR:HG21	2:B:810:SER:HB2	2.02	0.41
1:C:463:THR:O	1:C:465:PRO:HD3	2.20	0.41
1:A:238:ARG:HD3	1:A:238:ARG:HA	1.75	0.41
1:A:431:TYR:O	1:A:476:CYS:HA	2.21	0.41
1:A:671:ASN:ND2	2:B:813:LEU:HD21	2.35	0.41
1:A:790:LYS:HE2	1:A:790:LYS:HB3	1.92	0.41
2:B:308:LEU:HD23	2:B:308:LEU:HA	1.84	0.41
2:B:777:ASP:O	2:B:778:LEU:C	2.63	0.41
1:C:594:VAL:HG12	1:C:598:LEU:HD23	2.02	0.41
1:A:115:ARG:HB3	1:A:340:PRO:HD3	2.02	0.41
2:B:532:THR:OG1	2:B:533:GLY:N	2.54	0.41
2:B:533:GLY:O	2:B:733:ALA:N	2.54	0.41
1:C:119:LEU:HA	1:C:138:LEU:O	2.21	0.41
1:C:579:PHE:HB2	1:C:584:TRP:CZ2	2.56	0.41
1:C:719:GLU:O	1:C:721:SER:N	2.54	0.41
1:C:798:LEU:HD23	1:C:798:LEU:HA	1.71	0.41
1:C:830:THR:OG1	1:C:831:CYS:N	2.53	0.41
2:D:164:TYR:HE2	2:D:386:MET:HE2	1.85	0.41
2:D:806:ASN:O	2:D:807:GLU:HB2	2.20	0.41
1:A:580:GLN:NE2	2:B:812:GLN:OE1	2.54	0.41
1:A:624:LEU:O	1:A:627:ALA:N	2.53	0.41
1:A:720:LEU:O	1:A:723:MET:HG2	2.21	0.41
1:A:757:LEU:HA	1:A:757:LEU:HD13	1.81	0.41
2:B:204:LEU:C	2:B:205:LEU:HD22	2.45	0.41
2:B:428:THR:OG1	2:B:429:CYS:N	2.54	0.41
2:B:551:LEU:HD23	2:B:551:LEU:HA	1.86	0.41
1:C:115:ARG:HB3	1:C:340:PRO:HD3	2.02	0.41
1:C:242:LEU:HD12	1:C:243:SER:N	2.36	0.41
1:C:580:GLN:NE2	2:D:812:GLN:OE1	2.53	0.41
1:C:598:LEU:HD13	1:C:650:ALA:HB1	2.02	0.41
1:C:601:LEU:HD23	1:C:601:LEU:HA	1.80	0.41
1:C:720:LEU:O	1:C:723:MET:HG2	2.21	0.41
2:D:40:ILE:O	2:D:41:LEU:HD22	2.21	0.41
2:D:190:ILE:HD13	2:D:190:ILE:HA	1.81	0.41
2:D:423:ASP:OD2	2:D:425:LEU:HB3	2.21	0.41
2:D:428:THR:OG1	2:D:429:CYS:N	2.54	0.41
2:D:498:ILE:HA	2:D:498:ILE:HD13	1.84	0.41
2:D:533:GLY:O	2:D:733:ALA:N	2.54	0.41
2:D:553:PRO:HB2	2:D:649:ASN:ND2	2.36	0.41
2:D:772:TRP:O	2:D:773:LYS:C	2.63	0.41
2:D:818:MET:O	2:D:821:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1:NAG:O6	3:F:2:NAG:N2	2.45	0.41
1:A:119:LEU:HA	1:A:138:LEU:O	2.21	0.41
1:A:169:ASP:N	1:A:218:PHE:O	2.53	0.41
1:A:170:ASP:CG	1:A:171:HIS:N	2.79	0.41
1:A:714:PHE:HD1	1:A:714:PHE:HA	1.73	0.41
2:B:423:ASP:OD2	2:B:425:LEU:HB3	2.21	0.41
2:B:468:ILE:HA	2:B:468:ILE:HD13	1.79	0.41
2:B:553:PRO:HB2	2:B:649:ASN:ND2	2.36	0.41
2:B:749:VAL:HG12	2:B:750:THR:O	2.21	0.41
1:C:316:LEU:HG	1:C:317:LEU:HD12	2.03	0.41
2:D:335:LEU:HD12	2:D:335:LEU:HA	1.88	0.41
2:D:550:PHE:CZ	2:D:551:LEU:HG	2.56	0.41
2:D:615:ASN:C	2:D:617:SER:N	2.78	0.41
1:A:128:TYR:HB3	1:A:137:PHE:CD2	2.56	0.40
2:B:161:MET:HE2	2:B:169:PHE:CD2	2.55	0.40
2:B:550:PHE:CE2	2:B:821:VAL:HG12	2.57	0.40
1:C:240:ILE:HD11	1:C:268:TRP:CZ3	2.56	0.40
2:D:542:ASN:N	2:D:542:ASN:OD1	2.52	0.40
2:D:732:ASP:HB2	2:D:735:VAL:HG12	2.02	0.40
1:A:592:HIS:O	1:A:596:VAL:HG13	2.22	0.40
2:B:635:TRP:O	2:B:638:PHE:HB3	2.21	0.40
1:C:185:GLU:O	1:C:187:ARG:N	2.51	0.40
1:C:680:ARG:HA	1:C:681:PRO:HD3	1.91	0.40
2:D:550:PHE:CE2	2:D:821:VAL:HG12	2.57	0.40
1:A:481:ILE:O	1:A:484:LEU:HB3	2.22	0.40
1:A:704:THR:HG21	1:A:710:VAL:HG11	2.03	0.40
1:C:592:HIS:O	1:C:596:VAL:HG13	2.22	0.40
2:D:777:ASP:O	2:D:778:LEU:C	2.63	0.40
1:A:579:PHE:HB2	1:A:584:TRP:CZ2	2.56	0.40
1:A:692:ARG:O	1:A:693:LEU:HD23	2.20	0.40
1:A:822:ARG:O	1:A:824:ASN:N	2.55	0.40
2:B:40:ILE:O	2:B:41:LEU:HD22	2.21	0.40
2:B:465:LEU:HA	2:B:465:LEU:HD12	1.85	0.40
2:B:732:ASP:HB2	2:B:735:VAL:HG12	2.02	0.40
2:D:641:ILE:HD13	2:D:641:ILE:HA	1.88	0.40
2:D:749:VAL:HG12	2:D:750:THR:O	2.21	0.40
2:D:797:LEU:HD23	2:D:797:LEU:HA	1.75	0.40
1:A:587:VAL:HA	1:A:590:SER:OG	2.22	0.40
1:A:825:ALA:N	1:A:826:PRO:HD3	2.37	0.40
2:B:482:THR:OG1	2:B:483:ASN:N	2.55	0.40
1:C:587:VAL:HA	1:C:590:SER:OG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:436:CYS:N	2:D:455:LYS:O	2.29	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	791/959 (82%)	668 (84%)	123 (16%)	0	100	100
1	C	791/959 (82%)	668 (84%)	123 (16%)	0	100	100
2	B	781/883 (88%)	643 (82%)	138 (18%)	0	100	100
2	D	781/883 (88%)	642 (82%)	139 (18%)	0	100	100
All	All	3144/3684 (85%)	2621 (83%)	523 (17%)	0	100	100

There are no Ramachandran outliers to report.

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	545/826 (66%)	539 (99%)	6 (1%)	65	74
1	C	545/826 (66%)	539 (99%)	6 (1%)	65	74
2	B	552/762 (72%)	549 (100%)	3 (0%)	81	82
2	D	552/762 (72%)	549 (100%)	3 (0%)	81	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2194/3176 (69%)	2176 (99%)	18 (1%)	70	77

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	497	VAL
1	A	572	LEU
1	A	688	ILE
1	A	722	THR
1	A	765	CYS
1	A	794	SER
2	B	332	SER
2	B	410	THR
2	B	667	SER
1	C	497	VAL
1	C	572	LEU
1	C	688	ILE
1	C	722	THR
1	C	765	CYS
1	C	794	SER
2	D	332	SER
2	D	410	THR
2	D	667	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	162	HIS
1	A	171	HIS
1	A	294	ASN
1	A	301	HIS
1	A	425	HIS
1	A	530	GLN
1	A	695	ASN
1	A	731	ASN
1	A	740	GLN
1	A	763	GLN
2	B	95	GLN
2	B	153	GLN
2	B	180	GLN

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Mol	Chain	Res	Type
2	B	333	ASN
2	B	368	ASN
2	B	486	HIS
2	B	656	GLN
2	B	697	ASN
2	B	710	ASN
1	C	47	ASN
1	C	162	HIS
1	C	171	HIS
1	C	177	GLN
1	C	217	GLN
1	C	294	ASN
1	C	301	HIS
1	C	530	GLN
1	C	695	ASN
1	C	717	GLN
1	C	731	ASN
1	C	740	GLN
1	C	748	HIS
1	C	763	GLN
2	D	95	GLN
2	D	153	GLN
2	D	180	GLN
2	D	333	ASN
2	D	368	ASN
2	D	486	HIS
2	D	656	GLN
2	D	697	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	2,3	14,14,15	0.47	0	17,19,21	0.44	0
3	NAG	E	2	3	14,14,15	0.30	0	17,19,21	0.45	0
3	NAG	F	1	2,3	14,14,15	0.47	0	17,19,21	0.44	0
3	NAG	F	2	3	14,14,15	0.30	0	17,19,21	0.45	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	2,3	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	2,3	-	1/6/23/26	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 (6) torsion outliers are listed below:

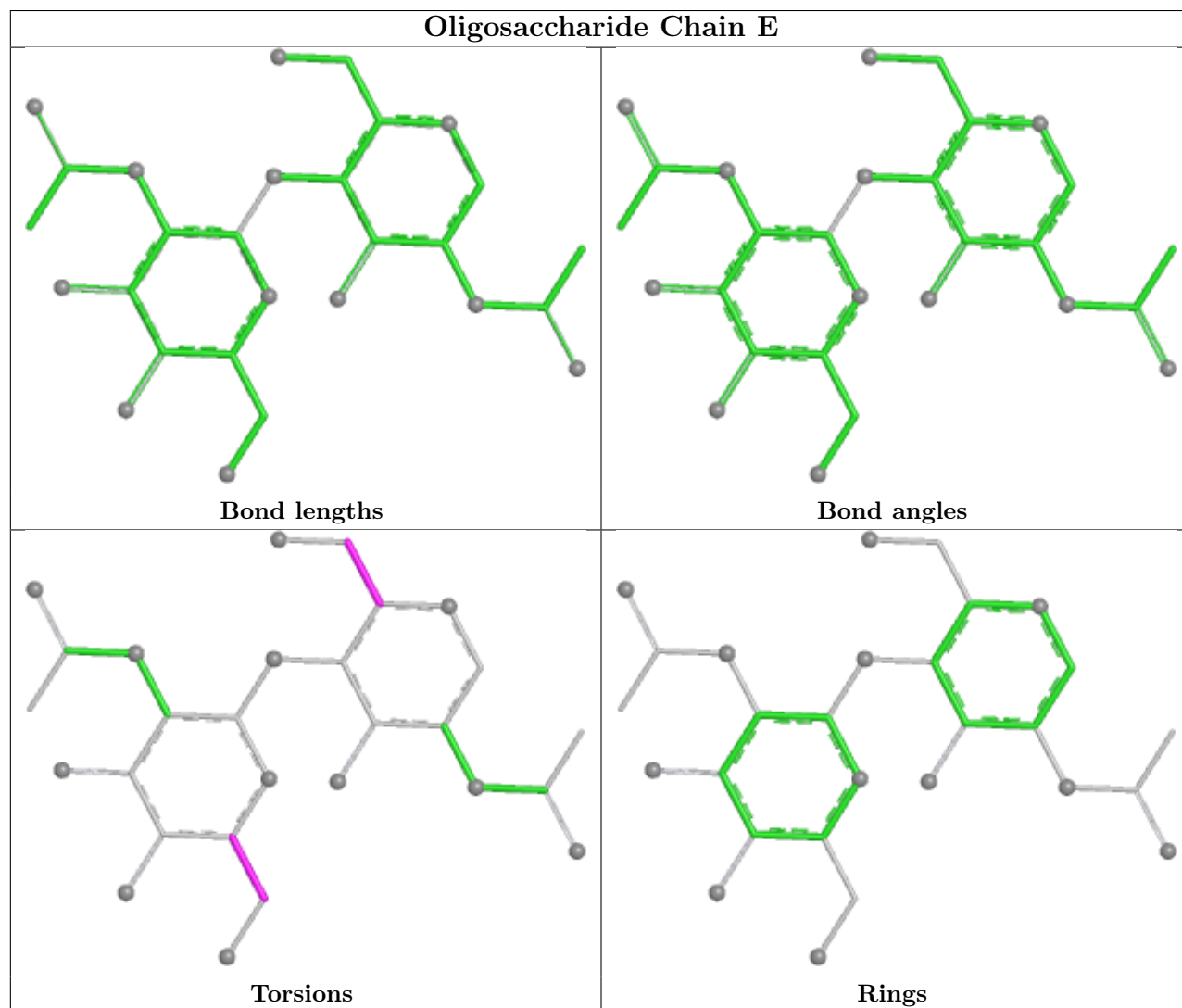
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6

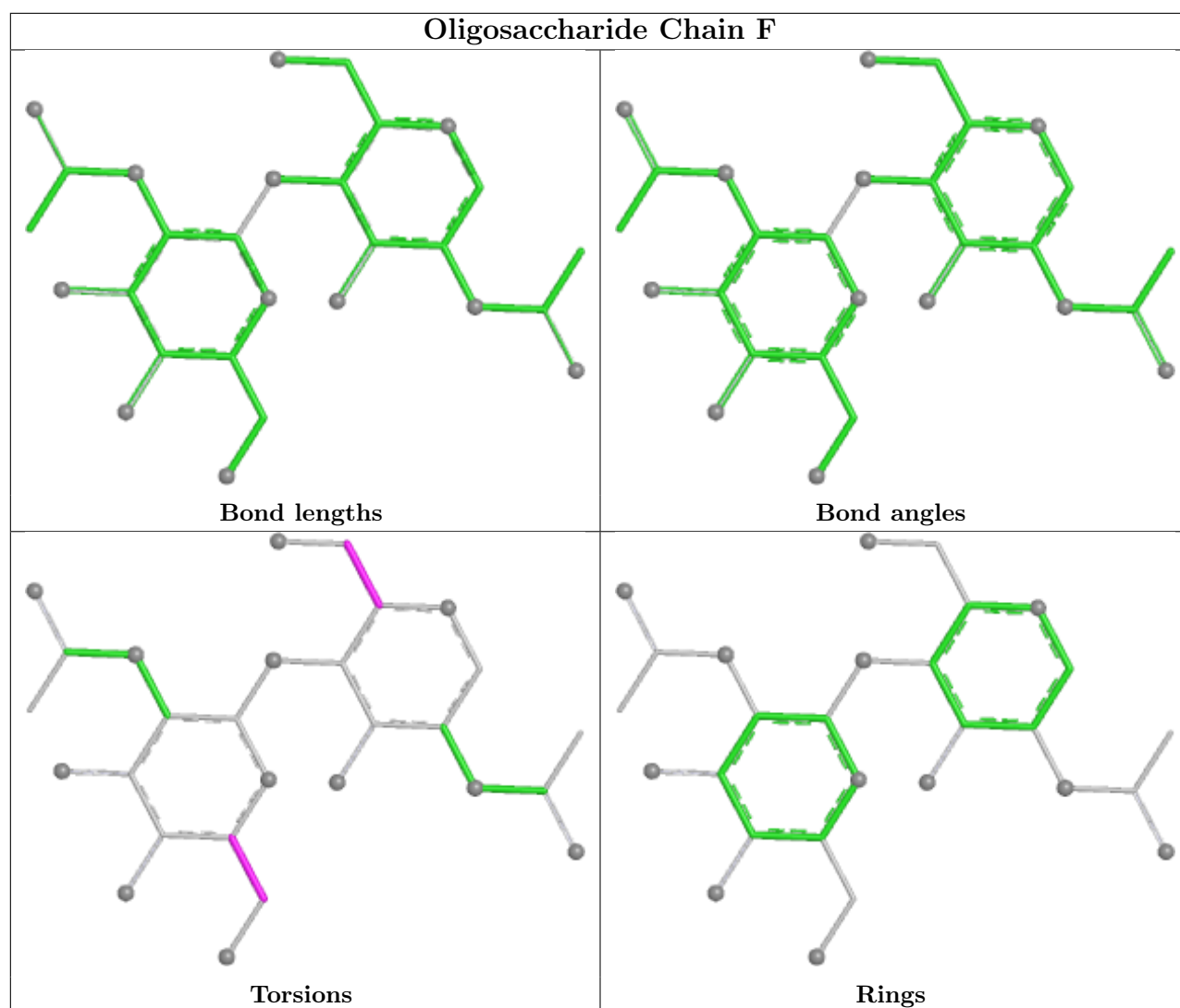
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	1	0
3	F	1	NAG	1	0

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





5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	903	2	14,14,15	0.90	1 (7%)	17,19,21	1.18	1 (5%)
4	NAG	C	1001	1	14,14,15	0.32	0	17,19,21	0.44	0
4	NAG	A	1001	1	14,14,15	0.33	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1002	1	14,14,15	0.30	0	17,19,21	0.54	0
4	NAG	D	904	2	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	D	903	2	14,14,15	0.91	1 (7%)	17,19,21	1.18	1 (5%)
4	NAG	A	1002	1	14,14,15	0.31	0	17,19,21	0.55	0
4	NAG	B	904	2	14,14,15	0.19	0	17,19,21	0.45	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
4	NAG	B	903	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1001	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1002	1	-	2/6/23/26	0/1/1/1
4	NAG	D	904	2	-	2/6/23/26	0/1/1/1
4	NAG	D	903	2	-	0/6/23/26	0/1/1/1
4	NAG	A	1002	1	-	2/6/23/26	0/1/1/1
4	NAG	B	904	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	903	NAG	O5-C1	3.13	1.48	1.43
4	B	903	NAG	O5-C1	3.12	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	903	NAG	C1-O5-C5	4.61	118.37	112.19
4	D	903	NAG	C1-O5-C5	4.57	118.32	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	NAG	O5-C5-C6-O6
4	C	1002	NAG	O5-C5-C6-O6
4	A	1002	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	1002	NAG	C4-C5-C6-O6
4	B	904	NAG	O5-C5-C6-O6
4	D	904	NAG	O5-C5-C6-O6
4	B	904	NAG	C4-C5-C6-O6
4	D	904	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

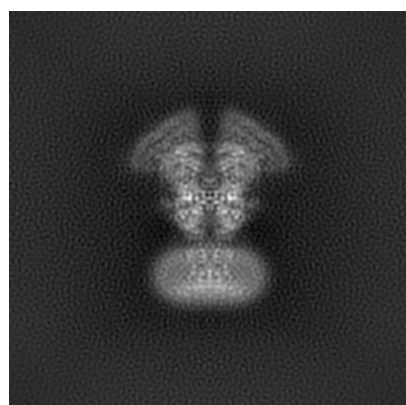
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21674. These allow visual inspection of the internal detail of the map and identification of artifacts.

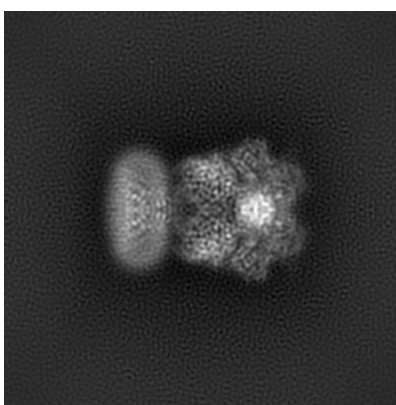
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

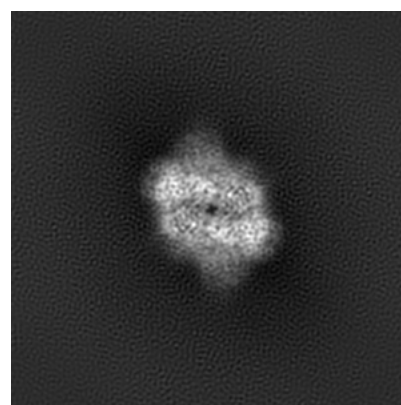
6.1.1 Primary map



X



Y

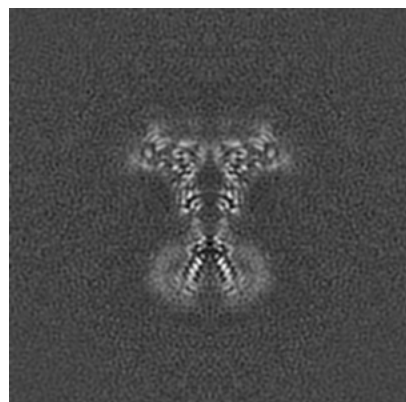


Z

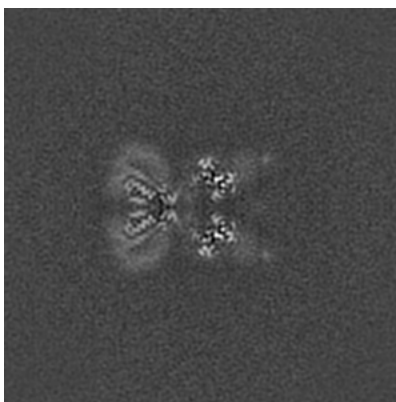
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

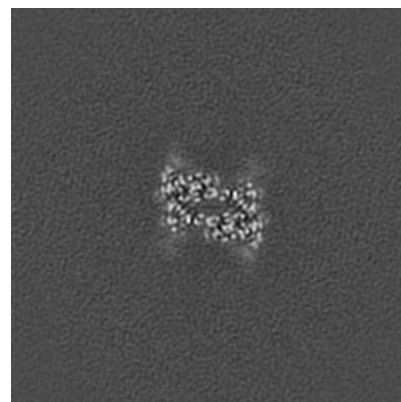
6.2.1 Primary map



X Index: 128



Y Index: 128

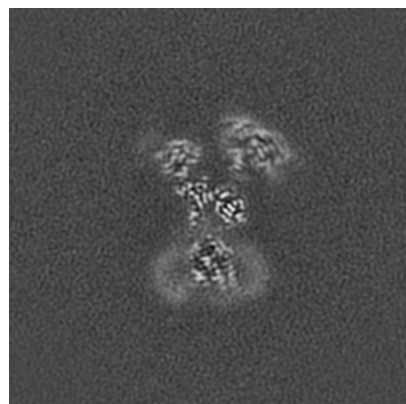


Z Index: 128

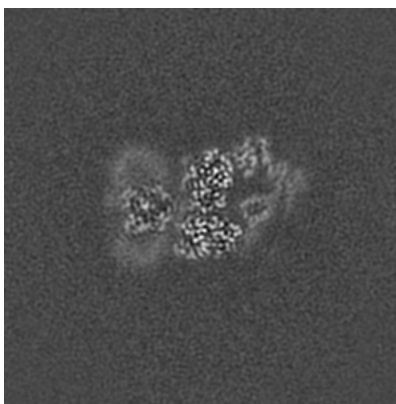
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

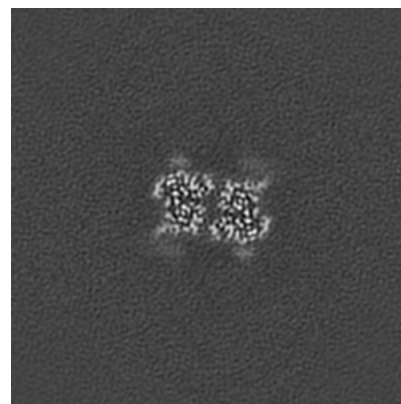
6.3.1 Primary map



X Index: 120



Y Index: 119

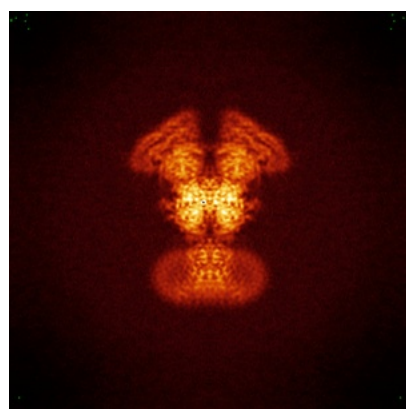


Z Index: 135

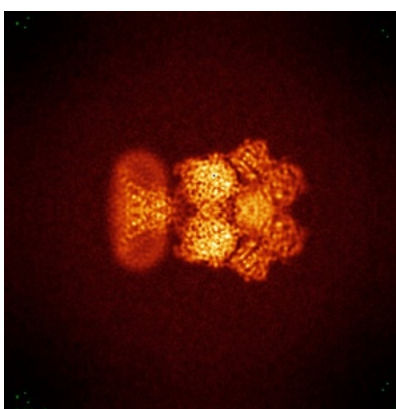
The images above show the largest variance slices of the map in three orthogonal directions.

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

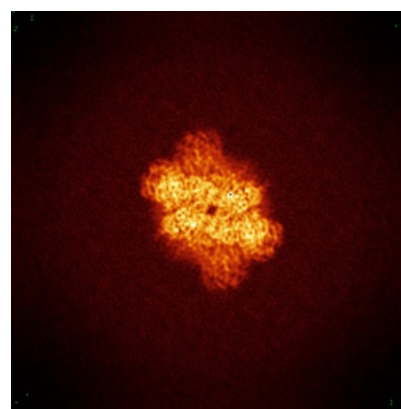
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

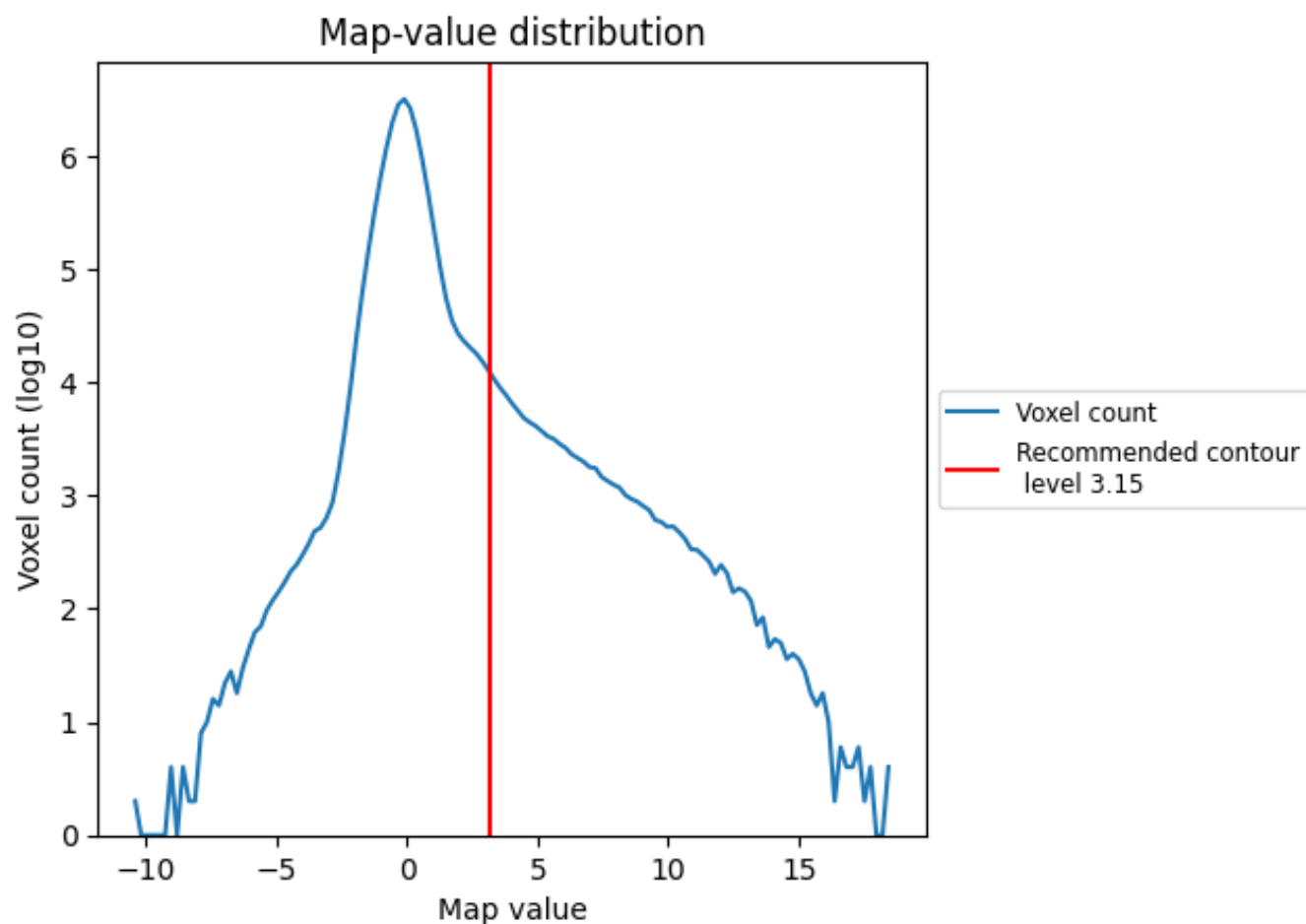
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

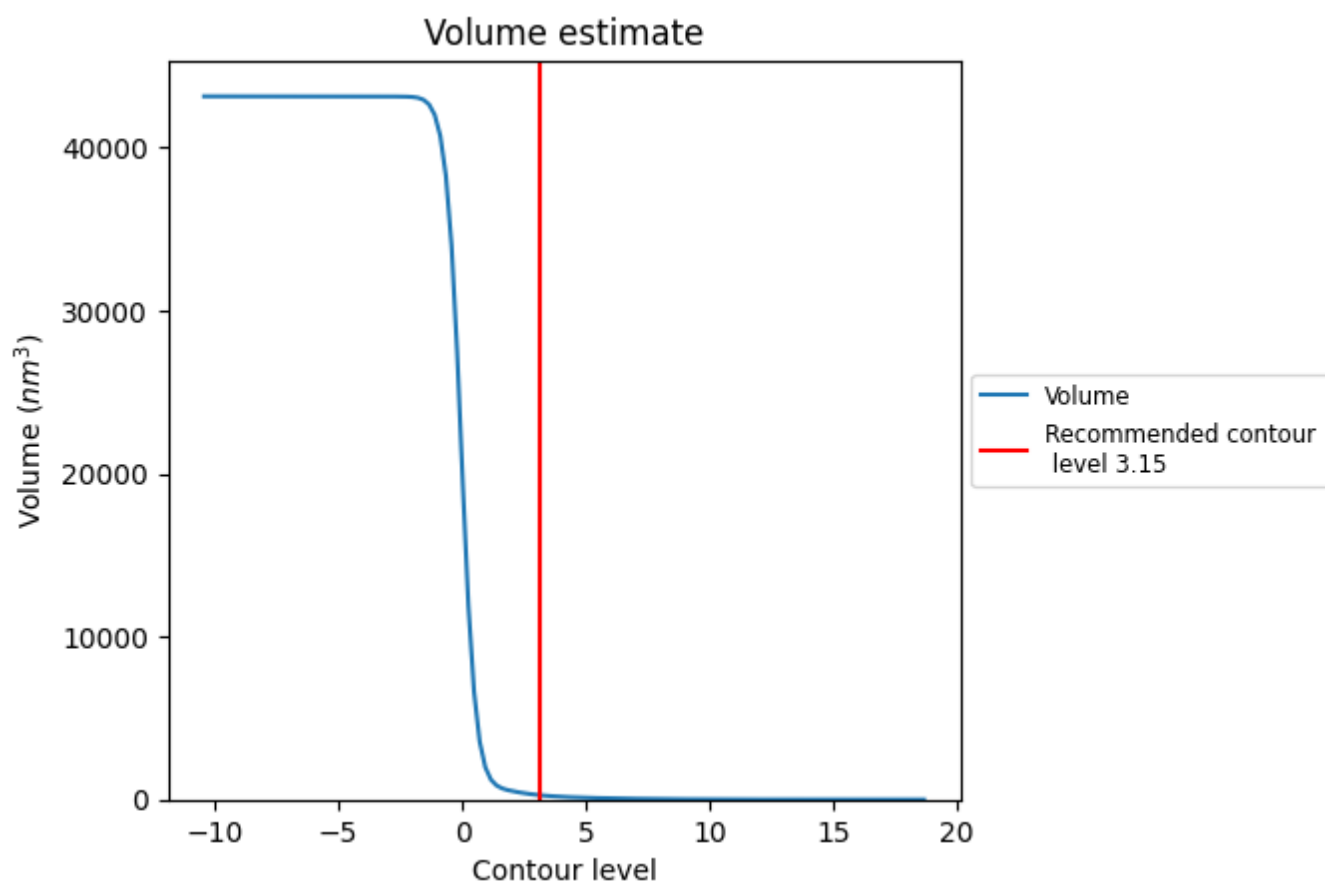
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

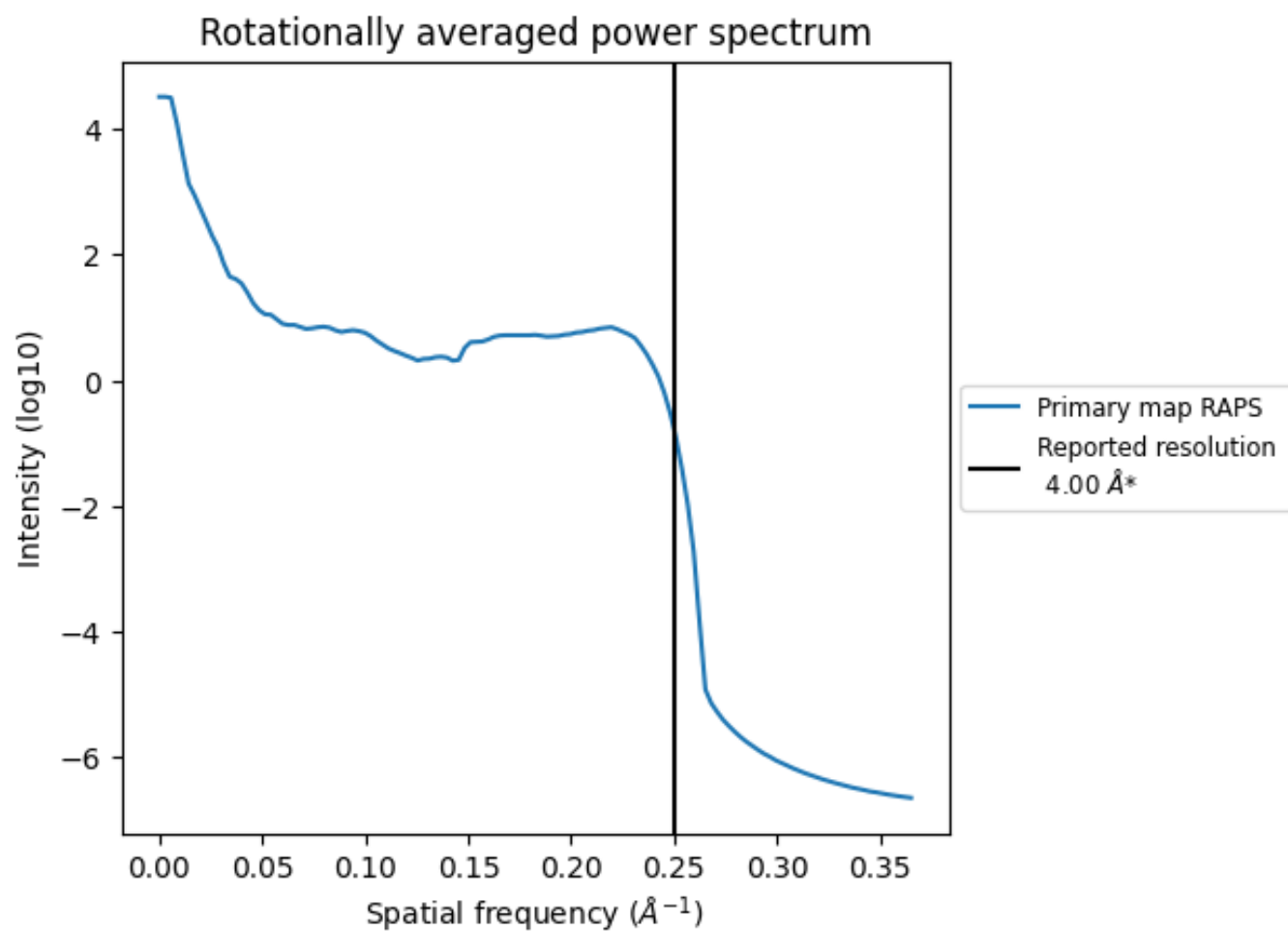
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 268 nm³; this corresponds to an approximate mass of 242 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 0.250 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

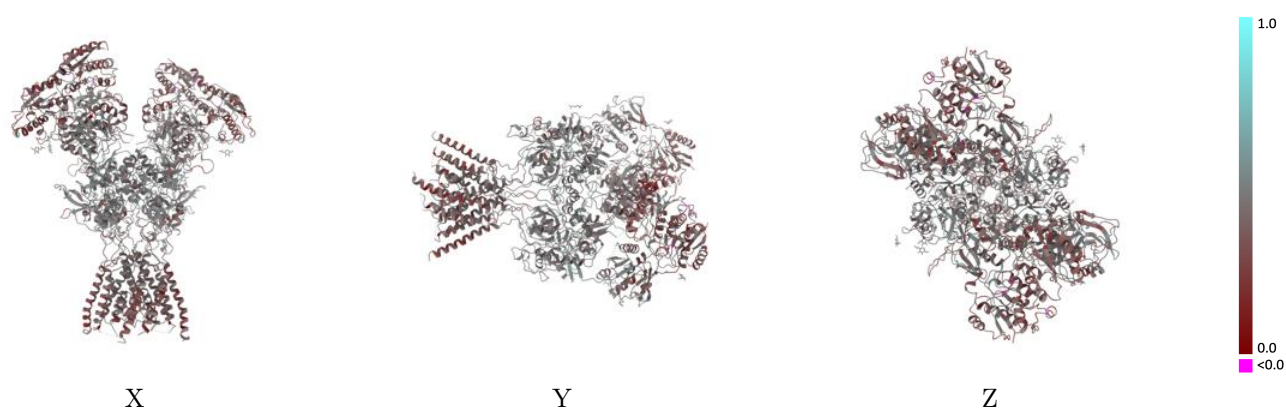
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21674 and PDB model 6WHS. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)

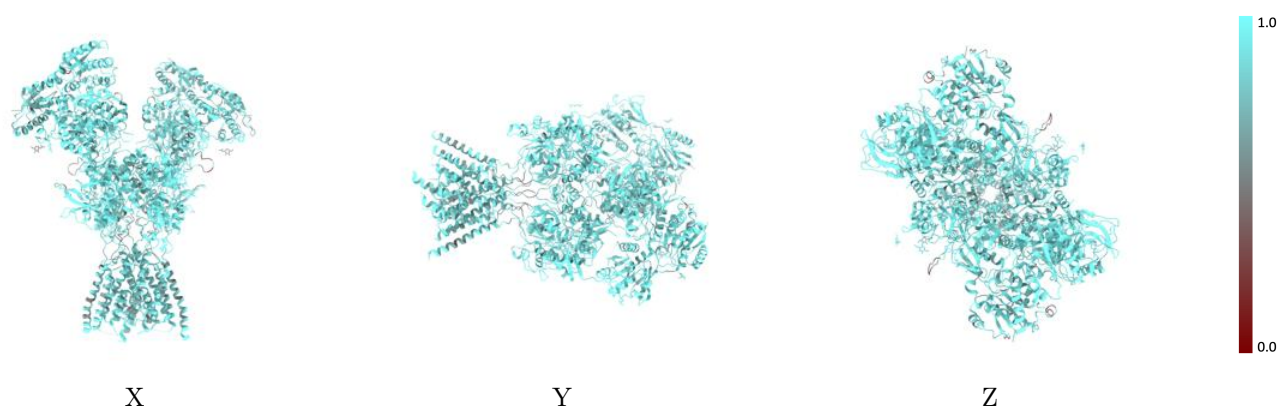
This section was not generated.

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



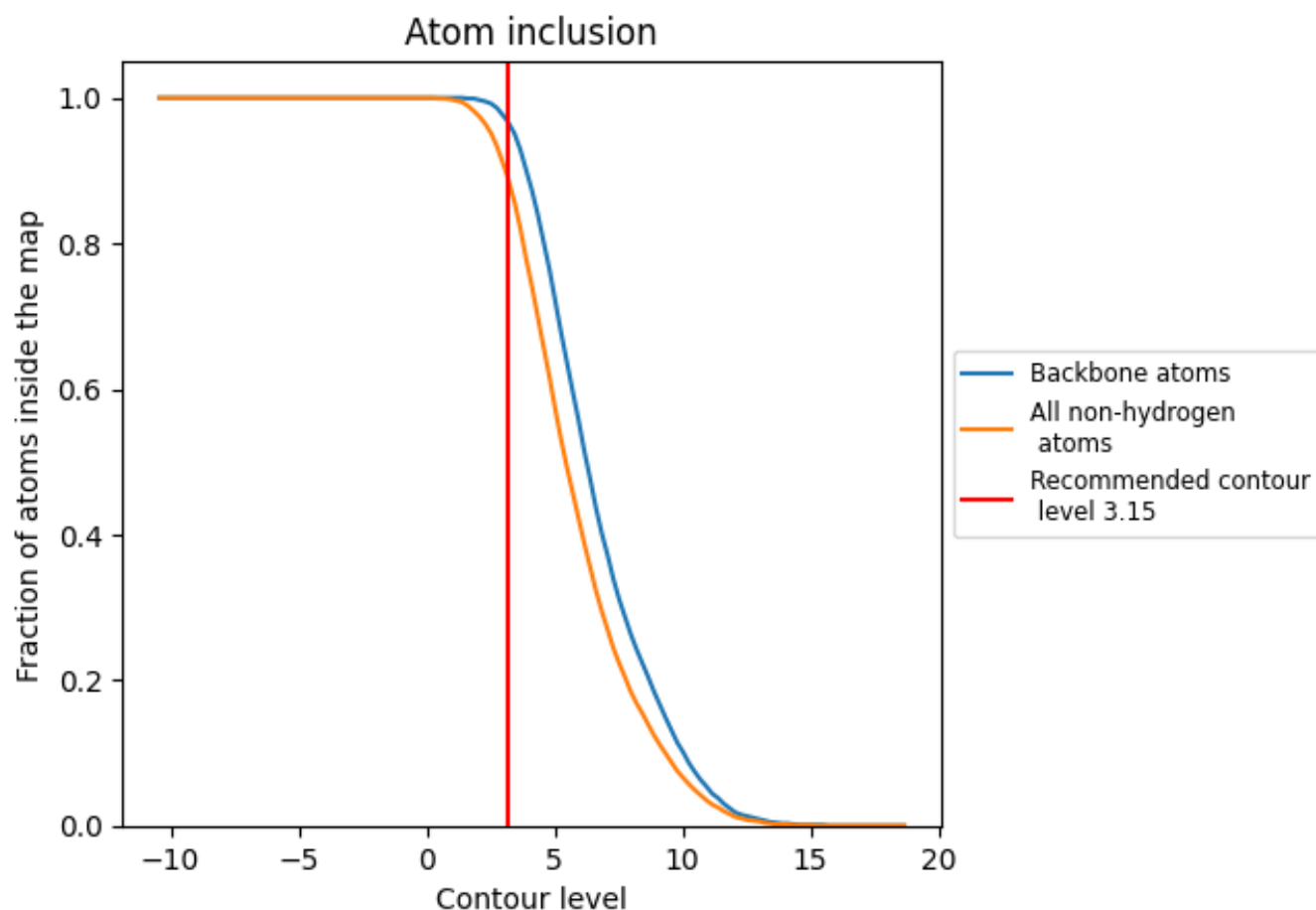
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 89% 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 (3.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8940	0.4210
A	0.9080	0.4240
B	0.8790	0.4180
C	0.9070	0.4250
D	0.8800	0.4190
E	0.8570	0.4780
F	0.8570	0.4880

1.0

0.0

<0.0