



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 12:10 PM UTC

PDB ID : 8GWK / pdb_00008gwk
EMDB ID : EMD-34314
Title : SARS-CoV-2 RNA E-RTC complex with RMP-nsp9 and GMPPNP
Authors : Yan, L.M.; Huang, Y.C.; Ge, J.; Liu, Z.Y.; Gao, Y.; Rao, Z.H.; Lou, Z.Y.
Deposited on : 2022-09-17
Resolution : 2.72 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:

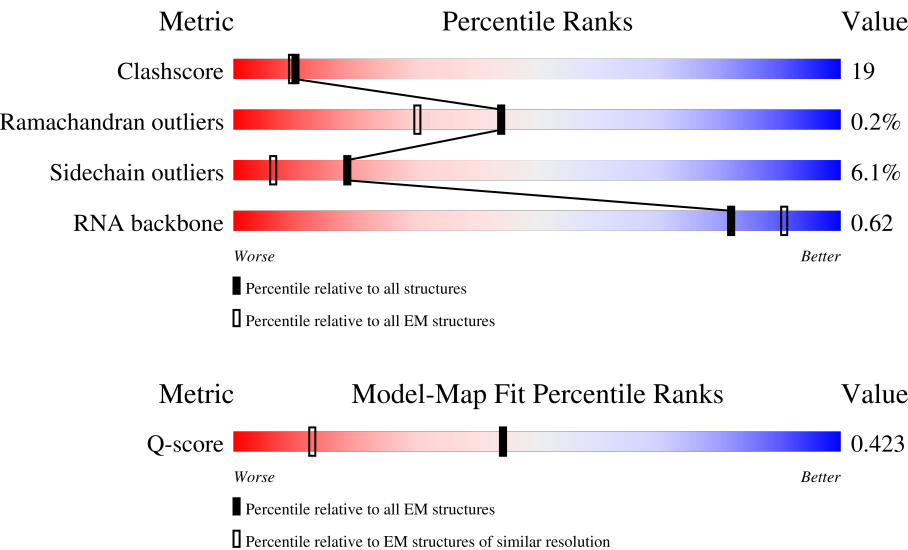
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.72 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	10355 (2.22 - 3.22)

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	932	
2	B	198	
2	D	198	

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Mol	Chain	Length	Quality of chain
3	C	83	70% 20% • 8%
4	I	25	56% 36% 8%
5	J	26	69% 31%
6	E	601	17% 46% 48% • •
6	F	601	8% 44% 51% • •
7	G	113	• 56% 37% 7%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 21949 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	931	Total	C	N	O	S	0	0
			7496	4787	1257	1398	54		

- Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	187	Total	C	N	O	S	0	0
			1400	873	241	275	11		
2	D	186	Total	C	N	O	S	0	0
			1418	892	243	272	11		

- Molecule 3 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	76	Total	C	N	O	S	0	0
			586	369	95	115	7		

- Molecule 4 is a RNA chain called primer.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	25	Total	C	N	O	P	0	0
			545	242	105	173	25		

- Molecule 5 is a RNA chain called template.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	26	Total	C	N	O	P	0	0
			545	244	92	183	26		

- Molecule 6 is a protein called Helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	585	Total	C	N	O	S	1	0
			4512	2878	751	848	35		
6	F	585	Total	C	N	O	S	1	0
			4508	2875	750	848	35		

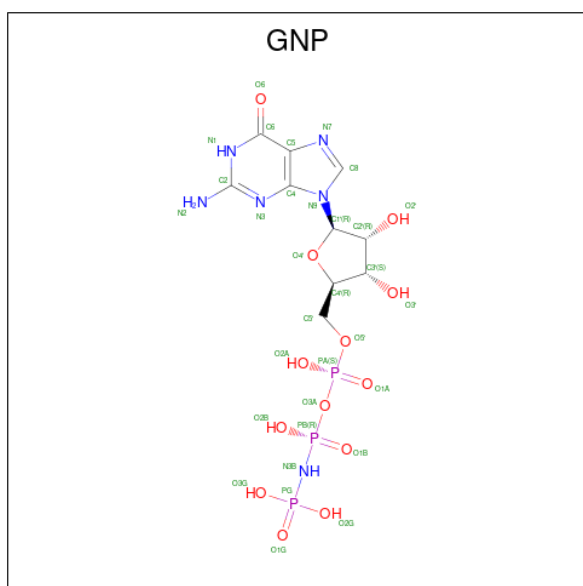
- Molecule 7 is a protein called Non-structural protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	113	Total	C	N	O	S	0	0
			868	549	150	164	5		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	A	2	Total	Zn	0
			2	2	
8	E	3	Total	Zn	0
			3	3	
8	F	3	Total	Zn	0
			3	3	

- Molecule 9 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

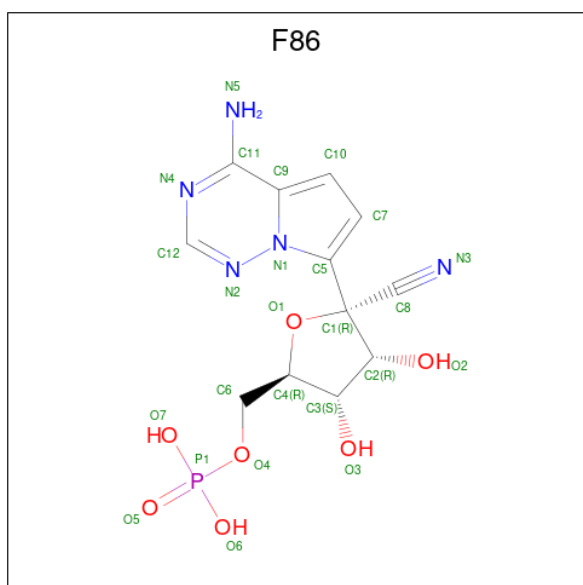


Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	

- Molecule 11 is [(2 {R},3 {S},4 {R},5 {R})-5-(4-azanylpyrrolo[2,1-f][1,2,4]triazin-7-yl)-5-cyano-3,4-bis(oxidanyl)oxolan-2-yl]methyl dihydrogen phosphate (CCD ID: F86) (formula: C₁₂H₁₄N₅O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	G	1	Total	C	N	O	P	0
			24	12	5	6	1	

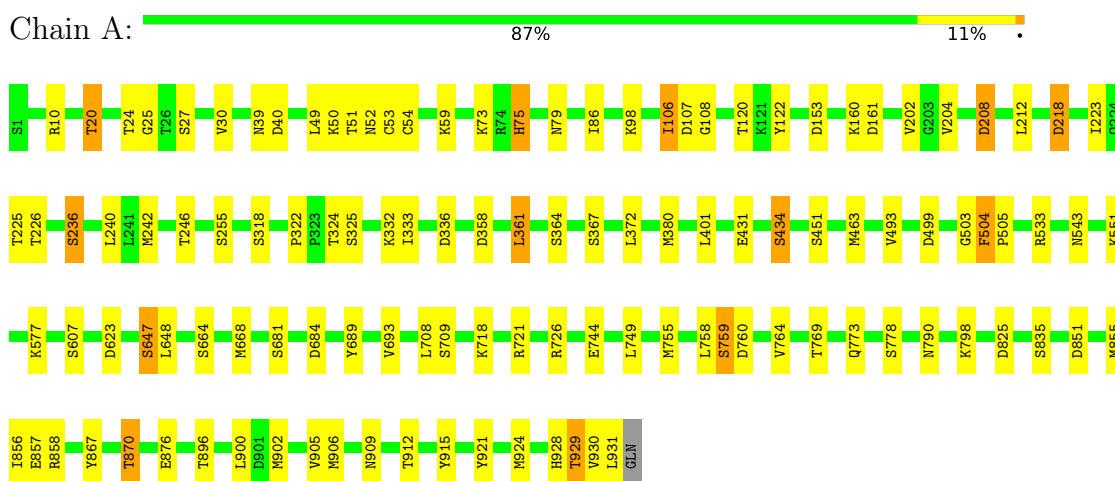
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	A	5	Total	O	0
			5	5	
12	G	1	Total	O	0
			1	1	

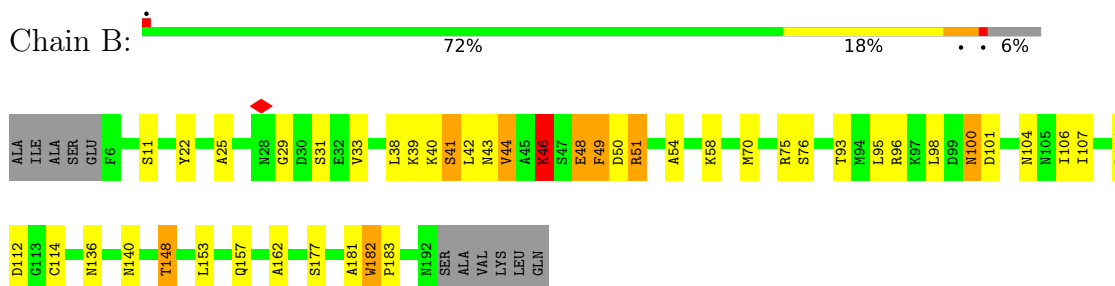
3 Residue-property plots

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.

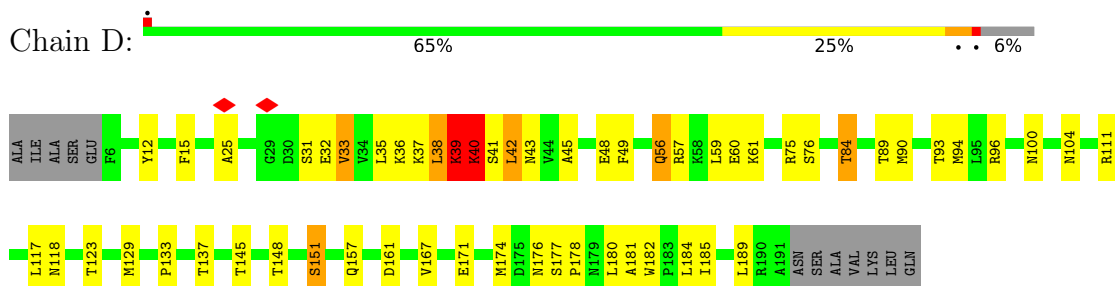
• Molecule 1: RNA-directed RNA polymerase



• Molecule 2: Non-structural protein 8



• Molecule 2: Non-structural protein 8



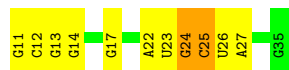
- Molecule 3: Non-structural protein 7

Chain C:  70% 20% 8%



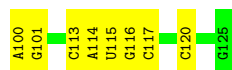
- Molecule 4: primer

Chain I:  56% 36% 8%



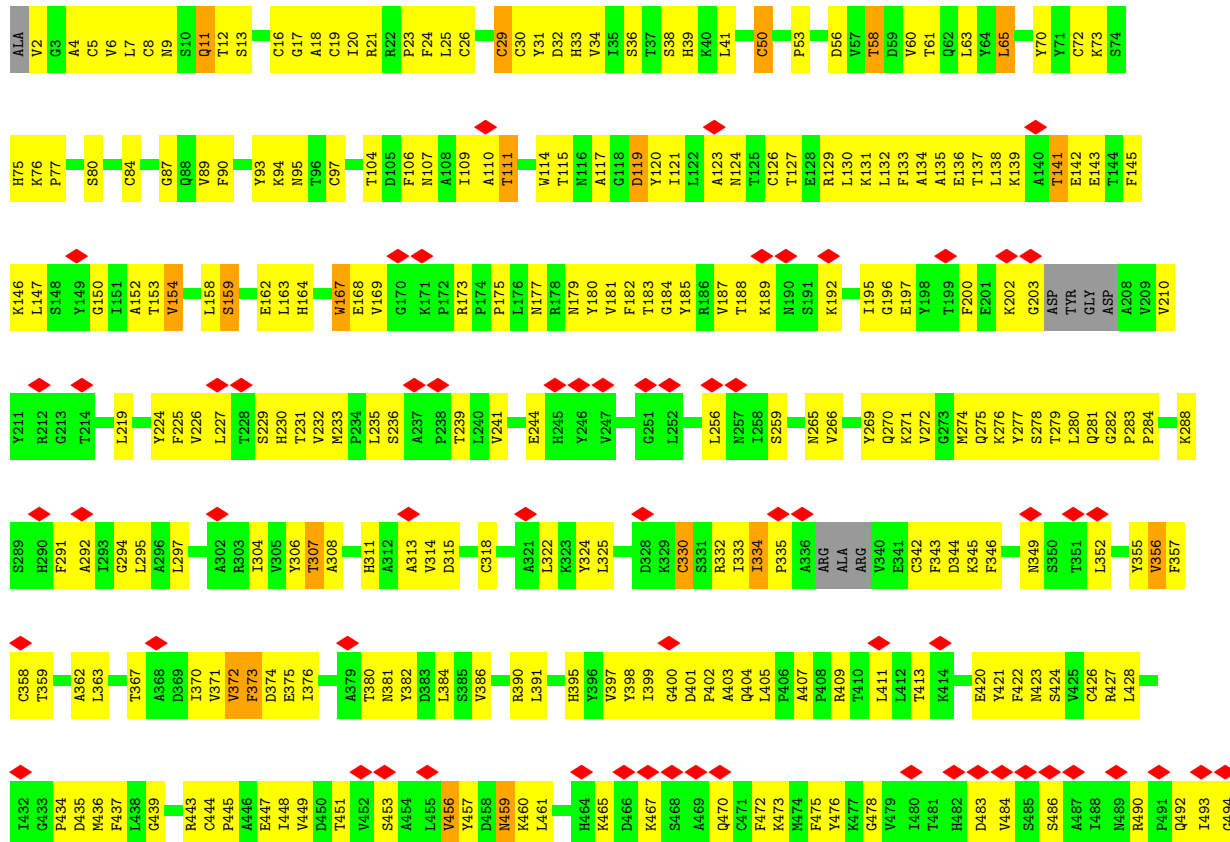
- Molecule 5: template

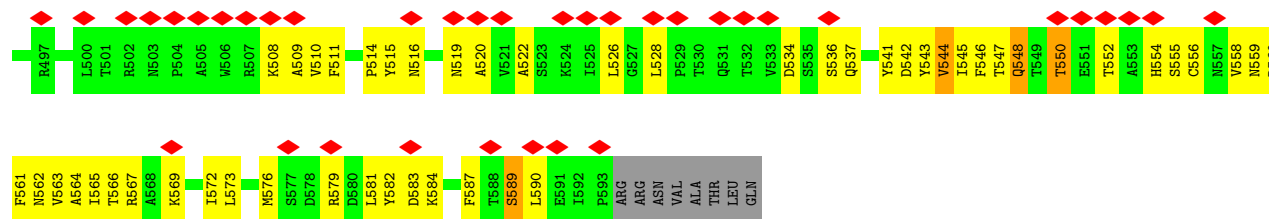
Chain J:  69% 31%



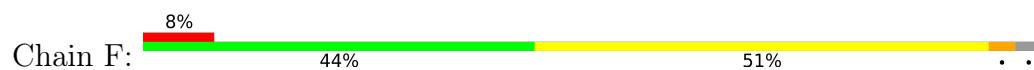
- Molecule 6: Helicase

Chain E:  17% 46% 48%

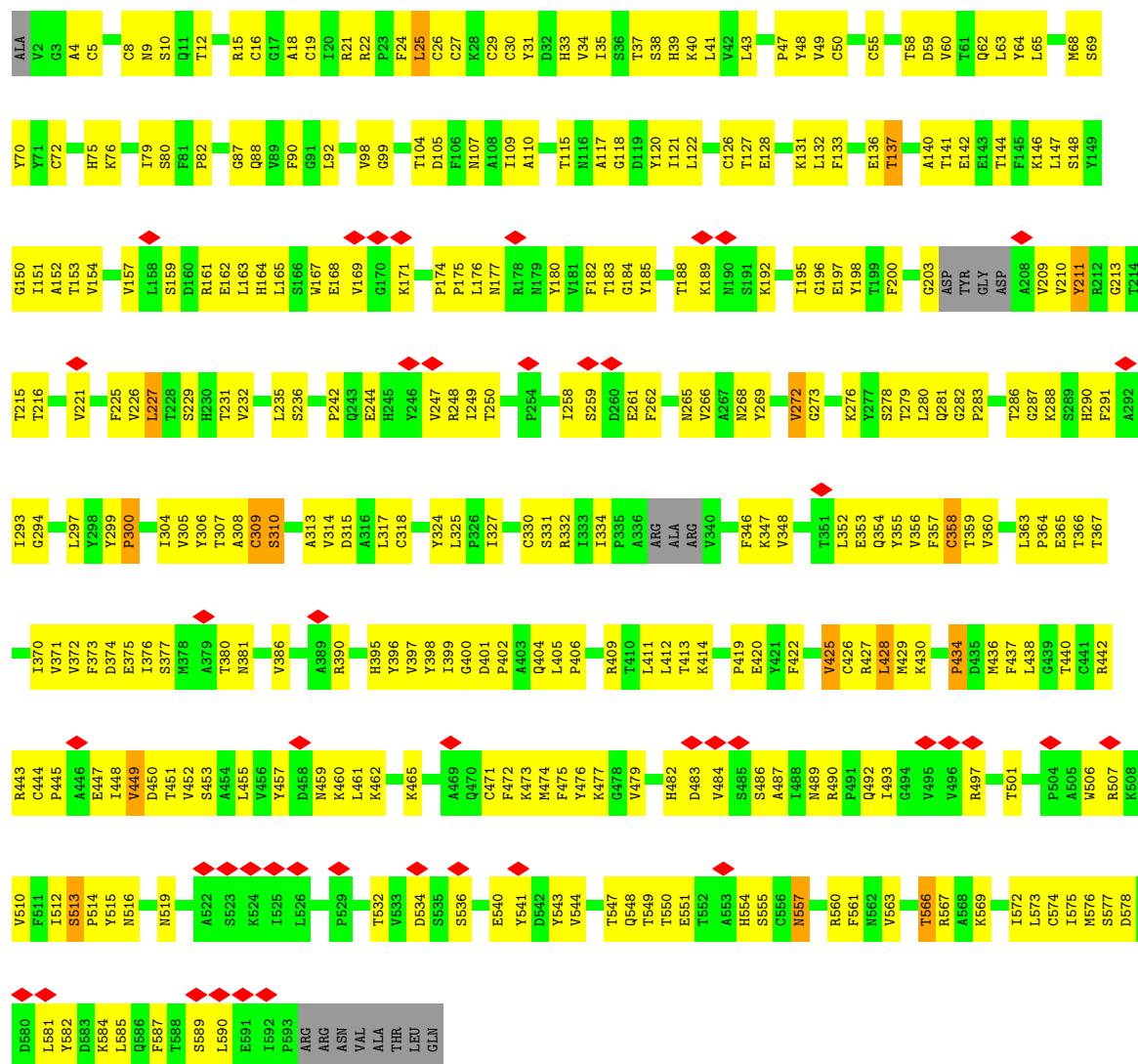




• Molecule 6: Helicase



Chain F:



• Molecule 7: Non-structural protein 9



Chain G:

Y87	L88	Y89	F90	I91	K92	L97	G104	R111	L112	Q113
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	779083	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	4.371	Depositor
Minimum map value	-2.392	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	430.08, 430.08, 430.08	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.96, 0.96, 0.96	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, ZN, F86, MG

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	0.24	1/7685 (0.0%)	0.48	4/10430 (0.0%)
2	B	0.42	2/1418 (0.1%)	0.66	2/1927 (0.1%)
2	D	0.37	1/1437 (0.1%)	0.81	6/1948 (0.3%)
3	C	0.21	0/589	0.50	0/793
4	I	0.16	0/611	0.37	0/953
5	J	0.14	0/606	0.30	0/940
6	E	0.21	0/4614	0.55	1/6287 (0.0%)
6	F	0.75	7/4610 (0.2%)	0.79	10/6283 (0.2%)
7	G	0.47	1/884 (0.1%)	0.73	5/1200 (0.4%)
All	All	0.42	12/22454 (0.1%)	0.61	28/30761 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	D	0	2
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	300	PRO	N-CD	-38.12	0.94	1.47
6	F	434	PRO	N-CD	24.49	1.82	1.47
6	F	434	PRO	CB-CG	-10.34	0.97	1.49
6	F	434	PRO	CG-CD	-8.32	1.22	1.50
7	G	2	ASN	N-CA	7.94	1.56	1.46
6	F	175	PRO	CG-CD	-7.34	1.25	1.50
6	F	300	PRO	CG-CD	-6.76	1.27	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	929	THR	CA-C	-6.19	1.44	1.53
6	F	300	PRO	CA-CB	-6.12	1.45	1.53
2	B	41	SER	CA-C	-5.75	1.44	1.52
2	B	48	GLU	CA-C	-5.25	1.45	1.52
2	D	38	LEU	CA-C	-5.03	1.45	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	434	PRO	CB-CG-CD	23.06	179.89	106.10
6	F	434	PRO	N-CD-CG	-21.56	70.86	103.20
6	F	434	PRO	CA-N-CD	-16.14	89.40	112.00
6	F	434	PRO	CA-CB-CG	-15.31	75.41	104.50
2	B	41	SER	N-CA-C	-14.37	95.87	113.41
1	A	503	GLY	N-CA-C	14.10	139.98	114.46
2	D	42	LEU	N-CA-C	13.18	125.38	111.14
6	F	300	PRO	CA-CB-CG	-12.94	79.91	104.50
2	D	39	LYS	N-CA-CB	-12.22	91.37	110.44
6	F	300	PRO	N-CD-CG	-11.83	85.45	103.20
2	D	41	SER	CB-CA-C	11.15	129.30	110.79
2	D	40	LYS	N-CA-C	-10.57	96.82	112.04
7	G	3	GLU	N-CA-C	10.05	125.99	110.42
1	A	929	THR	N-CA-C	9.77	122.93	110.33
6	F	300	PRO	N-CA-CB	-9.33	93.45	103.25
2	D	38	LEU	CB-CA-C	8.73	128.25	109.99
2	D	42	LEU	N-CA-CB	-8.56	97.65	110.07
2	B	46	LYS	N-CA-C	-6.85	104.92	113.55
6	E	167	TRP	CA-CB-CG	6.54	126.03	113.60
6	F	175	PRO	N-CD-CG	-6.41	93.59	103.20
7	G	6	PRO	CA-C-N	6.13	133.01	121.97
7	G	6	PRO	C-N-CA	6.13	133.01	121.97
7	G	1	ASN	O-C-N	-5.97	113.45	123.00
6	F	175	PRO	CA-N-CD	-5.87	103.78	112.00
1	A	928	HIS	N-CA-C	-5.73	98.60	110.80
6	F	577	SER	N-CA-C	-5.54	107.10	112.97
7	G	2	ASN	N-CA-CB	5.42	119.70	110.87
1	A	607	SER	CB-CA-C	-5.13	110.64	116.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	181	ALA	Peptide
2	B	182	TRP	Peptide
2	D	181	ALA	Peptide
2	D	37	LYS	Mainchain

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	7496	0	7239	75	0
2	B	1400	0	1372	35	0
2	D	1418	0	1427	43	0
3	C	586	0	615	14	0
4	I	545	0	272	19	0
5	J	545	0	281	9	0
6	E	4512	0	4434	328	0
6	F	4508	0	4423	284	0
7	G	868	0	878	40	0
8	A	2	0	0	0	0
8	E	3	0	0	0	0
8	F	3	0	0	0	0
9	A	32	0	13	8	0
10	A	1	0	0	0	0
11	G	24	0	0	1	0
12	A	5	0	0	1	0
12	G	1	0	0	0	0
All	All	21949	0	20954	825	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (825) 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)
6:E:141:THR:HG23	6:E:145:PHE:CE2	1.40	1.51
1:A:218:ASP:OD1	9:A:1003:GNP:O3G	1.58	1.21
2:D:38:LEU:O	2:D:42:LEU:HB2	1.38	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:141:THR:CG2	6:E:145:PHE:CE2	2.31	1.13
6:F:429:MET:CB	6:F:434:PRO:HD3	1.80	1.10
1:A:50:LYS:NZ	1:A:53:CYS:SG	2.25	1.10
6:F:62:GLN:NE2	6:F:63:LEU:HG	1.69	1.06
6:E:421:TYR:HA	6:E:427:ARG:NH2	1.70	1.05
6:F:19:CYS:SG	6:F:39:HIS:CE1	2.49	1.04
6:F:447:GLU:HB3	6:F:587:PHE:HE1	1.24	1.03
6:F:429:MET:HB3	6:F:434:PRO:HD3	1.35	1.02
6:E:124:ASN:HA	6:E:131:LYS:HE3	1.39	1.01
6:E:141:THR:CG2	6:E:145:PHE:HE2	1.72	1.01
6:E:421:TYR:CA	6:E:427:ARG:HH21	1.73	1.01
6:E:139:LYS:NZ	6:E:382:TYR:CD1	2.31	0.99
6:E:509:ALA:HB2	6:E:543:TYR:HD1	1.24	0.98
6:E:421:TYR:HA	6:E:427:ARG:HH21	0.85	0.98
6:E:139:LYS:NZ	6:E:382:TYR:CG	2.31	0.98
6:E:16:CYS:SG	6:E:33:HIS:HD2	1.88	0.97
6:F:413:THR:HB	6:F:414:LYS:HE2	1.46	0.97
6:E:447:GLU:OE2	6:E:447:GLU:N	1.99	0.95
6:E:167:TRP:HB2	6:E:173:ARG:HH11	1.31	0.94
6:F:62:GLN:HE21	6:F:63:LEU:HG	1.31	0.92
6:F:447:GLU:HB3	6:F:587:PHE:CE1	2.05	0.92
2:D:38:LEU:O	2:D:42:LEU:CB	2.18	0.92
6:F:26:CYS:SG	6:F:29:CYS:HB3	2.10	0.91
6:E:564:ALA:HA	6:E:567:ARG:HD3	1.52	0.91
6:E:141:THR:O	6:E:145:PHE:CD2	2.25	0.90
6:F:5:CYS:SG	6:F:8:CYS:HB2	2.11	0.90
6:E:181:VAL:HB	6:E:197:GLU:OE2	1.71	0.90
6:E:159:SER:H	6:E:162:GLU:HB2	1.39	0.87
6:E:30:CYS:O	6:E:34:VAL:HG12	1.76	0.85
3:C:67:ASP:OD2	3:C:70:LYS:HG2	1.77	0.84
6:E:129:ARG:HA	6:E:132:LEU:HD12	1.59	0.84
6:F:473:LYS:HG3	6:F:587:PHE:HB2	1.59	0.84
6:E:288:LYS:HZ3	6:E:400:GLY:H	1.26	0.84
6:F:16:CYS:SG	6:F:33:HIS:HD2	2.01	0.83
6:E:509:ALA:HB2	6:E:543:TYR:CD1	2.14	0.83
6:F:476:TYR:N	6:F:576:MET:O	2.11	0.82
6:E:17:GLY:HA3	6:E:41:LEU:HB3	1.62	0.81
6:E:120:TYR:HE1	6:E:124:ASN:HD21	1.29	0.81
6:E:333:ILE:HG22	6:E:349:ASN:H	1.45	0.81
6:E:311:HIS:CE1	6:E:342:CYS:HB3	2.16	0.80
6:E:239:THR:HG21	6:E:424:SER:HB2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:120:TYR:CE2	6:E:409:ARG:NH1	2.49	0.79
6:F:429:MET:HG2	6:F:434:PRO:HG3	1.63	0.79
6:E:311:HIS:CE1	6:E:315:ASP:OD2	2.36	0.79
6:F:413:THR:HB	6:F:414:LYS:CE	2.13	0.79
6:E:510:VAL:HG13	6:E:541:TYR:CD2	2.18	0.78
7:G:48:LEU:HD13	7:G:51:LEU:HD22	1.65	0.77
6:E:564:ALA:HA	6:E:567:ARG:HH11	1.49	0.76
6:F:413:THR:CB	6:F:414:LYS:HE2	2.16	0.76
6:F:115:THR:O	6:F:413:THR:OG1	2.04	0.76
6:F:244:GLU:HB3	6:F:276:LYS:H	1.48	0.76
6:E:358:CYS:SG	6:E:359:THR:N	2.54	0.76
6:F:282:GLY:HA3	6:F:288:LYS:HD2	1.68	0.76
1:A:120:THR:O	9:A:1003:GNP:N1	2.18	0.75
6:E:244:GLU:HB3	6:E:276:LYS:H	1.49	0.75
6:F:288:LYS:HZ3	6:F:400:GLY:H	1.33	0.74
6:E:239:THR:HG23	6:E:384:LEU:HD12	1.68	0.74
6:F:27:CYS:HB3	6:F:88:GLN:HG3	1.69	0.74
6:F:280:LEU:HD11	6:F:397:VAL:HG13	1.68	0.74
6:E:120:TYR:HE1	6:E:124:ASN:ND2	1.85	0.74
6:E:181:VAL:CB	6:E:197:GLU:OE2	2.35	0.74
6:E:124:ASN:ND2	6:E:421:TYR:O	2.21	0.73
6:F:429:MET:CG	6:F:434:PRO:HD3	2.18	0.73
6:F:548:GLN:OE1	6:F:576:MET:HG2	1.88	0.73
6:E:167:TRP:HB2	6:E:173:ARG:HD2	1.71	0.73
6:E:141:THR:HG23	6:E:145:PHE:HE2	0.92	0.73
6:E:104:THR:HA	6:E:107:ASN:HB2	1.71	0.72
6:F:62:GLN:CD	6:F:62:GLN:C	2.57	0.72
6:E:90:PHE:HD1	6:E:94:LYS:HE2	1.55	0.72
3:C:38:ASP:HB3	3:C:51:LYS:HE3	1.71	0.72
6:E:120:TYR:HE2	6:E:409:ARG:NH1	1.87	0.72
6:F:304:ILE:HG22	6:F:370:ILE:HB	1.70	0.72
6:F:429:MET:HB3	6:F:434:PRO:CD	2.17	0.71
6:E:510:VAL:HG13	6:E:541:TYR:CE2	2.25	0.71
6:E:154:VAL:HG21	6:E:163:LEU:HD13	1.73	0.71
6:E:476:TYR:N	6:E:576:MET:O	2.16	0.70
6:E:26:CYS:HB2	6:E:29:CYS:HB3	1.73	0.70
6:E:282:GLY:HA3	6:E:288:LYS:HD2	1.72	0.70
7:G:58:LYS:HG3	7:G:60:ASP:H	1.54	0.70
2:D:33:VAL:HA	2:D:36:LYS:HB2	1.72	0.70
2:D:133:PRO:HD2	2:D:137:THR:HG21	1.72	0.70
6:E:136:GLU:OE2	6:E:235:LEU:HD23	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:475:PHE:HA	6:F:576:MET:HB2	1.74	0.70
7:G:17:GLY:N	7:G:53:TRP:O	2.25	0.70
7:G:10:ARG:NH1	7:G:32:TYR:OH	2.25	0.70
7:G:6:PRO:O	7:G:7:VAL:HG12	1.92	0.69
6:F:460:LYS:HD3	6:F:461:LEU:HD22	1.75	0.69
3:C:67:ASP:OD2	3:C:70:LYS:CG	2.40	0.69
6:E:7:LEU:HD21	6:E:106:PHE:HB2	1.75	0.69
6:E:203:GLY:HA2	6:E:210:VAL:HG23	1.75	0.69
6:E:18:ALA:HB3	6:E:39:HIS:HA	1.75	0.68
6:E:490:ARG:HH21	6:E:493:ILE:HG21	1.59	0.68
6:F:364:PRO:HA	6:F:390:ARG:HH21	1.59	0.68
2:D:43:ASN:ND2	5:J:120:C:O3'	2.27	0.68
6:F:294:GLY:HA2	6:F:297:LEU:HB2	1.73	0.68
1:A:380:MET:CE	2:B:98:LEU:HD22	2.24	0.68
6:F:374:ASP:HA	6:F:399:ILE:HB	1.76	0.68
6:F:513:SER:OG	6:F:519:ASN:ND2	2.27	0.68
6:F:372:VAL:HG12	6:F:397:VAL:HG11	1.75	0.67
3:C:72:CYS:SG	2:D:111:ARG:NH2	2.67	0.67
6:F:419:PRO:HG3	6:F:560:ARG:HH12	1.60	0.67
6:F:544:VAL:HG11	6:F:567:ARG:HB3	1.75	0.67
6:F:445:PRO:HD3	6:F:569:LYS:HA	1.75	0.67
6:E:147:LEU:HD11	6:E:229:SER:HB3	1.78	0.66
6:E:544:VAL:HG23	6:E:572:ILE:HD13	1.76	0.66
7:G:70:GLU:OE1	7:G:92:LYS:HA	1.96	0.66
2:B:75:ARG:HH22	6:E:53:PRO:HB2	1.61	0.66
2:D:31:SER:OG	2:D:32:GLU:N	2.28	0.66
6:F:437:PHE:O	6:F:437:PHE:HD1	1.77	0.66
2:B:25:ALA:O	2:B:29:GLY:N	2.22	0.66
6:E:545:ILE:HG23	6:E:573:LEU:HD11	1.78	0.66
6:E:294:GLY:HA2	6:E:297:LEU:HB2	1.78	0.66
7:G:23:CYS:HB3	7:G:55:ARG:HG3	1.78	0.66
1:A:208:ASP:O	9:A:1003:GNP:O3'	2.13	0.65
6:F:37:THR:O	6:F:40:LYS:NZ	2.29	0.65
6:F:41:LEU:HD13	6:F:58:THR:HB	1.78	0.65
1:A:434:SER:OG	1:A:876:GLU:OE1	2.13	0.65
6:E:275:GLN:NE2	6:E:277:TYR:O	2.29	0.65
2:B:100:ASN:O	2:B:104:ASN:ND2	2.29	0.65
6:E:21:ARG:NH2	6:E:232:VAL:O	2.28	0.65
6:F:293:ILE:HG23	6:F:325:LEU:HD11	1.78	0.65
11:G:201:F86:N3	11:G:201:F86:O2	2.28	0.65
6:E:141:THR:HG23	6:E:145:PHE:CZ	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:453:SER:HB2	6:E:459:ASN:HA	1.78	0.65
6:E:472:PHE:HD2	6:E:590:LEU:HD23	1.62	0.65
6:F:373:PHE:O	6:F:399:ILE:N	2.29	0.65
6:F:279:THR:HG22	6:F:429:MET:HE3	1.78	0.65
6:F:358:CYS:SG	6:F:363:LEU:HB3	2.37	0.65
4:I:25:C:H2'	4:I:26:U:H6	1.61	0.65
6:F:151:ILE:H	6:F:168:GLU:HB2	1.61	0.65
6:E:72:CYS:H	6:E:75:HIS:HB2	1.62	0.65
6:E:567:ARG:N	6:E:567:ARG:HD2	2.10	0.65
6:E:473:LYS:HG3	6:E:587:PHE:HB2	1.78	0.64
6:E:159:SER:N	6:E:162:GLU:HB2	2.12	0.64
1:A:900:LEU:HD12	1:A:905:VAL:O	1.98	0.64
6:F:457:TYR:HB3	6:F:461:LEU:HD23	1.79	0.64
2:B:162:ALA:HB2	2:B:183:PRO:HD2	1.78	0.64
6:E:423:ASN:O	6:E:427:ARG:CZ	2.46	0.64
6:E:447:GLU:O	6:E:451:THR:OG1	2.11	0.64
6:F:118:GLY:O	6:F:122:LEU:HD12	1.95	0.64
6:F:231:THR:HG23	6:F:231:THR:O	1.98	0.64
6:F:331:SER:HB3	6:F:347:LYS:HZ2	1.63	0.64
6:E:423:ASN:O	6:E:427:ARG:NH1	2.31	0.64
6:F:373:PHE:HB3	6:F:376:ILE:HD11	1.79	0.64
6:F:429:MET:CA	6:F:434:PRO:HD3	2.28	0.64
6:E:311:HIS:ND1	6:E:315:ASP:OD2	2.30	0.63
6:E:445:PRO:HD3	6:E:569:LYS:HA	1.80	0.63
6:E:509:ALA:CB	6:E:543:TYR:HD1	2.07	0.63
6:E:401:ASP:HB3	6:E:404:GLN:HE21	1.63	0.63
6:F:306:TYR:HB2	6:F:357:PHE:HA	1.80	0.63
4:I:13:G:H2'	4:I:14:G:C8	2.33	0.63
6:E:133:PHE:O	6:E:137:THR:HG23	1.97	0.63
6:E:536:SER:O	6:E:567:ARG:NH2	2.32	0.63
6:F:9:ASN:ND2	6:F:9:ASN:O	2.32	0.63
6:F:447:GLU:CB	6:F:587:PHE:HE1	2.07	0.62
6:F:510:VAL:HB	6:F:541:TYR:CE2	2.33	0.62
6:F:581:LEU:HA	6:F:584:LYS:HB3	1.78	0.62
2:B:136:ASN:O	2:B:140:ASN:ND2	2.32	0.62
6:E:158:LEU:HD12	6:E:164:HIS:HE2	1.63	0.62
2:B:111:ARG:HB3	2:B:111:ARG:NH1	2.14	0.62
6:E:5:CYS:SG	6:E:6:VAL:N	2.73	0.62
6:E:363:LEU:HD12	6:E:390:ARG:HD3	1.82	0.62
6:E:423:ASN:OD1	6:E:426:CYS:N	2.32	0.62
6:E:182:PHE:O	6:E:197:GLU:HG2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:330:CYS:HA	6:E:355:TYR:HB2	1.82	0.62
6:E:265:ASN:HB3	6:E:269:TYR:CZ	2.35	0.61
6:E:373:PHE:HB2	6:E:376:ILE:HD11	1.80	0.61
6:F:126:CYS:SG	6:F:127:THR:N	2.70	0.61
6:E:158:LEU:HD12	6:E:164:HIS:NE2	2.16	0.61
6:E:374:ASP:HA	6:E:399:ILE:HB	1.81	0.61
6:E:402:PRO:HB3	6:E:426:CYS:HB2	1.81	0.61
6:F:386:VAL:O	6:F:390:ARG:HG2	2.00	0.61
7:G:30:ALA:HA	7:G:43:ALA:O	2.00	0.61
2:D:57:ARG:NH2	2:D:61:LYS:HD3	2.14	0.61
6:F:358:CYS:SG	6:F:359:THR:N	2.73	0.61
6:F:557:ASN:HB2	6:F:560:ARG:HB2	1.81	0.61
2:D:90:MET:O	2:D:94:MET:HG3	2.01	0.61
2:D:112:ASP:C	2:D:112:ASP:OD1	2.44	0.61
6:E:72:CYS:HB2	6:E:75:HIS:CG	2.35	0.61
6:F:366:THR:HG22	6:F:367:THR:H	1.66	0.61
6:E:124:ASN:CA	6:E:131:LYS:HE3	2.24	0.60
6:F:132:LEU:HD23	6:F:235:LEU:HB2	1.82	0.60
6:E:314:VAL:O	6:E:318:CYS:N	2.35	0.60
6:E:21:ARG:HG3	6:E:137:THR:HG22	1.84	0.60
6:E:119:ASP:OD1	6:E:119:ASP:N	2.31	0.60
6:E:278:SER:HB3	6:E:436:MET:SD	2.40	0.60
6:F:401:ASP:HB3	6:F:404:GLN:OE1	2.01	0.60
1:A:218:ASP:CG	9:A:1003:GNP:O3G	2.41	0.60
6:E:322:LEU:HD21	6:E:345:LYS:HB3	1.82	0.60
6:F:514:PRO:HB3	6:F:555:SER:HB2	1.84	0.60
6:E:39:HIS:NE2	6:E:110:ALA:HB1	2.17	0.60
4:I:13:G:H2'	4:I:14:G:H8	1.66	0.60
6:F:154:VAL:HG13	6:F:164:HIS:O	2.02	0.59
1:A:718:LYS:HZ1	1:A:721:ARG:HD3	1.66	0.59
6:E:235:LEU:N	6:E:235:LEU:HD22	2.17	0.59
6:E:150:GLY:HA2	6:E:168:GLU:OE1	2.03	0.59
6:F:331:SER:CB	6:F:347:LYS:HZ2	2.16	0.59
6:E:135:ALA:HB1	6:E:382:TYR:HD1	1.66	0.59
6:F:140:ALA:O	6:F:144:THR:HG23	2.03	0.59
1:A:52:ASN:ND2	12:A:1102:HOH:O	2.29	0.59
6:F:104:THR:HA	6:F:107:ASN:HB2	1.84	0.59
6:E:270:GLN:O	6:E:274:MET:HG3	2.03	0.59
2:B:40:LYS:HA	2:B:43:ASN:HB2	1.84	0.59
4:I:23:U:H2'	4:I:24:G:H8	1.66	0.59
6:E:407:ALA:O	6:E:409:ARG:NE	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:THR:HG22	1:A:226:THR:H	1.68	0.59
6:E:229:SER:OG	6:E:230:HIS:N	2.32	0.59
6:F:427:ARG:HH21	6:F:430:LYS:HB3	1.68	0.59
6:F:429:MET:HG2	6:F:434:PRO:HD3	1.84	0.59
4:I:25:C:H2'	4:I:26:U:C6	2.37	0.59
6:E:544:VAL:HG21	6:E:567:ARG:HB2	1.85	0.58
7:G:54:ALA:O	7:G:67:THR:OG1	2.21	0.58
6:F:306:TYR:HE1	6:F:355:TYR:HB3	1.68	0.58
6:E:420:GLU:O	6:E:427:ARG:NE	2.35	0.58
6:F:55:CYS:HB2	6:F:75:HIS:HE1	1.69	0.58
1:A:867:TYR:O	1:A:870:THR:OG1	2.21	0.58
4:I:11:G:H2'	4:I:12:C:C6	2.39	0.58
6:F:509:ALA:HB2	6:F:543:TYR:CD2	2.39	0.58
2:D:48:GLU:O	2:D:48:GLU:HG3	2.04	0.58
6:F:536:SER:HB2	6:F:567:ARG:HH22	1.68	0.58
6:F:422:PHE:HB2	6:F:426:CYS:SG	2.44	0.58
2:D:171:GLU:OE1	2:D:171:GLU:O	2.22	0.57
6:F:436:MET:HE1	6:F:438:LEU:HD13	1.84	0.57
6:E:136:GLU:CD	6:E:235:LEU:HD23	2.29	0.57
2:B:51:ARG:HA	2:B:51:ARG:HH11	1.70	0.57
6:F:72:CYS:SG	6:F:75:HIS:CG	2.97	0.57
6:E:124:ASN:HD22	6:E:427:ARG:HH22	1.52	0.57
6:E:380:THR:HG22	6:E:381:ASN:H	1.69	0.57
6:E:109:ILE:HD13	6:E:134:ALA:HB2	1.86	0.57
6:E:579:ARG:HH22	6:E:582:TYR:HB3	1.70	0.57
6:F:163:LEU:N	6:F:209:VAL:O	2.37	0.57
2:B:75:ARG:HH22	6:E:53:PRO:CB	2.17	0.57
5:J:113:C:H2'	5:J:114:A:C8	2.40	0.57
6:E:26:CYS:HB3	6:E:97:CYS:HB2	1.87	0.57
7:G:44:LEU:O	7:G:89:TYR:N	2.25	0.57
1:A:718:LYS:HZ1	1:A:721:ARG:CD	2.17	0.57
6:F:176:LEU:HB2	6:F:200:PHE:HB2	1.86	0.57
2:D:100:ASN:O	2:D:104:ASN:ND2	2.24	0.56
6:F:540:GLU:HA	6:F:567:ARG:HD3	1.87	0.56
1:A:909:ASN:OD1	1:A:912:THR:OG1	2.21	0.56
6:E:561:PHE:O	6:E:561:PHE:HD1	1.89	0.56
6:F:62:GLN:NE2	6:F:63:LEU:HA	2.21	0.56
6:E:546:PHE:HD1	6:E:547:THR:H	1.53	0.56
6:F:309:CYS:SG	6:F:310:SER:N	2.78	0.56
1:A:160:LYS:O	1:A:161:ASP:HB2	2.05	0.56
6:E:117:ALA:O	6:E:121:ILE:HG12	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:158:LEU:HD23	6:E:159:SER:OG	2.05	0.56
6:E:306:TYR:HB2	6:E:357:PHE:HA	1.87	0.56
6:E:550:THR:HG23	6:E:552:THR:H	1.71	0.56
6:F:161:ARG:HA	6:F:211:TYR:HE1	1.71	0.56
1:A:902:MET:HE3	6:E:93:TYR:HE2	1.69	0.56
6:E:404:GLN:C	6:E:405:LEU:HD12	2.31	0.56
6:F:128:GLU:O	6:F:131:LYS:HB2	2.06	0.56
6:E:141:THR:O	6:E:145:PHE:CG	2.58	0.56
6:E:556:CYS:HA	6:E:561:PHE:HD2	1.71	0.56
6:F:161:ARG:HA	6:F:211:TYR:CE1	2.40	0.56
6:F:165:LEU:HD22	6:F:209:VAL:HG23	1.87	0.56
7:G:70:GLU:O	7:G:89:TYR:HE2	1.89	0.56
2:D:32:GLU:HG2	2:D:33:VAL:HG23	1.88	0.56
6:E:120:TYR:CE1	6:E:124:ASN:OD1	2.59	0.56
6:E:141:THR:CG2	6:E:145:PHE:CZ	2.86	0.56
6:E:403:ALA:HA	6:E:559:ASN:HD22	1.71	0.56
6:F:287:GLY:HA2	6:F:442:ARG:HH21	1.71	0.56
6:E:123:ALA:O	6:E:131:LYS:HD3	2.05	0.55
6:E:315:ASP:CG	6:E:343:PHE:HB2	2.31	0.55
6:E:543:TYR:OH	6:E:573:LEU:HD23	2.06	0.55
6:F:154:VAL:HG11	6:F:163:LEU:HD23	1.88	0.55
2:B:50:ASP:OD1	4:I:17:G:H4'	2.06	0.55
4:I:12:C:H2'	4:I:13:G:H8	1.72	0.55
5:J:115:U:H2'	5:J:116:G:H8	1.71	0.55
6:E:120:TYR:CE1	6:E:124:ASN:ND2	2.72	0.55
1:A:380:MET:HE1	2:B:95:LEU:HD12	1.88	0.55
2:B:44:VAL:C	2:B:46:LYS:H	2.14	0.55
6:E:437:PHE:HD1	6:E:437:PHE:O	1.89	0.55
6:E:114:TRP:CD1	6:E:141:THR:HG21	2.42	0.55
7:G:58:LYS:HD2	7:G:59:SER:H	1.71	0.55
6:E:375:GLU:N	6:E:399:ILE:O	2.39	0.55
3:C:70:LYS:O	3:C:74:GLU:N	2.40	0.55
6:E:182:PHE:O	6:E:197:GLU:CG	2.53	0.55
6:E:333:ILE:HG22	6:E:349:ASN:N	2.19	0.55
6:E:306:TYR:HA	6:E:372:VAL:HG23	1.88	0.55
6:F:373:PHE:N	6:F:397:VAL:O	2.37	0.55
6:E:188:THR:HG22	6:E:189:LYS:H	1.71	0.55
6:E:279:THR:HA	6:E:398:TYR:CD1	2.41	0.55
6:F:163:LEU:O	6:F:209:VAL:N	2.36	0.55
6:E:139:LYS:HD2	6:E:232:VAL:HG21	1.89	0.54
6:F:288:LYS:NZ	6:F:400:GLY:H	2.02	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:24:G:H2'	4:I:25:C:H6	1.71	0.54
6:F:68:MET:SD	6:F:68:MET:N	2.81	0.54
6:F:64:TYR:HD2	6:F:76:LYS:HD2	1.72	0.54
1:A:332:LYS:NZ	2:B:104:ASN:OD1	2.40	0.54
2:B:112:ASP:N	2:B:112:ASP:OD1	2.39	0.54
6:F:486:SER:HB3	6:F:515:TYR:HB3	1.89	0.54
1:A:902:MET:HE1	6:E:11:GLN:HE21	1.71	0.54
6:F:287:GLY:HA2	6:F:442:ARG:NH2	2.22	0.54
4:I:26:U:H2'	4:I:27:A:H8	1.71	0.54
6:E:280:LEU:HA	6:E:436:MET:CG	2.38	0.54
6:F:24:PHE:O	6:F:25:LEU:HD23	2.08	0.54
6:F:203:GLY:HA2	6:F:210:VAL:HG23	1.89	0.54
6:F:490:ARG:HE	6:F:497:ARG:HH22	1.55	0.54
7:G:75:PHE:HD2	7:G:112:LEU:HD11	1.72	0.54
6:E:283:PRO:HB3	6:E:461:LEU:HD21	1.90	0.54
1:A:107:ASP:OD1	1:A:108:GLY:N	2.41	0.54
4:I:11:G:H2'	4:I:12:C:H6	1.72	0.54
6:E:334:ILE:HG13	6:E:335:PRO:HD2	1.90	0.54
6:F:479:VAL:O	6:F:489:ASN:ND2	2.40	0.54
1:A:902:MET:HE3	6:E:93:TYR:CE2	2.43	0.54
6:E:233:MET:SD	6:E:233:MET:N	2.80	0.53
6:E:443:ARG:O	6:E:569:LYS:HB3	2.09	0.53
6:F:117:ALA:O	6:F:121:ILE:HG12	2.08	0.53
6:F:281:GLN:HG2	6:F:434:PRO:HB3	1.90	0.53
6:F:48:TYR:OH	6:F:90:PHE:O	2.18	0.53
6:F:314:VAL:O	6:F:318:CYS:N	2.41	0.53
6:E:26:CYS:O	6:E:30:CYS:N	2.21	0.53
6:E:200:PHE:HZ	6:E:225:PHE:HD2	1.55	0.53
6:E:358:CYS:SG	6:E:362:ALA:HB3	2.49	0.53
6:E:375:GLU:OE1	6:E:537:GLN:NE2	2.41	0.53
6:F:184:GLY:C	6:F:195:ILE:HB	2.34	0.53
6:F:532:THR:O	6:F:536:SER:HB3	2.09	0.53
6:E:514:PRO:HD3	6:E:546:PHE:HE1	1.73	0.53
6:E:153:THR:HA	6:E:224:TYR:HB3	1.90	0.53
7:G:84:LYS:HB2	7:G:86:LYS:HE3	1.89	0.53
1:A:333:ILE:HG22	1:A:361:LEU:HD12	1.91	0.53
5:J:115:U:C2	5:J:116:G:C8	2.97	0.53
6:F:290:HIS:CE1	6:F:324:TYR:HH	2.21	0.53
6:E:120:TYR:CD1	6:E:124:ASN:OD1	2.62	0.53
6:E:311:HIS:ND1	6:E:315:ASP:CG	2.67	0.53
2:D:84:THR:O	2:D:84:THR:OG1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASP:OD1	1:A:153:ASP:N	2.42	0.53
6:E:399:ILE:HD12	6:E:399:ILE:H	1.74	0.53
1:A:647:SER:OG	1:A:648:LEU:N	2.40	0.53
2:B:38:LEU:HD23	2:B:41:SER:HB2	1.91	0.53
6:E:402:PRO:HG3	6:E:426:CYS:HA	1.91	0.53
6:F:288:LYS:NZ	6:F:400:GLY:O	2.42	0.53
6:E:177:ASN:HB2	6:E:179:ASN:OD1	2.09	0.52
6:E:536:SER:OG	6:E:567:ARG:NH2	2.42	0.52
6:F:184:GLY:N	6:F:196:GLY:O	2.40	0.52
7:G:16:ALA:HA	7:G:54:ALA:HA	1.90	0.52
7:G:47:ASP:OD2	7:G:86:LYS:HE2	2.09	0.52
2:B:39:LYS:O	2:B:43:ASN:HB2	2.08	0.52
6:E:145:PHE:CE2	6:E:411:LEU:HD11	2.44	0.52
6:F:148:SER:O	6:F:171:LYS:HD3	2.08	0.52
1:A:20:THR:HB	1:A:59:LYS:HZ1	1.74	0.52
6:E:265:ASN:HB3	6:E:269:TYR:CE2	2.44	0.52
6:F:34:VAL:HG11	6:F:60:VAL:HG21	1.91	0.52
1:A:120:THR:HG21	1:A:212:LEU:HB2	1.92	0.52
6:E:272:VAL:HG13	6:E:436:MET:HE1	1.92	0.52
6:E:554:HIS:O	6:E:560:ARG:NE	2.43	0.52
6:E:439:GLY:HA2	6:E:460:LYS:HE3	1.91	0.52
6:E:508:LYS:HE3	6:E:542:ASP:HB2	1.91	0.52
2:D:15:PHE:HA	2:D:45:ALA:HB1	1.91	0.52
6:F:282:GLY:H	6:F:401:ASP:HB2	1.75	0.52
2:D:151:SER:O	2:D:151:SER:OG	2.23	0.52
2:D:182:TRP:O	2:D:184:LEU:N	2.43	0.52
5:J:115:U:H2'	5:J:116:G:C8	2.45	0.52
6:E:422:PHE:N	6:E:426:CYS:SG	2.83	0.52
6:F:567:ARG:HG3	6:F:567:ARG:HH11	1.74	0.52
1:A:39:ASN:HD22	7:G:1:ASN:HB3	1.75	0.51
4:I:12:C:H2'	4:I:13:G:C8	2.44	0.51
6:E:280:LEU:HB2	6:E:398:TYR:C	2.35	0.51
6:E:453:SER:HB3	6:E:461:LEU:O	2.10	0.51
6:F:182:PHE:HA	6:F:227:LEU:HB3	1.92	0.51
7:G:51:LEU:C	7:G:52:LYS:HE2	2.36	0.51
6:E:141:THR:OG1	6:E:145:PHE:CZ	2.56	0.51
6:F:62:GLN:OE1	6:F:72:CYS:HA	2.09	0.51
2:B:11:SER:HB3	2:B:48:GLU:HB3	1.92	0.51
6:E:183:THR:HA	6:E:197:GLU:HA	1.91	0.51
6:F:352:LEU:HD23	6:F:352:LEU:H	1.75	0.51
6:F:402:PRO:HG3	6:F:426:CYS:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:185:TYR:HB2	6:F:192:LYS:NZ	2.25	0.51
6:F:332:ARG:HB2	6:F:346:PHE:HD2	1.76	0.51
7:G:77:THR:HB	7:G:111:ARG:O	2.11	0.51
1:A:380:MET:HE3	2:B:98:LEU:HD22	1.93	0.51
2:B:50:ASP:OD2	4:I:17:G:O2'	2.24	0.51
3:C:3:MET:O	3:C:6:VAL:HG12	2.11	0.51
6:F:314:VAL:HG21	6:F:358:CYS:O	2.11	0.51
6:F:359:THR:HG22	6:F:360:VAL:H	1.75	0.51
6:E:120:TYR:HE2	6:E:409:ARG:HH11	1.58	0.51
6:F:150:GLY:HA2	6:F:168:GLU:HB3	1.92	0.51
6:F:451:THR:HG22	6:F:585:LEU:HD22	1.93	0.51
6:F:516:ASN:HD22	6:F:516:ASN:H	1.59	0.51
6:F:548:GLN:OE1	6:F:576:MET:HA	2.11	0.51
3:C:27:LYS:O	3:C:31:GLN:HG3	2.11	0.50
6:E:272:VAL:HG12	6:E:278:SER:HB2	1.92	0.50
6:F:306:TYR:HA	6:F:372:VAL:HG23	1.93	0.50
6:F:402:PRO:HB3	6:F:426:CYS:SG	2.51	0.50
1:A:825:ASP:N	1:A:825:ASP:OD1	2.43	0.50
6:E:19:CYS:SG	6:E:39:HIS:HE1	2.18	0.50
6:F:174:PRO:HB2	6:F:180:TYR:CE2	2.46	0.50
6:F:183:THR:N	6:F:226:VAL:O	2.38	0.50
6:E:9:ASN:CG	6:E:9:ASN:O	2.54	0.50
6:E:11:GLN:HB2	6:E:93:TYR:CZ	2.46	0.50
6:E:60:VAL:HG13	6:E:61:THR:HG23	1.92	0.50
6:E:136:GLU:HG2	6:E:235:LEU:CD2	2.41	0.50
6:E:139:LYS:O	6:E:143:GLU:HG2	2.10	0.50
6:F:18:ALA:HB3	6:F:39:HIS:HA	1.94	0.50
6:F:244:GLU:HB3	6:F:276:LYS:N	2.24	0.50
6:F:447:GLU:O	6:F:451:THR:OG1	2.20	0.50
6:E:280:LEU:HA	6:E:436:MET:HG2	1.92	0.50
6:E:564:ALA:CA	6:E:567:ARG:HH11	2.24	0.50
6:F:429:MET:HG2	6:F:434:PRO:CD	2.41	0.50
6:E:11:GLN:HB2	6:E:93:TYR:CE2	2.46	0.50
6:F:26:CYS:O	6:F:30:CYS:N	2.30	0.50
7:G:44:LEU:HD22	7:G:89:TYR:HB2	1.93	0.50
6:E:271:LYS:HZ2	6:E:275:GLN:HG2	1.76	0.50
6:E:548:GLN:HG3	6:E:576:MET:SD	2.52	0.50
1:A:10:ARG:O	1:A:10:ARG:NH1	2.43	0.50
6:F:188:THR:HG22	6:F:189:LYS:H	1.76	0.50
6:F:540:GLU:HA	6:F:567:ARG:CD	2.41	0.50
7:G:55:ARG:NH2	7:G:64:THR:HG22	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:304:ILE:HA	6:F:370:ILE:O	2.11	0.50
6:E:150:GLY:HA3	6:E:173:ARG:HG3	1.93	0.49
1:A:798:LYS:NZ	1:A:798:LYS:HB3	2.26	0.49
6:E:288:LYS:NZ	6:E:400:GLY:H	2.03	0.49
6:E:370:ILE:HD11	6:E:397:VAL:HB	1.93	0.49
6:E:510:VAL:HG22	6:E:544:VAL:HG12	1.95	0.49
6:E:543:TYR:HE1	6:E:545:ILE:CG1	2.26	0.49
1:A:401:LEU:HD22	1:A:668:MET:HE1	1.94	0.49
6:E:76:LYS:NZ	6:E:80:SER:HB2	2.28	0.49
6:E:182:PHE:CG	6:E:200:PHE:HE2	2.29	0.49
6:E:244:GLU:HB3	6:E:276:LYS:N	2.23	0.49
6:E:266:VAL:HA	6:E:269:TYR:CD2	2.47	0.49
6:E:478:GLY:HA2	6:E:492:GLN:HE22	1.78	0.49
6:E:511:PHE:O	6:E:519:ASN:ND2	2.45	0.49
6:E:550:THR:CG2	6:E:552:THR:HG22	2.43	0.49
6:F:453:SER:HB2	6:F:459:ASN:HA	1.92	0.49
6:E:231:THR:O	6:E:233:MET:SD	2.70	0.49
6:F:50:CYS:HA	6:F:70:TYR:O	2.12	0.49
6:F:376:ILE:HG13	6:F:398:TYR:HB3	1.95	0.49
1:A:218:ASP:OD2	9:A:1003:GNP:O3A	2.31	0.49
2:D:56:GLN:HA	2:D:59:LEU:HB2	1.94	0.49
1:A:49:LEU:HD23	1:A:51:THR:HG23	1.94	0.49
6:E:126:CYS:SG	6:E:127:THR:N	2.84	0.49
6:F:215:THR:HG22	6:F:216:THR:H	1.77	0.49
6:F:265:ASN:HB3	6:F:269:TYR:CZ	2.47	0.49
6:F:548:GLN:HG3	6:F:561:PHE:HE2	1.78	0.49
3:C:77:ASP:H	2:D:96:ARG:HD2	1.76	0.49
6:E:473:LYS:O	6:E:589:SER:HA	2.13	0.49
6:E:522:ALA:O	6:E:526:LEU:N	2.35	0.49
6:E:7:LEU:HD11	6:E:106:PHE:CD2	2.47	0.49
6:E:279:THR:HA	6:E:398:TYR:HD1	1.75	0.49
6:F:372:VAL:HB	6:F:399:ILE:HD11	1.94	0.49
6:E:33:HIS:CG	6:E:106:PHE:HE1	2.31	0.49
6:E:373:PHE:O	6:E:399:ILE:N	2.46	0.49
6:E:563:VAL:O	6:E:567:ARG:HD3	2.13	0.49
6:F:62:GLN:NE2	6:F:63:LEU:CA	2.75	0.49
6:F:165:LEU:HD23	6:F:165:LEU:H	1.78	0.49
6:F:450:ASP:OD1	6:F:450:ASP:N	2.45	0.49
6:E:6:VAL:HG13	6:E:7:LEU:HG	1.95	0.48
6:E:115:THR:O	6:E:413:THR:OG1	2.30	0.48
6:E:167:TRP:CD2	6:E:173:ARG:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:55:ARG:NH2	7:G:65:ILE:O	2.40	0.48
6:F:332:ARG:HA	6:F:357:PHE:HB2	1.94	0.48
6:F:437:PHE:O	6:F:437:PHE:CD1	2.62	0.48
6:E:370:ILE:HD12	6:E:371:VAL:N	2.29	0.48
6:F:34:VAL:HG13	6:F:35:ILE:HD12	1.95	0.48
6:F:306:TYR:N	6:F:356:VAL:O	2.42	0.48
7:G:45:LEU:HB2	7:G:88:LEU:HB2	1.95	0.48
1:A:336:ASP:OD1	1:A:364:SER:O	2.30	0.48
6:F:159:SER:H	6:F:162:GLU:HB2	1.78	0.48
2:D:36:LYS:O	2:D:39:LYS:HB3	2.14	0.48
6:E:304:ILE:HA	6:E:370:ILE:HG23	1.94	0.48
6:E:423:ASN:O	6:E:427:ARG:NH2	2.47	0.48
6:F:25:LEU:HD22	6:F:29:CYS:SG	2.53	0.48
6:E:8:CYS:HB2	6:E:26:CYS:SG	2.53	0.48
6:E:58:THR:O	6:E:58:THR:OG1	2.29	0.48
6:E:486:SER:HB3	6:E:515:TYR:HB3	1.94	0.48
6:F:455:LEU:HA	6:F:584:LYS:NZ	2.28	0.48
6:F:465:LYS:HD2	6:F:465:LYS:N	2.29	0.48
1:A:223:ILE:CD1	7:G:104:GLY:HA2	2.44	0.48
1:A:769:THR:O	1:A:773:GLN:HG3	2.13	0.48
6:E:277:TYR:HE1	6:E:428:LEU:HD21	1.79	0.48
6:E:297:LEU:HD21	6:E:324:TYR:HB3	1.96	0.48
2:B:42:LEU:HD23	2:B:42:LEU:HA	1.60	0.48
4:I:23:U:H2'	4:I:24:G:C8	2.48	0.48
6:E:4:ALA:HA	6:E:11:GLN:HA	1.96	0.48
6:E:124:ASN:HD22	6:E:427:ARG:NH2	2.10	0.48
6:F:154:VAL:HG11	6:F:163:LEU:CD2	2.44	0.48
2:D:38:LEU:O	2:D:42:LEU:N	2.42	0.48
6:E:50:CYS:HA	6:E:70:TYR:O	2.14	0.48
6:E:111:THR:O	6:E:111:THR:OG1	2.29	0.48
6:F:4:ALA:HB1	6:F:9:ASN:HA	1.96	0.48
6:F:76:LYS:NZ	6:F:80:SER:HB2	2.28	0.48
6:F:330:CYS:HA	6:F:355:TYR:HB2	1.96	0.48
6:F:581:LEU:HD23	6:F:585:LEU:HD11	1.96	0.48
7:G:56:PHE:HB3	7:G:65:ILE:HD11	1.95	0.48
6:E:465:LYS:N	6:E:465:LYS:HD2	2.29	0.47
6:E:120:TYR:CE1	6:E:124:ASN:CG	2.92	0.47
6:E:404:GLN:O	6:E:405:LEU:HD12	2.14	0.47
6:F:105:ASP:O	6:F:109:ILE:HG13	2.13	0.47
2:D:12:TYR:HB2	2:D:49:PHE:CE1	2.49	0.47
6:E:546:PHE:HD1	6:E:547:THR:N	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:268:ASN:HD21	6:F:437:PHE:HE1	1.57	0.47
7:G:111:ARG:NH1	7:G:111:ARG:HA	2.29	0.47
6:F:276:LYS:O	6:F:395:HIS:HA	2.15	0.47
1:A:543:ASN:OD1	5:J:100:A:O2'	2.32	0.47
6:E:167:TRP:CB	6:E:173:ARG:HD2	2.41	0.47
6:F:62:GLN:NE2	6:F:63:LEU:CG	2.60	0.47
6:F:185:TYR:HB2	6:F:192:LYS:HZ2	1.78	0.47
6:F:412:LEU:HD12	6:F:412:LEU:O	2.14	0.47
2:D:40:LYS:HA	2:D:40:LYS:HD2	1.52	0.47
6:E:20:ILE:HG23	6:E:21:ARG:HG2	1.96	0.47
6:E:457:TYR:CZ	6:E:562:ASN:ND2	2.83	0.47
6:F:248:ARG:HG2	6:F:249:ILE:C	2.40	0.47
6:F:265:ASN:HB3	6:F:269:TYR:CE2	2.50	0.47
6:F:406:PRO:HB2	6:F:409:ARG:NH2	2.29	0.47
6:F:473:LYS:O	6:F:589:SER:HA	2.13	0.47
6:E:32:ASP:O	6:E:36:SER:HB2	2.14	0.47
6:E:152:ALA:HB3	6:E:225:PHE:HB2	1.97	0.47
6:E:244:GLU:O	6:E:275:GLN:HB2	2.14	0.47
6:E:288:LYS:O	6:E:292:ALA:N	2.44	0.47
6:E:370:ILE:HD12	6:E:371:VAL:H	1.80	0.47
6:E:483:ASP:OD2	6:E:484:VAL:HG23	2.14	0.47
6:F:49:VAL:HG12	6:F:58:THR:HG22	1.97	0.47
3:C:77:ASP:C	2:D:96:ARG:HB2	2.40	0.47
6:F:353:GLU:HG3	6:F:354:GLN:N	2.30	0.47
6:F:413:THR:C	6:F:414:LYS:HE2	2.40	0.47
4:I:26:U:H2'	4:I:27:A:C8	2.49	0.47
6:E:184:GLY:C	6:E:195:ILE:HB	2.39	0.47
6:E:475:PHE:HD1	6:E:576:MET:O	1.97	0.47
6:F:279:THR:HA	6:F:398:TYR:CD1	2.50	0.47
6:E:543:TYR:HE1	6:E:545:ILE:HG12	1.78	0.47
6:F:279:THR:HG22	6:F:429:MET:CE	2.44	0.47
6:F:473:LYS:HZ2	6:F:574:CYS:HB2	1.79	0.47
7:G:48:LEU:HB3	7:G:51:LEU:HD13	1.96	0.47
1:A:851:ASP:OD2	2:D:75:ARG:NH1	2.48	0.46
4:I:24:G:H2'	4:I:25:C:C6	2.50	0.46
6:E:136:GLU:CG	6:E:235:LEU:CD2	2.93	0.46
6:E:138:LEU:HD23	6:E:382:TYR:HE1	1.80	0.46
6:E:308:ALA:HB1	6:E:313:ALA:HB3	1.97	0.46
6:E:490:ARG:O	6:E:494:GLY:N	2.47	0.46
6:F:265:ASN:HA	6:F:291:PHE:CE2	2.51	0.46
1:A:75:HIS:CD2	1:A:79:ASN:HD22	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:PRO:O	1:A:325:SER:OG	2.30	0.46
2:D:25:ALA:HB1	2:D:35:LEU:HD22	1.96	0.46
6:E:141:THR:O	6:E:145:PHE:CE2	2.68	0.46
6:E:183:THR:N	6:E:226:VAL:O	2.44	0.46
6:E:200:PHE:CZ	6:E:225:PHE:HD2	2.33	0.46
6:E:276:LYS:O	6:E:395:HIS:HA	2.15	0.46
6:E:447:GLU:H	6:E:447:GLU:CD	2.14	0.46
2:D:89:THR:O	2:D:93:THR:HG23	2.14	0.46
1:A:218:ASP:CG	9:A:1003:GNP:N3B	2.73	0.46
5:J:114:A:C5	5:J:115:U:C5	3.04	0.46
6:E:25:LEU:HB3	6:E:30:CYS:HB2	1.98	0.46
6:E:288:LYS:NZ	6:E:400:GLY:O	2.48	0.46
6:F:188:THR:HG22	6:F:189:LYS:N	2.30	0.46
6:F:550:THR:HG23	6:F:554:HIS:HE1	1.81	0.46
1:A:236:SER:O	1:A:240:LEU:HB2	2.16	0.46
2:B:157:GLN:HG3	2:B:157:GLN:O	2.14	0.46
6:E:136:GLU:CD	6:E:235:LEU:CD2	2.89	0.46
6:E:510:VAL:CG1	6:E:541:TYR:CE2	2.96	0.46
6:F:473:LYS:CG	6:F:587:PHE:HB2	2.40	0.46
1:A:431:GLU:N	1:A:431:GLU:OE1	2.48	0.46
6:E:175:PRO:HD2	6:E:180:TYR:CE2	2.50	0.46
6:E:184:GLY:N	6:E:196:GLY:O	2.44	0.46
6:E:473:LYS:HD2	6:E:582:TYR:HD1	1.81	0.46
6:E:244:GLU:HB2	6:E:276:LYS:HG2	1.96	0.46
6:F:182:PHE:CG	6:F:200:PHE:HE2	2.34	0.46
6:E:76:LYS:HE3	6:E:77:PRO:O	2.16	0.46
6:E:467:LYS:HB2	6:E:467:LYS:HE2	1.74	0.46
6:F:268:ASN:HB2	6:F:291:PHE:CZ	2.50	0.46
6:F:447:GLU:OE1	6:F:587:PHE:HD1	1.99	0.46
6:E:187:VAL:HB	6:E:192:LYS:HD3	1.97	0.46
6:E:424:SER:HA	6:E:427:ARG:NH1	2.30	0.46
6:F:483:ASP:OD2	6:F:484:VAL:HG23	2.15	0.46
2:B:11:SER:CB	2:B:48:GLU:HB3	2.46	0.45
2:B:50:ASP:O	2:B:54:ALA:CB	2.64	0.45
3:C:44:ASP:OD2	3:C:46:THR:HG22	2.16	0.45
6:E:141:THR:C	6:E:145:PHE:CD2	2.93	0.45
6:F:561:PHE:O	6:F:563:VAL:N	2.49	0.45
3:C:2:LYS:HA	3:C:2:LYS:HD3	1.70	0.45
6:E:291:PHE:O	6:E:295:LEU:HD12	2.16	0.45
6:F:157:VAL:HG13	6:F:163:LEU:HD12	1.98	0.45
6:F:419:PRO:O	6:F:426:CYS:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:514:PRO:HB3	6:E:555:SER:HB2	1.99	0.45
6:F:131:LYS:HD3	6:F:131:LYS:HA	1.78	0.45
6:F:436:MET:HE3	6:F:437:PHE:N	2.31	0.45
6:F:540:GLU:C	6:F:541:TYR:HD1	2.25	0.45
1:A:726:ARG:NH1	1:A:744:GLU:OE1	2.45	0.45
2:D:12:TYR:CA	2:D:49:PHE:CE1	2.99	0.45
6:E:61:THR:HA	6:E:84:CYS:SG	2.56	0.45
6:F:299:TYR:HA	6:F:300:PRO:HD3	1.56	0.45
6:E:380:THR:HB	6:E:382:TYR:CZ	2.52	0.45
6:F:273:GLY:O	6:F:395:HIS:NE2	2.50	0.45
7:G:25:ASP:OD1	7:G:25:ASP:N	2.47	0.45
6:E:34:VAL:HG22	6:E:60:VAL:HG11	1.99	0.45
6:F:380:THR:HG22	6:F:381:ASN:H	1.81	0.45
6:F:581:LEU:HB3	6:F:585:LEU:HG	1.98	0.45
1:A:73:LYS:HD3	1:A:75:HIS:CD2	2.51	0.45
6:E:358:CYS:SG	6:E:363:LEU:HB3	2.57	0.45
6:E:420:GLU:O	6:E:427:ARG:HB3	2.16	0.45
6:F:365:GLU:HG2	6:F:390:ARG:NE	2.32	0.45
1:A:755:MET:HG2	1:A:764:VAL:HG22	1.99	0.45
2:D:94:MET:HE2	2:D:94:MET:HB3	1.89	0.45
6:E:90:PHE:CD1	6:E:94:LYS:HE2	2.44	0.45
7:G:23:CYS:CB	7:G:55:ARG:HG3	2.47	0.45
6:E:281:GLN:C	6:E:288:LYS:HZ1	2.26	0.44
6:F:55:CYS:SG	6:F:75:HIS:HE1	2.36	0.44
1:A:24:THR:OG1	1:A:25:GLY:N	2.50	0.44
1:A:361:LEU:HD22	1:A:361:LEU:H	1.82	0.44
6:E:332:ARG:HB3	6:E:344:ASP:OD1	2.16	0.44
6:E:435:ASP:C	6:E:436:MET:SD	3.00	0.44
6:F:540:GLU:HA	6:F:567:ARG:NE	2.32	0.44
1:A:242:MET:HG2	1:A:463:MET:HE2	1.98	0.44
6:E:139:LYS:HZ1	6:E:382:TYR:CB	2.30	0.44
6:E:456:VAL:HG21	6:E:559:ASN:OD1	2.17	0.44
6:F:404:GLN:OE1	6:F:404:GLN:N	2.51	0.44
6:F:443:ARG:O	6:F:569:LYS:HB3	2.18	0.44
1:A:718:LYS:HA	1:A:718:LYS:HD2	1.55	0.44
2:B:70:MET:HE3	6:F:92:LEU:HG	1.98	0.44
2:D:161:ASP:HA	2:D:184:LEU:HD23	1.99	0.44
6:E:56:ASP:O	6:E:56:ASP:CG	2.60	0.44
6:E:145:PHE:CE2	6:E:411:LEU:HD21	2.52	0.44
6:F:472:PHE:HD2	6:F:590:LEU:HD11	1.83	0.44
6:F:576:MET:SD	6:F:582:TYR:HB2	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:25:ASP:O	7:G:27:ASN:ND2	2.49	0.44
1:A:202:VAL:HB	1:A:223:ILE:HG12	1.99	0.44
1:A:380:MET:HE1	2:B:98:LEU:HD22	2.00	0.44
1:A:708:LEU:HD23	1:A:708:LEU:HA	1.82	0.44
6:F:183:THR:HA	6:F:197:GLU:HA	1.99	0.44
6:F:353:GLU:HG3	6:F:354:GLN:H	1.82	0.44
3:C:52:MET:HE3	3:C:52:MET:HB3	1.91	0.44
6:E:146:LYS:HD3	6:E:227:LEU:HD11	2.00	0.44
6:E:24:PHE:C	6:E:25:LEU:HD22	2.43	0.44
6:E:239:THR:HG23	6:E:384:LEU:CD1	2.44	0.44
2:B:31:SER:OG	2:B:33:VAL:HG12	2.18	0.44
2:D:117:LEU:HD12	2:D:129:MET:HB3	2.00	0.44
4:I:22:A:C6	4:I:23:U:C4	3.06	0.44
6:E:31:TYR:CE2	6:E:87:GLY:HA2	2.52	0.44
6:F:21:ARG:HD2	6:F:136:GLU:HB2	1.99	0.44
6:F:98:VAL:HG12	6:F:99:GLY:O	2.18	0.44
6:F:305:VAL:HB	6:F:371:VAL:HG12	1.99	0.44
6:F:396:TYR:HD2	6:F:398:TYR:HH	1.65	0.44
6:F:420:GLU:O	6:F:427:ARG:HB2	2.18	0.44
6:E:280:LEU:HA	6:E:436:MET:HG3	2.00	0.44
6:F:405:LEU:HD22	6:F:534:ASP:HA	1.99	0.44
6:F:429:MET:HG2	6:F:434:PRO:CG	2.39	0.44
6:F:551:GLU:OE1	6:F:578:ASP:HA	2.17	0.44
1:A:40:ASP:HB3	7:G:6:PRO:HB2	1.99	0.43
1:A:358:ASP:OD1	1:A:533:ARG:NH1	2.51	0.43
6:E:145:PHE:CD2	6:E:411:LEU:HD21	2.53	0.43
6:E:444:CYS:HB2	6:E:449:VAL:HG23	1.99	0.43
6:F:21:ARG:HG3	6:F:133:PHE:CE1	2.53	0.43
6:F:404:GLN:C	6:F:405:LEU:HD12	2.43	0.43
1:A:218:ASP:CG	9:A:1003:GNP:PG	3.01	0.43
1:A:336:ASP:OD1	1:A:364:SER:HA	2.18	0.43
6:E:142:GLU:HA	6:E:145:PHE:HD2	1.82	0.43
6:E:154:VAL:HG23	6:E:164:HIS:O	2.17	0.43
6:F:305:VAL:HG13	6:F:356:VAL:HB	2.00	0.43
1:A:504:PHE:HA	1:A:505:PRO:HA	1.90	0.43
2:D:171:GLU:OE2	2:D:176:ASN:ND2	2.51	0.43
6:E:581:LEU:HG	6:E:584:LYS:HE2	2.00	0.43
6:F:165:LEU:HB2	6:F:167:TRP:HE1	1.84	0.43
1:A:681:SER:O	1:A:684:ASP:OD1	2.36	0.43
5:J:116:G:H2'	5:J:117:C:C6	2.53	0.43
6:E:382:TYR:O	6:E:386:VAL:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:579:ARG:NH2	6:E:583:ASP:H	2.17	0.43
6:F:39:HIS:NE2	6:F:110:ALA:HB1	2.32	0.43
1:A:924:MET:HE3	1:A:924:MET:HB3	1.89	0.43
6:E:145:PHE:HE2	6:E:411:LEU:HD11	1.81	0.43
6:F:540:GLU:HA	6:F:567:ARG:HE	1.82	0.43
2:B:106:ILE:HG13	2:B:107:ILE:N	2.33	0.43
2:D:39:LYS:HA	2:D:42:LEU:HB3	2.00	0.43
6:E:526:LEU:HD12	6:E:528:LEU:HD12	2.00	0.43
6:F:55:CYS:CB	6:F:75:HIS:HE1	2.31	0.43
6:F:64:TYR:CD1	6:F:82:PRO:HA	2.52	0.43
6:F:153:THR:HG23	6:F:153:THR:O	2.17	0.43
6:F:226:VAL:HG12	6:F:227:LEU:N	2.33	0.43
7:G:91:ILE:H	7:G:91:ILE:HG13	1.53	0.43
6:F:176:LEU:HD23	6:F:176:LEU:H	1.84	0.43
6:F:185:TYR:HB3	6:F:192:LYS:HB3	2.00	0.43
6:F:425:VAL:HA	6:F:428:LEU:HB3	2.00	0.43
1:A:855:MET:HE2	1:A:858:ARG:HD3	2.00	0.43
2:D:61:LYS:HE2	2:D:61:LYS:HB2	1.73	0.43
6:F:279:THR:HA	6:F:398:TYR:HD1	1.83	0.43
6:E:73:LYS:HZ3	6:E:76:LYS:HG2	1.84	0.43
6:E:561:PHE:CE1	6:E:564:ALA:HB3	2.54	0.43
1:A:900:LEU:HD11	1:A:906:MET:HA	2.00	0.43
6:E:123:ALA:O	6:E:131:LYS:CE	2.67	0.43
6:F:177:ASN:OD1	6:F:177:ASN:N	2.51	0.43
7:G:75:PHE:CD2	7:G:112:LEU:HD11	2.53	0.43
6:E:177:ASN:ND2	6:E:516:ASN:OD1	2.52	0.42
6:E:181:VAL:HB	6:E:197:GLU:CD	2.40	0.42
6:E:405:LEU:HG	6:E:560:ARG:HG2	2.00	0.42
6:F:419:PRO:HD2	6:F:420:GLU:OE2	2.19	0.42
1:A:218:ASP:OD1	9:A:1003:GNP:PG	2.71	0.42
2:D:161:ASP:OD2	2:D:180:LEU:HB3	2.19	0.42
6:E:95:ASN:N	6:E:95:ASN:OD1	2.52	0.42
6:E:181:VAL:CG2	6:E:197:GLU:OE2	2.66	0.42
6:E:288:LYS:HE2	6:E:399:ILE:HG23	2.02	0.42
6:E:573:LEU:O	6:E:573:LEU:HD12	2.19	0.42
6:F:59:ASP:O	6:F:63:LEU:HD11	2.19	0.42
1:A:623:ASP:OD1	1:A:623:ASP:N	2.51	0.42
4:I:24:G:HO2'	4:I:25:C:P	2.43	0.42
6:E:136:GLU:HG2	6:E:235:LEU:HD21	1.99	0.42
6:E:158:LEU:HB3	6:E:162:GLU:HB3	2.01	0.42
6:E:185:TYR:HB3	6:E:192:LYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:311:HIS:HE1	6:E:315:ASP:OD2	1.97	0.42
6:F:19:CYS:SG	6:F:39:HIS:HE1	2.12	0.42
7:G:13:SER:OG	7:G:26:ASP:OD1	2.37	0.42
6:E:11:GLN:OE1	6:E:11:GLN:N	2.47	0.42
6:E:443:ARG:HD3	6:E:443:ARG:HA	1.79	0.42
6:F:313:ALA:O	6:F:317:LEU:HD12	2.20	0.42
6:F:548:GLN:CG	6:F:561:PHE:HE2	2.32	0.42
3:C:47:GLU:O	3:C:50:GLU:HG3	2.20	0.42
6:E:185:TYR:HB2	6:E:192:LYS:HD2	2.01	0.42
6:F:62:GLN:CD	6:F:63:LEU:N	2.76	0.42
6:F:62:GLN:C	6:F:62:GLN:OE1	2.62	0.42
6:F:120:TYR:OH	6:F:411:LEU:HB2	2.19	0.42
6:F:476:TYR:CG	6:F:477:LYS:N	2.84	0.42
6:F:507:ARG:C	6:F:507:ARG:HH11	2.26	0.42
2:B:148:THR:HG22	2:B:153:LEU:HD12	2.02	0.42
2:D:118:ASN:OD1	2:D:118:ASN:N	2.52	0.42
6:E:226:VAL:HG12	6:E:227:LEU:H	1.84	0.42
6:E:284:PRO:CB	6:E:566:THR:HG21	2.49	0.42
6:E:314:VAL:HG21	6:E:358:CYS:O	2.19	0.42
6:E:315:ASP:HA	6:E:318:CYS:HB2	2.01	0.42
6:F:133:PHE:O	6:F:137:THR:OG1	2.30	0.42
6:F:272:VAL:HG23	6:F:278:SER:HB2	2.02	0.42
6:F:330:CYS:HB3	6:F:355:TYR:HD2	1.84	0.42
6:F:492:GLN:HG2	6:F:549:THR:HG23	2.01	0.42
6:F:506:TRP:O	6:F:543:TYR:HE2	2.03	0.42
1:A:120:THR:HG22	1:A:122:TYR:H	1.84	0.42
6:E:281:GLN:HG2	6:E:434:PRO:CB	2.49	0.42
6:E:564:ALA:CA	6:E:567:ARG:HD3	2.38	0.42
6:F:283:PRO:HG2	6:F:460:LYS:NZ	2.34	0.42
6:F:434:PRO:C	6:F:436:MET:H	2.28	0.42
6:F:444:CYS:HB2	6:F:449:VAL:HG22	2.01	0.42
2:B:101:ASP:HA	2:B:104:ASN:HD22	1.83	0.42
6:F:152:ALA:HB3	6:F:225:PHE:HB2	2.01	0.42
6:F:315:ASP:HA	6:F:318:CYS:HB2	2.01	0.42
6:F:455:LEU:HA	6:F:584:LYS:HZ3	1.84	0.42
7:G:53:TRP:HE1	7:G:66:TYR:HD2	1.67	0.42
6:E:256:LEU:HD23	6:E:256:LEU:HA	1.85	0.42
6:E:332:ARG:HB2	6:E:346:PHE:HD2	1.84	0.42
6:F:146:LYS:HE3	6:F:147:LEU:HG	2.01	0.42
6:F:262:PHE:O	6:F:266:VAL:HG23	2.19	0.42
6:F:406:PRO:HB2	6:F:409:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:LEU:HD23	1:A:749:LEU:HA	1.84	0.42
1:A:759:SER:O	1:A:759:SER:OG	2.34	0.42
6:F:76:LYS:HZ1	6:F:80:SER:HB2	1.85	0.42
2:B:50:ASP:O	2:B:54:ALA:HB3	2.20	0.41
2:D:171:GLU:CD	2:D:176:ASN:HD22	2.28	0.41
2:D:184:LEU:O	2:D:185:ILE:HG13	2.20	0.41
6:E:401:ASP:HB3	6:E:404:GLN:NE2	2.32	0.41
6:F:268:ASN:HB2	6:F:291:PHE:HZ	1.85	0.41
3:C:27:LYS:HB3	3:C:27:LYS:HE2	1.58	0.41
6:E:41:LEU:HD12	6:E:41:LEU:HA	1.89	0.41
6:F:305:VAL:HA	6:F:356:VAL:HB	2.02	0.41
6:F:543:TYR:HE1	6:F:573:LEU:HD23	1.84	0.41
1:A:106:ILE:HD13	1:A:106:ILE:HA	1.83	0.41
6:E:352:LEU:HD23	6:E:352:LEU:H	1.85	0.41
6:E:470:GLN:N	6:E:470:GLN:OE1	2.53	0.41
6:F:308:ALA:HB1	6:F:375:GLU:OE2	2.20	0.41
6:F:374:ASP:OD1	6:F:375:GLU:N	2.53	0.41
7:G:56:PHE:CD1	7:G:56:PHE:C	2.97	0.41
7:G:56:PHE:O	7:G:65:ILE:HG12	2.20	0.41
1:A:915:TYR:O	1:A:921:TYR:OH	2.28	0.41
2:D:12:TYR:HA	2:D:49:PHE:CE1	2.56	0.41
5:J:116:G:H2'	5:J:117:C:H6	1.85	0.41
6:E:541:TYR:HB2	6:E:544:VAL:HG13	2.02	0.41
6:F:561:PHE:O	6:F:561:PHE:HD1	2.03	0.41
1:A:664:SER:O	1:A:664:SER:OG	2.39	0.41
1:A:855:MET:CE	1:A:858:ARG:HD3	2.50	0.41
6:E:139:LYS:NZ	6:E:382:TYR:CE1	2.84	0.41
6:E:548:GLN:H	6:E:548:GLN:HG2	1.46	0.41
6:F:377:SER:OG	6:F:405:LEU:O	2.31	0.41
6:F:452:VAL:O	6:F:457:TYR:HB2	2.20	0.41
6:F:547:THR:HA	6:F:575:ILE:HB	2.03	0.41
2:B:22:TYR:N	2:B:38:LEU:HD22	2.35	0.41
6:E:65:LEU:O	6:E:80:SER:HB3	2.21	0.41
6:F:15:ARG:HD2	6:F:24:PHE:HE1	1.86	0.41
6:F:198:TYR:HD2	6:F:213:GLY:HA2	1.85	0.41
6:F:231:THR:O	6:F:231:THR:CG2	2.68	0.41
6:F:297:LEU:HD21	6:F:324:TYR:HB3	2.03	0.41
2:B:58:LYS:HZ1	6:F:79:ILE:HG13	1.85	0.41
6:F:4:ALA:HA	6:F:10:SER:O	2.21	0.41
6:F:31:TYR:CZ	6:F:87:GLY:HA2	2.56	0.41
6:F:146:LYS:NZ	6:F:229:SER:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:43:LEU:HD23	6:F:47:PRO:HB3	2.03	0.41
7:G:18:THR:HA	7:G:52:LYS:H	1.86	0.41
1:A:98:LYS:HZ2	1:A:98:LYS:HG2	1.78	0.41
2:B:48:GLU:HB2	2:B:49:PHE:H	1.57	0.41
6:E:7:LEU:HD11	6:E:106:PHE:CG	2.56	0.41
6:E:23:PRO:HG2	6:E:25:LEU:HD21	2.03	0.41
6:E:120:TYR:CZ	6:E:409:ARG:NH1	2.88	0.41
6:E:202:LYS:HD2	6:E:520:ALA:HB1	2.03	0.41
6:E:528:LEU:HD13	6:E:545:ILE:HD12	2.02	0.41
6:F:258:ILE:HD13	6:F:266:VAL:HG22	2.01	0.41
6:F:448:ILE:HG21	6:F:566:THR:HA	2.02	0.41
6:F:462:LYS:HB3	6:F:462:LYS:HE3	1.66	0.41
6:F:482:HIS:ND1	6:F:487:ALA:HB2	2.36	0.41
6:F:541:TYR:HB2	6:F:544:VAL:HG12	2.03	0.41
2:D:174:MET:O	2:D:177:SER:OG	2.26	0.41
6:E:280:LEU:HD13	6:E:436:MET:HG3	2.03	0.41
6:F:490:ARG:HA	6:F:493:ILE:HB	2.03	0.41
6:F:544:VAL:HG22	6:F:572:ILE:HG13	2.03	0.41
1:A:855:MET:O	1:A:857:GLU:N	2.45	0.40
6:E:76:LYS:HZ2	6:E:80:SER:HB2	1.84	0.40
6:E:448:ILE:HD13	6:E:565:ILE:O	2.21	0.40
6:F:291:PHE:HE2	6:F:438:LEU:HD11	1.87	0.40
1:A:689:TYR:O	1:A:693:VAL:HG23	2.22	0.40
4:I:23:U:C2	4:I:24:G:C8	3.08	0.40
6:E:271:LYS:HA	6:E:274:MET:SD	2.61	0.40
6:F:334:ILE:H	6:F:348:VAL:HG13	1.86	0.40
6:F:510:VAL:HG13	6:F:512:ILE:HD11	2.03	0.40
6:E:7:LEU:HD23	6:E:130:LEU:HD11	2.02	0.40
6:E:453:SER:HB2	6:E:459:ASN:HD22	1.86	0.40
6:F:200:PHE:HZ	6:F:225:PHE:HD2	1.69	0.40
6:F:471:CYS:HA	6:F:572:ILE:HG22	2.02	0.40
7:G:29:LEU:N	7:G:45:LEU:O	2.54	0.40
2:B:96:ARG:NH1	2:B:96:ARG:HB3	2.37	0.40
2:D:177:SER:OG	2:D:178:PRO:HD3	2.22	0.40
6:E:123:ALA:O	6:E:131:LYS:CD	2.69	0.40
6:E:390:ARG:HB3	6:E:391:LEU:HD22	2.03	0.40
2:D:12:TYR:HB2	2:D:49:PHE:HE1	1.87	0.40
6:E:306:TYR:N	6:E:356:VAL:O	2.53	0.40
6:E:307:THR:HG22	6:E:308:ALA:H	1.86	0.40
6:F:242:PRO:O	6:F:276:LYS:HG2	2.22	0.40
6:F:281:GLN:HG2	6:F:434:PRO:CB	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:390:ARG:HG2	6:F:390:ARG:H	1.67	0.40
7:G:57:PRO:HA	7:G:64:THR:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	929/932 (100%)	871 (94%)	55 (6%)	3 (0%)	36	59
2	B	185/198 (93%)	170 (92%)	14 (8%)	1 (0%)	24	46
2	D	184/198 (93%)	167 (91%)	17 (9%)	0	100	100
3	C	74/83 (89%)	71 (96%)	3 (4%)	0	100	100
6	E	580/601 (96%)	508 (88%)	72 (12%)	0	100	100
6	F	580/601 (96%)	509 (88%)	71 (12%)	0	100	100
7	G	111/113 (98%)	91 (82%)	18 (16%)	2 (2%)	6	16
All	All	2643/2726 (97%)	2387 (90%)	250 (10%)	6 (0%)	44	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	7	VAL
1	A	504	PHE
2	B	49	PHE
1	A	930	VAL
1	A	856	ILE
7	G	70	GLU

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	822/823 (100%)	786 (96%)	36 (4%)	25	51
2	B	146/167 (87%)	136 (93%)	10 (7%)	14	33
2	D	150/167 (90%)	136 (91%)	14 (9%)	8	20
3	C	71/77 (92%)	69 (97%)	2 (3%)	38	67
6	E	499/523 (95%)	462 (93%)	37 (7%)	13	30
6	F	498/523 (95%)	462 (93%)	36 (7%)	13	31
7	G	94/94 (100%)	88 (94%)	6 (6%)	16	36
All	All	2280/2374 (96%)	2139 (94%)	141 (6%)	19	38

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	27	SER
1	A	30	VAL
1	A	54	CYS
1	A	75	HIS
1	A	86	ILE
1	A	106	ILE
1	A	204	VAL
1	A	208	ASP
1	A	218	ASP
1	A	236	SER
1	A	246	THR
1	A	255	SER
1	A	318	SER
1	A	324	THR
1	A	361	LEU
1	A	367	SER
1	A	372	LEU
1	A	434	SER
1	A	451	SER

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Mol	Chain	Res	Type
1	A	493	VAL
1	A	499	ASP
1	A	551	LYS
1	A	577	LYS
1	A	647	SER
1	A	709	SER
1	A	758	LEU
1	A	759	SER
1	A	760	ASP
1	A	778	SER
1	A	790	ASN
1	A	835	SER
1	A	870	THR
1	A	896	THR
1	A	929	THR
1	A	931	LEU
2	B	44	VAL
2	B	46	LYS
2	B	51	ARG
2	B	76	SER
2	B	93	THR
2	B	100	ASN
2	B	114	CYS
2	B	148	THR
2	B	177	SER
2	B	182	TRP
3	C	27	LYS
3	C	66	VAL
2	D	33	VAL
2	D	39	LYS
2	D	40	LYS
2	D	56	GLN
2	D	60	GLU
2	D	76	SER
2	D	84	THR
2	D	123	THR
2	D	145	THR
2	D	148	THR
2	D	151	SER
2	D	157	GLN
2	D	167	VAL
2	D	189	LEU

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Mol	Chain	Res	Type
6	E	2	VAL
6	E	11	GLN
6	E	12	THR
6	E	13	SER
6	E	29	CYS
6	E	38	SER
6	E	50	CYS
6	E	58	THR
6	E	63	LEU
6	E	65	LEU
6	E	89	VAL
6	E	111	THR
6	E	119	ASP
6	E	141	THR
6	E	154	VAL
6	E	159	SER
6	E	169	VAL
6	E	219	LEU
6	E	236	SER
6	E	241	VAL
6	E	259	SER
6	E	307	THR
6	E	325	LEU
6	E	330	CYS
6	E	334	ILE
6	E	356	VAL
6	E	367	THR
6	E	372	VAL
6	E	373	PHE
6	E	456	VAL
6	E	459	ASN
6	E	534	ASP
6	E	544	VAL
6	E	548	GLN
6	E	550	THR
6	E	558	VAL
6	E	589	SER
6	F	12	THR
6	F	22	ARG
6	F	25	LEU
6	F	38	SER
6	F	65	LEU

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Mol	Chain	Res	Type
6	F	69	SER
6	F	137	THR
6	F	141	THR
6	F	142	GLU
6	F	169	VAL
6	F	211	TYR
6	F	221	VAL
6	F	227	LEU
6	F	232	VAL
6	F	236	SER
6	F	247	VAL
6	F	250	THR
6	F	259	SER
6	F	261	GLU
6	F	272	VAL
6	F	286	THR
6	F	307	THR
6	F	309	CYS
6	F	310	SER
6	F	327	ILE
6	F	358	CYS
6	F	425	VAL
6	F	428	LEU
6	F	440	THR
6	F	449	VAL
6	F	474[A]	MET
6	F	474[B]	MET
6	F	501	THR
6	F	513	SER
6	F	557	ASN
6	F	566	THR
7	G	23	CYS
7	G	24	THR
7	G	77	THR
7	G	88	LEU
7	G	97	LEU
7	G	112	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN

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Mol	Chain	Res	Type
1	A	79	ASN
1	A	82	HIS
1	A	133	HIS
1	A	404	ASN
1	A	408	GLN
1	A	570	GLN
1	A	698	GLN
1	A	713	ASN
1	A	789	GLN
1	A	822	GLN
2	B	192	ASN
3	C	18	GLN
2	D	100	ASN
6	E	75	HIS
6	E	124	ASN
6	E	265	ASN
6	E	354	GLN
6	E	361	ASN
6	E	381	ASN
6	E	404	GLN
6	E	459	ASN
6	E	519	ASN
6	E	531	GLN
6	E	537	GLN
6	E	548	GLN
6	E	559	ASN
6	E	586	GLN
6	F	75	HIS
6	F	220	ASN
6	F	281	GLN
6	F	354	GLN
6	F	381	ASN
6	F	459	ASN
6	F	516	ASN
6	F	518	GLN
6	F	519	ASN
7	G	20	GLN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	I	24/25 (96%)	1 (4%)	1 (4%)
5	J	25/26 (96%)	1 (4%)	0
All	All	49/51 (96%)	2 (4%)	1 (2%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	I	25	C
5	J	101	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	I	24	G

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](#)

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 for Mogul analysis.

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
11	F86	G	201	7	19,26,27	5.40	6 (31%)	16,39,42	8.61	4 (25%)
9	GNP	A	1003	10	34,34,34	1.43	5 (14%)	47,54,54	0.93	2 (4%)

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
11	F86	G	201	7	-	3/6/33/34	0/3/3/3
9	GNP	A	1003	10	-	10/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	201	F86	C8-N3	20.55	1.44	1.14
11	G	201	F86	O1-C4	-6.39	1.29	1.43
11	G	201	F86	C11-N5	5.76	1.48	1.34
9	A	1003	GNP	PB-O3A	5.34	1.65	1.59
11	G	201	F86	O2-C2	4.38	1.51	1.42
11	G	201	F86	C9-N1	-4.18	1.33	1.39
9	A	1003	GNP	PG-N3B	3.24	1.71	1.63
9	A	1003	GNP	PB-O1B	3.10	1.50	1.46
9	A	1003	GNP	PG-O1G	2.79	1.50	1.46
11	G	201	F86	O3-C3	-2.57	1.36	1.43
9	A	1003	GNP	PB-O2B	-2.27	1.50	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	201	F86	C1-C8-N3	-34.01	110.37	176.59
9	A	1003	GNP	O2A-PA-O3A	2.88	115.06	107.27
11	G	201	F86	C9-N1-N2	-2.70	118.09	124.01
9	A	1003	GNP	O1B-PB-N3B	-2.65	107.88	111.77
11	G	201	F86	C12-N2-N1	2.64	122.55	113.69
11	G	201	F86	N2-C12-N4	-2.29	119.25	127.47

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1003	GNP	PG-N3B-PB-O1B
9	A	1003	GNP	C5'-O5'-PA-O3A
9	A	1003	GNP	C5'-O5'-PA-O1A
9	A	1003	GNP	C5'-O5'-PA-O2A
11	G	201	F86	O1-C1-C5-N1

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Mol	Chain	Res	Type	Atoms
9	A	1003	GNP	C3'-C4'-C5'-O5'
9	A	1003	GNP	O4'-C4'-C5'-O5'
11	G	201	F86	O1-C4-C6-O4
11	G	201	F86	C3-C4-C6-O4
9	A	1003	GNP	PB-O3A-PA-O5'
9	A	1003	GNP	PB-O3A-PA-O1A
9	A	1003	GNP	PA-O3A-PB-O2B
9	A	1003	GNP	C2'-C1'-N9-C4

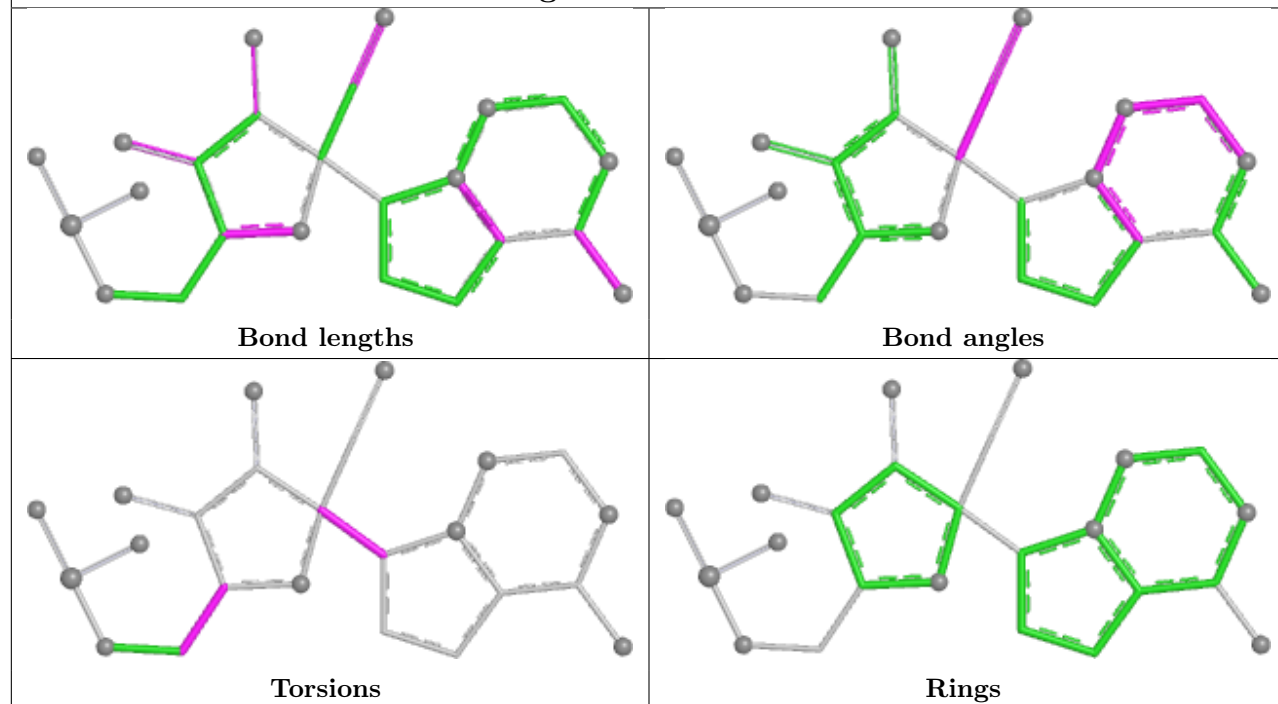
There are no ring outliers.

2 monomers are involved in 9 short contacts:

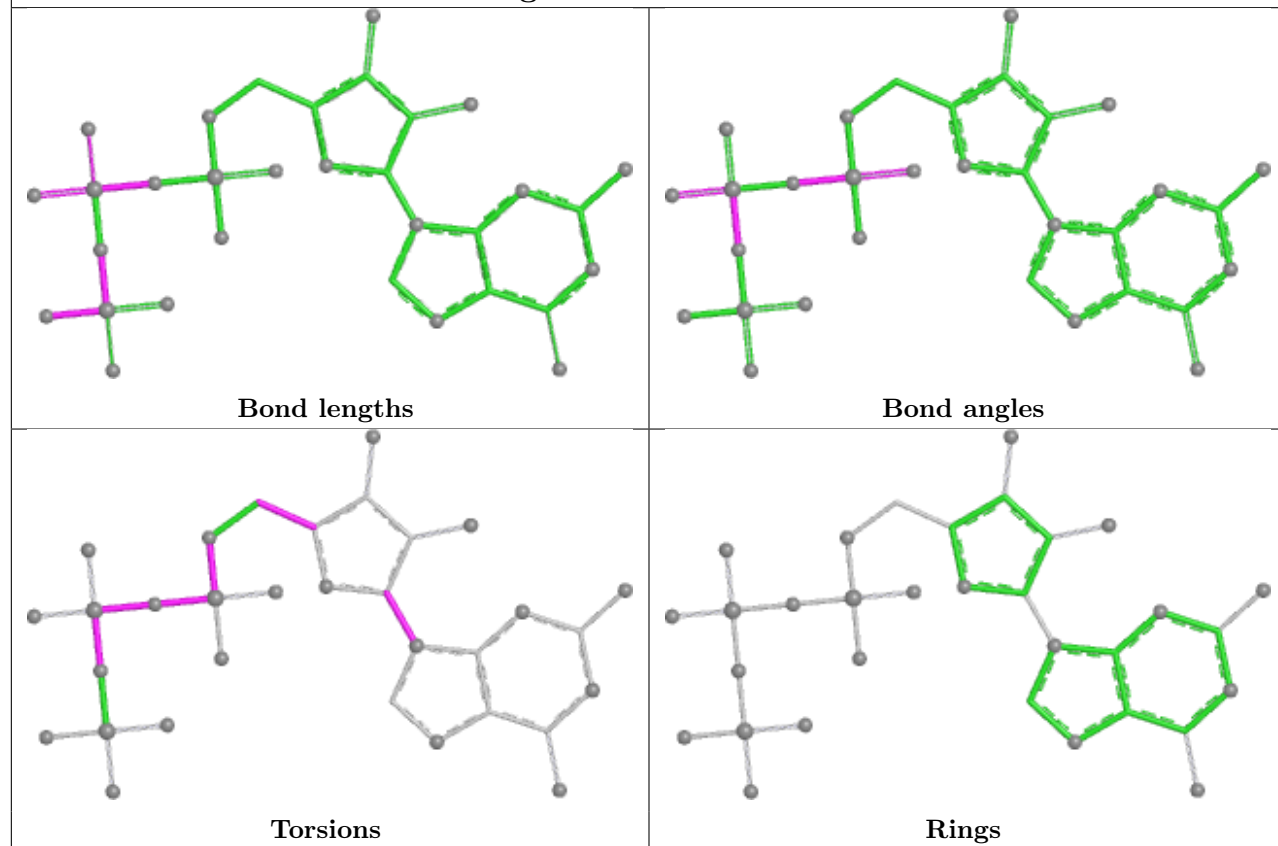
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	G	201	F86	1	0
9	A	1003	GNP	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand F86 G 201



Ligand GNP A 1003



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.

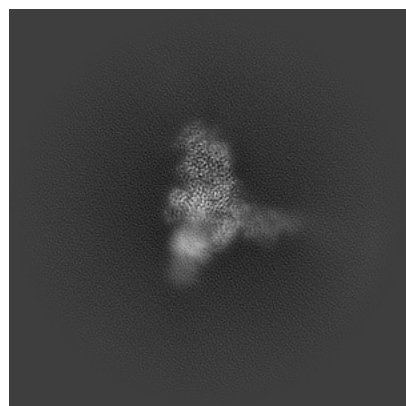
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34314. These allow visual inspection of the internal detail of the map and identification of artifacts.

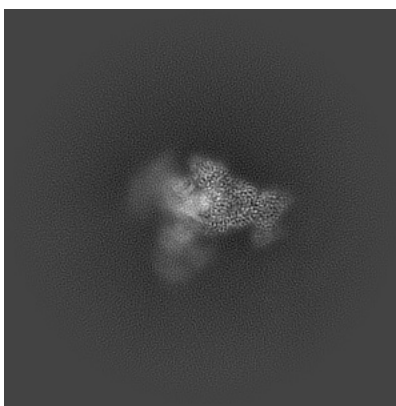
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

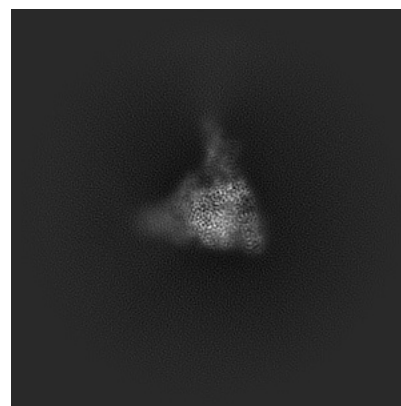
6.1.1 Primary map



X

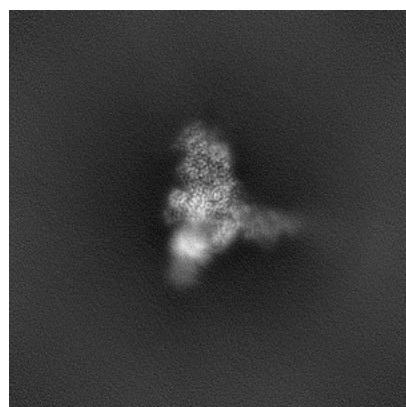


Y

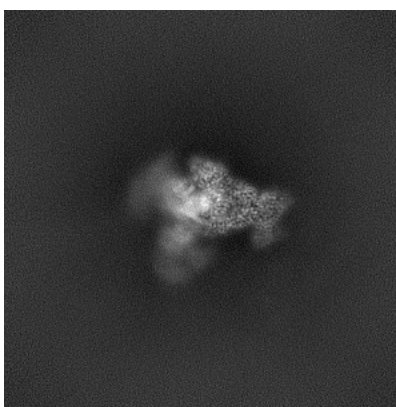


Z

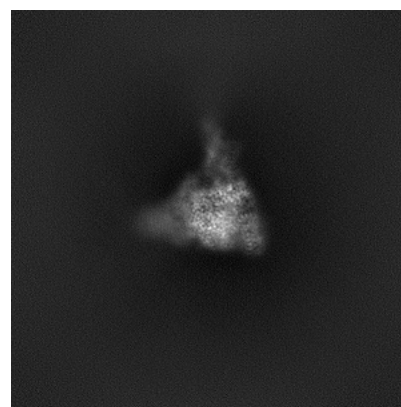
6.1.2 Raw map



X



Y

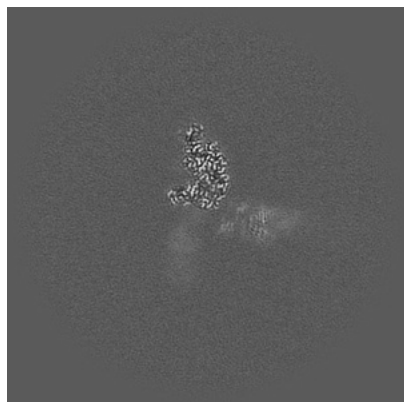


Z

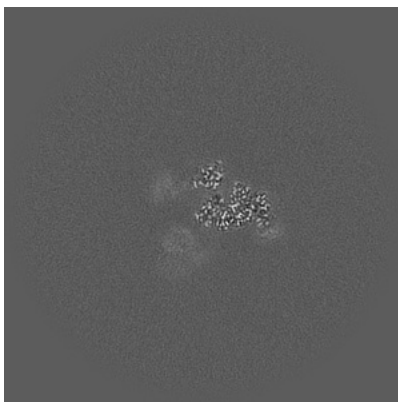
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

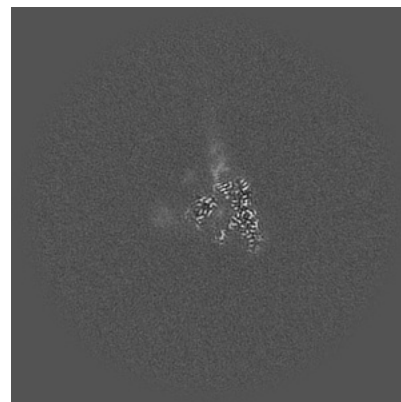
6.2.1 Primary map



X Index: 224



Y Index: 224

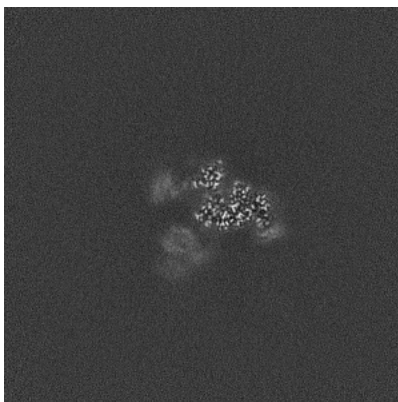


Z Index: 224

6.2.2 Raw map



X Index: 224



Y Index: 224

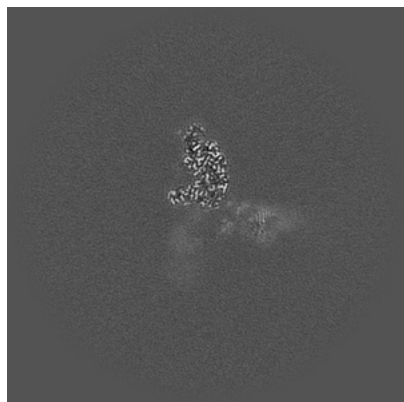


Z Index: 224

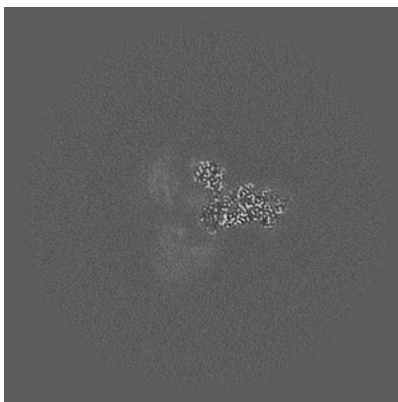
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

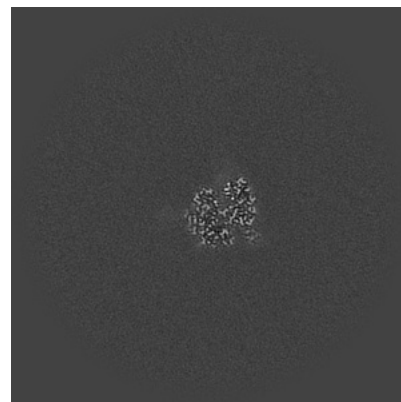
6.3.1 Primary map



X Index: 225



Y Index: 215

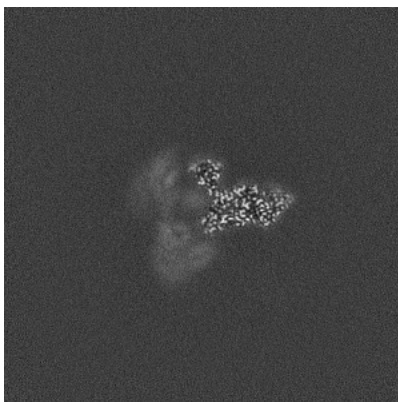


Z Index: 235

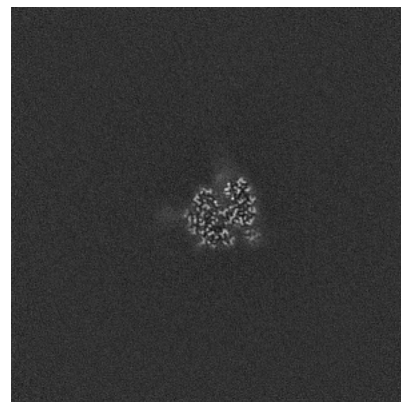
6.3.2 Raw map



X Index: 236



Y Index: 210

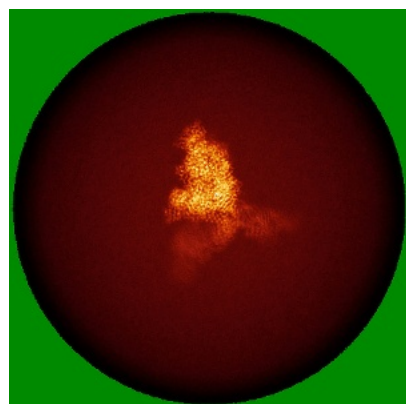


Z Index: 235

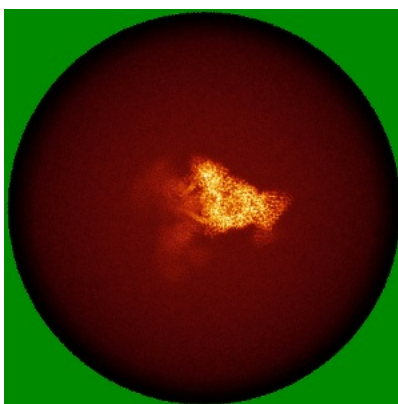
The images above show the largest variance slices of the map in three orthogonal directions.

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

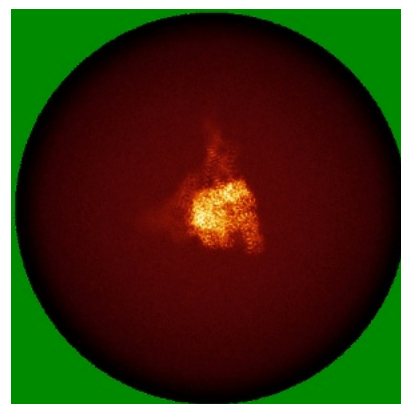
6.4.1 Primary map



X

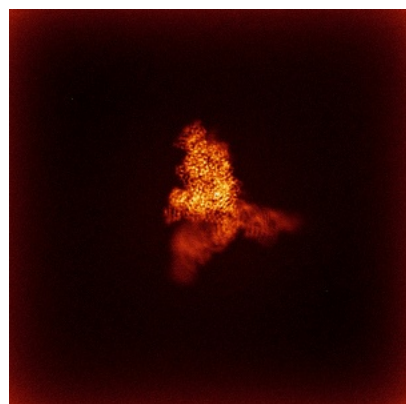


Y

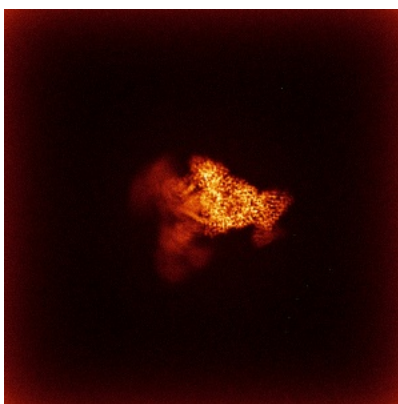


Z

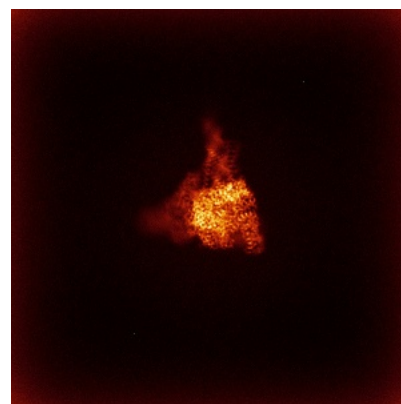
6.4.2 Raw map



X



Y

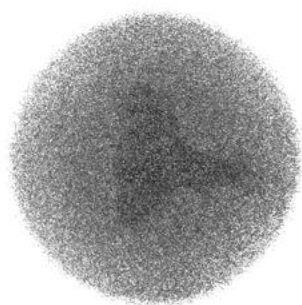


Z

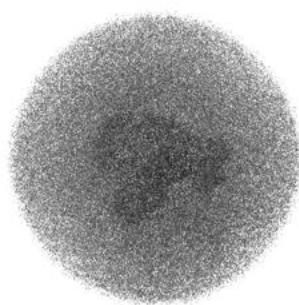
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

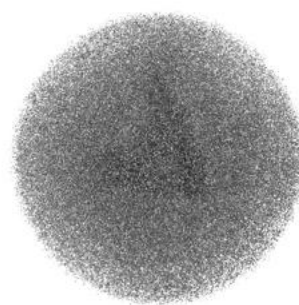
6.5.1 Primary map



X



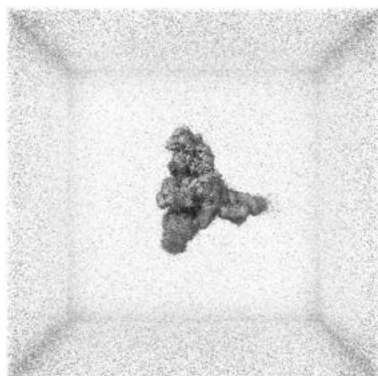
Y



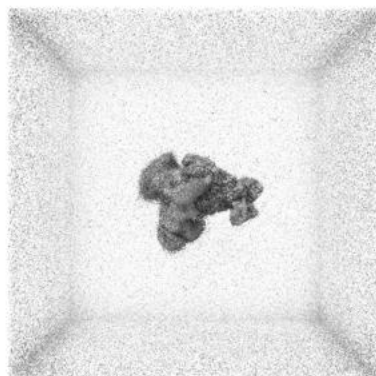
Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

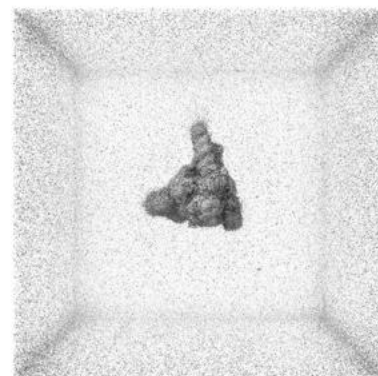
6.5.2 Raw map



X



Y



Z

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

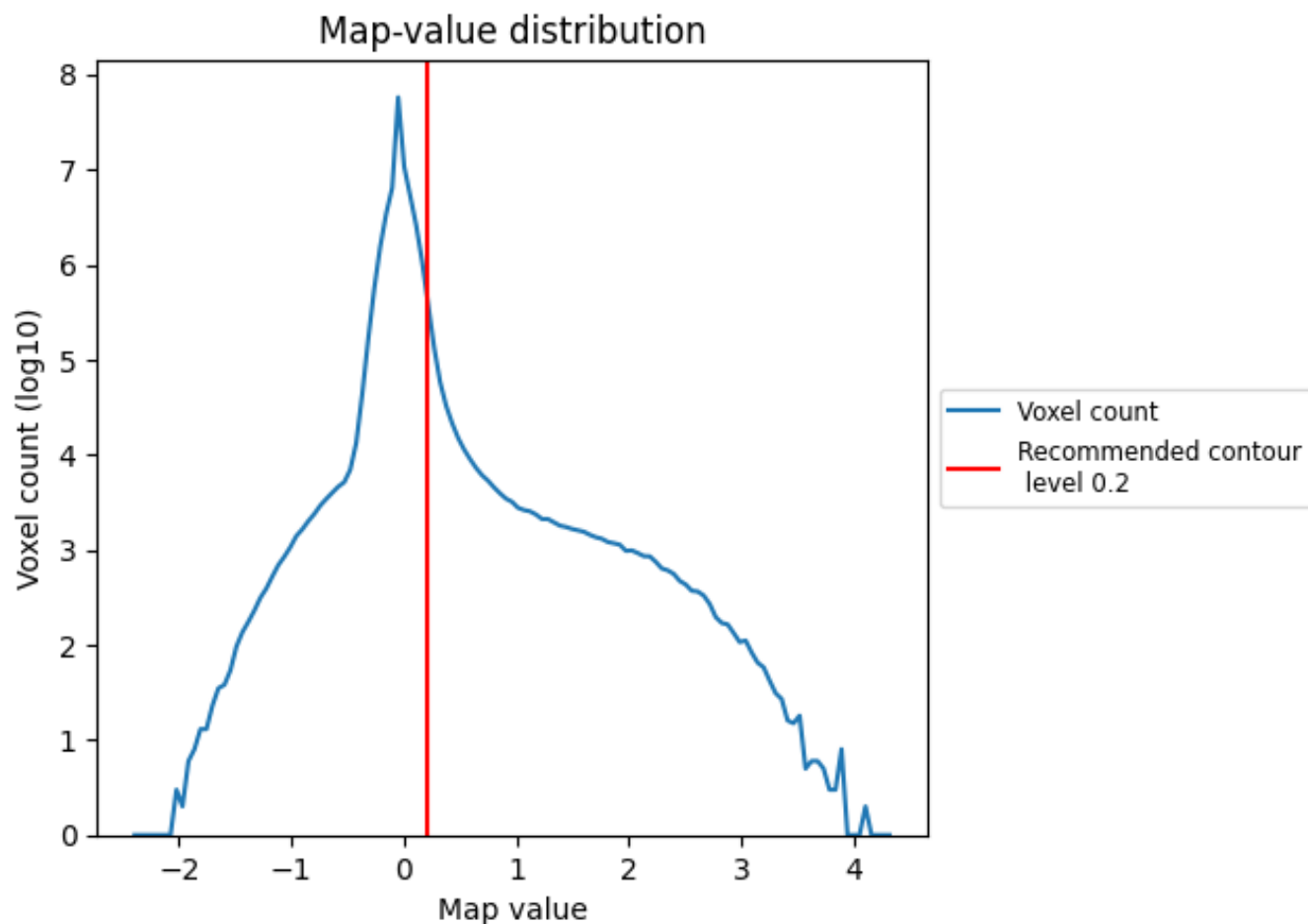
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

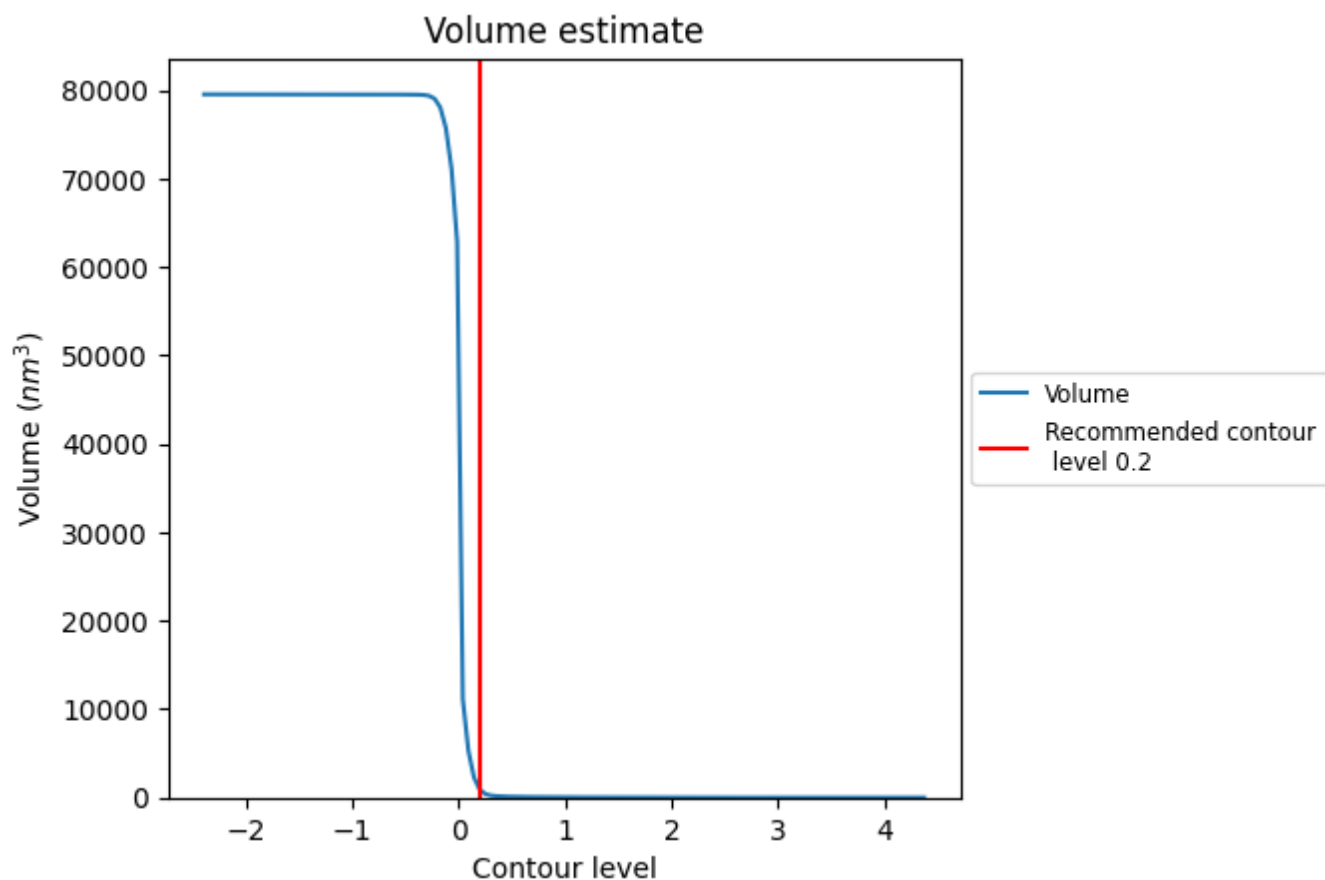
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

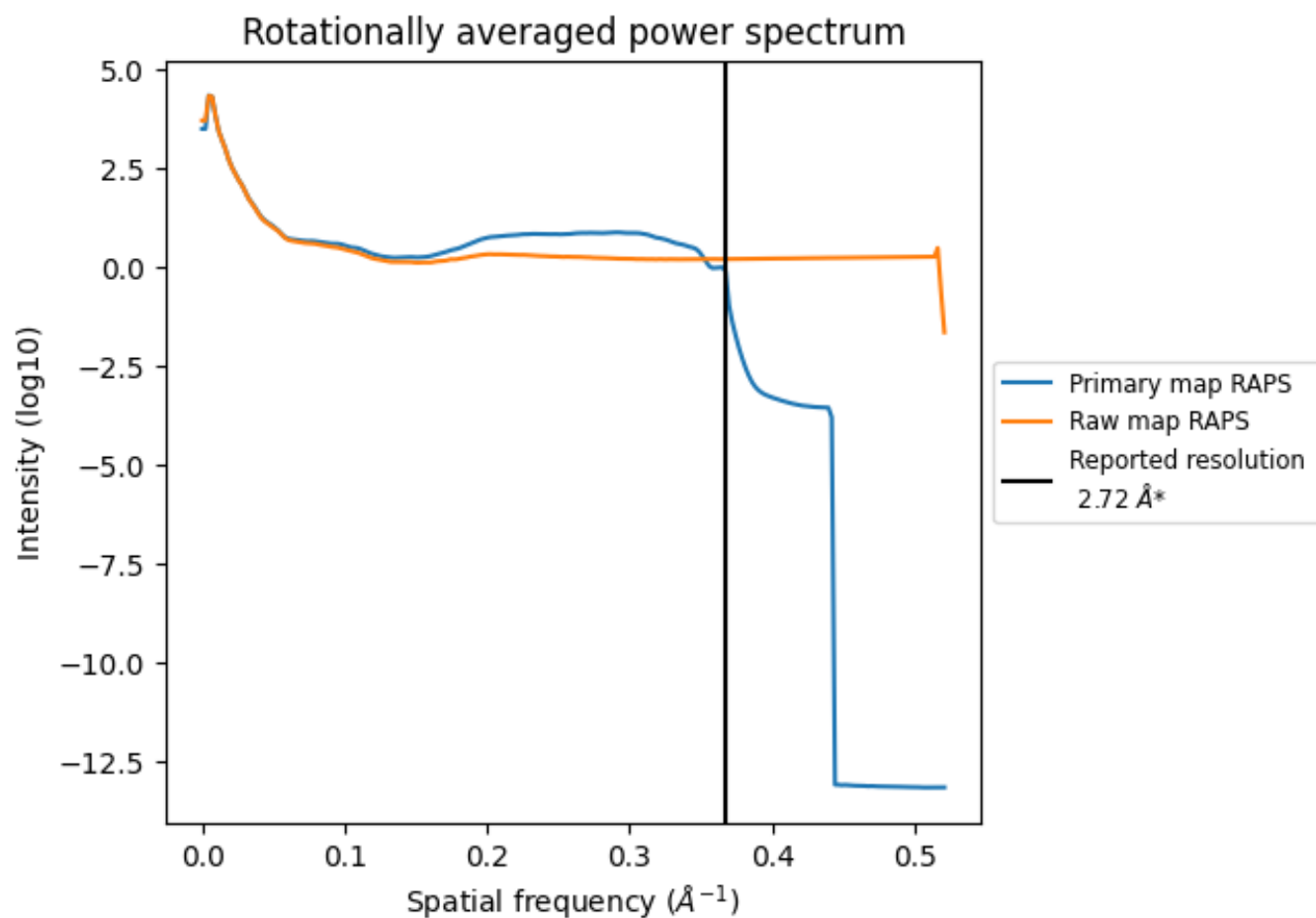
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 884 nm³; this corresponds to an approximate mass of 799 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 ⓘ

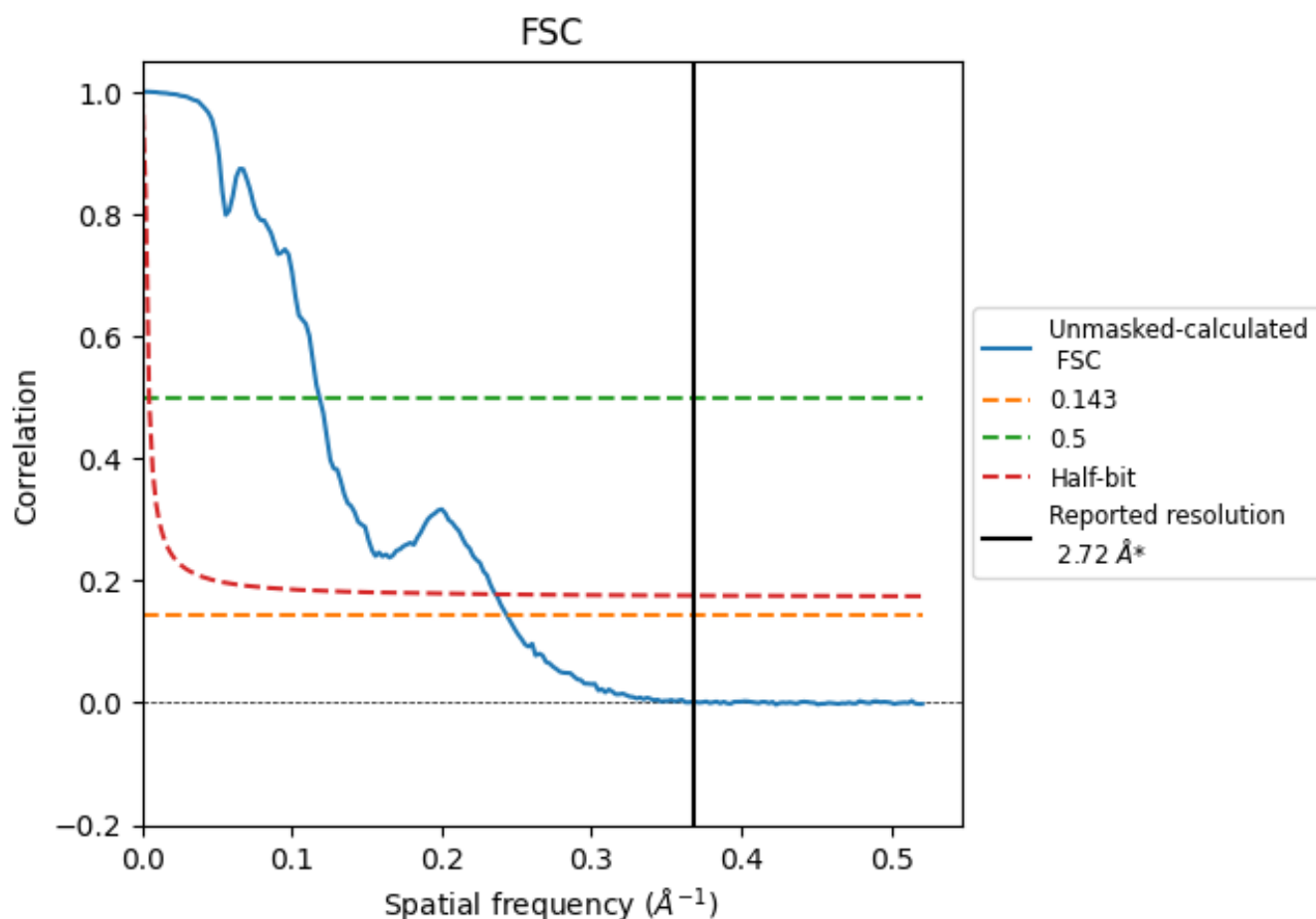


*Reported resolution corresponds to spatial frequency of 0.368 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.368 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.11	8.45	4.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.11 differs from the reported value 2.72 by more than 10 %

9 Map-model fit [i](#)

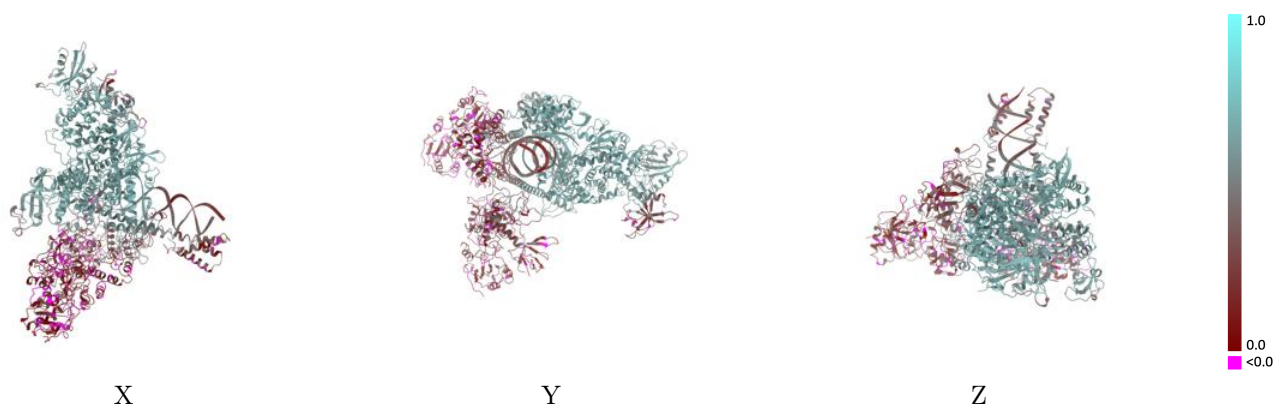
This section contains information regarding the fit between EMDB map EMD-34314 and PDB model 8GWK. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



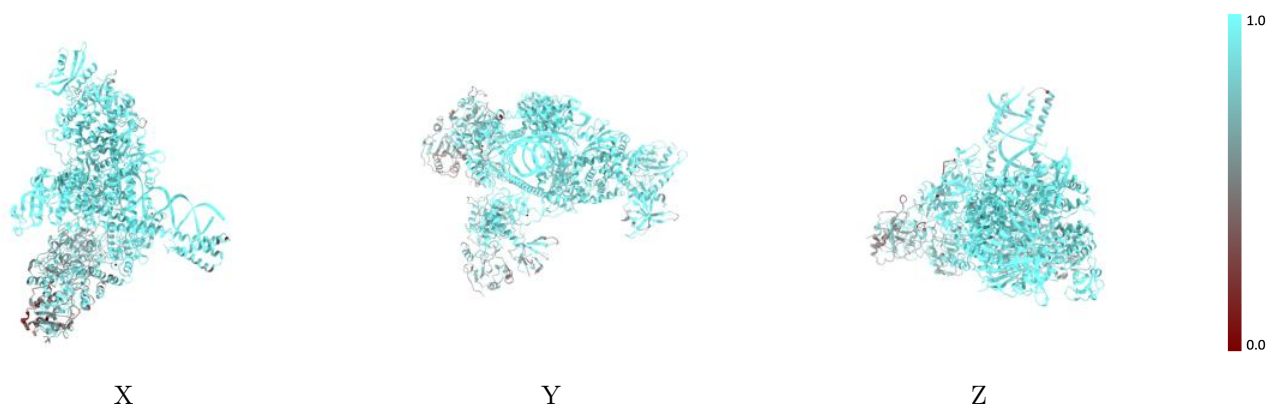
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



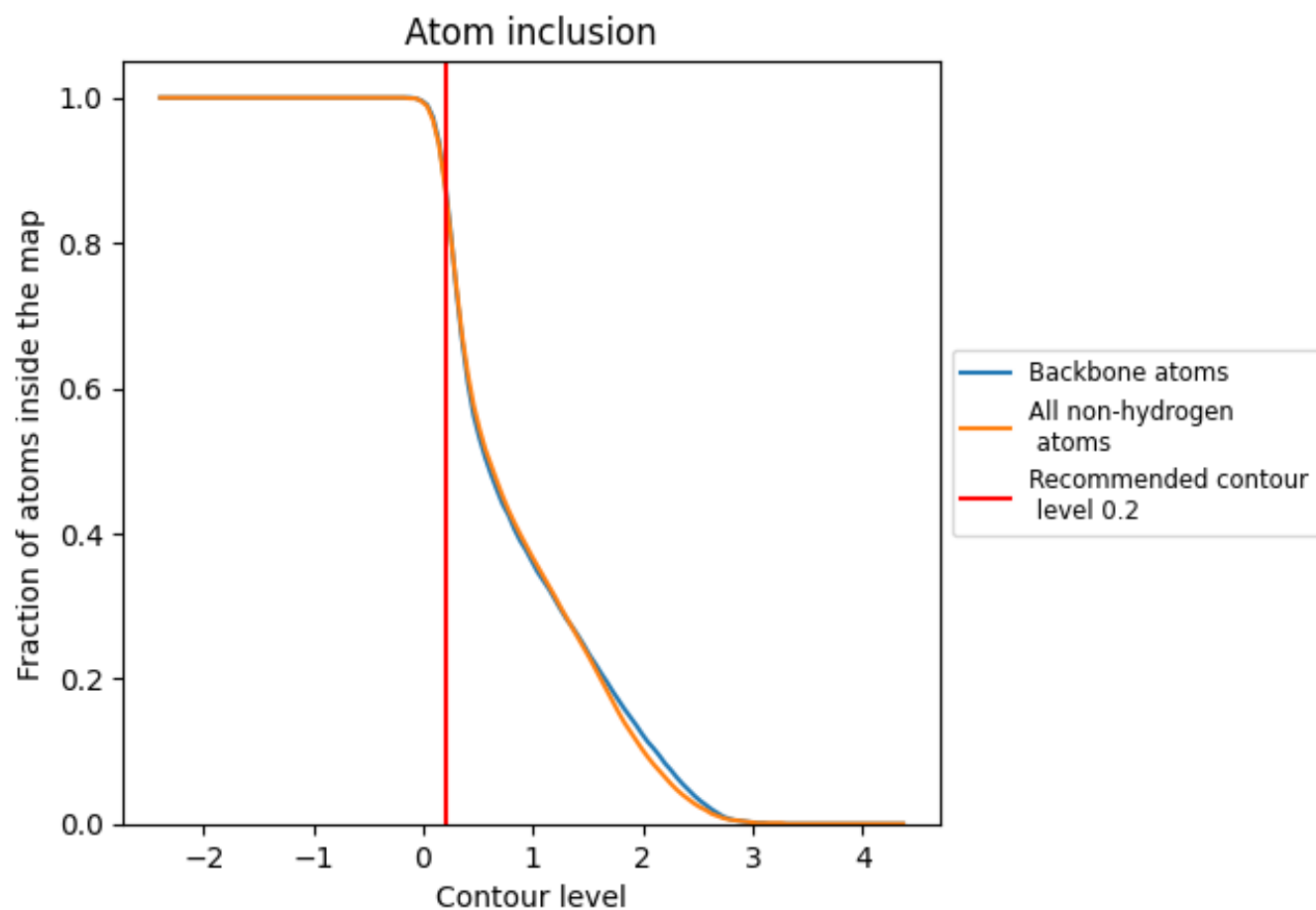
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8780	0.4230
A	0.9940	0.6360
B	0.9720	0.5360
C	0.9850	0.6120
D	0.9730	0.5080
E	0.6900	0.1670
F	0.7720	0.2390
G	0.8670	0.3680
I	0.9890	0.4620
J	0.9850	0.4700

1.0

0.0

<0.0