



Full wwPDB EM Validation Report ⓘ

Sep 28, 2026 – 12:29 PM EDT

PDB ID : 13FZ / pdb_000013fz
EMDB ID : EMD-77053
Title : Cryo-EM structure of human ZNFX1 dimer in complex with ssRNA and ATPgS
Authors : Wang, F.; He, Q.; Li, H.
Deposited on : 2026-05-05
Resolution : 3.37 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:

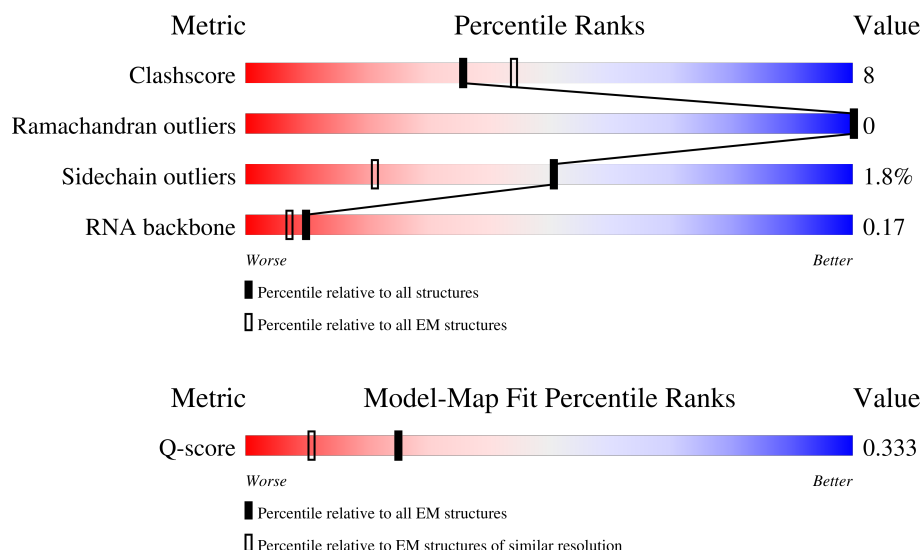
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.2
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.51

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 3.37 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	14287 (2.87 - 3.87)

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	1918	
1	C	1918	
2	B	60	

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Mol	Chain	Length	Quality of chain
2	D	60	5% 5% 12% 78%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 19220 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.

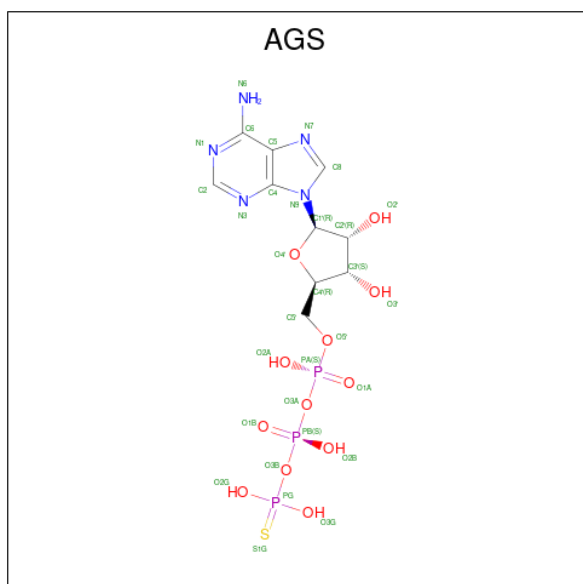
- Molecule 1 is a protein called NFX1-type zinc finger-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1149	Total	C	N	O	S	0	0
			9300	5887	1634	1714	65		
1	C	1149	Total	C	N	O	S	0	0
			9300	5887	1634	1714	65		

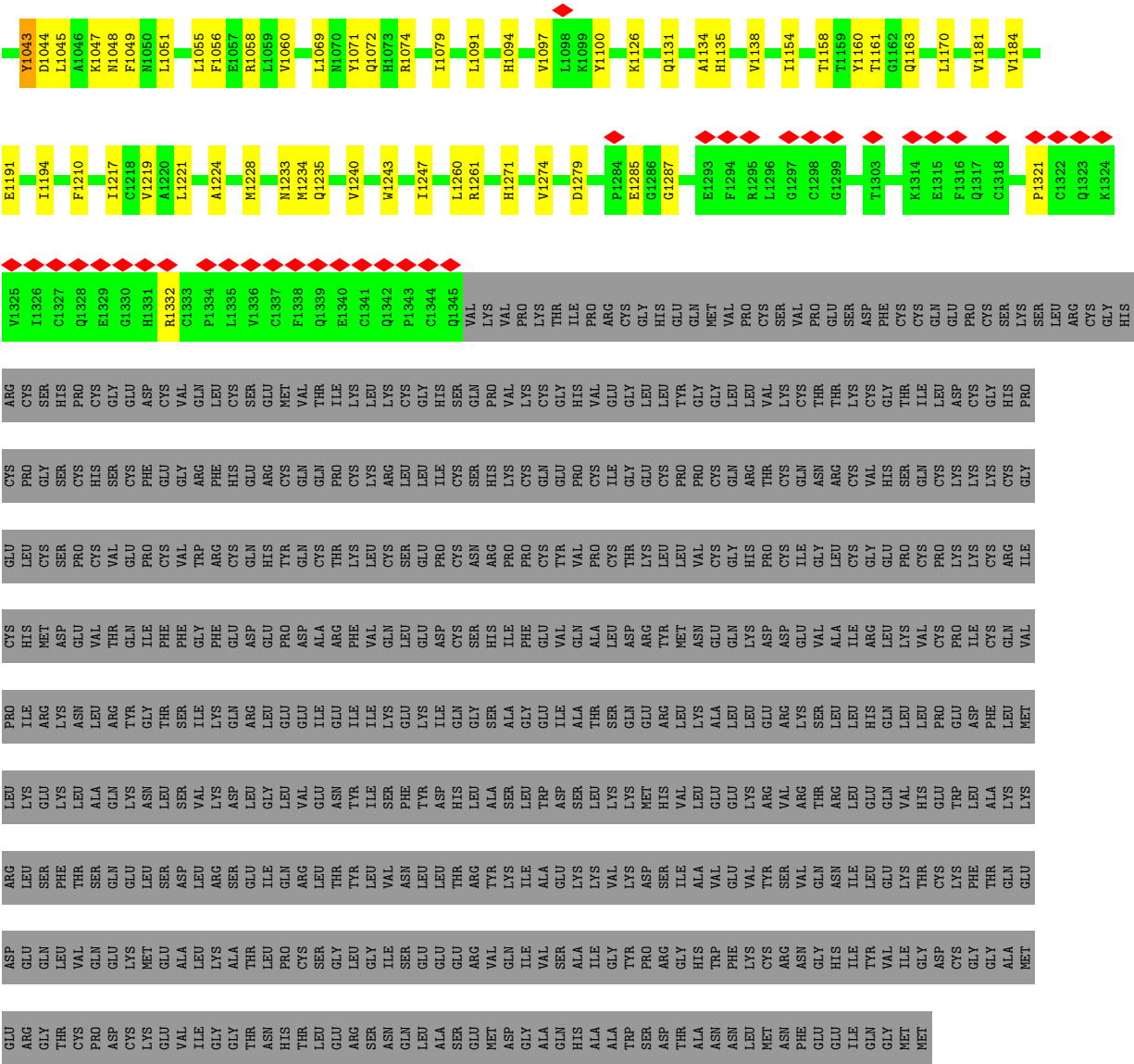
- Molecule 2 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	13	Total	C	N	O	P	0	0
			279	123	44	99	13		
2	D	13	Total	C	N	O	P	0	0
			279	123	44	99	13		

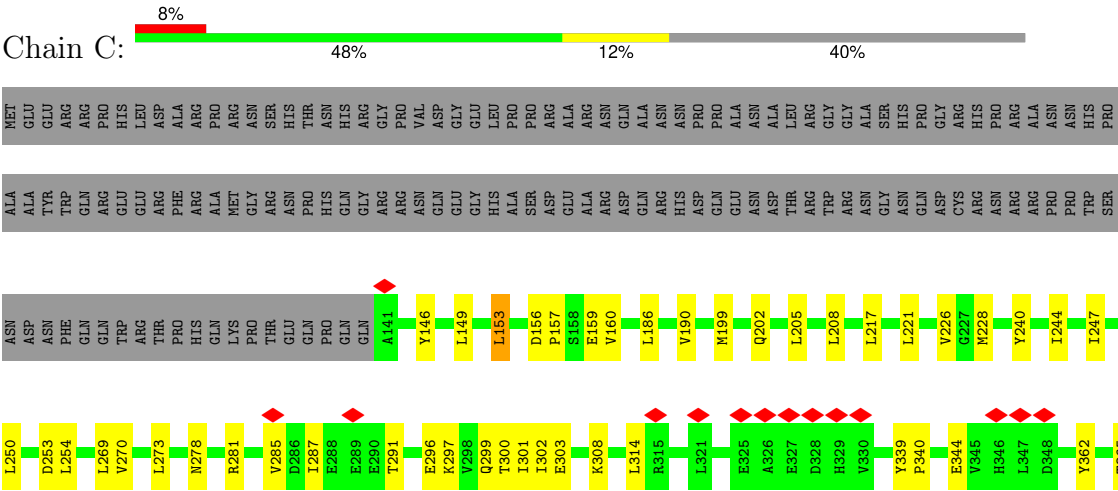
- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).

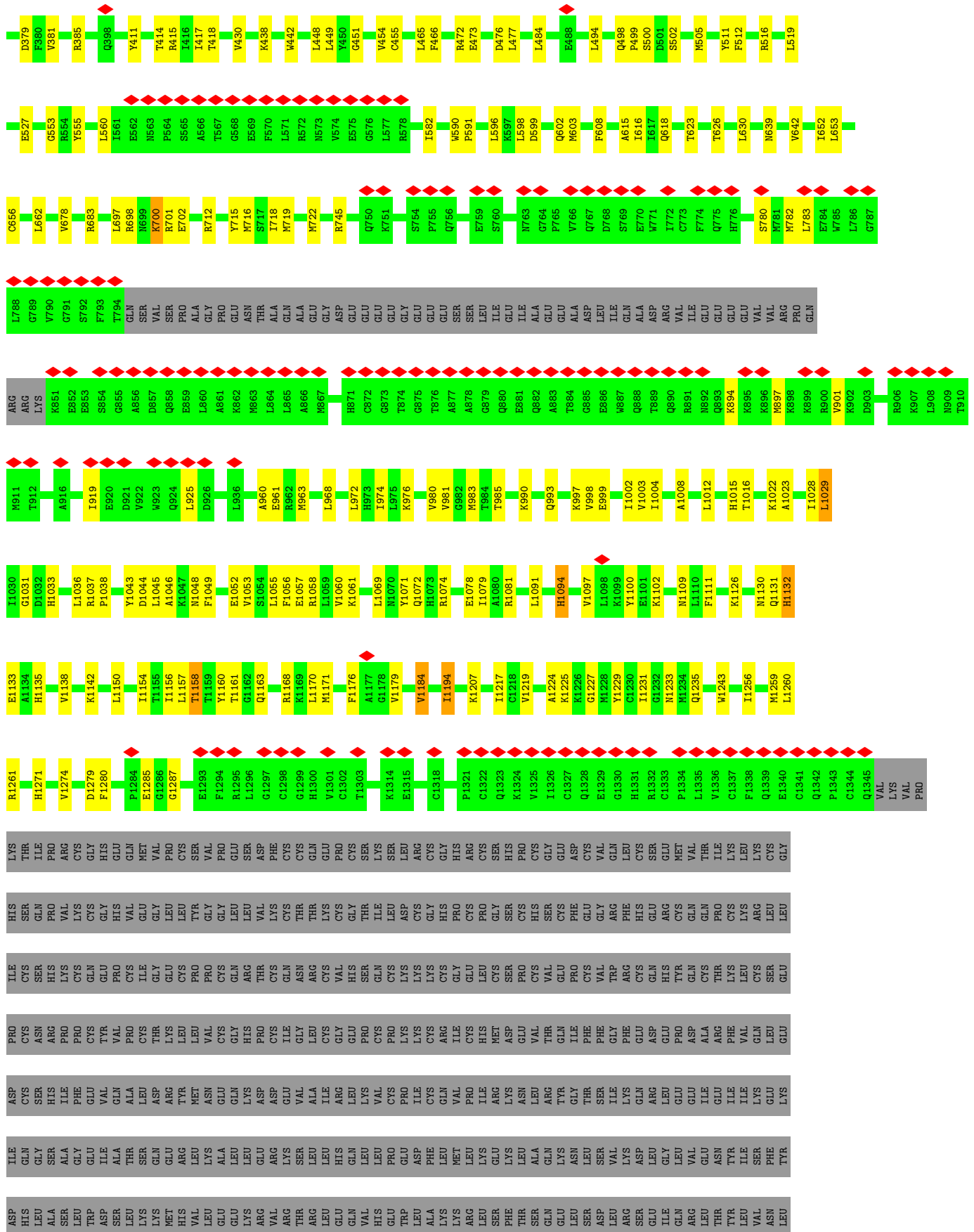


Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	



● Molecule 1: NFX1-type zinc finger-containing protein 1





ALA	SER	GLU	MET	ASP	GLY	ALA	GLN	HIS	ALA	ALA	TRP	SER	ASP	THR	ALA	ASN	ASN	LEU	MET	ASN	PHE	GLU	GLU	ILE	GLN	GLY	MET	MET
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Chain B: 5% 5% 12% 78%



Chain D: 5% 5% 12% 78%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	263896	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.224	Depositor
Minimum map value	-0.380	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.09	Depositor
Map size ($\text{\AA}$)	364.32, 364.32, 364.32	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.828, 0.828, 0.828	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: AGS

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	0.20	0/9485	0.43	0/12808
1	C	0.21	0/9485	0.44	0/12808
2	B	0.67	0/310	1.23	0/480
2	D	0.72	0/310	1.18	0/480
All	All	0.24	0/19590	0.48	0/26576

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	9300	0	9355	137	0
1	C	9300	0	9355	150	0
2	B	279	0	137	19	0
2	D	279	0	137	16	0
3	A	31	0	12	0	0
3	C	31	0	12	0	0
All	All	19220	0	19008	297	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 8.

All (297) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1260:LEU:HB3	1:C:1274:VAL:O	1.69	0.93
1:A:379:ASP:OD1	1:A:1045:LEU:HD12	1.69	0.91
1:A:990:LYS:HE3	2:B:8:G:H5'	1.65	0.78
1:C:199:MET:HE2	1:C:997:LYS:HE3	1.65	0.77
1:C:716:MET:HE2	2:D:13:U:H5''	1.65	0.77
1:C:379:ASP:OD1	1:C:1045:LEU:HD12	1.84	0.77
1:C:473:GLU:HB2	1:C:476:ASP:HB2	1.71	0.73
1:A:435:LYS:HG3	1:A:436:PRO:HD3	1.72	0.72
1:C:555:TYR:HD2	1:C:639:ASN:HD22	1.37	0.71
1:C:1260:LEU:CB	1:C:1274:VAL:O	2.38	0.71
1:C:1004:ILE:HG22	1:C:1028:ILE:HB	1.73	0.70
1:C:281:ARG:HH12	1:C:285:VAL:HA	1.57	0.70
1:A:1274:VAL:HG23	1:A:1279:ASP:HB2	1.75	0.69
1:C:990:LYS:HE3	2:D:8:G:H5'	1.74	0.68
1:A:281:ARG:HH12	1:A:285:VAL:HA	1.59	0.68
1:C:919:ILE:HG21	1:C:925:LEU:HD22	1.77	0.67
1:A:1160:TYR:HE1	2:B:2:G:H5'	1.60	0.67
1:A:972:LEU:HD21	1:A:997:LYS:HD2	1.75	0.66
1:A:414:THR:HG21	1:A:505:MET:HG2	1.77	0.65
1:C:745:ARG:HH21	1:C:780:SER:HB2	1.61	0.65
1:A:1004:ILE:HG22	1:A:1028:ILE:HB	1.78	0.64
1:C:308:LYS:HG2	1:C:314:LEU:HG	1.79	0.63
1:A:336:MET:HE3	1:A:374:ARG:HH12	1.63	0.63
1:A:308:LYS:HG2	1:A:314:LEU:HG	1.79	0.62
1:A:1160:TYR:HD1	2:B:3:U:OP2	1.82	0.62
1:A:1261:ARG:HH11	1:A:1271:HIS:HB3	1.64	0.62
1:C:700:LYS:HB3	1:C:700:LYS:NZ	2.14	0.62
1:A:415:ARG:HH12	1:A:502:SER:HA	1.64	0.62
1:A:716:MET:HE2	2:B:13:U:H5''	1.80	0.61
1:C:415:ARG:HH12	1:C:502:SER:HA	1.65	0.61
1:C:652:ILE:HG13	1:C:1002:ILE:HB	1.81	0.61
1:A:208:LEU:HD22	1:A:254:LEU:HD13	1.82	0.61
1:A:534:ARG:HE	1:A:540:ASN:HD22	1.49	0.61
1:A:202:GLN:HG3	1:A:961:GLU:HB3	1.83	0.60
1:C:623:THR:HA	1:C:1072:GLN:HA	1.84	0.60
1:C:698:ARG:HG2	1:C:974:ILE:CD1	2.31	0.60
1:A:449:LEU:HA	1:A:472:ARG:HD2	1.83	0.60
1:A:734:LYS:O	1:A:738:CYS:HB2	2.02	0.60
1:A:722:MET:HE1	1:A:960:ALA:HA	1.84	0.59
1:A:1138:VAL:HG21	1:A:1170:LEU:HG	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:ILE:HG13	1:A:1002:ILE:HB	1.85	0.59
1:C:414:THR:HG21	1:C:505:MET:HG2	1.82	0.59
1:A:270:VAL:HG21	1:A:302:ILE:HG21	1.84	0.59
1:A:653:LEU:HB3	1:A:1003:VAL:HG23	1.85	0.59
2:B:3:U:H1'	2:B:4:G:C2	2.38	0.59
1:C:449:LEU:HA	1:C:472:ARG:HD2	1.85	0.59
1:A:146:TYR:HE1	1:A:186:LEU:HD13	1.68	0.58
1:C:1078:GLU:HA	1:C:1081:ARG:HE	1.68	0.58
1:C:146:TYR:HE1	1:C:186:LEU:HD13	1.68	0.58
1:C:1102:LYS:HD3	1:C:1109:ASN:HD21	1.67	0.58
1:C:1071:TYR:HE2	1:C:1094:HIS:HA	1.69	0.58
1:C:498:GLN:HG3	1:C:500:SER:H	1.68	0.58
1:C:678:VAL:HG23	1:C:697:LEU:HD12	1.86	0.58
1:C:1160:TYR:HD1	2:D:3:U:OP2	1.87	0.58
2:D:3:U:H1'	2:D:4:G:C2	2.38	0.58
1:C:698:ARG:HG2	1:C:974:ILE:HD11	1.85	0.58
1:A:1036:LEU:HG	1:A:1219:VAL:HG21	1.87	0.57
1:C:1160:TYR:HE1	2:D:2:G:H5'	1.70	0.56
1:A:420:MET:HE1	1:A:429:LYS:HB2	1.86	0.56
1:A:716:MET:HE2	2:B:13:U:H4'	1.87	0.56
2:D:1:U:O2'	2:D:2:G:OP1	2.25	0.55
1:A:149:LEU:HB3	1:A:186:LEU:HD21	1.88	0.55
1:A:623:THR:HA	1:A:1072:GLN:HA	1.89	0.55
2:B:1:U:O2'	2:B:2:G:OP1	2.24	0.55
1:A:1016:THR:HG21	1:A:1055:LEU:HD22	1.87	0.55
1:A:1221:LEU:HD22	1:A:1228:MET:HE1	1.88	0.55
1:C:1016:THR:HG21	1:C:1055:LEU:HD22	1.87	0.55
1:C:202:GLN:HG3	1:C:961:GLU:HB3	1.89	0.54
1:C:712:ARG:NH1	2:D:13:U:OP1	2.41	0.54
1:C:448:LEU:HD23	1:C:477:LEU:HD11	1.90	0.54
1:A:498:GLN:HG3	1:A:500:SER:H	1.73	0.54
1:A:1285:GLU:HG2	1:A:1287:GLY:H	1.73	0.54
1:A:199:MET:HE2	1:A:997:LYS:HE2	1.90	0.54
1:A:417:ILE:HG22	1:A:418:THR:HG22	1.90	0.54
1:C:417:ILE:HG22	1:C:418:THR:HG22	1.90	0.53
1:C:1126:LYS:HE3	2:D:3:U:C5	2.42	0.53
1:C:244:ILE:HD13	1:C:247:ILE:HD12	1.91	0.53
1:A:1071:TYR:HE2	1:A:1094:HIS:HA	1.74	0.53
1:C:653:LEU:HD12	1:C:981:VAL:HB	1.90	0.53
1:C:653:LEU:HB3	1:C:1003:VAL:HG23	1.90	0.53
1:C:715:TYR:HE1	1:C:719:MET:HE3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1046:ALA:HB1	1:C:1052:GLU:HG2	1.91	0.52
1:C:1285:GLU:HG2	1:C:1287:GLY:H	1.75	0.52
1:A:430:VAL:HG21	1:A:484:LEU:HD12	1.90	0.52
1:C:616:ILE:HG13	1:C:1029:LEU:HD12	1.92	0.52
1:C:1111:PHE:CZ	1:C:1260:LEU:HA	2.45	0.52
1:C:722:MET:HE1	1:C:960:ALA:HA	1.91	0.52
1:C:362:TYR:HE2	1:C:1058:ARG:HH21	1.58	0.52
1:A:701:ARG:NH1	2:B:12:G:H5''	2.25	0.51
1:C:560:LEU:HD23	1:C:596:LEU:HD21	1.92	0.51
1:C:344:GLU:HG2	1:C:385:ARG:HD2	1.92	0.51
1:C:716:MET:HE2	2:D:13:U:C5'	2.38	0.51
1:C:228:MET:HE1	1:C:240:TYR:CG	2.46	0.51
1:C:972:LEU:HD22	1:C:997:LYS:HE2	1.91	0.51
1:C:553:GLY:HA3	1:C:642:VAL:HG13	1.93	0.51
1:A:652:ILE:HG22	1:A:980:VAL:HA	1.91	0.51
1:A:362:TYR:HE2	1:A:1058:ARG:HH21	1.59	0.51
1:C:287:ILE:HG23	1:C:291:THR:HB	1.93	0.51
1:A:1097:VAL:HA	1:A:1100:TYR:HD2	1.75	0.51
1:A:653:LEU:HD12	1:A:981:VAL:HB	1.92	0.50
1:C:465:LEU:HD23	1:C:494:LEU:HD12	1.92	0.50
1:A:709:MET:HE3	1:A:713:ARG:HG3	1.94	0.50
1:C:430:VAL:HG21	1:C:484:LEU:HD12	1.93	0.50
1:A:1072:GLN:HB3	1:A:1091:LEU:HD11	1.94	0.50
1:C:1008:ALA:HB3	1:C:1056:PHE:HD2	1.77	0.50
1:C:1036:LEU:HG	1:C:1219:VAL:HG21	1.94	0.50
1:C:1097:VAL:HA	1:C:1100:TYR:HD2	1.77	0.50
1:A:1045:LEU:HD22	1:A:1049:PHE:CD2	2.47	0.50
1:C:656:CYS:HB3	1:C:662:LEU:HB2	1.93	0.49
2:B:1:U:HO2'	2:B:2:G:P	2.35	0.49
1:C:455:CYS:O	1:C:505:MET:HA	2.12	0.49
1:C:608:PHE:HE1	1:C:615:ALA:HA	1.78	0.49
1:A:712:ARG:NH1	2:B:13:U:OP1	2.46	0.49
1:C:156:ASP:HB3	1:C:159:GLU:HB2	1.94	0.49
1:C:297:LYS:O	1:C:301:ILE:HG22	2.12	0.49
2:D:11:U:H5'	2:D:12:G:OP1	2.13	0.49
1:C:157:PRO:HA	1:C:160:VAL:HG12	1.95	0.49
1:A:156:ASP:HB3	1:A:159:GLU:HB2	1.95	0.49
1:C:652:ILE:HG22	1:C:980:VAL:HA	1.95	0.49
1:A:1134:ALA:HB1	1:A:1170:LEU:HD21	1.94	0.49
1:A:297:LYS:O	1:A:301:ILE:HG22	2.12	0.48
1:A:1260:LEU:HB3	1:A:1274:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:THR:HG21	2:B:4:G:OP1	2.13	0.48
1:C:626:THR:O	1:C:630:LEU:HD23	2.14	0.48
1:C:1079:ILE:HG21	1:C:1224:ALA:HB3	1.94	0.48
1:C:208:LEU:HD22	1:C:254:LEU:HD13	1.94	0.48
1:A:927:LEU:HA	1:A:930:ARG:HE	1.79	0.48
1:A:218:LYS:HG2	1:A:265:GLU:HG2	1.94	0.48
1:A:1210:PHE:HB3	2:B:2:G:OP1	2.14	0.48
1:A:1008:ALA:HB3	1:A:1056:PHE:HD2	1.78	0.48
1:C:281:ARG:HH22	1:C:285:VAL:HG13	1.78	0.48
1:C:451:GLY:O	1:C:512:PHE:HB3	2.14	0.48
1:C:454:VAL:HG13	1:C:505:MET:HB2	1.96	0.48
1:C:1217:ILE:HG21	1:C:1243:TRP:HE1	1.78	0.48
1:C:340:PRO:HD2	1:C:466:PHE:CE1	2.49	0.48
1:C:623:THR:HG23	1:C:1069:LEU:HD23	1.96	0.48
1:A:618:GLN:HA	1:A:1031:GLY:O	2.14	0.47
1:C:715:TYR:CD1	1:C:963:MET:HE1	2.49	0.47
1:A:225:VAL:O	1:A:228:MET:HB2	2.14	0.47
1:C:149:LEU:HB3	1:C:186:LEU:HD21	1.96	0.47
1:C:217:LEU:HD23	1:C:221:LEU:HD12	1.96	0.47
1:A:654:VAL:HG22	1:A:1004:ILE:HD11	1.95	0.47
1:A:1033:HIS:HD2	1:A:1060:VAL:HG21	1.80	0.47
1:A:1079:ILE:HG21	1:A:1224:ALA:HB3	1.97	0.47
1:C:582:ILE:HD13	1:C:591:PRO:HD3	1.96	0.47
1:A:454:VAL:HG13	1:A:505:MET:HB2	1.97	0.47
1:A:777:TRP:CE2	1:A:779:HIS:HB3	2.50	0.47
1:A:1234:MET:HE2	1:A:1247:ILE:HD11	1.97	0.47
1:C:1161:THR:HG21	2:D:4:G:OP1	2.14	0.47
1:A:152:LEU:HG	1:A:160:VAL:HG23	1.95	0.47
1:C:1157:LEU:HD23	1:C:1184:VAL:HG23	1.97	0.47
2:D:11:U:H4'	2:D:11:U:OP1	2.14	0.47
1:A:381:VAL:HG13	1:A:385:ARG:HE	1.80	0.47
1:A:313:THR:HA	1:A:315:ARG:HH12	1.80	0.46
1:A:473:GLU:HB2	1:A:476:ASP:HB2	1.97	0.46
1:A:897:MET:O	1:A:901:VAL:HG23	2.14	0.46
1:C:618:GLN:HA	1:C:1031:GLY:O	2.15	0.46
1:C:149:LEU:HD22	1:C:190:VAL:HG21	1.98	0.46
1:A:718:ILE:HD12	1:A:966:LEU:HD12	1.97	0.46
1:A:1012:LEU:HD23	1:A:1012:LEU:HA	1.76	0.46
1:C:615:ALA:HB3	1:C:1028:ILE:HG23	1.97	0.46
1:C:1158:THR:HB	1:C:1163:GLN:HG2	1.98	0.46
1:C:897:MET:O	1:C:901:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LEU:HD13	1:A:269:LEU:HD23	1.97	0.46
1:C:296:GLU:O	1:C:299:GLN:HG2	2.15	0.46
1:A:1126:LYS:NZ	2:B:3:U:O4	2.29	0.46
1:A:333:TYR:CE1	1:A:334:ARG:HD3	2.51	0.45
1:A:375:LEU:HB3	1:A:1051:LEU:HD12	1.99	0.45
1:A:420:MET:SD	1:A:427:VAL:HG23	2.56	0.45
1:A:1131:GLN:HG3	1:A:1135:HIS:NE2	2.32	0.45
1:C:718:ILE:O	1:C:722:MET:HG2	2.16	0.45
1:A:715:TYR:CD1	1:A:963:MET:HE1	2.51	0.45
1:A:465:LEU:HD21	1:A:493:LEU:HD22	1.98	0.45
1:C:1274:VAL:HG23	1:C:1279:ASP:HB2	1.99	0.45
1:C:1045:LEU:HD22	1:C:1049:PHE:CD2	2.52	0.45
1:A:680:VAL:HG13	1:A:694:LEU:HD13	1.97	0.45
1:A:1044:ASP:OD1	1:A:1048:ASN:ND2	2.50	0.45
1:A:1321:PRO:HB2	1:A:1332:ARG:HD3	1.99	0.45
1:C:1037:ARG:HG3	1:C:1038:PRO:HD2	1.99	0.45
1:A:623:THR:HG23	1:A:1069:LEU:HD23	1.99	0.45
1:A:718:ILE:HD13	1:A:962:ARG:HB3	1.99	0.45
1:C:700:LYS:HB2	1:C:702:GLU:OE1	2.16	0.45
1:C:712:ARG:CZ	2:D:13:U:OP1	2.65	0.45
1:C:1142:LYS:HG3	1:C:1176:PHE:HZ	1.82	0.45
1:A:1074:ARG:HD2	1:A:1191:GLU:HG3	1.98	0.44
1:C:438:LYS:HA	1:C:438:LYS:HE3	1.99	0.44
1:C:972:LEU:HD12	1:C:972:LEU:HA	1.88	0.44
1:A:206:HIS:CD2	1:A:210:ILE:HD11	2.52	0.44
1:C:339:TYR:HB3	1:C:466:PHE:CE1	2.51	0.44
1:C:999:GLU:HG3	1:C:1023:ALA:HB3	1.99	0.44
1:A:157:PRO:HA	1:A:160:VAL:HG12	1.99	0.44
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.74	0.44
1:A:716:MET:HE2	2:B:13:U:C5'	2.46	0.44
1:C:1156:ILE:HD13	1:C:1171:MET:HE1	1.99	0.44
1:A:149:LEU:HD22	1:A:190:VAL:HG21	1.99	0.44
1:C:590:TRP:CE3	1:C:591:PRO:HD2	2.53	0.44
1:C:1111:PHE:HZ	1:C:1259:MET:O	2.01	0.44
1:C:1111:PHE:HB3	1:C:1229:TYR:HD1	1.83	0.44
1:A:299:GLN:HA	1:A:302:ILE:HG22	2.00	0.44
1:C:376:LEU:HB3	1:C:519:LEU:HD21	2.00	0.44
1:C:449:LEU:HD13	1:C:511:TYR:HE1	1.83	0.44
1:A:455:CYS:HB3	1:A:506:VAL:HG13	1.99	0.44
2:D:3:U:O2'	2:D:4:G:O5'	2.33	0.44
1:A:728:GLU:HB3	1:A:952:TYR:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:ARG:NH1	2:B:10:G:C2	2.85	0.43
1:A:897:MET:SD	1:A:898:LYS:HD3	2.57	0.43
1:A:376:LEU:HB3	1:A:519:LEU:HD21	2.01	0.43
1:A:894:LYS:HA	1:A:894:LYS:HD3	1.87	0.43
1:A:1002:ILE:HG23	1:A:1026:HIS:HD2	1.82	0.43
1:A:340:PRO:HD2	1:A:466:PHE:CE1	2.54	0.43
1:C:270:VAL:HG21	1:C:302:ILE:HG21	1.99	0.43
1:C:1168:ARG:HA	1:C:1168:ARG:HD3	1.78	0.43
1:A:655:VAL:HG23	1:A:1005:VAL:HA	2.01	0.43
1:A:975:LEU:HD21	1:A:981:VAL:HG21	2.01	0.43
1:A:146:TYR:CE1	1:A:186:LEU:HD13	2.50	0.43
1:A:1261:ARG:HD2	1:A:1271:HIS:HB3	2.00	0.43
1:A:180:LYS:HE2	1:A:180:LYS:HB3	1.86	0.43
1:C:411:TYR:HD2	1:C:505:MET:HE3	1.83	0.43
1:C:1022:LYS:HD3	1:C:1022:LYS:HA	1.88	0.43
1:C:1033:HIS:HD2	1:C:1060:VAL:HG21	1.84	0.43
1:C:1072:GLN:HB3	1:C:1091:LEU:HD11	2.00	0.43
1:C:1130:ASN:HB3	1:C:1133:GLU:HB2	2.00	0.43
1:A:287:ILE:HG23	1:A:291:THR:HB	2.00	0.43
1:C:1057:GLU:O	1:C:1061:LYS:HB2	2.19	0.43
1:C:1217:ILE:HG21	1:C:1243:TRP:NE1	2.34	0.43
1:C:1132:HIS:CE1	1:C:1231:ILE:HD11	2.53	0.43
1:A:1217:ILE:HG21	1:A:1243:TRP:NE1	2.34	0.43
1:C:1044:ASP:O	1:C:1048:ASN:HB2	2.19	0.43
1:A:448:LEU:HD23	1:A:477:LEU:HD11	2.01	0.42
1:C:598:LEU:HD21	1:C:603:MET:HB2	2.00	0.42
1:A:206:HIS:NE2	1:A:210:ILE:HD11	2.34	0.42
2:B:3:U:H4'	2:B:4:G:OP1	2.19	0.42
1:A:656:CYS:HB3	1:A:662:LEU:HB2	2.01	0.42
1:A:716:MET:HE2	2:B:13:U:C4'	2.48	0.42
1:C:1150:LEU:HD12	1:C:1150:LEU:H	1.85	0.42
1:A:281:ARG:HA	1:A:281:ARG:HD2	1.76	0.42
1:A:339:TYR:HB3	1:A:466:PHE:CE1	2.54	0.42
1:C:299:GLN:HA	1:C:302:ILE:HG22	2.00	0.42
1:A:217:LEU:HD11	1:A:254:LEU:HD23	2.00	0.42
1:A:633:VAL:HG21	1:A:669:ILE:HD11	2.01	0.42
1:A:754:SER:HA	1:A:755:PRO:HD3	1.96	0.42
2:D:8:G:H2'	2:D:9:U:C6	2.55	0.42
1:A:254:LEU:HD12	1:A:254:LEU:HA	1.89	0.42
1:A:269:LEU:HD12	1:A:269:LEU:HA	1.85	0.42
1:C:512:PHE:CZ	1:C:516:ARG:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:782:MET:HE1	1:C:783:LEU:HD23	2.02	0.42
1:A:975:LEU:HD22	1:A:998:VAL:HG21	2.01	0.42
1:A:1158:THR:HB	1:A:1163:GLN:HG2	2.01	0.42
1:C:146:TYR:CE1	1:C:186:LEU:HD13	2.51	0.42
1:C:1194:ILE:HA	1:C:1227:GLY:O	2.20	0.42
1:A:728:GLU:HB3	1:A:952:TYR:CE2	2.55	0.41
1:A:1126:LYS:HE3	2:B:3:U:C5	2.55	0.41
1:A:1217:ILE:HG21	1:A:1243:TRP:HE1	1.85	0.41
1:C:269:LEU:HD12	1:C:269:LEU:HA	1.92	0.41
1:C:366:ALA:HB2	1:C:527:GLU:CD	2.45	0.41
1:C:448:LEU:HD12	1:C:448:LEU:HA	1.85	0.41
1:A:1233:ASN:OD1	1:A:1235:GLN:HB2	2.20	0.41
1:C:1138:VAL:HG22	1:C:1171:MET:HE2	2.02	0.41
1:A:701:ARG:HH12	1:A:705:ARG:HH12	1.68	0.41
1:C:1176:PHE:HB3	1:C:1179:VAL:HB	2.02	0.41
1:C:1274:VAL:HG21	1:C:1280:PHE:CD1	2.56	0.41
1:C:1012:LEU:HA	1:C:1012:LEU:HD23	1.75	0.41
1:A:199:MET:HE1	1:A:969:GLN:OE1	2.21	0.41
1:A:350:ARG:HH21	1:A:385:ARG:HH12	1.69	0.41
1:C:287:ILE:HD13	1:C:287:ILE:HA	1.92	0.41
1:C:1261:ARG:HD2	1:C:1271:HIS:HB3	2.02	0.41
1:C:1074:ARG:O	1:C:1225:LYS:HD3	2.20	0.41
1:C:1207:LYS:H	1:C:1207:LYS:HG2	1.66	0.41
1:C:1261:ARG:HA	1:C:1261:ARG:HD3	1.71	0.41
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.82	0.41
1:A:409:ARG:HG2	1:A:447:ARG:HG2	2.02	0.41
1:C:221:LEU:HD13	1:C:269:LEU:HD21	2.01	0.41
1:C:1053:VAL:HB	1:C:1057:GLU:HG2	2.02	0.41
1:A:990:LYS:CE	2:B:8:G:H5'	2.42	0.41
1:C:250:LEU:HA	1:C:253:ASP:OD2	2.20	0.41
1:C:1131:GLN:HG3	1:C:1135:HIS:NE2	2.36	0.41
1:A:143:LYS:HA	1:A:143:LYS:HD3	1.91	0.40
1:A:534:ARG:NE	1:A:540:ASN:HD22	2.14	0.40
1:A:1043:TYR:HB3	1:A:1047:LYS:HE3	2.03	0.40
1:A:1047:LYS:HB3	1:A:1047:LYS:HE2	1.60	0.40
1:C:300:THR:O	1:C:303:GLU:HG3	2.21	0.40
1:C:498:GLN:HA	1:C:499:PRO:HD3	1.94	0.40
1:C:968:LEU:HD11	1:C:993:GLN:HB3	2.03	0.40
1:C:985:THR:OG1	1:C:1015:HIS:HB3	2.21	0.40
1:A:263:VAL:O	1:A:267:SER:HB2	2.21	0.40
1:A:1240:VAL:HG11	1:A:1243:TRP:HD1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:VAL:HG11	1:C:484:LEU:HD11	2.03	0.40
1:C:153:LEU:HD23	1:C:153:LEU:HA	1.88	0.40
1:C:273:LEU:HD23	1:C:273:LEU:HA	1.90	0.40
1:C:894:LYS:HA	1:C:894:LYS:HD3	1.86	0.40
1:C:1233:ASN:OD1	1:C:1235:GLN:HB2	2.22	0.40
1:A:656:CYS:SG	1:A:661:ALA:HB3	2.62	0.40
1:C:442:TRP:CH2	1:C:477:LEU:HD12	2.57	0.40
1:C:716:MET:HE2	2:D:13:U:H4'	2.04	0.40
1:C:976:LYS:HE2	1:C:976:LYS:HB2	1.88	0.40
1:C:599:ASP:HB3	1:C:602:GLN:HG3	2.03	0.40
1:C:1131:GLN:HG3	1:C:1135:HIS:CE1	2.57	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	1145/1918 (60%)	1101 (96%)	44 (4%)	0	100	100
1	C	1145/1918 (60%)	1102 (96%)	43 (4%)	0	100	100
All	All	2290/3836 (60%)	2203 (96%)	87 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1042/1726 (60%)	1026 (98%)	16 (2%)	57	69
1	C	1042/1726 (60%)	1021 (98%)	21 (2%)	48	66
All	All	2084/3452 (60%)	2047 (98%)	37 (2%)	51	67

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	VAL
1	A	205	LEU
1	A	354	ARG
1	A	365	THR
1	A	381	VAL
1	A	524	GLU
1	A	592	SER
1	A	683	ARG
1	A	717	SER
1	A	911	MET
1	A	983	MET
1	A	1043	TYR
1	A	1154	ILE
1	A	1181	VAL
1	A	1184	VAL
1	A	1194	ILE
1	C	153	LEU
1	C	205	LEU
1	C	226	VAL
1	C	278	ASN
1	C	365	THR
1	C	381	VAL
1	C	683	ARG
1	C	700	LYS
1	C	701	ARG
1	C	983	MET
1	C	998	VAL
1	C	1029	LEU
1	C	1043	TYR
1	C	1094	HIS
1	C	1132	HIS
1	C	1154	ILE
1	C	1158	THR
1	C	1170	LEU
1	C	1184	VAL

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Mol	Chain	Res	Type
1	C	1194	ILE
1	C	1256	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
1	A	306	GLN
1	A	540	ASN
1	A	776	HIS
1	A	893	GLN
1	A	942	GLN
1	A	1063	ASN
1	A	1266	ASN
1	A	1267	HIS
1	C	264	GLN
1	C	393	GLN
1	C	487	ASN
1	C	498	GLN
1	C	699	ASN
1	C	871	HIS
1	C	1063	ASN
1	C	1070	ASN
1	C	1109	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	13/60 (21%)	7 (53%)	4 (30%)
2	D	13/60 (21%)	7 (53%)	3 (23%)
All	All	26/120 (21%)	14 (53%)	7 (26%)

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	G
2	B	3	U
2	B	4	G
2	B	10	G
2	B	11	U

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Mol	Chain	Res	Type
2	B	12	G
2	B	13	U
2	D	2	G
2	D	3	U
2	D	4	G
2	D	10	G
2	D	11	U
2	D	12	G
2	D	13	U

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1	U
2	B	3	U
2	B	9	U
2	B	12	G
2	D	1	U
2	D	3	U
2	D	12	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AGS	A	2000	-	32,33,33	0.52	1 (3%)	45,52,52	0.66	1 (2%)
3	AGS	C	2000	-	32,33,33	0.57	1 (3%)	45,52,52	0.72	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	A	2000	-	-	4/21/38/38	0/3/3/3
3	AGS	C	2000	-	-	5/21/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2000	AGS	PG-S1G	2.06	1.95	1.90
3	A	2000	AGS	PG-S1G	2.02	1.95	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	AGS	PB-O3B-PG	-3.45	120.53	133.17
3	C	2000	AGS	PB-O3B-PG	-3.39	120.75	133.17

There are no chirality outliers.

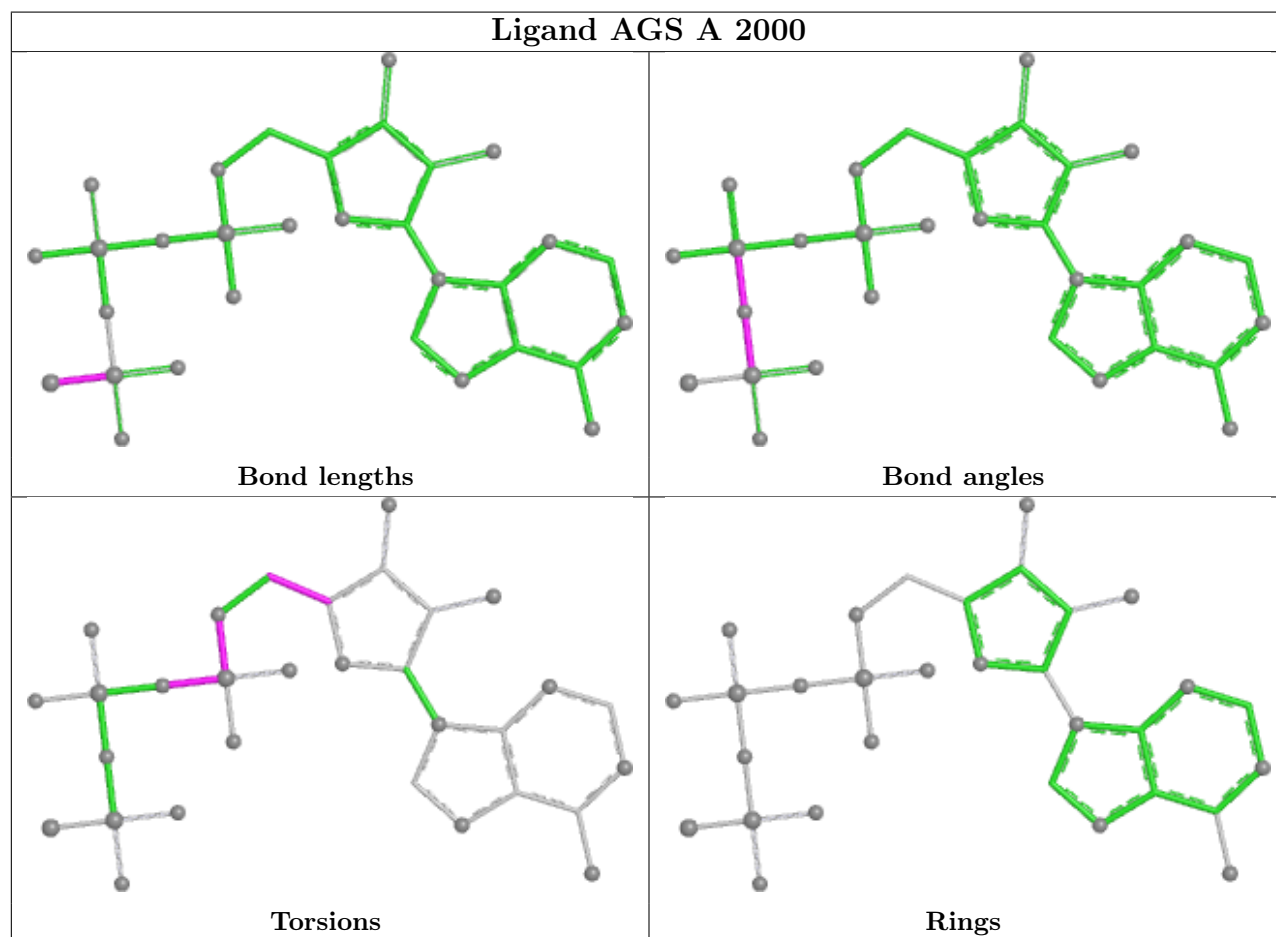
All (9) torsion outliers are listed below:

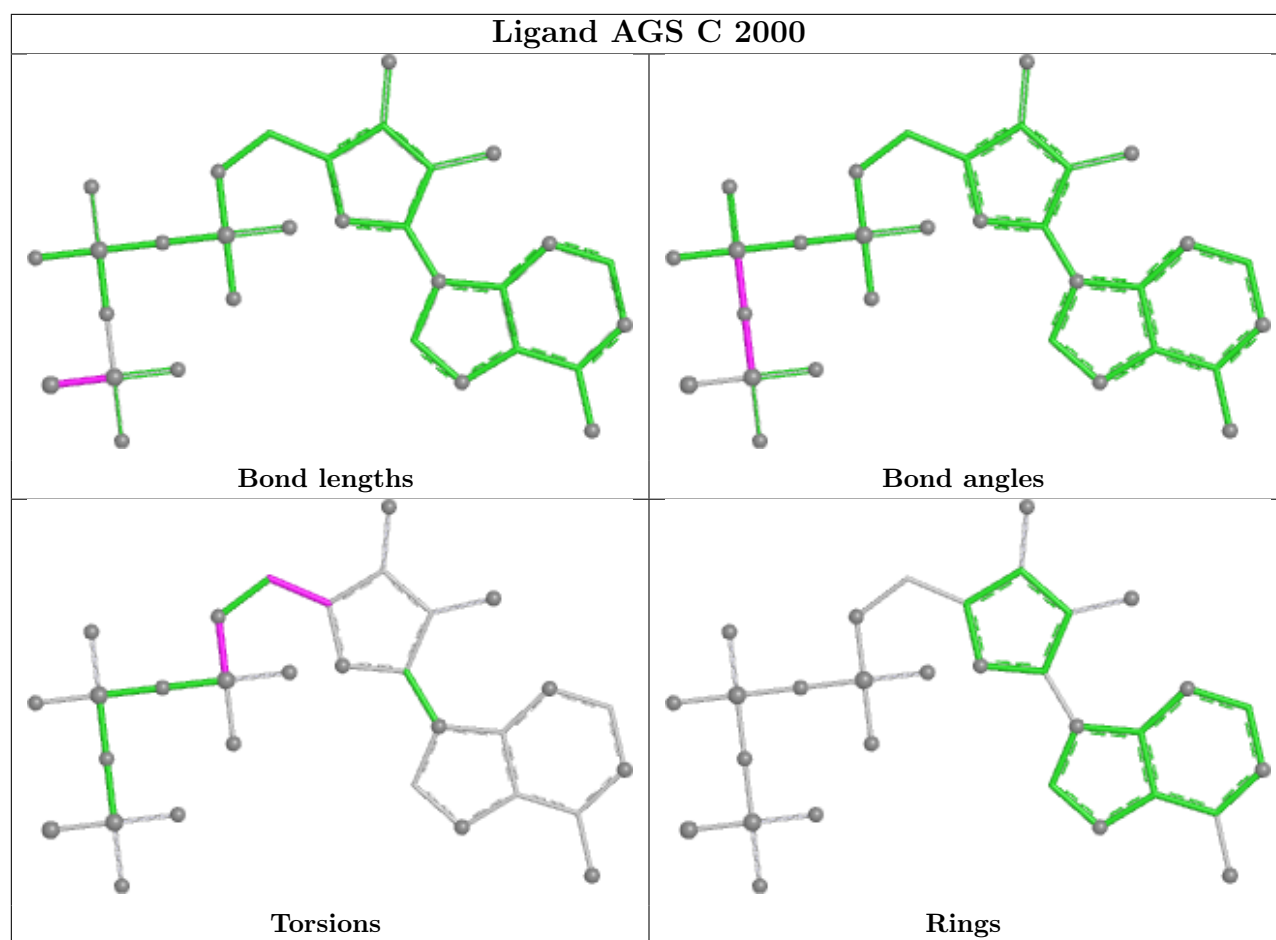
Mol	Chain	Res	Type	Atoms
3	C	2000	AGS	C5'-O5'-PA-O2A
3	C	2000	AGS	C5'-O5'-PA-O3A
3	C	2000	AGS	O4'-C4'-C5'-O5'
3	C	2000	AGS	C3'-C4'-C5'-O5'
3	A	2000	AGS	O4'-C4'-C5'-O5'
3	A	2000	AGS	C5'-O5'-PA-O2A
3	A	2000	AGS	C5'-O5'-PA-O3A
3	C	2000	AGS	C5'-O5'-PA-O1A
3	A	2000	AGS	PB-O3A-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

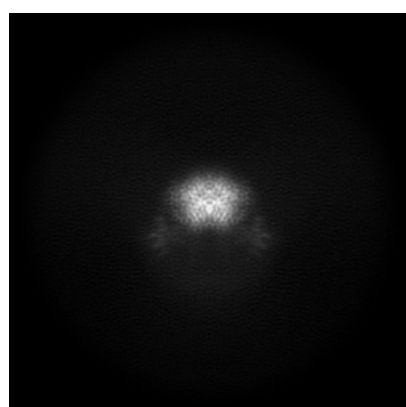
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-77053. These allow visual inspection of the internal detail of the map and identification of artifacts.

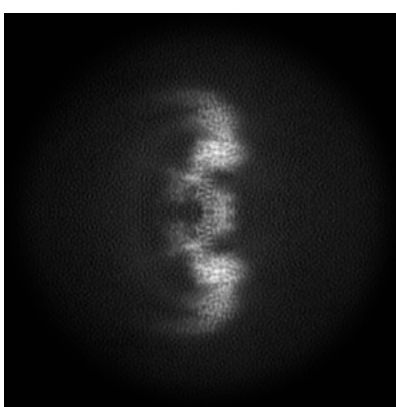
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

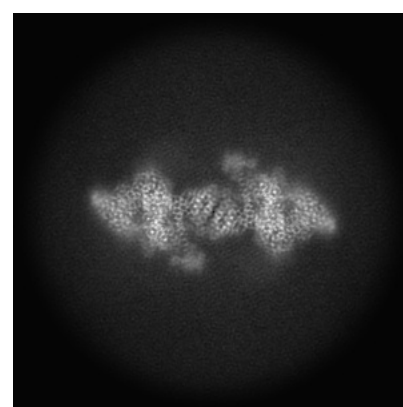
6.1.1 Primary map



X



Y

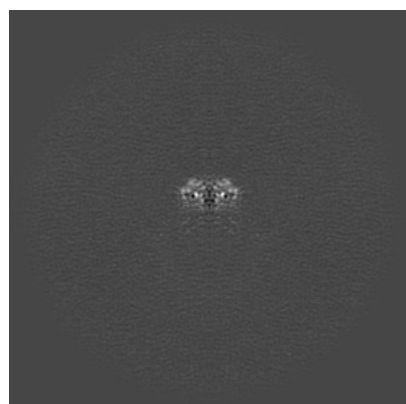


Z

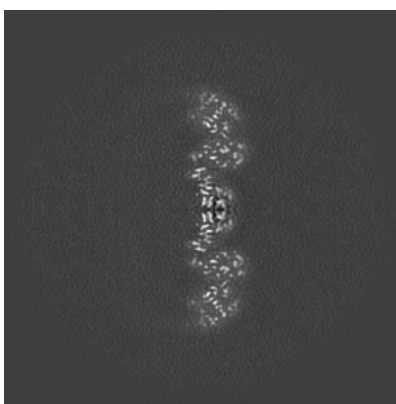
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

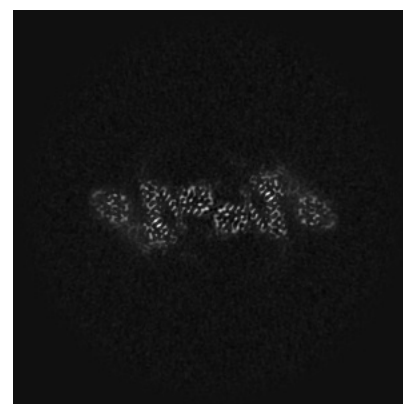
6.2.1 Primary map



X Index: 220



Y Index: 220

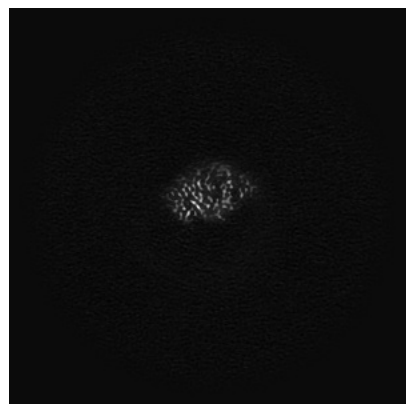


Z Index: 220

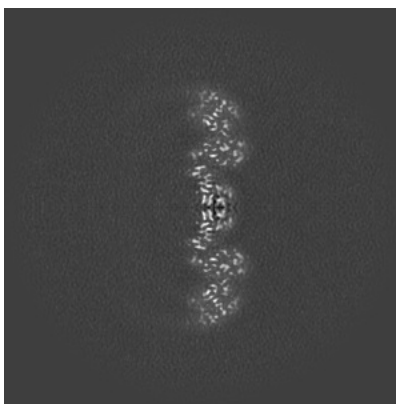
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

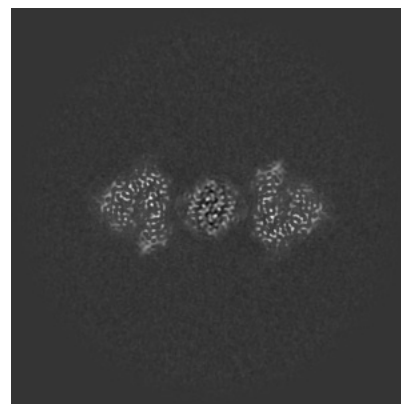
6.3.1 Primary map



X Index: 157



Y Index: 220

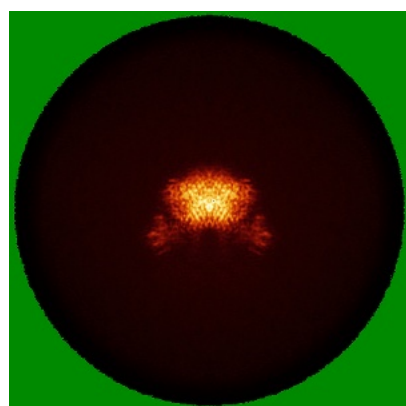


Z Index: 234

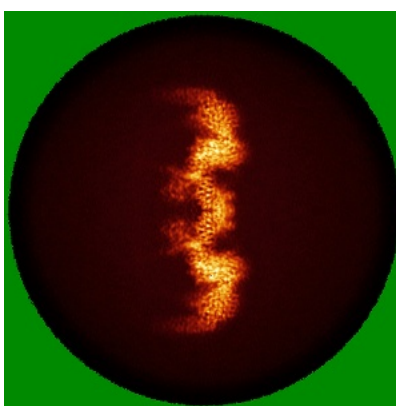
The images above show the largest variance slices of the map in three orthogonal directions.

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

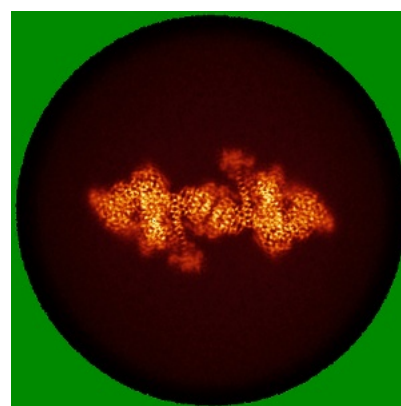
6.4.1 Primary map



X



Y

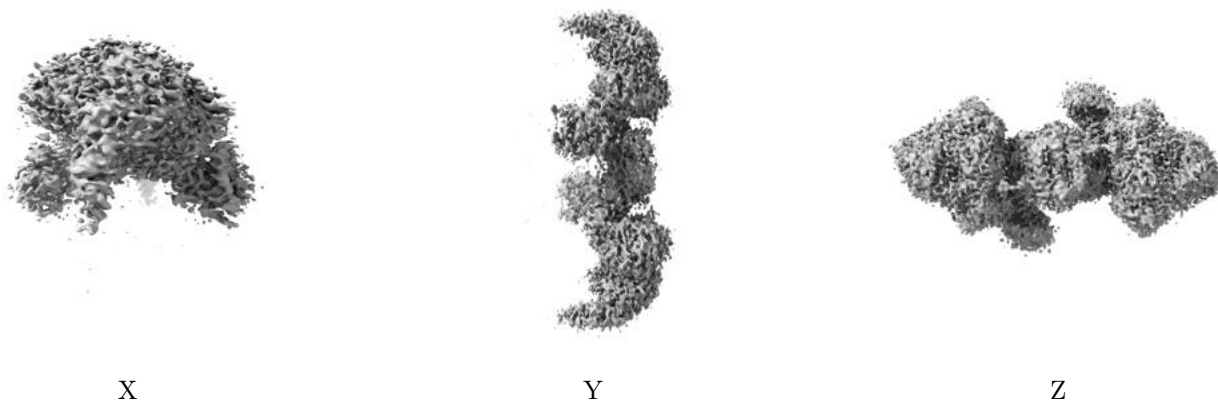


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

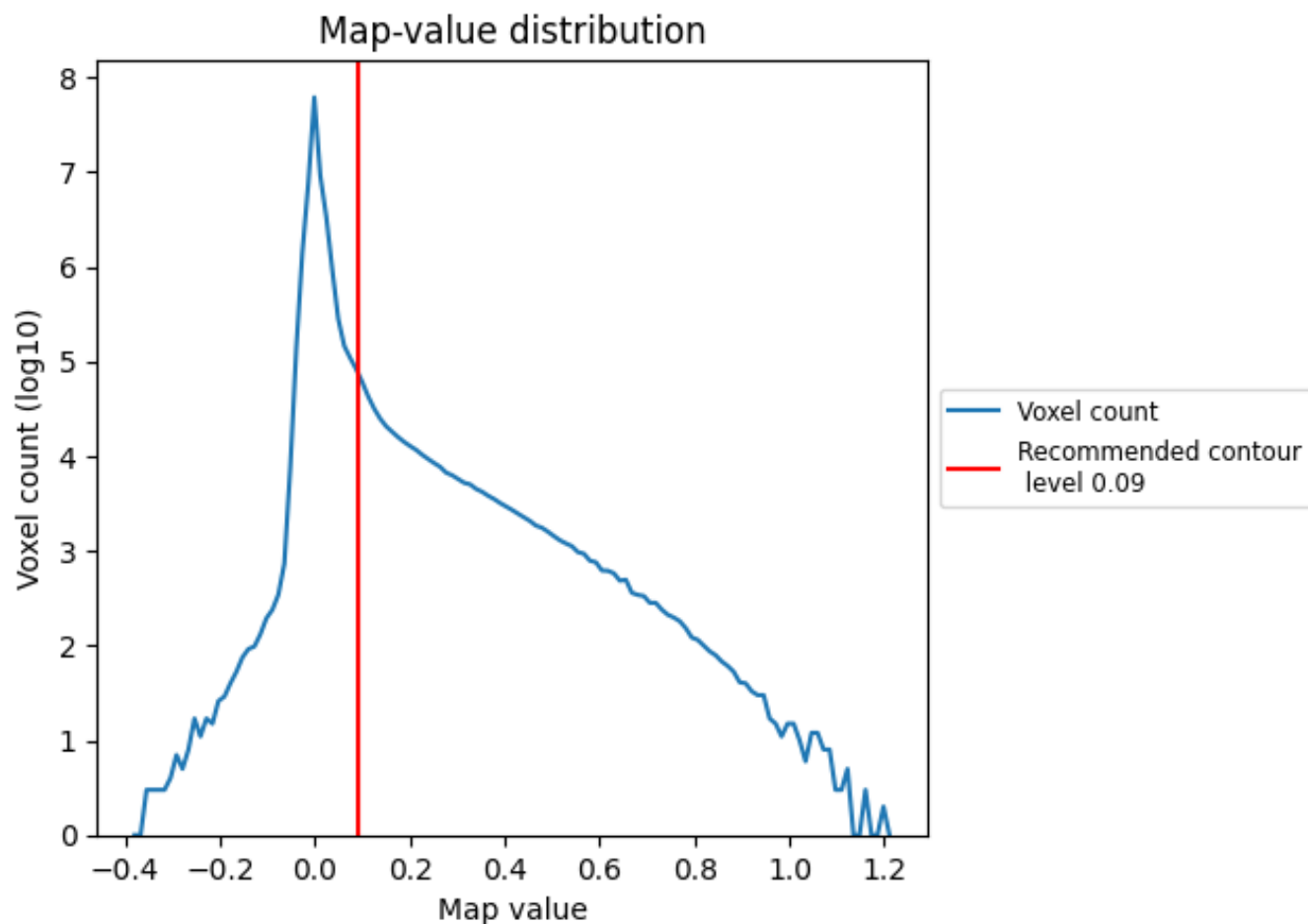
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

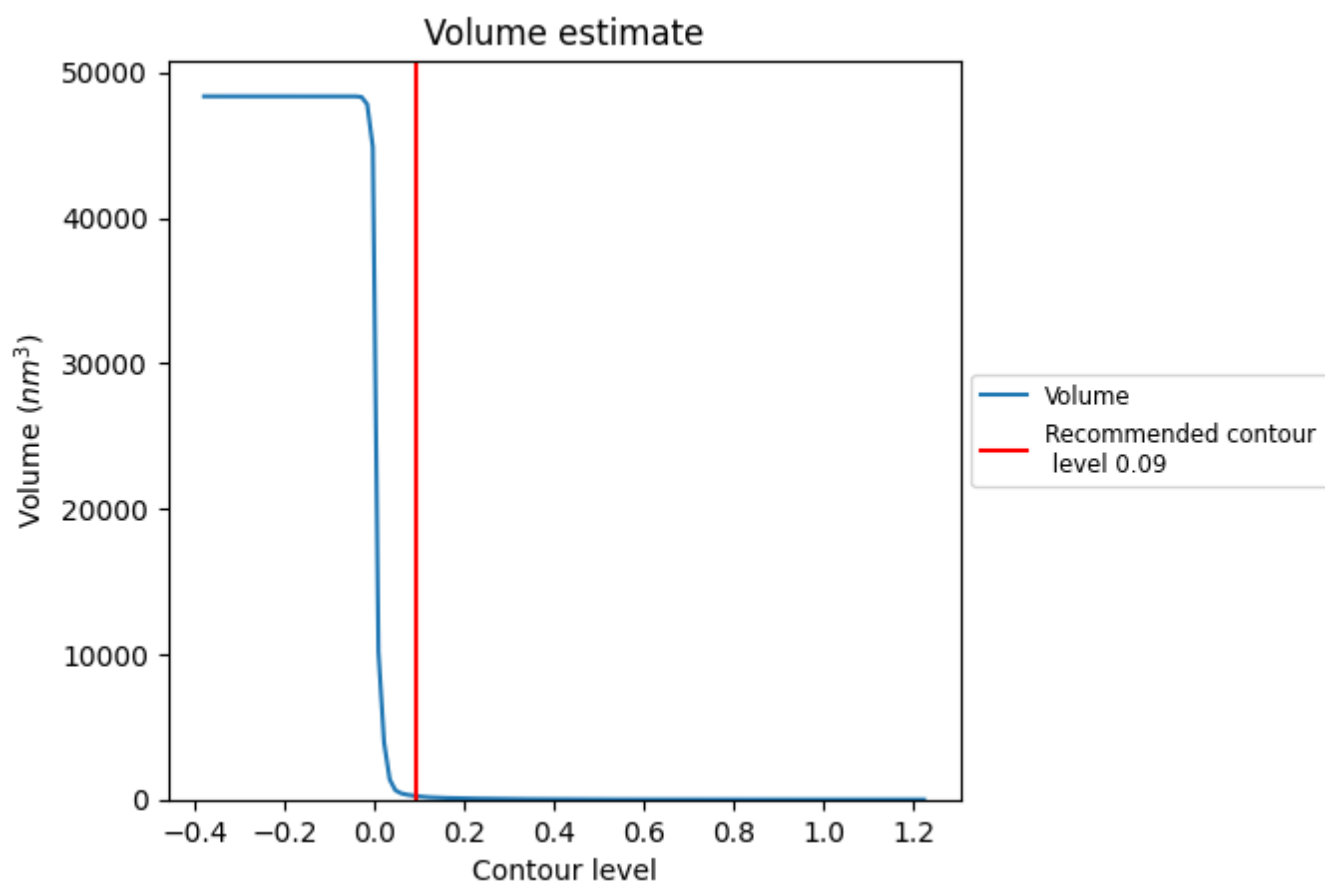
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

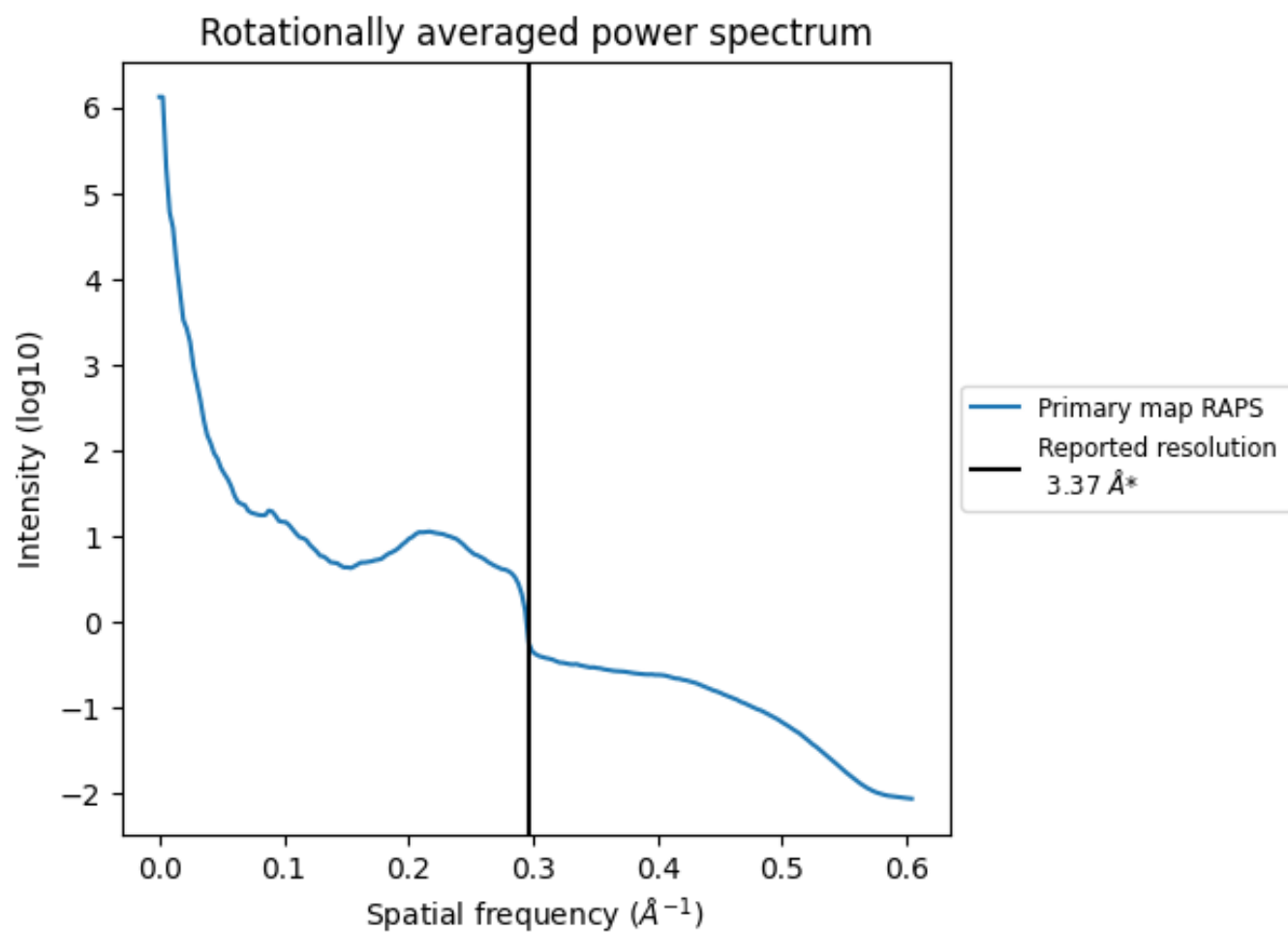
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 246 nm^3 ; this corresponds to an approximate mass of 223 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 0.297 Å⁻¹

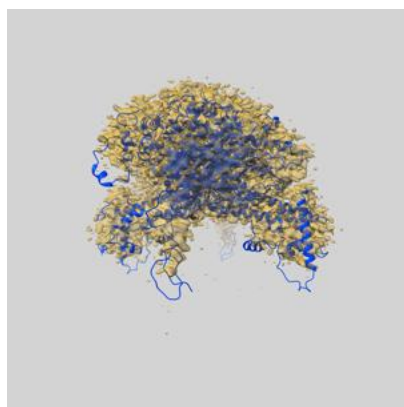
8 Fourier-Shell correlation ⓘ

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

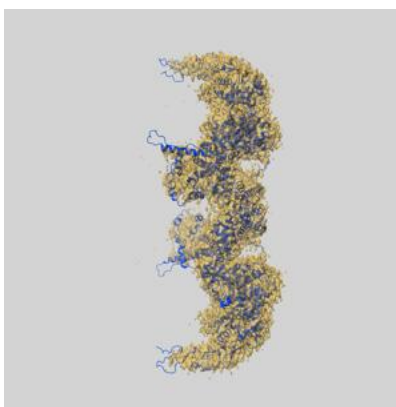
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-77053 and PDB model 13FZ. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

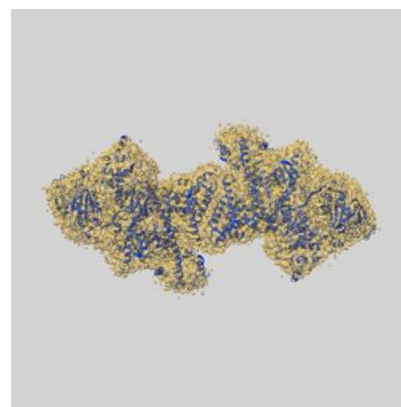
9.1 Map-model overlay [i](#)



X



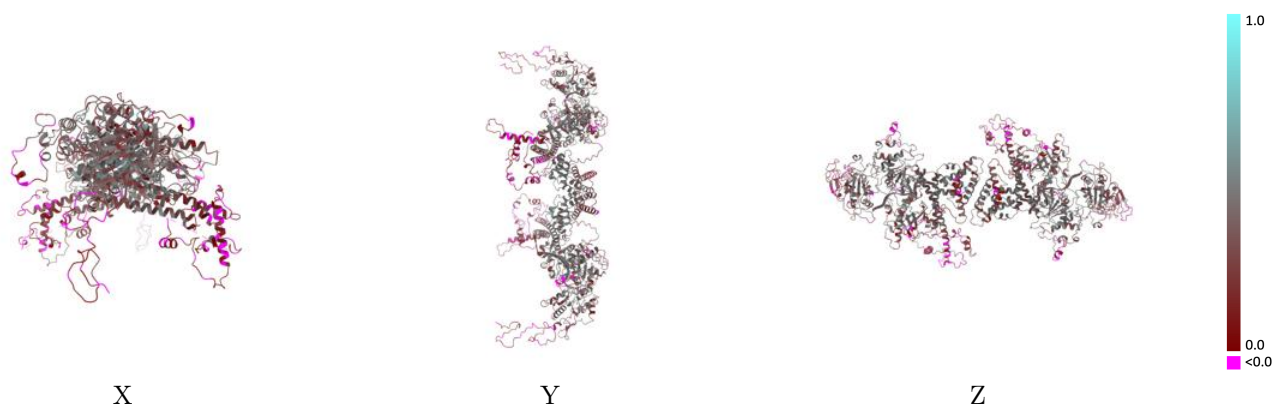
Y



Z

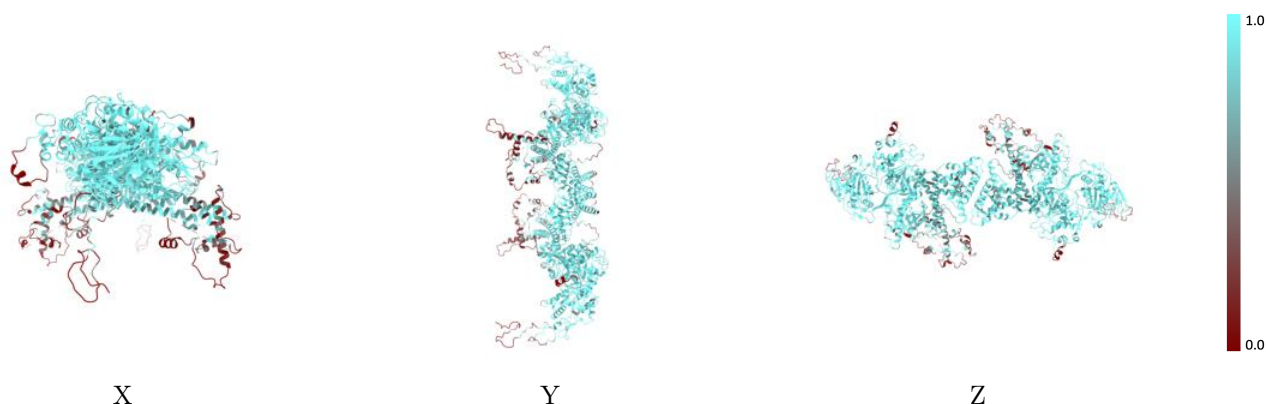
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



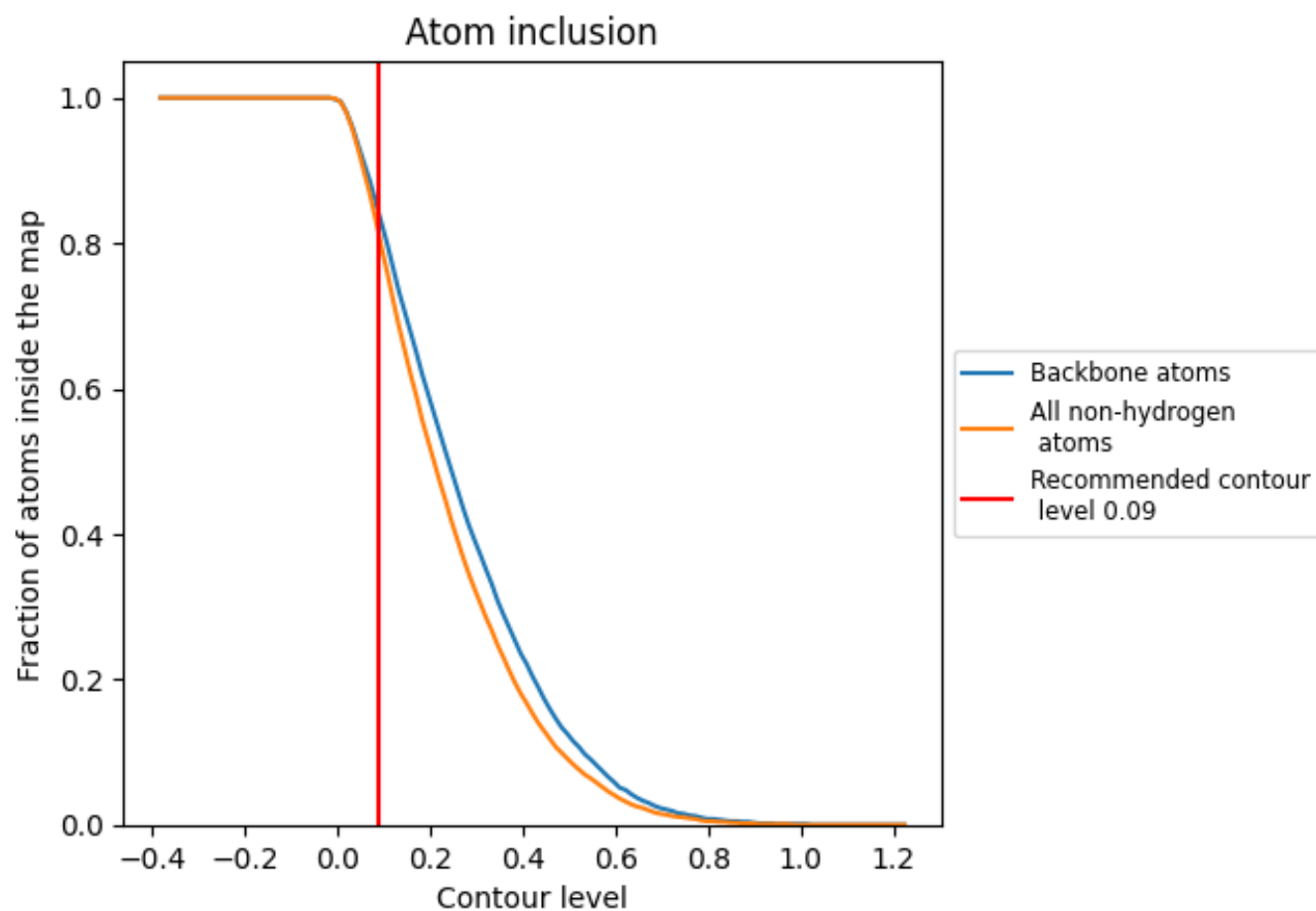
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 81% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8140	0.3330
A	0.8100	0.3300
B	0.8670	0.3900
C	0.8140	0.3330
D	0.8640	0.3710

