



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:10 AM UTC

PDB ID : 7BUD / pdb_00007bud
EMDB ID : EMD-30195
Title : Cryo-EM structure of Dengue virus serotype 2 complexed with Fab SIgN-3C at pH 8.0
Authors : Zhang, S.; Chew, S.V.; Lim, X.N.; Ng, T.S.; Kostyuchenko, V.A.; Lok, S.M.
Deposited on : 2020-04-06
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

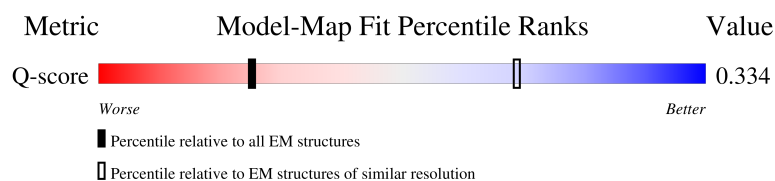
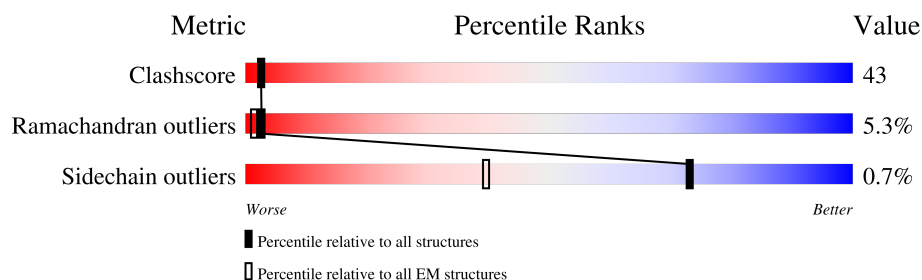
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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	G	132	30% 42% 55% ..
1	H	132	32% 42% 51% 5% .
2	I	107	32% 44% 54% .
2	L	107	30% 44% 53% ..

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Mol	Chain	Length	Quality of chain
3	A	495	25% 34% 60% • •
3	B	495	27% 36% 55% 8% •
3	C	495	26% 38% 51% 9% •
4	D	72	40% 40% 51% • 6%
4	E	72	35% 40% 56% • •
4	F	72	39% 43% 54% • •
5	J	2	50% 50% 50%
5	K	2	100% 50% 50%
5	M	2	100% 50% 50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16338 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 SIgN-3C Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	132	Total	C	N	O	S	0	0
			961	590	173	193	5		
1	H	132	Total	C	N	O	S	0	0
			976	604	174	193	5		

- Molecule 2 is a protein called SIgN-3C Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	107	Total	C	N	O	S	0	0
			834	526	139	167	2		
2	L	107	Total	C	N	O	S	0	0
			834	526	139	167	2		

- Molecule 3 is a protein called Dengue virus serotype 2 E protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	495	Total	C	N	O	S	0	0
			3644	2352	644	619	29		
3	A	495	Total	C	N	O	S	0	0
			3650	2356	645	619	30		
3	C	495	Total	C	N	O	S	0	0
			3638	2351	641	616	30		

- Molecule 4 is a protein called Dengue virus serotype 2 M protein.

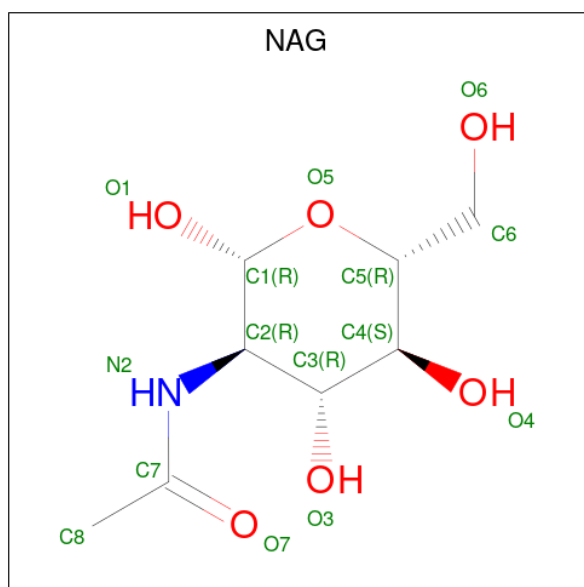
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	72	Total	C	N	O	S	0	0
			559	371	96	89	3		
4	D	72	Total	C	N	O	S	0	0
			560	372	96	89	3		
4	F	72	Total	C	N	O	S	0	0
			556	370	94	89	3		

- Molecule 5 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
5	J	2	Total	C	N	O	0	0
			28	16	2	10		
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	M	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

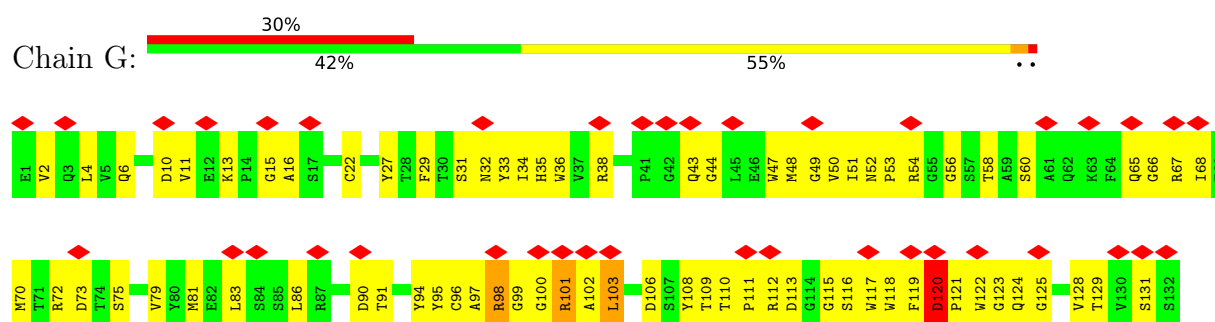


Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

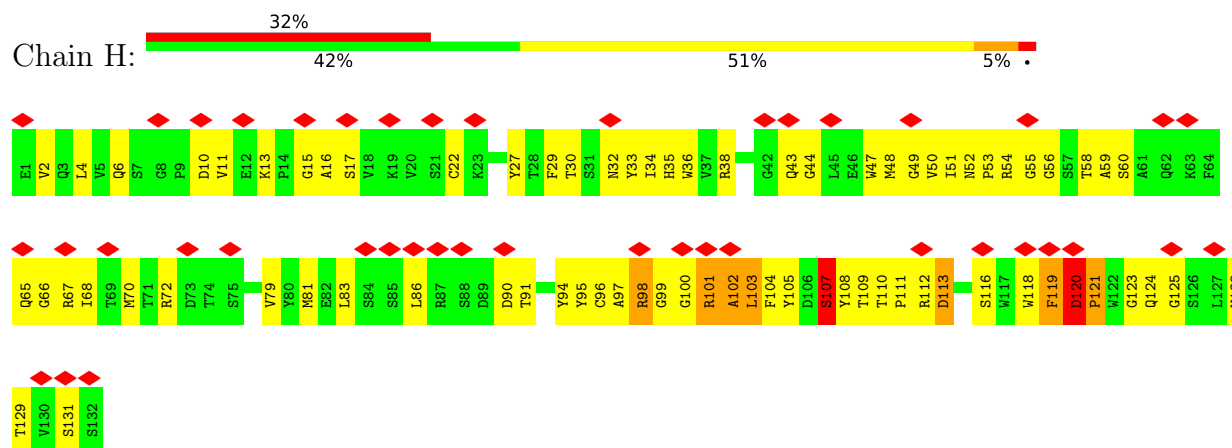
3 Residue-property plots

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.

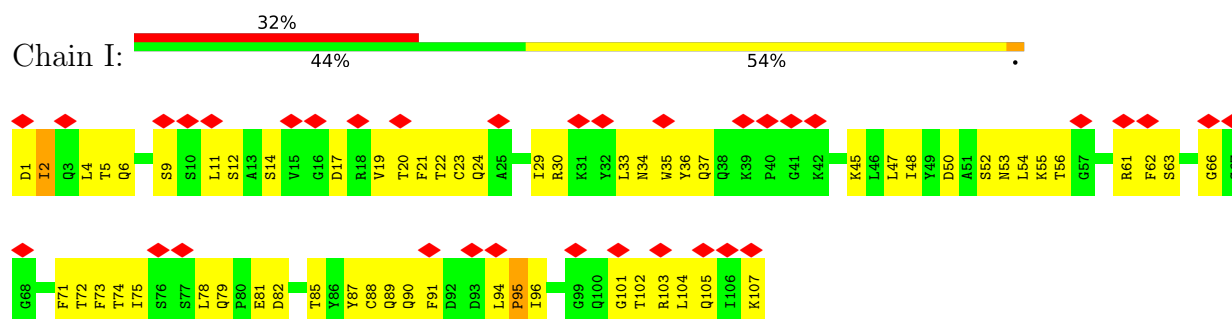
- Molecule 1: SIgN-3C Fab heavy chain



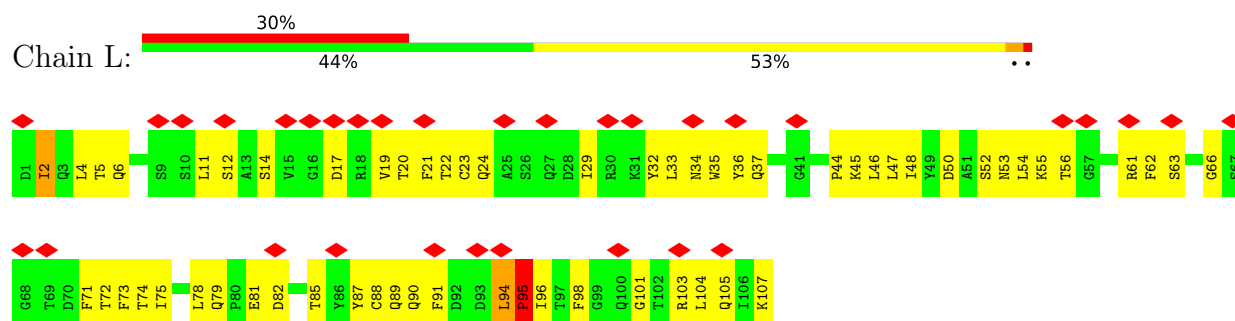
- Molecule 1: SIgN-3C Fab heavy chain



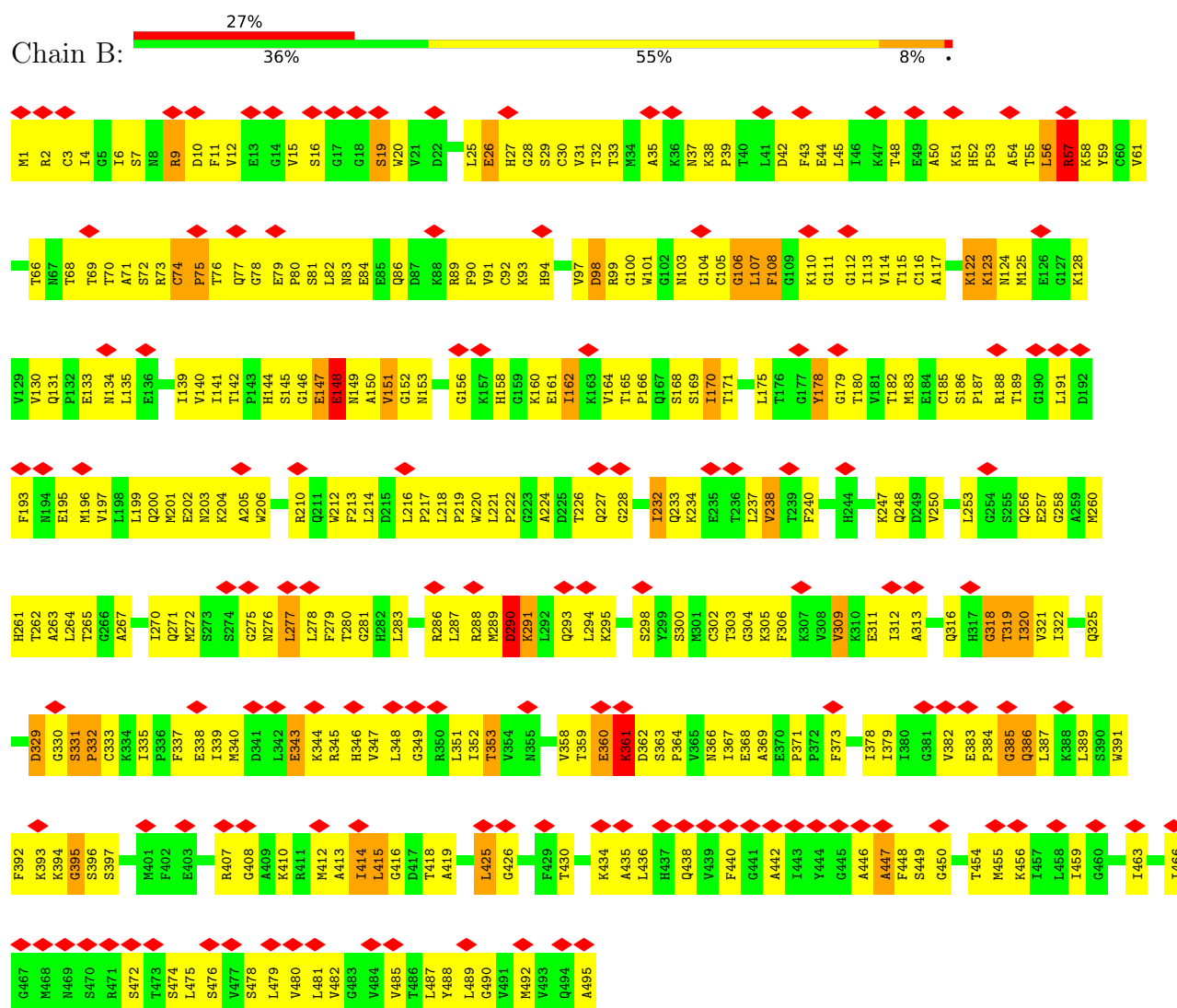
- Molecule 2: SIgN-3C Fab light chain



- Molecule 2: SIgN-3C Fab light chain

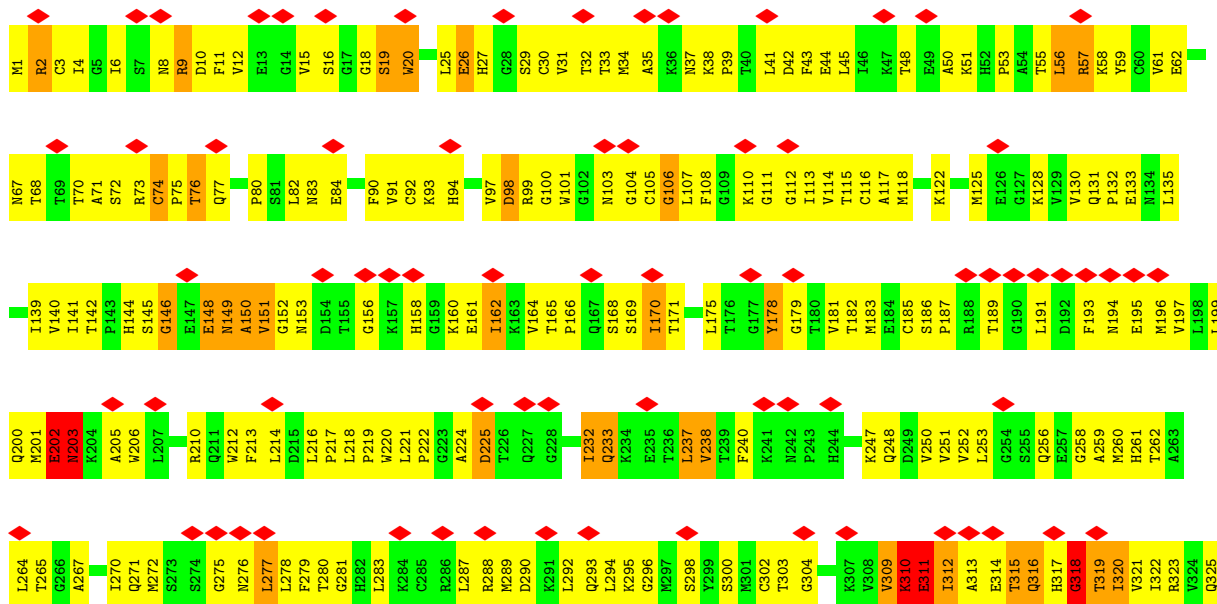


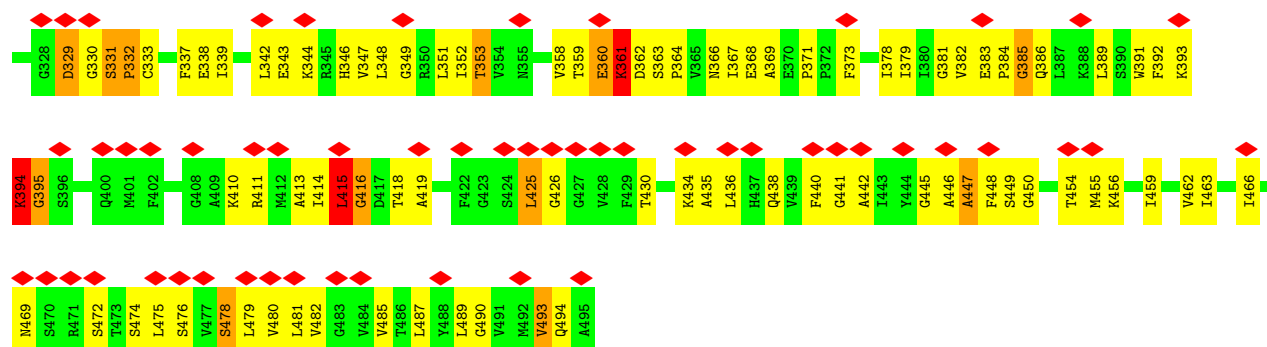
- Molecule 3: Dengue virus serotype 2 E protein



- Molecule 3: Dengue virus serotype 2 E protein

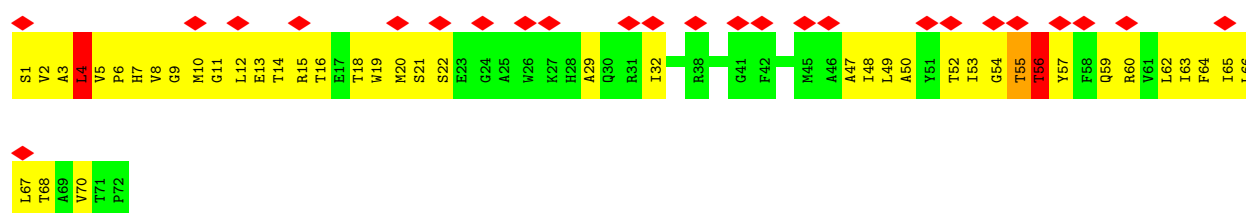






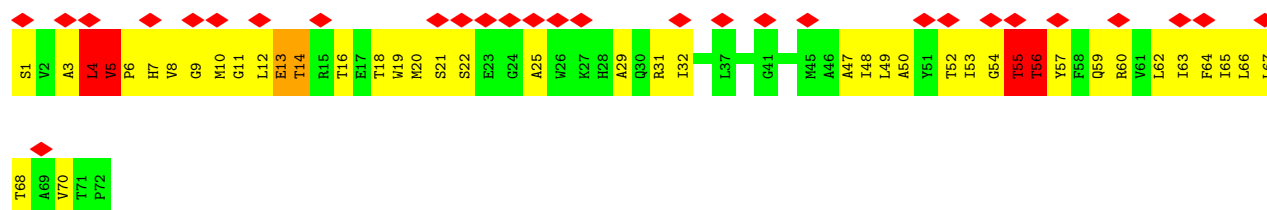
• Molecule 4: Dengue virus serotype 2 M protein

Chain E: 35% 40% 56%



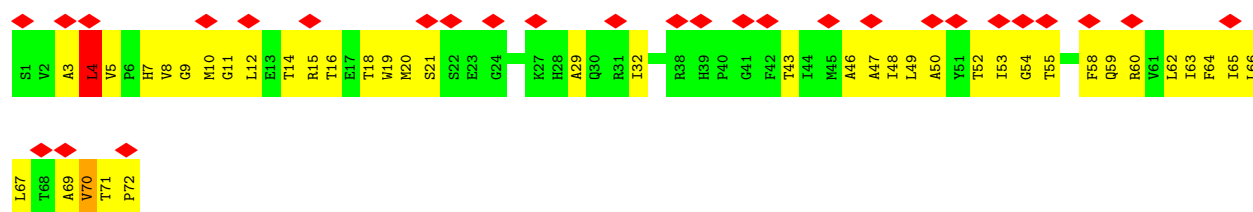
• Molecule 4: Dengue virus serotype 2 M protein

Chain D: 40% 40% 51% 6%



• Molecule 4: Dengue virus serotype 2 M protein

Chain F: 39% 43% 54%



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 50% 50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 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	9607	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 ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	12.013	Depositor
Minimum map value	-6.679	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.8	Depositor
Map size (Å)	696.32, 696.32, 696.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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	G	0.52	1/979 (0.1%)	0.90	7/1324 (0.5%)
1	H	0.51	0/997	0.96	8/1349 (0.6%)
2	I	0.46	0/852	0.78	1/1154 (0.1%)
2	L	0.45	0/852	0.78	1/1154 (0.1%)
3	A	0.51	0/3726	1.10	25/5040 (0.5%)
3	B	0.50	0/3720	0.94	14/5032 (0.3%)
3	C	0.50	0/3714	0.98	16/5022 (0.3%)
4	D	0.47	0/576	0.88	4/787 (0.5%)
4	E	0.43	0/575	0.87	2/786 (0.3%)
4	F	0.48	0/572	1.01	4/782 (0.5%)
All	All	0.50	1/16563 (0.0%)	0.97	82/22430 (0.4%)

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	G	0	4
1	H	0	3
3	A	0	24
3	B	0	24
3	C	0	29
4	D	0	4
4	E	0	3
4	F	0	1
All	All	0	92

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	116	SER	CA-CB	-5.43	1.44	1.53

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	74	CYS	CA-C-N	-14.89	101.23	119.84
3	A	74	CYS	C-N-CA	-14.89	101.23	119.84
3	A	314	GLU	CA-C-N	12.49	145.41	121.54
3	A	314	GLU	C-N-CA	12.49	145.41	121.54
3	A	396	SER	CA-C-N	-11.64	108.59	122.44
3	A	396	SER	C-N-CA	-11.64	108.59	122.44
2	L	95	PRO	N-CA-C	-11.48	88.82	112.47
2	I	95	PRO	N-CA-C	-11.47	88.84	112.47
3	A	396	SER	N-CA-C	10.70	133.59	110.80
3	A	309	VAL	CA-C-N	9.44	142.77	121.53
3	A	309	VAL	C-N-CA	9.44	142.77	121.53
1	H	102	ALA	CA-C-N	-9.16	104.05	121.54
1	H	102	ALA	C-N-CA	-9.16	104.05	121.54
3	C	311	GLU	CA-C-N	9.04	138.24	121.97
3	C	311	GLU	C-N-CA	9.04	138.24	121.97
3	C	149	ASN	N-CA-C	8.89	123.71	112.86
3	B	395	GLY	CA-C-N	-8.41	105.47	121.54
3	B	395	GLY	C-N-CA	-8.41	105.47	121.54
3	A	314	GLU	N-CA-C	8.34	120.06	110.97
1	H	107	SER	CA-C-N	8.19	133.12	120.75
1	H	107	SER	C-N-CA	8.19	133.12	120.75
3	C	415	LEU	N-CA-C	7.96	124.03	113.20
3	B	395	GLY	O-C-N	-7.45	115.41	122.86
1	H	120	ASP	C-N-CD	-7.35	94.85	125.00
1	G	120	ASP	C-N-CD	-7.28	95.16	125.00
3	B	309	VAL	CA-C-N	7.18	135.26	121.54
3	B	309	VAL	C-N-CA	7.18	135.26	121.54
3	C	20	TRP	CA-CB-CG	7.00	126.91	113.60
3	A	343	GLU	CB-CA-C	-6.91	107.57	115.79
1	G	115	GLY	CA-C-N	6.67	134.28	121.54
1	G	115	GLY	C-N-CA	6.67	134.28	121.54
3	A	75	PRO	N-CA-C	6.53	125.93	112.47
3	A	134	ASN	CA-C-N	6.51	133.40	121.94
3	A	134	ASN	C-N-CA	6.51	133.40	121.94
3	C	318	GLY	N-CA-C	6.30	117.47	111.67
1	G	103	LEU	CA-C-N	6.26	128.58	120.44
1	G	103	LEU	C-N-CA	6.26	128.58	120.44
1	H	98	ARG	N-CA-C	6.25	118.68	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	318	GLY	N-CA-C	6.24	117.41	111.67
3	C	20	TRP	N-CA-CB	-6.21	100.65	110.77
1	G	98	ARG	N-CA-C	6.21	118.62	109.69
4	F	4	LEU	CA-C-N	6.19	133.58	122.13
4	F	4	LEU	C-N-CA	6.19	133.58	122.13
3	C	415	LEU	CA-C-N	6.08	133.33	121.41
3	C	415	LEU	C-N-CA	6.08	133.33	121.41
3	B	148	GLU	CA-C-N	6.02	133.04	121.54
3	B	148	GLU	C-N-CA	6.02	133.04	121.54
3	C	232	ILE	CA-C-N	5.98	132.96	121.54
3	C	232	ILE	C-N-CA	5.98	132.96	121.54
3	A	20	TRP	CA-C-N	5.93	128.76	122.11
3	A	20	TRP	C-N-CA	5.93	128.76	122.11
3	A	57	ARG	CA-C-N	-5.89	114.49	122.86
3	A	57	ARG	C-N-CA	-5.89	114.49	122.86
1	G	115	GLY	O-C-N	5.84	130.29	122.70
3	A	385	GLY	CA-C-N	5.82	132.66	121.54
3	A	385	GLY	C-N-CA	5.82	132.66	121.54
3	A	108	PHE	N-CA-C	5.68	117.56	110.91
4	D	5	VAL	CA-C-N	-5.62	114.33	121.91
4	D	5	VAL	C-N-CA	-5.62	114.33	121.91
3	A	377	TYR	CA-CB-CG	5.43	123.67	113.90
1	H	101	ARG	CA-C-N	5.40	130.80	120.97
1	H	101	ARG	C-N-CA	5.40	130.80	120.97
3	B	57	ARG	CA-C-N	-5.38	115.23	122.86
3	B	57	ARG	C-N-CA	-5.38	115.23	122.86
3	C	20	TRP	CA-C-N	-5.27	115.21	122.69
3	C	20	TRP	C-N-CA	-5.27	115.21	122.69
3	B	108	PHE	N-CA-C	5.24	117.57	111.02
4	E	4	LEU	CA-C-N	5.19	131.73	122.13
4	E	4	LEU	C-N-CA	5.19	131.73	122.13
4	F	21	SER	CA-C-N	5.18	129.91	122.40
4	F	21	SER	C-N-CA	5.18	129.91	122.40
3	B	122	LYS	CA-C-N	5.08	131.25	121.54
3	B	122	LYS	C-N-CA	5.08	131.25	121.54
4	D	55	THR	O-C-N	-5.08	115.83	122.59
3	C	247	LYS	CA-C-N	5.08	131.24	121.54
3	C	247	LYS	C-N-CA	5.08	131.24	121.54
3	B	415	LEU	CA-C-N	-5.06	113.77	123.29
3	B	415	LEU	C-N-CA	-5.06	113.77	123.29
3	C	296	GLY	O-C-N	-5.06	116.12	122.70
3	A	122	LYS	CA-C-N	5.05	131.19	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	122	LYS	C-N-CA	5.05	131.19	121.54
4	D	4	LEU	O-C-N	-5.03	116.49	123.12

There are no chirality outliers.

All (92) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	106	GLY	Peptide
3	A	122	LYS	Peptide
3	A	133	GLU	Peptide
3	A	147	GLU	Peptide
3	A	148	GLU	Mainchain
3	A	178	TYR	Peptide
3	A	26	GLU	Peptide
3	A	277	LEU	Peptide
3	A	290	ASP	Peptide
3	A	315	THR	Mainchain
3	A	318	GLY	Peptide
3	A	329	ASP	Peptide
3	A	343	GLU	Peptide
3	A	346	HIS	Peptide
3	A	348	LEU	Peptide
3	A	349	GLY	Peptide
3	A	353	THR	Peptide
3	A	361	LYS	Peptide
3	A	395	GLY	Peptide
3	A	396	SER	Peptide
3	A	447	ALA	Peptide
3	A	56	LEU	Peptide
3	A	75	PRO	Peptide
3	A	9	ARG	Peptide
3	B	106	GLY	Peptide
3	B	122	LYS	Peptide
3	B	148	GLU	Mainchain
3	B	178	TYR	Peptide
3	B	19	SER	Peptide
3	B	26	GLU	Peptide
3	B	277	LEU	Peptide
3	B	290	ASP	Peptide
3	B	309	VAL	Mainchain
3	B	318	GLY	Peptide
3	B	329	ASP	Peptide

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Mol	Chain	Res	Type	Group
3	B	343	GLU	Peptide
3	B	346	HIS	Peptide
3	B	348	LEU	Peptide
3	B	349	GLY	Peptide
3	B	353	THR	Peptide
3	B	361	LYS	Peptide
3	B	385	GLY	Peptide,Mainchain
3	B	447	ALA	Peptide
3	B	56	LEU	Peptide
3	B	74	CYS	Peptide
3	B	75	PRO	Peptide
3	B	9	ARG	Peptide
3	C	106	GLY	Mainchain
3	C	107	LEU	Peptide
3	C	146	GLY	Peptide
3	C	148	GLU	Peptide,Mainchain
3	C	178	TYR	Peptide
3	C	18	GLY	Mainchain
3	C	202	GLU	Mainchain
3	C	203	ASN	Peptide
3	C	224	ALA	Peptide
3	C	237	LEU	Peptide
3	C	26	GLU	Mainchain
3	C	277	LEU	Peptide
3	C	309	VAL	Mainchain
3	C	310	LYS	Peptide
3	C	315	THR	Mainchain
3	C	318	GLY	Peptide
3	C	329	ASP	Peptide
3	C	346	HIS	Peptide
3	C	348	LEU	Peptide
3	C	349	GLY	Peptide
3	C	353	THR	Peptide
3	C	361	LYS	Peptide
3	C	394	LYS	Peptide
3	C	415	LEU	Peptide
3	C	447	ALA	Peptide
3	C	56	LEU	Peptide
3	C	74	CYS	Peptide
3	C	9	ARG	Peptide
4	D	4	LEU	Mainchain
4	D	5	VAL	Peptide

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Mol	Chain	Res	Type	Group
4	D	55	THR	Peptide
4	D	56	THR	Peptide
4	E	4	LEU	Mainchain
4	E	55	THR	Peptide
4	E	56	THR	Peptide
4	F	4	LEU	Mainchain
1	G	100	GLY	Peptide
1	G	101	ARG	Peptide
1	G	102	ALA	Peptide
1	G	106	ASP	Peptide
1	H	100	GLY	Peptide
1	H	103	LEU	Peptide
1	H	107	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	961	0	910	101	0
1	H	976	0	925	113	0
2	I	834	0	814	60	0
2	L	834	0	813	100	0
3	A	3650	0	3714	375	0
3	B	3644	0	3708	317	0
3	C	3638	0	3703	321	0
4	D	560	0	579	58	0
4	E	559	0	577	43	0
4	F	556	0	572	54	0
5	J	28	0	25	0	0
5	K	28	0	25	1	0
5	M	28	0	25	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
All	All	16338	0	16429	1398	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 43.

All (1398) 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:H:118:TRP:CZ2	2:L:98:PHE:HZ	1.20	1.60
1:H:118:TRP:CZ2	2:L:98:PHE:CZ	2.00	1.48
1:H:118:TRP:HZ2	2:L:98:PHE:CZ	1.30	1.44
1:G:120:ASP:HB2	1:G:121:PRO:CD	1.41	1.39
2:L:2:ILE:HG22	2:L:90:GLN:OE1	1.20	1.36
1:H:119:PHE:CG	2:L:45:LYS:O	1.82	1.33
1:G:4:LEU:HD12	1:G:121:PRO:O	1.21	1.30
1:H:119:PHE:O	2:L:45:LYS:HA	1.15	1.29
1:H:119:PHE:CD2	2:L:45:LYS:O	1.90	1.22
1:G:120:ASP:HB2	1:G:121:PRO:HD3	1.24	1.19
1:H:119:PHE:CG	2:L:45:LYS:C	2.17	1.19
1:G:4:LEU:CD1	1:G:121:PRO:O	1.91	1.17
1:G:120:ASP:CB	1:G:121:PRO:CD	2.20	1.16
1:H:118:TRP:CE2	2:L:98:PHE:HZ	1.64	1.15
2:L:91:PHE:CZ	2:L:94:LEU:HD21	1.81	1.14
2:I:91:PHE:CZ	2:I:94:LEU:HD21	1.85	1.11
1:G:97:ALA:HB2	1:G:122:TRP:CB	1.82	1.10
1:G:120:ASP:CB	1:G:121:PRO:HD3	1.78	1.08
3:C:58:LYS:HB3	3:C:221:LEU:HB3	1.38	1.05
2:L:2:ILE:CG2	2:L:90:GLN:OE1	2.05	1.04
1:G:120:ASP:HB2	1:G:121:PRO:HD2	1.06	1.01
1:H:120:ASP:CB	1:H:121:PRO:HD3	1.72	1.01
1:G:97:ALA:HB2	1:G:122:TRP:CA	1.90	1.00
1:H:120:ASP:HB3	1:H:121:PRO:HD3	1.01	1.00
3:B:78:GLY:H	3:A:56:LEU:HD22	1.24	1.00
1:G:96:CYS:O	1:G:122:TRP:O	1.79	1.00
2:L:2:ILE:HG22	2:L:90:GLN:CD	1.85	0.99
1:H:119:PHE:O	2:L:45:LYS:CA	2.11	0.98
3:A:452:SER:HA	3:A:494:GLN:HE22	1.25	0.98
1:H:119:PHE:CD1	2:L:45:LYS:O	2.14	0.98
1:H:33:TYR:O	1:H:98:ARG:HA	1.64	0.97
1:G:97:ALA:HB2	1:G:122:TRP:HA	1.47	0.97
3:B:78:GLY:HA2	3:A:56:LEU:HD13	1.42	0.96
1:G:33:TYR:O	1:G:98:ARG:HA	1.63	0.96
1:H:118:TRP:CE2	2:L:98:PHE:CZ	2.47	0.94
3:C:310:LYS:HG2	3:C:311:GLU:HB3	1.45	0.94
3:A:105:CYS:HA	1:H:111:PRO:HG3	1.48	0.93
1:H:33:TYR:HE2	1:H:101:ARG:HB2	1.32	0.92
1:G:4:LEU:CD1	1:G:122:TRP:C	2.42	0.92
2:L:91:PHE:HZ	2:L:94:LEU:HD21	1.34	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:101:TRP:CZ2	3:C:310:LYS:HD2	2.06	0.91
1:G:4:LEU:HD12	1:G:122:TRP:C	1.96	0.90
3:C:237:LEU:HD23	3:C:238:VAL:H	1.38	0.89
1:G:120:ASP:CB	1:G:121:PRO:HD2	1.96	0.89
1:H:120:ASP:HB3	1:H:121:PRO:CD	1.97	0.89
1:H:33:TYR:CE2	1:H:101:ARG:HB2	2.08	0.88
3:C:302:CYS:SG	3:C:303:THR:N	2.47	0.88
2:L:91:PHE:CZ	2:L:94:LEU:CD2	2.55	0.88
3:A:125:MET:HB3	3:A:199:LEU:HD11	1.57	0.87
3:C:200:GLN:NE2	3:C:272:MET:SD	2.47	0.87
3:C:125:MET:HB3	3:C:199:LEU:HD11	1.57	0.87
3:A:302:CYS:SG	3:A:303:THR:N	2.47	0.86
3:A:200:GLN:NE2	3:A:272:MET:SD	2.47	0.86
1:G:4:LEU:HD13	1:G:122:TRP:O	1.74	0.86
3:B:200:GLN:NE2	3:B:272:MET:SD	2.47	0.85
3:B:125:MET:HB3	3:B:199:LEU:HD11	1.57	0.85
3:A:4:ILE:HD13	3:A:9:ARG:HH22	1.41	0.85
3:C:4:ILE:HD13	3:C:9:ARG:HH22	1.41	0.85
2:I:91:PHE:CZ	2:I:94:LEU:CD2	2.59	0.85
1:G:96:CYS:O	1:G:122:TRP:CA	2.25	0.85
1:H:119:PHE:CE2	2:L:45:LYS:O	2.29	0.84
3:C:237:LEU:HD23	3:C:238:VAL:HG13	1.57	0.84
1:G:4:LEU:HD12	1:G:121:PRO:C	2.01	0.84
3:C:238:VAL:HG12	3:C:252:VAL:HA	1.58	0.84
2:I:91:PHE:HZ	2:I:94:LEU:HD21	1.39	0.83
3:B:4:ILE:HD13	3:B:9:ARG:HH22	1.41	0.83
2:I:34:ASN:O	2:I:88:CYS:HA	1.78	0.83
1:H:119:PHE:CE1	2:L:37:GLN:O	2.32	0.83
3:B:302:CYS:SG	3:B:303:THR:N	2.47	0.83
3:A:259:ALA:HB2	3:C:259:ALA:HB2	1.61	0.83
2:L:34:ASN:O	2:L:88:CYS:HA	1.78	0.83
3:A:267:ALA:HB2	4:D:7:HIS:HD2	1.43	0.82
3:B:91:VAL:O	3:B:116:CYS:HA	1.79	0.82
3:A:91:VAL:O	3:A:116:CYS:HA	1.79	0.82
3:A:138:THR:OG1	3:A:163:LYS:NZ	2.12	0.81
3:A:149:ASN:OD1	3:A:150:ALA:N	2.10	0.81
3:C:91:VAL:O	3:C:116:CYS:HA	1.79	0.81
2:L:91:PHE:CE1	2:L:94:LEU:HD21	2.16	0.81
3:A:105:CYS:HA	1:H:111:PRO:CG	2.10	0.81
3:B:267:ALA:HB2	4:E:7:HIS:CD2	2.15	0.81
3:B:100:GLY:O	3:B:104:GLY:N	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:34:ASN:HB2	2:L:89:GLN:HB3	1.61	0.81
2:L:91:PHE:CE1	2:L:94:LEU:CD2	2.63	0.80
1:H:119:PHE:C	2:L:45:LYS:HA	2.06	0.80
2:I:34:ASN:HB2	2:I:89:GLN:HB3	1.61	0.80
3:A:97:VAL:HG23	3:A:98:ASP:H	1.47	0.80
3:A:315:THR:HG22	3:A:316:GLN:H	1.46	0.80
2:I:91:PHE:CE1	2:I:94:LEU:HD21	2.16	0.80
3:B:56:LEU:HD13	3:A:78:GLY:HA2	1.64	0.80
3:A:267:ALA:HB2	4:D:7:HIS:CD2	2.17	0.80
3:A:100:GLY:O	3:A:104:GLY:N	2.13	0.80
3:C:100:GLY:O	3:C:104:GLY:N	2.13	0.80
3:B:97:VAL:HG23	3:B:98:ASP:H	1.47	0.79
3:C:2:ARG:HH22	3:C:158:HIS:HB2	1.47	0.79
1:G:96:CYS:O	1:G:122:TRP:C	2.26	0.79
2:I:91:PHE:CE1	2:I:94:LEU:CD2	2.65	0.79
4:E:55:THR:HB	4:E:60:ARG:HE	1.48	0.78
1:H:120:ASP:CB	1:H:121:PRO:CD	2.60	0.78
3:A:27:HIS:NE2	3:A:280:THR:O	2.16	0.78
1:G:2:VAL:HG13	1:G:98:ARG:HH22	1.48	0.78
3:B:50:ALA:H	3:B:276:ASN:HD22	1.32	0.78
1:H:32:ASN:HA	1:H:99:GLY:O	1.84	0.78
3:A:2:ARG:HH22	3:A:158:HIS:HB2	1.47	0.78
4:D:63:ILE:HA	4:D:66:LEU:HD22	1.66	0.78
3:C:50:ALA:H	3:C:276:ASN:HD22	1.32	0.78
4:D:55:THR:HB	4:D:60:ARG:HE	1.48	0.78
4:F:55:THR:HB	4:F:60:ARG:HE	1.48	0.78
3:A:70:THR:N	1:H:55:GLY:O	2.14	0.78
1:H:2:VAL:HG13	1:H:98:ARG:HH22	1.49	0.78
3:C:441:GLY:O	3:C:445:GLY:N	2.16	0.78
1:G:119:PHE:CB	2:I:36:TYR:HE1	1.98	0.78
3:B:2:ARG:HH22	3:B:158:HIS:HB2	1.47	0.77
3:C:97:VAL:HG23	3:C:98:ASP:H	1.47	0.77
3:C:27:HIS:HD2	3:C:45:LEU:HG	1.50	0.77
3:B:201:MET:HG3	3:B:202:GLU:H	1.48	0.77
3:C:56:LEU:HG	3:C:57:ARG:HG3	1.65	0.77
3:B:56:LEU:HG	3:B:57:ARG:HG3	1.65	0.77
3:A:57:ARG:HD3	3:A:213:PHE:CE2	2.20	0.77
3:A:50:ALA:H	3:A:276:ASN:HD22	1.31	0.77
1:G:32:ASN:HA	1:G:99:GLY:O	1.84	0.76
3:C:57:ARG:HD3	3:C:213:PHE:CE2	2.20	0.76
3:A:319:THR:O	3:A:369:ALA:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:359:THR:HG22	3:C:360:GLU:H	1.49	0.76
3:A:56:LEU:HG	3:A:57:ARG:HG3	1.65	0.76
3:A:359:THR:HG22	3:A:360:GLU:H	1.49	0.76
3:C:201:MET:HG3	3:C:202:GLU:H	1.49	0.76
3:A:429:PHE:HA	3:A:432:ILE:HG22	1.68	0.76
1:G:117:TRP:CB	2:I:89:GLN:HE22	1.97	0.76
3:C:232:ILE:O	3:C:233:GLN:HG2	1.86	0.76
3:B:57:ARG:HD3	3:B:213:PHE:CE2	2.20	0.76
3:B:78:GLY:N	3:A:56:LEU:HD22	1.99	0.75
3:B:319:THR:O	3:B:369:ALA:N	2.18	0.75
3:A:201:MET:HG3	3:A:202:GLU:H	1.49	0.75
3:B:359:THR:HG22	3:B:360:GLU:H	1.49	0.75
1:H:118:TRP:NE1	2:L:98:PHE:CZ	2.54	0.75
3:A:75:PRO:CB	3:A:77:GLN:HG2	2.16	0.75
4:D:65:ILE:O	4:D:68:THR:OG1	2.04	0.75
3:C:267:ALA:HB2	4:F:7:HIS:HD2	1.51	0.75
3:C:276:ASN:OD1	3:C:278:LEU:N	2.19	0.75
4:E:14:THR:HG23	4:E:16:THR:H	1.51	0.74
3:B:276:ASN:OD1	3:B:278:LEU:N	2.19	0.74
3:C:237:LEU:HA	3:C:253:LEU:HD22	1.68	0.74
3:A:237:LEU:HA	3:A:253:LEU:HD22	1.68	0.74
3:A:340:MET:O	3:A:377:TYR:HB3	1.87	0.74
3:C:319:THR:O	3:C:369:ALA:N	2.18	0.74
3:A:276:ASN:OD1	3:A:278:LEU:N	2.19	0.74
2:L:2:ILE:O	2:L:90:GLN:OE1	2.06	0.74
3:C:57:ARG:NH1	3:C:59:TYR:OH	2.21	0.74
3:B:237:LEU:HA	3:B:253:LEU:HD22	1.68	0.73
4:D:14:THR:HG23	4:D:16:THR:H	1.53	0.73
3:B:57:ARG:NH1	3:B:59:TYR:OH	2.21	0.73
4:E:55:THR:HA	4:E:60:ARG:HG3	1.71	0.73
3:A:57:ARG:NH1	3:A:59:TYR:OH	2.21	0.73
3:C:70:THR:OG1	3:C:114:VAL:O	2.07	0.73
1:G:4:LEU:HD13	1:G:122:TRP:C	2.09	0.73
4:D:5:VAL:O	4:D:7:HIS:N	2.21	0.73
3:A:148:GLU:CG	3:A:149:ASN:H	1.98	0.73
3:B:267:ALA:HB2	4:E:7:HIS:HD2	1.52	0.73
3:A:70:THR:OG1	3:A:114:VAL:O	2.07	0.73
1:H:119:PHE:CB	2:L:45:LYS:C	2.61	0.73
3:B:3:CYS:HB3	3:B:9:ARG:HH21	1.54	0.73
4:D:55:THR:HA	4:D:60:ARG:HG3	1.71	0.73
1:G:65:GLN:NE2	3:A:227:GLN:H	1.86	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:20:TRP:HA	3:A:287:LEU:O	1.88	0.72
3:C:58:LYS:CB	3:C:221:LEU:HB3	2.18	0.72
3:C:67:ASN:OD1	3:C:118:MET:HG3	1.89	0.72
4:F:55:THR:HA	4:F:60:ARG:HG3	1.71	0.72
3:A:343:GLU:HB2	3:A:344:LYS:HG2	1.71	0.72
1:G:97:ALA:CB	1:G:122:TRP:HA	2.18	0.72
3:A:232:ILE:HG22	3:A:233:GLN:H	1.52	0.71
3:C:3:CYS:HB3	3:C:9:ARG:HH21	1.54	0.71
3:C:493:VAL:HG23	3:C:494:GLN:HG2	1.71	0.71
3:A:3:CYS:HB3	3:A:9:ARG:HH21	1.54	0.71
3:C:27:HIS:CD2	3:C:45:LEU:HG	2.25	0.71
3:A:150:ALA:C	3:A:152:GLY:H	1.99	0.71
3:B:27:HIS:CD2	3:B:280:THR:H	2.09	0.70
3:C:73:ARG:H	3:C:80:PRO:HG3	1.56	0.70
3:B:150:ALA:C	3:B:152:GLY:H	1.99	0.70
4:F:66:LEU:O	4:F:69:ALA:N	2.24	0.70
1:H:107:SER:O	2:L:94:LEU:HD13	1.91	0.70
1:H:119:PHE:CE1	2:L:44:PRO:CB	2.74	0.70
3:B:73:ARG:H	3:B:80:PRO:HG3	1.56	0.70
2:I:21:PHE:O	2:I:72:THR:HA	1.92	0.70
3:A:73:ARG:H	3:A:80:PRO:HG3	1.56	0.70
1:H:119:PHE:CZ	2:L:37:GLN:N	2.59	0.70
3:B:227:GLN:HG3	1:H:66:GLY:HA2	1.73	0.70
3:C:12:VAL:HB	3:C:33:THR:HG22	1.73	0.70
3:C:150:ALA:C	3:C:152:GLY:H	1.99	0.70
3:B:89:ARG:HB2	3:A:86:GLN:HE21	1.56	0.70
3:A:396:SER:O	3:A:396:SER:OG	2.08	0.70
4:D:31:ARG:NH1	4:F:4:LEU:HD22	2.07	0.70
1:H:119:PHE:HB3	2:L:46:LEU:N	2.05	0.70
3:A:305:LYS:H	3:A:386:GLN:HG2	1.57	0.69
2:L:21:PHE:O	2:L:72:THR:HA	1.92	0.69
3:B:70:THR:OG1	3:B:114:VAL:O	2.07	0.69
3:C:394:LYS:HG3	3:C:395:GLY:H	1.56	0.69
1:H:6:GLN:NE2	1:H:96:CYS:SG	2.60	0.69
3:C:62:GLU:HB3	3:C:122:LYS:HB2	1.75	0.69
4:D:66:LEU:HG	4:F:66:LEU:HD13	1.75	0.69
3:A:75:PRO:HB2	3:A:77:GLN:N	2.07	0.69
3:C:39:PRO:HD2	3:C:292:LEU:HD23	1.75	0.69
3:C:434:LYS:O	3:C:438:GLN:HB2	1.93	0.69
4:F:64:PHE:O	4:F:67:LEU:N	2.26	0.69
3:A:12:VAL:HB	3:A:33:THR:HG22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:434:LYS:O	3:A:438:GLN:HB2	1.93	0.69
3:B:312:ILE:HG13	3:B:313:ALA:H	1.59	0.68
1:G:6:GLN:NE2	1:G:96:CYS:SG	2.60	0.68
3:A:312:ILE:HG13	3:A:313:ALA:H	1.59	0.68
3:C:267:ALA:HB2	4:F:7:HIS:CD2	2.27	0.68
3:C:320:ILE:HG13	3:C:369:ALA:O	1.94	0.68
3:C:446:ALA:HA	3:C:449:SER:HB2	1.76	0.68
4:F:19:TRP:HD1	4:F:20:MET:HG2	1.58	0.68
1:G:47:TRP:CE2	2:I:96:ILE:HD12	2.29	0.68
3:B:12:VAL:HB	3:B:33:THR:HG22	1.74	0.68
3:B:232:ILE:HG22	3:B:233:GLN:H	1.58	0.68
4:E:19:TRP:HD1	4:E:20:MET:HG2	1.58	0.68
1:G:4:LEU:HD12	1:G:122:TRP:CA	2.24	0.68
3:B:76:THR:HG23	3:B:107:LEU:HD21	1.75	0.68
3:B:434:LYS:O	3:B:438:GLN:HB2	1.93	0.68
3:C:312:ILE:HG13	3:C:313:ALA:H	1.59	0.68
3:B:320:ILE:HG13	3:B:369:ALA:O	1.94	0.68
3:B:450:GLY:HA2	4:E:10:MET:H	1.59	0.68
3:A:320:ILE:HG13	3:A:369:ALA:O	1.94	0.68
4:D:19:TRP:HD1	4:D:20:MET:HG2	1.58	0.68
1:H:118:TRP:CZ2	2:L:98:PHE:CE1	2.80	0.68
4:F:4:LEU:O	4:F:5:VAL:HG22	1.93	0.67
2:L:91:PHE:CE1	2:L:94:LEU:HD23	2.29	0.67
3:A:39:PRO:HD2	3:A:292:LEU:HD23	1.75	0.67
3:B:203:ASN:OD1	3:B:204:LYS:N	2.27	0.67
1:H:119:PHE:CD1	2:L:44:PRO:CB	2.78	0.67
3:A:19:SER:HB2	3:A:20:TRP:HE3	1.57	0.67
2:I:22:THR:HA	2:I:71:PHE:O	1.95	0.67
1:G:2:VAL:HG13	1:G:98:ARG:NH2	2.10	0.67
1:H:108:TYR:HB3	1:H:111:PRO:HD2	1.76	0.67
3:B:396:SER:OG	3:B:397:SER:N	2.18	0.67
4:D:70:VAL:HB	3:C:455:MET:SD	2.34	0.67
1:H:2:VAL:HG13	1:H:98:ARG:NH2	2.10	0.66
2:L:81:GLU:OE1	2:L:81:GLU:N	2.27	0.66
3:A:244:HIS:HB3	4:F:16:THR:HG22	1.78	0.66
3:A:459:ILE:O	3:A:463:ILE:HG22	1.96	0.66
1:G:33:TYR:HE2	1:G:101:ARG:HA	1.60	0.66
1:G:34:ILE:HA	1:G:97:ALA:O	1.95	0.66
3:C:310:LYS:HG2	3:C:311:GLU:CB	2.23	0.66
2:L:22:THR:HA	2:L:71:PHE:O	1.95	0.66
1:H:32:ASN:HB2	1:H:98:ARG:HD2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:LEU:CD1	1:G:122:TRP:CA	2.73	0.66
3:A:321:VAL:HA	3:A:367:ILE:O	1.96	0.66
3:C:321:VAL:HA	3:C:367:ILE:O	1.96	0.66
3:B:321:VAL:HA	3:B:367:ILE:O	1.96	0.65
1:G:32:ASN:HB2	1:G:98:ARG:HD2	1.78	0.65
3:B:186:SER:O	3:B:189:THR:OG1	2.13	0.65
3:C:311:GLU:CG	3:C:312:ILE:H	2.05	0.65
1:G:65:GLN:HE22	3:A:227:GLN:H	1.42	0.65
3:C:459:ILE:O	3:C:463:ILE:HG22	1.96	0.65
3:A:27:HIS:CD2	3:A:280:THR:O	2.50	0.65
1:H:34:ILE:HA	1:H:97:ALA:O	1.95	0.65
3:B:459:ILE:O	3:B:463:ILE:HG22	1.95	0.65
3:A:186:SER:O	3:A:189:THR:OG1	2.13	0.65
3:A:253:LEU:O	3:C:261:HIS:ND1	2.28	0.65
4:F:63:ILE:O	4:F:66:LEU:HB3	1.97	0.65
1:H:119:PHE:CE1	2:L:44:PRO:HB3	2.32	0.65
3:B:2:ARG:NH1	3:B:156:GLY:O	2.29	0.65
3:B:191:LEU:HB3	3:B:196:MET:HE3	1.79	0.65
1:H:119:PHE:CE1	2:L:45:LYS:O	2.50	0.65
3:C:191:LEU:HB3	3:C:196:MET:HE3	1.79	0.65
2:I:81:GLU:OE1	2:I:81:GLU:N	2.27	0.65
3:A:2:ARG:NH1	3:A:156:GLY:O	2.29	0.65
3:A:331:SER:O	3:A:333:CYS:N	2.30	0.65
3:A:384:PRO:C	3:A:386:GLN:H	2.05	0.64
3:C:90:PHE:HA	3:C:117:ALA:O	1.97	0.64
1:G:4:LEU:HB2	1:G:123:GLY:HA2	1.78	0.64
3:B:90:PHE:HA	3:B:117:ALA:O	1.97	0.64
3:B:305:LYS:HA	3:B:386:GLN:HG2	1.79	0.64
3:C:186:SER:O	3:C:189:THR:OG1	2.13	0.64
1:G:96:CYS:O	1:G:122:TRP:HA	1.98	0.64
3:C:2:ARG:NH1	3:C:156:GLY:O	2.29	0.64
3:C:309:VAL:O	3:C:310:LYS:HB2	1.98	0.64
1:G:96:CYS:O	1:G:122:TRP:CB	2.46	0.64
3:C:220:TRP:HE1	3:C:222:PRO:HG3	1.63	0.64
1:H:108:TYR:O	2:L:94:LEU:HD11	1.98	0.64
3:B:475:LEU:O	3:B:479:LEU:HB3	1.98	0.64
2:L:20:THR:HA	2:L:73:PHE:O	1.98	0.64
4:E:65:ILE:O	4:E:68:THR:OG1	2.16	0.63
3:A:34:MET:SD	3:A:352:ILE:HD12	2.39	0.63
3:A:191:LEU:HB3	3:A:196:MET:HE3	1.79	0.63
3:C:331:SER:O	3:C:333:CYS:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:175:LEU:HB2	3:A:179:GLY:HA3	1.80	0.63
4:D:4:LEU:O	4:D:5:VAL:HG13	1.98	0.63
3:C:416:GLY:O	3:C:419:ALA:N	2.24	0.63
3:C:475:LEU:O	3:C:479:LEU:HB3	1.98	0.63
3:B:220:TRP:HE1	3:B:222:PRO:HG3	1.63	0.63
3:B:331:SER:O	3:B:333:CYS:N	2.31	0.63
3:A:90:PHE:HA	3:A:117:ALA:O	1.98	0.63
3:C:27:HIS:CE1	3:C:279:PHE:HA	2.34	0.63
1:G:66:GLY:HA2	3:A:227:GLN:HG3	1.80	0.63
3:B:150:ALA:HB3	3:B:153:ASN:OD1	1.98	0.63
3:C:175:LEU:HB2	3:C:179:GLY:HA3	1.80	0.63
2:I:20:THR:HA	2:I:73:PHE:O	1.98	0.63
3:C:150:ALA:HB3	3:C:153:ASN:OD1	1.98	0.63
3:C:221:LEU:HD21	3:C:225:ASP:CB	2.28	0.63
3:A:377:TYR:CZ	3:A:388:LYS:HE3	2.34	0.63
1:H:119:PHE:CE1	2:L:44:PRO:CA	2.76	0.63
3:B:75:PRO:HB3	3:B:110:LYS:C	2.22	0.63
3:A:73:ARG:HG3	3:A:75:PRO:HG2	1.81	0.63
3:C:34:MET:SD	3:C:352:ILE:HD12	2.39	0.63
3:A:171:THR:HB	3:A:183:MET:O	1.99	0.62
3:A:475:LEU:O	3:A:479:LEU:HB3	1.98	0.62
3:C:99:ARG:HA	3:C:103:ASN:ND2	2.14	0.62
3:C:100:GLY:H	3:C:103:ASN:HB2	1.64	0.62
1:G:119:PHE:CB	2:I:36:TYR:CE1	2.80	0.62
1:H:36:TRP:CE2	1:H:81:MET:HB2	2.34	0.62
3:B:171:THR:HB	3:B:183:MET:O	1.99	0.62
4:D:56:THR:HG23	4:D:59:GLN:CB	2.29	0.62
1:G:38:ARG:HH22	1:G:90:ASP:HA	1.64	0.62
3:A:150:ALA:HB3	3:A:153:ASN:OD1	1.98	0.62
2:I:91:PHE:CE1	2:I:94:LEU:HD23	2.33	0.62
3:B:75:PRO:HA	3:B:111:GLY:HA2	1.82	0.62
1:H:38:ARG:HH22	1:H:90:ASP:HA	1.64	0.62
1:H:108:TYR:C	2:L:94:LEU:HD11	2.25	0.62
3:B:125:MET:HE1	3:B:260:MET:HE2	1.82	0.62
3:B:416:GLY:O	3:B:419:ALA:N	2.24	0.62
3:A:452:SER:HA	3:A:494:GLN:NE2	2.07	0.62
1:H:107:SER:O	2:L:94:LEU:CD1	2.48	0.62
1:G:36:TRP:CE2	1:G:81:MET:HB2	2.34	0.62
1:G:53:PRO:HD2	1:G:101:ARG:NH2	2.14	0.62
2:L:2:ILE:CG2	2:L:90:GLN:CD	2.65	0.62
3:B:50:ALA:H	3:B:276:ASN:ND2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:319:THR:C	3:B:369:ALA:O	2.43	0.62
3:B:479:LEU:O	3:B:482:VAL:N	2.33	0.62
3:A:82:LEU:HD23	3:A:84:GLU:H	1.64	0.62
3:A:149:ASN:CG	3:A:150:ALA:H	2.03	0.62
3:B:99:ARG:HA	3:B:103:ASN:ND2	2.14	0.62
3:B:238:VAL:H	3:B:253:LEU:HB2	1.65	0.62
3:A:99:ARG:HA	3:A:103:ASN:ND2	2.14	0.62
3:A:479:LEU:O	3:A:482:VAL:N	2.33	0.62
3:C:82:LEU:HD23	3:C:84:GLU:H	1.64	0.62
3:C:319:THR:C	3:C:369:ALA:O	2.42	0.62
1:G:32:ASN:N	1:G:101:ARG:HE	1.98	0.62
3:A:100:GLY:H	3:A:103:ASN:HB2	1.64	0.62
3:A:319:THR:C	3:A:369:ALA:O	2.43	0.61
3:A:455:MET:SD	4:F:70:VAL:HG13	2.39	0.61
2:I:21:PHE:HZ	2:I:104:LEU:HD11	1.65	0.61
3:B:175:LEU:HB2	3:B:179:GLY:HA3	1.80	0.61
3:B:224:ALA:HB3	3:A:81:SER:HB3	1.82	0.61
3:C:1:MET:C	3:C:3:CYS:H	2.08	0.61
2:L:21:PHE:HZ	2:L:104:LEU:HD11	1.65	0.61
3:A:19:SER:HB2	3:A:20:TRP:CE3	2.35	0.61
3:C:411:ARG:HG2	3:C:419:ALA:HB1	1.81	0.61
1:H:54:ARG:CZ	1:H:103:LEU:HD22	2.31	0.61
3:B:220:TRP:CD1	3:B:232:ILE:HD12	2.36	0.61
3:B:331:SER:OG	3:B:332:PRO:HD2	2.01	0.61
3:B:55:THR:HA	3:B:128:LYS:HG2	1.83	0.61
3:C:373:PHE:O	3:C:393:LYS:O	2.19	0.61
3:B:19:SER:HB2	3:B:20:TRP:HE3	1.65	0.61
3:C:50:ALA:H	3:C:276:ASN:ND2	1.98	0.61
3:C:178:TYR:HB3	3:C:293:GLN:HB2	1.83	0.61
4:F:54:GLY:O	4:F:55:THR:OG1	2.19	0.61
3:C:55:THR:HA	3:C:128:LYS:HG2	1.83	0.61
3:C:466:ILE:HD12	3:C:469:ASN:ND2	2.15	0.61
3:A:73:ARG:HG3	3:A:75:PRO:CG	2.31	0.61
3:A:220:TRP:HE1	3:A:222:PRO:HG3	1.63	0.61
3:C:15:VAL:HG21	3:C:19:SER:HA	1.83	0.61
3:B:139:ILE:O	3:B:162:ILE:HG22	2.00	0.61
3:B:166:PRO:HB3	3:B:187:PRO:HG2	1.81	0.61
3:B:385:GLY:O	3:B:387:LEU:N	2.34	0.60
3:C:171:THR:HB	3:C:183:MET:O	1.99	0.60
3:B:82:LEU:HD23	3:B:84:GLU:H	1.64	0.60
3:C:139:ILE:O	3:C:162:ILE:HG22	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:450:GLY:HA2	4:F:10:MET:H	1.66	0.60
3:C:479:LEU:O	3:C:482:VAL:N	2.33	0.60
1:H:116:SER:HB2	2:L:46:LEU:HD22	1.82	0.60
3:B:100:GLY:H	3:B:103:ASN:HB2	1.64	0.60
3:B:52:HIS:HB2	3:B:134:ASN:HD22	1.67	0.60
3:A:50:ALA:H	3:A:276:ASN:ND2	1.98	0.60
3:A:74:CYS:N	3:A:75:PRO:HD3	2.17	0.60
3:A:166:PRO:HB3	3:A:187:PRO:HG2	1.82	0.60
3:C:202:GLU:O	3:C:203:ASN:HB2	2.00	0.60
3:B:1:MET:SD	3:B:151:VAL:HA	2.41	0.60
3:A:103:ASN:O	1:H:102:ALA:HB1	2.02	0.60
3:A:139:ILE:O	3:A:162:ILE:HG22	2.00	0.60
3:C:321:VAL:HG12	3:C:368:GLU:HB3	1.83	0.60
3:C:166:PRO:HB3	3:C:187:PRO:HG2	1.82	0.60
3:C:331:SER:OG	3:C:332:PRO:HD2	2.01	0.60
3:B:2:ARG:NH2	3:B:158:HIS:HB2	2.16	0.60
3:B:25:LEU:HD13	3:B:45:LEU:HB2	1.83	0.60
3:B:321:VAL:HG12	3:B:368:GLU:HB3	1.83	0.60
3:A:331:SER:OG	3:A:332:PRO:HD2	2.01	0.60
3:B:178:TYR:HB3	3:B:293:GLN:HB2	1.83	0.60
3:A:373:PHE:O	3:A:393:LYS:O	2.19	0.60
3:A:416:GLY:O	3:A:419:ALA:N	2.24	0.60
1:G:109:THR:HG23	1:G:110:THR:H	1.66	0.60
3:B:50:ALA:HA	3:B:135:LEU:HA	1.84	0.60
3:A:73:ARG:C	3:A:75:PRO:HD3	2.26	0.60
3:A:270:ILE:HD11	3:A:278:LEU:HA	1.84	0.60
3:C:270:ILE:HD11	3:C:278:LEU:HA	1.84	0.60
3:A:55:THR:HA	3:A:128:LYS:HG2	1.83	0.59
3:C:148:GLU:H	3:C:149:ASN:HD22	1.49	0.59
3:B:373:PHE:O	3:B:393:LYS:O	2.19	0.59
1:G:60:SER:HB3	3:A:226:THR:HG23	1.84	0.59
3:B:149:ASN:OD1	3:B:150:ALA:N	2.35	0.59
3:B:224:ALA:N	3:A:73:ARG:HH12	2.00	0.59
3:C:25:LEU:HD13	3:C:45:LEU:HB2	1.83	0.59
3:B:139:ILE:O	3:B:161:GLU:C	2.46	0.59
3:B:20:TRP:HA	3:B:287:LEU:O	2.03	0.59
4:E:54:GLY:O	4:E:55:THR:OG1	2.19	0.59
3:C:139:ILE:O	3:C:161:GLU:C	2.46	0.59
4:E:8:VAL:HG23	4:E:9:GLY:H	1.67	0.59
3:A:131:GLN:O	3:A:133:GLU:N	2.30	0.59
3:A:178:TYR:HB3	3:A:293:GLN:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:321:VAL:HG12	3:A:368:GLU:HB3	1.83	0.59
3:C:382:VAL:HG23	3:C:383:GLU:H	1.68	0.59
3:B:83:ASN:OD1	3:B:84:GLU:N	2.36	0.59
3:A:2:ARG:NH2	3:A:158:HIS:HB2	2.16	0.59
4:D:54:GLY:O	4:D:55:THR:OG1	2.19	0.59
3:C:384:PRO:O	3:C:386:GLN:N	2.35	0.59
3:C:2:ARG:NH2	3:C:158:HIS:HB2	2.16	0.59
2:I:36:TYR:HB2	2:I:87:TYR:HB2	1.85	0.59
3:B:99:ARG:CZ	3:B:103:ASN:HB3	2.33	0.59
3:C:38:LYS:H	3:C:294:LEU:HD21	1.68	0.59
3:B:26:GLU:O	3:B:29:SER:OG	2.17	0.59
3:B:220:TRP:HB3	3:B:232:ILE:HB	1.83	0.59
3:A:25:LEU:HD13	3:A:45:LEU:HB2	1.83	0.59
3:A:83:ASN:OD1	3:A:84:GLU:N	2.36	0.59
3:A:382:VAL:HG23	3:A:383:GLU:H	1.68	0.59
3:C:415:LEU:O	3:C:418:THR:OG1	2.21	0.59
3:A:50:ALA:HA	3:A:135:LEU:HA	1.84	0.58
3:B:270:ILE:HD11	3:B:278:LEU:HA	1.84	0.58
3:A:99:ARG:CZ	3:A:103:ASN:HB3	2.33	0.58
2:L:4:LEU:HD11	2:L:23:CYS:HB3	1.85	0.58
1:G:15:GLY:N	1:G:86:LEU:O	2.30	0.58
2:I:52:SER:OG	2:I:53:ASN:ND2	2.36	0.58
2:L:52:SER:OG	2:L:53:ASN:ND2	2.36	0.58
2:I:4:LEU:HD11	2:I:23:CYS:HB3	1.85	0.58
3:B:7:SER:HA	3:B:316:GLN:HE21	1.68	0.58
2:L:36:TYR:HB2	2:L:87:TYR:HB2	1.85	0.58
3:A:139:ILE:O	3:A:161:GLU:C	2.46	0.58
3:C:50:ALA:HA	3:C:135:LEU:HA	1.84	0.58
3:B:38:LYS:H	3:B:294:LEU:HD21	1.68	0.58
3:A:138:THR:HG1	3:A:163:LYS:HZ2	1.47	0.58
1:H:15:GLY:N	1:H:86:LEU:O	2.30	0.58
1:H:119:PHE:CZ	2:L:45:LYS:O	2.57	0.58
3:A:1:MET:C	3:A:3:CYS:H	2.11	0.58
4:D:31:ARG:CZ	4:F:4:LEU:HD22	2.33	0.58
3:C:83:ASN:OD1	3:C:84:GLU:N	2.36	0.58
3:B:131:GLN:O	3:B:133:GLU:N	2.30	0.58
1:H:113:ASP:OD1	2:L:32:TYR:CE1	2.57	0.58
3:C:99:ARG:CZ	3:C:103:ASN:HB3	2.33	0.57
1:G:118:TRP:HA	1:G:122:TRP:CB	2.34	0.57
3:B:495:ALA:OXT	4:E:18:THR:N	2.31	0.57
3:A:203:ASN:OD1	3:A:204:LYS:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:58:LYS:HB2	3:B:221:LEU:HB3	1.86	0.57
3:B:382:VAL:HG23	3:B:383:GLU:H	1.68	0.57
3:B:387:LEU:HD21	3:B:389:LEU:HG	1.85	0.57
3:A:149:ASN:HB2	5:K:1:NAG:H2	1.86	0.57
4:D:8:VAL:HG23	4:D:9:GLY:H	1.69	0.57
4:E:56:THR:HG23	4:E:59:GLN:CB	2.35	0.57
3:A:27:HIS:H	3:A:45:LEU:HD23	1.70	0.57
3:B:101:TRP:HD1	3:B:108:PHE:CE2	2.23	0.57
3:B:320:ILE:HG12	3:B:371:PRO:HD3	1.86	0.57
3:A:26:GLU:O	3:A:29:SER:OG	2.17	0.57
3:C:384:PRO:C	3:C:386:GLN:H	2.11	0.57
3:A:101:TRP:HD1	3:A:108:PHE:CE2	2.23	0.57
3:C:131:GLN:O	3:C:133:GLU:N	2.30	0.57
1:G:32:ASN:HB3	1:G:98:ARG:HB3	1.87	0.57
3:B:148:GLU:CG	3:B:149:ASN:H	2.17	0.57
3:A:94:HIS:ND1	3:A:114:VAL:HG12	2.20	0.57
2:I:35:TRP:CE2	2:I:73:PHE:HB2	2.39	0.57
1:H:119:PHE:HB2	2:L:36:TYR:CE1	2.40	0.57
2:L:35:TRP:CE2	2:L:73:PHE:HB2	2.39	0.57
1:G:91:THR:HG23	1:G:129:THR:HA	1.86	0.57
3:B:6:ILE:HG21	3:B:30:CYS:SG	2.45	0.57
3:A:320:ILE:HG12	3:A:371:PRO:HD3	1.86	0.57
3:C:94:HIS:ND1	3:C:114:VAL:HG12	2.20	0.57
3:C:216:LEU:HD23	3:C:217:PRO:O	2.05	0.57
3:C:289:MET:O	3:C:292:LEU:HD13	2.04	0.57
3:A:6:ILE:HG21	3:A:30:CYS:SG	2.45	0.57
3:C:101:TRP:HD1	3:C:108:PHE:CE2	2.23	0.57
3:B:94:HIS:ND1	3:B:114:VAL:HG12	2.20	0.56
3:C:205:ALA:HB3	3:C:270:ILE:O	2.05	0.56
1:G:2:VAL:HG11	1:G:121:PRO:HG3	1.87	0.56
4:D:67:LEU:O	4:D:70:VAL:HG22	2.05	0.56
3:C:6:ILE:HG21	3:C:30:CYS:SG	2.45	0.56
3:C:320:ILE:HG12	3:C:371:PRO:HD3	1.86	0.56
1:G:4:LEU:CD1	1:G:122:TRP:HA	2.35	0.56
1:G:6:GLN:N	1:G:124:GLN:HE22	2.04	0.56
3:B:27:HIS:H	3:B:45:LEU:HD23	1.70	0.56
3:B:256:GLN:OE1	3:B:256:GLN:N	2.38	0.56
3:A:205:ALA:HB3	3:A:270:ILE:O	2.06	0.56
3:A:436:LEU:O	3:A:440:PHE:CB	2.54	0.56
3:C:62:GLU:O	3:C:122:LYS:N	2.31	0.56
3:C:256:GLN:N	3:C:256:GLN:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:276:ASN:OD1	3:C:277:LEU:N	2.38	0.56
1:H:91:THR:HG23	1:H:129:THR:HA	1.86	0.56
1:H:113:ASP:CG	2:L:32:TYR:CE1	2.83	0.56
2:L:55:LYS:HG3	2:L:56:THR:O	2.05	0.56
3:B:54:ALA:HB3	3:A:77:GLN:OE1	2.05	0.56
3:B:205:ALA:HB3	3:B:270:ILE:O	2.05	0.56
3:C:317:HIS:O	3:C:317:HIS:ND1	2.38	0.56
3:C:359:THR:C	3:C:361:LYS:H	2.13	0.56
1:G:47:TRP:CH2	1:G:49:GLY:HA2	2.41	0.56
3:B:56:LEU:HD22	3:A:78:GLY:H	1.71	0.56
3:A:289:MET:O	3:A:292:LEU:HD13	2.05	0.56
3:C:436:LEU:O	3:C:440:PHE:CB	2.54	0.56
3:A:446:ALA:HA	3:A:449:SER:HB3	1.88	0.56
1:G:119:PHE:O	2:I:45:LYS:HA	2.05	0.56
3:B:216:LEU:HD23	3:B:217:PRO:O	2.05	0.56
3:B:276:ASN:OD1	3:B:277:LEU:N	2.38	0.56
3:B:495:ALA:O	4:E:18:THR:HG23	2.06	0.56
3:A:38:LYS:H	3:A:294:LEU:HD21	1.68	0.56
3:A:359:THR:C	3:A:361:LYS:H	2.13	0.56
1:H:32:ASN:HB3	1:H:98:ARG:HB3	1.87	0.56
3:A:216:LEU:HD23	3:A:217:PRO:O	2.05	0.56
3:A:450:GLY:HA2	4:D:10:MET:H	1.71	0.56
3:B:300:SER:OG	3:B:333:CYS:SG	2.64	0.56
3:A:238:VAL:H	3:A:253:LEU:HB2	1.70	0.56
3:A:310:LYS:HD2	3:C:101:TRP:HH2	1.71	0.56
3:C:206:TRP:NE1	3:C:264:LEU:HD13	2.21	0.56
4:F:8:VAL:HG13	4:F:9:GLY:H	1.71	0.56
1:H:118:TRP:HH2	2:L:96:ILE:HG21	1.71	0.56
3:B:206:TRP:NE1	3:B:264:LEU:HD13	2.21	0.56
3:B:436:LEU:O	3:B:440:PHE:CB	2.54	0.56
3:C:73:ARG:N	3:C:80:PRO:HG3	2.21	0.56
1:G:52:ASN:ND2	1:G:101:ARG:HH12	2.03	0.55
2:I:55:LYS:HG3	2:I:56:THR:O	2.05	0.55
3:B:359:THR:C	3:B:361:LYS:H	2.13	0.55
3:A:206:TRP:NE1	3:A:264:LEU:HD13	2.21	0.55
1:H:119:PHE:CD1	2:L:44:PRO:HB2	2.42	0.55
3:A:256:GLN:N	3:A:256:GLN:OE1	2.38	0.55
3:A:383:GLU:H	3:A:386:GLN:HE22	1.53	0.55
3:C:237:LEU:CD2	3:C:238:VAL:HG13	2.32	0.55
1:H:47:TRP:CH2	1:H:49:GLY:HA2	2.41	0.55
3:A:276:ASN:OD1	3:A:277:LEU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:193:PHE:C	3:B:195:GLU:H	2.14	0.55
3:C:193:PHE:C	3:C:195:GLU:H	2.14	0.55
2:L:94:LEU:N	2:L:95:PRO:HD3	2.21	0.55
3:A:193:PHE:C	3:A:195:GLU:H	2.14	0.55
1:H:6:GLN:N	1:H:124:GLN:HE22	2.04	0.55
3:B:261:HIS:HA	3:B:264:LEU:HG	1.88	0.55
3:A:261:HIS:HA	3:A:264:LEU:HG	1.88	0.55
3:A:73:ARG:N	3:A:80:PRO:HG3	2.21	0.55
3:C:261:HIS:HA	3:C:264:LEU:HG	1.88	0.55
1:H:11:VAL:HG22	1:H:129:THR:HB	1.88	0.55
1:H:30:THR:O	1:H:103:LEU:HD21	2.07	0.55
2:I:5:THR:OG1	2:I:24:GLN:HB3	2.08	0.54
2:L:5:THR:OG1	2:L:24:GLN:HB3	2.07	0.54
1:G:4:LEU:CG	1:G:121:PRO:O	2.53	0.54
3:B:227:GLN:H	1:H:65:GLN:NE2	2.05	0.54
3:B:329:ASP:O	3:B:331:SER:N	2.41	0.54
1:H:119:PHE:HE1	2:L:44:PRO:CA	2.21	0.54
3:B:394:LYS:HG3	3:B:395:GLY:H	1.72	0.54
2:I:29:ILE:HD11	2:I:71:PHE:CE2	2.43	0.54
3:B:232:ILE:HG22	3:B:233:GLN:N	2.21	0.54
3:A:51:LYS:O	3:A:53:PRO:HD3	2.08	0.54
3:A:329:ASP:O	3:A:331:SER:N	2.41	0.54
4:F:64:PHE:O	4:F:67:LEU:HB3	2.08	0.54
2:I:94:LEU:N	2:I:95:PRO:HD3	2.21	0.54
3:B:330:GLY:O	3:B:331:SER:HB3	2.07	0.54
4:E:66:LEU:O	4:E:70:VAL:HG13	2.08	0.54
3:C:309:VAL:O	3:C:310:LYS:CB	2.55	0.54
4:F:14:THR:HG23	4:F:16:THR:H	1.72	0.54
1:G:11:VAL:HG22	1:G:129:THR:HB	1.88	0.54
3:A:101:TRP:HD1	3:A:108:PHE:CZ	2.26	0.54
3:C:101:TRP:HD1	3:C:108:PHE:CZ	2.26	0.54
3:C:258:GLY:O	3:C:261:HIS:N	2.41	0.54
3:B:101:TRP:HD1	3:B:108:PHE:CZ	2.26	0.54
3:B:258:GLY:O	3:B:261:HIS:N	2.41	0.54
3:C:26:GLU:O	3:C:29:SER:OG	2.17	0.54
3:C:330:GLY:O	3:C:331:SER:HB3	2.07	0.54
2:L:50:ASP:HB2	2:L:53:ASN:HD22	1.73	0.54
3:C:212:TRP:CE2	4:F:7:HIS:HB2	2.42	0.54
3:A:258:GLY:O	3:A:261:HIS:N	2.41	0.54
3:A:373:PHE:HB2	3:A:396:SER:HB3	1.90	0.54
3:B:73:ARG:N	3:B:80:PRO:HG3	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:300:SER:OG	3:C:333:CYS:SG	2.64	0.53
3:C:415:LEU:HD12	3:C:419:ALA:HB2	1.90	0.53
3:B:2:ARG:HB2	3:B:142:THR:HG21	1.90	0.53
3:A:139:ILE:O	3:A:161:GLU:O	2.26	0.53
3:C:2:ARG:HB2	3:C:142:THR:HG21	1.90	0.53
3:C:318:GLY:O	3:C:320:ILE:N	2.42	0.53
1:H:119:PHE:HB3	2:L:45:LYS:C	2.29	0.53
2:L:29:ILE:HD11	2:L:71:PHE:CE2	2.43	0.53
3:B:139:ILE:O	3:B:161:GLU:O	2.26	0.53
3:A:182:THR:OG1	3:A:288:ARG:HB2	2.09	0.53
3:C:182:THR:OG1	3:C:288:ARG:HB2	2.09	0.53
1:H:6:GLN:H	1:H:124:GLN:HE22	1.57	0.53
4:E:67:LEU:O	4:E:70:VAL:HG22	2.08	0.53
3:C:51:LYS:O	3:C:53:PRO:HD3	2.08	0.53
3:C:139:ILE:HB	3:C:162:ILE:HG23	1.90	0.53
1:H:34:ILE:HG13	1:H:79:VAL:HG21	1.90	0.53
1:H:36:TRP:CZ3	1:H:96:CYS:HB3	2.44	0.53
1:G:36:TRP:CZ3	1:G:96:CYS:HB3	2.44	0.53
2:I:50:ASP:HB2	2:I:53:ASN:HD22	1.73	0.53
3:B:139:ILE:HB	3:B:162:ILE:HG23	1.90	0.53
3:C:201:MET:SD	3:C:260:MET:HE1	2.49	0.53
3:C:329:ASP:O	3:C:331:SER:N	2.41	0.53
3:B:51:LYS:O	3:B:53:PRO:HD3	2.08	0.53
3:A:314:GLU:HA	3:A:320:ILE:HG22	1.90	0.53
4:F:14:THR:HG23	4:F:16:THR:N	2.24	0.53
3:A:151:VAL:HG21	3:C:108:PHE:HZ	1.73	0.53
3:A:318:GLY:O	3:A:320:ILE:N	2.42	0.53
3:C:139:ILE:O	3:C:161:GLU:O	2.26	0.53
3:A:319:THR:O	3:A:369:ALA:O	2.27	0.53
3:C:271:GLN:HG2	3:C:277:LEU:HD12	1.91	0.53
2:I:61:ARG:NH2	2:I:82:ASP:OD1	2.42	0.53
3:A:20:TRP:HB3	3:A:288:ARG:HG2	1.90	0.53
3:A:219:PRO:HA	3:A:233:GLN:HB2	1.91	0.53
3:A:311:GLU:O	3:A:322:ILE:HD12	2.09	0.53
3:B:89:ARG:HH21	3:A:86:GLN:NE2	2.07	0.52
3:B:319:THR:O	3:B:369:ALA:O	2.27	0.52
3:A:184:GLU:O	3:A:285:CYS:HA	2.09	0.52
3:A:220:TRP:CD1	3:A:232:ILE:HD12	2.44	0.52
3:A:436:LEU:O	3:A:440:PHE:HB3	2.09	0.52
3:C:27:HIS:HD2	3:C:45:LEU:CG	2.20	0.52
3:C:220:TRP:HB3	3:C:232:ILE:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:GLN:HG2	1:H:44:GLY:H	1.74	0.52
3:A:212:TRP:CE2	4:D:7:HIS:HB2	2.44	0.52
3:A:330:GLY:O	3:A:331:SER:HB3	2.07	0.52
4:F:64:PHE:CE1	4:F:67:LEU:HD23	2.45	0.52
1:H:118:TRP:NE1	2:L:98:PHE:CE1	2.77	0.52
2:I:37:GLN:HE21	2:I:45:LYS:HD3	1.75	0.52
3:B:115:THR:HB	3:B:248:GLN:NE2	2.25	0.52
3:B:191:LEU:HD21	3:B:281:GLY:HA2	1.92	0.52
3:B:318:GLY:O	3:B:320:ILE:N	2.42	0.52
3:C:115:THR:HB	3:C:248:GLN:NE2	2.25	0.52
3:C:219:PRO:HA	3:C:233:GLN:HB2	1.91	0.52
4:F:62:LEU:O	4:F:65:ILE:HG22	2.10	0.52
1:G:43:GLN:HG2	1:G:44:GLY:H	1.74	0.52
1:G:120:ASP:N	1:G:120:ASP:OD1	2.41	0.52
3:B:182:THR:OG1	3:B:288:ARG:HB2	2.09	0.52
3:A:139:ILE:HB	3:A:162:ILE:HG23	1.90	0.52
3:A:204:LYS:NZ	3:C:251:VAL:HG13	2.25	0.52
3:A:387:LEU:HD21	3:A:389:LEU:HG	1.91	0.52
4:D:56:THR:HG23	4:D:59:GLN:HB3	1.91	0.52
3:C:436:LEU:O	3:C:440:PHE:HB3	2.09	0.52
2:L:2:ILE:HG22	2:L:2:ILE:O	2.08	0.52
1:G:34:ILE:HG13	1:G:79:VAL:HG21	1.90	0.52
3:A:123:LYS:O	3:A:124:ASN:ND2	2.42	0.52
3:A:475:LEU:O	3:A:479:LEU:CB	2.58	0.52
3:C:271:GLN:O	3:C:277:LEU:HB2	2.10	0.52
3:A:75:PRO:HB3	3:A:77:GLN:HG2	1.88	0.52
3:A:232:ILE:HG22	3:A:233:GLN:N	2.23	0.52
4:D:62:LEU:O	4:D:65:ILE:HG22	2.10	0.52
3:B:201:MET:HE2	3:B:257:GLU:HG3	1.92	0.52
3:B:219:PRO:HA	3:B:233:GLN:HB2	1.91	0.52
3:B:271:GLN:HG2	3:B:277:LEU:HD12	1.92	0.52
3:A:384:PRO:O	3:A:386:GLN:N	2.30	0.52
4:D:62:LEU:O	4:D:66:LEU:HD13	2.10	0.52
3:C:73:ARG:O	3:C:74:CYS:HB2	2.08	0.52
3:C:319:THR:O	3:C:369:ALA:O	2.27	0.52
1:G:67:ARG:O	1:G:83:LEU:HD12	2.10	0.52
3:A:261:HIS:ND1	3:C:253:LEU:O	2.42	0.52
3:A:271:GLN:HG2	3:A:277:LEU:HD12	1.91	0.52
3:A:426:GLY:HA3	3:A:430:THR:OG1	2.10	0.52
3:C:15:VAL:HG22	3:C:16:SER:O	2.10	0.52
3:C:201:MET:O	3:C:203:ASN:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:ARG:O	1:H:83:LEU:HD12	2.10	0.52
2:L:37:GLN:HE21	2:L:45:LYS:HD3	1.75	0.52
3:B:144:HIS:O	3:B:145:SER:OG	2.25	0.52
3:B:224:ALA:HB2	3:A:73:ARG:HH11	1.73	0.52
3:B:426:GLY:HA3	3:B:430:THR:OG1	2.10	0.52
3:B:436:LEU:O	3:B:440:PHE:HB3	2.09	0.52
3:C:191:LEU:HD21	3:C:281:GLY:HA2	1.91	0.52
1:H:52:ASN:OD1	1:H:54:ARG:N	2.43	0.52
3:B:224:ALA:N	3:A:73:ARG:NH1	2.58	0.51
3:A:57:ARG:NH2	3:A:214:LEU:HA	2.25	0.51
3:A:271:GLN:O	3:A:277:LEU:HB2	2.10	0.51
3:C:411:ARG:HG3	3:C:415:LEU:HD11	1.92	0.51
3:C:426:GLY:HA3	3:C:430:THR:OG1	2.10	0.51
3:C:475:LEU:O	3:C:479:LEU:CB	2.58	0.51
1:G:6:GLN:H	1:G:124:GLN:HE22	1.57	0.51
3:A:2:ARG:HB2	3:A:142:THR:HG21	1.90	0.51
3:A:75:PRO:HB2	3:A:77:GLN:HG2	1.91	0.51
3:A:487:LEU:O	3:A:490:GLY:N	2.42	0.51
3:C:15:VAL:CG2	3:C:19:SER:HA	2.40	0.51
1:H:10:ASP:O	1:H:128:VAL:HA	2.10	0.51
1:H:22:CYS:HB2	1:H:36:TRP:CH2	2.45	0.51
1:H:32:ASN:CB	1:H:98:ARG:HD2	2.39	0.51
1:G:52:ASN:OD1	1:G:54:ARG:N	2.43	0.51
3:B:15:VAL:HG22	3:B:16:SER:O	2.10	0.51
3:B:463:ILE:HG23	3:B:482:VAL:CG1	2.40	0.51
3:A:463:ILE:HG23	3:A:482:VAL:CG1	2.40	0.51
4:D:29:ALA:O	4:D:32:ILE:HG13	2.10	0.51
3:A:115:THR:HB	3:A:248:GLN:NE2	2.24	0.51
4:D:4:LEU:HD23	4:F:72:PRO:HG3	1.92	0.51
4:D:14:THR:HG23	4:D:16:THR:N	2.24	0.51
1:G:10:ASP:O	1:G:128:VAL:HA	2.11	0.51
1:G:32:ASN:CB	1:G:98:ARG:HD2	2.39	0.51
4:E:62:LEU:O	4:E:65:ILE:HG22	2.10	0.51
3:A:178:TYR:CE1	3:A:295:LYS:HD2	2.46	0.51
3:A:315:THR:HG22	3:A:316:GLN:N	2.22	0.51
3:A:381:GLY:CA	3:A:386:GLN:HB2	2.40	0.51
2:L:33:LEU:HG	2:L:34:ASN:N	2.25	0.51
2:L:61:ARG:NH2	2:L:82:ASP:OD1	2.42	0.51
3:B:1:MET:HE1	3:B:366:ASN:HD21	1.75	0.51
3:B:141:ILE:HD12	3:B:175:LEU:HD11	1.93	0.51
3:A:191:LEU:HD21	3:A:281:GLY:HA2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:TYR:CE1	3:C:295:LYS:HD2	2.46	0.51
1:G:32:ASN:C	1:G:101:ARG:HH21	2.17	0.51
2:I:50:ASP:C	2:I:52:SER:H	2.19	0.51
3:B:19:SER:HB2	3:B:20:TRP:CE3	2.46	0.51
3:B:178:TYR:CE1	3:B:295:LYS:HD2	2.46	0.51
3:A:101:TRP:CE2	3:C:310:LYS:HD2	2.46	0.51
1:G:22:CYS:HB2	1:G:36:TRP:CH2	2.45	0.51
2:I:33:LEU:HG	2:I:34:ASN:N	2.25	0.51
3:B:1:MET:C	3:B:3:CYS:H	2.18	0.51
3:B:57:ARG:NH2	3:B:214:LEU:HA	2.25	0.51
3:C:57:ARG:NH2	3:C:214:LEU:HA	2.25	0.51
4:F:29:ALA:O	4:F:32:ILE:HG13	2.10	0.51
4:E:29:ALA:O	4:E:32:ILE:HG13	2.10	0.51
3:A:300:SER:OG	3:A:333:CYS:SG	2.64	0.51
3:C:57:ARG:NH2	3:C:214:LEU:HD23	2.26	0.51
3:B:57:ARG:NH2	3:B:214:LEU:HD23	2.26	0.51
3:A:359:THR:O	3:A:361:LYS:N	2.39	0.51
3:C:463:ILE:HG23	3:C:482:VAL:CG1	2.40	0.51
3:B:271:GLN:O	3:B:277:LEU:HB2	2.10	0.50
3:A:15:VAL:HG22	3:A:16:SER:O	2.10	0.50
3:C:141:ILE:HD12	3:C:175:LEU:HD11	1.93	0.50
3:C:150:ALA:C	3:C:152:GLY:N	2.66	0.50
2:I:61:ARG:NH1	2:I:79:GLN:OE1	2.45	0.50
3:A:25:LEU:HD12	3:A:45:LEU:HD22	1.94	0.50
3:A:57:ARG:NH2	3:A:214:LEU:HD23	2.26	0.50
3:A:416:GLY:O	3:A:418:THR:N	2.45	0.50
3:B:105:CYS:SG	3:B:106:GLY:N	2.84	0.50
3:B:475:LEU:O	3:B:479:LEU:CB	2.58	0.50
3:B:475:LEU:HD12	3:B:476:SER:N	2.27	0.50
3:A:73:ARG:O	3:A:74:CYS:SG	2.69	0.50
2:L:35:TRP:HB2	2:L:48:ILE:HB	1.93	0.50
3:B:416:GLY:O	3:B:418:THR:N	2.45	0.50
3:C:75:PRO:HG2	3:C:106:GLY:C	2.36	0.50
2:L:61:ARG:NH1	2:L:79:GLN:OE1	2.45	0.50
3:C:416:GLY:O	3:C:418:THR:N	2.45	0.50
3:B:396:SER:HG	3:B:397:SER:H	1.57	0.50
3:A:391:TRP:CG	3:A:392:PHE:N	2.80	0.50
3:A:453:TRP:CD1	4:D:25:ALA:HB2	2.47	0.50
3:C:391:TRP:CG	3:C:392:PHE:N	2.80	0.50
3:B:78:GLY:HA2	3:A:56:LEU:CD1	2.28	0.50
3:B:391:TRP:CG	3:B:392:PHE:N	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:141:ILE:HD12	3:A:175:LEU:HD11	1.93	0.50
3:C:25:LEU:HD12	3:C:45:LEU:HD22	1.94	0.50
3:C:58:LYS:HG2	3:C:221:LEU:HD22	1.93	0.50
3:C:314:GLU:OE1	3:C:391:TRP:HZ2	1.94	0.50
1:H:35:HIS:ND1	1:H:50:VAL:HB	2.27	0.50
2:I:35:TRP:HB2	2:I:48:ILE:HB	1.93	0.50
3:B:150:ALA:HB3	3:B:153:ASN:CG	2.37	0.50
3:A:133:GLU:O	3:A:134:ASN:C	2.54	0.50
3:A:270:ILE:CD1	3:A:278:LEU:HA	2.42	0.50
3:A:440:PHE:HZ	3:A:481:LEU:HD11	1.77	0.50
3:C:195:GLU:O	3:C:210:ARG:N	2.45	0.50
1:G:124:GLN:OE1	1:G:124:GLN:N	2.42	0.49
3:C:150:ALA:HB3	3:C:153:ASN:CG	2.37	0.49
3:C:270:ILE:CD1	3:C:278:LEU:HA	2.42	0.49
3:C:475:LEU:HD12	3:C:476:SER:N	2.26	0.49
4:F:43:THR:HG23	4:F:67:LEU:HD21	1.94	0.49
2:L:50:ASP:C	2:L:52:SER:H	2.19	0.49
3:B:359:THR:HG22	3:B:360:GLU:N	2.24	0.49
3:A:69:THR:HG22	1:H:72:ARG:HH12	1.77	0.49
3:A:144:HIS:O	3:A:145:SER:OG	2.25	0.49
3:B:197:VAL:HG11	3:B:213:PHE:CD2	2.48	0.49
3:B:270:ILE:CD1	3:B:278:LEU:HA	2.42	0.49
3:A:438:GLN:O	3:A:442:ALA:HB2	2.12	0.49
3:C:381:GLY:HA3	3:C:386:GLN:HB2	1.94	0.49
3:B:359:THR:O	3:B:361:LYS:N	2.39	0.49
3:B:487:LEU:O	3:B:490:GLY:N	2.42	0.49
4:E:47:ALA:HB2	4:E:64:PHE:HE1	1.78	0.49
3:A:76:THR:OG1	3:A:77:GLN:N	2.46	0.49
3:C:310:LYS:HE2	3:C:323:ARG:H	1.78	0.49
4:F:47:ALA:HB2	4:F:64:PHE:HE1	1.77	0.49
2:L:17:ASP:O	2:L:78:LEU:N	2.44	0.49
1:G:35:HIS:ND1	1:G:50:VAL:HB	2.27	0.49
1:G:113:ASP:OD1	1:G:113:ASP:N	2.45	0.49
3:B:15:VAL:HG13	3:B:16:SER:H	1.78	0.49
3:B:25:LEU:HD12	3:B:45:LEU:HD22	1.93	0.49
3:A:15:VAL:HG13	3:A:16:SER:H	1.78	0.49
3:A:212:TRP:CZ2	4:D:7:HIS:HB2	2.47	0.49
3:C:197:VAL:HG11	3:C:213:PHE:CD2	2.48	0.49
3:B:10:ASP:H	3:B:407:ARG:NH1	2.10	0.49
3:B:203:ASN:OD1	3:B:204:LYS:HG3	2.13	0.49
3:A:181:VAL:HG22	3:A:292:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:56:THR:O	4:D:59:GLN:N	2.42	0.49
3:C:316:GLN:C	3:C:317:HIS:CG	2.90	0.49
3:B:438:GLN:O	3:B:442:ALA:HB2	2.12	0.49
3:A:150:ALA:HB3	3:A:153:ASN:CG	2.37	0.49
3:A:197:VAL:HG11	3:A:213:PHE:CD2	2.48	0.49
4:D:47:ALA:HB2	4:D:64:PHE:HE1	1.78	0.49
3:C:169:SER:C	3:C:171:THR:H	2.20	0.49
3:C:181:VAL:HG22	3:C:292:LEU:HD11	1.95	0.49
3:B:440:PHE:HZ	3:B:481:LEU:HD11	1.77	0.49
4:E:3:ALA:C	4:E:4:LEU:HD12	2.38	0.49
3:A:169:SER:C	3:A:171:THR:H	2.20	0.49
3:A:310:LYS:HD2	3:C:101:TRP:CH2	2.48	0.49
3:A:452:SER:CA	3:A:494:GLN:HE22	2.12	0.49
3:C:197:VAL:HG11	3:C:213:PHE:CE2	2.48	0.49
4:F:70:VAL:O	4:F:71:THR:OG1	2.29	0.49
1:H:51:ILE:HG13	1:H:58:THR:HG22	1.95	0.49
2:L:4:LEU:HD22	2:L:90:GLN:HG3	1.94	0.49
1:G:35:HIS:HD1	1:G:50:VAL:HB	1.78	0.48
2:I:4:LEU:HD22	2:I:90:GLN:HG3	1.94	0.48
3:B:61:VAL:HG21	3:B:201:MET:HE1	1.94	0.48
3:A:152:GLY:O	3:A:153:ASN:OD1	2.31	0.48
3:A:164:VAL:HG21	3:A:185:CYS:SG	2.53	0.48
3:A:197:VAL:HG11	3:A:213:PHE:CE2	2.48	0.48
3:A:475:LEU:HD12	3:A:476:SER:N	2.27	0.48
4:D:3:ALA:C	4:D:4:LEU:HD12	2.38	0.48
3:C:15:VAL:HG13	3:C:16:SER:H	1.78	0.48
3:C:152:GLY:O	3:C:153:ASN:OD1	2.31	0.48
3:B:26:GLU:HA	3:B:45:LEU:HD23	1.95	0.48
3:B:76:THR:OG1	3:B:77:GLN:N	2.46	0.48
3:B:123:LYS:O	3:B:124:ASN:ND2	2.46	0.48
3:B:164:VAL:HG21	3:B:185:CYS:SG	2.53	0.48
3:B:98:ASP:HA	3:B:110:LYS:HA	1.95	0.48
3:A:26:GLU:HA	3:A:45:LEU:HD23	1.95	0.48
3:A:453:TRP:NE1	4:D:25:ALA:HB2	2.28	0.48
3:C:440:PHE:HZ	3:C:481:LEU:HD11	1.77	0.48
3:C:487:LEU:O	3:C:490:GLY:N	2.42	0.48
4:F:3:ALA:C	4:F:4:LEU:HD12	2.38	0.48
3:B:35:ALA:HB3	3:B:37:ASN:O	2.13	0.48
3:B:325:GLN:HE22	3:B:363:SER:C	2.21	0.48
3:A:69:THR:HB	1:H:56:GLY:HA3	1.96	0.48
3:C:61:VAL:HG21	3:C:201:MET:HE1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:105:CYS:SG	3:C:106:GLY:N	2.84	0.48
3:B:86:GLN:HA	3:A:230:ASN:OD1	2.14	0.48
4:E:56:THR:HG23	4:E:59:GLN:HB3	1.95	0.48
3:A:35:ALA:HB3	3:A:37:ASN:O	2.13	0.48
3:C:26:GLU:HA	3:C:45:LEU:HD23	1.95	0.48
3:C:76:THR:OG1	3:C:77:GLN:N	2.46	0.48
3:C:98:ASP:HA	3:C:110:LYS:HA	1.95	0.48
3:C:325:GLN:HE22	3:C:363:SER:C	2.22	0.48
3:C:438:GLN:O	3:C:442:ALA:HB2	2.12	0.48
3:B:1:MET:O	3:B:3:CYS:N	2.45	0.48
3:B:86:GLN:OE1	3:A:230:ASN:HA	2.14	0.48
3:B:311:GLU:O	3:B:322:ILE:HD12	2.14	0.48
4:D:67:LEU:HA	4:D:70:VAL:HG13	1.96	0.48
3:C:394:LYS:O	3:C:395:GLY:O	2.31	0.48
1:H:4:LEU:HB2	1:H:123:GLY:HA2	1.96	0.48
2:I:35:TRP:HA	2:I:87:TYR:O	2.13	0.48
3:B:226:THR:HG23	1:H:60:SER:CB	2.43	0.48
3:A:93:LYS:HD2	3:A:240:PHE:HD2	1.79	0.48
3:A:98:ASP:HA	3:A:110:LYS:HA	1.95	0.48
3:A:206:TRP:CD2	3:A:264:LEU:HD22	2.49	0.48
3:A:381:GLY:HA3	3:A:386:GLN:HB2	1.96	0.48
3:C:472:SER:C	3:C:474:SER:H	2.22	0.48
1:H:119:PHE:CZ	2:L:37:GLN:O	2.66	0.48
3:B:150:ALA:C	3:B:152:GLY:N	2.66	0.48
3:B:197:VAL:HG11	3:B:213:PHE:CE2	2.48	0.48
3:A:58:LYS:HB2	3:A:221:LEU:HB3	1.96	0.48
3:A:175:LEU:H	3:A:179:GLY:HA3	1.79	0.48
3:A:325:GLN:HE22	3:A:363:SER:C	2.22	0.48
3:C:93:LYS:HD2	3:C:240:PHE:HD2	1.79	0.48
3:B:169:SER:C	3:B:171:THR:H	2.20	0.48
4:E:7:HIS:HA	4:E:10:MET:HE3	1.96	0.48
3:A:180:THR:HG21	3:A:291:LYS:HD2	1.96	0.48
3:A:237:LEU:HA	3:A:253:LEU:CD2	2.41	0.48
4:D:7:HIS:HA	4:D:10:MET:HE3	1.96	0.48
3:C:394:LYS:HG3	3:C:395:GLY:N	2.27	0.48
1:G:16:ALA:O	1:G:86:LEU:HG	2.14	0.48
1:G:110:THR:O	1:G:112:ARG:N	2.47	0.48
3:B:478:SER:O	3:B:479:LEU:C	2.57	0.48
3:C:35:ALA:HB3	3:C:37:ASN:O	2.13	0.48
3:C:164:VAL:HG21	3:C:185:CYS:SG	2.53	0.48
3:C:206:TRP:CD2	3:C:264:LEU:HD22	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:14:SER:O	2:L:78:LEU:HD23	2.14	0.48
2:I:2:ILE:H	2:I:2:ILE:HG12	1.36	0.47
3:B:97:VAL:HG23	3:B:98:ASP:N	2.24	0.47
3:C:201:MET:C	3:C:203:ASN:H	2.21	0.47
3:C:435:ALA:O	3:C:438:GLN:HB3	2.14	0.47
4:F:7:HIS:HA	4:F:10:MET:HE3	1.96	0.47
2:I:14:SER:O	2:I:78:LEU:HD23	2.14	0.47
2:I:17:ASP:O	2:I:78:LEU:N	2.44	0.47
3:B:188:ARG:HD2	3:C:391:TRP:HA	1.96	0.47
3:B:226:THR:HG23	1:H:60:SER:HB3	1.96	0.47
3:A:61:VAL:HG21	3:A:201:MET:HE1	1.94	0.47
3:A:481:LEU:O	3:A:485:VAL:HG12	2.15	0.47
2:L:35:TRP:HA	2:L:87:TYR:O	2.14	0.47
1:G:108:TYR:HB3	1:G:111:PRO:HD2	1.95	0.47
3:B:98:ASP:HA	3:B:111:GLY:H	1.80	0.47
3:B:152:GLY:O	3:B:153:ASN:OD1	2.31	0.47
3:B:212:TRP:HE1	4:E:5:VAL:HG12	1.79	0.47
3:B:435:ALA:O	3:B:438:GLN:HB3	2.14	0.47
3:A:472:SER:C	3:A:474:SER:H	2.21	0.47
3:A:478:SER:O	3:A:479:LEU:C	2.57	0.47
3:C:316:GLN:O	3:C:317:HIS:CG	2.66	0.47
2:L:33:LEU:HD12	2:L:89:GLN:O	2.15	0.47
1:G:56:GLY:HA2	1:G:72:ARG:NH1	2.30	0.47
3:B:52:HIS:HB2	3:B:134:ASN:ND2	2.27	0.47
3:B:148:GLU:CG	3:B:149:ASN:N	2.77	0.47
3:A:15:VAL:HG13	3:A:16:SER:N	2.29	0.47
3:A:98:ASP:HA	3:A:111:GLY:H	1.79	0.47
3:A:463:ILE:O	3:A:466:ILE:HG22	2.14	0.47
3:C:98:ASP:HA	3:C:111:GLY:H	1.79	0.47
3:C:165:THR:HG23	3:C:168:SER:H	1.78	0.47
1:H:43:GLN:HG2	1:H:44:GLY:N	2.29	0.47
1:H:116:SER:OG	1:H:121:PRO:HD2	2.14	0.47
2:L:12:SER:C	2:L:107:LYS:HE3	2.40	0.47
3:B:15:VAL:HG13	3:B:16:SER:N	2.29	0.47
3:B:481:LEU:O	3:B:485:VAL:HG12	2.15	0.47
3:A:435:ALA:O	3:A:438:GLN:HB3	2.14	0.47
3:A:448:PHE:CG	3:A:448:PHE:O	2.67	0.47
3:C:1:MET:O	3:C:3:CYS:N	2.46	0.47
3:C:57:ARG:HH21	3:C:214:LEU:HD23	1.79	0.47
3:B:57:ARG:HH21	3:B:214:LEU:HD23	1.79	0.47
3:B:92:CYS:HA	3:B:115:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:170:ILE:C	3:B:183:MET:O	2.58	0.47
3:B:472:SER:C	3:B:474:SER:H	2.21	0.47
4:E:48:ILE:O	4:E:52:THR:HG23	2.15	0.47
3:C:39:PRO:HD3	3:C:293:GLN:O	2.15	0.47
3:C:58:LYS:O	3:C:58:LYS:HG3	2.15	0.47
3:C:237:LEU:HA	3:C:253:LEU:CD2	2.41	0.47
3:C:448:PHE:CG	3:C:448:PHE:O	2.67	0.47
1:H:56:GLY:HA2	1:H:72:ARG:NH1	2.30	0.47
2:L:35:TRP:HD1	2:L:48:ILE:HB	1.80	0.47
1:G:43:GLN:HG2	1:G:44:GLY:N	2.29	0.47
3:B:39:PRO:HD3	3:B:293:GLN:O	2.15	0.47
3:B:206:TRP:CD2	3:B:264:LEU:HD22	2.49	0.47
3:B:340:MET:HG2	3:B:347:VAL:CG2	2.45	0.47
3:A:92:CYS:HA	3:A:115:THR:O	2.15	0.47
3:A:105:CYS:SG	3:A:106:GLY:N	2.84	0.47
3:A:131:GLN:C	3:A:133:GLU:H	2.22	0.47
3:C:15:VAL:HG13	3:C:16:SER:N	2.29	0.47
3:C:170:ILE:C	3:C:183:MET:O	2.58	0.47
3:C:175:LEU:H	3:C:179:GLY:HA3	1.79	0.47
2:I:12:SER:C	2:I:107:LYS:HE3	2.40	0.47
2:I:33:LEU:HD12	2:I:89:GLN:O	2.15	0.47
3:B:488:TYR:CZ	3:B:492:MET:HG3	2.49	0.47
3:A:170:ILE:C	3:A:183:MET:O	2.58	0.47
3:A:195:GLU:O	3:A:210:ARG:N	2.45	0.47
3:A:385:GLY:N	3:A:386:GLN:OE1	2.48	0.47
3:C:378:ILE:HG22	3:C:389:LEU:O	2.15	0.47
4:F:48:ILE:O	4:F:52:THR:HG23	2.15	0.47
1:G:51:ILE:HG13	1:G:58:THR:HG22	1.95	0.47
3:C:238:VAL:CG1	3:C:252:VAL:HA	2.38	0.47
3:C:463:ILE:O	3:C:466:ILE:HG22	2.14	0.47
3:C:481:LEU:O	3:C:485:VAL:HG12	2.15	0.47
3:B:93:LYS:HD2	3:B:240:PHE:HD2	1.79	0.47
3:B:175:LEU:H	3:B:179:GLY:HA3	1.79	0.47
3:A:39:PRO:HD3	3:A:293:GLN:O	2.15	0.47
1:H:119:PHE:HE1	2:L:44:PRO:HA	1.80	0.47
3:A:359:THR:HG22	3:A:360:GLU:N	2.24	0.46
3:C:92:CYS:HA	3:C:115:THR:O	2.15	0.46
1:H:16:ALA:O	1:H:86:LEU:HG	2.14	0.46
1:H:102:ALA:C	1:H:103:LEU:HD12	2.39	0.46
2:I:35:TRP:HD1	2:I:48:ILE:HB	1.80	0.46
3:B:263:ALA:HB2	4:E:2:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:97:VAL:HG23	3:A:98:ASP:N	2.24	0.46
1:H:109:THR:HA	2:L:91:PHE:HE2	1.80	0.46
3:A:57:ARG:HH21	3:A:214:LEU:HD23	1.79	0.46
3:A:383:GLU:HB2	3:A:384:PRO:HD3	1.97	0.46
4:D:48:ILE:O	4:D:52:THR:HG23	2.15	0.46
2:L:54:LEU:HD21	2:L:62:PHE:O	2.15	0.46
2:I:54:LEU:HD21	2:I:62:PHE:O	2.15	0.46
3:B:81:SER:HB2	3:A:222:PRO:HG2	1.97	0.46
3:B:383:GLU:HB2	3:B:384:PRO:HD3	1.97	0.46
4:E:14:THR:HG23	4:E:16:THR:N	2.24	0.46
3:A:82:LEU:HD23	3:A:84:GLU:N	2.29	0.46
3:A:150:ALA:C	3:A:152:GLY:N	2.66	0.46
3:A:378:ILE:HG22	3:A:389:LEU:O	2.15	0.46
3:A:450:GLY:HA2	4:D:10:MET:N	2.29	0.46
3:C:383:GLU:HB2	3:C:384:PRO:HD3	1.97	0.46
3:C:478:SER:O	3:C:479:LEU:C	2.57	0.46
3:B:448:PHE:CG	3:B:448:PHE:O	2.67	0.46
3:A:115:THR:HB	3:A:248:GLN:HE21	1.80	0.46
3:B:378:ILE:HG22	3:B:389:LEU:O	2.15	0.46
3:B:463:ILE:O	3:B:466:ILE:HG22	2.15	0.46
3:A:262:THR:O	3:A:265:THR:HG22	2.16	0.46
3:C:343:GLU:CG	3:C:344:LYS:H	2.28	0.46
2:I:30:ARG:HH12	3:A:52:HIS:HE1	1.62	0.46
4:E:67:LEU:HD23	4:E:70:VAL:HG11	1.96	0.46
1:G:72:ARG:HH12	3:B:69:THR:HG22	1.81	0.46
3:B:337:PHE:CZ	3:B:378:ILE:HD11	2.51	0.46
3:B:373:PHE:HB2	3:B:396:SER:HA	1.98	0.46
3:A:105:CYS:HA	1:H:111:PRO:HG2	1.94	0.46
3:C:125:MET:SD	3:C:260:MET:SD	3.14	0.46
2:I:4:LEU:HD21	2:I:88:CYS:SG	2.56	0.46
2:I:35:TRP:CD1	2:I:48:ILE:HB	2.51	0.46
3:B:115:THR:HB	3:B:248:GLN:HE21	1.80	0.46
3:A:339:ILE:O	3:A:347:VAL:HG23	2.16	0.46
1:H:32:ASN:CA	1:H:99:GLY:O	2.62	0.46
2:L:4:LEU:HD21	2:L:88:CYS:SG	2.56	0.46
1:G:33:TYR:CE2	1:G:101:ARG:HA	2.46	0.46
3:B:44:GLU:HB3	3:B:140:VAL:HG23	1.98	0.46
3:B:339:ILE:O	3:B:347:VAL:HG23	2.16	0.46
3:A:44:GLU:HB3	3:A:140:VAL:HG23	1.98	0.46
3:A:68:THR:HG21	3:A:250:VAL:HG21	1.98	0.46
3:A:221:LEU:HA	3:A:222:PRO:HD3	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:384:PRO:C	3:A:386:GLN:N	2.73	0.46
3:B:82:LEU:HD23	3:B:84:GLU:N	2.29	0.45
3:A:217:PRO:O	3:A:218:LEU:HB2	2.16	0.45
3:A:358:VAL:HG12	3:A:359:THR:O	2.17	0.45
3:C:338:GLU:HB2	3:C:379:ILE:HG23	1.96	0.45
3:C:361:LYS:HG2	3:C:362:ASP:N	2.32	0.45
4:F:8:VAL:HG13	4:F:9:GLY:N	2.30	0.45
2:L:19:VAL:HG12	2:L:75:ILE:HB	1.99	0.45
3:A:75:PRO:O	3:A:107:LEU:HD22	2.15	0.45
3:A:125:MET:HE1	3:A:260:MET:HE2	1.97	0.45
3:C:68:THR:HG21	3:C:250:VAL:HG21	1.98	0.45
3:C:262:THR:O	3:C:265:THR:HG22	2.16	0.45
3:C:318:GLY:O	3:C:320:ILE:HG23	2.16	0.45
4:F:67:LEU:HA	4:F:70:VAL:HG23	1.97	0.45
3:B:68:THR:HG21	3:B:250:VAL:HG21	1.98	0.45
3:B:262:THR:O	3:B:265:THR:HG22	2.16	0.45
3:A:338:GLU:HB2	3:A:379:ILE:HG23	1.97	0.45
3:C:144:HIS:O	3:C:145:SER:OG	2.25	0.45
3:C:337:PHE:CZ	3:C:378:ILE:HD11	2.51	0.45
3:C:339:ILE:O	3:C:347:VAL:HG23	2.16	0.45
3:C:392:PHE:CE2	3:C:394:LYS:HA	2.51	0.45
3:B:195:GLU:O	3:B:210:ARG:N	2.45	0.45
3:B:312:ILE:HG13	3:B:313:ALA:N	2.30	0.45
3:B:447:ALA:O	3:B:448:PHE:HB3	2.17	0.45
4:D:21:SER:O	4:D:22:SER:OG	2.29	0.45
3:C:1:MET:HE1	3:C:146:GLY:O	2.16	0.45
3:C:44:GLU:HB3	3:C:140:VAL:HG23	1.98	0.45
3:C:217:PRO:O	3:C:218:LEU:HB2	2.16	0.45
3:C:358:VAL:HG12	3:C:359:THR:O	2.16	0.45
1:H:67:ARG:NH1	1:H:83:LEU:HD11	2.32	0.45
3:B:338:GLU:HB2	3:B:379:ILE:HG23	1.97	0.45
3:B:358:VAL:HG12	3:B:359:THR:O	2.17	0.45
3:A:165:THR:HG23	3:A:168:SER:H	1.82	0.45
3:A:320:ILE:HD11	3:A:369:ALA:HB3	1.98	0.45
3:C:320:ILE:HG12	3:C:371:PRO:CD	2.47	0.45
2:I:19:VAL:HG12	2:I:75:ILE:HB	1.99	0.45
3:B:131:GLN:C	3:B:133:GLU:H	2.22	0.45
3:B:320:ILE:HG12	3:B:371:PRO:CD	2.47	0.45
3:B:320:ILE:HD11	3:B:369:ALA:HB3	1.98	0.45
3:B:27:HIS:ND1	3:B:28:GLY:N	2.64	0.45
3:B:57:ARG:NH2	3:B:220:TRP:CZ3	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:286:ARG:NH2	3:C:342:LEU:HD22	2.32	0.45
4:E:56:THR:O	4:E:59:GLN:N	2.42	0.45
4:F:50:ALA:O	4:F:55:THR:HG22	2.17	0.45
3:B:237:LEU:HA	3:B:253:LEU:CD2	2.41	0.45
3:A:220:TRP:HB3	3:A:232:ILE:HB	1.99	0.45
4:F:46:ALA:HB3	4:F:67:LEU:HD22	1.99	0.45
2:L:35:TRP:CD1	2:L:48:ILE:HB	2.51	0.45
3:B:260:MET:SD	4:E:2:VAL:HG11	2.56	0.45
3:A:57:ARG:NH2	3:A:220:TRP:CZ3	2.85	0.45
3:A:320:ILE:HG12	3:A:371:PRO:CD	2.47	0.45
3:A:361:LYS:HG2	3:A:362:ASP:N	2.32	0.45
3:C:27:HIS:ND1	3:C:280:THR:N	2.65	0.45
3:C:315:THR:O	3:C:316:GLN:C	2.60	0.45
3:B:188:ARG:HH22	3:C:312:ILE:HD13	1.82	0.45
4:D:50:ALA:O	4:D:55:THR:HG22	2.17	0.45
3:C:381:GLY:CA	3:C:386:GLN:HB2	2.47	0.45
1:G:109:THR:HG23	1:G:110:THR:N	2.30	0.44
3:B:217:PRO:O	3:B:218:LEU:HB2	2.16	0.44
3:B:227:GLN:H	1:H:65:GLN:HE22	1.65	0.44
3:B:361:LYS:HG2	3:B:362:ASP:N	2.32	0.44
4:E:67:LEU:HD23	4:E:67:LEU:HA	1.85	0.44
3:A:384:PRO:HD2	3:A:386:GLN:NE2	2.33	0.44
3:C:57:ARG:NH2	3:C:220:TRP:CZ3	2.85	0.44
3:C:320:ILE:HD11	3:C:369:ALA:HB3	1.98	0.44
3:C:415:LEU:O	3:C:416:GLY:O	2.35	0.44
4:E:12:LEU:O	4:E:13:GLU:C	2.59	0.44
3:A:204:LYS:HE2	3:C:251:VAL:CG2	2.47	0.44
3:A:209:HIS:HB3	4:D:12:LEU:HD21	1.99	0.44
3:A:318:GLY:O	3:A:320:ILE:HG23	2.16	0.44
3:A:337:PHE:CZ	3:A:378:ILE:HD11	2.51	0.44
4:D:67:LEU:HD23	4:D:70:VAL:HG11	1.99	0.44
3:C:115:THR:HB	3:C:248:GLN:HE21	1.80	0.44
1:G:67:ARG:NH1	1:G:83:LEU:HD11	2.32	0.44
3:B:169:SER:O	3:B:170:ILE:HG12	2.17	0.44
3:A:289:MET:O	3:A:290:ASP:C	2.60	0.44
3:A:317:HIS:CE1	3:A:400:GLN:NE2	2.85	0.44
4:D:50:ALA:O	4:D:60:ARG:HG2	2.17	0.44
3:C:206:TRP:HZ2	4:F:19:TRP:CH2	2.36	0.44
2:L:12:SER:OG	2:L:105:GLN:HB2	2.17	0.44
2:L:35:TRP:CD2	2:L:73:PHE:HB2	2.52	0.44
3:B:289:MET:O	3:B:290:ASP:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:318:GLY:O	3:B:320:ILE:HG23	2.16	0.44
3:B:343:GLU:C	3:B:345:ARG:NH2	2.76	0.44
3:A:447:ALA:O	3:A:448:PHE:HB3	2.16	0.44
3:A:479:LEU:O	3:A:480:VAL:C	2.61	0.44
3:C:447:ALA:O	3:C:448:PHE:HB3	2.17	0.44
4:F:5:VAL:HG23	4:F:5:VAL:O	2.18	0.44
4:F:50:ALA:O	4:F:60:ARG:HG2	2.17	0.44
1:G:94:TYR:O	1:G:125:GLY:HA2	2.18	0.44
3:A:340:MET:HB2	3:A:377:TYR:HD2	1.82	0.44
3:A:414:ILE:HG22	3:A:415:LEU:N	2.32	0.44
3:A:455:MET:HG3	4:F:70:VAL:HG13	1.98	0.44
4:D:55:THR:HA	4:D:60:ARG:CG	2.46	0.44
3:C:312:ILE:HG13	3:C:313:ALA:N	2.30	0.44
1:H:48:MET:HE2	1:H:68:ILE:HD12	2.00	0.44
2:I:12:SER:OG	2:I:105:GLN:HB2	2.18	0.44
3:B:165:THR:HG23	3:B:168:SER:H	1.81	0.44
3:B:394:LYS:HG3	3:B:395:GLY:N	2.33	0.44
4:E:50:ALA:O	4:E:55:THR:HG22	2.17	0.44
3:A:463:ILE:HG23	3:A:482:VAL:HG11	2.00	0.44
3:C:463:ILE:HG23	3:C:482:VAL:HG11	2.00	0.44
4:F:70:VAL:HG12	4:F:71:THR:N	2.33	0.44
1:G:47:TRP:CG	2:I:96:ILE:HB	2.52	0.44
3:B:59:TYR:O	3:B:125:MET:N	2.51	0.44
3:A:410:LYS:O	3:A:413:ALA:C	2.61	0.44
3:C:320:ILE:HD12	3:C:320:ILE:O	2.18	0.44
3:C:479:LEU:O	3:C:480:VAL:C	2.60	0.44
1:H:110:THR:N	1:H:111:PRO:CD	2.81	0.44
1:G:4:LEU:HB2	1:G:123:GLY:CA	2.47	0.44
2:I:94:LEU:N	2:I:95:PRO:CD	2.81	0.44
3:B:2:ARG:H	3:B:151:VAL:C	2.26	0.44
3:B:81:SER:HB2	3:A:222:PRO:HB2	2.00	0.44
3:B:321:VAL:O	3:B:322:ILE:HD13	2.18	0.44
3:B:343:GLU:C	3:B:345:ARG:HH21	2.25	0.44
1:H:35:HIS:O	1:H:96:CYS:HA	2.18	0.44
1:G:48:MET:HE2	1:G:68:ILE:HD12	2.00	0.44
2:I:85:THR:OG1	2:I:103:ARG:HG2	2.18	0.44
3:B:320:ILE:O	3:B:320:ILE:HD12	2.18	0.44
3:A:3:CYS:CB	3:A:9:ARG:HH21	2.29	0.44
3:A:59:TYR:O	3:A:125:MET:N	2.51	0.44
1:H:53:PRO:O	1:H:72:ARG:NE	2.51	0.44
1:G:6:GLN:HE22	1:G:95:TYR:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:27:TYR:CE2	1:G:29:PHE:HA	2.53	0.43
1:G:53:PRO:O	1:G:72:ARG:NE	2.51	0.43
2:I:35:TRP:CD2	2:I:73:PHE:HB2	2.52	0.43
3:A:15:VAL:HG23	3:A:20:TRP:O	2.18	0.43
3:A:320:ILE:HD12	3:A:320:ILE:O	2.18	0.43
3:C:59:TYR:O	3:C:125:MET:N	2.51	0.43
3:C:71:ALA:O	3:C:113:ILE:HG13	2.18	0.43
3:C:410:LYS:O	3:C:413:ALA:C	2.61	0.43
3:C:20:TRP:HB3	3:C:425:LEU:HD23	1.99	0.43
4:E:11:GLY:O	4:E:12:LEU:HB2	2.19	0.43
4:D:11:GLY:O	4:D:12:LEU:HB2	2.19	0.43
3:C:169:SER:O	3:C:170:ILE:HG12	2.18	0.43
2:L:94:LEU:N	2:L:95:PRO:CD	2.81	0.43
3:B:75:PRO:HB3	3:B:111:GLY:N	2.33	0.43
3:B:410:LYS:O	3:B:413:ALA:C	2.61	0.43
3:A:71:ALA:O	3:A:113:ILE:HG13	2.18	0.43
4:D:12:LEU:O	4:D:13:GLU:C	2.61	0.43
2:L:33:LEU:HD22	2:L:71:PHE:CD2	2.53	0.43
3:A:34:MET:HE1	3:A:350:ARG:CZ	2.48	0.43
3:A:100:GLY:HA3	3:A:108:PHE:CD1	2.54	0.43
3:A:169:SER:O	3:A:170:ILE:HG12	2.18	0.43
3:C:82:LEU:HD23	3:C:84:GLU:N	2.29	0.43
1:H:6:GLN:HE22	1:H:95:TYR:HA	1.83	0.43
1:H:119:PHE:CB	2:L:36:TYR:CE1	2.91	0.43
3:B:146:GLY:HA2	3:B:366:ASN:OD1	2.19	0.43
3:B:463:ILE:HG23	3:B:482:VAL:HG11	2.00	0.43
4:E:6:PRO:O	4:E:8:VAL:HG13	2.19	0.43
4:E:50:ALA:O	4:E:60:ARG:HG2	2.17	0.43
3:A:277:LEU:HD23	3:A:277:LEU:HA	1.82	0.43
3:A:321:VAL:O	3:A:322:ILE:HD13	2.18	0.43
1:H:67:ARG:NH2	1:H:90:ASP:OD2	2.51	0.43
2:L:85:THR:OG1	2:L:103:ARG:HG2	2.18	0.43
2:I:37:GLN:HB3	2:I:47:LEU:HD11	2.00	0.43
3:B:75:PRO:CA	3:B:111:GLY:HA2	2.48	0.43
3:A:108:PHE:CD2	3:C:313:ALA:HB1	2.54	0.43
3:A:454:THR:OG1	3:A:455:MET:N	2.51	0.43
3:C:90:PHE:HD1	3:C:117:ALA:C	2.27	0.43
1:G:60:SER:CB	3:A:226:THR:HG23	2.48	0.43
1:G:67:ARG:NH2	1:G:90:ASP:OD2	2.51	0.43
3:B:436:LEU:O	3:B:440:PHE:HB2	2.19	0.43
3:A:436:LEU:O	3:A:440:PHE:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:GLY:HA3	3:C:108:PHE:CD1	2.54	0.43
3:C:321:VAL:O	3:C:322:ILE:HD13	2.18	0.43
1:H:27:TYR:CE2	1:H:29:PHE:HA	2.53	0.43
1:G:35:HIS:O	1:G:96:CYS:HA	2.18	0.43
2:I:33:LEU:HD22	2:I:71:PHE:CD2	2.53	0.43
3:B:72:SER:HB2	3:B:112:GLY:O	2.19	0.43
3:B:378:ILE:CG2	3:B:389:LEU:HB2	2.49	0.43
3:C:351:LEU:C	3:C:352:ILE:HD13	2.44	0.43
3:C:436:LEU:O	3:C:440:PHE:HB2	2.19	0.43
3:B:479:LEU:O	3:B:480:VAL:C	2.62	0.43
3:A:1:MET:HA	3:A:151:VAL:HA	2.01	0.43
3:A:38:LYS:H	3:A:294:LEU:CD2	2.32	0.43
3:A:53:PRO:HA	3:A:130:VAL:HG12	2.01	0.43
3:A:72:SER:HB2	3:A:112:GLY:O	2.19	0.43
3:A:312:ILE:HG13	3:A:313:ALA:N	2.30	0.43
3:C:162:ILE:HG23	3:C:162:ILE:O	2.19	0.43
3:C:359:THR:HG22	3:C:360:GLU:N	2.24	0.43
3:C:454:THR:OG1	3:C:455:MET:N	2.51	0.43
3:B:100:GLY:HA3	3:B:108:PHE:CD1	2.54	0.42
3:B:146:GLY:O	3:B:147:GLU:HB3	2.18	0.42
3:B:199:LEU:HD22	3:B:213:PHE:CE1	2.54	0.42
3:B:359:THR:C	3:B:361:LYS:N	2.77	0.42
3:A:1:MET:C	3:A:3:CYS:N	2.76	0.42
3:A:199:LEU:HD22	3:A:213:PHE:CE1	2.54	0.42
3:A:351:LEU:C	3:A:352:ILE:HD13	2.44	0.42
1:H:94:TYR:O	1:H:125:GLY:HA2	2.18	0.42
3:B:149:ASN:O	3:B:150:ALA:HB2	2.18	0.42
3:B:414:ILE:HG22	3:B:415:LEU:N	2.34	0.42
3:A:75:PRO:C	3:A:76:THR:HG1	2.27	0.42
3:A:146:GLY:HA2	3:A:366:ASN:OD1	2.19	0.42
3:A:257:GLU:O	3:A:260:MET:HB3	2.19	0.42
3:A:378:ILE:CG2	3:A:389:LEU:HB2	2.49	0.42
3:C:72:SER:HB2	3:C:112:GLY:O	2.19	0.42
4:F:46:ALA:HB1	4:F:67:LEU:HB2	2.01	0.42
1:H:119:PHE:HB3	2:L:46:LEU:CA	2.48	0.42
2:L:37:GLN:HB3	2:L:47:LEU:HD11	2.00	0.42
3:B:71:ALA:O	3:B:113:ILE:HG13	2.18	0.42
3:B:162:ILE:HG23	3:B:162:ILE:O	2.19	0.42
3:B:454:THR:OG1	3:B:455:MET:N	2.51	0.42
3:A:162:ILE:HG23	3:A:162:ILE:O	2.19	0.42
3:A:180:THR:CG2	3:A:291:LYS:HD2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:191:LEU:HD23	3:A:191:LEU:HA	1.83	0.42
3:A:475:LEU:O	3:A:478:SER:HB3	2.20	0.42
3:C:53:PRO:HA	3:C:130:VAL:HG12	2.01	0.42
3:C:140:VAL:HG12	3:C:160:LYS:O	2.20	0.42
3:C:146:GLY:HA2	3:C:366:ASN:OD1	2.18	0.42
3:C:289:MET:O	3:C:290:ASP:C	2.60	0.42
3:C:359:THR:O	3:C:361:LYS:N	2.39	0.42
4:F:19:TRP:CD1	4:F:20:MET:HG2	2.47	0.42
4:E:55:THR:HA	4:E:60:ARG:CG	2.46	0.42
3:A:125:MET:SD	3:A:199:LEU:HD21	2.60	0.42
3:B:125:MET:SD	3:B:199:LEU:HD21	2.60	0.42
3:A:140:VAL:HG12	3:A:160:LYS:O	2.20	0.42
3:A:180:THR:HG22	3:A:291:LYS:HB3	2.00	0.42
3:A:387:LEU:O	3:A:388:LYS:HG3	2.19	0.42
3:C:125:MET:SD	3:C:199:LEU:HD21	2.60	0.42
3:C:445:GLY:C	3:C:447:ALA:H	2.27	0.42
1:H:49:GLY:HA3	1:H:70:MET:HE1	2.01	0.42
3:B:53:PRO:HA	3:B:130:VAL:HG12	2.01	0.42
3:B:90:PHE:HD1	3:B:117:ALA:C	2.27	0.42
3:B:475:LEU:O	3:B:478:SER:HB3	2.20	0.42
3:A:2:ARG:H	3:A:151:VAL:C	2.27	0.42
3:A:359:THR:C	3:A:361:LYS:N	2.77	0.42
3:C:2:ARG:H	3:C:151:VAL:C	2.27	0.42
3:C:378:ILE:CG2	3:C:389:LEU:HB2	2.49	0.42
1:G:73:ASP:OD1	1:G:75:SER:OG	2.26	0.42
2:I:35:TRP:O	2:I:47:LEU:HB2	2.20	0.42
3:B:238:VAL:N	3:B:253:LEU:HB2	2.33	0.42
3:A:63:ALA:HA	3:A:121:CYS:HA	2.01	0.42
4:D:6:PRO:O	4:D:8:VAL:HG13	2.20	0.42
4:D:53:ILE:C	4:D:55:THR:HG23	2.45	0.42
4:D:66:LEU:HD11	4:F:66:LEU:HD22	2.02	0.42
3:C:221:LEU:HA	3:C:222:PRO:HD3	1.78	0.42
3:C:265:THR:HA	4:F:19:TRP:HB3	2.01	0.42
4:F:53:ILE:C	4:F:55:THR:HG23	2.45	0.42
3:B:48:THR:O	3:B:278:LEU:HB3	2.20	0.42
3:B:226:THR:OG1	1:H:59:ALA:HA	2.20	0.42
3:B:340:MET:HG2	3:B:347:VAL:HB	2.02	0.42
3:B:485:VAL:O	3:B:489:LEU:HB3	2.20	0.42
3:A:90:PHE:HD1	3:A:117:ALA:C	2.27	0.42
3:A:340:MET:HG2	3:A:347:VAL:HB	2.00	0.42
3:A:415:LEU:HD23	3:A:415:LEU:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:64:PHE:O	4:D:68:THR:HG23	2.20	0.42
3:C:27:HIS:HE1	3:C:279:PHE:HA	1.81	0.42
3:C:38:LYS:H	3:C:294:LEU:CD2	2.32	0.42
3:C:199:LEU:HD22	3:C:213:PHE:CE1	2.54	0.42
2:L:66:GLY:HA3	2:L:71:PHE:HA	2.02	0.42
3:B:11:PHE:CD1	3:B:32:THR:HB	2.55	0.42
3:A:74:CYS:HB2	3:A:99:ARG:HE	1.84	0.42
3:A:387:LEU:HD23	3:A:388:LYS:N	2.35	0.42
4:D:59:GLN:O	4:D:63:ILE:HG12	2.20	0.42
3:C:58:LYS:O	3:C:59:TYR:C	2.62	0.42
3:C:310:LYS:HE2	3:C:323:ARG:N	2.33	0.42
3:C:485:VAL:O	3:C:489:LEU:HB3	2.20	0.42
3:B:180:THR:HG22	3:B:291:LYS:HB3	2.01	0.42
3:B:283:LEU:HD12	3:B:283:LEU:C	2.45	0.42
3:A:283:LEU:C	3:A:283:LEU:HD12	2.45	0.42
4:D:1:SER:C	4:D:3:ALA:N	2.77	0.42
3:C:97:VAL:HG23	3:C:98:ASP:N	2.24	0.42
3:C:277:LEU:HA	3:C:277:LEU:HD23	1.82	0.42
2:L:6:GLN:OE1	2:L:101:GLY:N	2.38	0.42
1:G:49:GLY:HA3	1:G:70:MET:HE1	2.02	0.41
3:B:351:LEU:C	3:B:352:ILE:HD13	2.44	0.41
4:E:59:GLN:O	4:E:63:ILE:HG12	2.20	0.41
3:A:1:MET:O	3:A:3:CYS:N	2.51	0.41
3:A:340:MET:SD	3:A:345:ARG:HD2	2.60	0.41
3:A:363:SER:HA	3:A:364:PRO:HD3	1.82	0.41
3:A:463:ILE:HA	3:A:466:ILE:HG22	2.01	0.41
3:C:100:GLY:HA3	3:C:108:PHE:CE1	2.55	0.41
1:G:47:TRP:NE1	2:I:96:ILE:HD12	2.35	0.41
2:I:66:GLY:HA3	2:I:71:PHE:HA	2.02	0.41
3:B:448:PHE:CE1	3:B:459:ILE:HG21	2.55	0.41
4:E:1:SER:C	4:E:3:ALA:N	2.77	0.41
3:A:108:PHE:HD1	3:A:108:PHE:HA	1.70	0.41
3:A:294:LEU:HD12	3:A:297:MET:SD	2.60	0.41
3:A:480:VAL:HG23	3:A:481:LEU:H	1.85	0.41
3:A:485:VAL:O	3:A:489:LEU:HB3	2.20	0.41
4:D:67:LEU:HA	4:D:67:LEU:HD23	1.86	0.41
3:C:161:GLU:O	3:C:162:ILE:C	2.63	0.41
4:F:59:GLN:O	4:F:63:ILE:HG12	2.20	0.41
1:H:110:THR:HB	1:H:111:PRO:HD3	2.01	0.41
2:I:6:GLN:OE1	2:I:101:GLY:N	2.39	0.41
3:B:79:GLU:HA	3:B:80:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:161:GLU:O	3:B:162:ILE:C	2.63	0.41
3:B:247:LYS:HD2	3:B:247:LYS:HA	1.87	0.41
3:B:463:ILE:HA	3:B:466:ILE:HG22	2.01	0.41
4:E:53:ILE:C	4:E:55:THR:HG23	2.45	0.41
3:A:100:GLY:HA3	3:A:108:PHE:CE1	2.55	0.41
4:D:54:GLY:C	4:D:55:THR:HG1	2.26	0.41
3:C:463:ILE:HA	3:C:466:ILE:HG22	2.01	0.41
3:B:182:THR:O	3:B:287:LEU:HD12	2.21	0.41
3:A:175:LEU:CB	3:A:179:GLY:HA3	2.50	0.41
3:C:11:PHE:CD1	3:C:32:THR:HB	2.55	0.41
2:L:62:PHE:HD1	2:L:73:PHE:HZ	1.68	0.41
3:B:140:VAL:HG12	3:B:160:LYS:O	2.20	0.41
4:E:49:LEU:O	4:E:53:ILE:HG22	2.20	0.41
3:A:11:PHE:CD1	3:A:32:THR:HB	2.55	0.41
3:A:107:LEU:O	3:A:108:PHE:HB2	2.19	0.41
3:A:263:ALA:HA	4:D:6:PRO:HA	2.01	0.41
4:D:49:LEU:O	4:D:53:ILE:HG22	2.21	0.41
3:C:26:GLU:HB2	3:C:281:GLY:O	2.21	0.41
3:C:283:LEU:C	3:C:283:LEU:HD12	2.45	0.41
3:C:359:THR:C	3:C:361:LYS:N	2.77	0.41
2:I:63:SER:OG	2:I:74:THR:HB	2.21	0.41
3:B:38:LYS:H	3:B:294:LEU:CD2	2.32	0.41
3:B:188:ARG:NH1	3:C:312:ILE:HG21	2.36	0.41
3:B:446:ALA:HA	3:B:449:SER:HB3	2.02	0.41
3:B:456:LYS:O	3:B:459:ILE:HG22	2.21	0.41
3:A:303:THR:OG1	3:A:304:GLY:N	2.54	0.41
3:A:385:GLY:O	3:A:387:LEU:N	2.38	0.41
3:A:448:PHE:CE1	3:A:459:ILE:HG21	2.55	0.41
3:A:453:TRP:N	3:A:494:GLN:OE1	2.52	0.41
3:C:353:THR:O	3:C:353:THR:HG22	2.21	0.41
3:C:448:PHE:CE1	3:C:459:ILE:HG21	2.55	0.41
2:L:63:SER:OG	2:L:74:THR:HB	2.21	0.41
3:B:66:THR:O	3:B:68:THR:OG1	2.34	0.41
3:B:200:GLN:N	3:B:200:GLN:OE1	2.54	0.41
3:B:212:TRP:NE1	4:E:5:VAL:HG12	2.36	0.41
3:B:306:PHE:CZ	3:B:335:ILE:HG23	2.56	0.41
3:B:414:ILE:HD13	4:E:15:ARG:HE	1.86	0.41
3:A:26:GLU:HB2	3:A:281:GLY:O	2.21	0.41
3:A:48:THR:O	3:A:278:LEU:HB3	2.20	0.41
3:A:180:THR:CG2	3:A:291:LYS:HB3	2.51	0.41
3:A:238:VAL:N	3:A:253:LEU:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:306:PHE:CZ	3:A:335:ILE:HG23	2.56	0.41
4:D:66:LEU:O	4:D:70:VAL:HG13	2.21	0.41
3:C:363:SER:HA	3:C:364:PRO:HD3	1.82	0.41
4:F:66:LEU:O	4:F:67:LEU:C	2.64	0.41
3:B:43:PHE:CE2	3:B:287:LEU:HD22	2.56	0.41
4:D:56:THR:O	4:D:57:TYR:C	2.64	0.41
3:C:31:VAL:O	3:C:42:ASP:HA	2.21	0.41
3:C:270:ILE:HD13	3:C:278:LEU:HD12	2.03	0.41
3:C:456:LYS:O	3:C:459:ILE:HG22	2.21	0.41
4:F:11:GLY:O	4:F:12:LEU:HB2	2.18	0.41
1:G:13:LYS:HD3	1:G:131:SER:O	2.21	0.41
1:G:31:SER:HA	1:G:101:ARG:HD2	2.03	0.41
1:G:65:GLN:HE22	3:A:227:GLN:N	2.16	0.41
3:B:353:THR:O	3:B:353:THR:HG22	2.21	0.41
3:A:182:THR:O	3:A:287:LEU:HD12	2.21	0.41
3:A:408:GLY:O	3:A:412:MET:HG3	2.21	0.41
3:C:43:PHE:CE2	3:C:287:LEU:HD22	2.56	0.41
3:C:131:GLN:C	3:C:133:GLU:H	2.22	0.41
3:C:132:PRO:HD3	3:C:194:ASN:OD1	2.21	0.41
3:C:182:THR:O	3:C:287:LEU:HD12	2.21	0.41
3:C:303:THR:OG1	3:C:304:GLY:N	2.54	0.41
3:C:450:GLY:HA2	4:F:10:MET:N	2.33	0.41
1:H:13:LYS:HD3	1:H:131:SER:O	2.21	0.41
1:H:118:TRP:CD1	1:H:118:TRP:O	2.74	0.41
2:L:11:LEU:HD12	2:L:21:PHE:HE1	1.86	0.41
3:B:15:VAL:O	3:B:425:LEU:HD21	2.21	0.41
3:B:26:GLU:HB2	3:B:281:GLY:O	2.21	0.41
3:B:100:GLY:HA3	3:B:108:PHE:CE1	2.55	0.41
3:B:180:THR:CG2	3:B:291:LYS:HB3	2.51	0.41
3:B:257:GLU:O	3:B:260:MET:HB3	2.21	0.41
3:B:394:LYS:CG	3:B:395:GLY:H	2.34	0.41
4:E:56:THR:O	4:E:57:TYR:C	2.64	0.41
3:A:56:LEU:HG	3:A:56:LEU:O	2.21	0.41
4:D:63:ILE:O	4:D:66:LEU:HB2	2.21	0.41
3:C:15:VAL:O	3:C:425:LEU:HD21	2.21	0.41
3:C:385:GLY:O	3:C:386:GLN:C	2.62	0.41
2:I:11:LEU:HD12	2:I:21:PHE:HE1	1.86	0.40
3:B:27:HIS:CD2	3:B:279:PHE:HB3	2.56	0.40
3:B:31:VAL:O	3:B:42:ASP:HA	2.21	0.40
3:B:227:GLN:O	3:B:228:GLY:C	2.64	0.40
3:A:74:CYS:HB2	3:A:105:CYS:HG	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:200:GLN:OE1	3:A:200:GLN:N	2.54	0.40
3:C:1:MET:HE2	3:C:366:ASN:HD21	1.85	0.40
3:C:462:VAL:HG23	4:F:58:PHE:CZ	2.56	0.40
3:C:475:LEU:O	3:C:478:SER:HB3	2.20	0.40
1:H:17:SER:HA	1:H:83:LEU:O	2.21	0.40
1:G:32:ASN:CA	1:G:99:GLY:O	2.62	0.40
3:B:303:THR:OG1	3:B:304:GLY:N	2.54	0.40
3:B:478:SER:OG	3:B:479:LEU:N	2.55	0.40
3:A:43:PHE:CE2	3:A:287:LEU:HD22	2.56	0.40
3:A:161:GLU:O	3:A:162:ILE:C	2.63	0.40
3:A:456:LYS:O	3:A:459:ILE:HG22	2.21	0.40
3:C:200:GLN:OE1	3:C:200:GLN:N	2.54	0.40
3:C:267:ALA:O	4:F:18:THR:HB	2.22	0.40
3:C:275:GLY:O	3:C:276:ASN:HB2	2.21	0.40
2:L:35:TRP:O	2:L:47:LEU:HB2	2.20	0.40
3:B:199:LEU:O	3:B:205:ALA:HA	2.21	0.40
3:B:233:GLN:O	3:B:234:LYS:HB2	2.21	0.40
3:B:275:GLY:O	3:B:276:ASN:HB2	2.21	0.40
3:A:31:VAL:O	3:A:42:ASP:HA	2.21	0.40
3:A:233:GLN:O	3:A:234:LYS:HB2	2.22	0.40
3:A:267:ALA:O	4:D:18:THR:HB	2.21	0.40
3:A:353:THR:O	3:A:353:THR:HG22	2.21	0.40
3:A:456:LYS:HD2	3:A:490:GLY:HA2	2.03	0.40
3:C:48:THR:O	3:C:278:LEU:HB3	2.20	0.40
3:C:478:SER:OG	3:C:479:LEU:N	2.55	0.40
4:F:49:LEU:O	4:F:53:ILE:HG22	2.21	0.40
1:H:103:LEU:C	1:H:105:TYR:H	2.30	0.40
1:G:31:SER:C	1:G:101:ARG:HD2	2.47	0.40
2:I:9:SER:O	2:I:102:THR:HA	2.22	0.40
3:B:191:LEU:HD23	3:B:191:LEU:HA	1.83	0.40
3:B:363:SER:HA	3:B:364:PRO:HD3	1.82	0.40
3:B:408:GLY:O	3:B:412:MET:HG3	2.20	0.40
3:A:27:HIS:CE1	3:A:280:THR:O	2.73	0.40
3:A:99:ARG:HG2	3:A:103:ASN:CG	2.47	0.40
3:A:132:PRO:HD3	3:A:194:ASN:OD1	2.21	0.40
3:A:455:MET:CG	4:F:70:VAL:HG13	2.52	0.40
3:C:41:LEU:HD23	3:C:41:LEU:HA	1.84	0.40
3:C:272:MET:HE3	3:C:275:GLY:C	2.46	0.40
4:E:21:SER:O	4:E:22:SER:OG	2.29	0.40
3:A:270:ILE:HD13	3:A:278:LEU:HD12	2.03	0.40
3:A:272:MET:HE3	3:A:275:GLY:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:305:LYS:H	3:A:386:GLN:CG	2.30	0.40
3:C:8:ASN:HB2	4:F:15:ARG:NH1	2.36	0.40
3:C:175:LEU:CB	3:C:179:GLY:HA3	2.50	0.40
3:C:238:VAL:O	3:C:238:VAL:HG23	2.22	0.40
3:C:313:ALA:O	3:C:320:ILE:HA	2.22	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	H	130/132 (98%)	114 (88%)	12 (9%)	4 (3%)	3	22
2	L	105/107 (98%)	95 (90%)	7 (7%)	3 (3%)	3	23
3	A	41/495 (8%)	33 (80%)	7 (17%)	1 (2%)	4	27
3	B	417/495 (84%)	312 (75%)	81 (19%)	24 (6%)	1	14
3	C	493/495 (100%)	365 (74%)	95 (19%)	33 (7%)	1	12
4	D	70/72 (97%)	52 (74%)	14 (20%)	4 (6%)	1	14
4	F	70/72 (97%)	54 (77%)	15 (21%)	1 (1%)	9	39
All	All	1326/1868 (71%)	1025 (77%)	231 (17%)	70 (5%)	2	15

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	148	GLU
3	B	170	ILE
3	B	290	ASP
3	B	291	LYS
3	B	319	THR
3	B	360	GLU

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Mol	Chain	Res	Type
3	C	170	ILE
3	C	203	ASN
3	C	233	GLN
3	C	298	SER
3	C	310	LYS
3	C	311	GLU
3	C	319	THR
3	C	360	GLU
3	C	416	GLY
1	H	104	PHE
3	B	57	ARG
3	B	151	VAL
3	B	162	ILE
3	B	298	SER
3	B	386	GLN
4	D	13	GLU
4	D	56	THR
3	C	57	ARG
3	C	151	VAL
3	C	162	ILE
3	C	202	GLU
3	C	312	ILE
3	C	385	GLY
3	C	395	GLY
3	C	414	ILE
3	C	478	SER
1	H	112	ARG
1	H	121	PRO
2	L	94	LEU
3	B	74	CYS
3	B	320	ILE
3	A	447	ALA
3	C	19	SER
3	C	150	ALA
3	C	225	ASP
3	C	238	VAL
3	C	320	ILE
3	B	107	LEU
3	B	332	PRO
3	B	414	ILE
4	D	14	THR
3	C	10	ASP

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Mol	Chain	Res	Type
3	C	332	PRO
3	B	98	ASP
3	B	123	LYS
3	B	147	GLU
3	B	361	LYS
4	D	5	VAL
3	C	76	THR
3	C	98	ASP
3	C	316	GLN
3	C	361	LYS
3	C	394	LYS
2	L	95	PRO
3	B	238	VAL
3	B	344	LYS
3	C	2	ARG
3	B	232	ILE
3	C	493	VAL
3	B	331	SER
3	C	331	SER
4	F	70	VAL
2	L	2	ILE
1	H	120	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	101/109 (93%)	99 (98%)	2 (2%)	48	65
1	H	103/109 (94%)	101 (98%)	2 (2%)	50	66
2	I	94/94 (100%)	92 (98%)	2 (2%)	47	65
2	L	94/94 (100%)	94 (100%)	0	100	100
3	A	369/419 (88%)	368 (100%)	1 (0%)	86	84
3	B	369/419 (88%)	368 (100%)	1 (0%)	86	84
3	C	368/419 (88%)	367 (100%)	1 (0%)	86	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	56/60 (93%)	54 (96%)	2 (4%)	31	52
4	E	56/60 (93%)	55 (98%)	1 (2%)	51	67
4	F	55/60 (92%)	55 (100%)	0	100	100
All	All	1665/1843 (90%)	1653 (99%)	12 (1%)	73	79

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	103	LEU
1	G	120	ASP
2	I	1	ASP
2	I	2	ILE
3	B	425	LEU
4	E	56	THR
3	A	425	LEU
4	D	5	VAL
4	D	56	THR
3	C	425	LEU
1	H	113	ASP
1	H	119	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	65	GLN
2	I	34	ASN
2	I	37	GLN
2	I	53	ASN
3	B	103	ASN
3	B	124	ASN
3	B	317	HIS
3	B	400	GLN
4	E	7	HIS
4	E	59	GLN
3	A	52	HIS
3	A	86	GLN
3	A	103	ASN
3	A	124	ASN
3	A	400	GLN
4	D	7	HIS

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Mol	Chain	Res	Type
3	C	103	ASN
3	C	134	ASN
3	C	149	ASN
4	F	7	HIS
4	F	28	HIS
1	H	65	GLN
2	L	34	ASN
2	L	37	GLN
2	L	53	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 ⓘ

6 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	$\# Z > 2$
5	NAG	J	1	3,5	14,14,15	0.26	0	17,19,21	0.73	1 (5%)
5	NAG	J	2	5	14,14,15	0.19	0	17,19,21	0.38	0
5	NAG	K	1	3,5	14,14,15	0.28	0	17,19,21	0.74	1 (5%)
5	NAG	K	2	5	14,14,15	0.18	0	17,19,21	0.39	0
5	NAG	M	1	3,5	14,14,15	0.30	0	17,19,21	0.75	1 (5%)
5	NAG	M	2	5	14,14,15	0.17	0	17,19,21	0.39	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
5	NAG	J	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	4/6/23/26	0/1/1/1
5	NAG	K	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
5	NAG	M	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1	NAG	C1-O5-C5	2.57	115.63	112.19
5	K	1	NAG	C1-O5-C5	2.57	115.62	112.19
5	J	1	NAG	C1-O5-C5	2.54	115.58	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

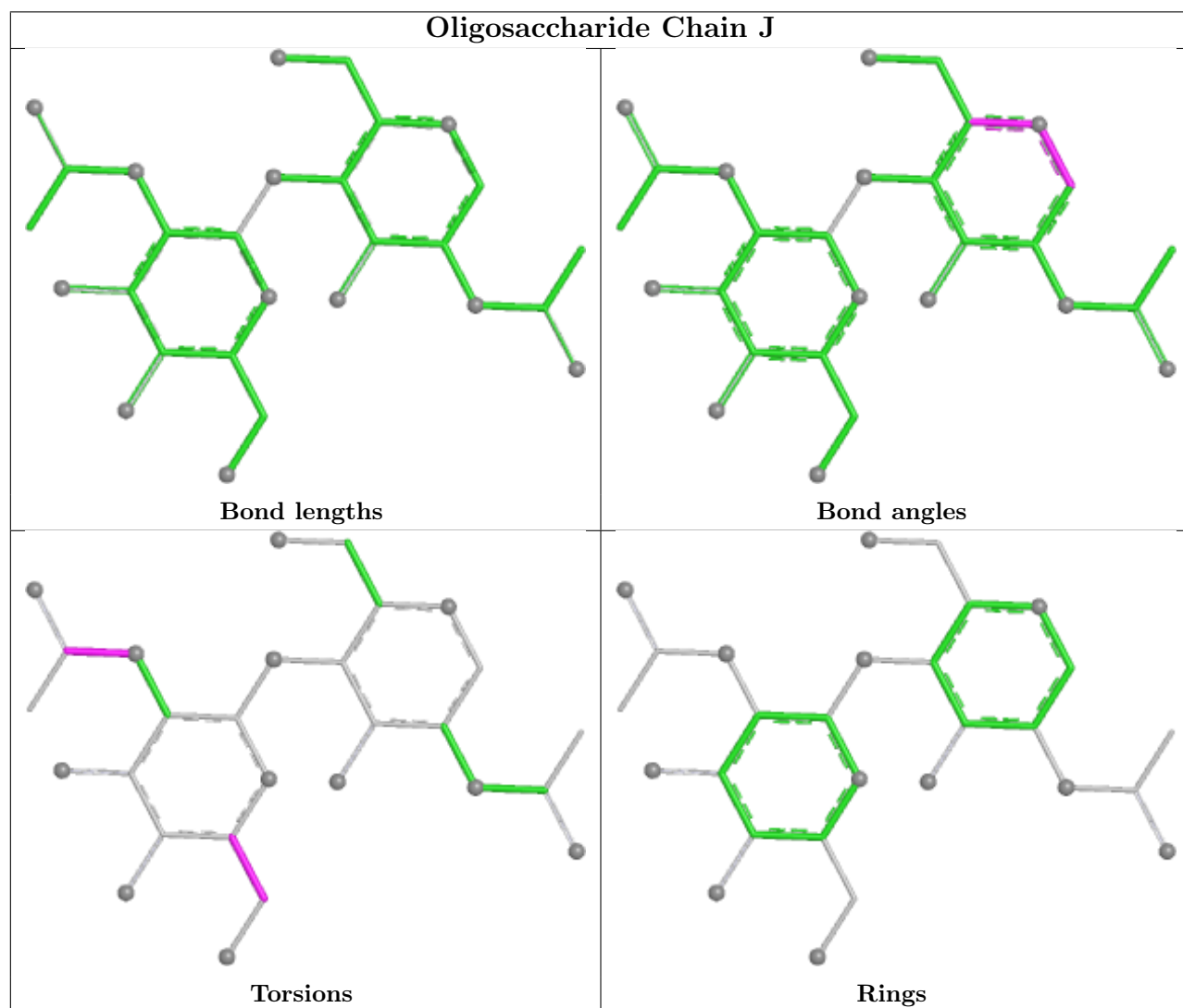
Mol	Chain	Res	Type	Atoms
5	K	2	NAG	C4-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	M	2	NAG	C8-C7-N2-C2
5	M	2	NAG	O7-C7-N2-C2

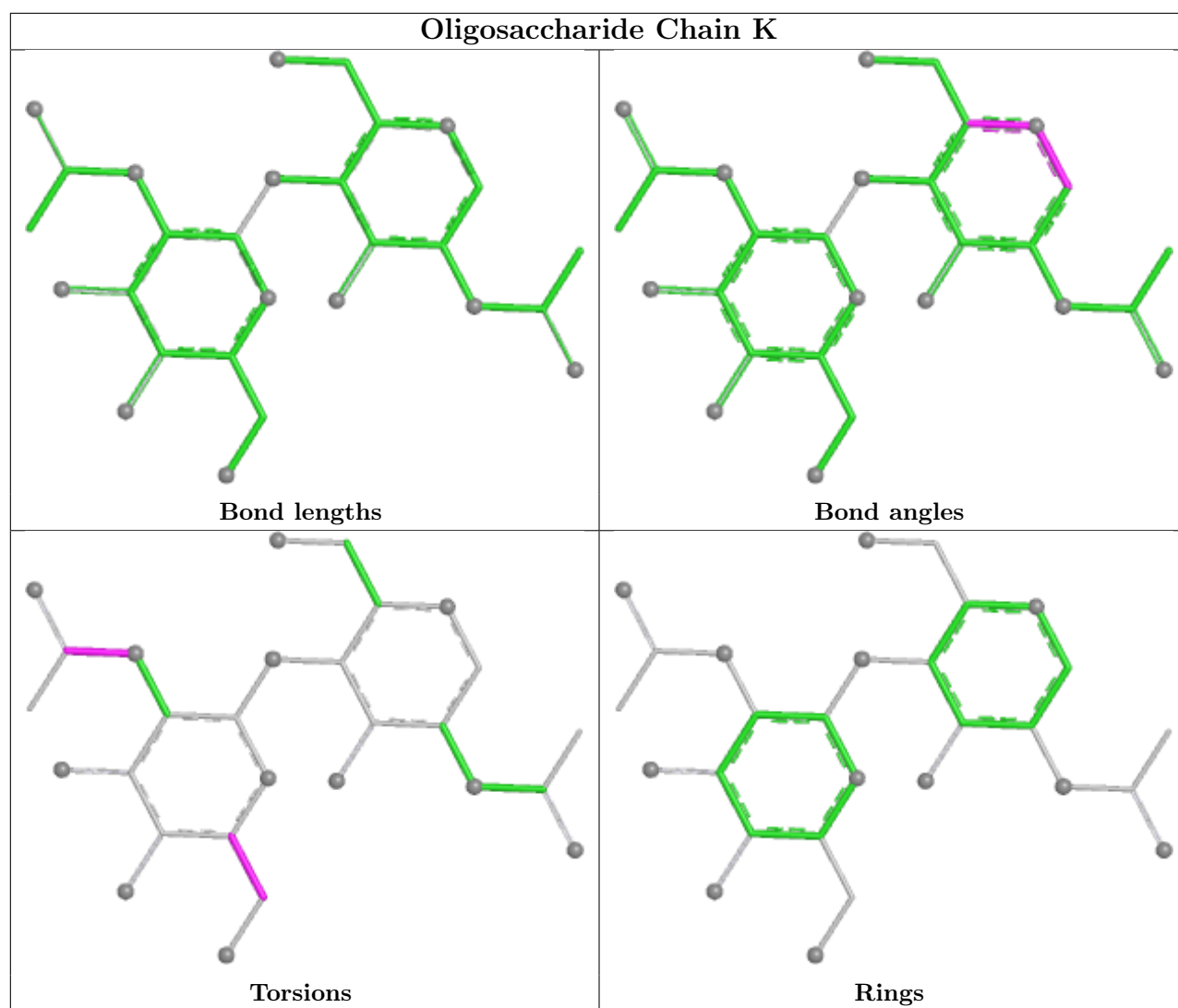
There are no ring outliers.

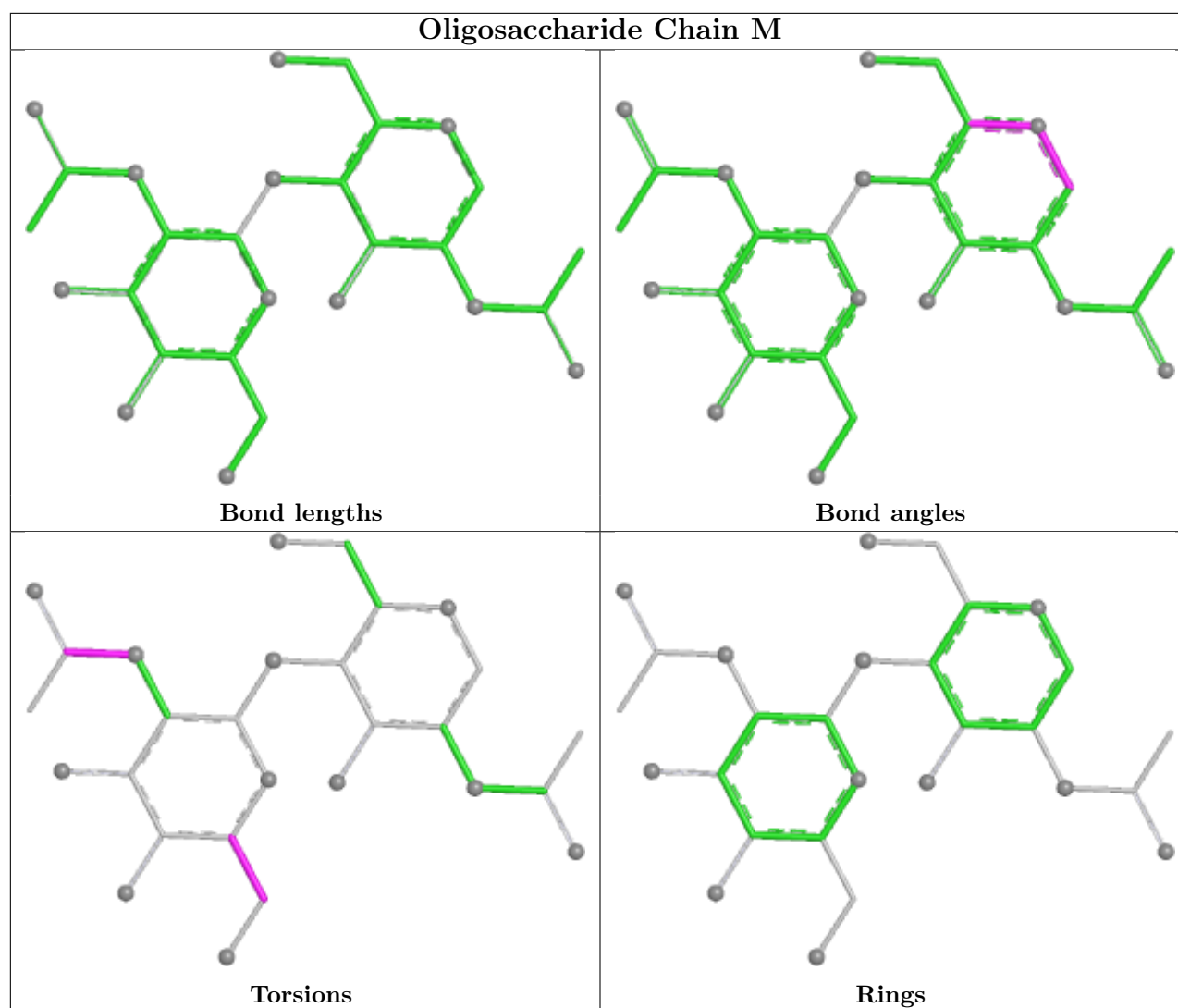
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	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](#)

3 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	$\# Z > 2$
6	NAG	A	501	3	14,14,15	0.34	0	17,19,21	0.50	0
6	NAG	C	501	3	14,14,15	0.55	0	17,19,21	0.55	0
6	NAG	B	501	3	14,14,15	0.40	0	17,19,21	0.57	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
6	NAG	A	501	3	-	1/6/23/26	0/1/1/1
6	NAG	C	501	3	-	4/6/23/26	0/1/1/1
6	NAG	B	501	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.

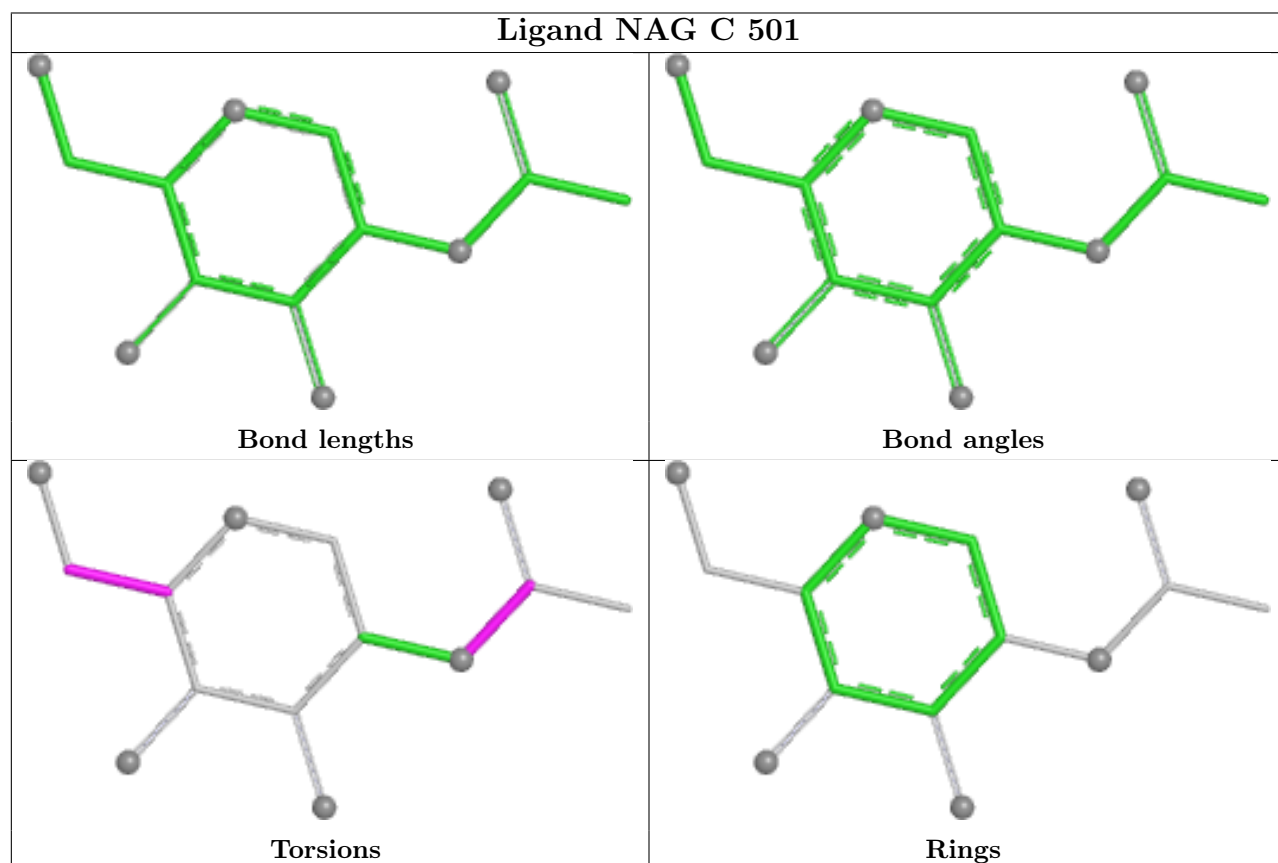
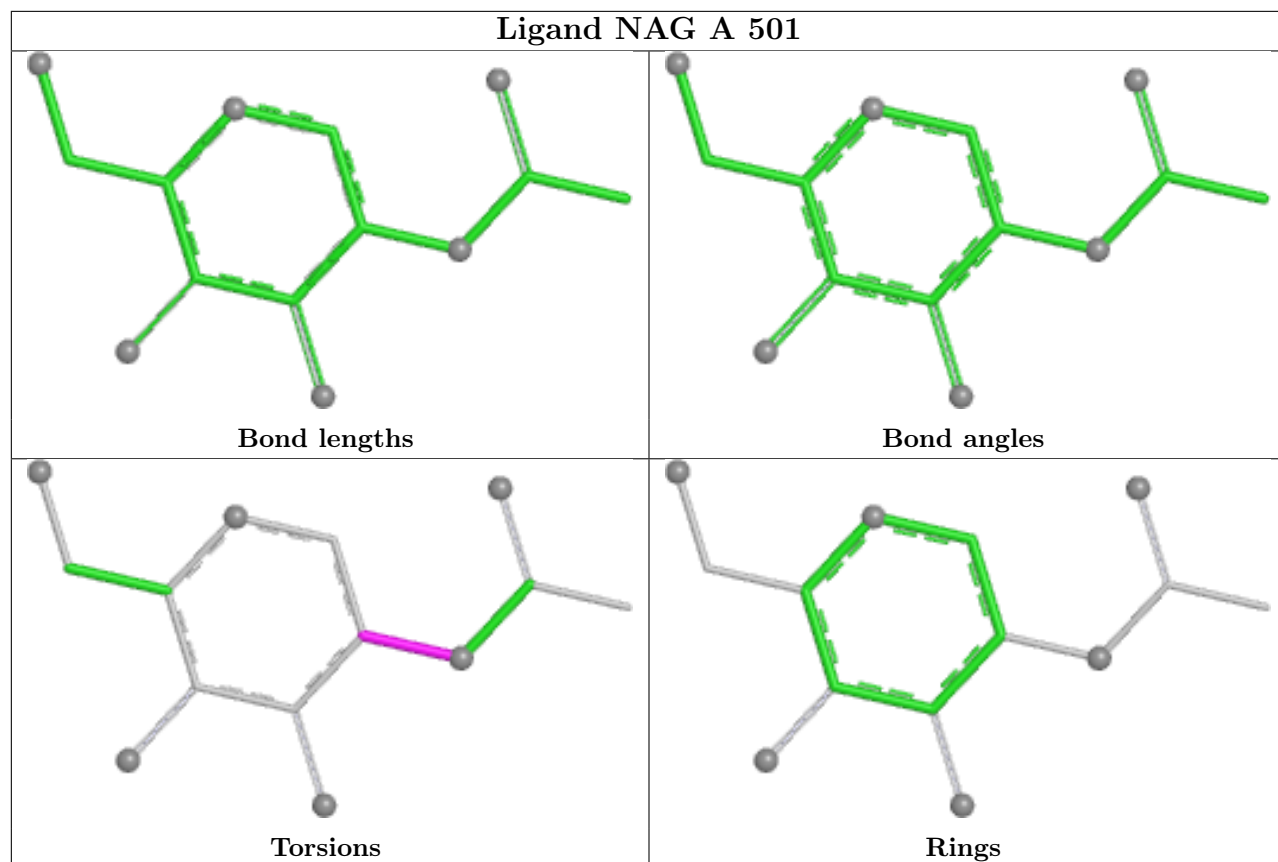
All (7) torsion outliers are listed below:

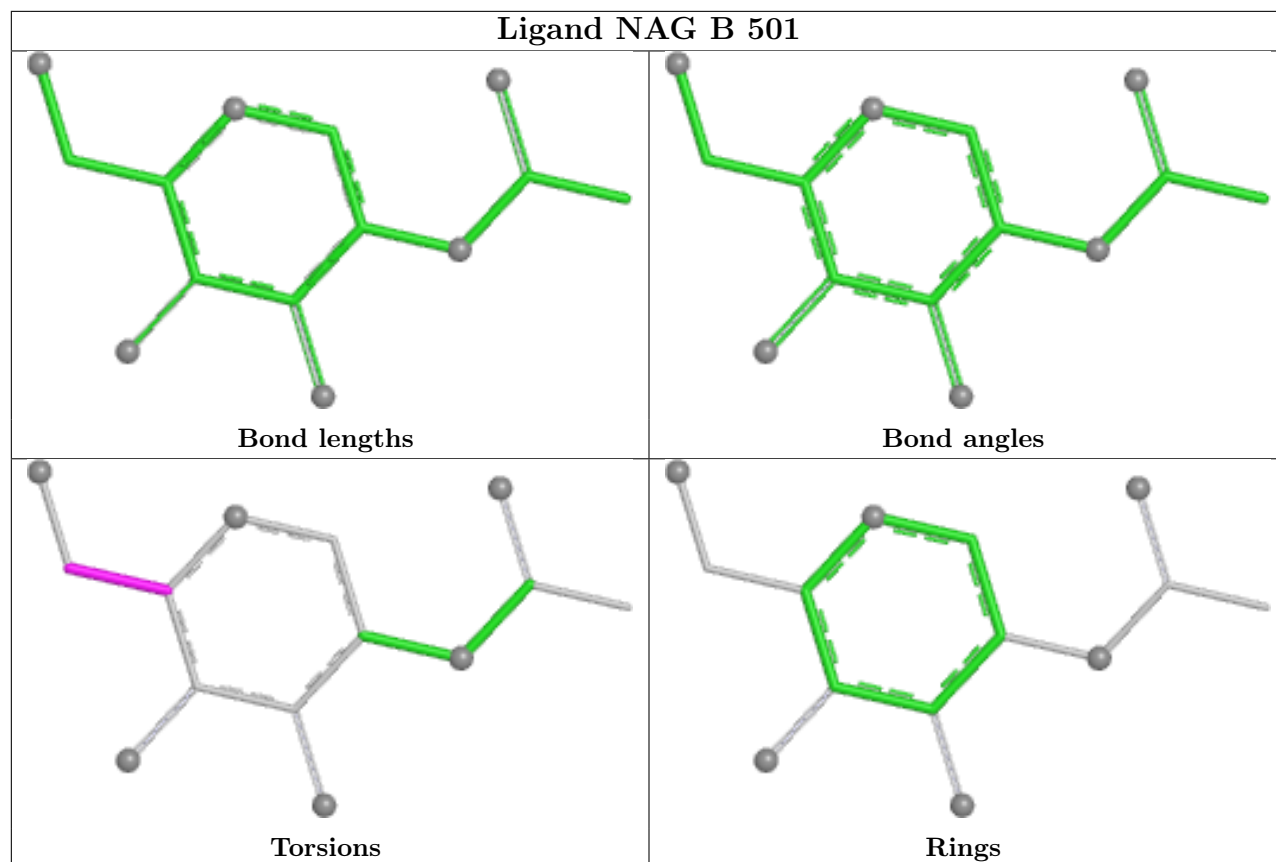
Mol	Chain	Res	Type	Atoms
6	C	501	NAG	O5-C5-C6-O6
6	C	501	NAG	C4-C5-C6-O6
6	B	501	NAG	O5-C5-C6-O6
6	C	501	NAG	C8-C7-N2-C2
6	C	501	NAG	O7-C7-N2-C2
6	B	501	NAG	C4-C5-C6-O6
6	A	501	NAG	C1-C2-N2-C7

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 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.

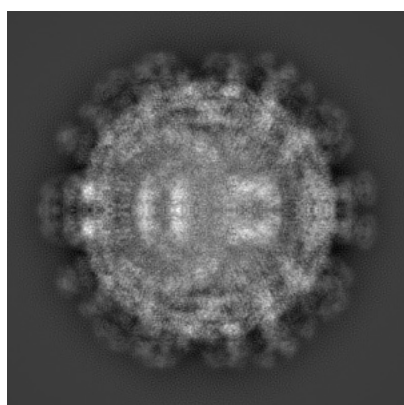
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30195. These allow visual inspection of the internal detail of the map and identification of artifacts.

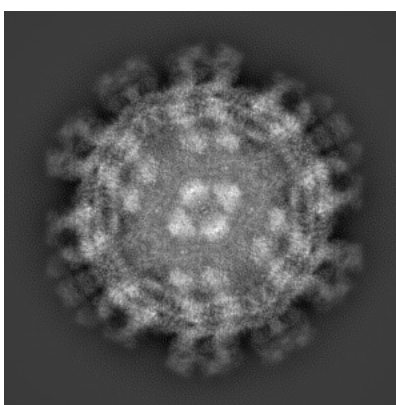
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

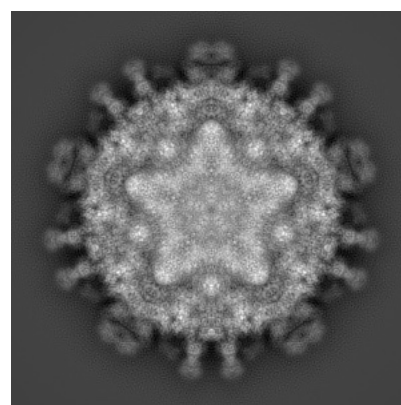
6.1.1 Primary map



X



Y

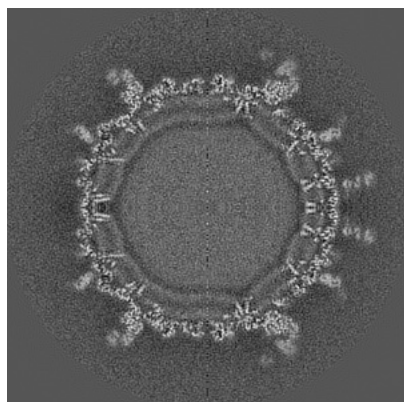


Z

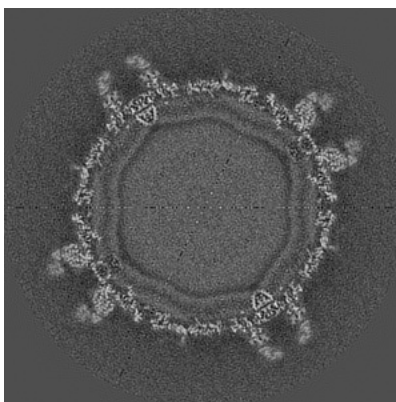
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

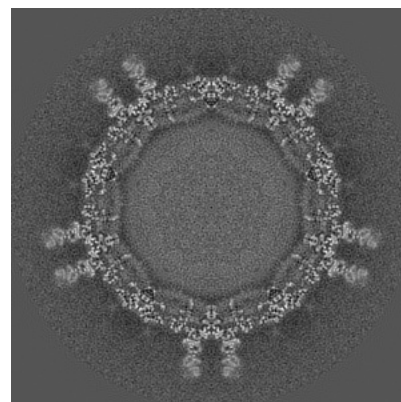
6.2.1 Primary map



X Index: 256



Y Index: 256

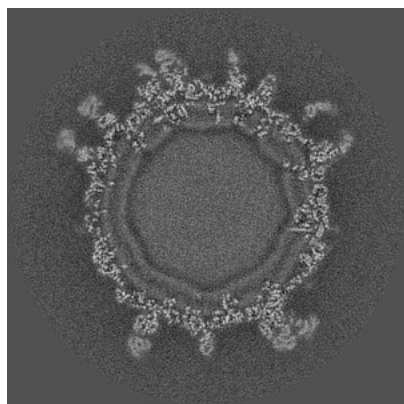


Z Index: 256

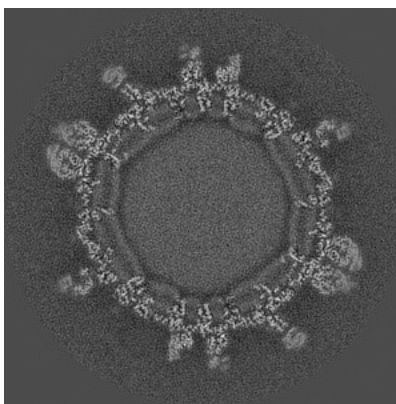
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

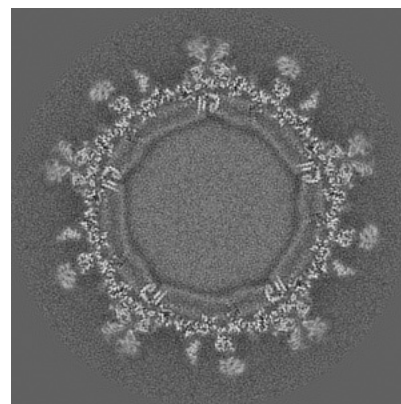
6.3.1 Primary map



X Index: 201



Y Index: 291

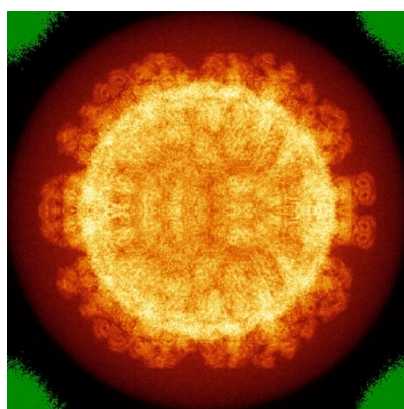


Z Index: 282

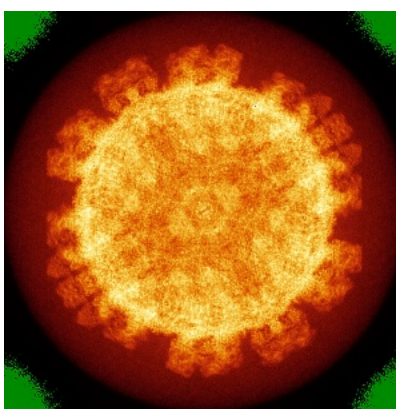
The images above show the largest variance slices of the map in three orthogonal directions.

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

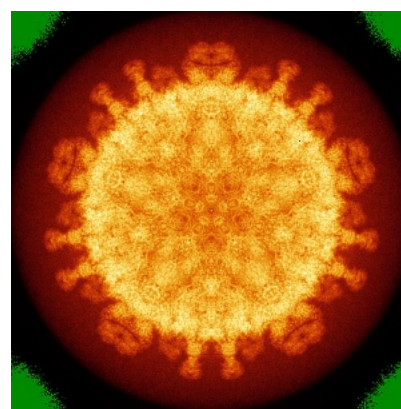
6.4.1 Primary map



X



Y

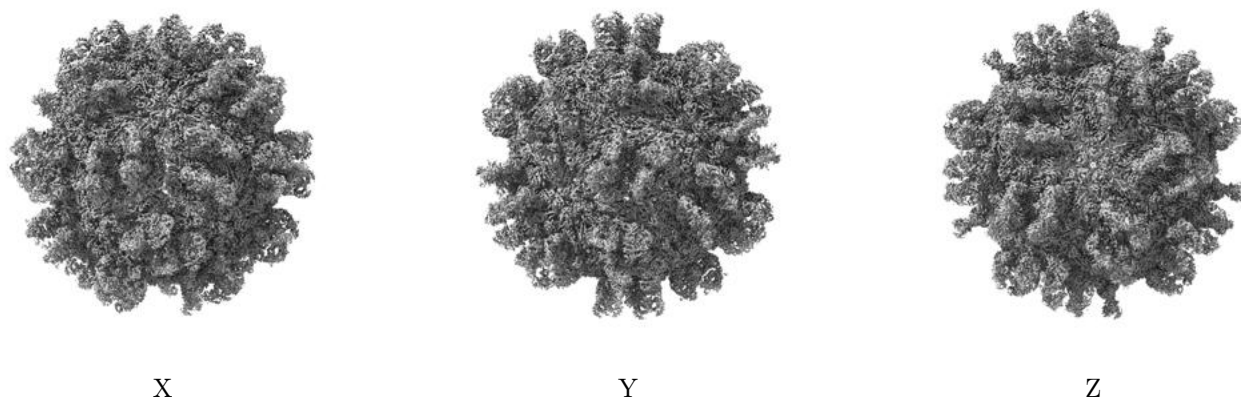


Z

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

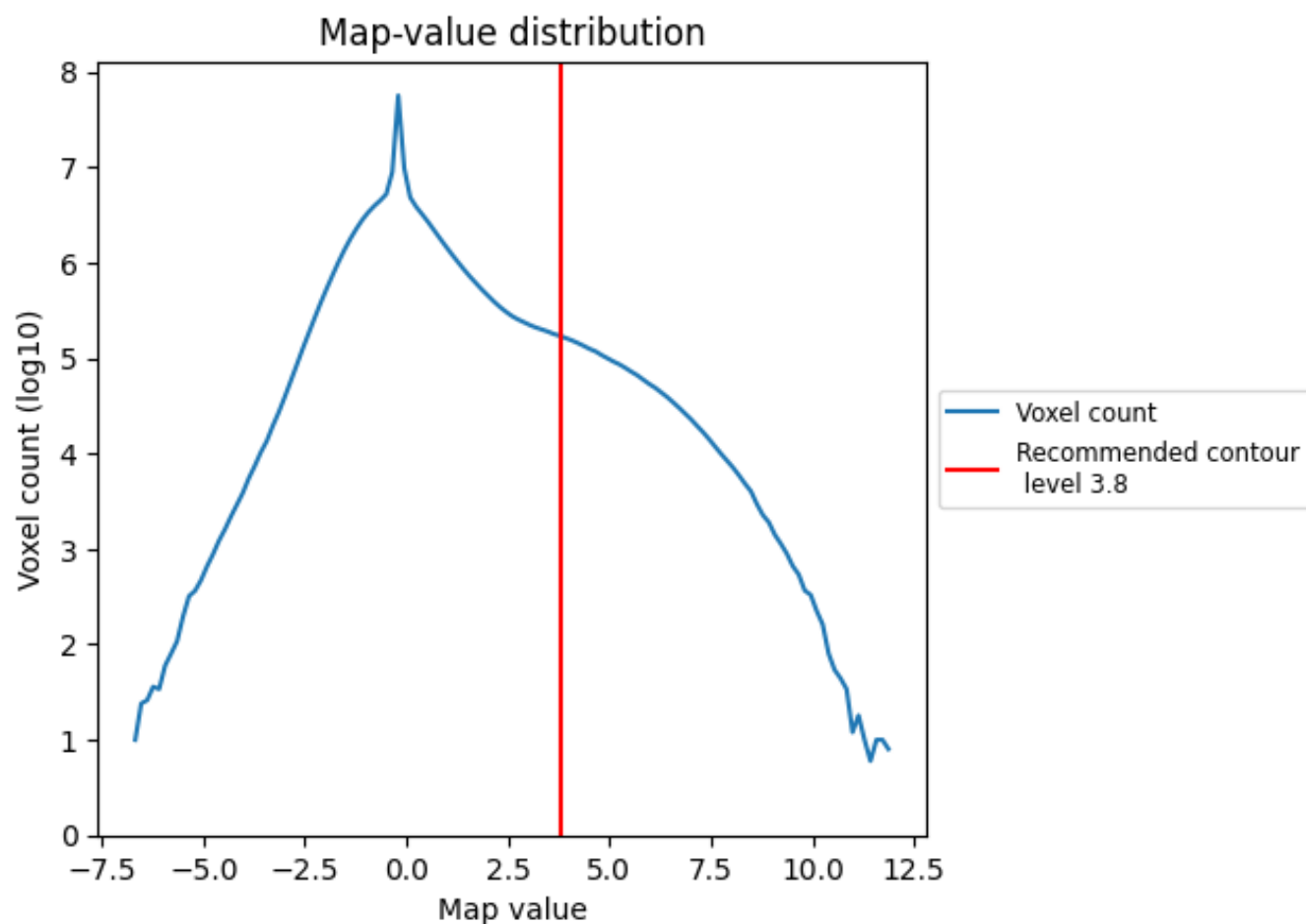
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

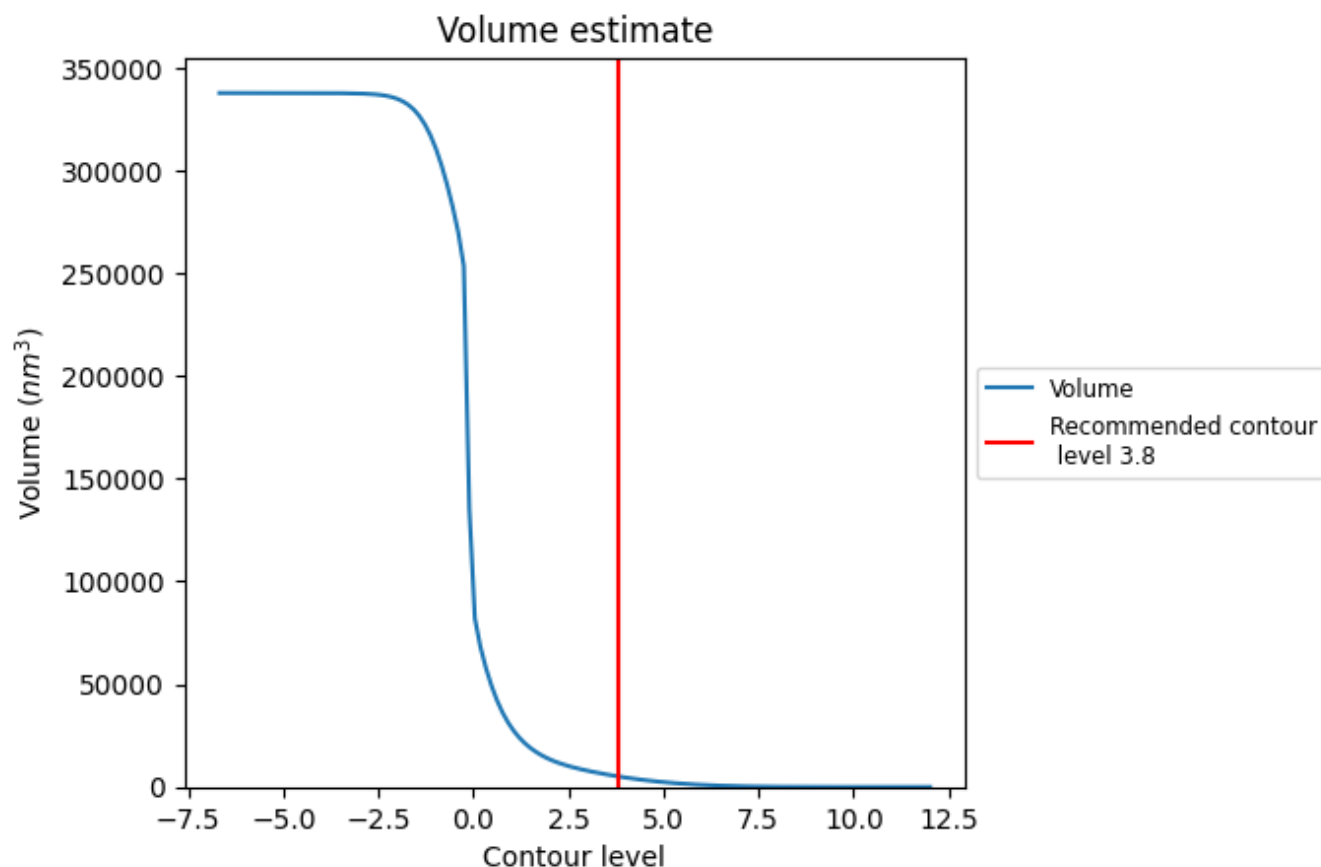
This section contains the results of statistical analysis of the map.

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.

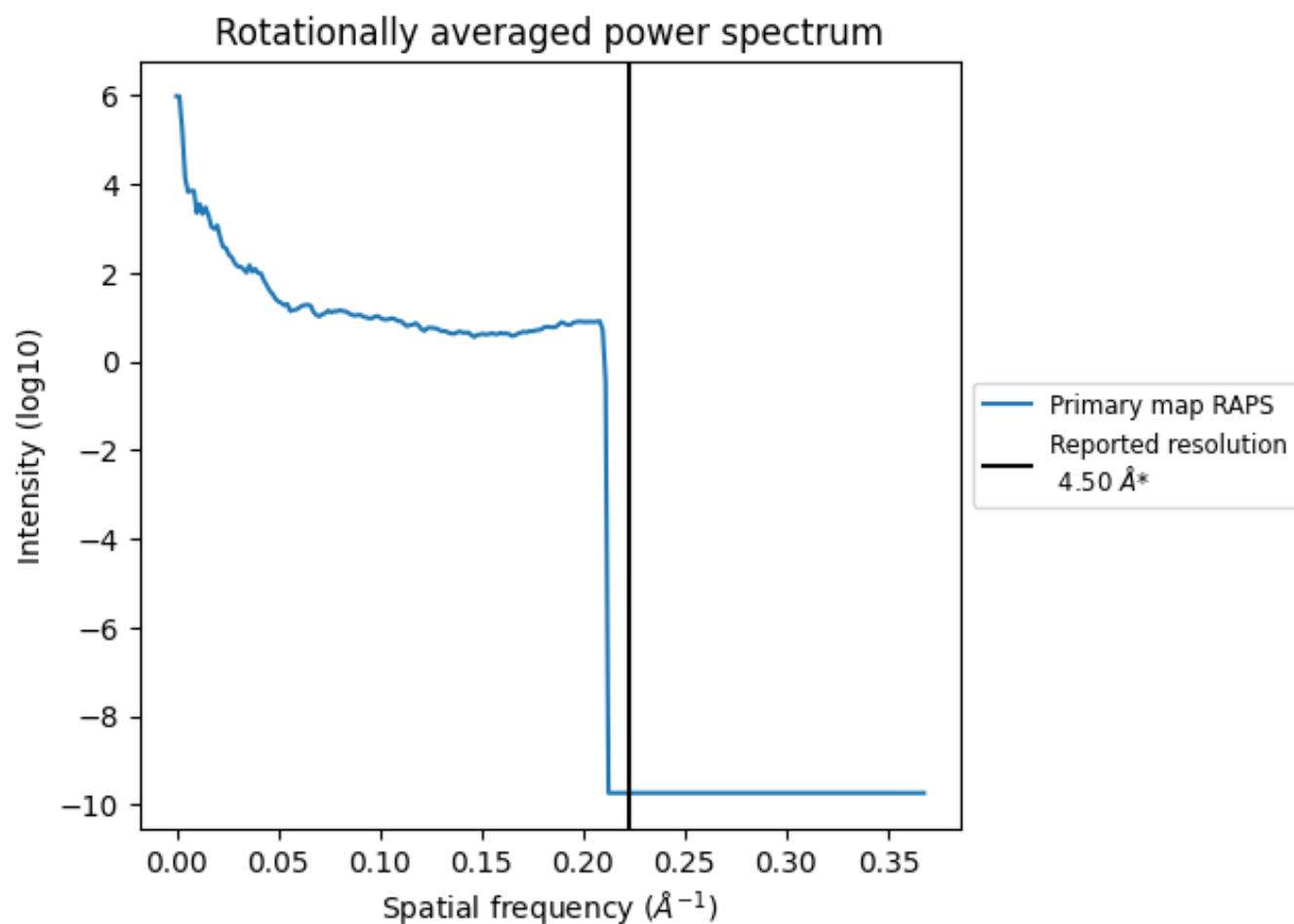
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5157 nm^3 ; this corresponds to an approximate mass of 4659 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 0.222 Å⁻¹

8 Fourier-Shell correlation ⓘ

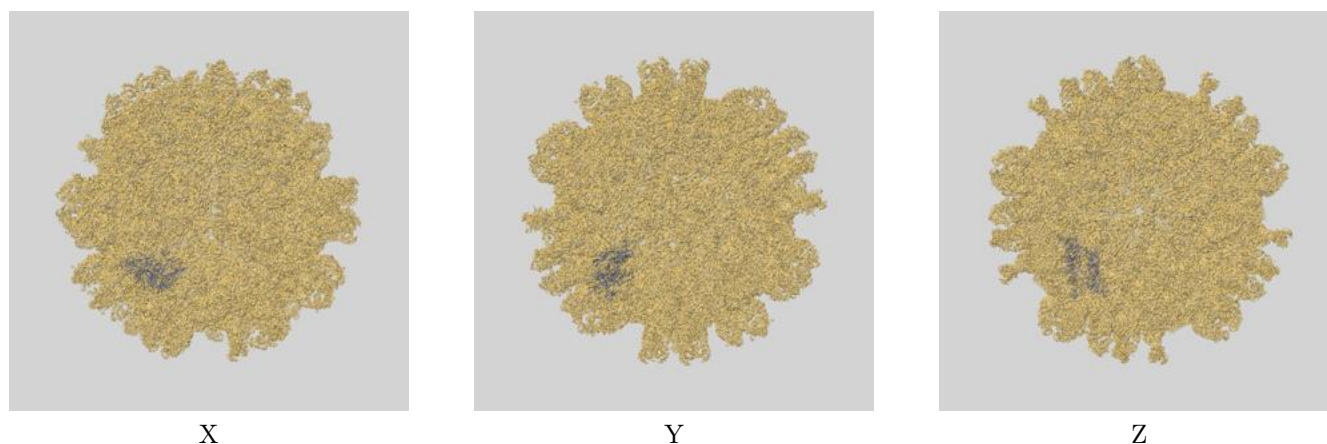
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

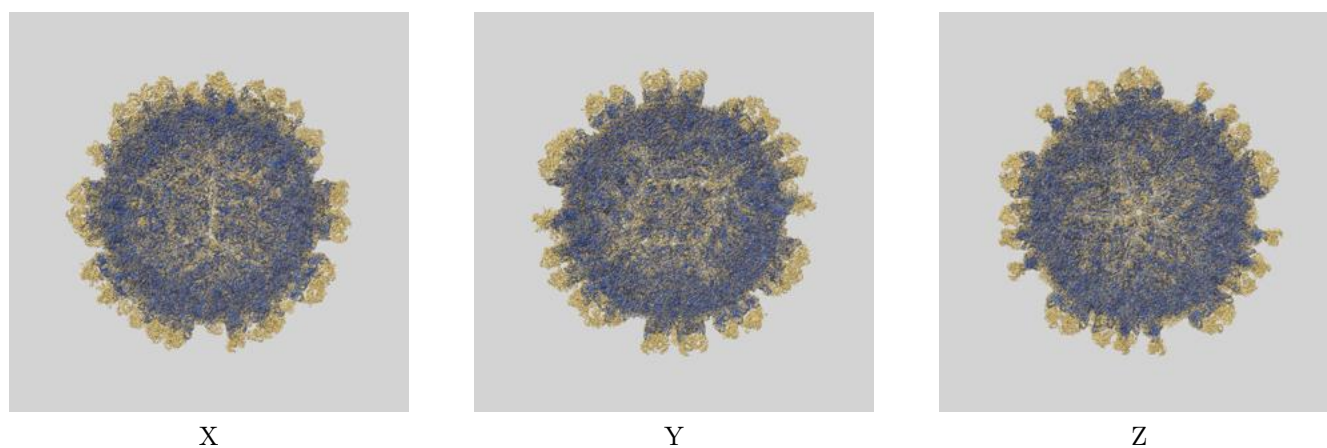
This section contains information regarding the fit between EMDB map EMD-30195 and PDB model 7BUD. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

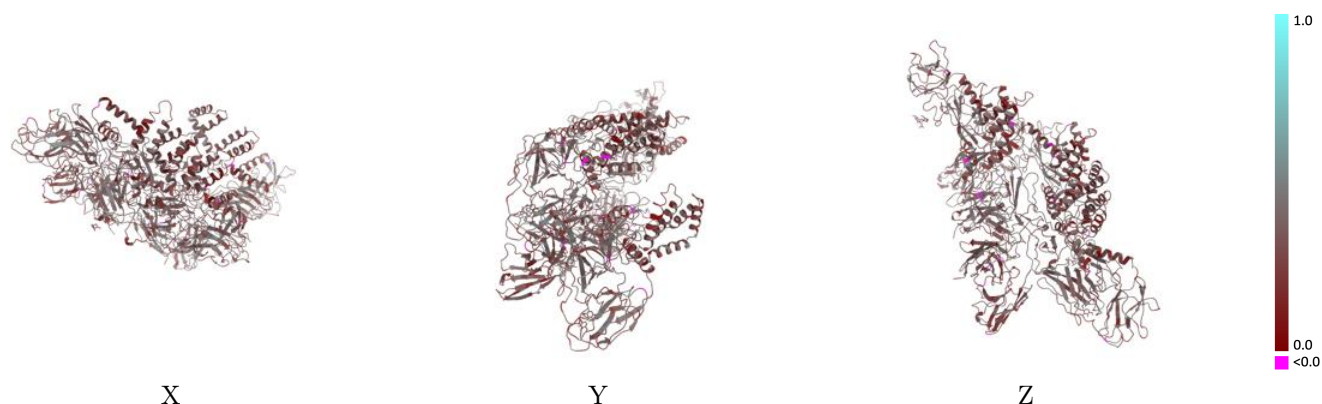


9.1.2 Map-model assembly overlay [i](#)



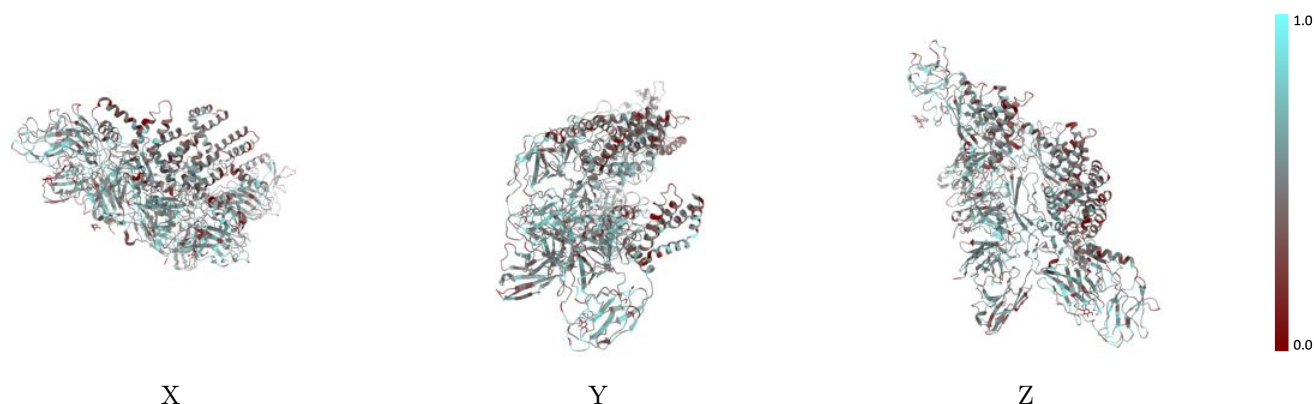
The images above show the 3D surface view of the map at the recommended contour level 3.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



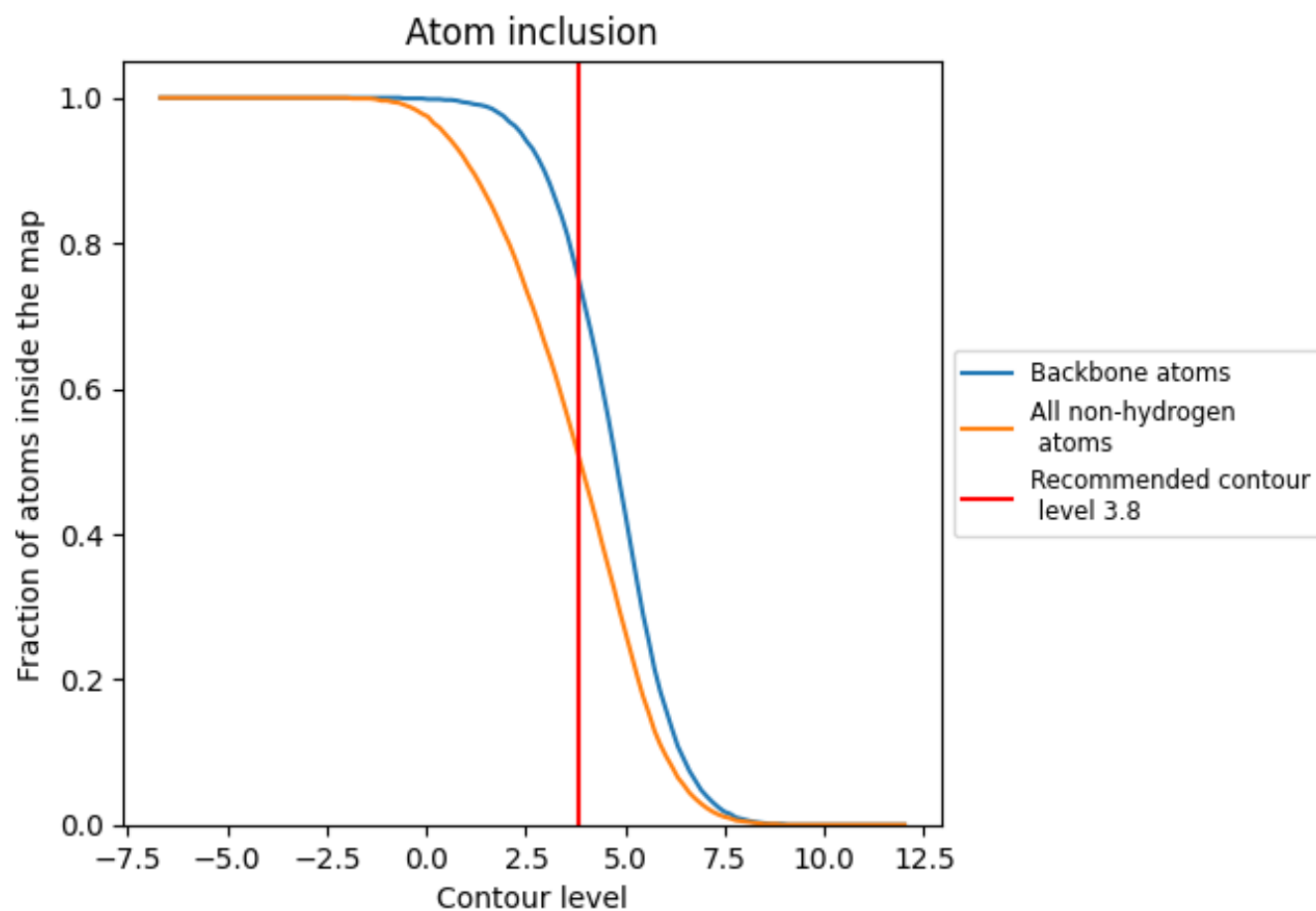
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 51% 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 (3.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5120	0.3340
A	0.5310	0.3450
B	0.5260	0.3430
C	0.5270	0.3410
D	0.4480	0.3190
E	0.4650	0.3330
F	0.4590	0.3250
G	0.5140	0.3120
H	0.5090	0.3130
I	0.4710	0.2950
J	0.3210	0.3090
K	0.1790	0.3030
L	0.4780	0.3140
M	0.1790	0.4080

