



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 09:58 PM UTC

PDB ID : 7BU8 / pdb_00007bu8
EMDB ID : EMD-30192
Title : Cryo-EM structure of zika virus complexed with Fab SIgN-3C at pH 6.5
Authors : Zhang, S.; Chew, S.V.; Lim, X.N.; Ng, T.S.; Kostyuchenko, V.A.; Lok, S.M.
Deposited on : 2020-04-05
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

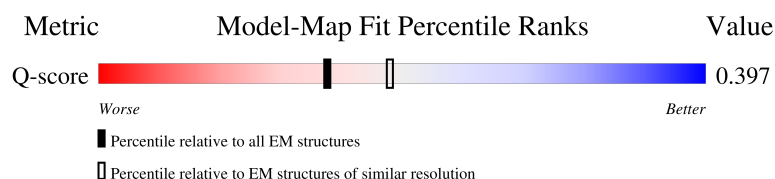
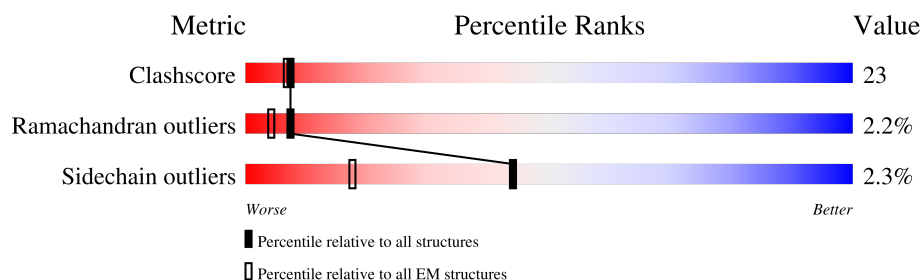
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	504	
1	B	504	
1	C	504	
2	D	75	

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Mol	Chain	Length	Quality of chain
2	E	75	
2	F	75	
3	G	132	
3	H	132	
3	J	132	
4	I	107	
4	K	107	
4	L	107	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 18731 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 Genome polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	504	Total	C	N	O	S	0	0
			3800	2392	660	717	31		
1	C	504	Total	C	N	O	S	0	0
			3808	2395	660	722	31		
1	B	504	Total	C	N	O	S	0	0
			3809	2395	660	723	31		

- Molecule 2 is a protein called Zika virus M protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	75	Total	C	N	O	S	0	0
			597	390	103	103	1		
2	E	75	Total	C	N	O	S	0	0
			600	391	105	103	1		
2	F	75	Total	C	N	O	S	0	0
			600	391	105	103	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	132	Total	C	N	O	S	0	0
			994	620	176	193	5		
3	H	132	Total	C	N	O	S	0	0
			985	612	175	193	5		
3	J	132	Total	C	N	O	S	0	0
			994	620	176	193	5		

- Molecule 4 is a protein called SIgN-3C Fab light chain.

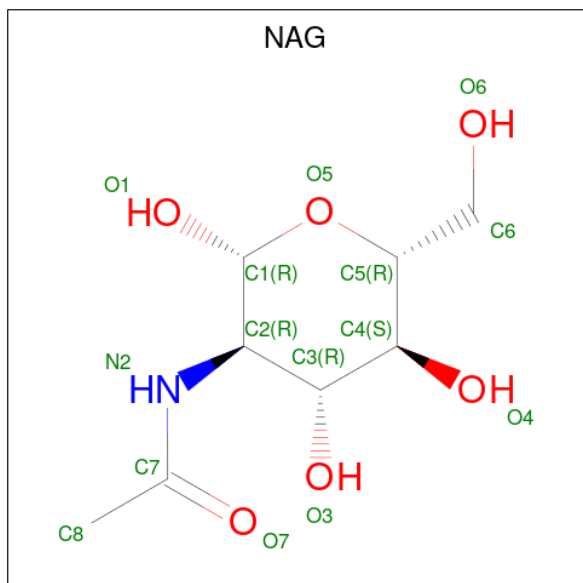
Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	107	Total	C	N	O	S	0	0
			834	526	139	167	2		

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

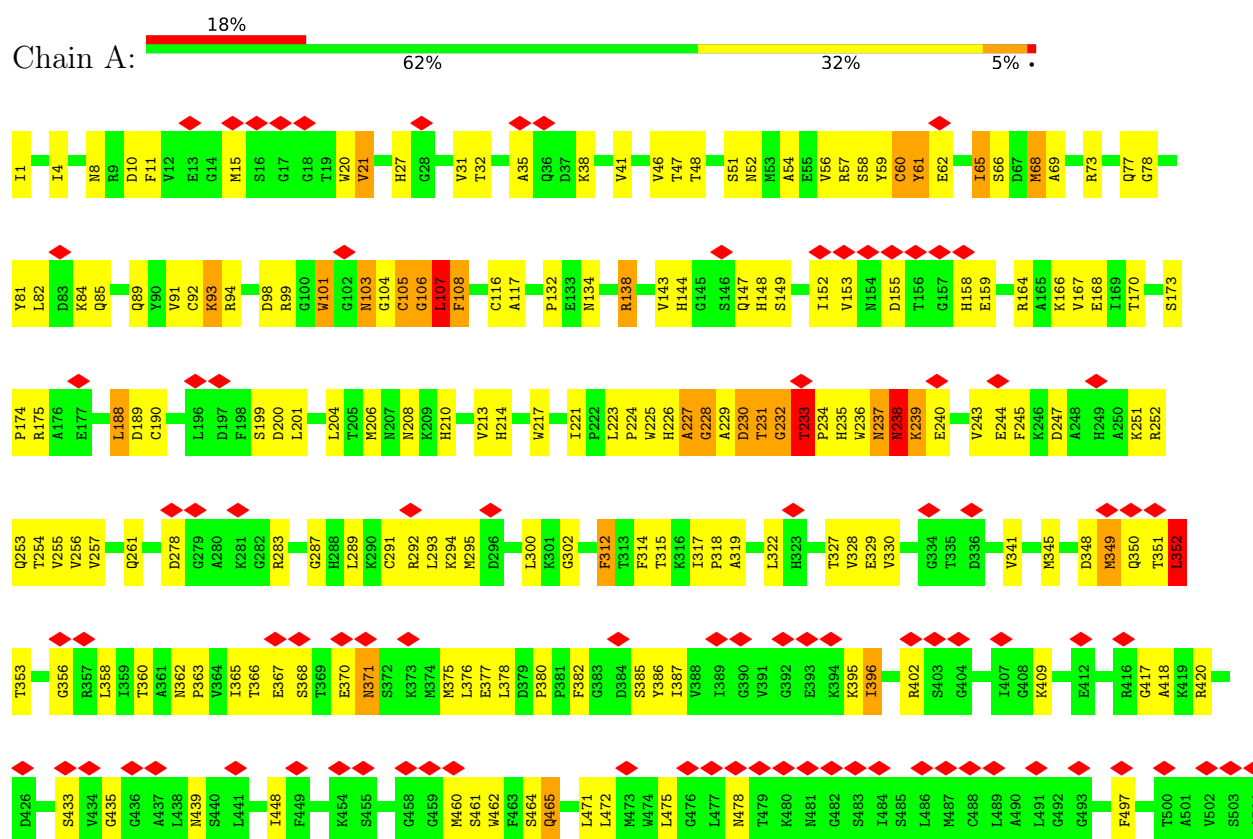


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

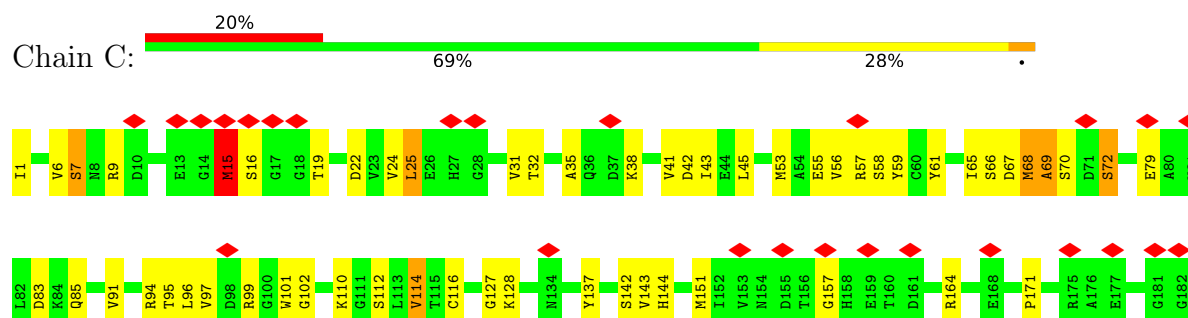
3 Residue-property plots

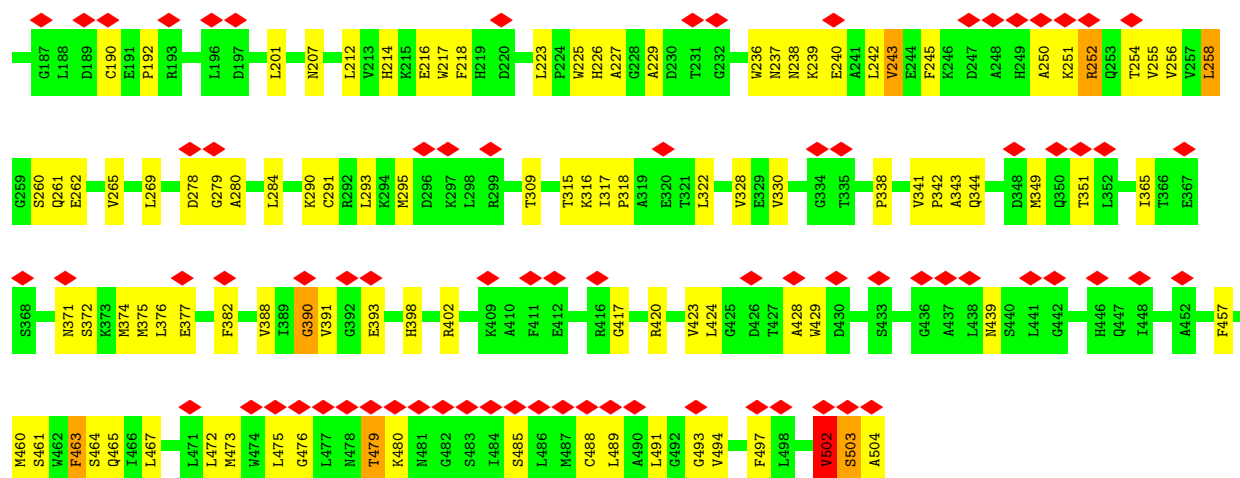
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Genome polyprotein

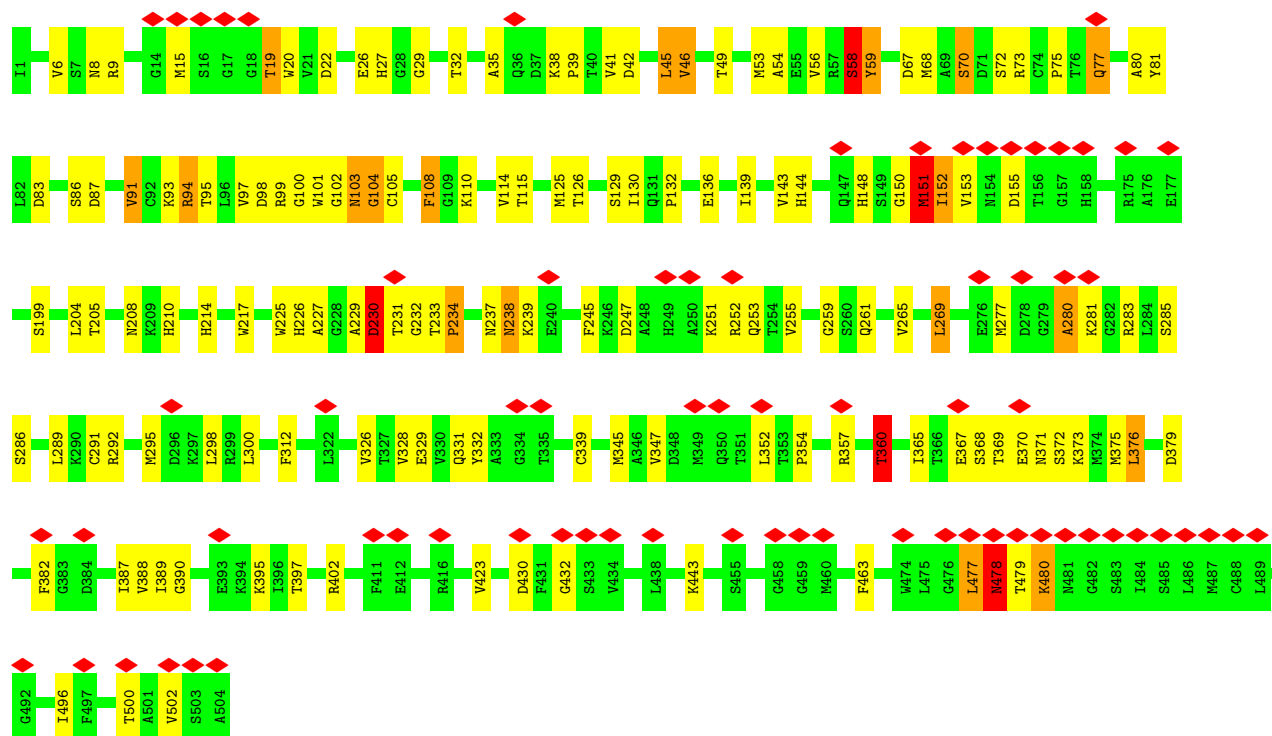


• Molecule 1: Genome polyprotein

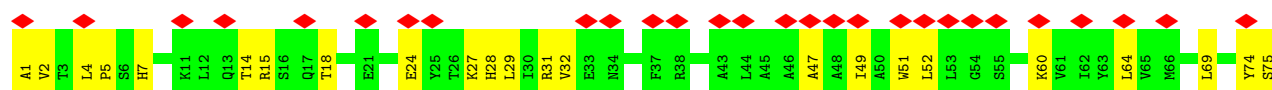




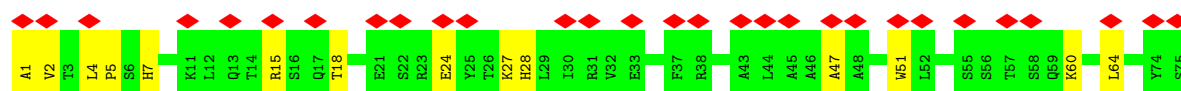
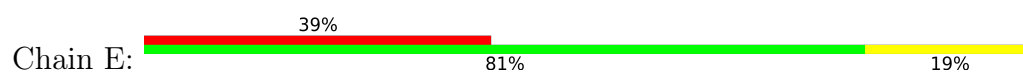
• Molecule 1: Genome polyprotein



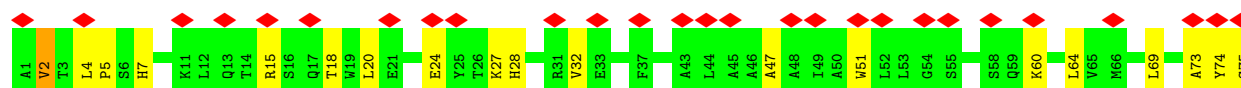
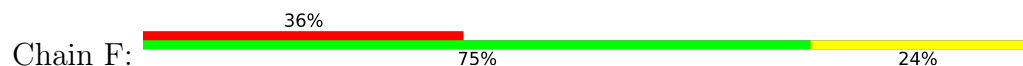
• Molecule 2: Zika virus M protein



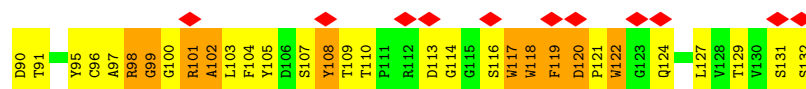
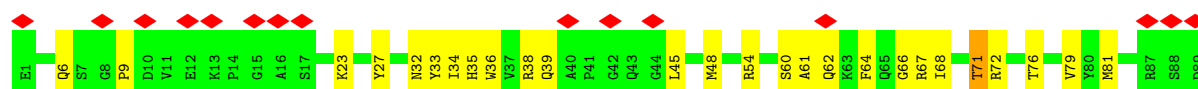
• Molecule 2: Zika virus M protein



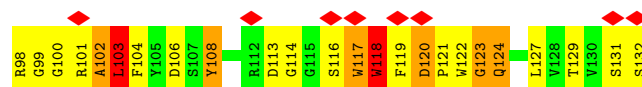
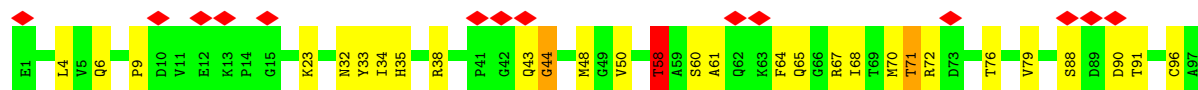
• Molecule 2: Zika virus M protein



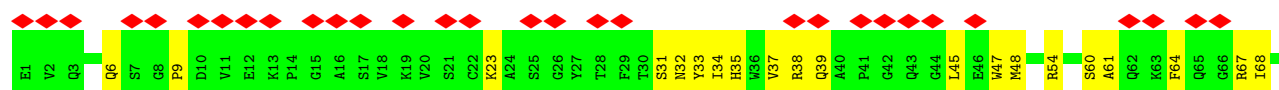
• Molecule 3: SIGN-3C Fab heavy chain



• Molecule 3: SIGN-3C Fab heavy chain

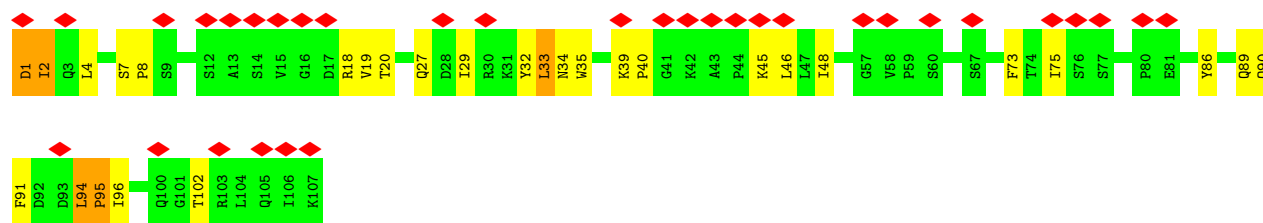


• Molecule 3: SIGN-3C Fab heavy chain

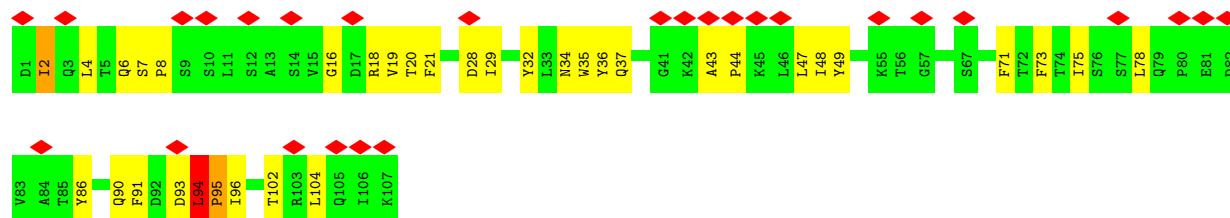


• Molecule 4: SIGN-3C Fab light chain

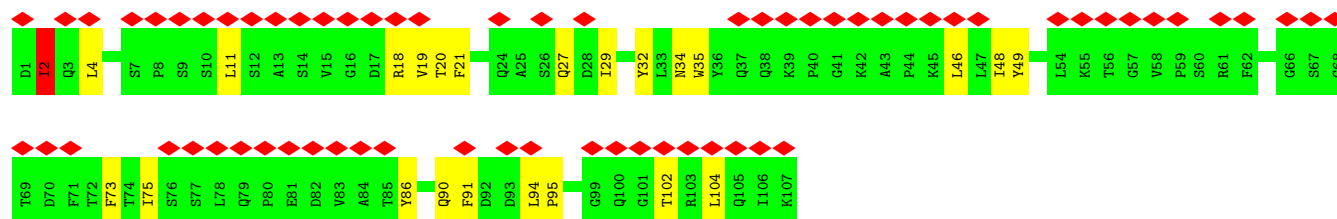
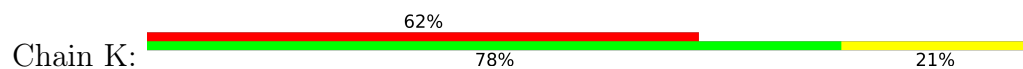




• Molecule 4: SIgN-3C Fab light chain



• Molecule 4: SIgN-3C Fab light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16300	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 ($e^-/\text{\AA}^2$)	30	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	20.944	Depositor
Minimum map value	-11.886	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3	Depositor
Map size (Å)	686.08, 686.08, 686.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.44	0/3879	1.00	23/5249 (0.4%)
1	B	0.54	1/3888 (0.0%)	1.11	20/5261 (0.4%)
1	C	0.43	0/3887	1.00	18/5261 (0.3%)
2	D	0.35	0/612	0.81	0/834
2	E	0.35	0/615	0.82	0/838
2	F	0.35	0/615	0.83	1/838 (0.1%)
3	G	0.75	2/1019 (0.2%)	1.06	13/1381 (0.9%)
3	H	0.45	0/1008	0.89	7/1365 (0.5%)
3	J	0.61	1/1019 (0.1%)	1.00	11/1381 (0.8%)
4	I	0.34	0/852	0.77	1/1154 (0.1%)
4	K	0.32	0/852	0.73	0/1154
4	L	0.31	0/852	0.78	2/1154 (0.2%)
All	All	0.47	4/19098 (0.0%)	0.98	96/25870 (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	A	0	9
1	B	0	13
1	C	0	13
3	H	0	1
3	J	0	2
4	I	0	2
4	K	0	2
All	All	0	42

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	234	PRO	N-CD	-19.76	1.20	1.47
3	G	101	ARG	CA-C	16.85	1.75	1.52
3	J	101	ARG	CA-C	14.16	1.71	1.52
3	G	109	THR	CA-C	10.56	1.64	1.53

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	PRO	N-CA-CB	-15.27	89.92	103.36
1	B	234	PRO	CA-N-CD	14.23	131.92	112.00
1	A	233	THR	CA-C-N	-13.77	102.63	119.84
1	A	233	THR	C-N-CA	-13.77	102.63	119.84
1	C	503	SER	N-CA-C	13.77	127.27	110.19
3	G	109	THR	N-CA-C	10.36	127.10	111.04
1	A	108	PHE	N-CA-C	-10.26	93.63	108.60
3	G	64	PHE	CB-CA-C	-9.94	92.66	110.35
1	C	317	ILE	N-CA-C	-9.92	100.10	108.63
3	J	101	ARG	CA-C-O	9.58	134.21	120.51
1	A	61	TYR	CB-CA-C	-8.90	92.71	110.42
3	J	100	GLY	CA-C-N	8.89	138.52	121.54
3	J	100	GLY	C-N-CA	8.89	138.52	121.54
1	C	502	VAL	N-CA-C	8.62	119.47	111.45
3	G	110	THR	N-CA-C	8.52	125.33	113.57
3	H	102	ALA	N-CA-C	-8.30	93.12	110.80
1	A	61	TYR	N-CA-C	8.08	128.02	110.80
3	J	106	ASP	N-CA-C	8.06	127.97	110.80
1	A	106	GLY	N-CA-C	8.05	127.25	112.27
1	A	93	LYS	N-CA-C	8.00	122.52	109.72
1	B	230	ASP	N-CA-C	7.99	127.82	110.80
3	G	101	ARG	CA-C-O	7.95	131.87	120.51
1	B	94	ARG	N-CA-C	7.62	121.65	109.24
1	B	75	PRO	N-CA-C	7.57	123.32	113.86
3	J	105	TYR	N-CA-C	7.52	120.66	108.41
1	B	77	GLN	N-CA-CB	7.36	123.82	112.41
4	L	94	LEU	CA-C-N	7.31	128.98	119.84
4	L	94	LEU	C-N-CA	7.31	128.98	119.84
1	B	285	SER	CA-C-N	6.80	134.53	121.54
1	B	285	SER	C-N-CA	6.80	134.53	121.54
1	A	230	ASP	N-CA-C	-6.79	92.81	107.49
3	G	108	TYR	CB-CA-C	6.67	123.69	110.42
3	H	88	SER	N-CA-C	-6.66	105.12	113.18
3	G	99	GLY	N-CA-C	-6.65	97.42	113.18
3	J	105	TYR	CA-C-N	6.59	134.12	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	105	TYR	C-N-CA	6.59	134.12	121.54
1	B	104	GLY	CA-C-N	-6.53	112.85	122.78
1	B	104	GLY	C-N-CA	-6.53	112.85	122.78
1	A	153	VAL	N-CA-C	6.50	117.00	110.23
1	B	360	THR	CA-C-N	6.47	131.66	121.56
1	B	360	THR	C-N-CA	6.47	131.66	121.56
1	A	319	ALA	N-CA-C	6.42	118.42	110.91
1	C	465	GLN	N-CA-CB	6.37	119.07	110.59
1	C	502	VAL	CA-C-N	6.32	132.28	121.29
1	C	502	VAL	C-N-CA	6.32	132.28	121.29
1	A	101	TRP	N-CA-C	-6.30	103.94	111.69
1	A	62	GLU	N-CA-CB	6.30	120.78	110.39
1	C	68	MET	CA-C-N	6.28	133.54	121.54
1	C	68	MET	C-N-CA	6.28	133.54	121.54
3	H	118	TRP	CA-C-N	-6.28	114.37	122.79
3	H	118	TRP	C-N-CA	-6.28	114.37	122.79
3	J	101	ARG	CB-CA-C	-6.19	98.10	110.42
1	C	465	GLN	N-CA-C	-6.10	106.38	113.88
3	G	110	THR	N-CA-CB	-6.09	100.58	110.39
1	B	58	SER	CA-C-N	6.06	133.12	121.54
1	B	58	SER	C-N-CA	6.06	133.12	121.54
1	B	280	ALA	N-CA-C	-6.01	106.60	112.97
3	G	109	THR	CA-C-O	6.00	127.19	120.89
3	G	108	TYR	CA-C-N	5.93	129.78	120.89
3	G	108	TYR	C-N-CA	5.93	129.78	120.89
1	C	56	VAL	CA-C-N	5.91	132.83	121.54
1	C	56	VAL	C-N-CA	5.91	132.83	121.54
1	A	251	LYS	CA-C-N	5.89	130.09	121.31
1	A	251	LYS	C-N-CA	5.89	130.09	121.31
3	J	88	SER	N-CA-C	-5.89	106.06	113.18
1	C	15	MET	CA-C-N	5.87	130.06	121.31
1	C	15	MET	C-N-CA	5.87	130.06	121.31
1	C	7	SER	CA-C-N	5.79	132.59	121.54
1	C	7	SER	C-N-CA	5.79	132.59	121.54
1	A	252	ARG	N-CA-C	5.78	118.44	110.35
1	A	107	LEU	N-CA-C	-5.73	98.60	110.80
1	A	60	CYS	CA-C-N	5.72	132.47	121.54
1	A	60	CYS	C-N-CA	5.72	132.47	121.54
1	B	232	GLY	N-CA-C	-5.65	93.95	111.07
1	A	367	GLU	CA-C-N	5.60	132.24	121.54
1	A	367	GLU	C-N-CA	5.60	132.24	121.54
1	A	208	ASN	N-CA-C	-5.51	105.55	114.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	SER	N-CA-C	5.50	119.16	111.90
1	C	463	PHE	N-CA-C	5.45	119.18	112.54
1	B	70	SER	N-CA-C	5.41	119.37	112.12
3	J	64	PHE	CB-CA-C	-5.39	102.01	110.85
1	B	234	PRO	N-CA-C	5.32	118.83	110.80
4	I	33	LEU	N-CA-C	-5.31	100.65	108.99
1	C	70	SER	N-CA-C	5.31	116.59	108.42
3	G	102	ALA	N-CA-C	-5.26	99.59	110.80
1	C	390	GLY	N-CA-C	5.24	125.59	113.18
3	G	119	PHE	N-CA-C	5.23	116.84	111.03
3	H	108	TYR	N-CA-C	-5.23	99.93	108.76
3	J	102	ALA	N-CA-CB	5.22	118.22	110.49
1	B	347	VAL	N-CA-C	-5.17	107.36	111.81
3	H	64	PHE	CB-CA-C	-5.17	103.12	111.18
3	G	104	PHE	N-CA-C	5.14	119.42	111.56
2	F	73	ALA	N-CA-C	5.13	119.40	111.56
3	H	58	THR	N-CA-CB	5.09	120.55	111.69
1	A	60	CYS	N-CA-C	-5.07	103.99	110.53
1	A	238	ASN	N-CA-CB	5.03	118.99	110.49

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	CYS	Peptide
1	A	152	ILE	Peptide
1	A	312	PHE	Peptide
1	A	322	LEU	Peptide
1	A	352	LEU	Peptide
1	A	366	THR	Peptide
1	A	395	LYS	Peptide
1	A	433	SER	Peptide
1	A	478	ASN	Peptide
1	B	15	MET	Peptide
1	B	150	GLY	Peptide
1	B	151	MET	Peptide
1	B	152	ILE	Peptide
1	B	20	TRP	Peptide
1	B	259	GLY	Peptide
1	B	269	LEU	Peptide
1	B	360	THR	Peptide
1	B	432	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	45	LEU	Peptide
1	B	477	LEU	Peptide
1	B	478	ASN	Peptide
1	B	58	SER	Peptide
1	C	15	MET	Peptide
1	C	16	SER	Peptide
1	C	242	LEU	Peptide
1	C	251	LYS	Peptide
1	C	258	LEU	Peptide
1	C	279	GLY	Peptide
1	C	351	THR	Peptide
1	C	45	LEU	Peptide
1	C	461	SER	Peptide
1	C	502	VAL	Peptide
1	C	6	VAL	Peptide
1	C	66	SER	Peptide
1	C	67	ASP	Peptide
3	H	101	ARG	Mainchain
4	I	29	ILE	Peptide
4	I	94	LEU	Peptide
3	J	117	TRP	Peptide
3	J	119	PHE	Peptide
4	K	29	ILE	Peptide
4	K	94	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3800	0	3755	203	0
1	B	3809	0	3761	163	0
1	C	3808	0	3761	117	0
2	D	597	0	619	72	0
2	E	600	0	624	12	0
2	F	600	0	624	67	0
3	G	994	0	941	130	0
3	H	985	0	933	117	0
3	J	994	0	941	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	834	0	811	69	0
4	K	834	0	814	27	0
4	L	834	0	814	69	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
All	All	18731	0	18437	864	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:117:TRP:CZ3	4:L:49:TYR:HB3	1.29	1.63
3:H:119:PHE:CE1	4:L:36:TYR:CD1	1.84	1.59
3:H:119:PHE:CE1	4:L:36:TYR:HD1	1.12	1.58
3:G:119:PHE:CD2	4:I:46:LEU:HD13	1.35	1.58
3:H:119:PHE:CD1	4:L:36:TYR:CE1	1.84	1.57
3:G:101:ARG:C	3:G:101:ARG:CA	1.75	1.53
1:A:229:ALA:CB	1:B:81:TYR:CD2	1.89	1.52
1:A:89:GLN:NE2	1:A:233:THR:CG2	1.71	1.51
1:B:477:LEU:HD12	1:B:478:ASN:N	1.32	1.43
3:G:119:PHE:CE2	4:I:46:LEU:HB2	1.53	1.41
1:A:229:ALA:HB2	1:B:81:TYR:CB	1.52	1.38
1:A:89:GLN:NE2	1:A:233:THR:HG21	1.08	1.37
1:B:477:LEU:CD1	1:B:478:ASN:H	1.37	1.36
4:K:2:ILE:HG22	4:K:90:GLN:NE2	1.08	1.36
1:A:229:ALA:CB	1:B:81:TYR:CG	2.10	1.35
3:H:119:PHE:CD1	4:L:36:TYR:HE1	1.28	1.34
1:B:230:ASP:CG	1:B:231:THR:H	1.25	1.34
1:A:229:ALA:HB2	1:B:81:TYR:CG	1.61	1.33
4:L:94:LEU:HB3	4:L:95:PRO:CD	1.57	1.33
3:H:4:LEU:O	3:H:123:GLY:HA2	1.32	1.28
3:G:119:PHE:CE2	4:I:46:LEU:CB	2.15	1.27
4:K:2:ILE:CG2	4:K:90:GLN:NE2	1.97	1.27
3:H:117:TRP:CZ3	4:L:49:TYR:CB	2.17	1.26
3:G:119:PHE:CZ	4:I:46:LEU:HA	1.72	1.25
4:I:1:ASP:N	4:I:95:PRO:HG2	1.53	1.24
3:H:119:PHE:CZ	4:L:36:TYR:HD1	1.54	1.24
1:A:232:GLY:O	1:A:234:PRO:HD3	1.33	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ALA:HB1	1:B:81:TYR:CD2	1.61	1.21
2:D:74:TYR:CE2	2:F:69:LEU:CD2	2.25	1.20
1:C:102:GLY:O	3:J:103:LEU:HD12	1.36	1.20
4:L:94:LEU:CB	4:L:95:PRO:CD	2.20	1.19
2:D:74:TYR:CE2	2:F:69:LEU:HG	1.77	1.19
1:C:102:GLY:O	3:J:103:LEU:CD1	1.91	1.18
3:G:113:ASP:HB2	3:G:117:TRP:CE2	1.79	1.17
3:H:6:GLN:H	3:H:124:GLN:NE2	1.42	1.16
4:L:2:ILE:HG22	4:L:90:GLN:NE2	1.57	1.16
3:G:113:ASP:HB2	3:G:117:TRP:NE1	1.59	1.15
2:D:74:TYR:CD2	2:F:69:LEU:HD23	1.79	1.15
3:G:119:PHE:CD2	4:I:46:LEU:CD1	2.30	1.13
2:D:74:TYR:CE2	2:F:69:LEU:CG	2.33	1.12
3:H:119:PHE:CD1	4:L:36:TYR:CD1	2.14	1.11
3:G:117:TRP:CD1	4:I:91:PHE:CE1	2.37	1.11
1:A:232:GLY:O	1:A:234:PRO:CD	1.98	1.11
3:H:6:GLN:N	3:H:124:GLN:HE22	1.48	1.11
3:H:118:TRP:O	3:H:122:TRP:CZ2	2.04	1.11
2:D:74:TYR:HE2	2:F:69:LEU:CD2	1.61	1.10
4:L:94:LEU:O	4:L:96:ILE:HG13	1.47	1.10
2:D:32:VAL:HG21	2:F:74:TYR:CZ	1.86	1.10
3:G:119:PHE:CE2	4:I:46:LEU:HD13	1.87	1.10
1:C:460:MET:HE3	1:C:464:SER:OG	1.48	1.10
4:I:1:ASP:H1	4:I:95:PRO:CG	1.64	1.10
4:L:93:ASP:O	4:L:94:LEU:HB2	1.34	1.10
1:A:229:ALA:HB2	1:B:81:TYR:HB3	1.33	1.09
2:D:74:TYR:HE2	2:F:69:LEU:CG	1.64	1.09
3:G:119:PHE:HE2	4:I:46:LEU:CB	1.56	1.09
4:L:94:LEU:CB	4:L:95:PRO:HD3	1.79	1.09
3:H:117:TRP:HZ3	4:L:49:TYR:CB	1.58	1.08
1:B:230:ASP:CG	1:B:231:THR:N	2.05	1.08
4:I:1:ASP:N	4:I:95:PRO:CG	2.15	1.08
3:H:6:GLN:N	3:H:124:GLN:NE2	2.02	1.07
4:I:32:TYR:HB3	4:I:91:PHE:HB2	1.30	1.07
2:D:74:TYR:CZ	2:F:32:VAL:HG21	1.89	1.06
1:B:231:THR:HG23	3:H:65:GLN:HA	1.34	1.06
4:I:1:ASP:H1	4:I:95:PRO:HG3	1.21	1.06
1:A:233:THR:O	1:A:234:PRO:C	1.94	1.05
3:H:120:ASP:HB3	3:H:121:PRO:HD3	1.06	1.05
2:D:32:VAL:HG21	2:F:74:TYR:CE2	1.93	1.04
3:H:120:ASP:N	3:H:122:TRP:HE1	1.55	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:119:PHE:HA	3:H:122:TRP:CZ2	1.94	1.03
3:G:119:PHE:O	3:G:122:TRP:CD1	2.10	1.02
3:H:58:THR:HG21	3:H:70:MET:HB2	1.39	1.02
4:K:2:ILE:HG22	4:K:90:GLN:CD	1.84	1.02
4:K:2:ILE:CG2	4:K:90:GLN:HE22	1.64	1.02
1:C:94:ARG:HG2	1:C:114:VAL:CG1	1.90	1.02
3:G:119:PHE:CZ	4:I:46:LEU:CA	2.42	1.02
4:L:93:ASP:O	4:L:94:LEU:CB	2.05	1.02
4:I:1:ASP:H2	4:I:95:PRO:HG2	1.12	1.01
3:H:120:ASP:HB3	3:H:121:PRO:CD	1.91	1.01
2:D:69:LEU:HG	2:F:74:TYR:CE2	1.96	1.00
3:G:120:ASP:HB3	3:G:121:PRO:HD3	1.42	1.00
1:A:104:GLY:N	3:H:103:LEU:CD1	2.26	0.99
2:D:32:VAL:CG2	2:F:74:TYR:CZ	2.46	0.99
3:G:119:PHE:O	3:G:122:TRP:NE1	1.96	0.98
2:D:74:TYR:CE2	2:F:69:LEU:HD23	1.92	0.98
4:L:2:ILE:HG22	4:L:90:GLN:HE22	1.27	0.97
3:H:120:ASP:H	3:H:122:TRP:HE1	1.11	0.97
1:A:104:GLY:HA2	3:H:103:LEU:HD12	1.46	0.97
1:A:229:ALA:HB3	1:B:81:TYR:CG	2.00	0.97
4:I:32:TYR:C	4:I:91:PHE:HD2	1.70	0.96
1:A:89:GLN:NE2	1:A:233:THR:HG22	1.78	0.95
1:A:98:ASP:O	1:A:99:ARG:HG2	1.65	0.95
1:B:73:ARG:HH21	1:B:77:GLN:CG	1.78	0.95
1:A:103:ASN:C	3:H:103:LEU:CD1	2.39	0.95
3:H:4:LEU:O	3:H:123:GLY:CA	2.15	0.94
4:L:94:LEU:O	4:L:96:ILE:N	2.00	0.94
3:G:118:TRP:HH2	4:I:96:ILE:HG21	1.32	0.94
1:A:460:MET:HG3	1:A:465:GLN:HG2	1.46	0.94
1:A:104:GLY:CA	3:H:103:LEU:HD12	1.97	0.93
1:A:81:TYR:HB3	1:B:229:ALA:CB	1.99	0.93
3:H:120:ASP:CB	3:H:121:PRO:HD3	1.96	0.93
1:A:229:ALA:HB3	1:B:81:TYR:CD2	2.03	0.93
3:G:119:PHE:CE2	4:I:46:LEU:CD1	2.51	0.93
3:G:119:PHE:CE2	4:I:46:LEU:CA	2.52	0.93
4:I:33:LEU:C	4:I:91:PHE:HE2	1.75	0.93
1:C:94:ARG:HG2	1:C:114:VAL:HG11	1.50	0.92
1:A:103:ASN:O	3:H:103:LEU:HD13	1.68	0.92
1:B:73:ARG:HH21	1:B:77:GLN:CD	1.78	0.92
1:C:94:ARG:HA	1:C:114:VAL:HB	1.49	0.92
1:A:231:THR:HG21	1:B:83:ASP:OD1	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:94:LEU:HB3	4:L:95:PRO:HD3	0.92	0.91
3:H:6:GLN:CA	3:H:124:GLN:NE2	2.33	0.91
3:G:119:PHE:CG	4:I:46:LEU:HD13	2.06	0.91
1:B:281:LYS:NZ	4:L:28:ASP:HB2	1.86	0.90
1:A:138:ARG:HG2	1:A:138:ARG:HH11	1.32	0.90
4:L:2:ILE:HG22	4:L:90:GLN:CD	1.96	0.90
2:D:69:LEU:HD23	2:F:74:TYR:CD2	2.07	0.89
3:G:99:GLY:CA	3:G:117:TRP:O	2.21	0.89
1:A:229:ALA:HB2	1:B:81:TYR:CD2	1.82	0.88
3:H:119:PHE:HD1	3:H:122:TRP:CZ2	1.90	0.88
1:B:99:ARG:NH2	1:B:105:CYS:SG	2.47	0.87
1:B:281:LYS:NZ	4:L:28:ASP:CB	2.37	0.87
3:G:113:ASP:CB	3:G:117:TRP:NE1	2.38	0.87
1:A:229:ALA:HB1	1:B:81:TYR:HD2	1.31	0.87
1:A:104:GLY:N	3:H:103:LEU:HD12	1.88	0.87
3:H:58:THR:CG2	3:H:70:MET:HB2	2.05	0.87
2:D:28:HIS:HB3	2:F:74:TYR:CE1	2.10	0.86
3:H:119:PHE:CE1	4:L:36:TYR:CE1	2.32	0.86
3:G:99:GLY:HA2	3:G:117:TRP:O	1.74	0.86
4:K:2:ILE:CG2	4:K:90:GLN:CD	2.42	0.86
1:B:225:TRP:HB2	1:B:237:ASN:HB2	1.57	0.86
1:A:103:ASN:C	3:H:103:LEU:HD13	2.01	0.85
4:I:1:ASP:N	4:I:1:ASP:OD1	2.09	0.84
1:A:61:TYR:OH	1:A:206:MET:SD	2.34	0.84
1:A:464:SER:HB3	2:F:75:SER:OG	1.77	0.84
3:G:120:ASP:CB	3:G:121:PRO:HD3	2.05	0.84
1:A:104:GLY:CA	3:H:103:LEU:CD1	2.56	0.84
3:H:118:TRP:O	3:H:122:TRP:CE2	2.30	0.84
1:A:226:HIS:O	1:A:227:ALA:CB	2.27	0.83
3:H:32:ASN:HB3	3:H:98:ARG:HB2	1.60	0.83
4:L:2:ILE:O	4:L:90:GLN:NE2	2.11	0.83
2:D:74:TYR:CD2	2:F:69:LEU:CD2	2.56	0.83
3:H:119:PHE:HA	3:H:122:TRP:HZ2	1.42	0.83
4:L:94:LEU:CB	4:L:95:PRO:HD2	2.08	0.83
1:A:226:HIS:O	1:A:227:ALA:HB3	1.78	0.83
1:A:460:MET:HG2	1:A:465:GLN:NE2	1.92	0.83
1:A:229:ALA:CB	1:B:81:TYR:CB	2.43	0.82
3:G:101:ARG:CA	3:G:102:ALA:N	2.42	0.82
3:G:119:PHE:HE2	4:I:46:LEU:HB2	0.69	0.82
1:B:226:HIS:O	1:B:227:ALA:HB3	1.78	0.81
3:G:113:ASP:CB	3:G:117:TRP:CE2	2.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:117:TRP:CG	4:I:91:PHE:HE1	1.98	0.81
4:K:2:ILE:HD13	4:K:27:GLN:HB2	1.63	0.81
1:B:281:LYS:HZ1	4:L:28:ASP:CB	1.92	0.81
3:G:101:ARG:C	3:G:101:ARG:CB	2.54	0.80
3:H:119:PHE:HA	3:H:122:TRP:CE2	2.16	0.80
2:D:74:TYR:CZ	2:F:32:VAL:CG2	2.64	0.80
1:A:11:PHE:HA	1:A:32:THR:O	1.81	0.80
1:A:232:GLY:HA3	3:G:66:GLY:HA2	1.62	0.80
3:G:117:TRP:CD1	4:I:91:PHE:HE1	1.99	0.79
1:A:11:PHE:HB3	1:A:32:THR:HB	1.64	0.79
1:A:225:TRP:NE1	1:A:237:ASN:HD22	1.80	0.79
4:I:32:TYR:C	4:I:91:PHE:CD2	2.60	0.79
3:H:119:PHE:CD1	3:H:122:TRP:CZ2	2.71	0.79
4:K:2:ILE:O	4:K:90:GLN:NE2	2.16	0.78
4:L:2:ILE:CG2	4:L:90:GLN:CD	2.56	0.78
3:H:6:GLN:HB2	3:H:124:GLN:HE21	1.49	0.78
1:A:229:ALA:CB	1:B:81:TYR:HD2	1.84	0.78
3:H:6:GLN:H	3:H:124:GLN:HE22	1.08	0.78
3:J:33:TYR:OH	3:J:108:TYR:CD2	2.38	0.77
1:B:93:LYS:HE3	1:B:245:PHE:HD2	1.49	0.77
3:G:118:TRP:CH2	4:I:96:ILE:HG21	2.18	0.77
1:A:232:GLY:O	1:A:234:PRO:N	2.17	0.77
1:A:233:THR:O	1:A:235:HIS:N	2.17	0.77
2:D:69:LEU:HG	2:F:74:TYR:CD2	2.19	0.77
3:G:117:TRP:CE2	4:I:91:PHE:CD1	2.73	0.77
3:H:6:GLN:C	3:H:124:GLN:NE2	2.42	0.77
1:A:89:GLN:HE22	1:A:233:THR:CG2	1.95	0.77
1:A:232:GLY:HA2	3:G:66:GLY:CA	2.14	0.77
1:A:68:MET:HE1	1:A:254:THR:HA	1.67	0.77
1:A:231:THR:HG21	1:B:83:ASP:CG	2.09	0.77
2:D:69:LEU:CD2	2:F:74:TYR:CD2	2.67	0.76
4:L:2:ILE:CG2	4:L:90:GLN:OE1	2.33	0.76
3:H:120:ASP:N	3:H:122:TRP:NE1	2.33	0.76
1:A:460:MET:HG3	1:A:465:GLN:CG	2.15	0.76
2:D:69:LEU:HG	2:F:74:TYR:HE2	1.45	0.76
1:C:315:THR:OG1	1:C:316:LYS:N	2.14	0.76
1:B:231:THR:HG23	3:H:65:GLN:CA	2.13	0.76
1:C:460:MET:CE	1:C:464:SER:OG	2.33	0.76
4:I:34:ASN:OD1	4:I:89:GLN:HB3	1.86	0.75
3:H:119:PHE:CZ	4:L:36:TYR:CD1	2.46	0.75
3:G:113:ASP:CG	3:G:117:TRP:HE1	1.94	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:119:PHE:CG	4:L:36:TYR:CE1	2.70	0.75
1:A:98:ASP:O	1:A:99:ARG:CG	2.33	0.75
1:A:138:ARG:HG2	1:A:138:ARG:NH1	1.99	0.75
3:G:119:PHE:CE2	4:I:46:LEU:CG	2.70	0.75
2:D:69:LEU:CG	2:F:74:TYR:CD2	2.70	0.75
1:A:104:GLY:HA2	3:H:103:LEU:CD1	2.16	0.75
2:D:74:TYR:HD2	2:F:69:LEU:HD23	1.44	0.75
1:A:232:GLY:CA	3:G:66:GLY:CA	2.65	0.74
1:B:477:LEU:HD12	1:B:478:ASN:CA	2.17	0.74
3:H:116:SER:O	3:H:117:TRP:C	2.29	0.74
1:A:461:SER:O	1:A:465:GLN:CG	2.36	0.74
3:G:117:TRP:NE1	4:I:91:PHE:CE1	2.54	0.74
1:B:231:THR:CG2	3:H:65:GLN:HA	2.17	0.74
3:H:120:ASP:H	3:H:122:TRP:NE1	1.83	0.74
1:B:94:ARG:HG2	1:B:114:VAL:HG23	1.70	0.74
4:L:94:LEU:HB2	4:L:95:PRO:HD2	1.70	0.74
1:A:81:TYR:HB3	1:B:229:ALA:HB3	1.70	0.73
1:A:81:TYR:HB3	1:B:229:ALA:HB2	1.68	0.72
1:C:94:ARG:CG	1:C:114:VAL:HG11	2.19	0.72
1:A:261:GLN:NE2	2:D:1:ALA:O	2.22	0.72
1:C:464:SER:CB	2:D:75:SER:OG	2.37	0.72
2:D:69:LEU:CG	2:F:74:TYR:CE2	2.71	0.72
3:G:33:TYR:OH	3:G:108:TYR:CD2	2.43	0.72
1:B:233:THR:CG2	1:B:234:PRO:HD2	2.20	0.72
4:I:2:ILE:HD12	4:I:27:GLN:HB2	1.72	0.72
3:H:119:PHE:HD1	4:L:36:TYR:HE1	0.78	0.72
3:G:119:PHE:C	3:G:122:TRP:HE1	1.97	0.72
3:G:120:ASP:HB3	3:G:121:PRO:CD	2.15	0.72
1:C:94:ARG:HG2	1:C:114:VAL:HG12	1.69	0.71
1:A:27:HIS:HE1	1:A:48:THR:H	1.34	0.71
1:B:281:LYS:HZ1	4:L:28:ASP:HB2	1.50	0.71
1:A:232:GLY:CA	3:G:66:GLY:HA2	2.20	0.71
2:D:28:HIS:C	2:F:74:TYR:HE1	1.99	0.70
2:D:28:HIS:HB3	2:F:74:TYR:CD1	2.25	0.70
1:A:69:ALA:HB2	1:A:84:LYS:HD2	1.71	0.70
1:A:21:VAL:O	1:A:293:LEU:HB3	1.90	0.70
3:J:32:ASN:HB3	3:J:98:ARG:HB2	1.72	0.70
4:K:32:TYR:HB3	4:K:91:PHE:HB3	1.74	0.70
1:B:332:TYR:O	1:B:371:ASN:HA	1.91	0.70
3:G:27:TYR:CZ	3:G:98:ARG:HD3	2.26	0.70
4:L:32:TYR:HB3	4:L:91:PHE:HB3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:TYR:HE2	2:F:69:LEU:HD21	1.57	0.69
4:I:33:LEU:C	4:I:91:PHE:CE2	2.66	0.69
3:G:117:TRP:CG	4:I:91:PHE:CE1	2.76	0.69
1:A:461:SER:O	1:A:465:GLN:HG3	1.92	0.69
1:C:245:PHE:HA	1:C:254:THR:O	1.93	0.69
3:G:68:ILE:HD11	3:G:81:MET:SD	2.33	0.69
2:D:69:LEU:HD23	2:F:74:TYR:HD2	1.55	0.69
3:H:6:GLN:HB2	3:H:124:GLN:NE2	2.07	0.68
2:D:74:TYR:OH	2:F:32:VAL:HG21	1.92	0.68
3:G:119:PHE:CE2	4:I:46:LEU:HA	2.16	0.68
1:B:93:LYS:HE3	1:B:245:PHE:CD2	2.29	0.68
3:H:99:GLY:O	3:H:117:TRP:O	2.12	0.68
3:H:6:GLN:O	3:H:124:GLN:NE2	2.27	0.68
3:G:117:TRP:NE1	4:I:91:PHE:CD1	2.62	0.68
1:B:104:GLY:HA2	3:G:101:ARG:NH2	2.09	0.67
1:B:101:TRP:O	1:B:102:GLY:C	2.36	0.67
1:B:72:SER:OG	1:B:99:ARG:NH1	2.28	0.67
1:A:138:ARG:HD3	1:A:168:GLU:HG2	1.76	0.67
2:D:74:TYR:CE2	2:F:69:LEU:HD21	2.30	0.67
1:C:85:GLN:NE2	1:C:94:ARG:HH11	1.93	0.67
1:B:97:VAL:O	1:B:110:LYS:HA	1.95	0.67
1:C:338:PRO:HA	1:C:365:ILE:O	1.95	0.66
1:C:65:ILE:HD13	1:C:243:VAL:HG21	1.77	0.66
2:D:32:VAL:HG23	2:F:74:TYR:CZ	2.28	0.66
3:G:107:SER:CB	4:I:94:LEU:HD11	2.25	0.66
1:A:214:HIS:H	2:D:7:HIS:HE1	1.43	0.66
1:C:217:TRP:NE1	2:F:5:PRO:O	2.28	0.66
4:K:2:ILE:CD1	4:K:27:GLN:HB2	2.25	0.66
1:A:58:SER:O	1:A:225:TRP:HA	1.96	0.66
3:G:118:TRP:O	3:G:122:TRP:CZ2	2.48	0.65
3:J:101:ARG:HD3	3:J:112:ARG:HG2	1.76	0.65
1:C:69:ALA:HB3	1:C:116:CYS:H	1.60	0.65
3:H:58:THR:HG21	3:H:70:MET:CB	2.22	0.65
4:I:35:TRP:HB2	4:I:48:ILE:HB	1.79	0.65
1:A:380:PRO:HG2	1:A:402:ARG:HD3	1.77	0.65
1:B:251:LYS:HG3	1:B:252:ARG:HG2	1.79	0.65
1:A:461:SER:O	1:A:465:GLN:HG2	1.97	0.65
1:B:214:HIS:H	2:E:7:HIS:HE1	1.43	0.65
4:I:34:ASN:HB3	4:I:91:PHE:HZ	1.62	0.65
3:H:119:PHE:HA	3:H:122:TRP:NE1	2.12	0.65
1:B:73:ARG:NH2	1:B:77:GLN:CG	2.55	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:GLY:HA2	1:C:420:ARG:HE	1.61	0.65
4:L:35:TRP:HB2	4:L:48:ILE:HB	1.79	0.65
1:B:93:LYS:HB3	1:B:245:PHE:CD2	2.32	0.64
1:B:230:ASP:OD2	1:B:231:THR:CB	2.45	0.64
3:H:6:GLN:CB	3:H:124:GLN:NE2	2.61	0.64
1:A:68:MET:CE	1:A:254:THR:HA	2.27	0.64
4:K:35:TRP:HB2	4:K:48:ILE:HB	1.79	0.64
1:A:81:TYR:CD2	1:B:229:ALA:HB3	2.33	0.64
2:D:28:HIS:O	2:F:74:TYR:CE1	2.51	0.64
1:A:238:ASN:C	1:A:240:GLU:H	2.05	0.64
2:D:28:HIS:O	2:F:74:TYR:HE1	1.78	0.64
1:B:226:HIS:O	1:B:227:ALA:CB	2.45	0.64
1:B:59:TYR:HB2	1:B:125:MET:HB3	1.78	0.64
1:B:281:LYS:HZ3	4:L:28:ASP:CB	2.11	0.63
2:D:74:TYR:CD2	2:F:69:LEU:CG	2.79	0.63
1:C:85:GLN:HE22	1:C:94:ARG:NH1	1.96	0.63
2:D:69:LEU:CD2	2:F:74:TYR:CE2	2.82	0.63
3:G:95:TYR:HB3	3:G:122:TRP:CE3	2.33	0.63
3:G:119:PHE:CD2	4:I:46:LEU:HD22	2.34	0.63
3:H:71:THR:HG23	3:H:72:ARG:N	2.13	0.63
3:H:119:PHE:HD1	4:L:36:TYR:CE1	1.68	0.63
1:C:102:GLY:O	3:J:103:LEU:HD13	1.95	0.63
3:G:113:ASP:CB	3:G:117:TRP:CZ2	2.81	0.63
1:C:252:ARG:HH21	3:J:54:ARG:HD3	1.64	0.62
1:B:277:MET:HB3	1:B:283:ARG:HB3	1.80	0.62
3:H:6:GLN:CB	3:H:124:GLN:HE21	2.11	0.62
3:H:119:PHE:C	3:H:122:TRP:HE1	2.07	0.62
1:C:475:LEU:HD13	2:D:52:LEU:HD23	1.82	0.62
3:H:99:GLY:HA2	3:H:117:TRP:O	1.99	0.62
3:G:71:THR:HG23	3:G:72:ARG:N	2.13	0.62
1:A:98:ASP:C	1:A:99:ARG:HG2	2.24	0.62
3:H:116:SER:C	3:H:118:TRP:N	2.56	0.62
3:H:6:GLN:CA	3:H:124:GLN:HE22	2.04	0.62
1:B:41:VAL:HG12	1:B:143:VAL:HG12	1.81	0.62
3:G:119:PHE:HZ	4:I:46:LEU:CA	2.12	0.62
1:A:68:MET:HA	1:A:116:CYS:O	1.99	0.61
1:B:70:SER:HA	1:B:115:THR:HA	1.81	0.61
4:K:2:ILE:HB	4:K:90:GLN:OE1	1.99	0.61
1:C:464:SER:HB2	2:D:75:SER:HA	1.82	0.61
1:A:170:THR:HG23	1:A:173:SER:H	1.65	0.61
1:C:424:LEU:HB2	1:C:428:ALA:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ALA:HB3	1:B:129:SER:HB3	1.81	0.61
1:A:89:GLN:CD	1:A:233:THR:CG2	2.67	0.61
1:C:58:SER:HB2	1:C:226:HIS:HB3	1.83	0.61
1:B:281:LYS:HZ3	4:L:28:ASP:HB3	1.64	0.61
4:I:34:ASN:CG	4:I:91:PHE:CZ	2.79	0.61
1:C:423:VAL:HG11	2:F:15:ARG:HG2	1.82	0.61
2:D:69:LEU:CG	2:F:74:TYR:HD2	2.13	0.61
4:I:4:LEU:HD22	4:I:90:GLN:HG3	1.82	0.61
3:H:6:GLN:H	3:H:124:GLN:CD	2.08	0.61
4:L:4:LEU:HD22	4:L:90:GLN:HG3	1.82	0.61
3:G:116:SER:O	3:G:117:TRP:C	2.44	0.61
3:G:119:PHE:HZ	4:I:45:LYS:C	2.07	0.61
1:B:245:PHE:HB3	1:B:253:GLN:HE21	1.66	0.61
4:K:4:LEU:HD22	4:K:90:GLN:HG3	1.82	0.61
1:A:460:MET:HG3	1:A:465:GLN:CD	2.26	0.60
1:B:357:ARG:HB3	1:B:379:ASP:HB3	1.83	0.60
1:B:104:GLY:H	3:G:101:ARG:NH2	1.99	0.60
3:H:114:GLY:HA2	3:H:117:TRP:HE3	1.66	0.60
1:B:281:LYS:NZ	4:L:28:ASP:HB3	2.15	0.60
1:C:85:GLN:HE22	1:C:94:ARG:HH11	1.48	0.60
1:B:27:HIS:NE2	1:B:46:VAL:O	2.35	0.60
3:G:99:GLY:HA3	3:G:117:TRP:O	1.99	0.60
3:H:43:GLN:O	3:H:44:GLY:O	2.19	0.60
1:C:464:SER:CB	2:D:75:SER:HG	2.15	0.60
3:H:117:TRP:CZ3	4:L:49:TYR:CA	2.83	0.60
1:A:15:MET:HE3	1:A:35:ALA:HB2	1.84	0.60
1:A:82:LEU:CD1	1:A:84:LYS:HB2	2.32	0.60
1:A:103:ASN:C	3:H:103:LEU:HD11	2.25	0.60
4:K:2:ILE:HG22	4:K:2:ILE:O	2.01	0.60
1:A:27:HIS:HE1	1:A:48:THR:N	2.00	0.60
1:A:81:TYR:CB	1:B:229:ALA:HB3	2.32	0.59
1:A:85:GLN:HG2	1:A:92:CYS:SG	2.42	0.59
3:G:113:ASP:CB	3:G:117:TRP:HE1	2.15	0.59
3:G:114:GLY:H	3:G:117:TRP:CD1	2.19	0.59
1:A:238:ASN:O	1:A:240:GLU:N	2.34	0.59
1:B:73:ARG:NH2	1:B:77:GLN:HB2	2.17	0.59
3:G:33:TYR:OH	3:G:108:TYR:HD2	1.85	0.59
1:A:460:MET:CG	1:A:465:GLN:NE2	2.64	0.59
1:C:171:PRO:HB3	1:C:192:PRO:HB2	1.84	0.59
1:A:174:PRO:HB2	1:A:175:ARG:HG3	1.85	0.59
1:B:100:GLY:HA2	1:B:108:PHE:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLU:HG3	1:A:166:LYS:HE3	1.85	0.58
1:C:374:MET:HE2	1:C:376:LEU:HD11	1.85	0.58
3:G:100:GLY:O	3:G:101:ARG:C	2.46	0.58
3:G:119:PHE:HD2	4:I:46:LEU:HD22	1.68	0.58
1:B:73:ARG:HH21	1:B:77:GLN:HG3	1.65	0.58
1:B:230:ASP:OD2	1:B:231:THR:HB	2.02	0.58
1:A:89:GLN:CD	1:A:233:THR:HG21	2.14	0.58
1:A:232:GLY:HA2	3:G:66:GLY:N	2.18	0.58
2:D:74:TYR:CE1	2:F:32:VAL:CG2	2.87	0.58
3:G:6:GLN:NE2	3:G:96:CYS:SG	2.75	0.58
3:H:6:GLN:C	3:H:124:GLN:HE21	2.12	0.58
1:B:9:ARG:HH21	1:B:32:THR:HG21	1.69	0.58
1:B:94:ARG:CG	1:B:114:VAL:HG23	2.33	0.58
1:C:503:SER:OG	1:C:504:ALA:N	2.34	0.58
1:B:477:LEU:HD12	1:B:478:ASN:H	0.50	0.58
1:A:46:VAL:HG12	1:A:47:THR:HG23	1.85	0.57
3:H:117:TRP:CE3	4:L:49:TYR:CB	2.86	0.57
1:B:39:PRO:HD2	1:B:298:LEU:HB3	1.86	0.57
1:A:65:ILE:HD13	1:A:257:VAL:HG22	1.85	0.57
1:A:232:GLY:H	3:G:66:GLY:H	1.53	0.57
1:A:217:TRP:CG	2:D:7:HIS:HD1	2.23	0.57
3:G:120:ASP:CB	3:G:121:PRO:CD	2.79	0.57
1:B:463:PHE:O	1:B:463:PHE:HD1	1.88	0.57
1:B:22:ASP:HA	1:B:292:ARG:HA	1.87	0.57
1:A:99:ARG:NH1	1:A:105:CYS:SG	2.78	0.57
2:D:29:LEU:HA	2:F:74:TYR:OH	2.05	0.57
3:J:6:GLN:NE2	3:J:96:CYS:SG	2.76	0.57
3:G:32:ASN:ND2	3:G:98:ARG:HD2	2.20	0.56
4:I:34:ASN:HB3	4:I:91:PHE:CZ	2.39	0.56
3:H:35:HIS:O	3:H:96:CYS:HA	2.05	0.56
1:A:104:GLY:CA	3:H:103:LEU:HD13	2.35	0.56
1:C:476:GLY:HA3	1:C:488:CYS:HB3	1.87	0.56
3:G:35:HIS:O	3:G:96:CYS:HA	2.06	0.56
1:A:98:ASP:O	1:A:99:ARG:CD	2.53	0.56
1:B:281:LYS:CE	4:L:28:ASP:HB2	2.34	0.56
3:G:116:SER:C	3:G:118:TRP:N	2.56	0.56
3:G:118:TRP:CD1	3:G:122:TRP:HZ2	2.23	0.56
1:A:231:THR:CG2	1:B:83:ASP:OD1	2.50	0.56
1:A:417:GLY:HA2	1:A:420:ARG:HE	1.71	0.56
1:A:232:GLY:CA	3:G:66:GLY:N	2.69	0.56
3:H:6:GLN:CA	3:H:124:GLN:HE21	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:TRP:O	3:J:101:ARG:NH1	2.38	0.56
3:J:35:HIS:O	3:J:96:CYS:HA	2.05	0.56
1:A:1:ILE:HD12	1:A:144:HIS:HA	1.86	0.56
1:C:463:PHE:CE2	1:C:467:LEU:HD11	2.40	0.56
1:C:464:SER:HB3	2:D:75:SER:OG	2.04	0.56
3:G:98:ARG:NE	3:G:121:PRO:HG2	2.20	0.56
3:G:113:ASP:HB3	3:G:117:TRP:CZ2	2.40	0.56
1:A:1:ILE:HD13	1:A:147:GLN:HB3	1.88	0.56
1:A:101:TRP:CD1	1:A:101:TRP:N	2.72	0.56
1:B:430:ASP:HB3	1:B:443:LYS:HD2	1.88	0.56
1:B:108:PHE:HD1	1:B:108:PHE:C	2.13	0.56
1:C:72:SER:HA	1:C:99:ARG:HH22	1.71	0.56
2:D:69:LEU:CD2	2:F:74:TYR:HD2	2.15	0.56
1:B:73:ARG:NH2	1:B:77:GLN:CD	2.59	0.56
1:B:217:TRP:NE1	2:E:5:PRO:O	2.35	0.56
1:B:230:ASP:OD2	1:B:231:THR:N	2.30	0.56
3:H:98:ARG:O	3:H:118:TRP:HA	2.06	0.55
3:H:119:PHE:CA	3:H:122:TRP:HZ2	2.14	0.55
1:A:351:THR:O	1:A:353:THR:N	2.36	0.55
2:D:74:TYR:CE1	2:F:32:VAL:HG23	2.40	0.55
3:G:118:TRP:O	3:G:122:TRP:CE2	2.59	0.55
4:L:94:LEU:O	4:L:96:ILE:CG1	2.38	0.55
1:A:132:PRO:HD3	1:A:199:SER:HB2	1.89	0.55
1:B:73:ARG:NH2	1:B:77:GLN:HG3	2.21	0.55
3:H:6:GLN:NE2	3:H:96:CYS:SG	2.75	0.55
3:H:33:TYR:O	3:H:98:ARG:HA	2.06	0.55
1:B:144:HIS:HB3	1:B:360:THR:HG23	1.89	0.55
3:H:122:TRP:CD1	3:H:122:TRP:N	2.73	0.55
1:A:300:LEU:HB3	1:A:362:ASN:HD22	1.72	0.55
3:H:32:ASN:OD1	3:H:100:GLY:HA2	2.06	0.55
3:H:119:PHE:HD1	3:H:122:TRP:CH2	2.24	0.55
1:C:472:LEU:HD23	1:C:475:LEU:HD12	1.89	0.55
1:A:225:TRP:NE1	1:A:237:ASN:ND2	2.52	0.55
3:G:119:PHE:O	3:G:122:TRP:HD1	1.84	0.55
1:A:238:ASN:C	1:A:240:GLU:N	2.63	0.54
1:B:104:GLY:CA	3:G:101:ARG:NH2	2.70	0.54
1:B:93:LYS:HB3	1:B:245:PHE:CE2	2.43	0.54
1:B:382:PHE:HA	1:B:402:ARG:HD3	1.90	0.54
1:C:391:VAL:HG12	1:C:393:GLU:H	1.72	0.54
1:C:42:ASP:OD1	1:C:42:ASP:N	2.35	0.54
3:G:118:TRP:CD1	3:G:118:TRP:C	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:GLN:HB2	1:C:388:VAL:HB	1.88	0.54
2:D:69:LEU:CG	2:F:74:TYR:HE2	2.16	0.54
4:I:34:ASN:CB	4:I:91:PHE:HZ	2.21	0.54
1:C:502:VAL:N	1:C:503:SER:O	2.41	0.54
1:B:68:MET:O	3:G:72:ARG:NH2	2.37	0.54
1:B:87:ASP:OD1	1:B:87:ASP:O	2.24	0.54
1:A:69:ALA:CB	1:A:84:LYS:HD2	2.37	0.54
1:C:137:TYR:HE2	1:C:192:PRO:HB3	1.73	0.54
2:D:32:VAL:HG23	2:F:74:TYR:CE1	2.43	0.54
1:B:108:PHE:C	1:B:108:PHE:CD1	2.86	0.54
4:L:86:TYR:HB2	4:L:102:THR:HB	1.90	0.54
4:K:2:ILE:HG21	4:K:90:GLN:CD	2.31	0.54
1:A:41:VAL:HG22	1:A:143:VAL:HG22	1.89	0.53
1:C:473:MET:HA	1:C:488:CYS:HB2	1.89	0.53
1:A:81:TYR:CG	1:B:229:ALA:HB3	2.43	0.53
1:C:1:ILE:HG22	1:C:142:SER:HB3	1.89	0.53
1:C:475:LEU:O	1:C:479:THR:OG1	2.25	0.53
1:B:104:GLY:HA2	3:G:101:ARG:HH21	1.73	0.53
1:B:214:HIS:H	2:E:7:HIS:CE1	2.26	0.53
4:I:33:LEU:N	4:I:91:PHE:CD2	2.75	0.53
1:A:435:GLY:HA3	1:A:439:ASN:HB2	1.90	0.53
4:L:2:ILE:HG21	4:L:90:GLN:OE1	2.08	0.53
1:A:51:SER:OG	1:A:134:ASN:OD1	2.25	0.53
3:G:97:ALA:HB2	3:G:122:TRP:CD2	2.44	0.53
1:A:4:ILE:HG21	1:C:101:TRP:HD1	1.74	0.53
1:A:341:VAL:HB	1:A:363:PRO:HG2	1.90	0.53
3:H:119:PHE:CA	3:H:122:TRP:HE1	2.21	0.53
1:A:200:ASP:OD2	1:A:214:HIS:ND1	2.42	0.53
1:A:350:GLN:O	1:A:350:GLN:HG3	2.08	0.53
1:C:342:PRO:HG2	1:C:390:GLY:HA2	1.91	0.53
4:I:34:ASN:CG	4:I:91:PHE:HZ	2.16	0.53
4:I:86:TYR:HB2	4:I:102:THR:HB	1.90	0.53
1:C:343:ALA:HA	1:C:388:VAL:O	2.09	0.53
1:A:232:GLY:H	3:G:66:GLY:N	2.06	0.53
2:D:28:HIS:HB3	2:F:74:TYR:HE1	1.70	0.53
1:B:73:ARG:HH21	1:B:77:GLN:CB	2.20	0.53
3:G:97:ALA:CB	3:G:121:PRO:O	2.57	0.53
3:J:114:GLY:HA2	3:J:117:TRP:HB3	1.90	0.53
4:K:86:TYR:HB2	4:K:102:THR:HB	1.90	0.53
1:A:58:SER:HB2	1:A:226:HIS:HB3	1.91	0.52
1:C:15:MET:HB2	1:C:35:ALA:HB1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:121:PRO:O	3:G:122:TRP:CD1	2.61	0.52
1:A:460:MET:CG	1:A:465:GLN:CD	2.82	0.52
3:H:119:PHE:HA	3:H:122:TRP:HE1	1.75	0.52
3:J:108:TYR:N	3:J:108:TYR:CD1	2.72	0.52
1:A:21:VAL:O	1:A:293:LEU:CB	2.57	0.52
1:C:457:PHE:HE2	1:C:491:LEU:HD21	1.72	0.52
1:C:96:LEU:HB3	1:C:110:LYS:HB3	1.91	0.52
3:H:23:LYS:NZ	3:H:76:THR:O	2.43	0.52
1:C:217:TRP:CG	2:F:7:HIS:HD1	2.27	0.52
1:A:148:HIS:HA	1:A:375:MET:HG2	1.91	0.52
2:D:74:TYR:CE1	2:F:28:HIS:HB3	2.45	0.52
1:A:418:ALA:HB1	1:A:497:PHE:HZ	1.73	0.52
1:B:390:GLY:HA3	1:B:395:LYS:HA	1.92	0.52
3:G:67:ARG:NH2	3:G:90:ASP:OD2	2.43	0.52
1:A:59:TYR:CE1	1:A:225:TRP:HB3	2.44	0.52
1:A:103:ASN:O	3:H:103:LEU:CD1	2.46	0.52
1:B:104:GLY:N	3:G:101:ARG:NH2	2.57	0.52
1:B:332:TYR:OH	1:B:339:CYS:SG	2.68	0.52
1:A:20:TRP:HE1	1:A:292:ARG:HD3	1.74	0.52
1:A:232:GLY:HA2	3:G:66:GLY:HA3	1.92	0.52
1:B:49:THR:O	1:B:136:GLU:N	2.43	0.52
1:B:329:GLU:HA	1:B:375:MET:HA	1.91	0.52
1:A:73:ARG:NH2	1:A:77:GLN:HB3	2.25	0.52
1:B:388:VAL:HG12	1:B:397:THR:HG22	1.90	0.51
3:G:23:LYS:NZ	3:G:76:THR:O	2.43	0.51
1:C:9:ARG:HD2	1:C:32:THR:HG23	1.92	0.51
3:G:95:TYR:HB3	3:G:122:TRP:HE3	1.73	0.51
1:A:59:TYR:HE1	1:A:225:TRP:HB3	1.75	0.51
2:D:28:HIS:C	2:F:74:TYR:CE1	2.86	0.51
3:J:23:LYS:NZ	3:J:76:THR:O	2.43	0.51
1:A:189:ASP:OD2	1:A:294:LYS:NZ	2.44	0.51
3:H:58:THR:HG22	3:H:70:MET:SD	2.51	0.51
1:A:82:LEU:HD13	1:A:84:LYS:HB2	1.91	0.51
1:C:79:GLU:OE2	1:C:94:ARG:HD3	2.09	0.51
1:B:233:THR:HG23	1:B:234:PRO:HD2	1.90	0.51
1:B:477:LEU:HD12	1:B:478:ASN:HA	1.93	0.51
4:K:2:ILE:HG22	4:K:90:GLN:HE22	0.70	0.51
1:A:117:ALA:HB2	1:A:255:VAL:HG11	1.93	0.51
1:A:144:HIS:HB3	1:A:360:THR:HG23	1.92	0.51
1:C:493:GLY:O	1:C:497:PHE:HB2	2.11	0.51
1:B:104:GLY:H	3:G:101:ARG:HH22	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLU:O	1:A:256:VAL:HB	2.11	0.51
2:D:32:VAL:CG2	2:F:74:TYR:OH	2.59	0.50
1:B:73:ARG:HG3	1:B:80:ALA:HA	1.93	0.50
4:L:93:ASP:O	4:L:94:LEU:CG	2.59	0.50
3:J:101:ARG:O	3:J:101:ARG:HG3	2.11	0.50
1:A:287:GLY:H	2:D:14:THR:HG21	1.76	0.50
1:B:93:LYS:HB3	1:B:245:PHE:HD2	1.75	0.50
1:C:1:ILE:HD13	1:C:144:HIS:HA	1.93	0.50
1:A:247:ASP:HA	1:A:253:GLN:HA	1.93	0.50
1:A:314:PHE:HA	1:A:330:VAL:HA	1.92	0.50
1:C:472:LEU:HD21	2:D:49:ILE:HG12	1.93	0.50
4:K:34:ASN:HD22	4:K:49:TYR:HA	1.76	0.50
2:D:74:TYR:OH	2:F:32:VAL:CG2	2.57	0.50
1:B:104:GLY:O	1:B:105:CYS:C	2.51	0.50
1:B:233:THR:HG22	1:B:234:PRO:HD2	1.91	0.50
3:J:91:THR:HG23	3:J:129:THR:HA	1.94	0.50
1:A:66:SER:C	1:A:68:MET:H	2.19	0.50
1:A:217:TRP:NE1	2:D:5:PRO:O	2.42	0.50
1:B:45:LEU:HA	1:B:139:ILE:HG22	1.94	0.50
3:H:103:LEU:C	3:H:103:LEU:HD22	2.37	0.50
1:B:312:PHE:HD2	1:B:389:ILE:HG22	1.77	0.49
3:G:71:THR:CG2	3:G:72:ARG:N	2.75	0.49
3:G:91:THR:HG23	3:G:129:THR:HA	1.94	0.49
4:K:2:ILE:CG2	4:K:90:GLN:OE1	2.58	0.49
1:A:106:GLY:O	1:A:107:LEU:O	2.29	0.49
1:C:95:THR:O	1:C:112:SER:HA	2.11	0.49
1:B:132:PRO:HD3	1:B:199:SER:HB3	1.94	0.49
1:B:496:ILE:O	1:B:500:THR:OG1	2.27	0.49
4:L:94:LEU:HB2	4:L:95:PRO:CD	2.22	0.49
1:A:349:MET:HE2	1:A:352:LEU:HD11	1.93	0.49
1:C:9:ARG:NH1	1:C:377:GLU:OE2	2.46	0.49
1:C:24:VAL:HG22	1:C:290:LYS:HG3	1.94	0.49
3:J:67:ARG:NH2	3:J:90:ASP:OD2	2.43	0.49
1:C:85:GLN:NE2	1:C:94:ARG:NH1	2.55	0.49
3:G:97:ALA:HB2	3:G:121:PRO:O	2.13	0.49
3:H:50:VAL:O	3:H:58:THR:HG22	2.12	0.49
3:H:58:THR:CG2	3:H:70:MET:SD	3.00	0.49
1:A:155:ASP:HA	1:A:158:HIS:HB3	1.95	0.49
1:B:345:MET:HE2	1:B:387:ILE:HG12	1.94	0.49
3:G:114:GLY:N	3:G:117:TRP:CD1	2.81	0.49
3:H:91:THR:HG23	3:H:129:THR:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:GLY:HA3	1:C:164:ARG:HH21	1.78	0.49
1:B:58:SER:H	1:B:226:HIS:HB3	1.76	0.49
3:H:71:THR:CG2	3:H:72:ARG:N	2.75	0.49
4:L:34:ASN:HD22	4:L:49:TYR:HA	1.76	0.49
4:K:2:ILE:C	4:K:90:GLN:HE22	2.19	0.49
2:D:27:LYS:HB2	2:F:2:VAL:HG11	1.95	0.49
3:G:117:TRP:CE2	4:I:91:PHE:CE1	3.00	0.49
3:G:119:PHE:CD2	4:I:46:LEU:CG	2.92	0.49
4:L:94:LEU:C	4:L:96:ILE:N	2.64	0.49
2:F:51:TRP:HA	2:F:60:LYS:HD2	1.95	0.49
3:G:119:PHE:HZ	4:I:46:LEU:N	2.10	0.48
3:H:119:PHE:CG	4:L:36:TYR:CD1	2.91	0.48
1:A:81:TYR:CD2	1:B:229:ALA:CB	2.96	0.48
2:D:74:TYR:CD2	2:F:69:LEU:HB3	2.48	0.48
1:B:280:ALA:C	1:B:281:LYS:HG2	2.38	0.48
1:B:423:VAL:HG11	2:E:15:ARG:HG2	1.95	0.48
1:A:8:ASN:HD21	2:D:15:ARG:HH11	1.60	0.48
1:C:212:LEU:HD11	1:C:284:LEU:HD11	1.95	0.48
1:B:42:ASP:OD1	1:B:42:ASP:N	2.44	0.48
3:G:121:PRO:O	3:G:122:TRP:CG	2.66	0.48
4:L:29:ILE:HD11	4:L:71:PHE:HE2	1.78	0.48
1:A:68:MET:HE3	1:A:255:VAL:HG13	1.94	0.48
1:A:236:TRP:O	1:A:237:ASN:O	2.32	0.48
1:B:477:LEU:CG	1:B:478:ASN:H	2.15	0.48
3:H:118:TRP:O	3:H:122:TRP:HZ2	1.83	0.48
1:A:328:VAL:HG21	1:A:387:ILE:HD13	1.95	0.48
2:D:51:TRP:HA	2:D:60:LYS:HD2	1.95	0.48
4:L:2:ILE:HB	4:L:90:GLN:OE1	2.13	0.48
1:C:91:VAL:O	1:C:116:CYS:HA	2.12	0.48
1:C:429:TRP:HE1	1:C:439:ASN:HA	1.78	0.48
1:A:327:THR:HG22	1:A:377:GLU:HG3	1.95	0.48
1:B:73:ARG:NH2	1:B:77:GLN:CB	2.77	0.48
4:I:1:ASP:CA	4:I:95:PRO:HG2	2.38	0.48
1:A:91:VAL:O	1:A:116:CYS:HA	2.14	0.48
1:A:175:ARG:HA	1:A:188:LEU:O	2.14	0.48
1:A:236:TRP:C	1:A:237:ASN:O	2.55	0.48
3:J:31:SER:C	3:J:102:ALA:HB3	2.38	0.48
1:A:228:GLY:HA3	1:B:73:ARG:HH12	1.79	0.48
1:B:19:THR:OG1	1:B:295:MET:N	2.43	0.48
1:A:229:ALA:HB2	1:B:81:TYR:HB2	1.77	0.47
1:C:32:THR:HG22	1:C:42:ASP:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:MET:HG3	1:C:128:LYS:HE2	1.95	0.47
4:I:33:LEU:CA	4:I:91:PHE:CE2	2.97	0.47
1:A:370:GLU:HG3	1:A:371:ASN:H	1.80	0.47
1:C:97:VAL:HG13	1:C:250:ALA:HB1	1.96	0.47
1:C:278:ASP:OD1	1:C:278:ASP:N	2.46	0.47
1:B:479:THR:OG1	1:B:480:LYS:N	2.40	0.47
3:G:54:ARG:NH2	3:G:103:LEU:O	2.47	0.47
3:G:33:TYR:HE2	3:G:107:SER:O	1.97	0.47
1:C:57:ARG:HD3	1:C:227:ALA:HA	1.95	0.47
3:G:98:ARG:O	3:G:118:TRP:HB3	2.14	0.47
3:G:117:TRP:CE2	4:I:91:PHE:HD1	2.25	0.47
3:H:103:LEU:C	3:H:103:LEU:CD2	2.87	0.47
4:L:29:ILE:HD11	4:L:71:PHE:CE2	2.49	0.47
1:B:101:TRP:O	1:B:103:ASN:N	2.46	0.47
1:B:352:LEU:HD12	1:B:354:PRO:HD3	1.97	0.47
2:E:51:TRP:HA	2:E:60:LYS:HD2	1.95	0.47
3:G:118:TRP:O	3:G:122:TRP:NE1	2.47	0.47
1:A:38:LYS:H	1:A:300:LEU:HD11	1.80	0.47
1:A:60:CYS:O	1:A:223:LEU:HD23	2.14	0.47
1:A:105:CYS:HB3	3:H:108:TYR:CD1	2.49	0.47
1:C:245:PHE:HB3	1:C:255:VAL:HA	1.96	0.47
1:B:99:ARG:NH2	3:G:108:TYR:OH	2.47	0.47
1:B:332:TYR:O	1:B:371:ASN:CA	2.61	0.47
3:G:119:PHE:CZ	4:I:46:LEU:N	2.82	0.47
3:G:119:PHE:CA	3:G:122:TRP:HE1	2.27	0.47
3:H:122:TRP:CH2	4:L:36:TYR:CE1	3.03	0.47
1:C:151:MET:HB3	1:C:164:ARG:HH12	1.79	0.47
1:B:238:ASN:O	1:B:239:LYS:HB2	2.13	0.47
2:D:28:HIS:CB	2:F:74:TYR:CE1	2.91	0.47
3:G:113:ASP:CG	3:G:117:TRP:NE1	2.62	0.47
3:H:113:ASP:N	3:H:113:ASP:OD1	2.46	0.47
1:A:382:PHE:HZ	1:A:409:LYS:HD3	1.80	0.47
1:B:151:MET:HE2	1:B:375:MET:HE1	1.96	0.47
1:B:87:ASP:OD1	1:B:87:ASP:C	2.56	0.46
1:B:101:TRP:C	1:B:103:ASN:N	2.69	0.46
1:B:217:TRP:CG	2:E:7:HIS:HD1	2.32	0.46
1:C:25:LEU:H	1:C:25:LEU:HG	1.51	0.46
2:D:74:TYR:HD2	2:F:69:LEU:HB3	1.79	0.46
3:J:119:PHE:CD2	4:K:46:LEU:HD13	2.50	0.46
1:A:101:TRP:CD1	1:A:101:TRP:H	2.33	0.46
1:A:138:ARG:HH11	1:A:138:ARG:CG	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:HIS:NE2	1:C:229:ALA:O	2.48	0.46
1:C:309:THR:HA	1:C:391:VAL:HG22	1.98	0.46
3:G:9:PRO:HB3	3:G:127:LEU:HB3	1.98	0.46
1:C:22:ASP:OD1	1:C:22:ASP:N	2.49	0.46
3:G:34:ILE:HG13	3:G:79:VAL:HG21	1.98	0.46
4:I:34:ASN:HB2	4:I:48:ILE:O	2.16	0.46
1:C:382:PHE:HA	1:C:402:ARG:HG2	1.98	0.46
1:B:22:ASP:HA	1:B:291:CYS:O	2.16	0.46
3:J:9:PRO:HB3	3:J:127:LEU:HB3	1.98	0.46
1:A:52:ASN:HB2	1:A:134:ASN:HD21	1.81	0.46
1:A:54:ALA:HB1	1:B:77:GLN:HB3	1.97	0.46
1:A:93:LYS:HG2	1:A:94:ARG:N	2.31	0.46
1:A:278:ASP:OD2	1:A:283:ARG:NE	2.49	0.46
1:B:247:ASP:HA	1:B:253:GLN:HA	1.98	0.46
1:A:224:PRO:HG3	1:A:239:LYS:HA	1.98	0.46
1:C:61:TYR:HB2	1:C:261:GLN:HB2	1.97	0.46
3:G:60:SER:OG	3:G:61:ALA:N	2.49	0.46
2:D:47:ALA:HA	2:D:64:LEU:HD21	1.98	0.46
1:B:53:MET:HG2	1:B:130:ILE:HG22	1.98	0.46
1:C:83:ASP:OD1	1:C:83:ASP:N	2.48	0.46
1:B:368:SER:OG	1:B:369:THR:N	2.43	0.45
3:G:98:ARG:HE	3:G:121:PRO:CG	2.29	0.45
3:G:119:PHE:CD2	4:I:46:LEU:CD2	2.99	0.45
4:I:34:ASN:CB	4:I:91:PHE:CZ	2.99	0.45
3:H:120:ASP:C	3:H:122:TRP:HD1	2.24	0.45
1:C:238:ASN:O	1:C:240:GLU:N	2.49	0.45
1:B:67:ASP:OD1	1:B:67:ASP:N	2.47	0.45
3:G:33:TYR:HH	3:G:108:TYR:HD2	1.51	0.45
1:A:15:MET:HE1	1:A:295:MET:HG3	1.99	0.45
1:A:358:LEU:HA	1:A:378:LEU:HA	1.97	0.45
3:G:105:TYR:H	3:G:108:TYR:HE2	1.65	0.45
3:J:54:ARG:NH2	3:J:103:LEU:O	2.49	0.45
1:C:328:VAL:O	1:C:375:MET:HA	2.17	0.45
2:D:74:TYR:HE1	2:F:28:HIS:O	2.00	0.45
3:J:6:GLN:O	3:J:124:GLN:NE2	2.50	0.45
3:J:60:SER:OG	3:J:61:ALA:N	2.49	0.45
1:A:350:GLN:C	1:A:352:LEU:H	2.25	0.45
1:C:214:HIS:H	2:F:7:HIS:HE1	1.65	0.45
1:B:8:ASN:HB3	1:B:29:GLY:HA3	1.99	0.45
2:E:47:ALA:HA	2:E:64:LEU:HD21	1.98	0.45
1:A:190:CYS:HA	1:A:291:CYS:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:THR:HB	1:C:295:MET:HB2	1.97	0.45
1:B:331:GLN:HA	1:B:372:SER:O	2.16	0.45
2:F:47:ALA:HA	2:F:64:LEU:HD21	1.98	0.45
1:C:480:LYS:O	1:C:485:SER:OG	2.32	0.45
1:C:493:GLY:O	1:C:497:PHE:CB	2.65	0.45
3:H:6:GLN:C	3:H:124:GLN:HE22	2.14	0.45
3:H:34:ILE:HG13	3:H:79:VAL:HG21	1.98	0.45
3:J:34:ILE:HG13	3:J:79:VAL:HG21	1.98	0.45
1:C:55:GLU:HG2	1:C:128:LYS:HG2	1.99	0.45
1:C:207:ASN:OD1	1:C:207:ASN:N	2.47	0.45
3:H:9:PRO:HB3	3:H:127:LEU:HB3	1.98	0.45
3:H:67:ARG:NH2	3:H:90:ASP:OD2	2.50	0.45
3:H:99:GLY:CA	3:H:117:TRP:O	2.64	0.45
4:L:6:GLN:NE2	4:L:86:TYR:O	2.38	0.45
1:C:365:ILE:HD12	1:C:372:SER:HB2	2.00	0.45
1:B:98:ASP:O	1:B:110:LYS:N	2.45	0.45
3:H:60:SER:OG	3:H:61:ALA:N	2.49	0.45
1:A:315:THR:OG1	1:A:329:GLU:OE1	2.35	0.44
1:B:331:GLN:HA	1:B:373:LYS:HA	1.99	0.44
1:A:189:ASP:HB2	1:A:292:ARG:HB2	1.99	0.44
1:C:463:PHE:CD2	1:C:463:PHE:O	2.70	0.44
1:C:494:VAL:HA	1:C:497:PHE:HB3	1.98	0.44
1:B:73:ARG:HH21	1:B:77:GLN:HB2	1.81	0.44
1:B:100:GLY:HA2	1:B:108:PHE:HB2	1.97	0.44
1:A:201:LEU:HA	1:A:213:VAL:O	2.18	0.44
3:G:119:PHE:HA	3:G:122:TRP:HE1	1.83	0.44
3:G:6:GLN:O	3:G:124:GLN:NE2	2.50	0.44
3:J:48:MET:HE2	3:J:68:ILE:HD12	2.00	0.44
2:D:31:ARG:HG3	2:F:4:LEU:HB2	2.00	0.44
4:I:33:LEU:CA	4:I:91:PHE:HE2	2.31	0.44
1:A:327:THR:HA	1:A:376:LEU:O	2.18	0.44
1:A:345:MET:HG2	1:A:380:PRO:HA	2.00	0.44
1:C:225:TRP:HB2	1:C:237:ASN:HB3	2.00	0.44
4:K:2:ILE:CB	4:K:90:GLN:OE1	2.66	0.44
1:A:89:GLN:CD	1:A:233:THR:HG22	2.38	0.44
1:A:230:ASP:OD1	3:G:62:GLN:NE2	2.51	0.44
3:G:97:ALA:CB	3:G:122:TRP:CE2	3.01	0.44
4:L:18:ARG:HA	4:L:75:ILE:O	2.18	0.44
1:A:302:GLY:C	1:A:362:ASN:HD21	2.26	0.44
1:B:477:LEU:O	1:B:479:THR:N	2.50	0.44
3:J:33:TYR:O	3:J:98:ARG:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:PRO:HG2	1:C:398:HIS:NE2	2.33	0.43
3:G:118:TRP:NE1	4:I:89:GLN:OE1	2.47	0.43
4:K:18:ARG:HA	4:K:75:ILE:O	2.18	0.43
1:C:315:THR:HG1	1:C:316:LYS:H	1.62	0.43
1:C:463:PHE:O	1:C:463:PHE:CG	2.70	0.43
1:B:365:ILE:HG22	1:B:367:GLU:H	1.83	0.43
3:G:95:TYR:HB3	3:G:122:TRP:CZ3	2.52	0.43
1:A:78:GLY:HA2	1:B:56:VAL:HG23	2.01	0.43
1:A:101:TRP:CD1	1:A:108:PHE:CZ	3.06	0.43
1:A:348:ASP:OD1	1:A:348:ASP:N	2.52	0.43
1:C:488:CYS:SG	1:C:489:LEU:N	2.91	0.43
1:B:35:ALA:HB3	1:B:38:LYS:HB2	1.99	0.43
1:B:148:HIS:HA	1:B:375:MET:HG2	2.00	0.43
1:A:237:ASN:O	1:A:239:LYS:HG2	2.18	0.43
4:L:2:ILE:HG22	4:L:2:ILE:O	2.19	0.43
1:A:300:LEU:HD23	1:A:362:ASN:HB2	2.00	0.43
3:G:32:ASN:CG	3:G:98:ARG:HD2	2.43	0.43
3:H:32:ASN:ND2	3:H:98:ARG:HD2	2.34	0.43
3:G:48:MET:HE2	3:G:68:ILE:HD12	2.00	0.43
4:L:2:ILE:CB	4:L:90:GLN:OE1	2.66	0.43
1:A:61:TYR:CZ	1:A:206:MET:SD	3.12	0.43
1:A:158:HIS:CD2	1:A:164:ARG:HG3	2.53	0.43
1:B:27:HIS:HB3	1:B:286:SER:HA	2.01	0.43
1:A:149:SER:O	3:J:112:ARG:NH2	2.51	0.43
1:A:350:GLN:C	1:A:352:LEU:N	2.77	0.43
1:C:15:MET:SD	1:C:38:LYS:NZ	2.78	0.43
1:C:371:ASN:OD1	1:C:371:ASN:N	2.49	0.43
3:H:48:MET:HE2	3:H:68:ILE:HD12	2.00	0.43
1:C:41:VAL:HB	1:C:143:VAL:HG22	2.00	0.42
1:C:491:LEU:HA	1:C:494:VAL:HG12	2.01	0.42
1:A:232:GLY:N	3:G:66:GLY:N	2.67	0.42
1:C:127:GLY:HA3	1:C:218:PHE:CZ	2.55	0.42
4:I:18:ARG:HA	4:I:75:ILE:O	2.18	0.42
1:C:420:ARG:HB3	1:C:428:ALA:HB1	2.00	0.42
3:G:27:TYR:CE2	3:G:98:ARG:HD3	2.52	0.42
1:C:226:HIS:HB2	1:C:236:TRP:CZ3	2.55	0.42
1:A:52:ASN:O	1:A:134:ASN:ND2	2.53	0.42
1:A:385:SER:OG	1:A:386:TYR:N	2.52	0.42
1:C:260:SER:OG	1:C:262:GLU:OE1	2.32	0.42
1:C:341:VAL:HB	1:C:374:MET:HE1	2.01	0.42
1:B:91:VAL:HB	1:B:239:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:43:ALA:HA	4:L:44:PRO:HD3	1.91	0.42
1:A:10:ASP:O	1:A:31:VAL:HA	2.19	0.42
2:F:24:GLU:HG2	2:F:27:LYS:HE2	2.02	0.42
3:H:117:TRP:CD2	3:H:117:TRP:N	2.88	0.42
1:C:31:VAL:O	1:C:42:ASP:HA	2.19	0.42
3:J:119:PHE:CG	4:K:46:LEU:HD13	2.54	0.42
1:A:204:LEU:O	1:A:210:HIS:HA	2.19	0.42
1:C:7:SER:HB2	1:C:322:LEU:HD11	2.01	0.42
1:B:247:ASP:OD1	1:B:247:ASP:N	2.46	0.42
3:J:131:SER:OG	3:J:132:SER:N	2.53	0.42
1:C:59:TYR:HD1	1:C:223:LEU:HB2	1.85	0.42
1:B:230:ASP:OD2	1:B:231:THR:OG1	2.38	0.42
3:G:98:ARG:HB3	3:G:99:GLY:H	1.59	0.42
3:G:131:SER:OG	3:G:132:SER:N	2.53	0.42
3:J:31:SER:O	3:J:102:ALA:HB3	2.20	0.42
4:K:20:THR:HA	4:K:73:PHE:O	2.20	0.42
2:D:74:TYR:CD1	2:F:28:HIS:HB3	2.55	0.42
1:B:463:PHE:HD2	2:E:28:HIS:HB2	1.85	0.42
3:H:99:GLY:C	3:H:117:TRP:O	2.62	0.42
3:H:131:SER:OG	3:H:132:SER:N	2.53	0.42
1:A:312:PHE:HB3	1:A:396:ILE:HD12	2.01	0.41
1:B:126:THR:HB	1:B:205:THR:HB	2.02	0.41
1:B:376:LEU:H	1:B:376:LEU:HG	1.67	0.41
4:L:20:THR:HA	4:L:73:PHE:O	2.20	0.41
2:D:74:TYR:HE2	2:F:69:LEU:HG	1.26	0.41
3:J:37:VAL:HG22	3:J:47:TRP:HA	2.02	0.41
1:A:65:ILE:HG23	1:A:117:ALA:HB1	2.01	0.41
1:A:472:LEU:HD23	1:A:475:LEU:HD12	2.01	0.41
1:C:201:LEU:HD23	1:C:212:LEU:HB3	2.01	0.41
1:C:256:VAL:HG12	1:C:258:LEU:H	1.84	0.41
1:B:237:ASN:O	1:B:239:LYS:N	2.54	0.41
1:B:265:VAL:O	1:B:269:LEU:HB2	2.19	0.41
1:B:369:THR:OG1	1:B:370:GLU:N	2.52	0.41
3:H:4:LEU:O	3:H:123:GLY:N	2.53	0.41
1:A:93:LYS:CB	1:A:245:PHE:HD2	2.32	0.41
1:A:461:SER:OG	1:A:462:TRP:N	2.54	0.41
2:D:24:GLU:HG2	2:D:27:LYS:HE2	2.02	0.41
2:D:28:HIS:CB	2:F:74:TYR:HE1	2.31	0.41
1:B:26:GLU:OE1	2:E:15:ARG:NH1	2.53	0.41
2:F:4:LEU:HG	2:F:5:PRO:HD3	2.02	0.41
3:H:102:ALA:O	3:H:103:LEU:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:98:ARG:HE	3:J:121:PRO:HG2	1.84	0.41
1:A:351:THR:C	1:A:353:THR:H	2.28	0.41
2:D:4:LEU:HG	2:D:5:PRO:HD3	2.02	0.41
2:D:69:LEU:HB3	2:F:74:TYR:HD2	1.85	0.41
2:E:24:GLU:HG2	2:E:27:LYS:HE2	2.02	0.41
4:I:19:VAL:HG12	4:I:75:ILE:HB	2.02	0.41
1:A:190:CYS:HB3	1:A:289:LEU:HD11	2.03	0.41
1:A:217:TRP:CZ3	1:A:221:ILE:HD11	2.56	0.41
1:C:97:VAL:O	1:C:110:LYS:HA	2.20	0.41
1:C:190:CYS:HA	1:C:291:CYS:HA	2.01	0.41
3:G:38:ARG:HH22	3:G:90:ASP:HA	1.86	0.41
4:L:2:ILE:HG21	4:L:90:GLN:CD	2.42	0.41
4:K:19:VAL:HG12	4:K:75:ILE:HB	2.02	0.41
1:A:98:ASP:N	1:A:98:ASP:OD1	2.54	0.41
4:I:20:THR:HA	4:I:73:PHE:O	2.20	0.41
4:I:33:LEU:N	4:I:91:PHE:CE2	2.88	0.41
3:H:122:TRP:CZ2	4:L:36:TYR:HE1	2.38	0.41
2:E:4:LEU:HG	2:E:5:PRO:HD3	2.02	0.41
3:G:101:ARG:C	3:G:101:ARG:CG	2.94	0.41
4:I:7:SER:HA	4:I:8:PRO:HA	1.90	0.41
3:H:116:SER:CB	3:H:120:ASP:HB2	2.50	0.41
3:H:117:TRP:CH2	4:L:48:ILE:O	2.74	0.41
1:A:11:PHE:CA	1:A:32:THR:O	2.62	0.41
1:A:167:VAL:HG11	1:A:188:LEU:HD11	2.03	0.41
1:A:244:GLU:HG3	2:F:20:LEU:HD23	2.03	0.41
1:C:94:ARG:CA	1:C:114:VAL:HB	2.35	0.41
1:B:151:MET:O	1:B:153:VAL:N	2.50	0.41
1:B:204:LEU:O	1:B:210:HIS:HA	2.21	0.41
4:L:7:SER:HA	4:L:8:PRO:HA	1.90	0.41
3:J:38:ARG:HH22	3:J:90:ASP:HA	1.86	0.41
3:J:39:GLN:HB2	3:J:45:LEU:HD23	2.03	0.41
1:C:214:HIS:H	2:F:7:HIS:CE1	2.39	0.41
3:G:36:TRP:HA	3:G:95:TYR:O	2.21	0.41
4:L:21:PHE:HZ	4:L:104:LEU:HD11	1.86	0.41
4:L:37:GLN:HB3	4:L:47:LEU:HD11	2.03	0.41
3:G:39:GLN:HB2	3:G:45:LEU:HD23	2.03	0.40
3:H:38:ARG:HH22	3:H:90:ASP:HA	1.86	0.40
2:D:69:LEU:CB	2:F:74:TYR:HD2	2.33	0.40
1:B:6:VAL:HG23	1:B:8:ASN:H	1.85	0.40
3:H:116:SER:HB3	3:H:120:ASP:HB2	2.03	0.40
4:K:21:PHE:HZ	4:K:104:LEU:HD11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASP:C	1:A:99:ARG:CG	2.91	0.40
1:A:101:TRP:H	1:A:101:TRP:HD1	1.69	0.40
1:C:59:TYR:CD1	1:C:223:LEU:HB2	2.56	0.40
4:I:39:LYS:HA	4:I:40:PRO:HD3	1.96	0.40
4:L:16:GLY:N	4:L:78:LEU:O	2.51	0.40
4:L:19:VAL:HG12	4:L:75:ILE:HB	2.02	0.40
1:A:91:VAL:HG11	1:A:243:VAL:HG21	2.03	0.40
1:A:345:MET:HB3	1:A:356:GLY:HA3	2.03	0.40
1:C:214:HIS:NE2	1:C:216:GLU:OE1	2.55	0.40
1:C:265:VAL:O	1:C:269:LEU:HD12	2.22	0.40
3:J:33:TYR:OH	3:J:108:TYR:CE2	2.73	0.40
4:K:11:LEU:HD12	4:K:21:PHE:HE1	1.87	0.40
1:A:175:ARG:HA	1:A:189:ASP:HA	2.04	0.40
1:C:43:ILE:HD13	1:C:293:LEU:HD21	2.04	0.40
1:B:39:PRO:HG3	1:B:300:LEU:HG	2.03	0.40
1:B:261:GLN:HE22	2:E:1:ALA:HB1	1.86	0.40
4:I:2:ILE:CD1	4:I:27:GLN:HB2	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/504 (100%)	413 (82%)	74 (15%)	15 (3%)	3	25
1	B	502/504 (100%)	392 (78%)	98 (20%)	12 (2%)	4	29
1	C	502/504 (100%)	417 (83%)	78 (16%)	7 (1%)	9	37
2	D	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
2	E	73/75 (97%)	65 (89%)	8 (11%)	0	100	100
2	F	73/75 (97%)	65 (89%)	8 (11%)	0	100	100
3	G	130/132 (98%)	112 (86%)	14 (11%)	4 (3%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	130/132 (98%)	109 (84%)	14 (11%)	7 (5%)	1	16
3	J	130/132 (98%)	113 (87%)	13 (10%)	4 (3%)	3	25
4	I	105/107 (98%)	93 (89%)	11 (10%)	1 (1%)	12	43
4	K	105/107 (98%)	92 (88%)	11 (10%)	2 (2%)	6	32
4	L	105/107 (98%)	91 (87%)	12 (11%)	2 (2%)	6	32
All	All	2430/2454 (99%)	2028 (84%)	348 (14%)	54 (2%)	7	30

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	ALA
1	A	233	THR
1	A	237	ASN
1	A	238	ASN
1	A	239	LYS
1	A	352	LEU
1	C	68	MET
1	C	239	LYS
1	B	152	ILE
1	B	230	ASP
1	B	478	ASN
3	G	118	TRP
3	H	44	GLY
3	H	103	LEU
3	H	104	PHE
4	L	94	LEU
4	L	95	PRO
3	J	101	ARG
3	J	107	SER
1	A	68	MET
1	A	107	LEU
1	A	371	ASN
1	C	252	ARG
1	C	280	ALA
1	B	59	TYR
1	B	238	ASN
1	B	480	LYS
1	B	502	VAL
3	G	98	ARG
3	H	123	GLY

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Mol	Chain	Res	Type
3	J	106	ASP
4	K	2	ILE
1	C	69	ALA
1	B	46	VAL
3	G	122	TRP
3	H	106	ASP
3	H	118	TRP
3	H	120	ASP
1	A	368	SER
1	C	349	MET
3	J	108	TYR
1	A	57	ARG
1	A	232	GLY
1	C	243	VAL
1	B	103	ASN
1	A	228	GLY
1	B	151	MET
1	B	155	ASP
1	B	208	ASN
1	A	318	PRO
3	G	120	ASP
4	I	95	PRO
4	K	95	PRO
1	A	317	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	407/410 (99%)	393 (97%)	14 (3%)	32	55
1	B	410/410 (100%)	401 (98%)	9 (2%)	45	63
1	C	410/410 (100%)	405 (99%)	5 (1%)	63	72
2	D	63/64 (98%)	61 (97%)	2 (3%)	34	56
2	E	64/64 (100%)	62 (97%)	2 (3%)	35	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	64/64 (100%)	62 (97%)	2 (3%)	35	57
3	G	105/109 (96%)	103 (98%)	2 (2%)	50	66
3	H	104/109 (95%)	99 (95%)	5 (5%)	23	47
3	J	105/109 (96%)	104 (99%)	1 (1%)	68	74
4	I	94/94 (100%)	92 (98%)	2 (2%)	47	64
4	K	94/94 (100%)	93 (99%)	1 (1%)	65	73
4	L	94/94 (100%)	92 (98%)	2 (2%)	47	64
All	All	2014/2031 (99%)	1967 (98%)	47 (2%)	44	63

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	56	VAL
1	A	65	ILE
1	A	103	ASN
1	A	138	ARG
1	A	188	LEU
1	A	231	THR
1	A	238	ASN
1	A	349	MET
1	A	365	ILE
1	A	396	ILE
1	A	448	ILE
1	A	465	GLN
1	A	471	LEU
1	C	25	LEU
1	C	72	SER
1	C	114	VAL
1	C	330	VAL
1	C	479	THR
2	D	2	VAL
2	D	18	THR
1	B	19	THR
1	B	91	VAL
1	B	95	THR
1	B	108	PHE
1	B	255	VAL
1	B	289	LEU
1	B	326	VAL

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Mol	Chain	Res	Type
1	B	328	VAL
1	B	376	LEU
2	E	2	VAL
2	E	18	THR
2	F	2	VAL
2	F	18	THR
3	G	71	THR
3	G	117	TRP
4	I	1	ASP
4	I	2	ILE
3	H	58	THR
3	H	71	THR
3	H	103	LEU
3	H	117	TRP
3	H	124	GLN
4	L	2	ILE
4	L	94	LEU
3	J	109	THR
4	K	2	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	163	ASN
1	A	237	ASN
1	A	266	HIS
1	A	362	ASN
1	A	446	HIS
1	A	465	GLN
1	A	481	ASN
1	C	36	GLN
1	C	85	GLN
1	C	103	ASN
1	C	134	ASN
1	C	144	HIS
1	C	147	GLN
1	C	266	HIS
1	C	323	HIS
1	C	401	HIS
2	D	17	GLN
2	D	39	ASN

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Mol	Chain	Res	Type
1	B	52	ASN
1	B	144	HIS
1	B	147	GLN
1	B	148	HIS
1	B	158	HIS
1	B	210	HIS
1	B	253	GLN
1	B	323	HIS
2	E	39	ASN
2	F	39	ASN
3	G	62	GLN
4	I	38	GLN
3	H	65	GLN
3	H	124	GLN
4	L	34	ASN
3	J	32	ASN
3	J	65	GLN
4	K	34	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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	$\# Z > 2$
5	NAG	B	601	1	14,14,15	0.46	0	17,19,21	0.54	0
5	NAG	A	601	1	14,14,15	0.74	1 (7%)	17,19,21	0.55	0
5	NAG	C	601	1	14,14,15	0.32	0	17,19,21	0.49	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	B	601	1	-	2/6/23/26	0/1/1/1
5	NAG	A	601	1	-	2/6/23/26	0/1/1/1
5	NAG	C	601	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	NAG	C1-C2	2.45	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

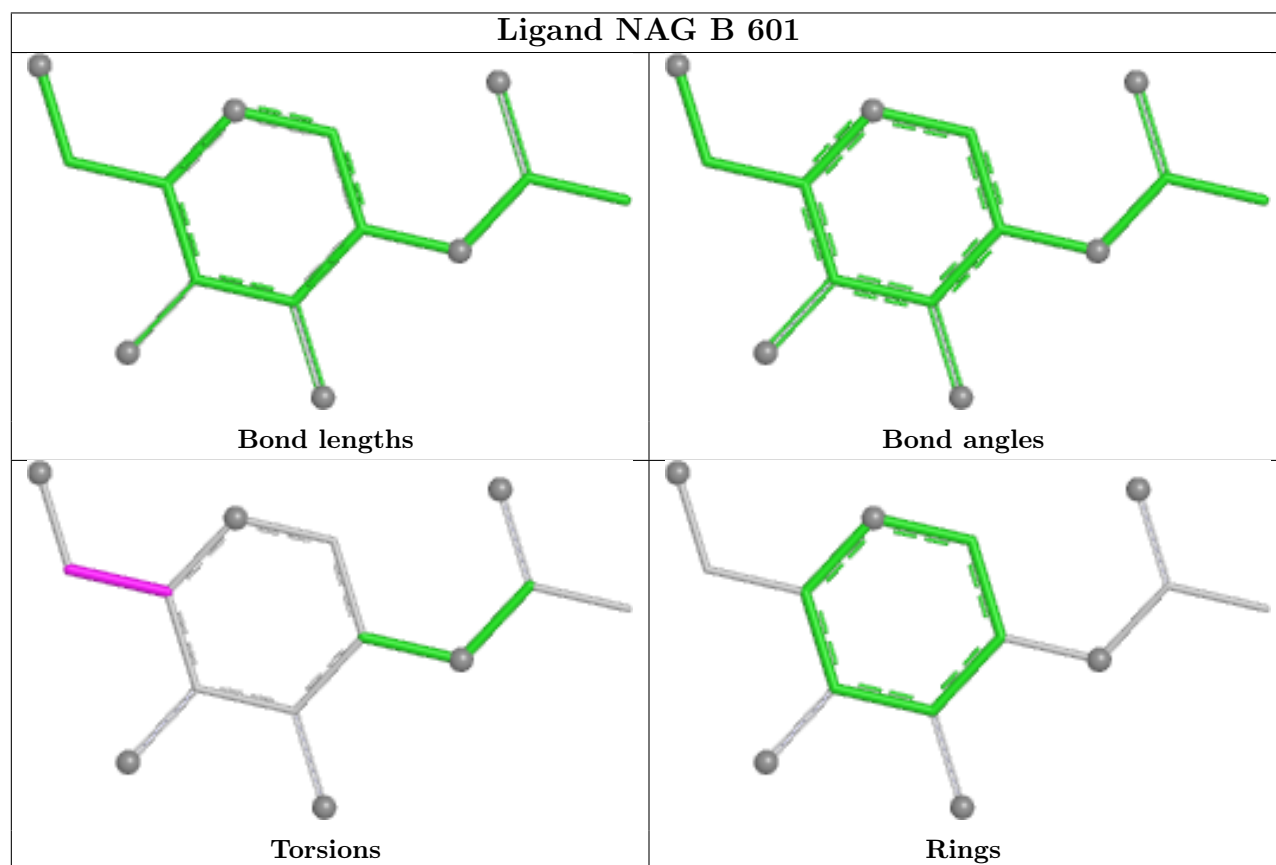
Mol	Chain	Res	Type	Atoms
5	A	601	NAG	O5-C5-C6-O6
5	B	601	NAG	O5-C5-C6-O6
5	A	601	NAG	C4-C5-C6-O6
5	B	601	NAG	C4-C5-C6-O6

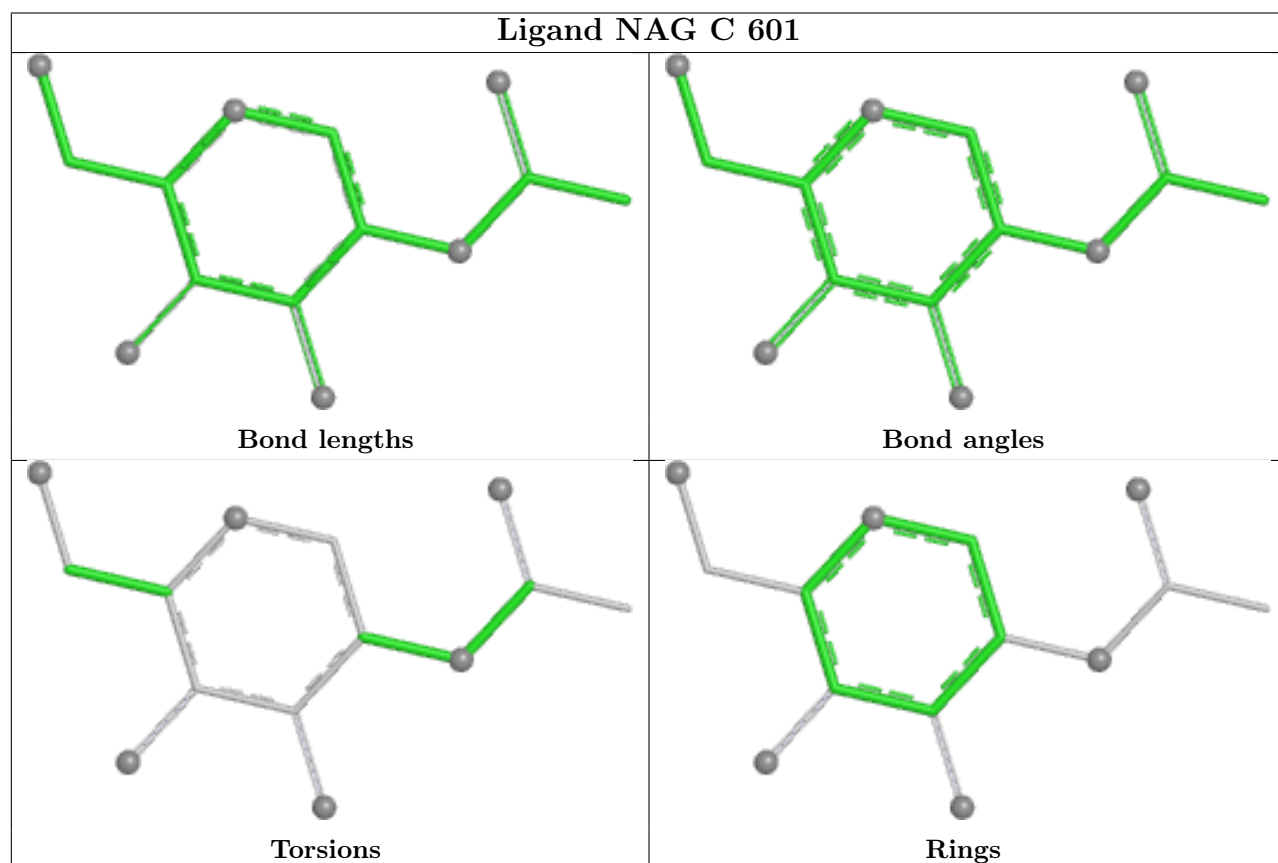
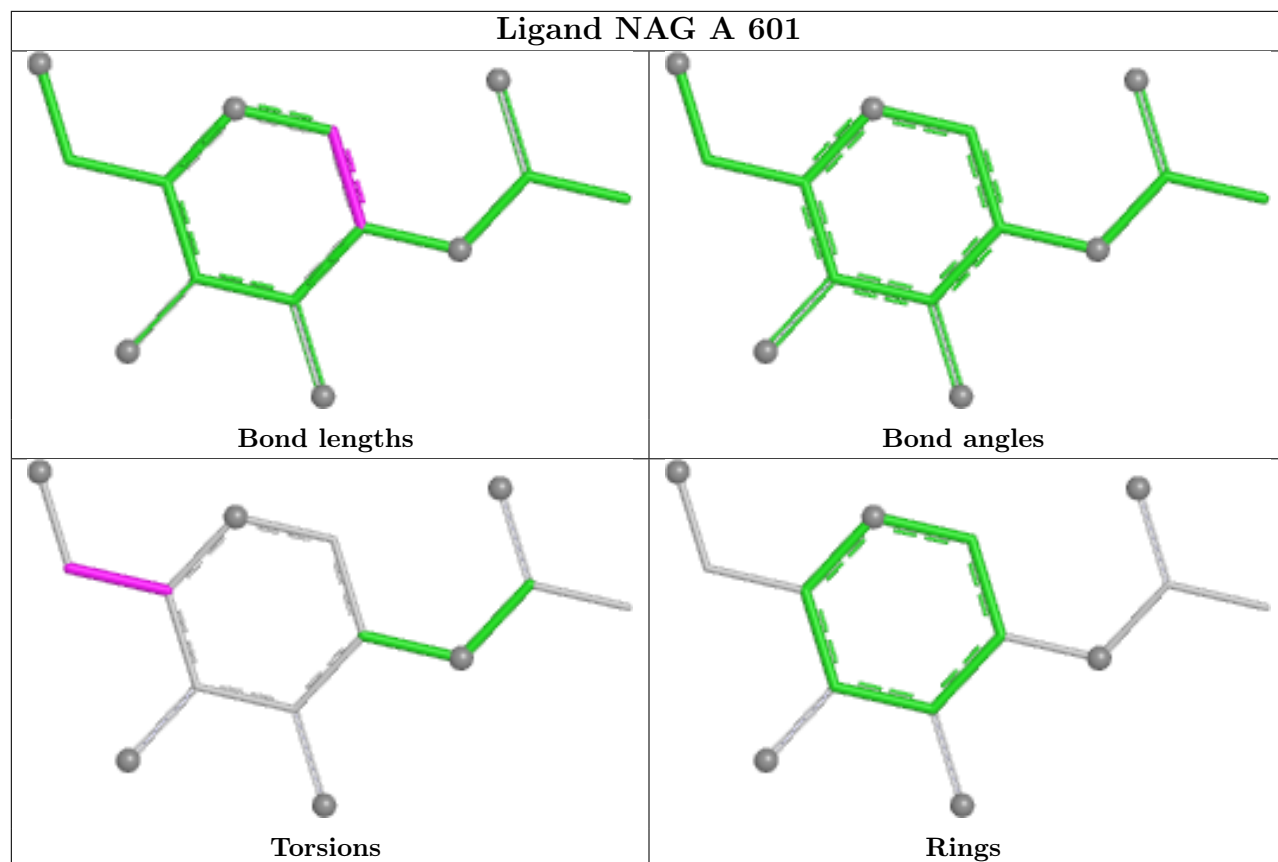
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

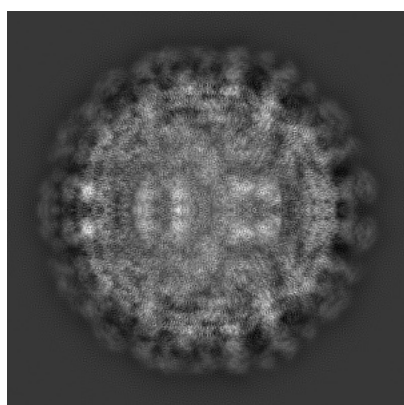
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30192. These allow visual inspection of the internal detail of the map and identification of artifacts.

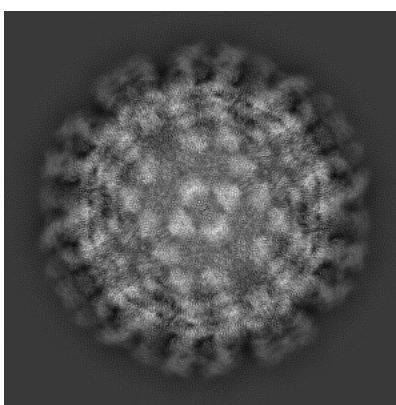
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

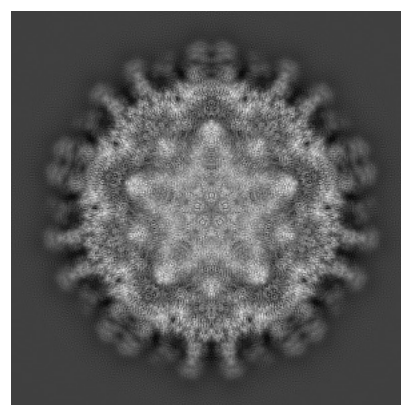
6.1.1 Primary map



X



Y

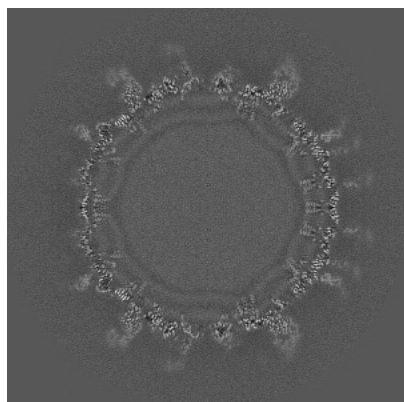


Z

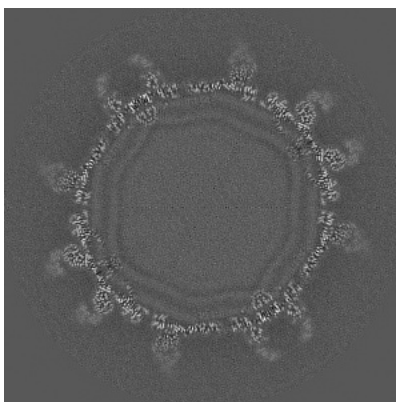
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

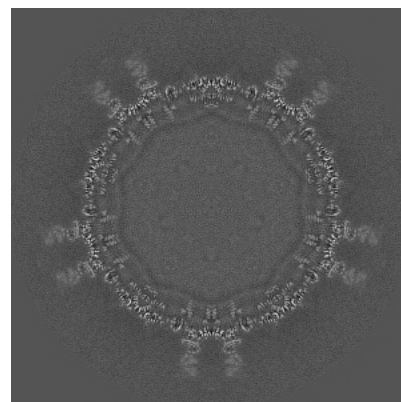
6.2.1 Primary map



X Index: 256



Y Index: 256

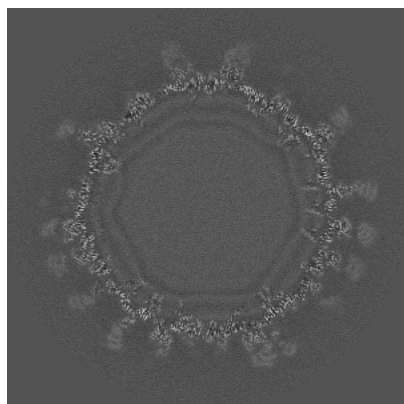


Z Index: 256

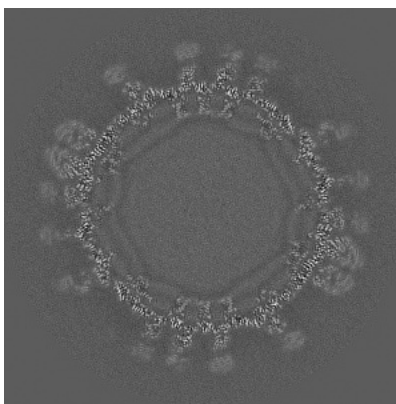
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

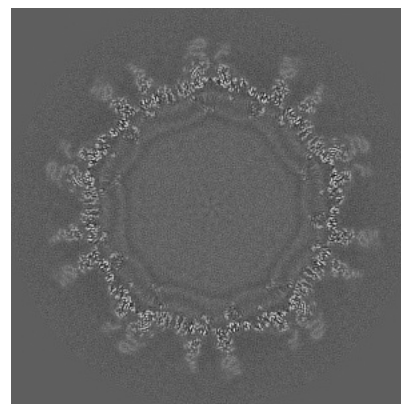
6.3.1 Primary map



X Index: 242



Y Index: 295

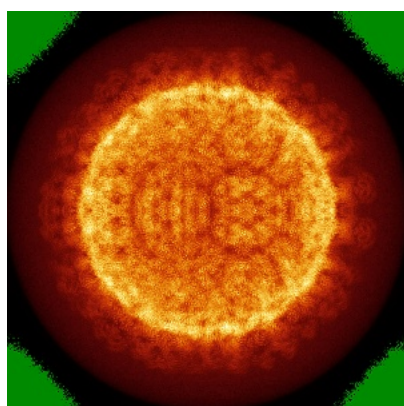


Z Index: 277

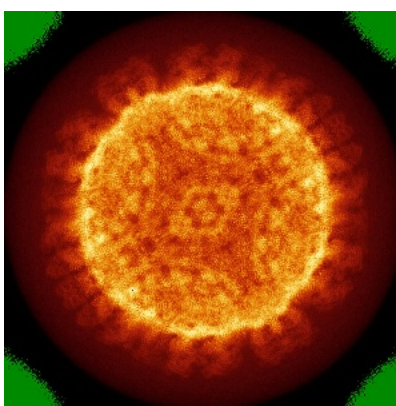
The images above show the largest variance slices of the map in three orthogonal directions.

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

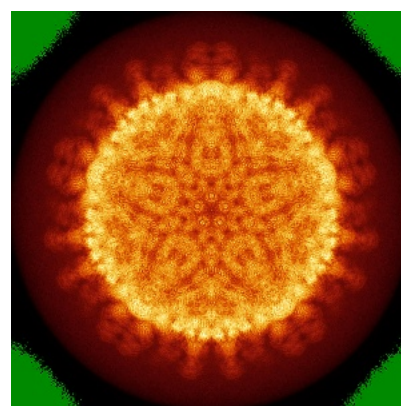
6.4.1 Primary map



X



Y

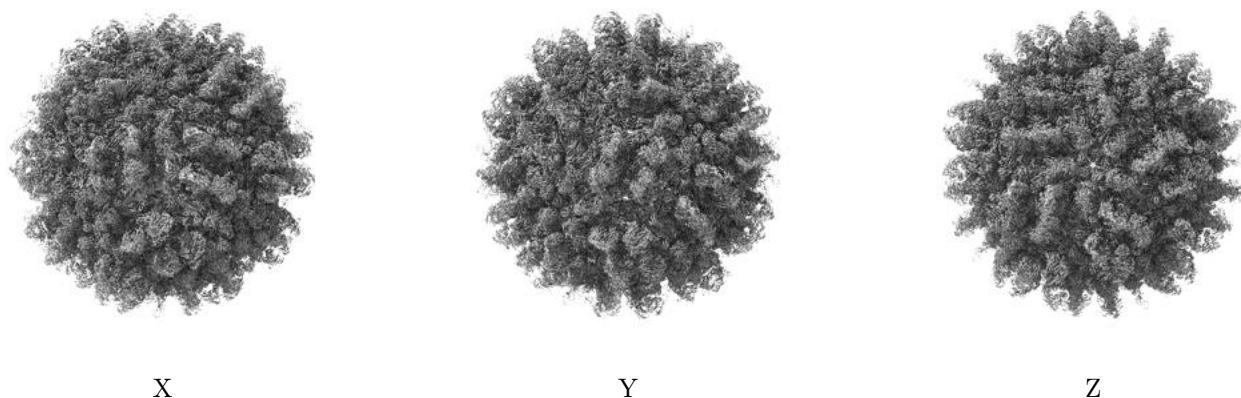


Z

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

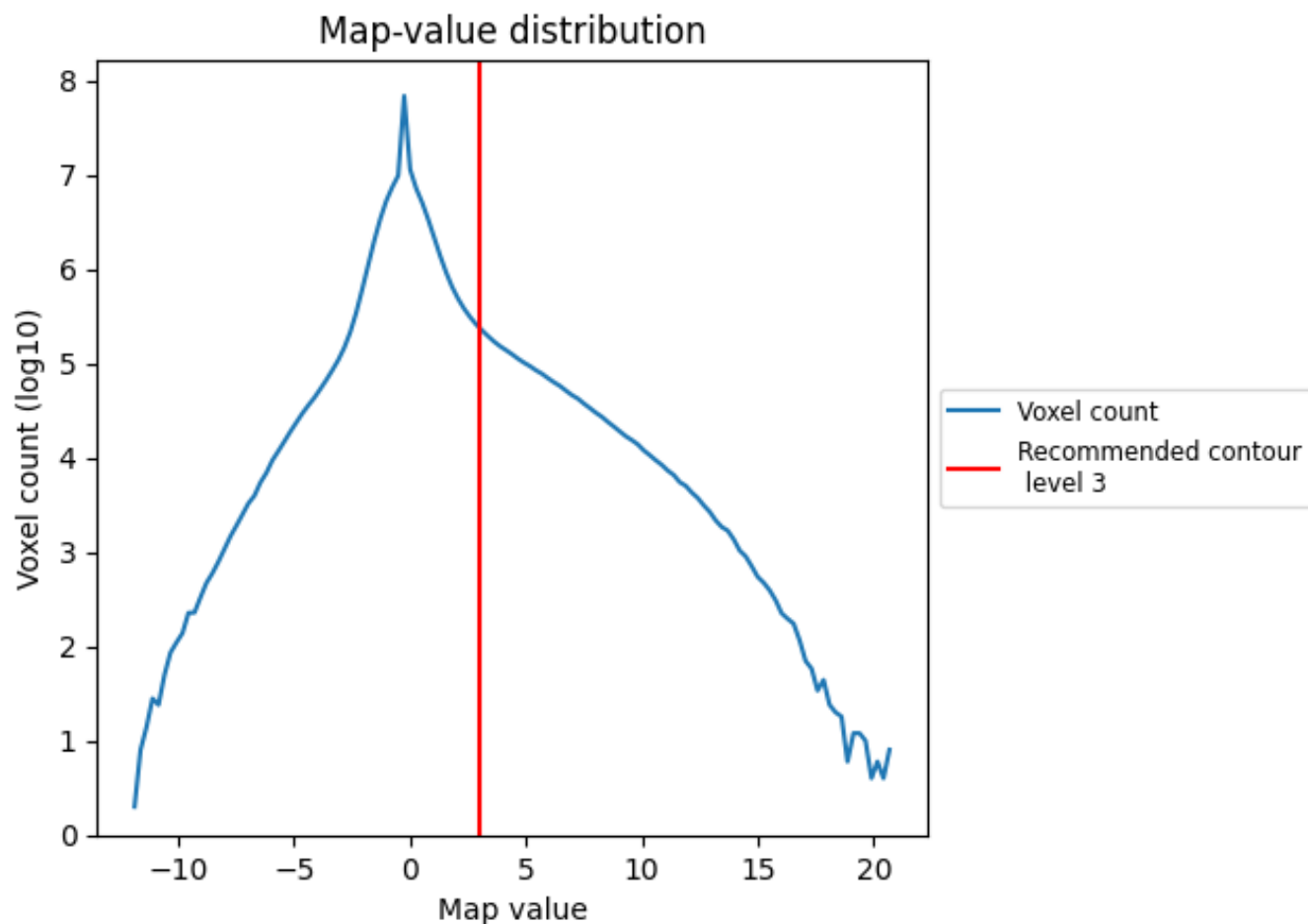
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

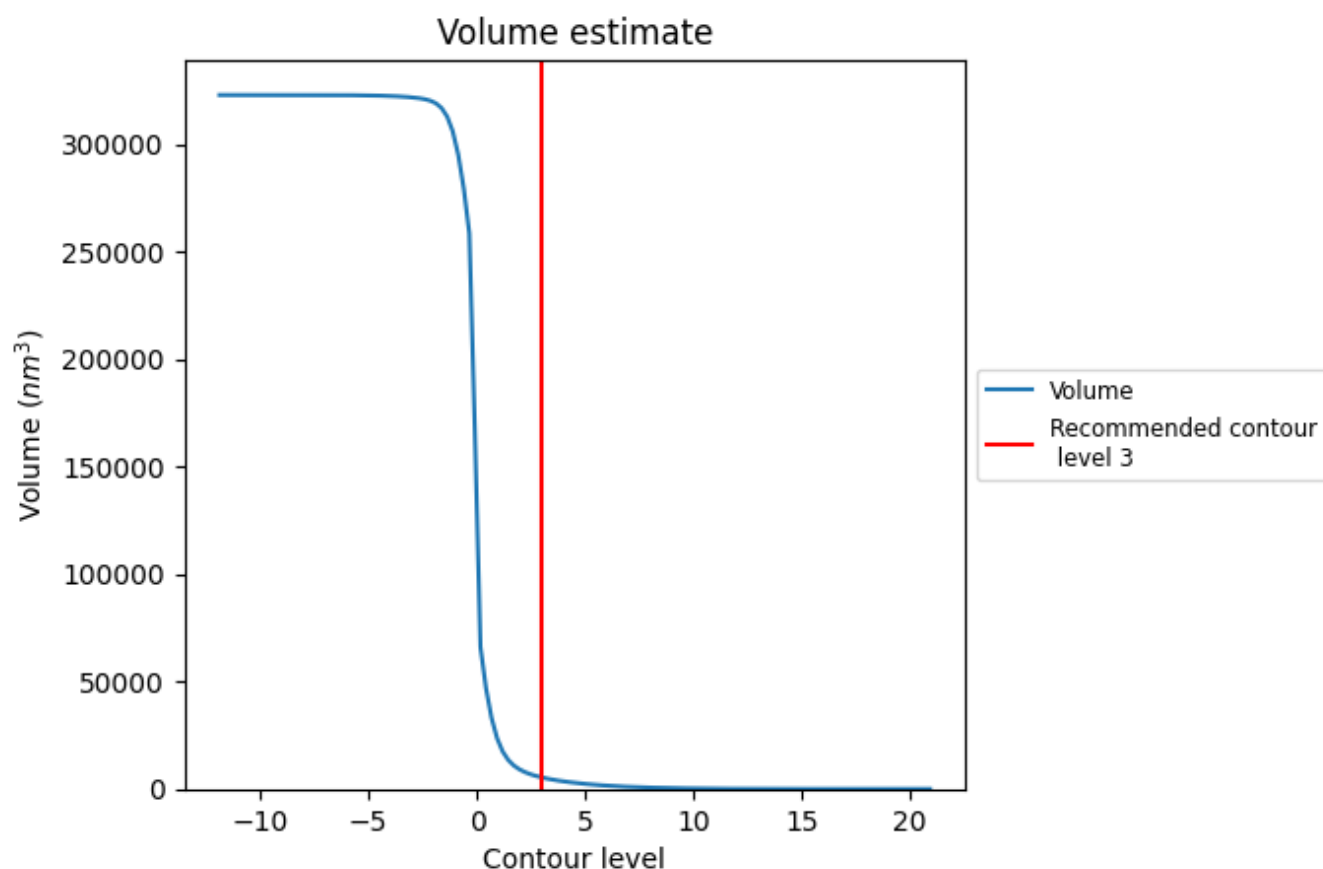
This section contains the results of statistical analysis of the map.

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.

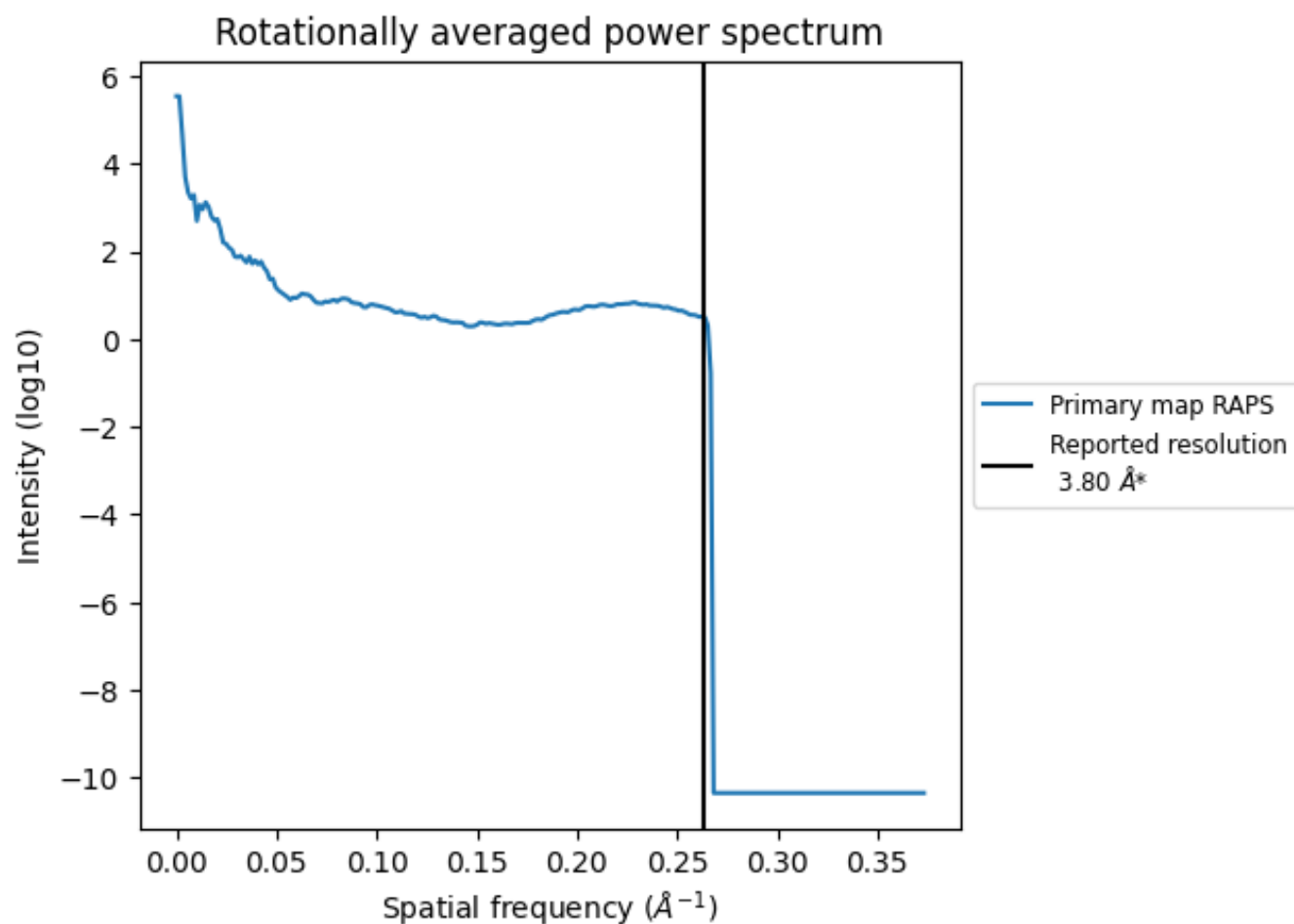
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5364 nm^3 ; this corresponds to an approximate mass of 4845 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 0.263 Å⁻¹

8 Fourier-Shell correlation

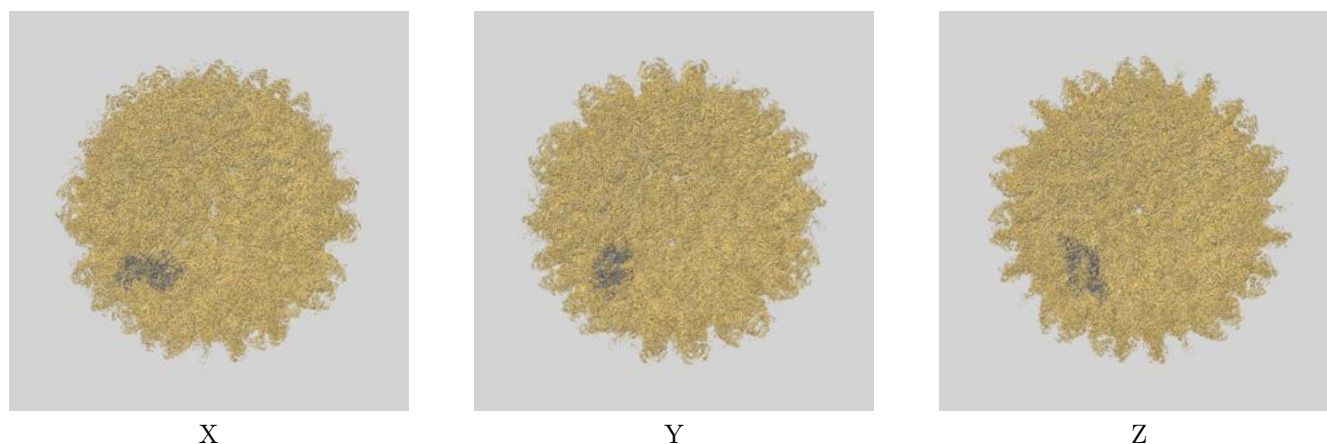
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

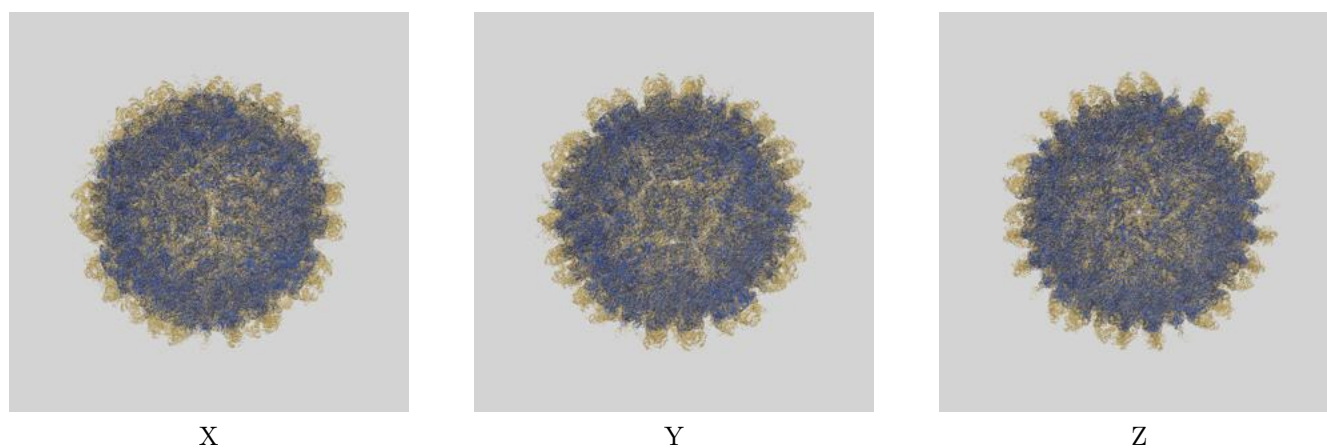
This section contains information regarding the fit between EMDB map EMD-30192 and PDB model 7BU8. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

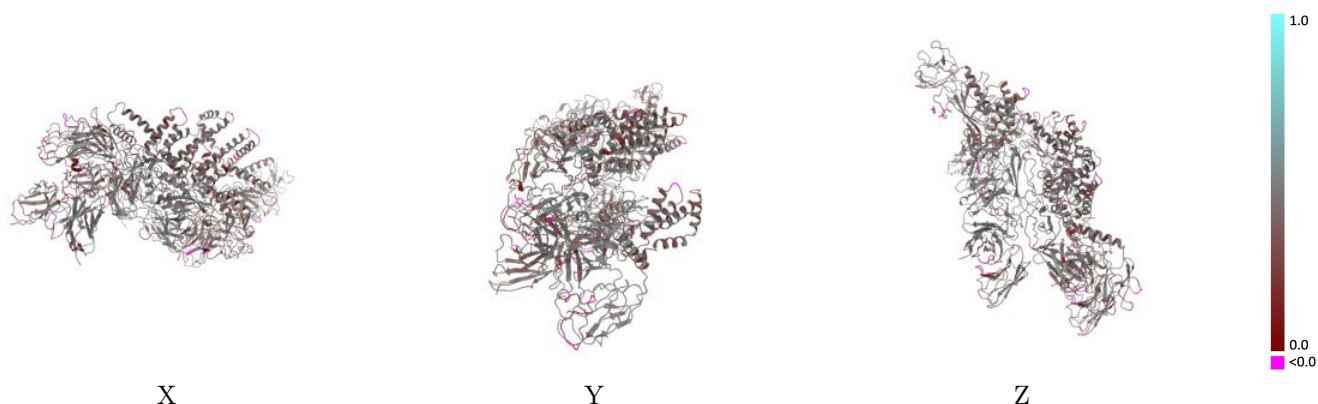


9.1.2 Map-model assembly overlay [i](#)



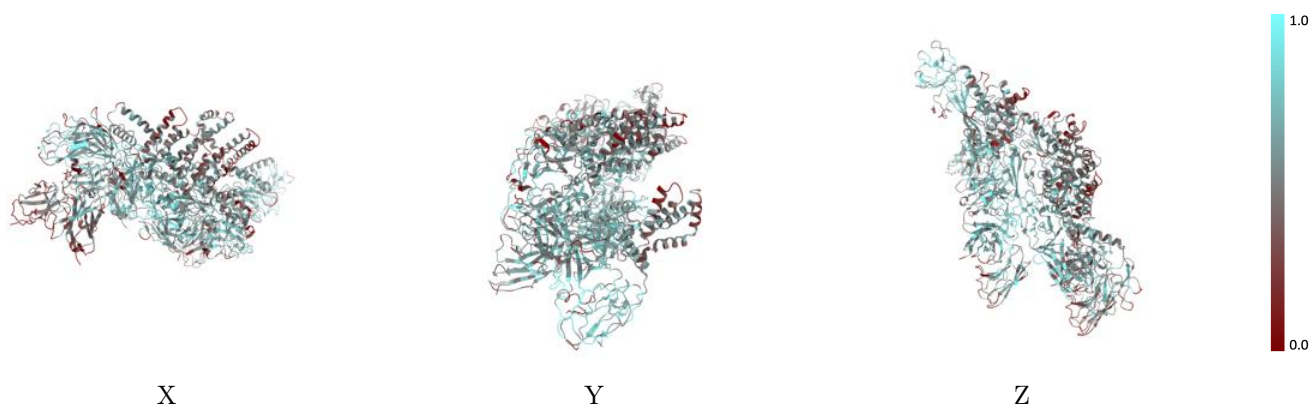
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



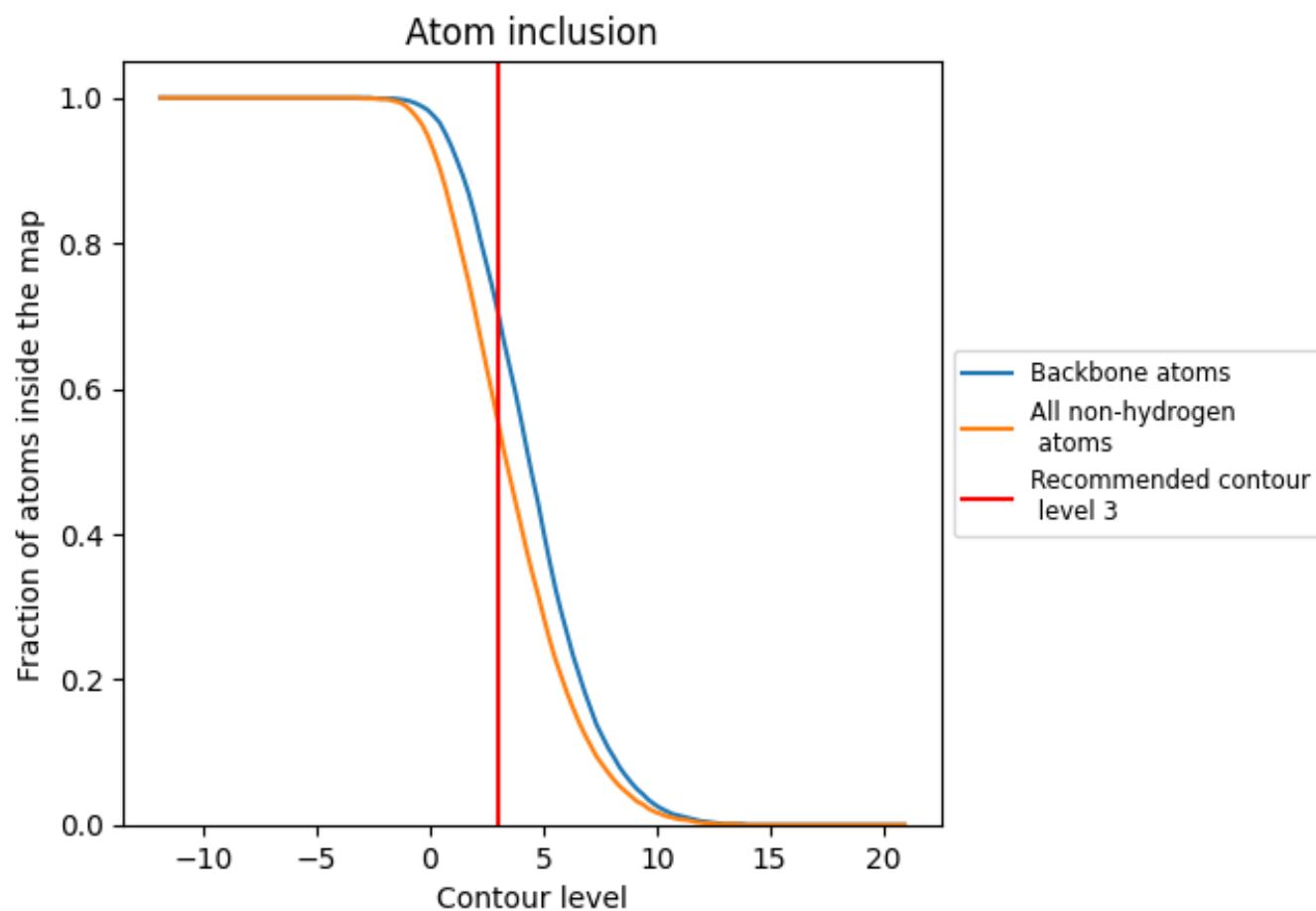
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 56% 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) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5550	0.3970
A	0.5920	0.4090
B	0.6240	0.4070
C	0.5720	0.3840
D	0.4790	0.3980
E	0.4780	0.3940
F	0.4860	0.3930
G	0.5950	0.4170
H	0.5870	0.4190
I	0.5050	0.3660
J	0.4090	0.3970
K	0.3280	0.3730
L	0.5170	0.3740

