



Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 09:25 PM EST

PDB ID : 6VVZ
EMDB ID : EMD-21408
Title : Mycobacterium tuberculosis RNAP S456L mutant transcription initiation intermediate structure with Sorangicin
Authors : Lilic, M.; Boyaci, H.; Chen, J.; Darst, S.A.; Campbell, E.A.
Deposited on : 2020-02-18
Resolution : 3.72 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

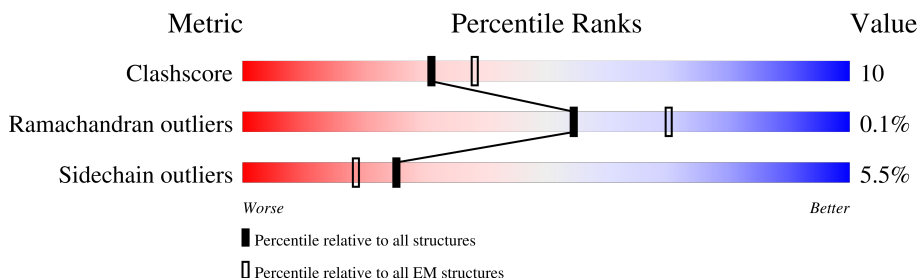
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.72 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	347	
1	B	347	
2	C	1179	
3	D	1326	
4	E	110	
5	F	531	
6	J	111	
7	M	162	

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Mol	Chain	Length	Quality of chain
8	P	90	<div><div><div></div><div></div><div></div></div><div>7%58%11%31%</div></div>
9	O	90	<div><div><div></div><div></div><div></div></div><div>60%12%28%</div></div>

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 29860 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	225	Total	C	N	O	S	0	0
			1716	1080	296	338	2		
1	B	237	Total	C	N	O	S	0	0
			1759	1112	298	346	3		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0
			8577	5377	1504	1657	39		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	456	LEU	SER	engineered mutation	UNP V9Z879
C	1179	LEU	-	expression tag	UNP V9Z879
C	1180	ALA	-	expression tag	UNP V9Z879
C	1181	ARG	-	expression tag	UNP V9Z879
C	1182	HIS	-	expression tag	UNP V9Z879
C	1183	GLY	-	expression tag	UNP V9Z879
C	1184	GLY	-	expression tag	UNP V9Z879
C	1185	SER	-	expression tag	UNP V9Z879

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1266	Total	C	N	O	S	0	0
			9873	6184	1794	1853	42		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP A5U053

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	ALA	-	expression tag	UNP A5U053
D	1317	HIS	-	expression tag	UNP A5U053
D	1318	HIS	-	expression tag	UNP A5U053
D	1319	HIS	-	expression tag	UNP A5U053
D	1320	HIS	-	expression tag	UNP A5U053
D	1321	HIS	-	expression tag	UNP A5U053
D	1322	HIS	-	expression tag	UNP A5U053
D	1323	HIS	-	expression tag	UNP A5U053
D	1324	HIS	-	expression tag	UNP A5U053

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			649	414	108	127		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	GLY	-	expression tag	UNP A0A0T9N9K3

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	319	Total	C	N	O	S	0	0
			2503	1563	456	475	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P9WGI0
F	-1	PRO	-	expression tag	UNP P9WGI0
F	0	HIS	-	expression tag	UNP P9WGI0

- Molecule 6 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	108	Total	C	N	O	S	0	0
			875	540	165	167	3		

- Molecule 7 is a protein called RNA polymerase-binding transcription factor CarD.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	159	Total	C	N	O	S	0	0
			1241	777	224	239	1		

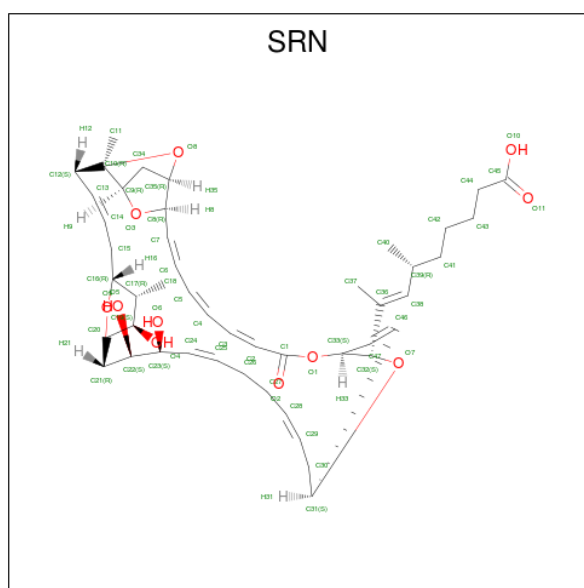
- Molecule 8 is a DNA chain called DNA (62-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	62	Total	C	N	O	P	0	0
			1270	601	239	368	62		

- Molecule 9 is a DNA chain called DNA (65-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	65	Total	C	N	O	P	0	0
			1336	633	243	395	65		

- Molecule 10 is SORANGICIN A (three-letter code: SRN) (formula: $C_{47}H_{66}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
10	C	1	Total	C	O	0
			58	47	11	

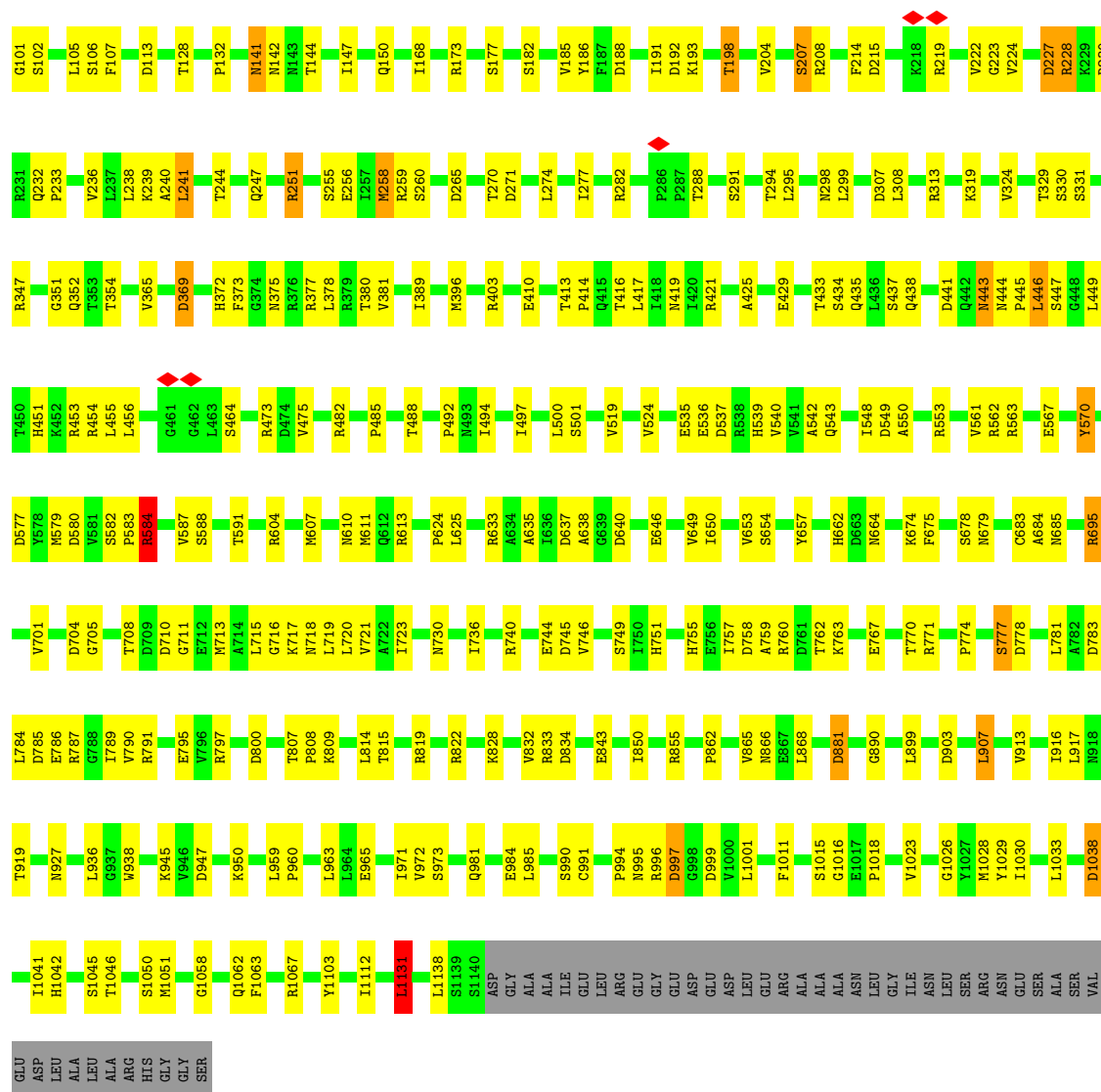
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	D	2	Total	Zn	0
			2	2	

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

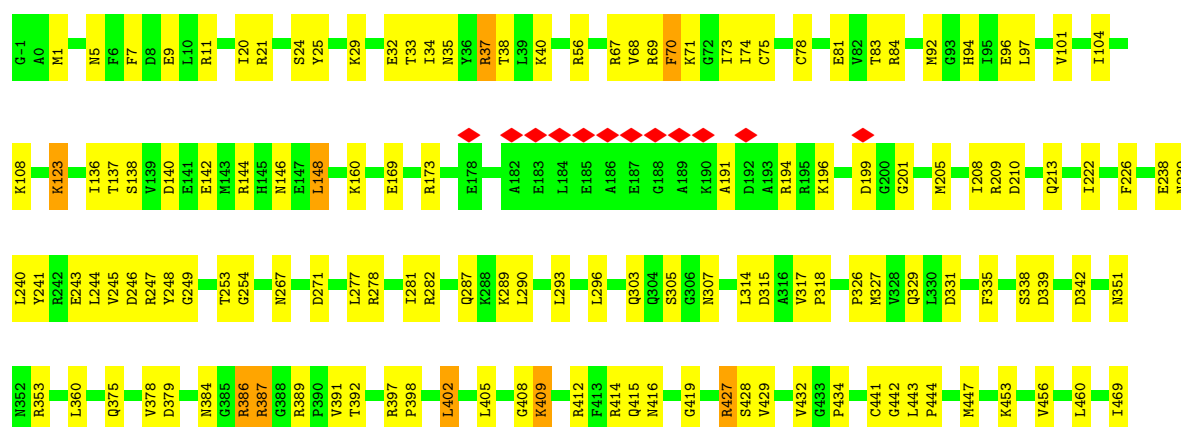
Mol	Chain	Residues	Atoms		AltConf
12	D	1	Total	Mg	0
			1	1	

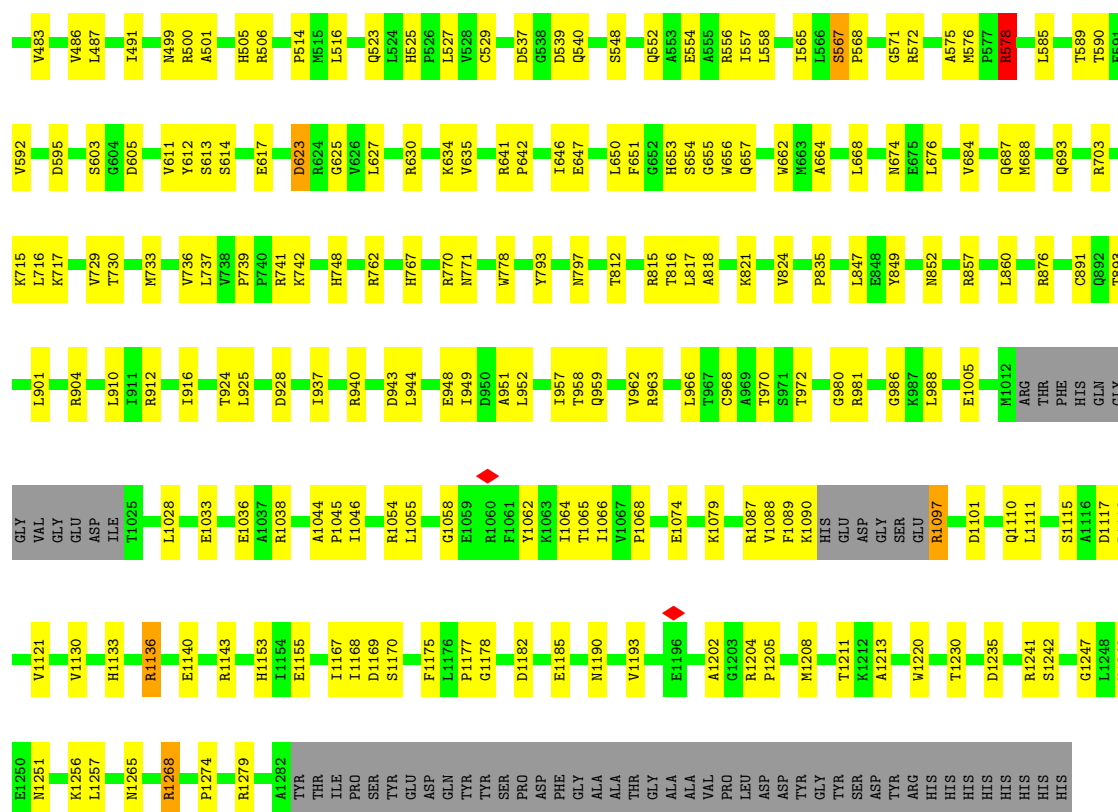




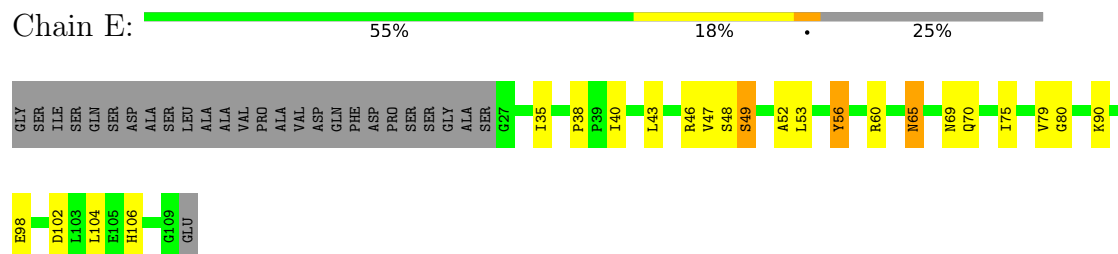
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D: 70% 25% 5%

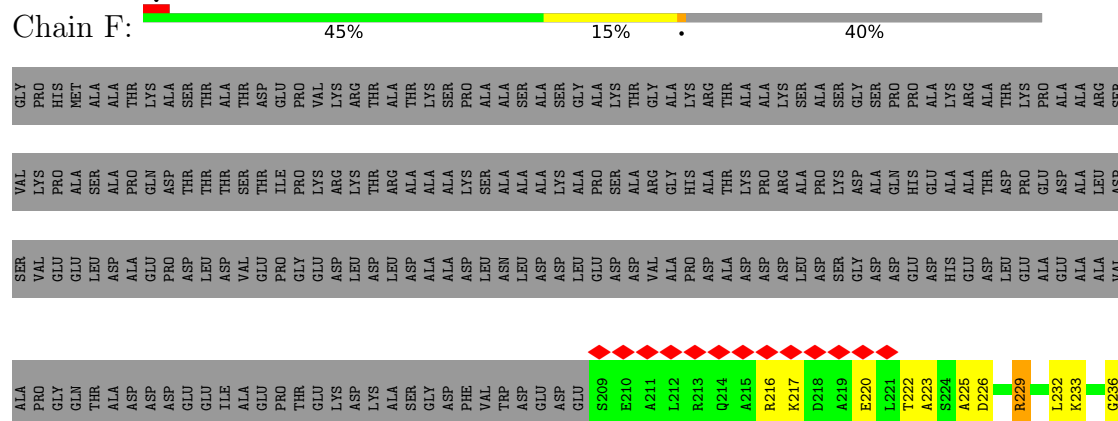




- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor SigA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47371	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 ($e^-/\text{\AA}^2$)	71	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.038	Depositor
Minimum map value	-0.711	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.394	Depositor
Map size (\AA)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

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

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	0/1742	0.56	0/2370
1	B	0.39	0/1786	0.54	0/2435
2	C	0.45	0/8736	0.58	4/11851 (0.0%)
3	D	0.42	0/10037	0.54	2/13570 (0.0%)
4	E	0.41	0/662	0.57	0/901
5	F	0.35	0/2534	0.48	1/3418 (0.0%)
6	J	0.35	0/891	0.54	0/1203
7	M	0.35	0/1257	0.60	0/1700
8	P	0.83	0/1424	1.04	1/2192 (0.0%)
9	O	0.84	0/1497	1.04	2/2310 (0.1%)
All	All	0.47	0/30566	0.62	10/41950 (0.0%)

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	148	LEU	CA-CB-CG	6.61	130.50	115.30
8	P	120	DA	O4'-C1'-N9	6.43	112.50	108.00
9	O	20	DT	O4'-C1'-N1	5.88	112.12	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	266	LEU	CA-CB-CG	5.56	128.08	115.30
2	C	241	LEU	CA-CB-CG	5.44	127.81	115.30
2	C	584	ARG	CA-CB-CG	5.33	125.13	113.40
9	O	42	DT	P-O3'-C3'	5.27	126.03	119.70
3	D	140	ASP	CB-CG-OD2	5.21	122.98	118.30
2	C	1131	LEU	CA-CB-CG	5.12	127.08	115.30
2	C	258	MET	CA-CB-CG	5.04	121.86	113.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	15	THR	Peptide
2	C	282	ARG	Peptide
3	D	501	ALA	Peptide
3	D	578	ARG	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	1716	0	1756	47	0
1	B	1759	0	1783	41	0
2	C	8577	0	8496	202	0
3	D	9873	0	9938	197	0
4	E	649	0	645	14	0
5	F	2503	0	2518	56	0
6	J	875	0	850	26	0
7	M	1241	0	1259	28	0
8	P	1270	0	695	8	0
9	O	1336	0	732	7	0
10	C	58	0	63	11	0
11	D	2	0	0	0	0
12	D	1	0	0	0	0
All	All	29860	0	28735	566	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 10.

All (566) 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)
10:C:1201:SRN:C10	10:C:1201:SRN:C12	1.76	1.59
10:C:1201:SRN:O3	10:C:1201:SRN:C8	1.79	1.29
10:C:1201:SRN:O3	10:C:1201:SRN:C9	1.81	1.28
3:D:144:ARG:O	3:D:148:LEU:HB2	1.57	1.04
10:C:1201:SRN:C10	10:C:1201:SRN:C13	2.50	0.90
5:F:386:LEU:O	5:F:390:LEU:HB3	1.84	0.78
3:D:1169:ASP:HB2	3:D:1202:ALA:H	1.51	0.76
10:C:1201:SRN:C12	10:C:1201:SRN:C9	2.55	0.76
2:C:147:ILE:HG12	7:M:47:ARG:H	1.52	0.74
10:C:1201:SRN:C12	10:C:1201:SRN:C11	2.63	0.74
5:F:492:ILE:O	5:F:496:TYR:HB2	1.93	0.68
5:F:500:ARG:NH2	8:P:126:DG:N7	2.43	0.67
7:M:22:ILE:HA	7:M:35:LEU:HA	1.75	0.66
2:C:548:ILE:HG23	2:C:550:ALA:H	1.59	0.66
3:D:676:LEU:HD12	3:D:715:LYS:HB3	1.79	0.65
2:C:1051:MET:SD	6:J:10:ARG:NH1	2.70	0.65
3:D:739:PRO:HG2	3:D:742:LYS:HB2	1.80	0.64
1:A:2:LEU:HB3	1:B:143:GLY:HA2	1.78	0.64
3:D:824:VAL:HG11	3:D:852:ASN:HA	1.80	0.63
1:B:183:VAL:HA	1:B:188:ASP:H	1.62	0.63
2:C:74:ALA:HA	2:C:77:ARG:HE	1.64	0.63
3:D:924:THR:HG23	3:D:980:GLY:HA2	1.80	0.63
2:C:774:PRO:HD2	2:C:834:ASP:HB2	1.80	0.62
3:D:529:CYS:HB2	3:D:578:ARG:HH22	1.64	0.62
3:D:360:LEU:HD21	5:F:329:ILE:HG21	1.80	0.62
5:F:280:ASP:HB2	6:J:105:ILE:HD13	1.80	0.62
5:F:220:GLU:O	5:F:229:ARG:NH1	2.32	0.61
1:A:6:ARG:HH22	1:B:217:GLU:HB3	1.65	0.61
2:C:150:GLN:HG3	7:M:44:LEU:HB3	1.83	0.61
2:C:583:PRO:HG2	2:C:584:ARG:HH21	1.67	0.60
2:C:62:GLU:HG3	2:C:70:TRP:HB2	1.83	0.60
3:D:646:ILE:O	3:D:650:LEU:HB2	2.02	0.60
3:D:688:MET:HB3	3:D:693:GLN:HE21	1.66	0.60
3:D:891:CYS:SG	3:D:963:ARG:NH2	2.75	0.60
2:C:102:SER:O	2:C:141:ASN:ND2	2.33	0.60
3:D:525:HIS:HE1	3:D:527:LEU:HD12	1.66	0.60
2:C:633:ARG:NH1	2:C:637:ASP:OD2	2.35	0.60
2:C:347:ARG:NH2	2:C:354:THR:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:881:ASP:N	2:C:881:ASP:OD1	2.33	0.59
2:C:771:ARG:NH2	2:C:781:LEU:O	2.36	0.59
3:D:243:GLU:HB3	3:D:247:ARG:HH21	1.66	0.59
2:C:1023:VAL:HA	3:D:730:THR:HG21	1.84	0.59
2:C:403:ARG:NH1	2:C:416:THR:O	2.35	0.59
3:D:71:LYS:O	6:J:27:ARG:NH1	2.36	0.59
3:D:108:LYS:O	3:D:386:ARG:NH1	2.35	0.59
2:C:453:ARG:NH2	2:C:501:SER:O	2.35	0.59
3:D:952:LEU:HD22	3:D:957:ILE:HD11	1.85	0.59
1:B:56:ILE:HG23	1:B:136:VAL:HG22	1.85	0.58
3:D:96:GLU:O	3:D:351:ASN:ND2	2.36	0.58
1:A:153:ARG:NH2	2:C:783:ASP:OD2	2.35	0.58
5:F:500:ARG:NH1	8:P:127:DT:O4	2.36	0.58
6:J:58:ASN:ND2	6:J:60:MET:SD	2.77	0.58
2:C:369:ASP:O	2:C:375:ASN:ND2	2.35	0.58
3:D:67:ARG:NH1	6:J:17:GLU:OE2	2.37	0.58
2:C:683:CYS:SG	2:C:684:ALA:N	2.76	0.57
2:C:938:TRP:HB2	2:C:1026:GLY:HA2	1.86	0.57
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.87	0.57
5:F:216:ARG:O	5:F:220:GLU:HB2	2.03	0.57
2:C:784:LEU:HA	2:C:790:VAL:HA	1.86	0.57
2:C:443:ASN:OD1	2:C:443:ASN:N	2.37	0.57
1:B:71:GLU:HG2	1:B:75:GLU:HB3	1.87	0.57
2:C:855:ARG:NH1	2:C:862:PRO:O	2.37	0.57
3:D:491:ILE:HG23	3:D:514:PRO:HG2	1.85	0.57
2:C:185:VAL:O	2:C:319:LYS:NZ	2.38	0.57
2:C:421:ARG:HH12	8:P:103:DT:H5"	1.70	0.57
6:J:85:LEU:HD12	6:J:88:ARG:HE	1.70	0.57
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.85	0.57
3:D:427:ARG:NH1	3:D:540:GLN:OE1	2.38	0.57
3:D:1058:GLY:H	3:D:1062:TYR:HA	1.69	0.57
3:D:1140:GLU:HA	3:D:1143:ARG:HD2	1.87	0.56
1:B:182:ARG:HG3	1:B:186:ARG:H	1.70	0.56
2:C:38:ARG:NH1	2:C:972:VAL:O	2.39	0.56
2:C:454:ARG:NH1	10:C:1201:SRN:O6	2.37	0.56
3:D:83:THR:OG1	3:D:84:ARG:N	2.36	0.56
2:C:758:ASP:N	2:C:758:ASP:OD1	2.35	0.56
2:C:1042:HIS:NE2	2:C:1063:PHE:O	2.37	0.56
3:D:245:VAL:O	3:D:249:GLY:HA3	2.05	0.56
3:D:1089:PHE:O	3:D:1097:ARG:N	2.39	0.56
2:C:380:THR:OG1	2:C:381:VAL:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:604:ARG:NH1	2:C:607:MET:SD	2.79	0.56
2:C:610:ASN:OD1	2:C:613:ARG:NH2	2.38	0.56
3:D:101:VAL:O	3:D:314:LEU:N	2.35	0.56
3:D:1204:ARG:NH1	3:D:1205:PRO:O	2.38	0.56
1:B:106:THR:HA	1:B:124:HIS:HA	1.87	0.56
2:C:173:ARG:NH1	2:C:437:SER:OG	2.39	0.56
2:C:635:ALA:HB2	2:C:713:MET:HG2	1.88	0.56
3:D:1087:ARG:NH1	3:D:1110:GLN:OE1	2.39	0.56
1:A:142:ARG:NH2	1:B:230:GLU:OE1	2.38	0.56
2:C:38:ARG:HG2	2:C:973:SER:HB3	1.88	0.56
2:C:959:LEU:HD22	2:C:960:PRO:HD2	1.87	0.56
2:C:1050:SER:OG	2:C:1051:MET:N	2.38	0.56
3:D:74:ILE:HD12	6:J:42:VAL:HG13	1.87	0.56
3:D:1274:PRO:HG3	4:E:79:VAL:HG11	1.88	0.56
5:F:248:GLU:OE2	6:J:101:ARG:NH2	2.38	0.56
3:D:24:SER:OG	3:D:25:TYR:N	2.39	0.55
3:D:1055:LEU:HA	3:D:1064:ILE:HG23	1.88	0.55
1:B:71:GLU:OE2	1:B:79:ASN:ND2	2.38	0.55
2:C:265:ASP:OD1	2:C:265:ASP:N	2.39	0.55
1:B:18:ARG:HG3	1:B:197:GLU:HB2	1.89	0.55
2:C:482:ARG:NH2	2:C:536:GLU:OE1	2.38	0.55
2:C:785:ASP:OD2	2:C:787:ARG:NH1	2.39	0.55
3:D:290:LEU:HA	3:D:293:LEU:HD12	1.89	0.55
3:D:641:ARG:HB2	3:D:657:GLN:HE21	1.70	0.55
1:A:225:LEU:O	1:B:205:ARG:NH1	2.39	0.55
4:E:65:ASN:O	4:E:69:ASN:ND2	2.40	0.55
2:C:185:VAL:HG12	2:C:204:VAL:HG22	1.89	0.55
3:D:144:ARG:NH1	3:D:226:PHE:O	2.39	0.55
1:A:9:LEU:HB2	1:B:221:LEU:HB3	1.89	0.55
2:C:613:ARG:NH1	10:C:1201:SRN:O5	2.39	0.55
3:D:20:ILE:HD13	3:D:318:PRO:HD3	1.89	0.55
1:A:53:SER:HA	1:A:164:VAL:HG23	1.89	0.55
2:C:1067:ARG:NH2	3:D:419:GLY:O	2.39	0.55
3:D:1190:ASN:HA	3:D:1193:VAL:HG12	1.87	0.55
2:C:519:VAL:HA	2:C:524:VAL:HA	1.88	0.55
3:D:387:ARG:NH1	5:F:225:ALA:O	2.40	0.55
3:D:605:ASP:OD1	3:D:605:ASP:N	2.40	0.54
3:D:928:ASP:OD1	3:D:940:ARG:N	2.40	0.54
5:F:501:GLU:OE1	8:P:128:DC:N4	2.39	0.54
3:D:329:GLN:HG2	6:J:11:LEU:HD21	1.90	0.54
1:A:71:GLU:HB3	1:A:75:GLU:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:168:ILE:HB	2:C:173:ARG:HD2	1.89	0.54
2:C:188:ASP:OD1	2:C:188:ASP:N	2.41	0.54
3:D:68:VAL:HB	6:J:20:ARG:HH21	1.72	0.54
3:D:642:PRO:HG2	3:D:647:GLU:HB2	1.90	0.54
3:D:387:ARG:HH22	5:F:225:ALA:HA	1.73	0.54
3:D:767:HIS:O	3:D:771:ASN:ND2	2.41	0.54
7:M:115:ASP:HA	7:M:119:GLY:H	1.71	0.54
2:C:740:ARG:O	2:C:744:GLU:HB2	2.08	0.54
2:C:822:ARG:NH1	2:C:828:LYS:O	2.40	0.54
3:D:69:ARG:NH2	5:F:485:GLN:OE1	2.40	0.53
3:D:138:SER:HG	3:D:253:THR:HG1	1.55	0.53
3:D:904:ARG:HB3	3:D:910:LEU:HD13	1.90	0.53
7:M:95:LYS:HZ3	7:M:104:VAL:HA	1.73	0.53
2:C:50:VAL:O	2:C:633:ARG:NH2	2.40	0.53
2:C:494:ILE:HD13	3:D:860:LEU:HB3	1.89	0.53
2:C:1131:LEU:HD23	3:D:402:LEU:HD22	1.90	0.53
2:C:654:SER:HG	2:C:657:TYR:H	1.57	0.53
2:C:808:PRO:HA	2:C:832:VAL:HG12	1.89	0.53
2:C:1015:SER:OG	2:C:1016:GLY:N	2.42	0.53
3:D:37:ARG:NH2	9:O:44:DT:OP1	2.41	0.53
3:D:245:VAL:O	3:D:249:GLY:CA	2.56	0.53
5:F:322:GLN:OE1	5:F:325:ASN:ND2	2.41	0.53
7:M:11:TYR:O	7:M:15:GLY:N	2.42	0.53
2:C:736:ILE:HD11	2:C:916:ILE:HD12	1.90	0.53
4:E:48:SER:OG	4:E:49:SER:N	2.41	0.53
2:C:721:VAL:HG11	2:C:1028:MET:HB2	1.91	0.53
3:D:1168:ILE:HA	3:D:1177:PRO:HA	1.91	0.53
7:M:6:GLY:H	7:M:19:VAL:HG23	1.73	0.53
1:A:57:ASP:OD1	1:A:57:ASP:N	2.41	0.53
5:F:326:LEU:HA	5:F:329:ILE:HD12	1.91	0.53
2:C:224:VAL:HB	2:C:232:GLN:HG3	1.91	0.53
2:C:403:ARG:HD2	2:C:417:LEU:HA	1.90	0.53
2:C:582:SER:OG	2:C:583:PRO:O	2.26	0.53
3:D:1235:ASP:OD1	3:D:1235:ASP:N	2.36	0.52
2:C:256:GLU:HG2	2:C:259:ARG:HH11	1.73	0.52
2:C:563:ARG:HB3	2:C:567:GLU:HB2	1.91	0.52
2:C:678:SER:OG	2:C:679:ASN:N	2.43	0.52
2:C:814:LEU:O	2:C:819:ARG:NH2	2.41	0.52
5:F:295:LEU:O	5:F:299:ASN:ND2	2.39	0.52
3:D:191:ALA:HA	3:D:194:ARG:HE	1.74	0.52
2:C:150:GLN:HB2	2:C:414:PRO:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:451:HIS:HD2	10:C:1201:SRN:H23	1.73	0.52
1:B:36:ASN:ND2	2:C:1015:SER:O	2.41	0.52
2:C:232:GLN:NE2	2:C:233:PRO:O	2.43	0.52
2:C:236:VAL:HG12	2:C:277:ILE:HG12	1.92	0.52
2:C:809:LYS:HB2	2:C:833:ARG:HB2	1.91	0.52
5:F:289:ASP:O	5:F:293:ASN:ND2	2.43	0.52
2:C:434:SER:OG	2:C:435:GLN:N	2.42	0.52
3:D:1068:PRO:HD3	3:D:1074:GLU:HA	1.91	0.52
2:C:425:ALA:O	2:C:429:GLU:HB2	2.09	0.52
7:M:18:LEU:HB2	7:M:38:LYS:HE3	1.92	0.52
3:D:38:THR:HG23	3:D:40:LYS:H	1.74	0.52
5:F:392:ARG:NH1	5:F:393:GLU:O	2.43	0.52
7:M:74:LEU:HG	7:M:75:ARG:HG3	1.92	0.52
1:A:186:ARG:NH1	1:B:149:ALA:O	2.43	0.52
2:C:1045:SER:OG	2:C:1046:THR:N	2.43	0.52
5:F:293:ASN:HA	5:F:296:LEU:HD12	1.91	0.52
2:C:113:ASP:HB2	2:C:132:PRO:HD2	1.91	0.51
2:C:144:THR:O	7:M:52:ASN:ND2	2.42	0.51
2:C:232:GLN:HE22	2:C:236:VAL:HB	1.74	0.51
3:D:613:SER:N	3:D:617:GLU:OE1	2.42	0.51
1:A:100:GLN:NE2	1:A:132:GLY:O	2.42	0.51
2:C:485:PRO:O	3:D:857:ARG:NH2	2.42	0.51
3:D:173:ARG:HH21	3:D:201:GLY:HA2	1.74	0.51
3:D:412:ARG:NH1	3:D:415:GLN:OE1	2.41	0.51
3:D:1170:SER:HA	3:D:1175:PHE:HB2	1.92	0.51
5:F:328:LEU:HD23	5:F:351:ILE:HD11	1.93	0.51
7:M:24:THR:HB	7:M:31:GLN:HB3	1.93	0.51
1:A:64:THR:OG1	1:A:65:THR:N	2.42	0.51
1:A:99:LYS:NZ	1:A:109:ASP:OD2	2.40	0.51
1:A:144:ARG:NH1	1:B:27:GLU:OE2	2.43	0.51
3:D:101:VAL:HG13	3:D:375:GLN:HE22	1.76	0.51
3:D:326:PRO:O	3:D:338:SER:OG	2.29	0.51
4:E:60:ARG:NH2	4:E:80:GLY:O	2.44	0.51
5:F:502:ARG:NH1	5:F:505:GLN:OE1	2.43	0.51
6:J:34:THR:HA	6:J:62:GLY:HA2	1.93	0.51
1:A:3:ILE:O	1:B:144:ARG:NH2	2.42	0.51
1:B:128:LEU:HD11	1:B:134:LEU:HD22	1.93	0.51
3:D:35:ASN:HD22	3:D:38:THR:HG22	1.76	0.51
3:D:331:ASP:OD1	3:D:331:ASP:N	2.42	0.51
2:C:664:ASN:N	2:C:664:ASN:OD1	2.44	0.51
2:C:758:ASP:HB3	2:C:868:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:215:ASP:HB2	2:C:223:GLY:HA3	1.93	0.51
2:C:351:GLY:O	2:C:352:GLN:NE2	2.44	0.51
2:C:207:SER:OG	2:C:307:ASP:O	2.28	0.50
2:C:740:ARG:NH1	2:C:744:GLU:OE1	2.43	0.50
2:C:749:SER:OG	2:C:751:HIS:NE2	2.43	0.50
3:D:966:LEU:HD11	3:D:1155:GLU:HG2	1.93	0.50
5:F:238:VAL:HG21	5:F:297:GLU:HB3	1.93	0.50
3:D:1036:GLU:HB3	3:D:1038:ARG:HG2	1.92	0.50
2:C:214:PHE:HD1	2:C:224:VAL:HG13	1.75	0.50
2:C:587:VAL:HG22	2:C:591:THR:HB	1.92	0.50
2:C:759:ALA:O	2:C:866:ASN:N	2.39	0.50
2:C:945:LYS:HA	2:C:965:GLU:HA	1.93	0.50
5:F:463:VAL:O	5:F:466:THR:OG1	2.28	0.50
1:A:102:PRO:HD3	1:A:130:ASP:HA	1.93	0.50
3:D:444:PRO:HG2	3:D:447:MET:HB3	1.93	0.50
1:A:99:LYS:HG2	1:A:105:VAL:HG22	1.94	0.50
1:A:153:ARG:HD2	2:C:797:ARG:HE	1.76	0.50
5:F:260:THR:O	5:F:264:THR:OG1	2.26	0.50
5:F:311:THR:OG1	5:F:312:GLY:N	2.44	0.50
5:F:449:ASP:OD1	5:F:449:ASP:N	2.40	0.50
1:B:199:LYS:HG3	1:B:201:SER:H	1.77	0.50
2:C:271:ASP:HA	2:C:274:LEU:HB2	1.93	0.50
2:C:625:LEU:HA	2:C:971:ILE:HG22	1.94	0.50
2:C:1138:LEU:HB2	3:D:9:GLU:HB3	1.94	0.50
3:D:137:THR:OG1	3:D:267:ASN:ND2	2.38	0.50
3:D:169:GLU:HB3	3:D:208:ILE:HD13	1.93	0.50
1:A:43:LEU:HA	1:A:171:VAL:HG11	1.94	0.50
1:B:102:PRO:HB3	1:B:130:ASP:HA	1.93	0.50
2:C:45:ARG:HH12	2:C:47:PRO:HG3	1.77	0.50
2:C:71:ARG:NH1	2:C:82:PRO:O	2.45	0.50
2:C:762:THR:OG1	2:C:763:LYS:N	2.44	0.50
3:D:527:LEU:HD11	3:D:717:LYS:HB2	1.94	0.50
2:C:542:ALA:HB3	2:C:579:MET:HG3	1.93	0.49
2:C:611:MET:HG3	2:C:1033:LEU:HD21	1.94	0.49
2:C:723:ILE:O	2:C:919:THR:OG1	2.30	0.49
2:C:760:ARG:HG2	2:C:865:VAL:HG22	1.94	0.49
3:D:278:ARG:HB3	3:D:282:ARG:HH21	1.76	0.49
3:D:500:ARG:NH2	3:D:539:ASP:OD2	2.45	0.49
7:M:71:PHE:HA	7:M:74:LEU:HD22	1.94	0.49
2:C:650:ILE:HG21	2:C:653:VAL:HG13	1.94	0.49
2:C:705:GLY:N	2:C:708:THR:OG1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:907:LEU:HD11	2:C:1001:LEU:HB3	1.94	0.49
1:B:41:THR:HG21	1:B:215:LEU:HG	1.94	0.49
2:C:947:ASP:OD1	2:C:947:ASP:N	2.41	0.49
3:D:589:THR:HG21	3:D:688:MET:HG2	1.94	0.49
1:A:10:SER:OG	1:A:22:VAL:O	2.31	0.49
1:A:155:SER:OG	1:A:156:GLY:N	2.44	0.49
1:A:173:LYS:HB3	1:A:197:GLU:HB3	1.94	0.49
1:B:97:LEU:HB3	1:B:136:VAL:HB	1.95	0.49
1:B:200:ASN:OD1	1:B:200:ASN:N	2.39	0.49
3:D:651:PHE:HE2	3:D:655:GLY:HA2	1.76	0.49
2:C:240:ALA:HA	2:C:274:LEU:HD22	1.93	0.49
2:C:288:THR:HG23	2:C:291:SER:HB3	1.94	0.49
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.42	0.49
2:C:354:THR:HA	2:C:365:VAL:H	1.77	0.49
3:D:554:GLU:O	3:D:558:LEU:HB2	2.13	0.49
5:F:336:ASP:OD1	5:F:338:THR:OG1	2.28	0.49
3:D:432:VAL:HG13	3:D:434:PRO:HD3	1.95	0.49
5:F:344:SER:O	5:F:348:THR:OG1	2.31	0.48
6:J:88:ARG:HG2	6:J:89:ARG:HG2	1.95	0.48
3:D:1208:MET:HG3	3:D:1213:ALA:HB2	1.95	0.48
1:B:104:GLU:HA	1:B:127:THR:HA	1.94	0.48
2:C:646:GLU:OE1	2:C:662:HIS:ND1	2.46	0.48
3:D:767:HIS:CE1	3:D:771:ASN:HD21	2.32	0.48
2:C:101:GLY:O	2:C:142:ASN:ND2	2.47	0.48
2:C:715:LEU:N	2:C:1029:TYR:OH	2.46	0.48
3:D:222:ILE:HG13	3:D:244:LEU:HD12	1.95	0.48
2:C:789:ILE:HD13	2:C:850:ILE:HD13	1.95	0.48
1:B:28:PRO:HA	1:B:29:GLY:HA2	1.58	0.48
2:C:90:LEU:O	2:C:94:SER:N	2.44	0.48
3:D:329:GLN:HA	3:D:335:PHE:HA	1.95	0.48
3:D:568:PRO:O	3:D:1153:HIS:NE2	2.35	0.48
1:A:183:VAL:HG13	1:A:185:GLN:H	1.78	0.48
2:C:927:ASN:OD1	2:C:927:ASN:N	2.46	0.48
3:D:246:ASP:N	3:D:246:ASP:OD1	2.42	0.48
3:D:912:ARG:HG3	3:D:916:ILE:HD12	1.96	0.48
7:M:115:ASP:HB3	7:M:120:LEU:HD13	1.94	0.48
2:C:783:ASP:O	2:C:791:ARG:NH2	2.47	0.48
2:C:807:THR:O	2:C:833:ARG:N	2.47	0.48
3:D:384:ASN:ND2	3:D:391:VAL:O	2.40	0.48
1:A:83:LEU:HA	1:A:120:ASN:HD21	1.78	0.48
1:A:151:GLN:NE2	2:C:795:GLU:OE2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:GLU:HG3	1:B:21:PHE:HE1	1.78	0.48
2:C:755:HIS:NE2	2:C:843:GLU:OE1	2.40	0.48
2:C:770:THR:OG1	2:C:771:ARG:N	2.46	0.48
6:J:90:SER:OG	6:J:92:GLU:OE1	2.31	0.48
7:M:88:ARG:O	7:M:92:ASN:ND2	2.47	0.48
1:A:104:GLU:HG3	1:A:124:HIS:HD2	1.78	0.48
1:A:219:PHE:HE1	1:B:34:LEU:HB2	1.78	0.48
3:D:585:LEU:O	3:D:589:THR:OG1	2.27	0.48
1:A:184:GLU:OE1	1:A:186:ARG:NH2	2.44	0.47
2:C:607:MET:O	2:C:611:MET:HB2	2.14	0.47
2:C:1058:GLY:O	2:C:1062:GLN:NE2	2.47	0.47
3:D:405:LEU:O	3:D:412:ARG:N	2.46	0.47
4:E:52:ALA:O	4:E:56:TYR:HB2	2.14	0.47
7:M:34:TYR:HB3	7:M:47:ARG:HG3	1.96	0.47
7:M:70:VAL:O	7:M:109:ARG:NH1	2.45	0.47
7:M:132:ARG:O	7:M:136:VAL:HB	2.13	0.47
2:C:313:ARG:HG3	2:C:331:SER:HA	1.96	0.47
2:C:372:HIS:NE2	2:C:537:ASP:OD2	2.46	0.47
2:C:435:GLN:HA	10:C:1201:SRN:H5	1.97	0.47
2:C:455:LEU:HD21	2:C:500:LEU:HG	1.96	0.47
5:F:297:GLU:HA	5:F:300:LEU:HD12	1.96	0.47
2:C:429:GLU:OE2	2:C:433:THR:OG1	2.32	0.47
2:C:454:ARG:HE	2:C:497:ILE:HG22	1.79	0.47
3:D:389:ARG:HH12	5:F:226:ASP:HB2	1.80	0.47
2:C:994:PRO:HB3	2:C:999:ASP:H	1.79	0.47
3:D:136:ILE:HA	3:D:254:GLY:HA2	1.96	0.47
5:F:305:SER:HA	5:F:308:LYS:HD2	1.97	0.47
1:A:56:ILE:HB	1:A:59:VAL:HG22	1.97	0.47
2:C:473:ARG:NH1	2:C:492:PRO:O	2.45	0.47
3:D:943:ASP:OD2	3:D:981:ARG:NE	2.46	0.47
4:E:38:PRO:HG2	4:E:43:LEU:HD11	1.97	0.47
4:E:40:ILE:HA	4:E:43:LEU:HB2	1.97	0.47
6:J:15:SER:OG	6:J:16:TYR:N	2.47	0.47
2:C:446:LEU:HB2	2:C:713:MET:HE1	1.95	0.47
2:C:675:PHE:N	2:C:685:ASN:OD1	2.44	0.47
3:D:408:GLY:O	3:D:414:ARG:NH1	2.47	0.47
3:D:537:ASP:N	3:D:537:ASP:OD1	2.38	0.47
3:D:1033:GLU:HB2	3:D:1038:ARG:HB2	1.97	0.47
3:D:327:MET:HG2	3:D:335:PHE:HD2	1.80	0.47
3:D:968:CYS:SG	3:D:970:THR:OG1	2.72	0.47
2:C:543:GLN:NE2	2:C:580:ASP:OD2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:1201:SRN:O3	10:C:1201:SRN:C35	2.55	0.47
3:D:386:ARG:HH21	3:D:1230:THR:HG21	1.79	0.47
3:D:1054:ARG:HB3	3:D:1065:THR:HB	1.95	0.47
7:M:10:VAL:HA	7:M:16:ALA:HA	1.96	0.47
1:A:18:ARG:HH12	2:C:996:ARG:HH12	1.62	0.47
2:C:144:THR:OG1	7:M:52:ASN:ND2	2.47	0.47
2:C:535:GLU:O	2:C:539:HIS:ND1	2.48	0.47
2:C:717:LYS:NZ	2:C:746:VAL:O	2.42	0.47
3:D:428:SER:OG	3:D:429:VAL:N	2.46	0.47
2:C:704:ASP:OD2	2:C:710:ASP:N	2.44	0.46
3:D:1055:LEU:N	3:D:1101:ASP:OD1	2.43	0.46
7:M:87:ARG:HH22	9:O:51:DG:H8	1.63	0.46
3:D:592:VAL:HG21	3:D:630:ARG:HH21	1.80	0.46
3:D:611:VAL:HG12	3:D:634:LYS:HB2	1.96	0.46
1:B:56:ILE:HG12	1:B:136:VAL:HG13	1.96	0.46
3:D:73:ILE:HD12	6:J:45:ALA:HB2	1.97	0.46
3:D:241:TYR:OH	3:D:254:GLY:O	2.29	0.46
9:O:22:DG:H2'	9:O:23:DT:H71	1.97	0.46
3:D:812:THR:HB	3:D:815:ARG:HH21	1.80	0.46
1:B:69:VAL:HG12	1:B:128:LEU:HG	1.98	0.46
2:C:239:LYS:HB3	2:C:270:THR:HA	1.96	0.46
3:D:469:ILE:HD11	5:F:452:SER:HB2	1.98	0.46
3:D:487:LEU:HD23	3:D:516:LEU:HD11	1.97	0.46
5:F:381:ARG:NH2	8:P:104:DC:O3'	2.48	0.46
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.51	0.46
4:E:47:VAL:HG21	4:E:53:LEU:HB2	1.98	0.46
4:E:98:GLU:HB3	4:E:104:LEU:HD11	1.97	0.46
2:C:238:LEU:HD13	2:C:241:LEU:HD23	1.96	0.46
2:C:797:ARG:N	2:C:800:ASP:OD2	2.41	0.46
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.97	0.46
3:D:1167:ILE:O	3:D:1178:GLY:N	2.48	0.46
2:C:329:THR:OG1	2:C:330:SER:N	2.49	0.46
2:C:995:ASN:N	2:C:995:ASN:OD1	2.42	0.46
3:D:32:GLU:HG2	5:F:367:ARG:HD3	1.98	0.46
3:D:74:ILE:HG12	3:D:81:GLU:HB2	1.97	0.46
1:A:149:ALA:N	1:A:165:ASP:OD1	2.48	0.46
3:D:1044:ALA:N	3:D:1115:SER:O	2.48	0.46
6:J:36:ASN:OD1	6:J:36:ASN:N	2.40	0.46
3:D:142:GLU:O	3:D:146:ASN:ND2	2.40	0.46
3:D:392:THR:HA	3:D:398:PRO:HA	1.97	0.46
3:D:958:THR:OG1	3:D:959:GLN:OE1	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:35:LEU:N	7:M:48:VAL:O	2.44	0.46
2:C:89:VAL:HG11	2:C:389:ILE:HG22	1.99	0.45
2:C:449:LEU:HD13	2:C:638:ALA:HA	1.98	0.45
2:C:809:LYS:H	2:C:832:VAL:HA	1.80	0.45
2:C:981:GLN:N	2:C:984:GLU:OE1	2.44	0.45
3:D:271:ASP:OD1	3:D:303:GLN:NE2	2.47	0.45
3:D:305:SER:OG	3:D:307:ASN:ND2	2.49	0.45
3:D:1045:PRO:O	3:D:1111:LEU:N	2.43	0.45
1:A:184:GLU:O	1:A:185:GLN:NE2	2.49	0.45
2:C:191:ILE:HA	2:C:198:THR:HA	1.99	0.45
3:D:627:LEU:HD13	3:D:668:LEU:HD12	1.97	0.45
5:F:461:GLN:OE1	5:F:476:ARG:NH2	2.46	0.45
2:C:106:SER:OG	2:C:107:PHE:N	2.49	0.45
2:C:717:LYS:HG3	2:C:746:VAL:HG12	1.97	0.45
2:C:760:ARG:N	2:C:767:GLU:OE1	2.42	0.45
3:D:612:TYR:HB2	3:D:635:VAL:HG12	1.98	0.45
5:F:470:ARG:HG2	5:F:496:TYR:HE1	1.81	0.45
2:C:227:ASP:OD1	2:C:228:ARG:NH1	2.49	0.45
2:C:577:ASP:OD1	2:C:577:ASP:N	2.49	0.45
2:C:294:THR:O	2:C:298:ASN:N	2.48	0.45
3:D:277:LEU:HB3	3:D:296:LEU:HD22	1.98	0.45
2:C:730:ASN:ND2	2:C:917:LEU:O	2.41	0.45
2:C:464:SER:OG	8:P:96:DC:OP1	2.27	0.45
3:D:1046:ILE:HA	3:D:1110:GLN:HA	1.99	0.45
1:A:24:GLU:HB3	1:A:191:LYS:HG3	1.97	0.45
3:D:1220:TRP:NE1	3:D:1241:ARG:O	2.50	0.45
5:F:217:LYS:HD3	5:F:217:LYS:HA	1.77	0.45
2:C:757:ILE:HD12	2:C:757:ILE:HA	1.81	0.45
3:D:1182:ASP:OD2	3:D:1185:GLU:N	2.49	0.45
2:C:716:GLY:N	2:C:1029:TYR:OH	2.43	0.44
3:D:56:ARG:HG2	6:J:13:ALA:H	1.82	0.44
3:D:97:LEU:HD11	3:D:317:VAL:HG23	1.98	0.44
2:C:649:VAL:HA	2:C:695:ARG:HA	1.98	0.44
2:C:719:LEU:HD22	2:C:1030:ILE:HD11	1.99	0.44
2:C:777:SER:OG	2:C:778:ASP:N	2.49	0.44
3:D:409:LYS:HA	3:D:414:ARG:HD2	1.99	0.44
1:A:100:GLN:HE22	1:A:133:LYS:HB2	1.82	0.44
2:C:990:SER:OG	2:C:991:CYS:N	2.50	0.44
1:A:91:GLU:H	1:A:91:GLU:HG2	1.57	0.44
1:B:150:VAL:HG13	1:B:155:SER:HB3	1.99	0.44
3:D:505:HIS:CD2	3:D:1005:GLU:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:972:THR:O	3:D:972:THR:OG1	2.31	0.44
3:D:981:ARG:HD3	3:D:986:GLY:HA2	2.00	0.44
3:D:443:LEU:HD12	3:D:443:LEU:HA	1.83	0.44
5:F:276:ALA:HB1	6:J:109:ARG:HH12	1.82	0.44
5:F:336:ASP:OD1	6:J:89:ARG:NH2	2.40	0.44
2:C:570:TYR:HD1	2:C:570:TYR:HA	1.71	0.44
2:C:701:VAL:HG11	2:C:711:GLY:HA2	1.99	0.44
5:F:236:GLY:HA2	5:F:301:ARG:HH21	1.83	0.44
7:M:112:TRP:O	7:M:116:GLN:HB2	2.17	0.44
1:A:8:THR:OG1	1:A:24:GLU:O	2.32	0.44
3:D:901:LEU:HD21	3:D:949:ILE:HD12	1.98	0.44
3:D:1257:LEU:HD12	3:D:1257:LEU:HA	1.89	0.44
1:A:61:HIS:CD2	1:A:63:PHE:H	2.36	0.43
3:D:342:ASP:N	3:D:342:ASP:OD1	2.50	0.43
3:D:703:ARG:HE	3:D:703:ARG:HB3	1.63	0.43
3:D:816:THR:HG22	3:D:821:LYS:HA	2.00	0.43
3:D:1133:HIS:HA	3:D:1136:ARG:HH21	1.83	0.43
5:F:353:GLN:HE21	5:F:353:GLN:HB3	1.68	0.43
2:C:604:ARG:NH2	2:C:890:GLY:O	2.52	0.43
3:D:674:ASN:ND2	3:D:684:VAL:H	2.16	0.43
3:D:988:LEU:HD12	3:D:988:LEU:HA	1.88	0.43
1:B:39:ARG:NH1	3:D:623:ASP:OD2	2.39	0.43
2:C:563:ARG:N	2:C:567:GLU:O	2.51	0.43
3:D:7:PHE:H	3:D:1256:LYS:NZ	2.16	0.43
3:D:674:ASN:HD21	3:D:684:VAL:H	1.67	0.43
3:D:737:LEU:N	3:D:793:TYR:OH	2.48	0.43
5:F:306:LEU:HD23	5:F:306:LEU:HA	1.80	0.43
2:C:71:ARG:HH11	2:C:82:PRO:HG2	1.83	0.43
2:C:255:SER:OG	2:C:258:MET:N	2.40	0.43
2:C:410:GLU:HG2	7:M:56:VAL:HG23	2.00	0.43
3:D:937:ILE:HD11	3:D:951:ALA:HB1	2.00	0.43
3:D:1249:LYS:HB2	3:D:1249:LYS:HE2	1.84	0.43
8:P:134:DC:H2''	8:P:135:DA:H5'	2.00	0.43
3:D:654:SER:O	3:D:656:TRP:N	2.51	0.43
1:A:213:LYS:HA	1:B:223:ARG:HG3	1.99	0.43
3:D:278:ARG:HA	3:D:278:ARG:HD3	1.77	0.43
3:D:817:LEU:HA	3:D:817:LEU:HD23	1.85	0.43
2:C:413:THR:HG22	2:C:416:THR:HG23	2.00	0.43
3:D:460:LEU:HB3	3:D:486:VAL:HG11	2.00	0.43
3:D:944:LEU:HA	3:D:948:GLU:HG3	2.01	0.43
3:D:1118:PRO:HA	3:D:1121:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:502:ARG:HA	5:F:502:ARG:HD2	1.89	0.43
1:B:62:GLU:HG2	1:B:64:THR:H	1.83	0.43
3:D:70:PHE:HB3	3:D:73:ILE:HD11	2.01	0.43
2:C:720:LEU:HD23	2:C:913:VAL:HA	2.01	0.42
3:D:196:LYS:HA	3:D:199:ASP:HB2	2.00	0.42
1:B:99:LYS:HD3	1:B:105:VAL:HG22	2.01	0.42
2:C:177:SER:HB3	2:C:378:LEU:HD11	2.00	0.42
2:C:488:THR:O	2:C:610:ASN:ND2	2.44	0.42
9:O:22:DG:H2''	9:O:23:DT:H5'	2.00	0.42
3:D:11:ARG:HA	3:D:1242:SER:HA	2.01	0.42
3:D:339:ASP:OD2	3:D:397:ARG:NH1	2.38	0.42
3:D:506:ARG:HE	3:D:506:ARG:HB3	1.63	0.42
5:F:233:LYS:HE2	5:F:233:LYS:HB3	1.78	0.42
7:M:145:THR:OG1	7:M:146:ASP:N	2.51	0.42
1:A:95:MET:HG3	1:A:138:LEU:HB2	2.02	0.42
2:C:295:LEU:HA	2:C:298:ASN:HB2	2.01	0.42
3:D:29:LYS:HB2	3:D:29:LYS:HE3	1.83	0.42
1:B:63:PHE:HD2	3:D:603:SER:HB3	1.84	0.42
2:C:960:PRO:HG2	2:C:963:LEU:HD12	2.01	0.42
1:A:213:LYS:NZ	1:B:233:GLU:OE2	2.42	0.42
2:C:713:MET:HE3	2:C:713:MET:HB3	1.93	0.42
2:C:771:ARG:HH21	2:C:781:LEU:HB3	1.84	0.42
3:D:94:HIS:HA	3:D:318:PRO:HA	2.01	0.42
3:D:552:GLN:O	3:D:556:ARG:HB2	2.20	0.42
3:D:893:THR:O	3:D:963:ARG:NH1	2.53	0.42
2:C:182:SER:OG	2:C:186:TYR:OH	2.37	0.42
2:C:646:GLU:HB3	2:C:662:HIS:HD1	1.85	0.42
5:F:459:GLN:NE2	5:F:522:VAL:O	2.53	0.42
3:D:353:ARG:NH1	5:F:319:ASP:OD1	2.41	0.42
3:D:736:VAL:HG12	3:D:818:ALA:HB2	2.02	0.42
5:F:489:LEU:HB3	5:F:503:ILE:HB	2.02	0.42
2:C:1011:PHE:HA	2:C:1018:PRO:HA	2.02	0.42
3:D:101:VAL:HG11	3:D:378:VAL:HG11	2.00	0.42
3:D:222:ILE:HD12	3:D:240:LEU:HD12	2.01	0.42
5:F:302:LEU:N	9:O:54:DT:O2	2.53	0.42
7:M:26:THR:HB	7:M:31:GLN:HE21	1.85	0.42
1:A:182:ARG:HH12	3:D:625:GLY:H	1.68	0.41
2:C:84:GLY:N	2:C:87:GLU:OE1	2.49	0.41
3:D:567:SER:HB2	3:D:571:GLY:H	1.84	0.41
2:C:438:GLN:OE1	2:C:451:HIS:NE2	2.54	0.41
3:D:210:ASP:HA	3:D:213:GLN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:590:THR:HA	3:D:687:GLN:HG3	2.01	0.41
5:F:522:VAL:HG23	5:F:523:LEU:HG	2.01	0.41
2:C:444:ASN:N	2:C:444:ASN:OD1	2.53	0.41
3:D:662:TRP:CZ3	3:D:664:ALA:HB2	2.55	0.41
1:A:120:ASN:OD1	1:A:120:ASN:N	2.52	0.41
2:C:445:PRO:HB3	2:C:640:ASP:HB2	2.02	0.41
3:D:453:LYS:HA	3:D:456:VAL:HG12	2.01	0.41
3:D:556:ARG:NH2	4:E:35:ILE:O	2.48	0.41
3:D:557:ILE:HG21	4:E:53:LEU:HD12	2.02	0.41
3:D:762:ARG:HA	3:D:762:ARG:HD3	1.84	0.41
4:E:46:ARG:NH1	4:E:102:ASP:OD1	2.54	0.41
6:J:99:LYS:HA	6:J:99:LYS:HD3	1.88	0.41
2:C:1112:ILE:HG13	3:D:548:SER:HA	2.03	0.41
4:E:75:ILE:HD12	4:E:75:ILE:HA	1.96	0.41
6:J:52:GLY:O	6:J:64:LEU:N	2.54	0.41
6:J:58:ASN:HB3	6:J:60:MET:HG2	2.01	0.41
7:M:121:SER:OG	8:P:107:DA:OP1	2.34	0.41
1:A:90:ASP:HA	1:A:142:ARG:HG3	2.03	0.41
1:B:80:LEU:HD13	1:B:138:LEU:HD21	2.03	0.41
2:C:719:LEU:HD13	2:C:1030:ILE:HG12	2.02	0.41
2:C:903:ASP:OD1	2:C:903:ASP:N	2.46	0.41
2:C:441:ASP:OD2	2:C:447:SER:OG	2.38	0.41
1:B:33:THR:OG1	1:B:34:LEU:N	2.53	0.41
1:B:38:LEU:HD12	1:B:38:LEU:HA	1.84	0.41
2:C:771:ARG:HD2	2:C:786:GLU:HA	2.03	0.41
7:M:95:LYS:HZ2	7:M:104:VAL:HG22	1.85	0.41
2:C:192:ASP:N	2:C:192:ASP:OD1	2.52	0.41
2:C:444:ASN:HD22	2:C:715:LEU:HD22	1.86	0.41
2:C:562:ARG:HD3	3:D:847:LEU:HD11	2.03	0.41
2:C:899:LEU:HD13	2:C:899:LEU:HA	1.96	0.41
3:D:281:ILE:HA	3:D:289:LYS:HG3	2.02	0.41
3:D:567:SER:OG	3:D:572:ARG:O	2.39	0.41
3:D:717:LYS:HE3	3:D:717:LYS:HB3	1.79	0.41
3:D:1167:ILE:HD13	3:D:1167:ILE:HA	1.96	0.41
5:F:264:THR:O	5:F:267:SER:OG	2.30	0.41
5:F:527:LEU:HD23	5:F:527:LEU:HA	1.91	0.41
2:C:251:ARG:HD3	2:C:251:ARG:HA	1.81	0.41
3:D:33:THR:OG1	3:D:34:ILE:N	2.54	0.41
3:D:97:LEU:HA	3:D:351:ASN:HD21	1.86	0.41
3:D:123:LYS:HB2	3:D:123:LYS:HE2	1.88	0.41
3:D:1087:ARG:HG3	3:D:1089:PHE:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:229:ARG:HA	5:F:232:LEU:HD12	2.03	0.41
6:J:64:LEU:HD23	6:J:66:GLU:H	1.86	0.41
9:O:45:DG:H2'	9:O:46:DT:H71	2.03	0.41
1:A:40:ARG:NH1	2:C:903:ASP:HB3	2.36	0.40
1:A:97:LEU:HB3	1:A:136:VAL:HG13	2.03	0.40
1:A:161:ARG:HA	1:A:161:ARG:HD3	1.78	0.40
1:B:159:ILE:H	1:B:159:ILE:HG13	1.74	0.40
3:D:716:LEU:HD23	3:D:716:LEU:HA	1.87	0.40
3:D:876:ARG:HD3	3:D:876:ARG:HA	1.88	0.40
3:D:1190:ASN:HA	3:D:1190:ASN:HD22	1.65	0.40
5:F:372:MET:HA	5:F:375:VAL:HG22	2.03	0.40
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.91	0.40
2:C:244:THR:H	2:C:247:GLN:HB2	1.86	0.40
2:C:256:GLU:O	2:C:260:SER:OG	2.36	0.40
2:C:674:LYS:HA	2:C:674:LYS:HD2	1.92	0.40
2:C:997:ASP:OD1	2:C:997:ASP:N	2.53	0.40
5:F:222:THR:OG1	5:F:223:ALA:N	2.53	0.40
6:J:83:ASP:OD1	6:J:83:ASP:N	2.52	0.40
9:O:72:DG:H1'	9:O:73:DC:H5'	2.02	0.40
2:C:69:ARG:O	2:C:73:SER:OG	2.27	0.40
2:C:96:ILE:O	2:C:105:LEU:N	2.46	0.40
2:C:624:PRO:HA	2:C:718:ASN:HD21	1.86	0.40
3:D:1089:PHE:HD1	3:D:1090:LYS:HB2	1.86	0.40
3:D:1265:ASN:OD1	3:D:1268:ARG:NH2	2.52	0.40
5:F:488:THR:OG1	5:F:491:GLU:OE1	2.28	0.40
6:J:32:TYR:N	6:J:40:PHE:O	2.44	0.40
3:D:1079:LYS:HA	3:D:1079:LYS:HD3	1.77	0.40
5:F:252:ARG:HG3	6:J:101:ARG:HH21	1.87	0.40
1:B:95:MET:N	1:B:138:LEU:O	2.55	0.40
1:B:107:ALA:N	1:B:123:MET:O	2.54	0.40
2:C:93:LEU:HD13	2:C:93:LEU:HA	1.91	0.40
2:C:446:LEU:HD23	2:C:613:ARG:HB3	2.03	0.40
2:C:549:ASP:OD1	2:C:553:ARG:N	2.55	0.40
2:C:1038:ASP:HA	2:C:1041:ILE:HG22	2.04	0.40
4:E:90:LYS:HD3	4:E:90:LYS:HA	1.87	0.40
7:M:25:ARG:NH1	7:M:26:THR:O	2.55	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	223/347 (64%)	205 (92%)	18 (8%)	0	100	100
1	B	235/347 (68%)	215 (92%)	20 (8%)	0	100	100
2	C	1109/1179 (94%)	1009 (91%)	100 (9%)	0	100	100
3	D	1260/1326 (95%)	1184 (94%)	75 (6%)	1 (0%)	51	83
4	E	81/110 (74%)	75 (93%)	6 (7%)	0	100	100
5	F	317/531 (60%)	306 (96%)	11 (4%)	0	100	100
6	J	106/111 (96%)	95 (90%)	10 (9%)	1 (1%)	17	53
7	M	157/162 (97%)	148 (94%)	9 (6%)	0	100	100
All	All	3488/4113 (85%)	3237 (93%)	249 (7%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	238	GLU
6	J	78	PRO

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	194/297 (65%)	182 (94%)	12 (6%)	18	49
1	B	194/297 (65%)	182 (94%)	12 (6%)	18	49
2	C	930/997 (93%)	884 (95%)	46 (5%)	25	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	1042/1103 (94%)	991 (95%)	51 (5%)	25	55
4	E	69/89 (78%)	64 (93%)	5 (7%)	14	45
5	F	259/429 (60%)	250 (96%)	9 (4%)	36	63
6	J	92/97 (95%)	78 (85%)	14 (15%)	3	17
7	M	129/131 (98%)	119 (92%)	10 (8%)	12	42
All	All	2909/3440 (85%)	2750 (94%)	159 (6%)	25	53

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	10	SER
1	A	18	ARG
1	A	74	THR
1	A	98	ARG
1	A	117	THR
1	A	144	ARG
1	A	147	VAL
1	A	171	VAL
1	A	187	THR
1	A	194	LEU
1	A	223	ARG
1	B	12	ASP
1	B	61	HIS
1	B	74	THR
1	B	84	VAL
1	B	98	ARG
1	B	111	VAL
1	B	123	MET
1	B	124	HIS
1	B	125	ILE
1	B	175	THR
1	B	177	LYS
1	B	213	LYS
2	C	69	ARG
2	C	77	ARG
2	C	81	ASN
2	C	100	SER
2	C	128	THR
2	C	141	ASN

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Mol	Chain	Res	Type
2	C	193	LYS
2	C	198	THR
2	C	207	SER
2	C	208	ARG
2	C	219	ARG
2	C	222	VAL
2	C	227	ASP
2	C	228	ARG
2	C	230	ARG
2	C	251	ARG
2	C	299	LEU
2	C	308	LEU
2	C	324	VAL
2	C	369	ASP
2	C	373	PHE
2	C	377	ARG
2	C	396	MET
2	C	419	ASN
2	C	443	ASN
2	C	446	LEU
2	C	456	LEU
2	C	475	VAL
2	C	540	VAL
2	C	561	VAL
2	C	570	TYR
2	C	584	ARG
2	C	588	SER
2	C	695	ARG
2	C	745	ASP
2	C	777	SER
2	C	815	THR
2	C	881	ASP
2	C	907	LEU
2	C	936	LEU
2	C	950	LYS
2	C	985	LEU
2	C	997	ASP
2	C	1038	ASP
2	C	1103	TYR
2	C	1131	LEU
3	D	1	MET
3	D	5	ASN

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Mol	Chain	Res	Type
3	D	21	ARG
3	D	37	ARG
3	D	70	PHE
3	D	75	CYS
3	D	78	CYS
3	D	92	MET
3	D	123	LYS
3	D	160	LYS
3	D	205	MET
3	D	209	ARG
3	D	239	ASN
3	D	248	TYR
3	D	287	GLN
3	D	315	ASP
3	D	386	ARG
3	D	387	ARG
3	D	402	LEU
3	D	409	LYS
3	D	416	ASN
3	D	427	ARG
3	D	441	CYS
3	D	483	VAL
3	D	499	ASN
3	D	567	SER
3	D	576	MET
3	D	578	ARG
3	D	595	ASP
3	D	614	SER
3	D	623	ASP
3	D	653	HIS
3	D	729	VAL
3	D	733	MET
3	D	741	ARG
3	D	748	HIS
3	D	770	ARG
3	D	797	ASN
3	D	849	TYR
3	D	925	LEU
3	D	962	VAL
3	D	1028	LEU
3	D	1066	ILE
3	D	1088	VAL

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Mol	Chain	Res	Type
3	D	1097	ARG
3	D	1117	ASP
3	D	1130	VAL
3	D	1136	ARG
3	D	1211	THR
3	D	1268	ARG
3	D	1279	ARG
4	E	49	SER
4	E	56	TYR
4	E	65	ASN
4	E	70	GLN
4	E	106	HIS
5	F	229	ARG
5	F	269	ARG
5	F	279	ARG
5	F	309	ARG
5	F	313	ARG
5	F	332	VAL
5	F	352	ARG
5	F	353	GLN
5	F	459	GLN
6	J	6	LEU
6	J	9	SER
6	J	16	TYR
6	J	21	ASN
6	J	27	ARG
6	J	57	ARG
6	J	76	LYS
6	J	83	ASP
6	J	88	ARG
6	J	102	LEU
6	J	104	LEU
6	J	108	ARG
6	J	109	ARG
6	J	110	ARG
7	M	19	VAL
7	M	25	ARG
7	M	37	LEU
7	M	38	LYS
7	M	44	LEU
7	M	74	LEU
7	M	85	TRP

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Mol	Chain	Res	Type
7	M	95	LYS
7	M	115	ASP
7	M	121	SER

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

Mol	Chain	Res	Type
1	A	61	HIS
1	A	119	HIS
1	A	124	HIS
1	B	151	GLN
1	B	226	ASN
2	C	81	ASN
2	C	141	ASN
2	C	142	ASN
2	C	232	GLN
2	C	298	ASN
2	C	352	GLN
2	C	543	GLN
2	C	612	GLN
2	C	920	HIS
2	C	1035	HIS
3	D	5	ASN
3	D	35	ASN
3	D	239	ASN
3	D	287	GLN
3	D	307	ASN
3	D	368	ASN
3	D	416	ASN
3	D	505	HIS
3	D	544	HIS
3	D	657	GLN
3	D	693	GLN
3	D	767	HIS
3	D	797	ASN
3	D	1145	GLN
3	D	1190	ASN
4	E	65	ASN
4	E	69	ASN
5	F	234	GLN
5	F	293	ASN
5	F	353	GLN

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Mol	Chain	Res	Type
5	F	377	ASN
5	F	388	GLN
6	J	58	ASN
7	M	14	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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$
10	SRN	C	1201	-	60,62,62	5.04	33 (55%)	62,84,84	1.52	11 (17%)

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
10	SRN	C	1201	-	-	17/52/105/105	0/4/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1201	SRN	O3-C8	19.41	1.79	1.44
10	C	1201	SRN	O3-C9	16.16	1.81	1.45
10	C	1201	SRN	C34-C9	-10.70	1.29	1.52
10	C	1201	SRN	C3-C2	9.51	1.59	1.34
10	C	1201	SRN	C34-C35	-8.58	1.33	1.52
10	C	1201	SRN	C4-C5	8.17	1.57	1.36
10	C	1201	SRN	C13-C14	6.70	1.60	1.31
10	C	1201	SRN	C6-C7	6.07	1.57	1.33
10	C	1201	SRN	C24-C25	6.02	1.57	1.31
10	C	1201	SRN	C8-C7	-5.85	1.30	1.50
10	C	1201	SRN	C12-C13	-5.80	1.30	1.50
10	C	1201	SRN	O7-C32	5.58	1.52	1.43
10	C	1201	SRN	C10-C9	-5.07	1.43	1.53
10	C	1201	SRN	C28-C29	5.07	1.61	1.31
10	C	1201	SRN	O8-C12	4.83	1.51	1.43
10	C	1201	SRN	C5-C6	4.71	1.57	1.44
10	C	1201	SRN	C3-C4	4.57	1.57	1.44
10	C	1201	SRN	C11-C10	-4.38	1.44	1.53
10	C	1201	SRN	C35-C8	-4.32	1.46	1.53
10	C	1201	SRN	C46-C47	4.09	1.45	1.33
10	C	1201	SRN	C33-C47	-3.79	1.43	1.49
10	C	1201	SRN	O7-C31	3.60	1.53	1.44
10	C	1201	SRN	C30-C29	3.55	1.61	1.50
10	C	1201	SRN	C2-C1	3.45	1.56	1.48
10	C	1201	SRN	O1-C33	3.44	1.51	1.46
10	C	1201	SRN	O1-C1	3.41	1.41	1.34
10	C	1201	SRN	C23-C24	3.02	1.55	1.50
10	C	1201	SRN	C31-C46	2.98	1.55	1.50
10	C	1201	SRN	C15-C14	2.59	1.58	1.50
10	C	1201	SRN	O8-C35	2.32	1.50	1.44
10	C	1201	SRN	C22-C21	2.25	1.56	1.52
10	C	1201	SRN	C17-C16	2.19	1.57	1.53
10	C	1201	SRN	O6-C23	-2.08	1.39	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1201	SRN	C23-C24-C25	-3.28	117.48	124.79
10	C	1201	SRN	C8-C7-C6	-3.16	119.43	125.61
10	C	1201	SRN	C32-C33-C47	-3.12	107.46	110.64
10	C	1201	SRN	C35-O8-C12	2.87	117.92	112.81
10	C	1201	SRN	C37-C36-C32	2.85	120.61	115.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1201	SRN	C3-C4-C5	-2.83	118.50	124.81
10	C	1201	SRN	C6-C5-C4	-2.80	118.58	124.81
10	C	1201	SRN	C18-C17-C19	-2.77	107.97	111.36
10	C	1201	SRN	C9-C34-C35	2.65	111.39	103.73
10	C	1201	SRN	C20-C19-C17	2.58	114.31	111.02
10	C	1201	SRN	C43-C44-C45	-2.18	108.98	114.47

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	1201	SRN	C2-C1-O1-C33
10	C	1201	SRN	C29-C30-C31-C46
10	C	1201	SRN	C29-C30-C31-O7
10	C	1201	SRN	C25-C26-C27-C28
10	C	1201	SRN	C10-C12-C13-C14
10	C	1201	SRN	O2-C1-O1-C33
10	C	1201	SRN	C39-C41-C42-C43
10	C	1201	SRN	O1-C1-C2-C3
10	C	1201	SRN	O2-C1-C2-C3
10	C	1201	SRN	C13-C14-C15-C16
10	C	1201	SRN	C26-C27-C28-C29
10	C	1201	SRN	O8-C12-C13-C14
10	C	1201	SRN	C33-C32-C36-C38
10	C	1201	SRN	C43-C44-C45-O10
10	C	1201	SRN	C43-C44-C45-O11
10	C	1201	SRN	C28-C29-C30-C31
10	C	1201	SRN	C38-C39-C41-C42

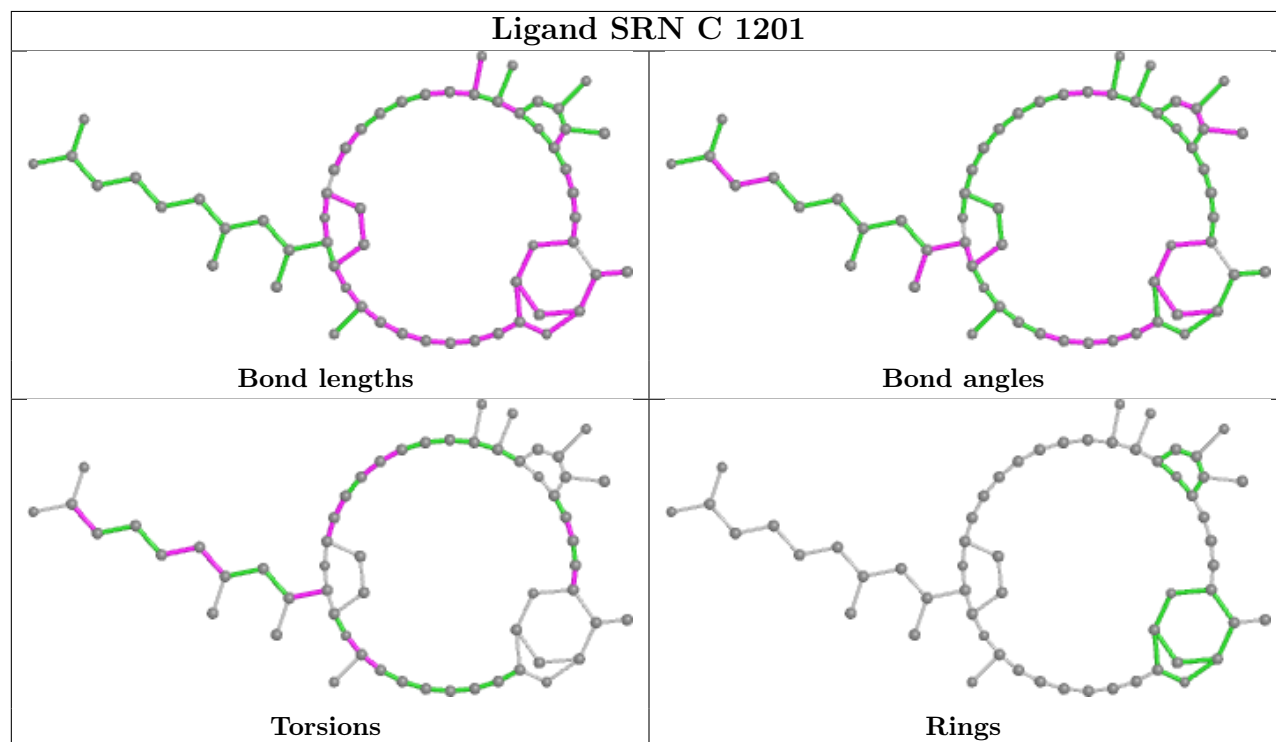
There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1201	SRN	11	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.



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.

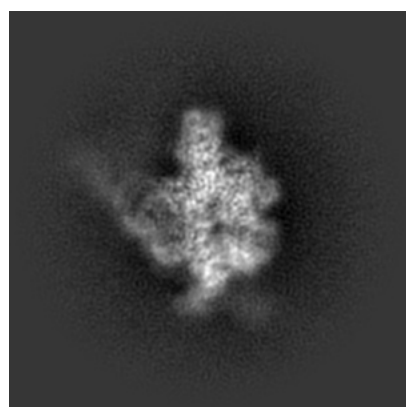
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21408. These allow visual inspection of the internal detail of the map and identification of artifacts.

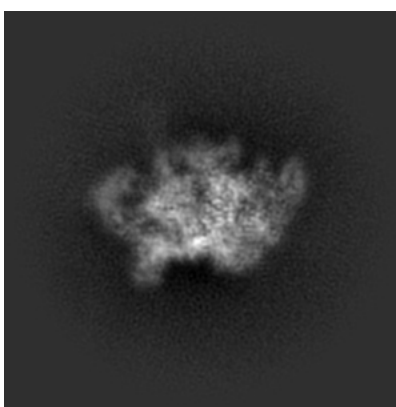
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

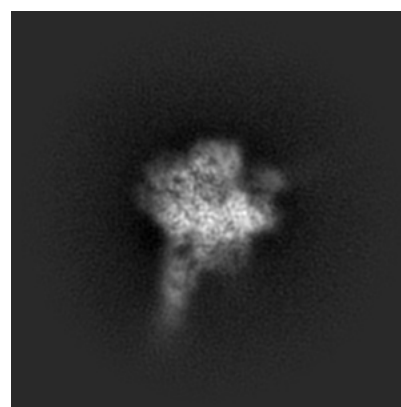
6.1.1 Primary map



X



Y

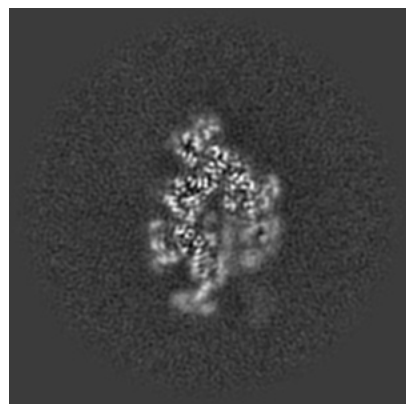


Z

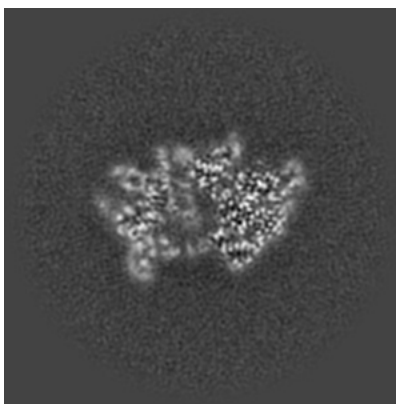
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

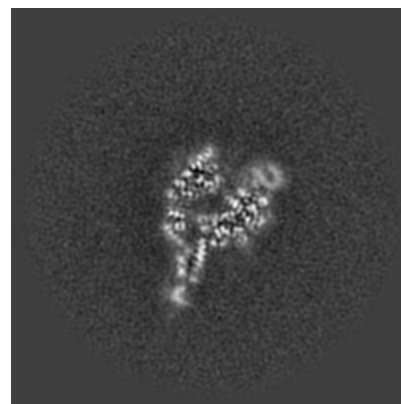
6.2.1 Primary map



X Index: 128



Y Index: 128

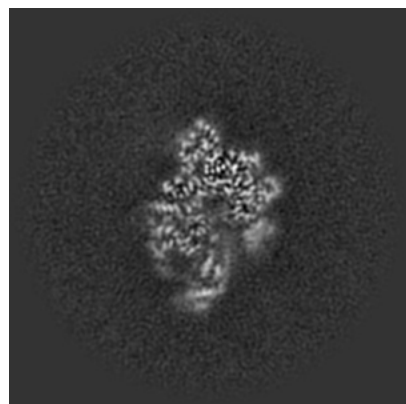


Z Index: 128

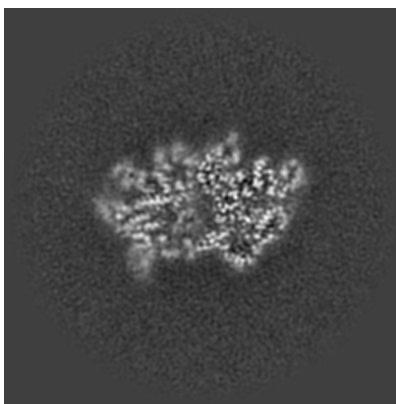
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

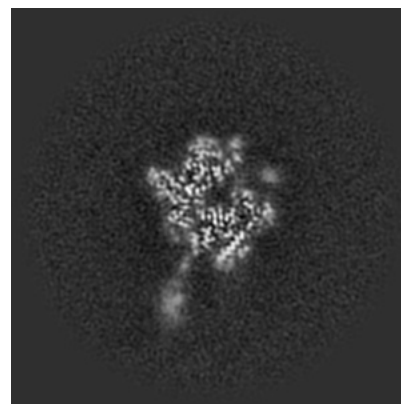
6.3.1 Primary map



X Index: 122



Y Index: 125



Z Index: 137

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.394. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

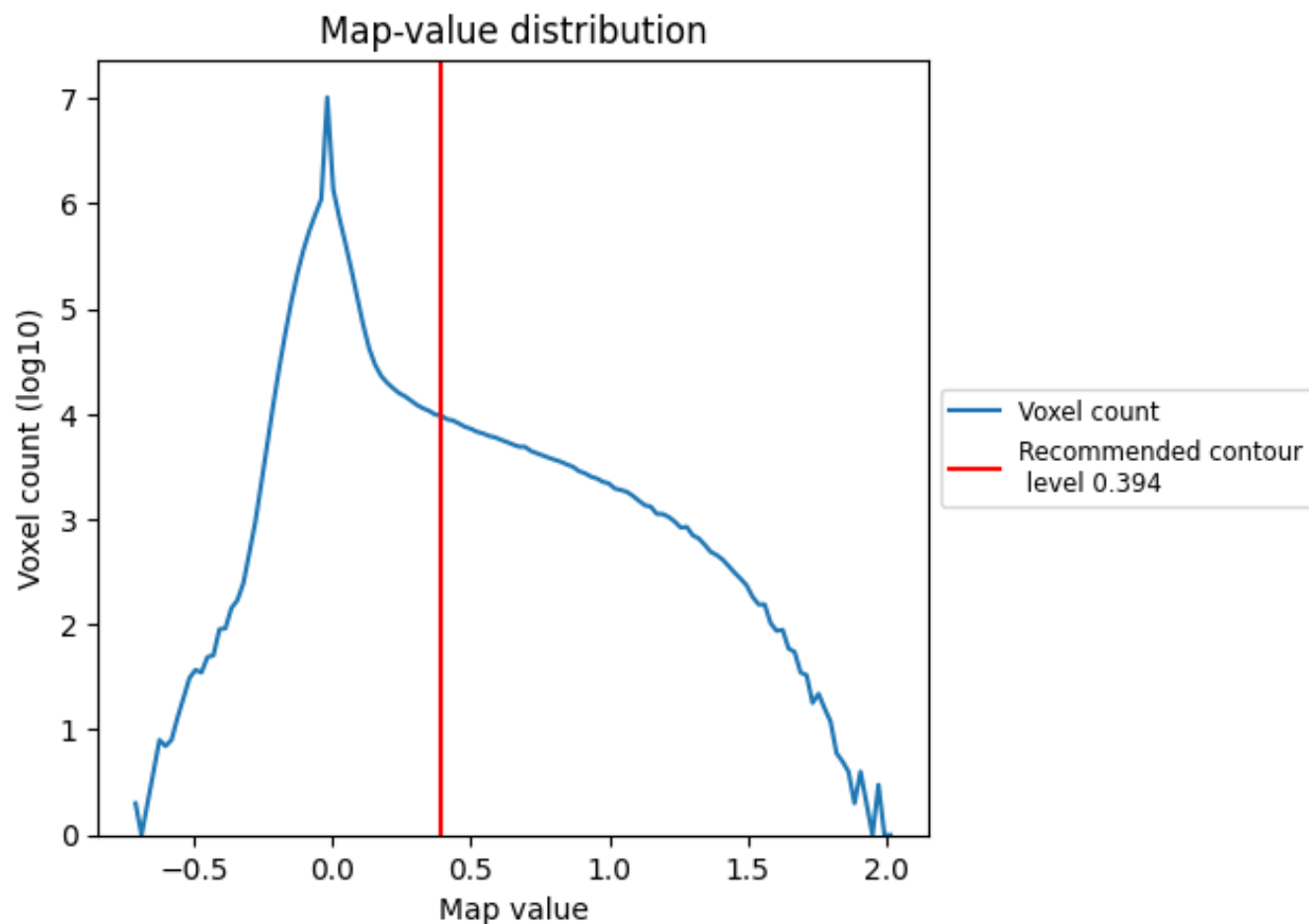
6.5 Mask visualisation

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

7 Map analysis [i](#)

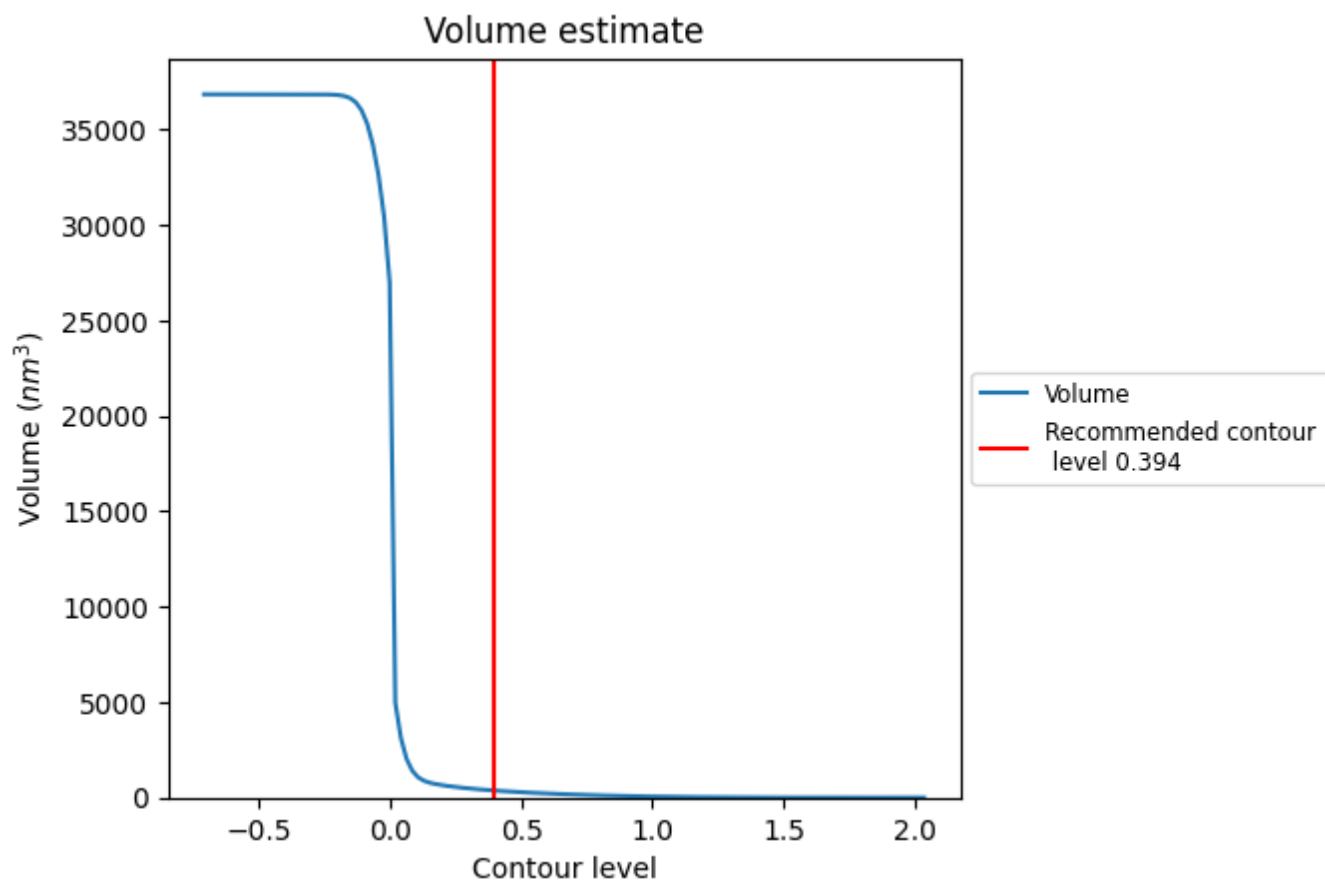
This section contains the results of statistical analysis of the map.

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.

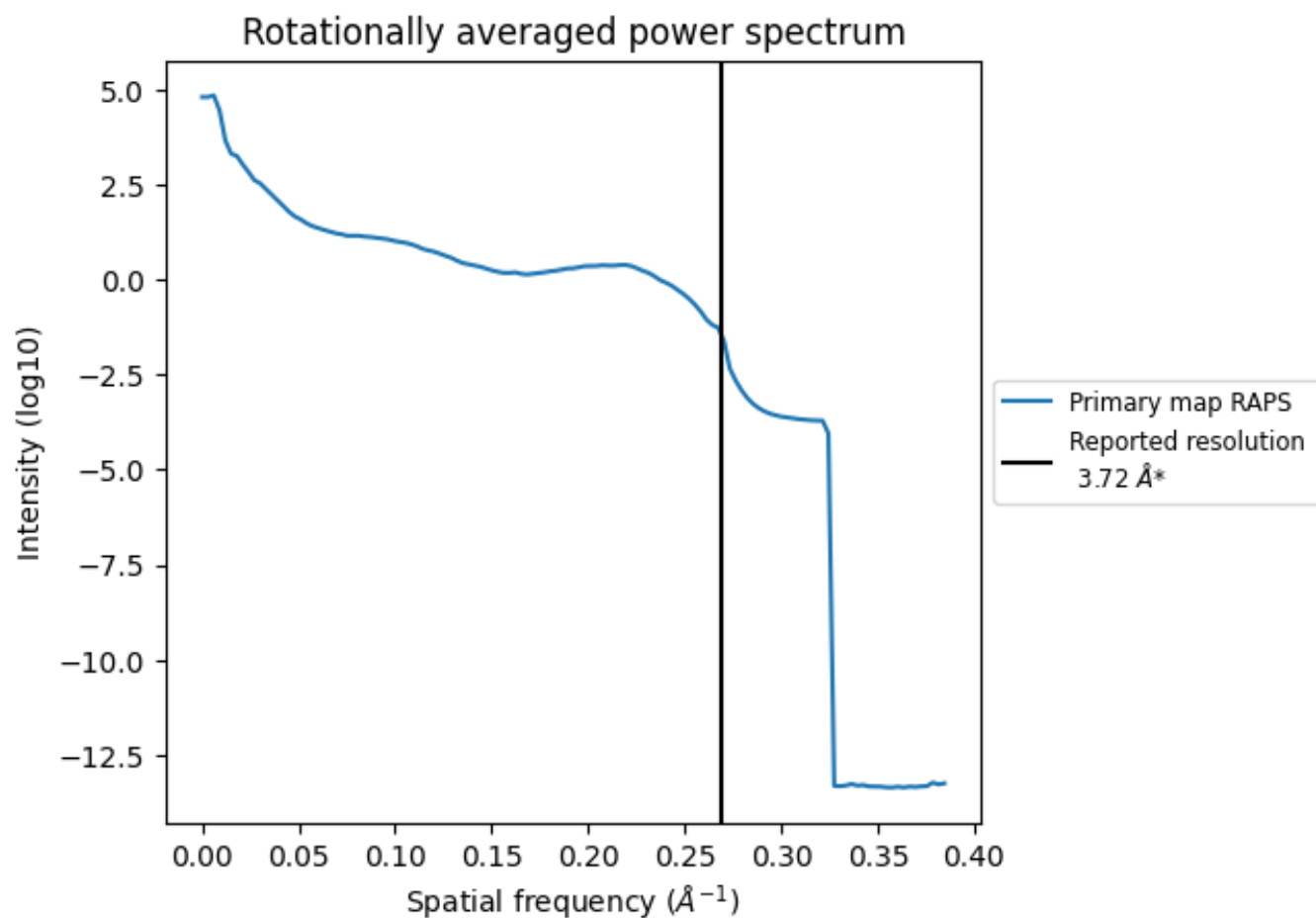
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 372 nm³; this corresponds to an approximate mass of 336 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 0.269 Å⁻¹

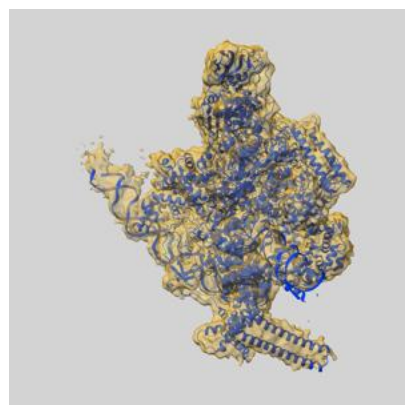
8 Fourier-Shell correlation ⓘ

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

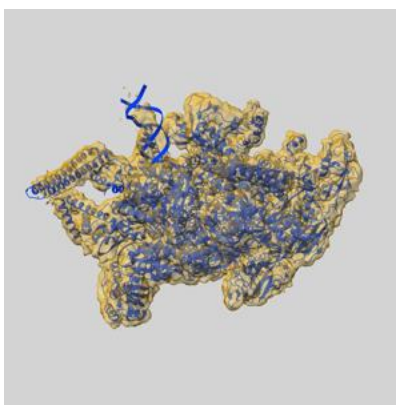
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21408 and PDB model 6VVZ. Per-residue inclusion information can be found in section 3 on page 8.

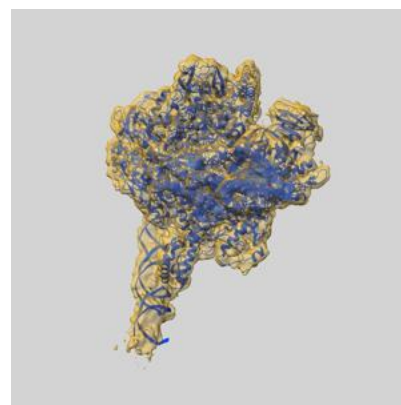
9.1 Map-model overlay [i](#)



X



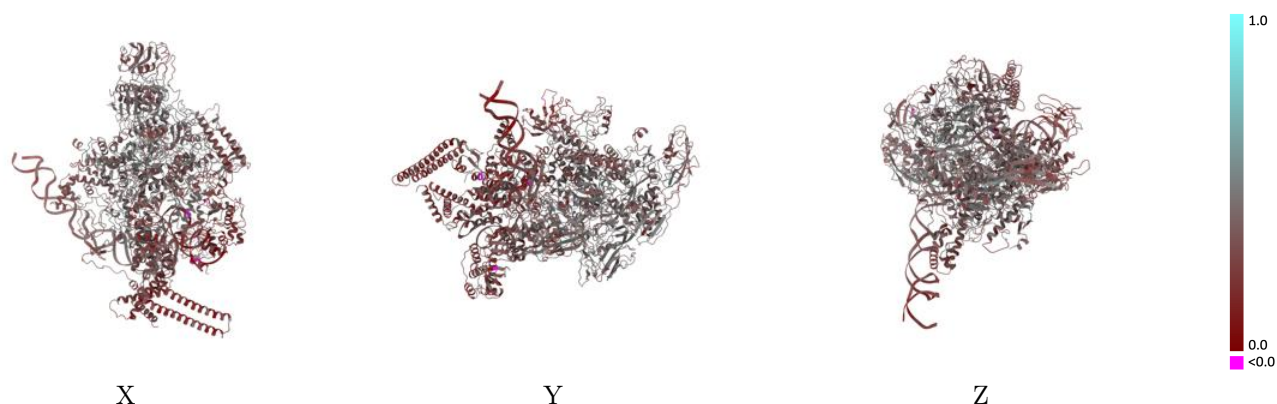
Y



Z

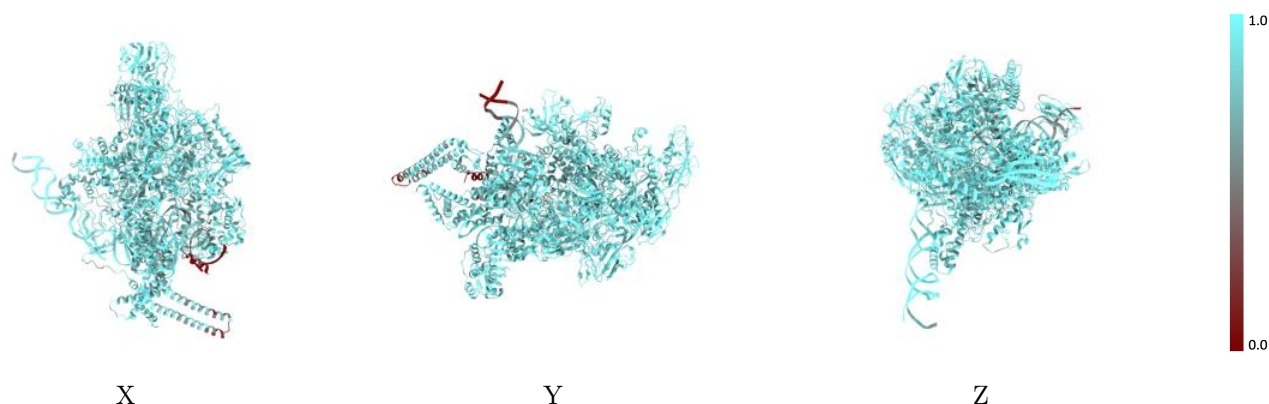
The images above show the 3D surface view of the map at the recommended contour level 0.394 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



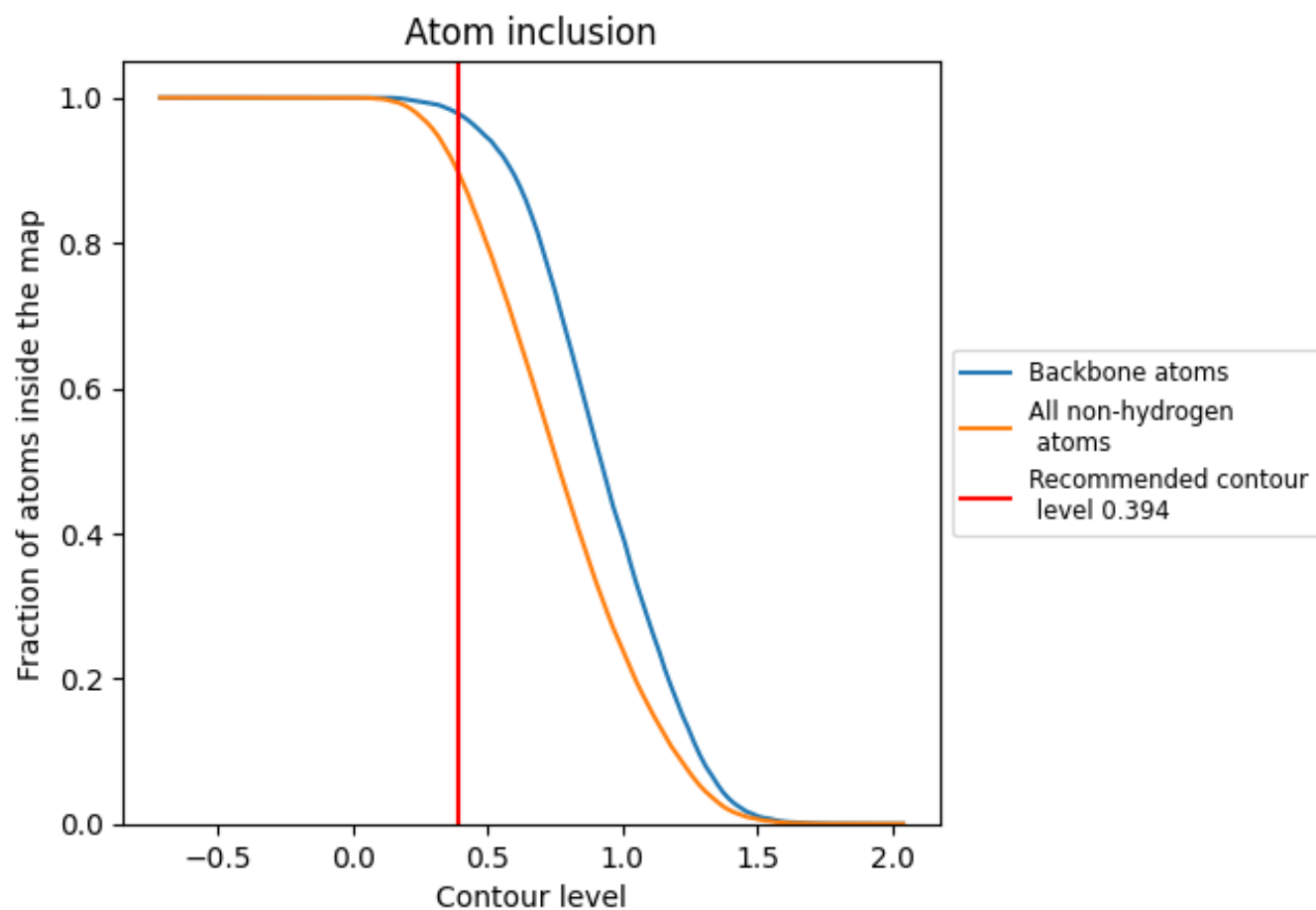
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.394).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 90% 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 (0.394) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8955	<div><div></div></div> 0.3610
A	<div><div></div></div> 0.9352	<div><div></div></div> 0.4150
B	<div><div></div></div> 0.9307	<div><div></div></div> 0.3790
C	<div><div></div></div> 0.9118	<div><div></div></div> 0.3930
D	<div><div></div></div> 0.8943	<div><div></div></div> 0.3710
E	<div><div></div></div> 0.8961	<div><div></div></div> 0.3850
F	<div><div></div></div> 0.8531	<div><div></div></div> 0.3050
J	<div><div></div></div> 0.8751	<div><div></div></div> 0.3270
M	<div><div></div></div> 0.8836	<div><div></div></div> 0.2670
O	<div><div></div></div> 0.8533	<div><div></div></div> 0.2680
P	<div><div></div></div> 0.8465	<div><div></div></div> 0.2720

1.0

0.0

<0.0