Full wwPDB EM Validation Report

Mar 30, 2025 – 12:57 AM JST

PDB ID	:	8ZIT
EMDB ID	:	EMD-60129
Title	:	DUF4297-HerA complex with DNA and ATPgamaS
Authors	:	Yu, Y.; Chen, Q.
Deposited on	:	2024-05-14
Resolution	:	3.76 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:

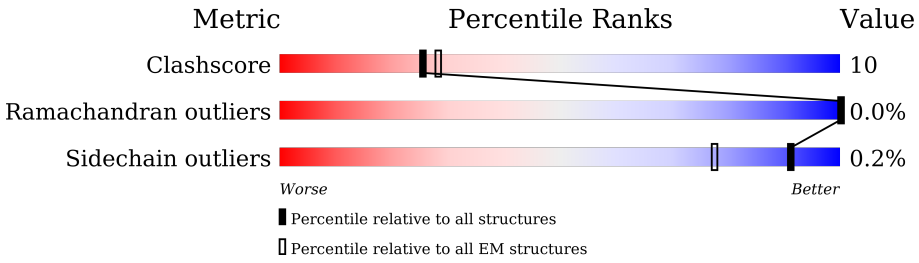
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 3.76 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	397	72% 25%
1	B	397	39% 56%
1	C	397	73% 24%
1	D	397	38% 5% 57%
1	E	397	70% 27%
1	F	397	37% 7% 57%
1	G	397	75% 23%
1	H	397	35% 9% 57%

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Mol	Chain	Length	Quality of chain
1	I	397	73% 24%
1	J	397	36% 8% 56%
1	K	397	68% 29%
1	L	397	37% 7% 56%
2	M	617	79% 16% 5%
2	N	617	77% 15% 8%
2	O	617	72% 21% 7%
2	P	617	78% 17% 5%
2	Q	617	74% 21% 5%
2	R	617	80% 15% 5%
3	U	16	12% 88%
4	V	17	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 107777 atoms, of which 52462 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 DUF4297.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	387	Total	C	H	N	O	S	0	0
			5979	2004	2846	544	577	8		
1	B	173	Total	C	H	N	O	S	0	0
			2841	921	1400	261	254	5		
1	C	386	Total	C	H	N	O	S	0	0
			6007	1992	2890	541	576	8		
1	D	172	Total	C	H	N	O	S	0	0
			2850	915	1418	259	253	5		
1	E	387	Total	C	H	N	O	S	0	0
			5979	2004	2846	544	577	8		
1	F	172	Total	C	H	N	O	S	0	0
			2837	915	1405	259	253	5		
1	G	387	Total	C	H	N	O	S	0	0
			5979	2004	2846	544	577	8		
1	H	172	Total	C	H	N	O	S	0	0
			2841	915	1409	259	253	5		
1	I	386	Total	C	H	N	O	S	0	0
			6007	1992	2890	541	576	8		
1	J	175	Total	C	H	N	O	S	0	0
			2871	928	1418	263	257	5		
1	K	386	Total	C	H	N	O	S	0	0
			6007	1992	2890	541	576	8		
1	L	173	Total	C	H	N	O	S	0	0
			2850	921	1409	261	254	5		

- Molecule 2 is a protein called HerA.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	M	586	Total	C	H	N	O	S	0	0
			9048	2897	4496	778	864	13		
2	N	568	Total	C	H	N	O	S	0	0
			8742	2793	4353	747	836	13		
2	O	576	Total	C	H	N	O	S	0	0
			8905	2855	4424	762	851	13		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	P	586	Total	C	H	N	O	S	0	0
			9048	2897	4496	778	864	13		
2	Q	585	Total	C	H	N	O	S	0	0
			9014	2891	4471	776	863	13		
2	R	586	Total	C	H	N	O	S	0	0
			9029	2897	4477	778	864	13		

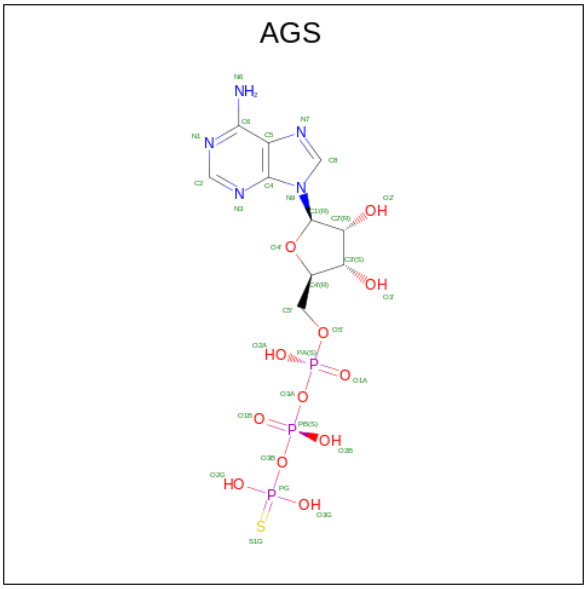
- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	16	Total	C	N	O	P	0	0
			328	160	56	96	16		

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	17	Total	C	N	O	P	0	0
			345	170	58	101	16		

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms							AltConf
5	M	1	Total	C	H	N	O	P	S	0
			44	10	13	5	12	3	1	
5	N	1	Total	C	H	N	O	P	S	0
			44	10	13	5	12	3	1	
5	O	1	Total	C	H	N	O	P	S	0
			44	10	13	5	12	3	1	
5	P	1	Total	C	H	N	O	P	S	0
			44	10	13	5	12	3	1	
5	Q	1	Total	C	H	N	O	P	S	0
			44	10	13	5	12	3	1	
5	R	1	Total	C	H	N	O	P	S	0
			44	10	13	5	12	3	1	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

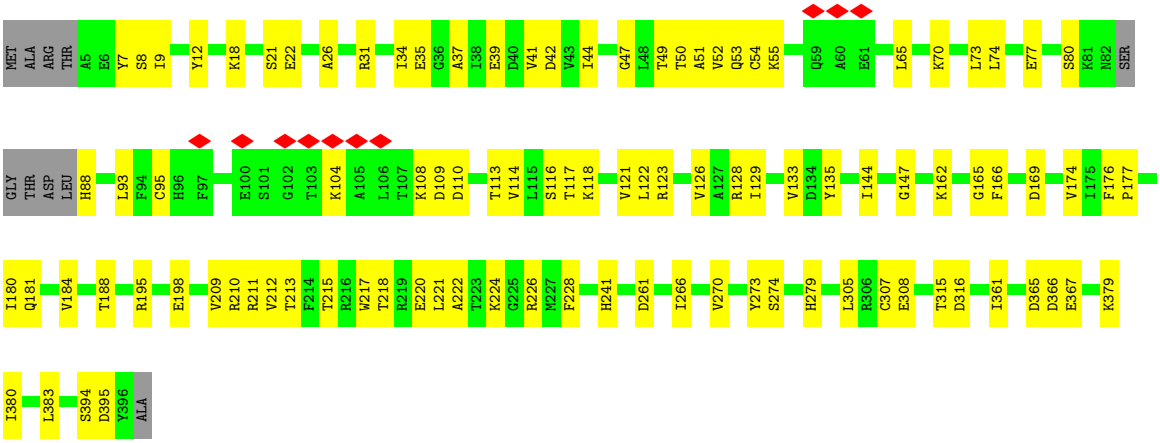
Mol	Chain	Residues	Atoms		AltConf
6	M	1	Total	Mg	0
			1	1	
6	N	1	Total	Mg	0
			1	1	
6	O	1	Total	Mg	0
			1	1	
6	P	1	Total	Mg	0
			1	1	
6	Q	1	Total	Mg	0
			1	1	
6	R	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

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.

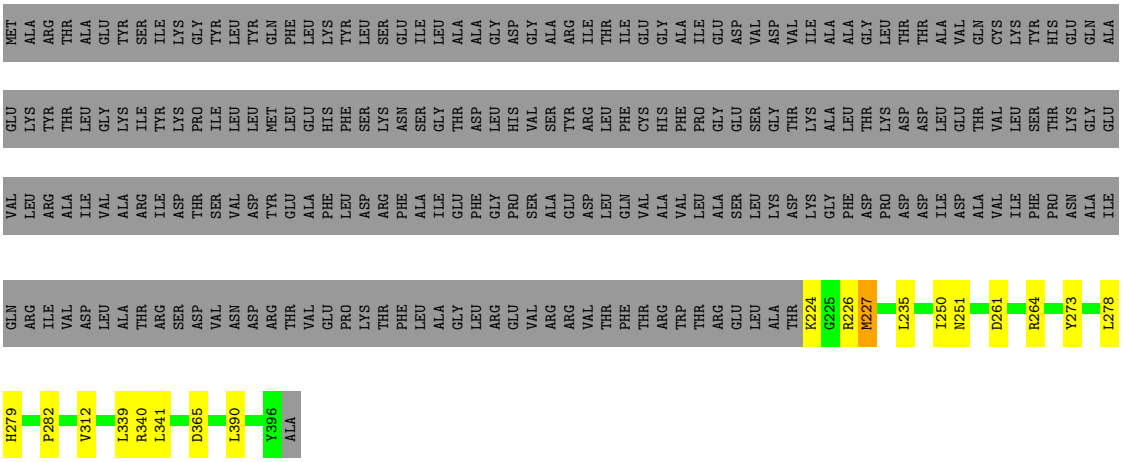
• Molecule 1: DUF4297

Chain A:



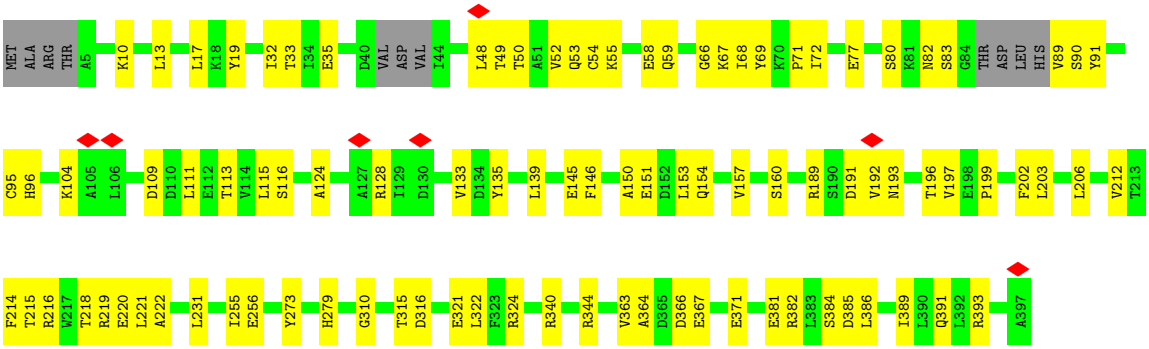
• Molecule 1: DUF4297

Chain B:



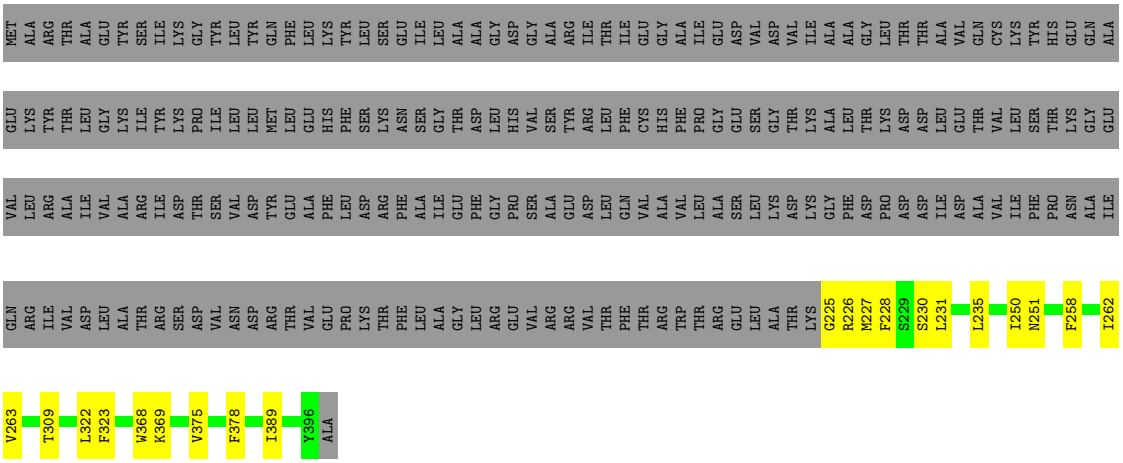
• Molecule 1: DUF4297

Chain C:



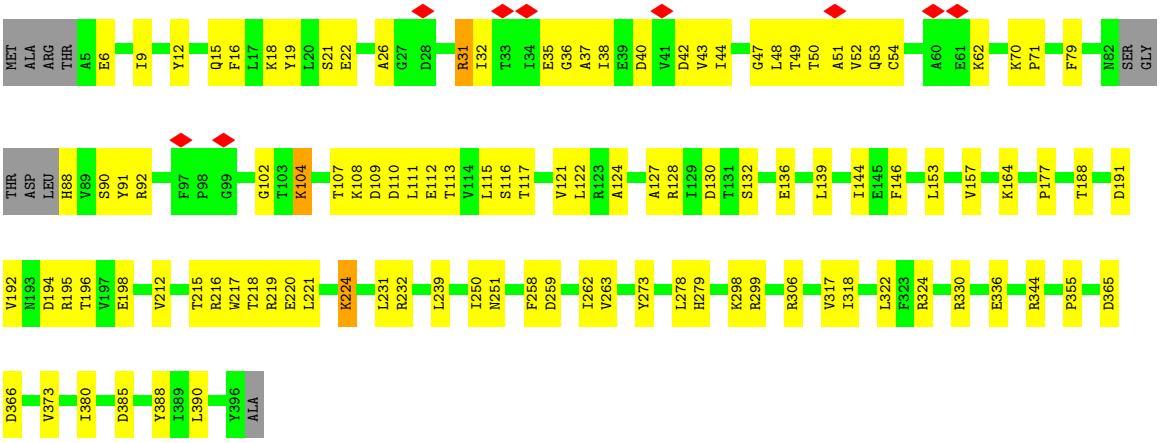
• Molecule 1: DUF4297

Chain D:



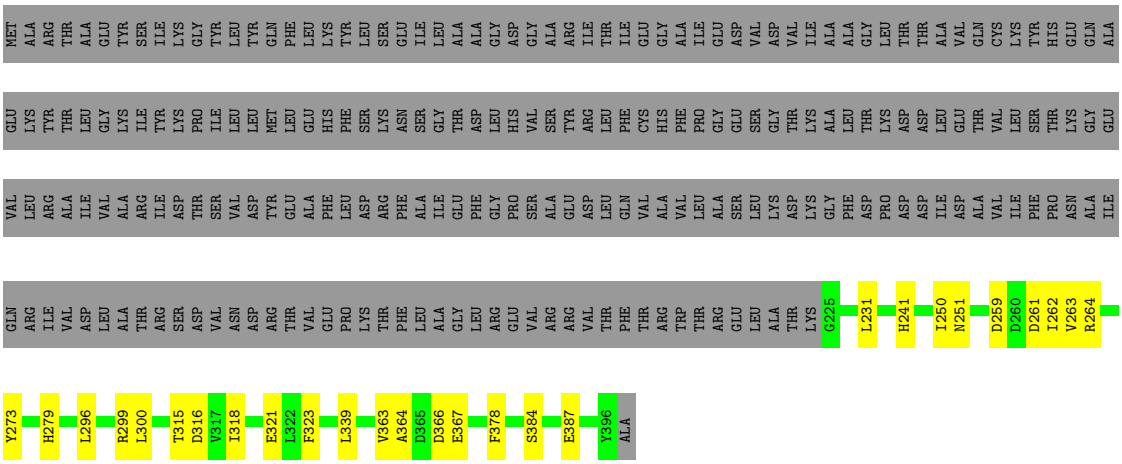
• Molecule 1: DUF4297

Chain E:



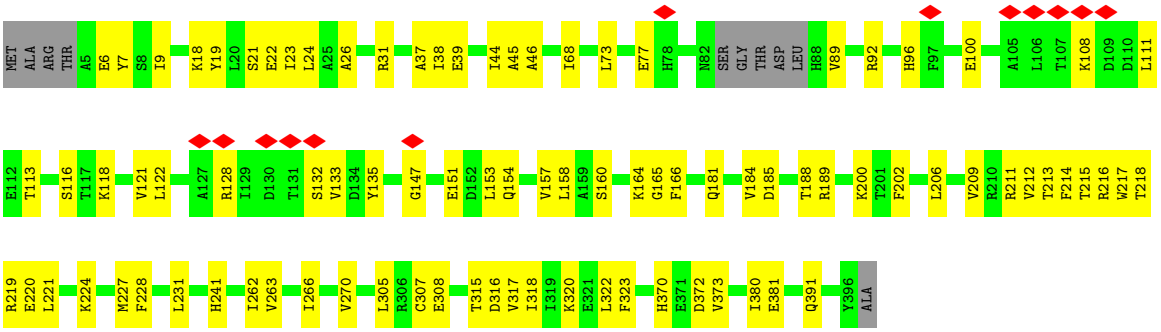
• Molecule 1: DUF4297

Chain F:



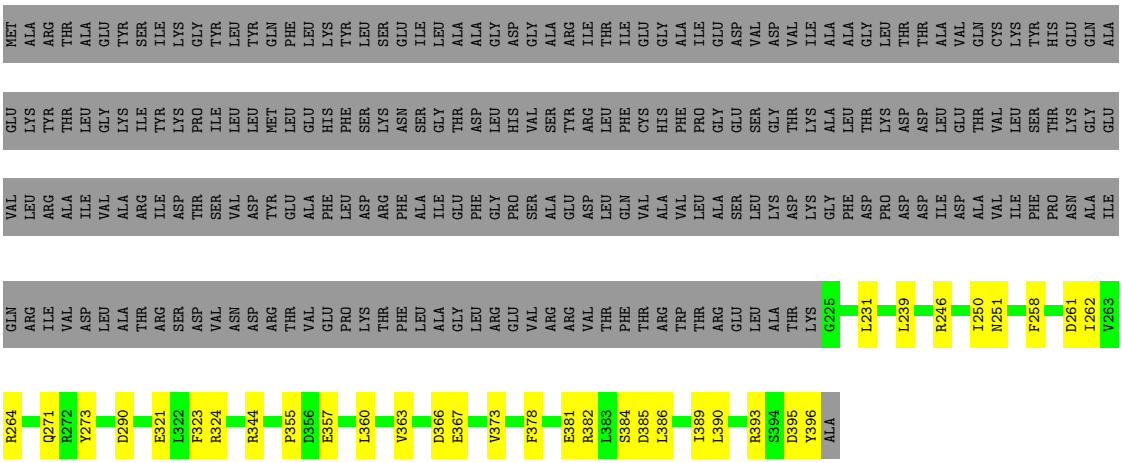
• Molecule 1: DUF4297

Chain G:



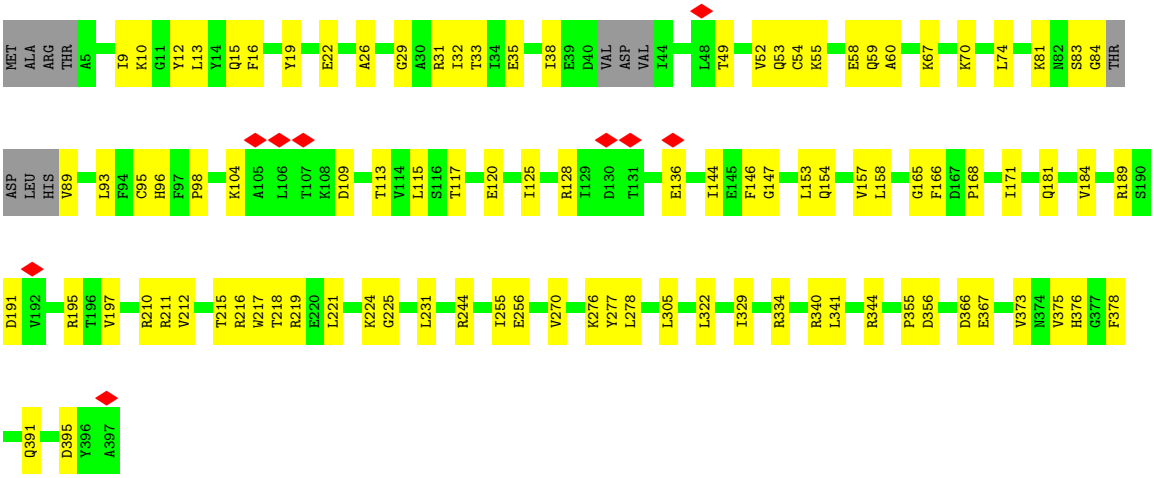
• Molecule 1: DUF4297

Chain H:



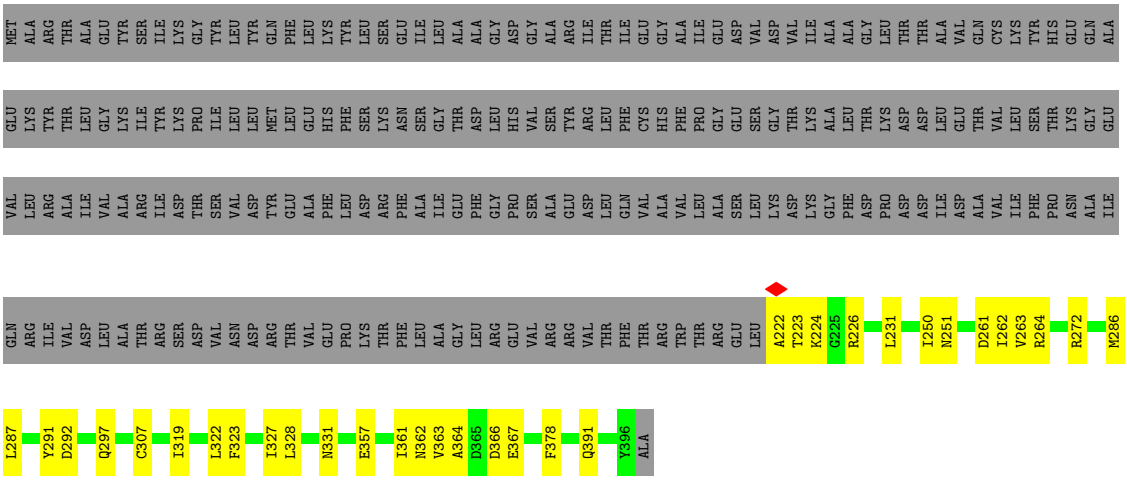
• Molecule 1: DUF4297

Chain I:



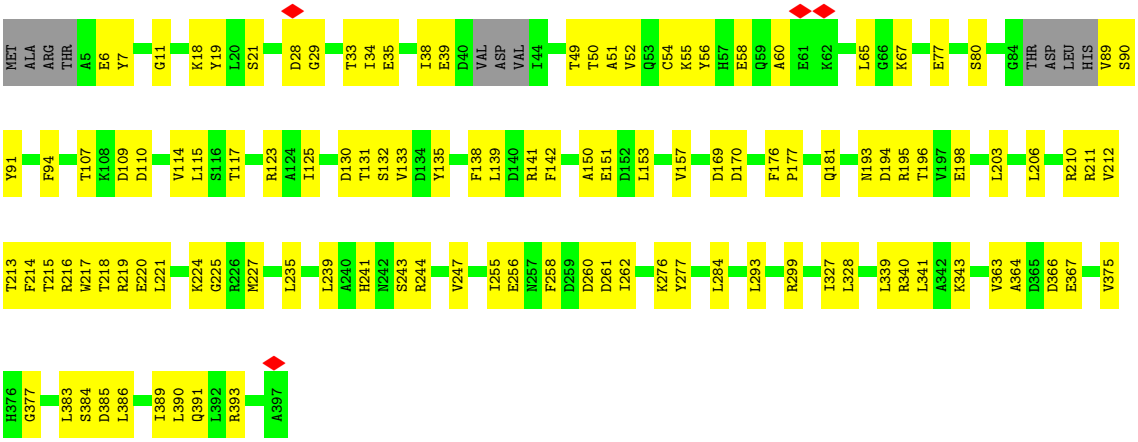
• Molecule 1: DUF4297

Chain J:



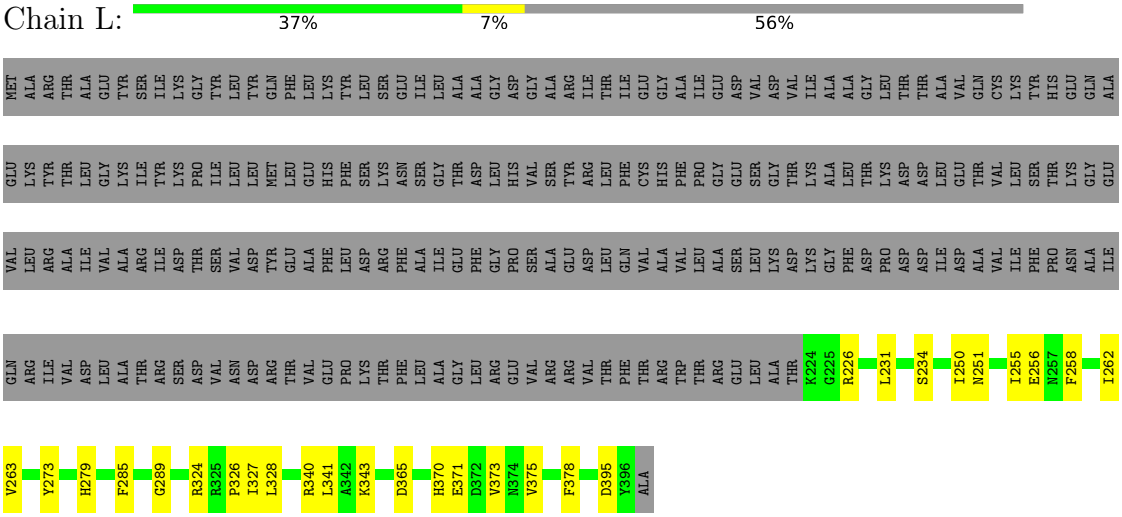
• Molecule 1: DUF4297

Chain K:



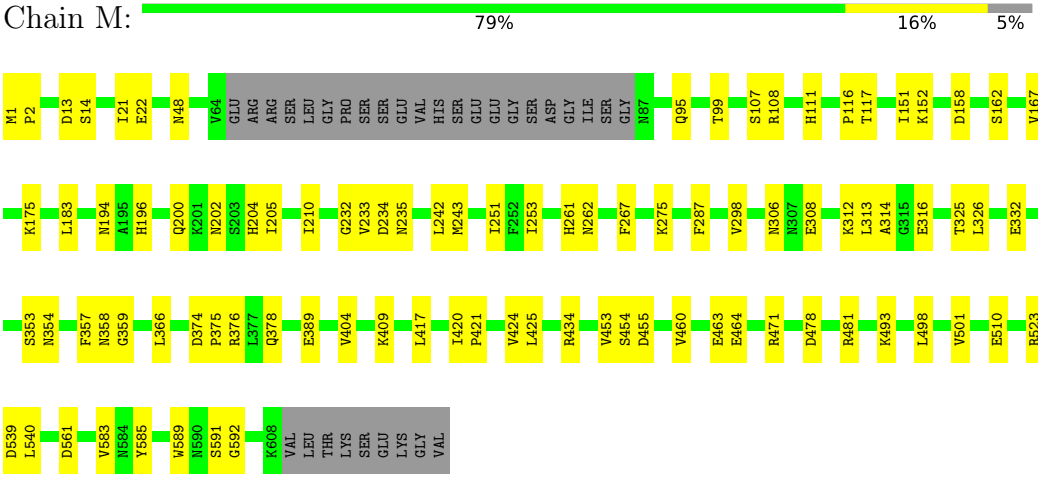
• Molecule 1: DUF4297

Chain L:



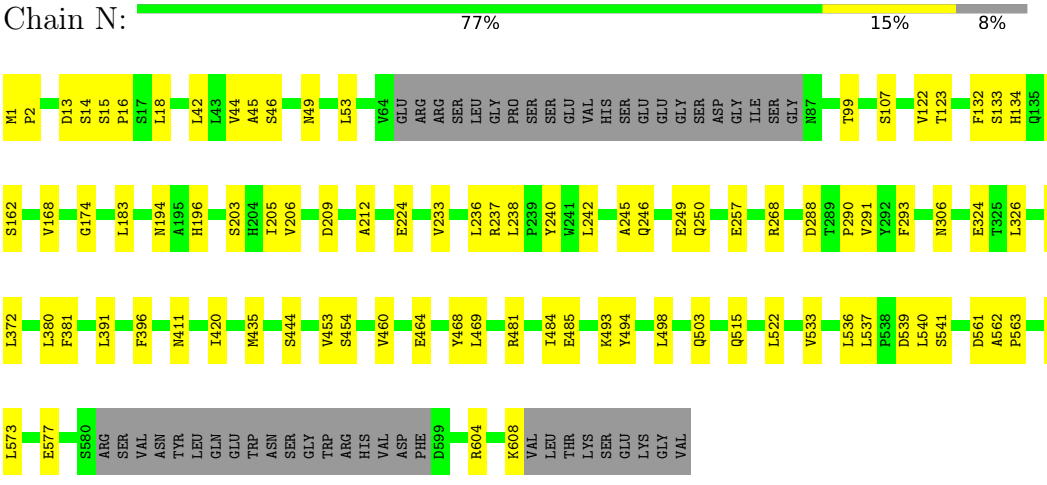
• Molecule 2: HerA

Chain M:



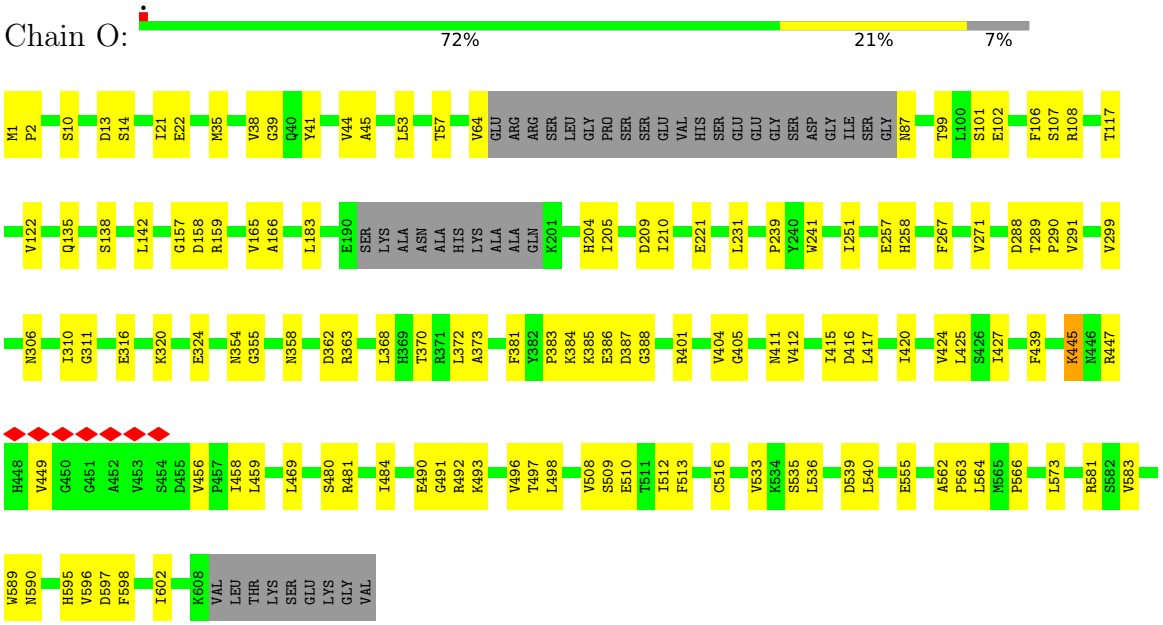
• Molecule 2: HerA

Chain N:



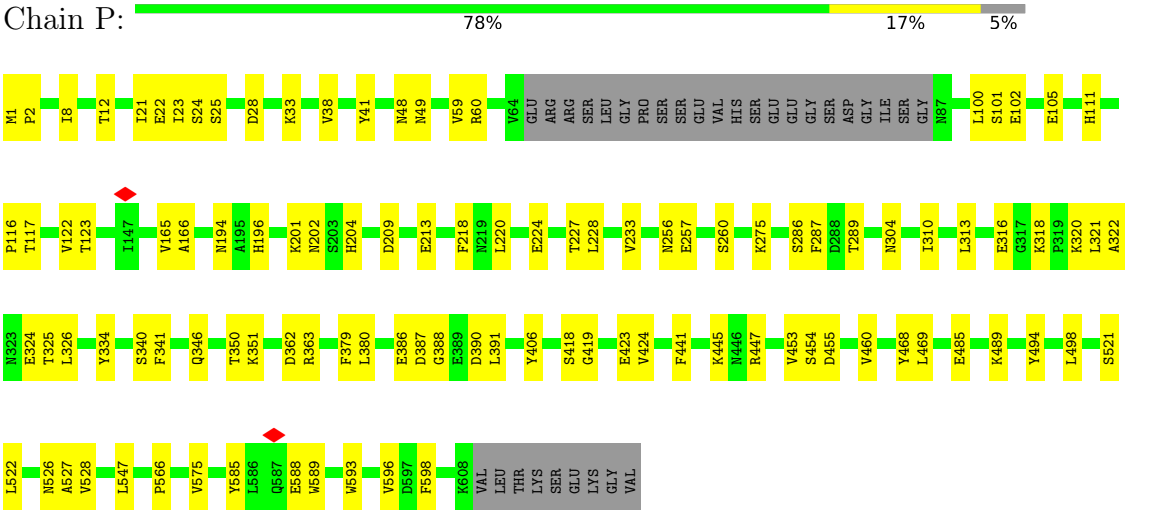
• Molecule 2: HerA

Chain O:



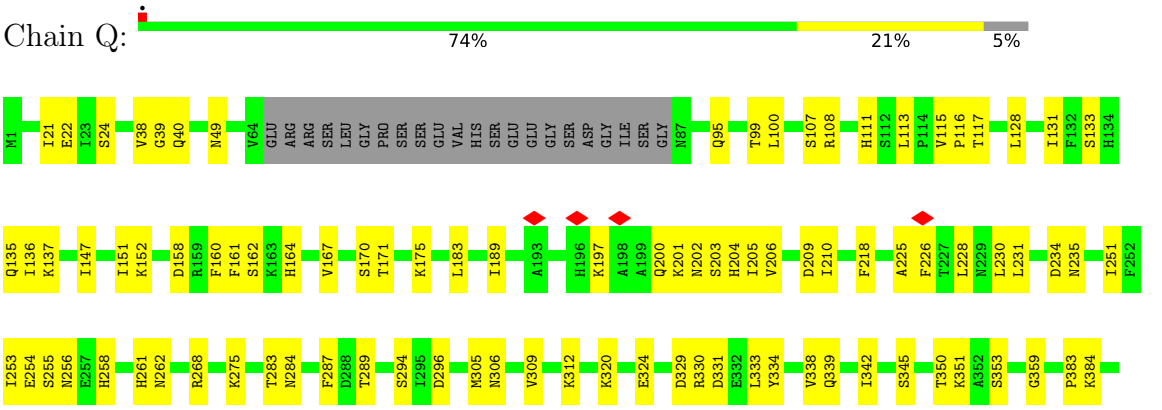
• Molecule 2: HerA

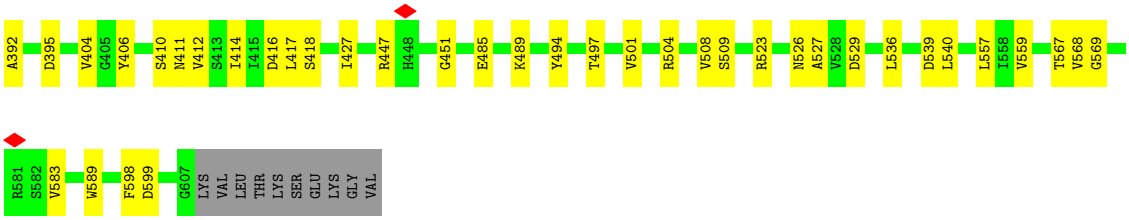
Chain P:



• Molecule 2: HerA

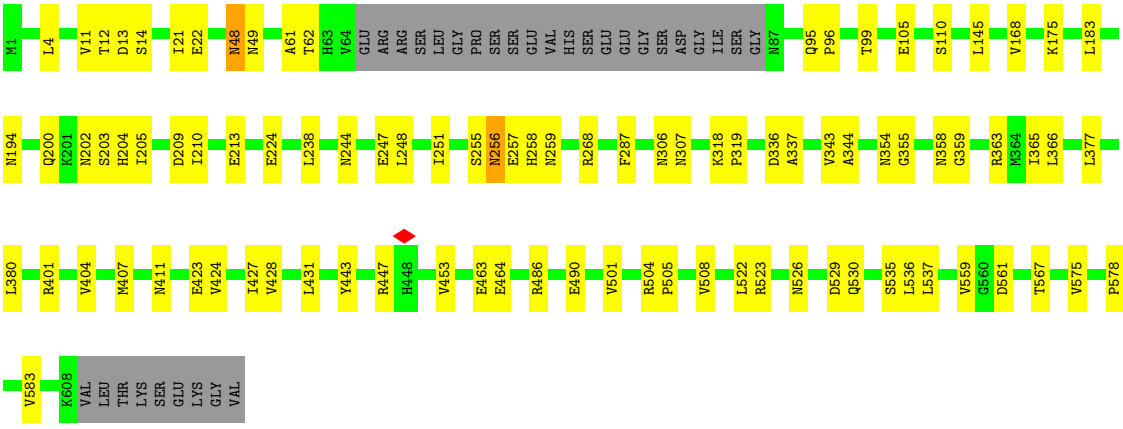
Chain Q:





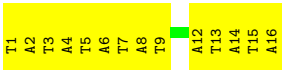
• Molecule 2: HerA

Chain R:



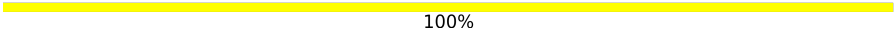
• Molecule 3: DNA (5'-D(P*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*A)-3')

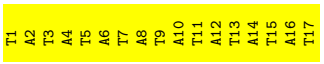
Chain U:



• Molecule 4: DNA (5'-D(*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*T)-3')

Chain V:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88914	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	63.01	Depositor
Minimum defocus (nm)	456	Depositor
Maximum defocus (nm)	2902	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.984	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.0121	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, 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	0.42	0/3195	0.45	0/4315
1	B	0.51	0/1472	0.46	0/1981
1	C	0.42	0/3177	0.46	0/4286
1	D	0.50	0/1463	0.47	0/1970
1	E	0.43	0/3195	0.46	1/4315 (0.0%)
1	F	0.51	0/1463	0.46	0/1970
1	G	0.41	0/3195	0.45	0/4315
1	H	0.53	0/1463	0.47	0/1970
1	I	0.43	0/3177	0.46	0/4286
1	J	0.52	0/1484	0.47	0/1998
1	K	0.44	0/3177	0.44	0/4286
1	L	0.52	0/1472	0.48	0/1981
2	M	0.54	0/4654	0.49	0/6316
2	N	0.52	0/4483	0.47	0/6081
2	O	0.50	0/4581	0.47	0/6217
2	P	0.52	0/4654	0.48	0/6316
2	Q	0.49	0/4645	0.48	0/6305
2	R	0.53	0/4654	0.48	1/6316 (0.0%)
3	U	0.77	0/367	1.06	0/564
4	V	0.81	0/386	1.08	0/594
All	All	0.49	0/56357	0.48	2/76382 (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
2	R	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	48	ASN	C-N-CA	5.19	134.67	121.70
1	E	31	ARG	NE-CZ-NH1	-5.07	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	R	256	ASN	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	3133	2846	3152	84	0
1	B	1441	1400	1455	17	0
1	C	3117	2890	3135	76	0
1	D	1432	1418	1442	18	0
1	E	3133	2846	3152	89	0
1	F	1432	1405	1442	16	0
1	G	3133	2846	3152	78	0
1	H	1432	1409	1442	21	0
1	I	3117	2890	3135	72	0
1	J	1453	1418	1467	23	0
1	K	3117	2890	3135	86	0
1	L	1441	1409	1455	17	0
2	M	4552	4496	4494	73	0
2	N	4389	4353	4350	65	0
2	O	4481	4424	4421	86	0
2	P	4552	4496	4495	80	0
2	Q	4543	4471	4481	92	0
2	R	4552	4477	4494	74	0
3	U	328	0	185	48	0
4	V	345	0	198	36	0
5	M	31	13	12	1	0
5	N	31	13	12	3	0
5	O	31	13	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	31	13	12	1	0
5	Q	31	13	12	1	0
5	R	31	13	12	3	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0
6	P	1	0	0	0	0
6	Q	1	0	0	0	0
6	R	1	0	0	0	0
All	All	55315	52462	54754	1110	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 (1110) 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:E:37:ALA:HA	1:E:51:ALA:HB1	1.29	1.09
3:U:7:DT:H2"	3:U:8:DA:H5"	1.43	1.00
5:Q:701:AGS:S1G	5:Q:701:AGS:O2B	2.24	0.94
1:C:391:GLN:OE1	2:N:49:ASN:ND2	2.01	0.93
1:A:215:THR:HG22	1:A:218:THR:HG23	1.53	0.91
1:K:49:THR:O	1:K:89:VAL:N	2.04	0.91
5:N:701:AGS:S1G	5:N:701:AGS:O2B	2.30	0.89
3:U:12:DA:H5'	3:U:12:DA:H8	1.35	0.88
1:A:39:GLU:OE1	1:A:39:GLU:N	2.08	0.86
2:R:238:LEU:HD21	2:R:431:LEU:HD23	1.58	0.86
4:V:7:DT:H2"	4:V:8:DA:H5'	1.58	0.86
2:R:202:ASN:OD1	2:R:204:HIS:NE2	2.09	0.85
5:R:701:AGS:S1G	5:R:701:AGS:O2B	2.34	0.84
1:K:151:GLU:N	1:K:151:GLU:OE1	2.10	0.84
1:J:366:ASP:OD1	1:J:367:GLU:N	2.10	0.83
1:E:113:THR:O	1:E:116:SER:OG	1.95	0.83
4:V:4:DA:H2'	4:V:5:DT:H71	1.59	0.83
2:O:205:ILE:HG23	2:O:412:VAL:HG23	1.59	0.83
3:U:12:DA:H5'	3:U:12:DA:C8	2.14	0.83
2:N:306:ASN:ND2	2:N:361:PHE:O	2.12	0.82
1:A:12:TYR:OH	1:A:37:ALA:HB3	1.80	0.82
1:G:113:THR:O	1:G:116:SER:OG	1.95	0.82
1:G:39:GLU:N	1:G:39:GLU:OE1	2.13	0.81
2:M:158:ASP:O	2:M:162:SER:OG	1.99	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:ILE:HG21	1:E:42:ASP:HB2	1.63	0.80
1:E:259:ASP:O	1:E:299:ARG:NH2	2.14	0.80
1:A:53:GLN:NE2	1:A:54:CYS:O	2.13	0.80
1:E:31:ARG:NH2	1:E:198:GLU:OE2	2.15	0.80
2:P:321:LEU:N	2:P:325:THR:O	2.15	0.80
1:K:77:GLU:O	1:K:80:SER:OG	2.00	0.79
1:E:37:ALA:CA	1:E:51:ALA:HB1	2.12	0.79
2:N:99:THR:OG1	2:N:107:SER:OG	2.00	0.79
1:A:37:ALA:HB2	1:A:52:VAL:O	1.83	0.78
1:G:22:GLU:O	1:G:26:ALA:N	2.16	0.78
1:E:50:THR:HG22	1:E:88:HIS:CB	2.14	0.78
2:N:158:ASP:O	2:N:162:SER:OG	2.01	0.78
2:O:316:GLU:OE2	2:O:320:LYS:NZ	2.16	0.78
1:K:366:ASP:OD1	1:K:367:GLU:N	2.17	0.78
4:V:15:DT:H2”	4:V:16:DA:C8	2.19	0.78
1:E:212:VAL:HG21	1:E:231:LEU:HD11	1.67	0.77
1:H:261:ASP:OD1	1:H:264:ARG:NH2	2.17	0.77
2:M:275:LYS:NZ	2:M:287:PHE:O	2.18	0.77
1:C:371:GLU:OE2	1:C:371:GLU:N	2.17	0.76
2:M:194:ASN:OD1	2:M:196:HIS:N	2.17	0.76
3:U:7:DT:C2’	3:U:8:DA:H5”	2.15	0.76
1:G:19:TYR:O	1:G:23:ILE:HD12	1.85	0.76
2:R:175:LYS:NZ	5:R:701:AGS:O2G	2.16	0.76
2:R:354:ASN:OD1	2:R:355:GLY:N	2.18	0.76
1:E:53:GLN:NE2	1:E:54:CYS:O	2.19	0.76
2:O:41:TYR:OH	2:O:566:PRO:O	2.04	0.76
2:P:346:GLN:OE1	2:P:351:LYS:NZ	2.19	0.76
2:Q:306:ASN:OD1	2:Q:359:GLY:N	2.19	0.76
4:V:3:DT:H2”	4:V:4:DA:C5’	2.16	0.76
4:V:7:DT:H2”	4:V:8:DA:C5’	2.15	0.76
1:I:212:VAL:HG21	1:I:231:LEU:HD11	1.68	0.75
2:M:332:GLU:N	2:M:332:GLU:OE2	2.19	0.75
1:K:224:LYS:O	1:K:227:MET:N	2.20	0.75
1:I:35:GLU:HB3	1:I:52:VAL:HB	1.68	0.75
1:G:200:LYS:O	1:G:200:LYS:NZ	2.15	0.74
2:O:64:VAL:O	2:O:87:ASN:N	2.20	0.74
4:V:8:DA:H2’	4:V:9:DT:H72	1.69	0.74
1:C:77:GLU:O	1:C:80:SER:OG	2.02	0.74
1:F:366:ASP:OD1	1:F:367:GLU:N	2.19	0.74
1:G:9:ILE:HD11	1:G:217:TRP:HE1	1.52	0.74
2:R:358:ASN:OD1	2:R:359:GLY:N	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:589:TRP:CD1	2:N:203:SER:HA	2.22	0.74
1:E:18:LYS:O	1:E:21:SER:OG	2.05	0.74
2:Q:209:ASP:OD1	2:Q:210:ILE:N	2.21	0.74
3:U:8:DA:H2'	3:U:9:DT:H72	1.70	0.74
2:M:242:LEU:O	2:M:434:ARG:NH2	2.20	0.73
2:O:209:ASP:OD1	2:O:210:ILE:N	2.20	0.73
1:C:113:THR:O	1:C:116:SER:OG	2.02	0.73
2:N:203:SER:O	2:N:411:ASN:ND2	2.21	0.73
1:E:258:PHE:CE2	1:E:262:ILE:HD13	2.24	0.73
1:G:111:LEU:HD21	1:G:135:TYR:HB3	1.71	0.73
2:P:387:ASP:OD1	2:P:388:GLY:N	2.21	0.73
1:G:111:LEU:HD21	1:G:135:TYR:CB	2.18	0.73
2:M:389:GLU:OE1	2:M:389:GLU:N	2.22	0.73
1:J:261:ASP:OD1	1:J:264:ARG:NH2	2.23	0.72
1:E:153:LEU:O	1:E:157:VAL:HG23	1.90	0.72
2:Q:167:VAL:HB	2:Q:501:VAL:HG12	1.71	0.72
2:Q:183:LEU:HD22	2:Q:205:ILE:HD13	1.71	0.72
2:Q:345:SER:OG	2:Q:350:THR:O	2.06	0.72
1:D:227:MET:O	1:D:230:SER:OG	2.05	0.72
4:V:8:DA:C2'	4:V:9:DT:H72	2.20	0.72
2:R:306:ASN:ND2	2:R:307:ASN:OD1	2.22	0.71
2:P:322:ALA:HB2	2:P:341:PHE:N	2.03	0.71
4:V:12:DA:C8	4:V:13:DT:H72	2.25	0.71
1:A:215:THR:CG2	1:A:218:THR:HG23	2.21	0.71
1:L:231:LEU:O	1:L:234:SER:OG	2.07	0.71
2:M:183:LEU:HD22	2:M:205:ILE:HD13	1.73	0.71
2:O:138:SER:O	2:O:157:GLY:N	2.24	0.71
2:O:458:ILE:HB	2:O:496:VAL:HG22	1.72	0.71
2:O:267:PHE:O	2:O:271:VAL:HG23	1.91	0.70
1:G:219:ARG:HB2	1:G:224:LYS:HE2	1.71	0.70
1:H:344:ARG:NH2	1:H:366:ASP:OD1	2.25	0.70
2:Q:158:ASP:O	2:Q:162:SER:OG	2.02	0.70
1:I:58:GLU:N	1:I:58:GLU:OE1	2.25	0.70
1:I:366:ASP:OD1	1:I:367:GLU:N	2.24	0.70
2:O:142:LEU:O	2:O:142:LEU:HD23	1.90	0.70
1:C:221:LEU:HD23	1:C:222:ALA:N	2.06	0.70
1:K:241:HIS:O	2:R:48:ASN:ND2	2.25	0.70
2:P:33:LYS:NZ	2:Q:113:LEU:O	2.23	0.70
1:K:219:ARG:HG3	1:K:224:LYS:NZ	2.06	0.69
1:H:231:LEU:HD21	1:H:378:PHE:CE1	2.26	0.69
1:A:77:GLU:O	1:A:80:SER:OG	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:99:THR:OG1	2:O:107:SER:OG	2.11	0.69
4:V:11:DT:H2'	4:V:12:DA:C8	2.26	0.69
1:G:219:ARG:O	1:G:224:LYS:HE3	1.93	0.69
1:A:162:LYS:NZ	1:A:166:PHE:O	2.26	0.69
1:K:7:TYR:CZ	1:K:39:GLU:HG2	2.28	0.69
1:C:109:ASP:O	1:C:113:THR:HG23	1.93	0.68
1:I:35:GLU:N	1:I:35:GLU:OE2	2.26	0.68
2:Q:189:ILE:HD11	2:Q:226:PHE:CZ	2.28	0.68
2:Q:128:LEU:HD22	2:Q:151:ILE:HD13	1.74	0.68
1:A:80:SER:HB3	1:A:129:ILE:HG23	1.75	0.68
1:K:35:GLU:OE2	1:K:50:THR:OG1	2.07	0.68
1:B:227:MET:SD	1:B:227:MET:N	2.65	0.68
1:D:231:LEU:HD13	1:D:378:PHE:HE1	1.58	0.68
2:R:256:ASN:HB3	2:R:259:ASN:HB3	1.75	0.67
1:K:210:ARG:HD2	1:K:210:ARG:O	1.94	0.67
2:M:460:VAL:HB	2:M:498:LEU:HD23	1.76	0.67
2:P:41:TYR:OH	2:P:566:PRO:O	2.12	0.67
2:R:13:ASP:OD1	2:R:14:SER:N	2.28	0.67
2:R:443:TYR:OH	2:R:447:ARG:NH2	2.27	0.67
2:M:169:GLY:O	2:M:175:LYS:NZ	2.23	0.67
1:K:35:GLU:HG2	1:K:52:VAL:HB	1.75	0.67
2:N:238:LEU:O	2:N:380:LEU:HD12	1.94	0.67
3:U:8:DA:H2'	3:U:9:DT:C7	2.24	0.67
1:E:102:GLY:H	1:E:146:PHE:HB2	1.58	0.67
2:N:194:ASN:OD1	2:N:196:HIS:N	2.26	0.67
2:P:589:TRP:O	2:Q:201:LYS:NZ	2.27	0.67
1:J:361:ILE:HG22	1:J:362:ASN:OD1	1.94	0.67
2:M:417:LEU:HD13	2:M:425:LEU:HD11	1.76	0.67
1:E:194:ASP:HB2	1:E:196:THR:HG22	1.77	0.67
2:R:363:ARG:NH2	4:V:1:DT:O5'	2.27	0.67
2:P:100:LEU:HD12	2:P:105:GLU:O	1.95	0.67
2:Q:99:THR:OG1	2:Q:107:SER:OG	2.11	0.67
1:C:366:ASP:OD1	1:C:367:GLU:N	2.26	0.66
1:D:227:MET:SD	1:D:227:MET:N	2.68	0.66
1:J:297:GLN:NE2	1:J:307:CYS:SG	2.68	0.66
1:K:115:LEU:HD23	1:K:115:LEU:O	1.96	0.66
2:P:423:GLU:HG3	2:P:424:VAL:HG13	1.78	0.66
2:Q:526:ASN:OD1	2:Q:527:ALA:N	2.29	0.66
3:U:7:DT:H2"	3:U:8:DA:C8	2.30	0.66
1:E:51:ALA:O	1:E:90:SER:N	2.29	0.66
1:A:366:ASP:OD1	1:A:367:GLU:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:GLU:N	1:C:151:GLU:OE1	2.27	0.66
1:C:384:SER:OG	1:C:393:ARG:NH1	2.29	0.66
1:F:261:ASP:OD1	1:F:264:ARG:NH2	2.29	0.66
2:M:561:ASP:OD2	2:R:523:ARG:NH1	2.29	0.65
1:A:209:VAL:O	1:A:210:ARG:HD2	1.96	0.65
2:O:555:GLU:OE2	2:P:111:HIS:NE2	2.29	0.65
1:K:133:VAL:HG21	1:K:135:TYR:CE1	2.32	0.65
2:N:453:VAL:HG12	2:N:454:SER:H	1.62	0.65
1:E:136:GLU:OE1	1:E:136:GLU:N	2.28	0.65
1:I:191:ASP:O	1:I:195:ARG:NH1	2.30	0.65
3:U:6:DA:H2"	3:U:7:DT:C6	2.32	0.65
1:C:214:PHE:HA	1:C:218:THR:HG21	1.77	0.65
2:M:170:SER:OG	2:M:171:THR:N	2.29	0.65
1:K:18:LYS:O	1:K:21:SER:OG	2.13	0.64
2:M:354:ASN:N	3:U:12:DA:OP1	2.28	0.64
2:R:486:ARG:NE	2:R:490:GLU:OE2	2.28	0.64
1:A:95:CYS:O	1:A:147:GLY:N	2.29	0.64
1:G:9:ILE:HD11	1:G:217:TRP:NE1	2.13	0.64
2:N:372:LEU:HD23	2:N:381:PHE:CD2	2.32	0.64
2:O:306:ASN:O	2:O:358:ASN:ND2	2.31	0.64
2:R:183:LEU:HD22	2:R:205:ILE:HD13	1.80	0.63
1:H:366:ASP:OD1	1:H:367:GLU:N	2.29	0.63
1:I:136:GLU:OE1	1:I:136:GLU:N	2.31	0.63
1:A:222:ALA:O	1:A:226:ARG:NH2	2.31	0.63
2:P:25:SER:OG	2:P:28:ASP:OD1	2.16	0.63
2:Q:228:LEU:HD21	2:Q:414:ILE:HD12	1.79	0.63
2:M:526:ASN:OD1	2:M:527:ALA:N	2.32	0.63
1:E:112:GLU:HA	1:E:115:LEU:HD12	1.80	0.63
2:N:237:ARG:O	2:N:238:LEU:HD22	1.99	0.63
1:G:241:HIS:O	2:P:48:ASN:ND2	2.31	0.63
1:H:381:GLU:OE2	1:H:382:ARG:NH1	2.31	0.63
1:A:54:CYS:SG	1:A:55:LYS:N	2.71	0.63
2:M:116:PRO:O	2:M:117:THR:OG1	2.15	0.63
1:A:9:ILE:HD11	1:A:217:TRP:CD1	2.34	0.63
2:O:101:SER:OG	2:O:102:GLU:N	2.31	0.63
1:K:33:THR:OG1	1:K:195:ARG:O	2.16	0.62
2:M:420:ILE:CG2	2:M:424:VAL:HG23	2.28	0.62
2:M:108:ARG:O	2:M:111:HIS:NE2	2.32	0.62
2:R:210:ILE:HD12	2:R:464:GLU:HB2	1.81	0.62
3:U:3:DT:H2"	3:U:4:DA:OP2	1.99	0.62
1:I:32:ILE:O	1:I:197:VAL:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:59:GLN:N	1:I:59:GLN:OE1	2.32	0.62
1:E:47:GLY:O	1:E:50:THR:OG1	2.17	0.62
1:I:38:ILE:HG21	1:I:53:GLN:OE1	1.99	0.62
1:K:107:THR:OG1	1:K:109:ASP:OD1	2.17	0.62
2:O:324:GLU:OE1	2:O:324:GLU:N	2.33	0.62
3:U:3:DT:H2"	3:U:4:DA:H8	1.65	0.62
2:M:306:ASN:OD1	2:M:359:GLY:N	2.32	0.62
2:O:513:PHE:O	2:O:516:CYS:N	2.26	0.62
4:V:5:DT:H2"	4:V:6:DA:O5'	1.98	0.62
4:V:14:DA:C8	4:V:15:DT:H72	2.34	0.62
1:K:117:THR:OG1	1:K:123:ARG:NH1	2.33	0.62
1:K:150:ALA:O	1:K:153:LEU:N	2.33	0.62
2:O:416:ASP:OD1	2:O:417:LEU:N	2.33	0.62
1:C:385:ASP:OD1	1:C:386:LEU:N	2.32	0.62
2:Q:200:GLN:NE2	2:Q:410:SER:O	2.32	0.62
1:E:344:ARG:NH2	1:E:366:ASP:OD2	2.33	0.61
1:A:181:GLN:O	1:A:181:GLN:NE2	2.33	0.61
2:N:573:LEU:HD13	5:N:701:AGS:C2	2.30	0.61
1:A:126:VAL:HG13	1:A:129:ILE:HD12	1.81	0.61
1:K:384:SER:OG	1:K:393:ARG:NH1	2.34	0.61
2:O:204:HIS:ND1	2:O:411:ASN:OD1	2.33	0.61
3:U:4:DA:H2"	3:U:5:DT:OP2	2.00	0.61
1:G:216:ARG:HA	1:G:219:ARG:NH1	2.16	0.61
1:E:130:ASP:OD2	1:E:132:SER:OG	2.17	0.61
1:A:37:ALA:HA	1:A:51:ALA:HB1	1.82	0.61
1:E:50:THR:HG22	1:E:88:HIS:HB3	1.82	0.61
1:I:210:ARG:HD2	1:I:210:ARG:O	2.00	0.60
2:R:175:LYS:N	5:R:701:AGS:O1B	2.32	0.60
1:K:193:ASN:O	1:K:195:ARG:NH1	2.33	0.60
1:I:340:ARG:O	1:I:341:LEU:HD12	2.00	0.60
1:K:220:GLU:HA	1:K:220:GLU:OE1	2.00	0.60
1:C:221:LEU:HD23	1:C:222:ALA:H	1.67	0.60
1:L:373:VAL:O	1:L:375:VAL:HG23	2.02	0.60
2:M:170:SER:O	2:M:175:LYS:NZ	2.34	0.60
2:O:231:LEU:HD12	2:O:415:ILE:CD1	2.32	0.60
2:O:404:VAL:O	2:O:411:ASN:ND2	2.35	0.60
2:R:244:ASN:N	2:R:247:GLU:OE2	2.34	0.60
1:C:216:ARG:NH1	1:C:216:ARG:HB3	2.15	0.60
1:K:211:ARG:HB2	1:K:377:GLY:O	2.01	0.60
2:N:245:ALA:N	2:N:288:ASP:OD1	2.35	0.60
1:A:224:LYS:HG3	1:A:228:PHE:HE2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:99:THR:OG1	2:M:107:SER:OG	2.20	0.60
2:N:249:GLU:OE2	2:N:268:ARG:NH2	2.35	0.60
1:K:54:CYS:SG	1:K:55:LYS:N	2.75	0.59
1:A:65:LEU:HD11	1:A:114:VAL:HG22	1.84	0.59
2:P:390:ASP:OD1	2:P:391:LEU:N	2.35	0.59
1:K:247:VAL:HG13	1:K:284:LEU:HD11	1.84	0.59
2:P:194:ASN:OD1	2:P:196:HIS:N	2.35	0.59
1:A:80:SER:CB	1:A:129:ILE:HG23	2.33	0.59
1:D:231:LEU:HD13	1:D:378:PHE:CE1	2.37	0.59
4:V:3:DT:H2"	4:V:4:DA:H5'	1.85	0.59
1:K:181:GLN:OE1	1:K:215:THR:HG21	2.03	0.59
2:Q:275:LYS:NZ	2:Q:289:THR:O	2.34	0.59
1:G:24:LEU:HD21	1:G:160:SER:HB2	1.85	0.59
1:E:239:LEU:HD11	1:E:390:LEU:HD22	1.85	0.59
1:E:36:GLY:HA2	1:E:52:VAL:HG12	1.84	0.59
1:E:108:LYS:O	1:E:111:LEU:N	2.36	0.58
1:H:360:LEU:HD23	1:H:363:VAL:HG13	1.86	0.58
1:L:327:ILE:C	1:L:328:LEU:HD12	2.24	0.58
2:M:353:SER:OG	3:U:12:DA:OP1	2.20	0.58
2:N:522:LEU:HD12	2:N:522:LEU:N	2.19	0.58
2:M:358:ASN:OD1	2:M:359:GLY:N	2.36	0.58
2:N:242:LEU:HD22	2:N:435:MET:HE2	1.85	0.58
2:P:165:VAL:HG12	2:P:166:ALA:N	2.19	0.58
2:Q:447:ARG:O	2:Q:451:GLY:N	2.36	0.58
1:D:369:LYS:HG3	1:D:375:VAL:HG21	1.84	0.58
1:J:223:THR:HA	1:J:226:ARG:NH2	2.19	0.58
3:U:4:DA:C8	3:U:5:DT:H72	2.39	0.58
2:R:404:VAL:HG12	2:R:404:VAL:O	2.04	0.58
2:N:236:LEU:HG	2:N:238:LEU:HD23	1.85	0.58
2:N:604:ARG:NH2	2:N:608:LYS:O	2.35	0.58
2:P:304:ASN:ND2	2:P:334:TYR:O	2.37	0.58
1:A:220:GLU:HA	1:A:220:GLU:OE1	2.04	0.57
2:Q:416:ASP:OD1	2:Q:418:SER:N	2.37	0.57
1:I:109:ASP:O	1:I:113:THR:HG23	2.04	0.57
3:U:2:DA:H2"	3:U:3:DT:OP2	2.03	0.57
1:A:273:TYR:O	1:A:279:HIS:ND1	2.38	0.57
1:B:273:TYR:OH	1:B:390:LEU:O	2.22	0.57
1:C:220:GLU:HA	1:C:220:GLU:OE1	2.05	0.57
2:O:108:ARG:NH2	2:O:564:LEU:O	2.33	0.57
2:O:583:VAL:HG22	2:P:453:VAL:HG22	1.87	0.57
1:A:224:LYS:HG3	1:A:228:PHE:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:313:LEU:HD23	2:M:314:ALA:O	2.05	0.57
2:Q:416:ASP:OD1	2:Q:417:LEU:N	2.37	0.57
1:L:324:ARG:O	1:L:340:ARG:NH2	2.38	0.57
1:F:384:SER:O	1:F:387:GLU:N	2.36	0.57
1:K:258:PHE:CZ	1:K:262:ILE:HD12	2.40	0.57
1:K:194:ASP:OD1	1:K:196:THR:HG22	2.04	0.56
2:O:372:LEU:HD23	2:O:381:PHE:CD2	2.41	0.56
2:Q:189:ILE:HD11	2:Q:226:PHE:HZ	1.69	0.56
4:V:3:DT:H2'	4:V:4:DA:H8	1.70	0.56
1:E:198:GLU:N	1:E:198:GLU:OE1	2.37	0.56
2:P:116:PRO:O	2:P:117:THR:OG1	2.21	0.56
2:R:194:ASN:N	2:R:224:GLU:OE2	2.33	0.56
1:E:306:ARG:NH1	1:F:321:GLU:OE2	2.38	0.56
1:K:198:GLU:OE1	1:K:198:GLU:N	2.38	0.56
2:P:257:GLU:O	2:P:260:SER:OG	2.22	0.56
2:Q:345:SER:OG	2:Q:350:THR:OG1	2.02	0.56
2:P:322:ALA:HB2	2:P:341:PHE:CA	2.35	0.56
2:M:13:ASP:OD1	2:M:14:SER:N	2.39	0.56
1:E:31:ARG:HD3	1:E:196:THR:OG1	2.05	0.56
1:A:210:ARG:HE	1:A:210:ARG:HA	1.70	0.56
1:C:115:LEU:O	1:C:115:LEU:HD23	2.05	0.56
1:I:181:GLN:NE2	1:I:215:THR:HG21	2.20	0.56
2:N:122:VAL:HG12	2:N:123:THR:N	2.21	0.56
2:O:387:ASP:OD1	2:O:388:GLY:N	2.39	0.56
4:V:6:DA:H2"	4:V:7:DT:H5'	1.87	0.56
1:E:218:THR:HA	1:E:221:LEU:HD13	1.88	0.56
2:O:490:GLU:O	2:O:492:ARG:N	2.39	0.56
2:R:200:GLN:NE2	2:R:411:ASN:OD1	2.38	0.56
1:B:261:ASP:OD1	1:B:264:ARG:NH2	2.39	0.56
2:P:310:ILE:HG23	2:P:318:LYS:C	2.27	0.55
2:R:424:VAL:HG12	2:R:428:VAL:HG23	1.88	0.55
1:A:241:HIS:O	2:M:48:ASN:ND2	2.39	0.55
2:Q:210:ILE:HG22	2:Q:210:ILE:O	2.05	0.55
1:A:307:CYS:SG	1:A:308:GLU:N	2.79	0.55
2:R:423:GLU:HG3	2:R:424:VAL:HG23	1.87	0.55
2:R:504:ARG:NH1	2:R:529:ASP:OD2	2.40	0.55
1:A:109:ASP:OD1	1:A:110:ASP:N	2.40	0.55
1:C:215:THR:H	1:C:218:THR:HG22	1.72	0.55
1:E:50:THR:HG22	1:E:88:HIS:HB2	1.88	0.55
1:J:223:THR:H	1:J:226:ARG:HH12	1.55	0.55
2:M:357:PHE:HE2	2:R:366:LEU:HD23	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:493:LYS:NZ	2:R:213:GLU:OE2	2.38	0.55
2:O:183:LEU:HD22	2:O:205:ILE:CD1	2.36	0.55
1:E:35:GLU:OE1	1:E:50:THR:OG1	2.13	0.55
1:E:117:THR:O	1:E:117:THR:HG23	2.06	0.55
2:M:167:VAL:HB	2:M:501:VAL:HG12	1.88	0.55
1:A:117:THR:HG21	1:A:123:ARG:HB2	1.89	0.55
3:U:3:DT:H2"	3:U:4:DA:C8	2.42	0.55
1:G:24:LEU:O	1:G:164:LYS:NZ	2.34	0.55
1:I:215:THR:OG1	1:I:217:TRP:N	2.39	0.55
1:C:273:TYR:O	1:C:279:HIS:ND1	2.39	0.55
1:H:246:ARG:NE	1:H:357:GLU:OE2	2.36	0.55
2:O:354:ASN:OD1	2:O:355:GLY:N	2.40	0.55
2:O:401:ARG:O	2:O:405:GLY:N	2.38	0.55
2:P:386:GLU:OE1	2:P:386:GLU:N	2.38	0.55
2:R:363:ARG:NH1	4:V:1:DT:O5'	2.40	0.55
3:U:7:DT:H2"	3:U:8:DA:H8	1.70	0.55
1:C:212:VAL:HG11	1:C:231:LEU:CD1	2.38	0.54
1:E:107:THR:HG23	1:E:109:ASP:OD1	2.07	0.54
2:O:598:PHE:O	2:O:602:ILE:HG22	2.07	0.54
1:C:214:PHE:HE1	1:C:389:ILE:HD11	1.71	0.54
1:F:231:LEU:HD21	1:F:378:PHE:CE1	2.43	0.54
1:G:73:LEU:HD13	1:G:122:LEU:HD12	1.89	0.54
2:P:325:THR:HG22	2:P:326:LEU:N	2.23	0.54
1:E:121:VAL:HG13	1:E:122:LEU:HD22	1.89	0.54
1:E:224:LYS:HD2	1:E:224:LYS:C	2.28	0.54
1:F:259:ASP:OD1	1:F:299:ARG:NH1	2.39	0.54
2:M:404:VAL:HG12	2:M:404:VAL:O	2.08	0.54
2:N:453:VAL:HG12	2:N:454:SER:N	2.21	0.54
2:O:258:HIS:O	2:O:258:HIS:ND1	2.40	0.54
1:E:188:THR:O	1:E:188:THR:HG23	2.08	0.54
1:I:355:PRO:O	1:I:373:VAL:HG22	2.08	0.54
2:O:35:MET:SD	2:O:122:VAL:HG11	2.48	0.54
2:Q:22:GLU:OE2	2:Q:24:SER:OG	2.22	0.54
1:G:307:CYS:SG	1:G:308:GLU:N	2.80	0.54
1:K:327:ILE:C	1:K:328:LEU:HD12	2.28	0.54
2:N:537:LEU:HD21	2:N:541:SER:O	2.08	0.54
2:N:481:ARG:O	2:N:485:GLU:N	2.39	0.54
1:A:116:SER:OG	1:A:118:LYS:NZ	2.41	0.54
1:E:218:THR:CA	1:E:221:LEU:HD13	2.38	0.54
1:F:241:HIS:NE2	1:H:271:GLN:OE1	2.41	0.54
1:K:38:ILE:HB	1:K:52:VAL:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:90:SER:OG	1:K:91:TYR:N	2.41	0.54
1:K:214:PHE:HE1	1:K:389:ILE:HD11	1.71	0.54
2:O:362:ASP:OD2	2:O:363:ARG:N	2.40	0.54
1:J:223:THR:HG22	1:J:226:ARG:HH22	1.73	0.53
1:L:289:GLY:O	1:L:343:LYS:NZ	2.41	0.53
1:I:29:GLY:O	1:I:31:ARG:NH1	2.41	0.53
1:I:153:LEU:O	1:I:157:VAL:HG23	2.08	0.53
2:Q:251:ILE:HD11	2:Q:427:ILE:HD13	1.90	0.53
2:R:343:VAL:HG12	2:R:344:ALA:N	2.22	0.53
1:A:198:GLU:N	1:A:198:GLU:OE2	2.41	0.53
1:E:177:PRO:HB3	1:E:218:THR:HG23	1.89	0.53
1:E:218:THR:H	1:E:221:LEU:HD13	1.72	0.53
2:N:203:SER:OG	2:N:411:ASN:ND2	2.40	0.53
1:C:150:ALA:O	1:C:153:LEU:N	2.41	0.53
1:D:309:THR:O	1:D:309:THR:HG22	2.07	0.53
2:R:209:ASP:OD2	2:R:213:GLU:N	2.41	0.53
1:C:212:VAL:HG21	1:C:231:LEU:CD2	2.39	0.53
1:I:216:ARG:HA	1:I:219:ARG:NH1	2.22	0.53
3:U:5:DT:H2"	3:U:6:DA:N7	2.24	0.53
1:A:35:GLU:HB3	1:A:51:ALA:HA	1.91	0.53
1:A:117:THR:HG23	1:A:117:THR:O	2.08	0.53
2:P:588:GLU:O	2:Q:202:ASN:ND2	2.42	0.53
1:E:9:ILE:HD11	1:E:217:TRP:NE1	2.23	0.53
1:K:19:TYR:CE2	1:K:34:ILE:HG23	2.44	0.53
2:P:526:ASN:OD1	2:P:527:ALA:N	2.41	0.53
3:U:6:DA:H2'	3:U:7:DT:H72	1.90	0.53
1:K:215:THR:HG22	1:K:218:THR:HG23	1.90	0.53
1:K:219:ARG:HG3	1:K:224:LYS:HZ1	1.74	0.53
3:U:1:DT:H2"	3:U:2:DA:C8	2.44	0.53
3:U:13:DT:H2"	3:U:14:DA:H8	1.73	0.53
4:V:13:DT:H2"	4:V:14:DA:H8	1.74	0.53
1:H:384:SER:OG	1:H:393:ARG:NH1	2.42	0.53
2:P:441:PHE:HE1	2:P:445:LYS:HZ1	1.57	0.53
4:V:3:DT:H2"	4:V:4:DA:O4'	2.09	0.52
1:G:37:ALA:HB1	1:G:39:GLU:OE1	2.09	0.52
1:G:111:LEU:HD21	1:G:135:TYR:HB2	1.90	0.52
1:I:54:CYS:SG	1:I:55:LYS:N	2.82	0.52
1:G:266:ILE:O	1:G:270:VAL:HG22	2.10	0.52
2:M:1:MET:N	2:M:2:PRO:CD	2.72	0.52
1:A:49:THR:O	1:A:88:HIS:N	2.43	0.52
1:I:35:GLU:HB3	1:I:52:VAL:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:340:ARG:C	1:K:341:LEU:HD12	2.29	0.52
2:Q:305:MET:SD	2:Q:330:ARG:NH1	2.82	0.52
2:R:238:LEU:HD23	2:R:380:LEU:HD13	1.91	0.52
3:U:3:DT:OP2	3:U:3:DT:H6	1.91	0.52
3:U:15:DT:H2"	3:U:16:DA:OP2	2.09	0.52
1:B:312:VAL:HG12	1:B:312:VAL:O	2.10	0.52
1:D:227:MET:HG2	1:D:228:PHE:HD1	1.75	0.52
2:P:526:ASN:OD1	2:P:528:VAL:N	2.41	0.52
5:P:701:AGS:O2B	5:P:701:AGS:S1G	2.68	0.52
1:A:80:SER:OG	1:A:128:ARG:NH1	2.43	0.52
2:M:453:VAL:CG1	2:R:583:VAL:HG22	2.39	0.52
3:U:6:DA:C2'	3:U:7:DT:H72	2.40	0.52
1:E:355:PRO:O	1:E:373:VAL:HG22	2.09	0.52
1:I:189:ARG:O	1:I:195:ARG:NH2	2.43	0.52
1:L:370:HIS:CD2	1:L:371:GLU:H	2.28	0.52
2:Q:228:LEU:HD23	2:Q:230:LEU:HD21	1.92	0.52
2:R:377:LEU:CD2	2:R:424:VAL:HG21	2.39	0.52
1:G:96:HIS:ND1	1:G:147:GLY:O	2.43	0.52
1:I:32:ILE:HG22	1:I:33:THR:N	2.25	0.52
2:Q:205:ILE:HG22	2:Q:206:VAL:N	2.25	0.52
2:Q:392:ALA:O	2:Q:395:ASP:N	2.40	0.52
1:A:210:ARG:HA	1:A:210:ARG:NE	2.22	0.52
1:C:189:ARG:NH1	1:C:191:ASP:O	2.43	0.52
1:L:250:ILE:HG22	1:L:251:ASN:N	2.25	0.52
3:U:6:DA:O5'	3:U:6:DA:H8	1.93	0.52
1:E:48:LEU:O	1:E:50:THR:HG23	2.10	0.52
1:F:315:THR:HG23	1:F:316:ASP:N	2.25	0.52
1:G:7:TYR:HE2	1:G:39:GLU:HB3	1.75	0.52
1:J:272:ARG:NH1	1:J:391:GLN:O	2.43	0.52
1:J:357:GLU:N	1:J:357:GLU:OE1	2.42	0.52
2:M:591:SER:OG	2:M:592:GLY:N	2.41	0.52
2:N:242:LEU:HD11	2:N:396:PHE:CE2	2.45	0.52
2:O:596:VAL:HG23	2:P:406:TYR:CE1	2.44	0.52
1:D:258:PHE:CE2	1:D:262:ILE:HD13	2.44	0.51
1:E:38:ILE:CG2	1:E:42:ASP:HB2	2.37	0.51
1:E:218:THR:N	1:E:221:LEU:HD13	2.25	0.51
1:E:278:LEU:HD11	2:O:117:THR:OG1	2.08	0.51
2:M:417:LEU:HD13	2:M:425:LEU:CD1	2.39	0.51
5:M:701:AGS:O3G	2:N:493:LYS:NZ	2.43	0.51
1:B:282:PRO:O	1:B:340:ARG:NH2	2.44	0.51
2:M:234:ASP:OD2	2:M:235:ASN:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:316:GLU:HG2	2:M:326:LEU:HD11	1.92	0.51
2:P:313:LEU:HD21	2:P:351:LYS:N	2.25	0.51
2:Q:338:VAL:HG12	2:Q:339:GLN:N	2.25	0.51
2:Q:404:VAL:HG12	2:Q:404:VAL:O	2.10	0.51
1:B:339:LEU:HD12	1:B:341:LEU:HD11	1.92	0.51
1:K:110:ASP:O	1:K:114:VAL:HG23	2.10	0.51
1:K:214:PHE:HE2	1:K:227:MET:SD	2.34	0.51
2:Q:329:ASP:OD1	2:Q:330:ARG:N	2.44	0.51
2:R:256:ASN:O	2:R:258:HIS:N	2.43	0.51
1:A:41:VAL:HG23	1:A:41:VAL:O	2.09	0.51
1:B:224:LYS:C	1:B:224:LYS:HD3	2.31	0.51
1:B:365:ASP:OD2	1:B:365:ASP:N	2.42	0.51
1:H:250:ILE:HG22	1:H:251:ASN:N	2.25	0.51
2:O:539:ASP:O	2:O:540:LEU:HD12	2.10	0.51
2:Q:320:LYS:HG2	2:Q:342:ILE:HD13	1.93	0.51
2:Q:411:ASN:O	2:Q:412:VAL:HG23	2.10	0.51
2:R:256:ASN:O	2:R:259:ASN:N	2.44	0.51
1:G:188:THR:HG23	1:G:188:THR:O	2.10	0.51
1:G:373:VAL:HG23	1:G:373:VAL:O	2.11	0.51
1:A:110:ASP:O	1:A:114:VAL:HG23	2.09	0.51
1:C:324:ARG:O	1:C:340:ARG:NH2	2.43	0.51
1:I:120:GLU:OE1	1:I:120:GLU:N	2.38	0.51
1:I:219:ARG:HB2	1:I:219:ARG:CZ	2.40	0.51
2:P:1:MET:HB3	2:P:2:PRO:HD3	1.92	0.51
3:U:8:DA:H5"	3:U:8:DA:H8	1.76	0.51
1:C:216:ARG:HB3	1:C:216:ARG:HH11	1.74	0.51
1:I:255:ILE:HG22	1:I:256:GLU:N	2.26	0.51
2:N:539:ASP:OD1	2:N:540:LEU:N	2.43	0.51
2:Q:234:ASP:OD2	2:Q:235:ASN:N	2.44	0.51
1:C:111:LEU:HD13	1:C:135:TYR:HB3	1.92	0.51
2:O:221:GLU:N	2:O:221:GLU:OE1	2.43	0.51
2:P:286:SER:OG	2:P:289:THR:OG1	1.99	0.51
1:G:108:LYS:HE3	1:G:111:LEU:HD23	1.91	0.51
1:C:157:VAL:O	1:C:160:SER:OG	2.26	0.51
1:D:250:ILE:HG22	1:D:251:ASN:N	2.26	0.51
1:H:250:ILE:HG22	1:H:251:ASN:H	1.76	0.51
1:K:235:LEU:HD12	1:K:389:ILE:HG22	1.92	0.51
1:A:34:ILE:HG22	1:A:35:GLU:N	2.25	0.50
1:C:111:LEU:HD23	1:C:111:LEU:O	2.11	0.50
1:L:231:LEU:HD11	1:L:378:PHE:CE1	2.46	0.50
1:A:22:GLU:O	1:A:26:ALA:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:THR:HG23	1:E:196:THR:O	2.11	0.50
1:L:273:TYR:O	1:L:279:HIS:ND1	2.44	0.50
2:M:453:VAL:HG12	2:M:454:SER:N	2.25	0.50
2:N:46:SER:O	2:N:46:SER:OG	2.29	0.50
2:R:575:VAL:HG13	2:R:575:VAL:O	2.11	0.50
1:C:58:GLU:N	1:C:58:GLU:OE1	2.44	0.50
2:M:325:THR:HG22	2:M:326:LEU:N	2.26	0.50
1:C:212:VAL:HG21	1:C:231:LEU:HD22	1.94	0.50
1:I:96:HIS:ND1	1:I:147:GLY:O	2.45	0.50
1:I:344:ARG:NH2	1:I:366:ASP:OD1	2.42	0.50
1:J:250:ILE:HG22	1:J:251:ASN:N	2.27	0.50
2:O:290:PRO:O	2:O:291:VAL:HG13	2.10	0.50
1:E:324:ARG:NH1	1:E:336:GLU:OE1	2.43	0.50
2:M:232:GLY:N	2:M:235:ASN:OD1	2.41	0.50
2:N:13:ASP:OD1	2:N:14:SER:N	2.39	0.50
2:P:256:ASN:OD1	2:P:257:GLU:N	2.41	0.50
2:R:105:GLU:N	2:R:105:GLU:OE1	2.45	0.50
1:G:322:LEU:HD23	1:G:323:PHE:CE1	2.47	0.50
1:K:385:ASP:OD1	1:K:386:LEU:N	2.45	0.50
2:N:573:LEU:HD11	2:N:577:GLU:OE2	2.11	0.50
2:Q:100:LEU:HD22	2:Q:131:ILE:HD11	1.94	0.50
2:R:99:THR:HG23	2:R:110:SER:HB2	1.93	0.50
1:E:111:LEU:HD22	1:E:139:LEU:HD11	1.93	0.50
1:K:221:LEU:HD12	1:K:221:LEU:H	1.77	0.50
2:M:308:GLU:HA	2:M:341:PHE:CE1	2.47	0.50
2:Q:523:ARG:NH1	2:R:561:ASP:OD1	2.45	0.50
1:G:215:THR:O	1:G:219:ARG:NH1	2.45	0.50
4:V:3:DT:H2"	4:V:4:DA:O5'	2.10	0.50
4:V:13:DT:H2"	4:V:14:DA:C8	2.47	0.50
1:E:112:GLU:OE2	1:E:112:GLU:N	2.45	0.50
1:K:58:GLU:N	1:K:58:GLU:OE2	2.45	0.50
2:M:202:ASN:OD1	2:M:204:HIS:NE2	2.41	0.50
1:C:82:ASN:O	1:C:83:SER:OG	2.26	0.49
1:E:32:ILE:O	1:E:196:THR:N	2.45	0.49
2:Q:116:PRO:O	2:Q:117:THR:OG1	2.27	0.49
1:B:278:LEU:HD12	1:B:278:LEU:H	1.77	0.49
1:E:104:LYS:O	1:E:144:ILE:HG22	2.11	0.49
2:M:478:ASP:OD1	2:M:481:ARG:NH2	2.40	0.49
2:N:464:GLU:OE2	2:N:503:GLN:NE2	2.45	0.49
1:E:49:THR:O	1:E:49:THR:HG22	2.11	0.49
1:G:100:GLU:N	1:G:100:GLU:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:395:ASP:OD2	1:L:395:ASP:N	2.46	0.49
2:Q:583:VAL:HG22	2:R:453:VAL:HG22	1.95	0.49
1:A:44:ILE:HD12	1:A:44:ILE:H	1.77	0.49
1:C:52:VAL:HG22	1:C:53:GLN:N	2.27	0.49
1:I:278:LEU:CD2	2:Q:115:VAL:HG21	2.42	0.49
1:K:391:GLN:OE1	2:R:49:ASN:ND2	2.38	0.49
1:G:214:PHE:HB2	1:G:380:ILE:HD13	1.94	0.49
2:Q:170:SER:OG	2:Q:171:THR:N	2.46	0.49
2:R:424:VAL:HG12	2:R:424:VAL:O	2.13	0.49
4:V:6:DA:C2'	4:V:7:DT:H5'	2.43	0.49
1:C:50:THR:HG23	1:C:50:THR:O	2.13	0.49
1:C:189:ARG:NH2	1:C:193:ASN:OD1	2.46	0.49
2:M:233:VAL:CG2	2:M:420:ILE:HD11	2.43	0.49
2:O:310:ILE:HG22	2:O:311:GLY:N	2.27	0.49
1:A:188:THR:HG23	1:A:188:THR:O	2.13	0.49
1:G:6:GLU:O	1:G:7:TYR:HB3	2.11	0.49
1:G:44:ILE:HD12	1:G:46:ALA:HB2	1.95	0.49
1:I:22:GLU:O	1:I:26:ALA:N	2.46	0.49
1:K:210:ARG:NH1	1:K:375:VAL:O	2.46	0.49
2:M:313:LEU:HD22	2:M:316:GLU:OE1	2.13	0.49
2:M:523:ARG:NH1	2:N:561:ASP:OD1	2.46	0.49
2:R:535:SER:OG	2:R:536:LEU:N	2.46	0.49
1:A:212:VAL:HG22	1:A:213:THR:N	2.27	0.49
1:G:270:VAL:HG21	1:G:305:LEU:HD13	1.94	0.49
2:O:257:GLU:OE2	2:O:257:GLU:N	2.46	0.49
2:Q:345:SER:CB	2:Q:350:THR:HG1	2.17	0.49
1:I:95:CYS:O	1:I:146:PHE:HA	2.12	0.49
2:P:165:VAL:HG12	2:P:166:ALA:H	1.78	0.49
1:C:95:CYS:O	1:C:146:PHE:HA	2.13	0.48
1:G:154:GLN:HE22	1:G:221:LEU:HD11	1.78	0.48
2:Q:294:SER:OG	2:Q:296:ASP:OD2	2.31	0.48
1:A:49:THR:HG22	1:A:88:HIS:N	2.27	0.48
1:E:70:LYS:HB2	1:E:71:PRO:HD3	1.94	0.48
1:K:339:LEU:HD12	1:K:341:LEU:HD11	1.95	0.48
2:R:257:GLU:HA	2:R:257:GLU:OE2	2.13	0.48
4:V:11:DT:C5'	4:V:11:DT:H6	2.25	0.48
1:A:34:ILE:O	1:A:195:ARG:NH1	2.46	0.48
1:A:218:THR:HA	1:A:221:LEU:HD23	1.94	0.48
1:I:278:LEU:HD21	2:Q:115:VAL:HG21	1.96	0.48
1:K:33:THR:OG1	1:K:195:ARG:HB3	2.13	0.48
2:N:469:LEU:HD21	2:N:484:ILE:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:205:ILE:CG2	2:O:412:VAL:HG23	2.38	0.48
2:P:325:THR:HG22	2:P:326:LEU:H	1.78	0.48
2:R:11:VAL:HG12	2:R:13:ASP:H	1.78	0.48
3:U:4:DA:OP2	3:U:4:DA:H8	1.96	0.48
1:C:32:ILE:N	1:C:196:THR:OG1	2.46	0.48
1:H:395:ASP:OD2	1:H:396:TYR:N	2.46	0.48
1:J:222:ALA:O	1:J:223:THR:OG1	2.27	0.48
2:M:421:PRO:HG2	2:M:424:VAL:HG22	1.94	0.48
2:O:57:THR:HG23	2:O:57:THR:O	2.13	0.48
1:F:262:ILE:HG23	1:F:263:VAL:N	2.28	0.48
1:K:247:VAL:HG13	1:K:284:LEU:CD1	2.43	0.48
2:N:242:LEU:HD11	2:N:396:PHE:HE2	1.78	0.48
2:P:227:THR:HG22	2:P:228:LEU:H	1.78	0.48
2:Q:228:LEU:HD21	2:Q:414:ILE:CD1	2.43	0.48
1:K:216:ARG:HH21	1:K:217:TRP:HE1	1.60	0.48
2:P:522:LEU:HD12	2:P:522:LEU:N	2.28	0.48
2:R:318:LYS:HB3	2:R:319:PRO:CD	2.44	0.48
1:E:298:LYS:HE2	1:F:318:ILE:HD11	1.96	0.48
1:K:153:LEU:O	1:K:157:VAL:HG23	2.13	0.48
2:M:151:ILE:HG22	2:M:152:LYS:N	2.27	0.48
1:G:370:HIS:HB3	1:G:373:VAL:HG22	1.95	0.48
2:N:209:ASP:OD1	2:N:212:ALA:N	2.46	0.48
2:O:165:VAL:HG12	2:O:166:ALA:N	2.28	0.48
1:C:363:VAL:HG12	1:C:364:ALA:N	2.29	0.48
1:G:181:GLN:OE1	1:G:215:THR:HG21	2.13	0.48
1:K:130:ASP:OD1	1:K:132:SER:N	2.42	0.48
2:P:593:TRP:CZ2	2:Q:406:TYR:CD1	3.02	0.48
1:F:296:LEU:O	1:F:300:LEU:HD13	2.13	0.48
2:O:562:ALA:N	2:O:563:PRO:CD	2.77	0.48
1:A:73:LEU:HD13	1:A:122:LEU:HD12	1.94	0.47
1:B:339:LEU:CD1	1:B:341:LEU:HD11	2.43	0.47
1:C:19:TYR:OH	1:C:35:GLU:HB2	2.14	0.47
1:I:81:LYS:HA	1:I:81:LYS:HE3	1.96	0.47
2:P:227:THR:HG22	2:P:228:LEU:N	2.29	0.47
2:P:453:VAL:HG22	2:P:454:SER:H	1.79	0.47
2:Q:197:LYS:HD2	2:Q:225:ALA:HB3	1.96	0.47
2:R:12:THR:HG21	2:R:22:GLU:OE1	2.14	0.47
2:N:391:LEU:N	2:N:391:LEU:HD12	2.29	0.47
2:O:417:LEU:HD22	2:O:420:ILE:HD12	1.96	0.47
2:R:401:ARG:HB3	2:R:407:MET:HG3	1.95	0.47
3:U:5:DT:H2"	3:U:6:DA:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ALA:HB2	1:A:52:VAL:C	2.32	0.47
1:C:59:GLN:OE1	1:C:59:GLN:N	2.46	0.47
1:E:38:ILE:HB	1:E:40:ASP:O	2.13	0.47
1:I:211:ARG:HG3	1:I:211:ARG:O	2.13	0.47
2:O:490:GLU:O	2:O:493:LYS:HG2	2.14	0.47
2:Q:329:ASP:OD1	2:Q:331:ASP:N	2.46	0.47
2:R:145:LEU:HD22	2:R:567:THR:HG21	1.96	0.47
2:R:537:LEU:HD21	2:R:559:VAL:HG22	1.97	0.47
3:U:15:DT:H2"	3:U:16:DA:H8	1.78	0.47
4:V:16:DA:H8	4:V:16:DA:OP2	1.96	0.47
1:C:133:VAL:HG21	1:C:135:TYR:CE1	2.49	0.47
1:G:317:VAL:HG12	1:G:318:ILE:N	2.28	0.47
1:H:321:GLU:OE2	1:H:324:ARG:NE	2.47	0.47
2:O:210:ILE:HG22	2:O:210:ILE:O	2.14	0.47
2:P:589:TRP:CD2	2:Q:203:SER:HB3	2.50	0.47
2:Q:38:VAL:HG12	2:Q:39:GLY:N	2.29	0.47
1:A:121:VAL:HG13	1:A:122:LEU:HD22	1.97	0.47
1:E:6:GLU:OE1	1:E:6:GLU:HA	2.15	0.47
2:P:340:SER:OG	2:P:341:PHE:N	2.46	0.47
2:R:501:VAL:O	2:R:501:VAL:HG23	2.15	0.47
1:B:224:LYS:O	1:B:226:ARG:HD3	2.14	0.47
2:M:21:ILE:HG22	2:M:22:GLU:N	2.29	0.47
1:A:365:ASP:OD1	1:A:366:ASP:N	2.47	0.47
1:I:395:ASP:OD2	1:I:395:ASP:N	2.45	0.47
2:P:453:VAL:HG22	2:P:454:SER:N	2.29	0.47
2:P:460:VAL:HB	2:P:498:LEU:HD23	1.97	0.47
2:Q:164:HIS:N	2:Q:164:HIS:CD2	2.82	0.47
2:Q:598:PHE:O	2:Q:599:ASP:C	2.51	0.47
1:E:217:TRP:C	1:E:219:ARG:H	2.18	0.47
1:G:212:VAL:HG11	1:G:231:LEU:HD11	1.97	0.47
1:G:227:MET:HG3	1:G:228:PHE:N	2.30	0.47
1:I:9:ILE:HG23	1:I:10:LYS:N	2.30	0.47
1:J:323:PHE:CD1	1:J:323:PHE:N	2.80	0.47
2:Q:283:THR:OG1	2:Q:284:ASN:ND2	2.48	0.47
3:U:14:DA:N9	3:U:15:DT:H72	2.29	0.47
1:C:215:THR:O	1:C:219:ARG:HG2	2.14	0.47
2:M:233:VAL:HG21	2:M:420:ILE:HD11	1.97	0.47
2:R:61:ALA:O	2:R:62:THR:HG23	2.15	0.47
1:B:250:ILE:HG22	1:B:251:ASN:N	2.30	0.47
1:G:212:VAL:HG12	1:G:213:THR:N	2.30	0.47
2:O:1:MET:HB3	2:O:2:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:VAL:O	1:A:52:VAL:HG23	2.16	0.46
1:C:219:ARG:HH22	1:C:382:ARG:HH11	1.61	0.46
1:E:250:ILE:HG22	1:E:251:ASN:N	2.30	0.46
1:E:273:TYR:O	1:E:279:HIS:ND1	2.47	0.46
1:K:109:ASP:OD1	1:K:110:ASP:N	2.48	0.46
2:Q:333:LEU:HD11	2:Q:339:GLN:NE2	2.30	0.46
3:U:4:DA:H2'	3:U:5:DT:H72	1.97	0.46
1:C:54:CYS:SG	1:C:55:LYS:N	2.89	0.46
2:M:261:HIS:ND1	2:M:262:ASN:N	2.63	0.46
2:M:453:VAL:HG12	2:R:583:VAL:HG22	1.96	0.46
2:O:581:ARG:HD2	2:O:581:ARG:O	2.15	0.46
3:U:16:DA:OP2	3:U:16:DA:H8	1.98	0.46
1:C:202:PHE:CD2	1:C:203:LEU:HD23	2.50	0.46
1:G:154:GLN:O	1:G:158:LEU:HD23	2.15	0.46
2:P:233:VAL:HG12	2:P:233:VAL:O	2.15	0.46
2:P:350:THR:HG22	2:P:350:THR:O	2.15	0.46
2:Q:40:GLN:NE2	2:Q:147:ILE:O	2.48	0.46
4:V:9:DT:H2"	4:V:10:DA:H8	1.80	0.46
1:G:121:VAL:HG13	1:G:122:LEU:HD22	1.97	0.46
2:O:590:ASN:OD1	2:P:201:LYS:NZ	2.46	0.46
2:Q:151:ILE:HG22	2:Q:152:LYS:N	2.31	0.46
1:A:270:VAL:HG21	1:A:305:LEU:HD13	1.97	0.46
1:C:115:LEU:HD12	1:C:135:TYR:HE2	1.79	0.46
1:G:270:VAL:HG21	1:G:305:LEU:CD1	2.45	0.46
1:G:380:ILE:HG22	1:G:381:GLU:N	2.29	0.46
1:I:54:CYS:HG	1:I:55:LYS:N	2.14	0.46
1:G:181:GLN:HA	1:G:184:VAL:HG12	1.98	0.46
1:K:60:ALA:HB2	1:K:67:LYS:NZ	2.31	0.46
1:L:365:ASP:N	1:L:365:ASP:OD1	2.46	0.46
2:N:533:VAL:O	2:N:536:LEU:N	2.49	0.46
2:O:573:LEU:HD21	5:O:701:AGS:C4	2.45	0.46
2:P:59:VAL:HG12	2:P:60:ARG:N	2.31	0.46
3:U:5:DT:H1'	3:U:6:DA:C8	2.51	0.46
1:C:215:THR:N	1:C:218:THR:HG22	2.31	0.46
1:D:323:PHE:CD1	1:D:323:PHE:N	2.83	0.46
1:I:276:LYS:HG2	1:I:277:TYR:N	2.30	0.46
1:J:262:ILE:HG23	1:J:263:VAL:N	2.31	0.46
2:O:204:HIS:CD2	2:O:456:VAL:HG13	2.51	0.46
2:Q:494:TYR:N	2:Q:494:TYR:CD1	2.83	0.46
2:R:343:VAL:HG12	2:R:344:ALA:H	1.79	0.46
1:C:321:GLU:OE1	1:C:324:ARG:NE	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:ASP:OD1	1:E:110:ASP:N	2.48	0.46
1:H:389:ILE:C	1:H:390:LEU:HD12	2.37	0.46
1:K:28:ASP:OD1	1:K:29:GLY:N	2.48	0.46
2:N:444:SER:HB3	2:N:494:TYR:HD1	1.81	0.46
2:N:566:PRO:O	2:N:567:THR:OG1	2.30	0.46
2:O:288:ASP:OD2	2:O:289:THR:N	2.49	0.46
1:D:227:MET:HG2	1:D:228:PHE:CD1	2.51	0.46
1:G:216:ARG:HA	1:G:219:ARG:HH11	1.81	0.46
1:I:83:SER:OG	1:I:84:GLY:N	2.47	0.46
1:J:286:MET:O	1:J:287:LEU:HD23	2.16	0.46
2:O:299:VAL:HG21	2:O:368:LEU:HD22	1.98	0.46
2:P:485:GLU:OE2	2:P:489:LYS:NZ	2.47	0.46
2:R:247:GLU:HG2	2:R:427:ILE:HD11	1.98	0.46
2:R:424:VAL:O	2:R:427:ILE:HG22	2.16	0.46
1:H:239:LEU:HD13	1:H:273:TYR:CE2	2.51	0.46
1:K:6:GLU:HA	1:K:6:GLU:OE1	2.16	0.46
1:K:130:ASP:OD1	1:K:131:THR:N	2.49	0.46
2:O:53:LEU:HD22	2:O:106:PHE:HE2	1.81	0.46
2:P:8:ILE:O	2:P:23:ILE:HG12	2.15	0.46
1:E:22:GLU:O	1:E:26:ALA:N	2.47	0.45
2:N:290:PRO:O	2:N:291:VAL:HG13	2.16	0.45
2:O:459:LEU:HD12	2:O:497:THR:O	2.16	0.45
2:R:424:VAL:O	2:R:428:VAL:HG23	2.15	0.45
3:U:6:DA:H2"	3:U:7:DT:C5	2.51	0.45
1:A:34:ILE:HD12	1:A:195:ARG:HB3	1.97	0.45
1:G:220:GLU:HA	1:G:220:GLU:OE2	2.16	0.45
1:I:211:ARG:O	1:I:211:ARG:CG	2.64	0.45
1:J:331:ASN:O	1:J:331:ASN:ND2	2.49	0.45
2:N:1:MET:HB3	2:N:2:PRO:HD3	1.97	0.45
2:P:224:GLU:N	2:P:224:GLU:OE1	2.49	0.45
1:E:215:THR:OG1	1:E:216:ARG:N	2.49	0.45
1:G:18:LYS:O	1:G:21:SER:OG	2.23	0.45
1:H:360:LEU:HD23	1:H:363:VAL:CG1	2.46	0.45
1:K:215:THR:CG2	1:K:218:THR:HG23	2.45	0.45
2:M:95:GLN:NE2	2:M:540:LEU:O	2.49	0.45
2:N:324:GLU:OE2	2:N:324:GLU:N	2.49	0.45
2:O:370:THR:O	2:O:373:ALA:N	2.50	0.45
2:P:324:GLU:OE1	2:P:325:THR:OG1	2.30	0.45
2:R:336:ASP:OD1	2:R:337:ALA:N	2.49	0.45
2:R:522:LEU:N	2:R:522:LEU:HD12	2.31	0.45
1:A:42:ASP:OD1	1:A:44:ILE:HB	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ALA:O	1:C:128:ARG:NH1	2.43	0.45
2:O:412:VAL:O	2:O:412:VAL:HG13	2.16	0.45
2:R:4:LEU:N	2:R:4:LEU:HD12	2.31	0.45
3:U:12:DA:C2	3:U:13:DT:C4	3.04	0.45
1:A:211:ARG:HH12	1:A:379:LYS:HD3	1.82	0.45
1:E:258:PHE:CZ	1:E:262:ILE:HD13	2.51	0.45
1:G:315:THR:OG1	1:G:316:ASP:N	2.49	0.45
1:K:65:LEU:HD23	1:K:65:LEU:O	2.15	0.45
1:K:239:LEU:HD11	1:K:390:LEU:HD22	1.99	0.45
2:M:338:VAL:HG12	2:M:339:GLN:N	2.31	0.45
2:M:353:SER:OG	2:M:354:ASN:N	2.50	0.45
1:C:310:GLY:HA3	1:C:322:LEU:HD13	1.98	0.45
1:I:115:LEU:O	1:I:117:THR:HG23	2.17	0.45
2:P:12:THR:HG21	2:P:22:GLU:OE1	2.16	0.45
1:I:340:ARG:C	1:I:341:LEU:HD12	2.37	0.45
1:K:293:LEU:HD11	1:K:343:LYS:HG3	1.99	0.45
2:O:510:GLU:OE1	2:O:510:GLU:N	2.38	0.45
3:U:2:DA:H2"	3:U:3:DT:H71	1.98	0.45
3:U:8:DA:H4'	3:U:8:DA:OP1	2.17	0.45
1:E:15:GLN:O	1:E:19:TYR:CD1	2.70	0.45
1:G:151:GLU:OE1	1:G:151:GLU:N	2.38	0.45
1:I:12:TYR:CE2	1:I:217:TRP:HH2	2.34	0.45
1:K:363:VAL:HG12	1:K:364:ALA:N	2.31	0.45
2:M:171:THR:OG1	2:N:515:GLN:OE1	2.32	0.45
2:O:411:ASN:ND2	2:O:411:ASN:O	2.50	0.45
2:O:508:VAL:HG12	2:O:509:SER:N	2.32	0.45
2:Q:268:ARG:HA	2:Q:287:PHE:HE2	1.82	0.45
1:A:215:THR:HG22	1:A:218:THR:CG2	2.34	0.45
1:C:67:LYS:HD3	1:C:67:LYS:N	2.32	0.45
1:G:391:GLN:OE1	2:P:49:ASN:ND2	2.46	0.45
2:M:353:SER:HG	3:U:12:DA:P	2.38	0.45
2:P:310:ILE:HG23	2:P:318:LYS:O	2.17	0.45
2:R:21:ILE:HG22	2:R:22:GLU:N	2.31	0.45
1:A:266:ILE:O	1:A:270:VAL:HG22	2.17	0.44
1:G:215:THR:O	1:G:218:THR:HG22	2.17	0.44
1:I:31:ARG:O	1:I:32:ILE:HD13	2.17	0.44
1:I:49:THR:HB	1:I:89:VAL:HG23	2.00	0.44
1:K:260:ASP:OD1	1:K:299:ARG:NH1	2.46	0.44
2:N:132:PHE:O	2:N:136:ILE:HD12	2.17	0.44
2:P:575:VAL:HG23	2:P:575:VAL:O	2.17	0.44
3:U:14:DA:C8	3:U:15:DT:H72	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ASP:N	1:A:169:ASP:OD2	2.51	0.44
1:B:273:TYR:O	1:B:279:HIS:ND1	2.51	0.44
1:C:203:LEU:HD22	1:C:206:LEU:HD21	2.00	0.44
1:E:278:LEU:HD12	1:E:278:LEU:H	1.81	0.44
1:F:363:VAL:HG12	1:F:364:ALA:N	2.32	0.44
1:G:9:ILE:HD11	1:G:217:TRP:CD1	2.52	0.44
1:K:125:ILE:HD12	1:K:125:ILE:H	1.81	0.44
2:P:41:TYR:O	2:P:123:THR:OG1	2.29	0.44
1:A:74:LEU:HA	1:A:77:GLU:OE1	2.17	0.44
1:A:113:THR:O	1:A:116:SER:OG	2.26	0.44
1:C:111:LEU:HD22	1:C:135:TYR:CG	2.52	0.44
1:I:218:THR:O	1:I:221:LEU:HB3	2.17	0.44
2:N:194:ASN:N	2:N:224:GLU:OE2	2.45	0.44
2:O:385:LYS:HG2	2:O:386:GLU:N	2.32	0.44
2:Q:95:GLN:HE22	2:Q:540:LEU:HD11	1.81	0.44
4:V:5:DT:C2	4:V:6:DA:C8	3.04	0.44
1:A:93:LEU:HD21	1:A:95:CYS:HB2	1.99	0.44
1:E:36:GLY:HA2	1:E:195:ARG:HH22	1.82	0.44
1:E:79:PHE:N	1:E:91:TYR:OH	2.50	0.44
1:G:7:TYR:HE1	1:G:9:ILE:HD13	1.82	0.44
1:G:89:VAL:HG13	1:G:89:VAL:O	2.17	0.44
1:K:38:ILE:HD13	1:K:51:ALA:HB1	1.99	0.44
1:L:285:PHE:O	1:L:341:LEU:HD12	2.18	0.44
2:O:251:ILE:HG12	2:O:427:ILE:HD13	1.98	0.44
2:O:424:VAL:HA	2:O:427:ILE:HD12	1.99	0.44
2:P:23:ILE:HG22	2:P:24:SER:N	2.33	0.44
2:Q:230:LEU:O	2:Q:231:LEU:HG	2.17	0.44
2:R:210:ILE:HD12	2:R:464:GLU:CB	2.45	0.44
2:R:255:SER:O	2:R:256:ASN:C	2.55	0.44
3:U:7:DT:C3'	3:U:8:DA:H5"	2.48	0.44
1:E:52:VAL:HG13	1:E:52:VAL:O	2.18	0.44
2:M:455:ASP:OD1	2:M:455:ASP:N	2.50	0.44
2:P:101:SER:OG	2:P:102:GLU:N	2.51	0.44
2:Q:133:SER:O	2:Q:135:GLN:N	2.51	0.44
2:Q:218:PHE:HB3	2:Q:226:PHE:HE1	1.83	0.44
2:Q:261:HIS:ND1	2:Q:262:ASN:OD1	2.48	0.44
1:A:8:SER:O	1:A:8:SER:OG	2.32	0.44
1:A:18:LYS:O	1:A:21:SER:OG	2.29	0.44
1:C:202:PHE:HD2	1:C:203:LEU:HD23	1.82	0.44
1:E:262:ILE:HG23	1:E:263:VAL:N	2.33	0.44
1:G:185:ASP:OD1	1:G:189:ARG:NE	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:290:ASP:OD1	1:H:290:ASP:N	2.48	0.44
1:L:258:PHE:CE2	1:L:262:ILE:HD13	2.53	0.44
4:V:8:DA:C2'	4:V:9:DT:C7	2.93	0.44
1:E:62:LYS:HE3	1:E:62:LYS:HA	2.00	0.44
1:G:44:ILE:HG13	1:G:45:ALA:N	2.32	0.44
1:I:70:LYS:O	1:I:74:LEU:HD13	2.18	0.44
1:L:231:LEU:HD11	1:L:378:PHE:CZ	2.52	0.44
2:N:122:VAL:HG12	2:N:123:THR:H	1.83	0.44
2:Q:312:LYS:HB2	2:Q:351:LYS:HG2	2.00	0.44
1:A:274:SER:HA	1:A:279:HIS:HD1	1.83	0.44
1:C:58:GLU:HB2	1:C:96:HIS:HB3	2.00	0.44
1:C:89:VAL:HG12	1:C:89:VAL:O	2.18	0.44
1:G:214:PHE:HB2	1:G:380:ILE:CD1	2.47	0.44
1:J:231:LEU:HD22	1:J:378:PHE:HE1	1.83	0.44
1:G:77:GLU:O	1:G:128:ARG:NH1	2.44	0.44
2:O:44:VAL:HG12	2:O:45:ALA:N	2.33	0.44
2:O:583:VAL:HG22	2:P:453:VAL:CG2	2.48	0.44
2:R:526:ASN:O	2:R:530:GLN:HG3	2.17	0.44
4:V:14:DA:H2'	4:V:15:DT:H72	1.98	0.44
1:A:34:ILE:HG22	1:A:35:GLU:H	1.83	0.43
1:D:322:LEU:HD23	1:D:323:PHE:HE1	1.82	0.43
1:G:224:LYS:HG2	1:G:228:PHE:CE2	2.53	0.43
1:K:261:ASP:OD1	1:K:262:ILE:N	2.51	0.43
2:Q:598:PHE:HE2	2:R:401:ARG:HG2	1.83	0.43
1:A:315:THR:OG1	1:A:316:ASP:N	2.51	0.43
1:B:235:LEU:HD12	1:B:235:LEU:N	2.33	0.43
1:C:344:ARG:NH2	1:C:366:ASP:OD1	2.47	0.43
1:D:389:ILE:O	1:D:389:ILE:HG22	2.17	0.43
1:I:216:ARG:HA	1:I:219:ARG:HH12	1.82	0.43
2:P:49:ASN:OD1	2:P:49:ASN:N	2.50	0.43
2:P:362:ASP:OD1	2:P:363:ARG:N	2.51	0.43
2:Q:508:VAL:HG12	2:Q:509:SER:N	2.33	0.43
1:C:212:VAL:HG11	1:C:231:LEU:HD13	1.99	0.43
1:C:255:ILE:HG22	1:C:256:GLU:N	2.34	0.43
2:M:583:VAL:HG13	2:M:585:TYR:CE1	2.53	0.43
2:O:484:ILE:HG23	2:O:498:LEU:HD11	2.00	0.43
2:P:122:VAL:HG12	2:P:123:THR:N	2.33	0.43
2:P:468:TYR:O	2:P:469:LEU:HG	2.19	0.43
2:Q:204:HIS:CD2	2:Q:204:HIS:N	2.86	0.43
1:D:322:LEU:HD23	1:D:323:PHE:CE1	2.54	0.43
2:M:253:ILE:HD11	2:M:267:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:15:SER:OG	2:N:18:LEU:N	2.51	0.43
1:D:225:GLY:N	1:D:227:MET:SD	2.92	0.43
1:E:37:ALA:HB2	1:E:52:VAL:C	2.39	0.43
1:E:43:VAL:HG23	1:E:44:ILE:HD13	1.99	0.43
1:H:355:PRO:O	1:H:373:VAL:HG13	2.17	0.43
1:K:243:SER:O	1:K:244:ARG:HG3	2.19	0.43
2:M:210:ILE:HD12	2:M:464:GLU:HB2	1.99	0.43
2:N:183:LEU:HD22	2:N:205:ILE:HD13	1.99	0.43
2:N:567:THR:HG22	2:N:568:VAL:N	2.33	0.43
2:P:21:ILE:HG22	2:P:22:GLU:N	2.34	0.43
2:P:220:LEU:HD13	2:P:224:GLU:HG2	2.00	0.43
2:P:447:ARG:NH2	2:P:455:ASP:OD2	2.52	0.43
2:Q:136:ILE:HG22	2:Q:137:LYS:N	2.33	0.43
1:B:340:ARG:C	1:B:341:LEU:HD12	2.39	0.43
1:C:17:LEU:HD13	1:C:154:GLN:OE1	2.18	0.43
1:C:111:LEU:HD22	1:C:135:TYR:CD2	2.53	0.43
1:G:118:LYS:N	1:G:118:LYS:HD2	2.34	0.43
4:V:3:DT:H2'	4:V:4:DA:C8	2.51	0.43
1:C:115:LEU:HD12	1:C:135:TYR:CE2	2.53	0.43
1:K:203:LEU:HD12	1:K:206:LEU:HD21	2.00	0.43
1:K:224:LYS:CG	1:K:225:GLY:N	2.81	0.43
2:Q:539:ASP:OD1	2:Q:540:LEU:N	2.51	0.43
1:C:10:LYS:O	1:C:13:LEU:HG	2.18	0.43
1:C:197:VAL:HG23	1:C:197:VAL:O	2.19	0.43
1:E:194:ASP:OD1	1:E:194:ASP:N	2.50	0.43
2:P:585:TYR:OH	2:Q:497:THR:HG23	2.19	0.43
2:Q:160:PHE:O	2:Q:161:PHE:HB2	2.18	0.43
4:V:4:DA:C4	4:V:5:DT:C5	3.06	0.43
4:V:16:DA:H2'	4:V:17:DT:H72	2.01	0.43
1:E:221:LEU:HD12	1:E:221:LEU:H	1.84	0.43
2:M:539:ASP:OD1	2:M:540:LEU:N	2.52	0.43
2:N:44:VAL:HG12	2:N:45:ALA:N	2.34	0.43
2:N:168:VAL:O	2:N:168:VAL:HG23	2.19	0.43
1:C:66:GLY:O	1:C:69:TYR:CD2	2.72	0.43
1:C:69:TYR:O	1:C:72:ILE:HD12	2.19	0.43
1:I:224:LYS:HG3	1:I:225:GLY:N	2.34	0.43
1:K:216:ARG:HE	1:K:216:ARG:HB3	1.72	0.43
2:N:246:GLN:NE2	2:N:250:GLN:OE1	2.51	0.43
2:P:494:TYR:N	2:P:494:TYR:CD1	2.85	0.43
2:Q:95:GLN:NE2	2:Q:540:LEU:HD11	2.34	0.43
2:Q:170:SER:O	2:Q:175:LYS:NZ	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:248:LEU:HA	2:R:251:ILE:HG22	2.01	0.43
2:R:365:ILE:HG13	2:R:366:LEU:N	2.34	0.43
3:U:4:DA:H2"	3:U:5:DT:C6	2.53	0.43
1:C:32:ILE:HG22	1:C:33:THR:N	2.34	0.42
1:E:164:LYS:O	1:E:164:LYS:HD3	2.18	0.42
1:F:323:PHE:N	1:F:323:PHE:CD1	2.84	0.42
1:K:169:ASP:OD2	1:K:170:ASP:N	2.52	0.42
2:P:209:ASP:OD2	2:P:213:GLU:N	2.49	0.42
1:A:176:PHE:N	1:A:177:PRO:CD	2.83	0.42
1:D:235:LEU:N	1:D:235:LEU:HD12	2.34	0.42
1:E:36:GLY:CA	1:E:195:ARG:NH2	2.82	0.42
1:E:365:ASP:OD1	1:E:365:ASP:N	2.53	0.42
1:I:165:GLY:O	1:I:166:PHE:CD1	2.72	0.42
1:I:244:ARG:NH2	1:I:356:ASP:HB3	2.35	0.42
2:M:313:LEU:HD23	2:M:314:ALA:N	2.34	0.42
2:M:374:ASP:OD2	2:M:376:ARG:NH2	2.51	0.42
2:N:174:GLY:HA2	5:N:701:AGS:PA	2.59	0.42
2:N:460:VAL:HB	2:N:498:LEU:HD23	2.00	0.42
2:N:468:TYR:O	2:N:469:LEU:HG	2.18	0.42
2:P:218:PHE:N	2:P:218:PHE:CD2	2.86	0.42
1:A:8:SER:HB2	1:A:55:LYS:CD	2.48	0.42
1:A:104:LYS:O	1:A:144:ILE:HG22	2.19	0.42
1:B:224:LYS:HD3	1:B:224:LYS:O	2.19	0.42
1:E:317:VAL:HG12	1:E:318:ILE:N	2.34	0.42
1:G:209:VAL:CG1	1:G:211:ARG:HG2	2.49	0.42
1:G:215:THR:HG23	1:G:218:THR:H	1.84	0.42
1:G:218:THR:HG23	1:G:219:ARG:N	2.34	0.42
1:K:224:LYS:O	1:K:225:GLY:C	2.58	0.42
2:O:13:ASP:OD1	2:O:14:SER:N	2.52	0.42
2:Q:228:LEU:HD23	2:Q:230:LEU:CD2	2.50	0.42
2:Q:504:ARG:NE	2:Q:529:ASP:OD2	2.49	0.42
2:M:200:GLN:NE2	2:M:409:LYS:O	2.41	0.42
2:M:471:ARG:NH2	2:M:510:GLU:OE2	2.53	0.42
2:O:439:PHE:CD1	2:O:439:PHE:C	2.93	0.42
3:U:1:DT:H2"	3:U:2:DA:OP2	2.19	0.42
1:A:394:SER:OG	1:A:395:ASP:N	2.52	0.42
1:C:145:GLU:OE2	1:C:146:PHE:O	2.38	0.42
1:D:262:ILE:HG23	1:D:263:VAL:N	2.33	0.42
1:E:220:GLU:HA	1:E:220:GLU:OE2	2.19	0.42
1:H:385:ASP:OD1	1:H:386:LEU:N	2.53	0.42
1:I:32:ILE:O	1:I:197:VAL:HG22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:275:LYS:NZ	2:P:287:PHE:O	2.50	0.42
2:Q:108:ARG:O	2:Q:111:HIS:NE2	2.52	0.42
2:Q:557:LEU:HD12	2:Q:567:THR:O	2.19	0.42
1:B:224:LYS:O	1:B:226:ARG:NH1	2.53	0.42
1:I:322:LEU:HD23	1:I:322:LEU:O	2.19	0.42
2:M:583:VAL:HG13	2:M:585:TYR:HE1	1.84	0.42
2:N:240:TYR:OH	2:N:293:PHE:O	2.20	0.42
2:Q:324:GLU:OE2	2:Q:324:GLU:N	2.52	0.42
4:V:12:DA:H2'	4:V:13:DT:H72	2.02	0.42
1:A:42:ASP:OD1	1:A:44:ILE:N	2.51	0.42
1:G:153:LEU:O	1:G:157:VAL:HG23	2.20	0.42
1:J:327:ILE:C	1:J:328:LEU:HD12	2.40	0.42
2:O:447:ARG:HA	2:O:447:ARG:NE	2.35	0.42
1:C:199:PRO:O	1:C:202:PHE:HB3	2.19	0.42
1:J:231:LEU:HD22	1:J:378:PHE:CE1	2.55	0.42
1:K:35:GLU:OE2	1:K:51:ALA:N	2.53	0.42
1:K:213:THR:HG23	1:K:213:THR:O	2.20	0.42
2:M:267:PHE:CE2	2:M:298:VAL:HG11	2.55	0.42
2:O:21:ILE:HG22	2:O:22:GLU:N	2.35	0.42
2:Q:254:GLU:O	2:Q:255:SER:C	2.58	0.42
1:C:273:TYR:N	1:C:273:TYR:CD1	2.87	0.42
1:C:315:THR:HG23	1:C:316:ASP:N	2.35	0.42
1:G:185:ASP:OD1	1:G:189:ARG:NH2	2.52	0.42
1:I:215:THR:OG1	1:I:217:TRP:HB2	2.20	0.42
1:K:224:LYS:O	1:K:227:MET:HB3	2.20	0.42
2:Q:228:LEU:HA	2:Q:410:SER:HB3	2.02	0.42
2:Q:312:LYS:CB	2:Q:351:LYS:HG2	2.50	0.42
3:U:2:DA:C2'	3:U:3:DT:H71	2.50	0.42
1:E:90:SER:O	1:E:92:ARG:HG3	2.20	0.42
1:I:93:LEU:HD22	1:I:144:ILE:HG23	2.02	0.42
2:N:326:LEU:N	2:N:326:LEU:HD23	2.35	0.42
2:O:595:HIS:ND1	2:O:597:ASP:OD1	2.53	0.42
2:Q:253:ILE:HG23	2:Q:256:ASN:ND2	2.35	0.42
2:Q:485:GLU:OE2	2:Q:489:LYS:NZ	2.50	0.42
2:Q:536:LEU:CD2	2:Q:559:VAL:HG11	2.50	0.42
3:U:14:DA:N6	4:V:2:DA:N6	2.68	0.42
1:C:139:LEU:HD23	1:C:139:LEU:C	2.39	0.41
1:E:12:TYR:O	1:E:16:PHE:CD2	2.73	0.41
1:E:124:ALA:O	1:E:127:ALA:HB3	2.19	0.41
1:E:322:LEU:O	1:E:322:LEU:HD23	2.20	0.41
1:E:330:ARG:NH2	2:O:10:SER:OG	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:ILE:O	1:G:38:ILE:HG13	2.19	0.41
1:I:270:VAL:HG11	1:I:305:LEU:HD23	2.02	0.41
2:N:233:VAL:HG22	2:N:420:ILE:HD11	2.02	0.41
2:O:38:VAL:HG12	2:O:39:GLY:N	2.34	0.41
2:O:535:SER:OG	2:O:536:LEU:N	2.53	0.41
2:P:204:HIS:CE1	2:P:406:TYR:CE2	3.08	0.41
2:Q:589:TRP:CD1	2:R:203:SER:HA	2.55	0.41
3:U:3:DT:OP2	3:U:3:DT:H2'	2.19	0.41
1:A:47:GLY:O	1:A:50:THR:OG1	2.26	0.41
1:A:361:ILE:HG21	1:A:380:ILE:HD11	2.01	0.41
1:G:92:ARG:NH1	1:G:92:ARG:HB2	2.35	0.41
1:H:258:PHE:CE2	1:H:262:ILE:HD13	2.55	0.41
1:K:89:VAL:HB	1:K:141:ARG:HH22	1.86	0.41
1:K:133:VAL:HG21	1:K:135:TYR:CZ	2.55	0.41
2:M:243:MET:SD	2:M:251:ILE:HD12	2.60	0.41
2:M:375:PRO:HA	2:M:378:GLN:HG2	2.02	0.41
2:O:469:LEU:HD13	2:O:512:ILE:HD13	2.01	0.41
1:A:7:TYR:HE1	1:A:39:GLU:HG2	1.86	0.41
1:I:13:LEU:O	1:I:16:PHE:N	2.54	0.41
1:I:52:VAL:HG22	1:I:53:GLN:N	2.36	0.41
1:I:278:LEU:HD12	1:I:278:LEU:H	1.85	0.41
1:L:326:PRO:HG2	1:L:328:LEU:HD11	2.01	0.41
2:M:366:LEU:HD23	2:N:357:PHE:CE2	2.54	0.41
2:Q:21:ILE:HG22	2:Q:22:GLU:N	2.35	0.41
2:R:213:GLU:OE1	2:R:578:PRO:HB2	2.20	0.41
1:G:318:ILE:HG22	1:G:320:LYS:H	1.85	0.41
1:I:219:ARG:HA	1:I:224:LYS:HD2	2.03	0.41
1:K:7:TYR:CE1	1:K:39:GLU:HG2	2.55	0.41
1:F:273:TYR:O	1:F:279:HIS:ND1	2.53	0.41
1:G:68:ILE:O	1:G:68:ILE:HG23	2.20	0.41
1:K:340:ARG:O	1:K:341:LEU:HD12	2.20	0.41
2:N:122:VAL:CG1	2:N:123:THR:N	2.84	0.41
2:O:135:GLN:O	2:O:135:GLN:HG2	2.20	0.41
2:O:533:VAL:O	2:O:533:VAL:HG12	2.20	0.41
2:P:320:LYS:HA	2:P:326:LEU:HA	2.03	0.41
2:R:268:ARG:HG2	2:R:287:PHE:CE2	2.55	0.41
3:U:6:DA:H2"	3:U:7:DT:C7	2.50	0.41
1:G:202:PHE:CE2	1:G:206:LEU:HD22	2.55	0.41
1:H:323:PHE:N	1:H:323:PHE:CD1	2.88	0.41
1:I:15:GLN:NE2	1:I:19:TYR:CE1	2.89	0.41
1:I:378:PHE:N	1:I:378:PHE:CD1	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:319:ILE:N	1:J:319:ILE:HD13	2.35	0.41
1:K:261:ASP:OD2	1:K:383:LEU:HD12	2.21	0.41
2:M:312:LYS:O	2:M:312:LYS:HG2	2.20	0.41
2:P:316:GLU:O	2:P:318:LYS:N	2.48	0.41
2:R:505:PRO:O	2:R:508:VAL:N	2.53	0.41
1:A:180:ILE:O	1:A:184:VAL:HG23	2.20	0.41
2:N:42:LEU:O	2:N:53:LEU:HD12	2.21	0.41
2:O:290:PRO:O	2:O:291:VAL:CG1	2.69	0.41
2:O:480:SER:O	2:O:481:ARG:C	2.59	0.41
2:P:596:VAL:HB	2:P:598:PHE:CE1	2.56	0.41
2:Q:309:VAL:HG13	2:Q:353:SER:C	2.41	0.41
2:R:168:VAL:HG23	2:R:168:VAL:O	2.19	0.41
2:R:463:GLU:HA	2:R:501:VAL:CG2	2.51	0.41
1:A:261:ASP:OD1	1:A:383:LEU:HD12	2.20	0.41
1:A:270:VAL:HG21	1:A:305:LEU:CD1	2.50	0.41
1:C:206:LEU:C	1:C:206:LEU:HD12	2.40	0.41
1:I:154:GLN:O	1:I:158:LEU:HG	2.21	0.41
1:J:322:LEU:HD23	1:J:323:PHE:HE1	1.85	0.41
1:K:176:PHE:HB3	1:K:177:PRO:HD3	2.02	0.41
1:K:276:LYS:HG2	1:K:277:TYR:N	2.36	0.41
2:N:15:SER:HB2	2:N:16:PRO:HD2	2.03	0.41
2:N:205:ILE:CG2	2:N:206:VAL:N	2.83	0.41
2:O:239:PRO:HB2	2:O:241:TRP:CD1	2.56	0.41
2:O:445:LYS:O	2:O:449:VAL:HG23	2.21	0.41
1:A:70:LYS:HD2	1:A:122:LEU:HD11	2.02	0.41
1:A:118:LYS:N	1:A:118:LYS:CD	2.83	0.41
1:C:68:ILE:O	1:C:71:PRO:HD2	2.21	0.41
1:C:90:SER:OG	1:C:91:TYR:N	2.54	0.41
1:C:192:VAL:O	1:C:192:VAL:HG13	2.21	0.41
1:C:216:ARG:N	1:C:381:GLU:OE2	2.53	0.41
1:D:368:TRP:N	1:D:368:TRP:CD1	2.85	0.41
1:E:12:TYR:O	1:E:15:GLN:HG2	2.21	0.41
1:E:232:ARG:NH1	1:E:388:TYR:CE1	2.89	0.41
1:F:250:ILE:HG22	1:F:251:ASN:N	2.36	0.41
1:F:339:LEU:H	1:F:339:LEU:HD23	1.86	0.41
1:G:133:VAL:CG1	1:G:135:TYR:CZ	3.03	0.41
1:G:262:ILE:HG23	1:G:263:VAL:N	2.35	0.41
1:G:372:ASP:N	1:G:372:ASP:OD1	2.53	0.41
1:I:391:GLN:OE1	2:Q:49:ASN:ND2	2.54	0.41
1:J:222:ALA:O	1:J:224:LYS:HD2	2.21	0.41
1:K:56:TYR:HA	1:K:94:PHE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:212:VAL:HG22	1:K:213:THR:N	2.35	0.41
1:L:255:ILE:HG22	1:L:256:GLU:N	2.36	0.41
2:M:463:GLU:HA	2:M:501:VAL:CG2	2.51	0.41
2:N:257:GLU:HA	2:N:257:GLU:OE2	2.21	0.41
2:O:490:GLU:O	2:O:491:GLY:C	2.57	0.41
2:R:238:LEU:HD21	2:R:431:LEU:CD2	2.38	0.41
4:V:10:DA:H2"	4:V:11:DT:O5'	2.21	0.41
1:E:221:LEU:HD12	1:E:221:LEU:N	2.36	0.41
1:E:380:ILE:HD11	1:E:385:ASP:HB2	2.02	0.41
1:G:165:GLY:O	1:G:166:PHE:CD1	2.74	0.41
1:I:60:ALA:HB3	1:I:98:PRO:HD2	2.02	0.41
1:I:181:GLN:O	1:I:184:VAL:HG22	2.21	0.41
1:K:139:LEU:HD23	1:K:139:LEU:C	2.41	0.41
1:K:255:ILE:HG22	1:K:256:GLU:N	2.36	0.41
2:N:562:ALA:HB3	2:N:563:PRO:CD	2.51	0.41
2:O:589:TRP:HA	2:P:202:ASN:HB3	2.03	0.41
2:Q:210:ILE:O	2:Q:210:ILE:CG2	2.69	0.41
2:R:11:VAL:HG12	2:R:12:THR:N	2.36	0.41
4:V:11:DT:H2"	4:V:12:DA:O4'	2.20	0.41
1:C:48:LEU:HG	1:C:49:THR:N	2.37	0.40
4:V:7:DT:H2'	4:V:8:DA:C8	2.56	0.40
1:A:108:LYS:HD3	1:A:108:LYS:HA	1.94	0.40
1:A:174:VAL:HG22	1:A:174:VAL:O	2.21	0.40
1:A:279:HIS:CD2	1:A:279:HIS:N	2.89	0.40
1:E:191:ASP:OD1	1:E:192:VAL:N	2.54	0.40
1:I:35:GLU:HB3	1:I:52:VAL:CG1	2.52	0.40
1:I:125:ILE:HA	1:I:128:ARG:HD2	2.02	0.40
1:J:291:TYR:CD1	1:J:292:ASP:N	2.89	0.40
1:L:262:ILE:HG23	1:L:263:VAL:N	2.36	0.40
2:Q:200:GLN:HG3	2:Q:410:SER:O	2.21	0.40
3:U:4:DA:C2'	3:U:5:DT:H72	2.51	0.40
3:U:6:DA:O5'	3:U:6:DA:C8	2.72	0.40
1:G:132:SER:O	1:G:132:SER:OG	2.38	0.40
1:K:11:GLY:HA2	1:K:56:TYR:HB3	2.03	0.40
1:K:138:PHE:O	1:K:142:PHE:N	2.55	0.40
2:O:417:LEU:HD13	2:O:425:LEU:HD11	2.03	0.40
2:P:38:VAL:HG12	2:P:547:LEU:HD11	2.03	0.40
1:E:37:ALA:N	1:E:52:VAL:H	2.19	0.40
1:G:370:HIS:ND1	1:G:372:ASP:OD1	2.52	0.40
1:I:329:ILE:HD11	1:I:334:ARG:HB3	2.02	0.40
1:J:363:VAL:HG12	1:J:364:ALA:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:21:ILE:CG2	2:M:22:GLU:N	2.84	0.40
2:N:133:SER:OG	2:N:134:HIS:N	2.53	0.40
2:O:383:PRO:O	2:O:384:LYS:HD3	2.22	0.40
2:P:521:SER:C	2:P:522:LEU:HD12	2.42	0.40
4:V:10:DA:C2'	4:V:11:DT:H72	2.52	0.40
1:A:133:VAL:CG1	1:A:135:TYR:CZ	3.05	0.40
1:A:162:LYS:O	1:A:165:GLY:N	2.54	0.40
1:G:219:ARG:HG3	1:G:220:GLU:N	2.36	0.40
1:G:317:VAL:CG1	1:G:318:ILE:N	2.85	0.40
1:I:67:LYS:N	1:I:67:LYS:HD3	2.36	0.40
1:I:168:PRO:HA	1:I:171:ILE:HD12	2.04	0.40
1:I:375:VAL:HG12	1:I:376:HIS:N	2.37	0.40
2:O:158:ASP:OD1	2:O:159:ARG:N	2.55	0.40
2:O:417:LEU:CD2	2:O:420:ILE:HD12	2.52	0.40
2:P:379:PHE:CD2	2:P:380:LEU:N	2.89	0.40
2:P:418:SER:OG	2:P:419:GLY:N	2.55	0.40
2:Q:333:LEU:O	2:Q:334:TYR:C	2.60	0.40
2:Q:383:PRO:O	2:Q:384:LYS:HD3	2.22	0.40
2:Q:568:VAL:HG12	2:Q:569:GLY:N	2.36	0.40
2:R:95:GLN:HG3	2:R:96:PRO:HD2	2.04	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	383/397 (96%)	357 (93%)	26 (7%)	0	100	100
1	B	171/397 (43%)	159 (93%)	12 (7%)	0	100	100
1	C	380/397 (96%)	357 (94%)	23 (6%)	0	100	100
1	D	170/397 (43%)	161 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	383/397 (96%)	362 (94%)	21 (6%)	0	100	100
1	F	170/397 (43%)	160 (94%)	10 (6%)	0	100	100
1	G	383/397 (96%)	363 (95%)	20 (5%)	0	100	100
1	H	170/397 (43%)	164 (96%)	6 (4%)	0	100	100
1	I	380/397 (96%)	350 (92%)	30 (8%)	0	100	100
1	J	173/397 (44%)	158 (91%)	15 (9%)	0	100	100
1	K	380/397 (96%)	357 (94%)	23 (6%)	0	100	100
1	L	171/397 (43%)	158 (92%)	13 (8%)	0	100	100
2	M	582/617 (94%)	534 (92%)	48 (8%)	0	100	100
2	N	562/617 (91%)	513 (91%)	49 (9%)	0	100	100
2	O	570/617 (92%)	513 (90%)	57 (10%)	0	100	100
2	P	582/617 (94%)	525 (90%)	57 (10%)	0	100	100
2	Q	581/617 (94%)	515 (89%)	65 (11%)	1 (0%)	44	73
2	R	582/617 (94%)	523 (90%)	59 (10%)	0	100	100
All	All	6773/8466 (80%)	6229 (92%)	543 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Q	258	HIS

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	339/346 (98%)	338 (100%)	1 (0%)	91	94
1	B	159/346 (46%)	158 (99%)	1 (1%)	84	90
1	C	336/346 (97%)	335 (100%)	1 (0%)	91	94
1	D	158/346 (46%)	157 (99%)	1 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	339/346 (98%)	336 (99%)	3 (1%)	75 84
1	F	158/346 (46%)	158 (100%)	0	100 100
1	G	339/346 (98%)	338 (100%)	1 (0%)	91 94
1	H	158/346 (46%)	158 (100%)	0	100 100
1	I	336/346 (97%)	335 (100%)	1 (0%)	91 94
1	J	160/346 (46%)	160 (100%)	0	100 100
1	K	336/346 (97%)	336 (100%)	0	100 100
1	L	159/346 (46%)	158 (99%)	1 (1%)	84 90
2	M	499/525 (95%)	499 (100%)	0	100 100
2	N	482/525 (92%)	482 (100%)	0	100 100
2	O	493/525 (94%)	492 (100%)	1 (0%)	92 95
2	P	499/525 (95%)	499 (100%)	0	100 100
2	Q	498/525 (95%)	498 (100%)	0	100 100
2	R	499/525 (95%)	499 (100%)	0	100 100
All	All	5947/7302 (81%)	5936 (100%)	11 (0%)	91 95

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	B	227	MET
1	C	104	LYS
1	D	226	ARG
1	E	104	LYS
1	E	128	ARG
1	E	224	LYS
1	G	31	ARG
1	I	104	LYS
1	L	226	ARG
2	O	445	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	193	ASN

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Mol	Chain	Res	Type
1	C	376	HIS
1	D	376	HIS
1	E	78	HIS
1	E	193	ASN
1	F	362	ASN
1	G	53	GLN
1	G	59	GLN
1	G	193	ASN
1	G	374	ASN
1	H	376	HIS
1	I	181	GLN
1	I	279	HIS
1	J	331	ASN
1	K	59	GLN
1	K	78	HIS
1	L	370	HIS
2	M	49	ASN
2	M	134	HIS
2	M	246	GLN
2	M	442	HIS
2	M	466	HIS
2	M	570	HIS
2	N	63	HIS
2	N	200	GLN
2	N	262	ASN
2	N	411	ASN
2	N	448	HIS
2	N	503	GLN
2	O	134	HIS
2	O	164	HIS
2	O	269	HIS
2	O	584	ASN
2	P	196	HIS
2	P	204	HIS
2	P	402	GLN
2	P	442	HIS
2	P	467	ASN
2	P	590	ASN
2	Q	49	ASN
2	Q	95	GLN
2	Q	164	HIS
2	Q	204	HIS

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Mol	Chain	Res	Type
2	Q	235	ASN
2	Q	279	ASN
2	Q	284	ASN
2	Q	358	ASN
2	Q	369	HIS
2	R	63	HIS
2	R	442	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
5	AGS	Q	701	-	26,33,33	1.83	3 (11%)	26,52,52	1.75	4 (15%)
5	AGS	N	701	6	26,33,33	1.80	2 (7%)	26,52,52	1.69	4 (15%)
5	AGS	M	701	6	26,33,33	1.86	3 (11%)	26,52,52	1.59	4 (15%)
5	AGS	O	701	6	26,33,33	1.82	3 (11%)	26,52,52	1.77	4 (15%)
5	AGS	P	701	6	26,33,33	1.82	3 (11%)	26,52,52	1.65	4 (15%)
5	AGS	R	701	-	26,33,33	1.80	2 (7%)	26,52,52	1.75	4 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AGS	Q	701	-	-	5/17/38/38	0/3/3/3
5	AGS	N	701	6	-	3/17/38/38	0/3/3/3
5	AGS	M	701	6	-	3/17/38/38	0/3/3/3
5	AGS	O	701	6	-	6/17/38/38	0/3/3/3
5	AGS	P	701	6	-	2/17/38/38	0/3/3/3
5	AGS	R	701	-	-	6/17/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	701	AGS	PG-S1G	7.68	2.07	1.90
5	P	701	AGS	PG-S1G	7.64	2.07	1.90
5	O	701	AGS	PG-S1G	7.61	2.07	1.90
5	N	701	AGS	PG-S1G	7.58	2.07	1.90
5	Q	701	AGS	PG-S1G	7.57	2.07	1.90
5	R	701	AGS	PG-S1G	7.56	2.07	1.90
5	Q	701	AGS	PG-O3G	-2.31	1.47	1.54
5	M	701	AGS	C2'-C1'	-2.28	1.50	1.53
5	N	701	AGS	PG-O3G	-2.23	1.47	1.54
5	P	701	AGS	PG-O3G	-2.16	1.48	1.54
5	R	701	AGS	PG-O3G	-2.15	1.48	1.54
5	M	701	AGS	PG-O3G	-2.15	1.48	1.54
5	P	701	AGS	C5-C4	2.14	1.46	1.40
5	O	701	AGS	PG-O3G	-2.14	1.48	1.54
5	O	701	AGS	C5-C4	2.07	1.46	1.40
5	Q	701	AGS	C2'-C1'	-2.02	1.50	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Q	701	AGS	PA-O3A-PB	-5.37	114.40	132.83
5	N	701	AGS	PA-O3A-PB	-5.24	114.86	132.83
5	R	701	AGS	PA-O3A-PB	-5.09	115.37	132.83
5	O	701	AGS	PA-O3A-PB	-4.90	116.02	132.83
5	M	701	AGS	PA-O3A-PB	-4.62	116.97	132.83
5	P	701	AGS	PA-O3A-PB	-4.48	117.46	132.83
5	O	701	AGS	N3-C2-N1	-3.80	122.73	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	701	AGS	N3-C2-N1	-3.79	122.75	128.68
5	M	701	AGS	N3-C2-N1	-3.71	122.88	128.68
5	N	701	AGS	N3-C2-N1	-3.63	123.01	128.68
5	Q	701	AGS	N3-C2-N1	-3.60	123.05	128.68
5	P	701	AGS	N3-C2-N1	-3.53	123.17	128.68
5	R	701	AGS	C3'-C2'-C1'	3.07	105.59	100.98
5	O	701	AGS	C4-C5-N7	-2.91	106.36	109.40
5	P	701	AGS	C3'-C2'-C1'	2.86	105.29	100.98
5	R	701	AGS	C4-C5-N7	-2.63	106.66	109.40
5	Q	701	AGS	C3'-C2'-C1'	2.59	104.87	100.98
5	P	701	AGS	C4-C5-N7	-2.58	106.70	109.40
5	N	701	AGS	C4-C5-N7	-2.49	106.81	109.40
5	M	701	AGS	C4-C5-N7	-2.22	107.09	109.40
5	Q	701	AGS	C4-C5-N7	-2.21	107.09	109.40
5	N	701	AGS	C3'-C2'-C1'	2.20	104.28	100.98
5	O	701	AGS	C3'-C2'-C1'	2.16	104.22	100.98
5	M	701	AGS	C3'-C2'-C1'	2.05	104.06	100.98

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	701	AGS	C5'-O5'-PA-O3A
5	N	701	AGS	PB-O3B-PG-O2G
5	N	701	AGS	C5'-O5'-PA-O1A
5	O	701	AGS	C5'-O5'-PA-O1A
5	O	701	AGS	O4'-C4'-C5'-O5'
5	P	701	AGS	C5'-O5'-PA-O1A
5	Q	701	AGS	PB-O3B-PG-O2G
5	Q	701	AGS	C5'-O5'-PA-O3A
5	R	701	AGS	PB-O3B-PG-O2G
5	R	701	AGS	PB-O3B-PG-O3G
5	R	701	AGS	C5'-O5'-PA-O2A
5	R	701	AGS	C5'-O5'-PA-O3A
5	R	701	AGS	C3'-C4'-C5'-O5'
5	O	701	AGS	C3'-C4'-C5'-O5'
5	R	701	AGS	O4'-C4'-C5'-O5'
5	O	701	AGS	C5'-O5'-PA-O3A
5	M	701	AGS	C5'-O5'-PA-O1A
5	O	701	AGS	C5'-O5'-PA-O2A
5	Q	701	AGS	C5'-O5'-PA-O1A
5	N	701	AGS	PB-O3B-PG-O3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	Q	701	AGS	PB-O3B-PG-O3G
5	M	701	AGS	C3'-C4'-C5'-O5'
5	O	701	AGS	PG-O3B-PB-O1B
5	Q	701	AGS	PG-O3B-PB-O1B
5	P	701	AGS	C5'-O5'-PA-O3A

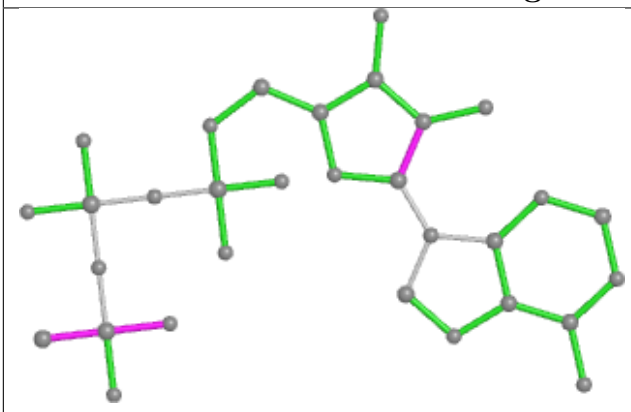
There are no ring outliers.

6 monomers are involved in 10 short contacts:

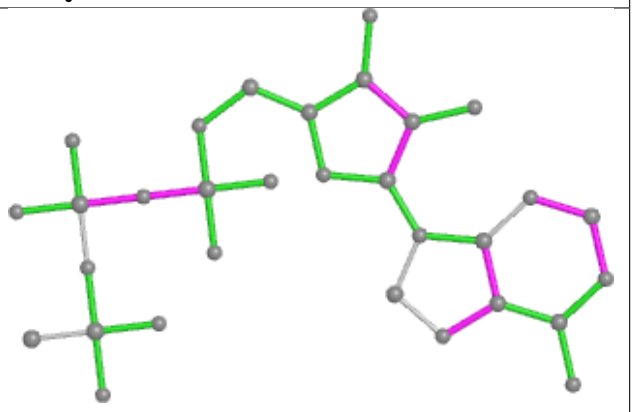
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Q	701	AGS	1	0
5	N	701	AGS	3	0
5	M	701	AGS	1	0
5	O	701	AGS	1	0
5	P	701	AGS	1	0
5	R	701	AGS	3	0

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 then 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.

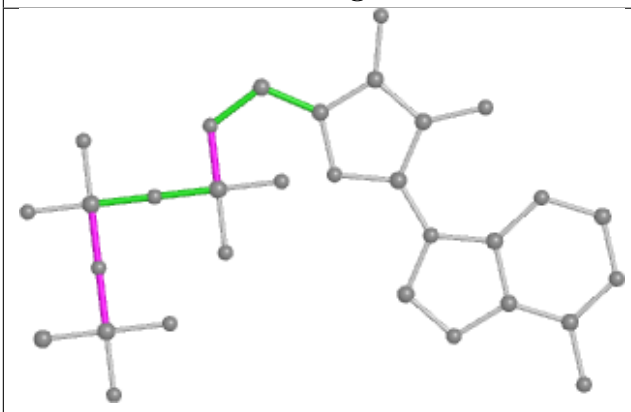
Ligand AGS Q 701



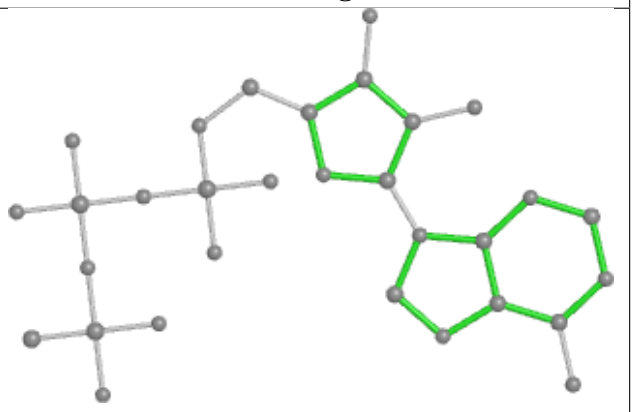
Bond lengths



Bond angles

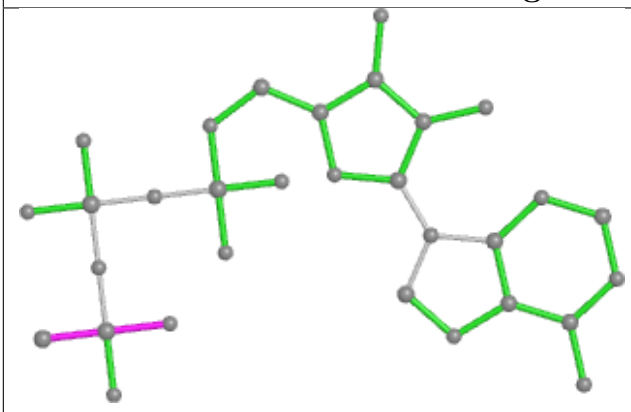


Torsions

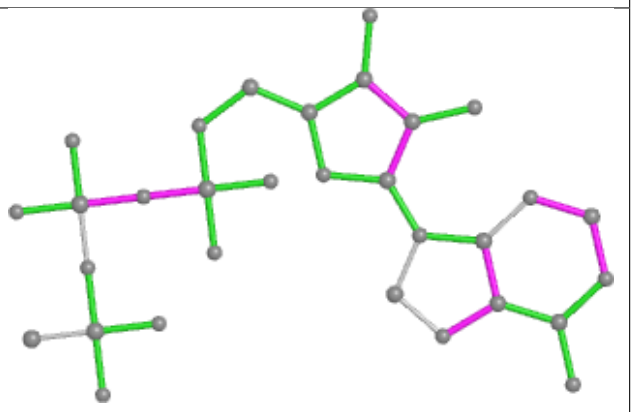


Rings

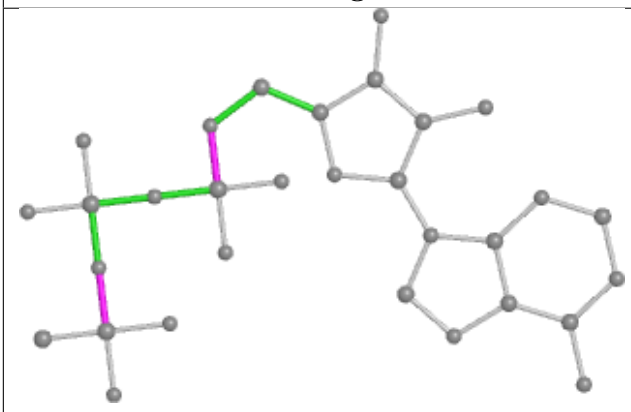
Ligand AGS N 701



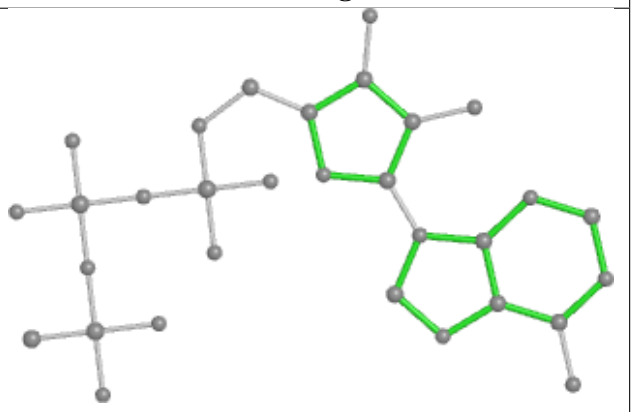
Bond lengths



Bond angles

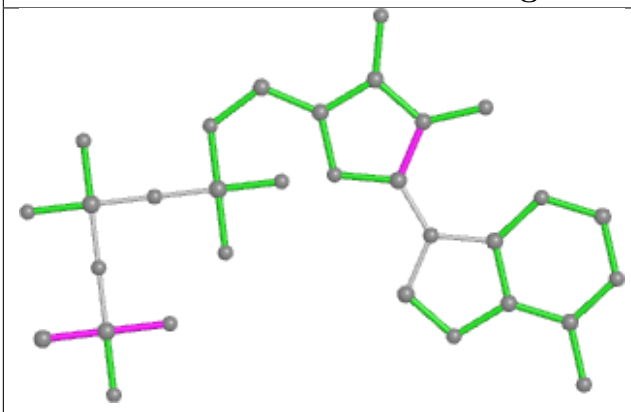


Torsions

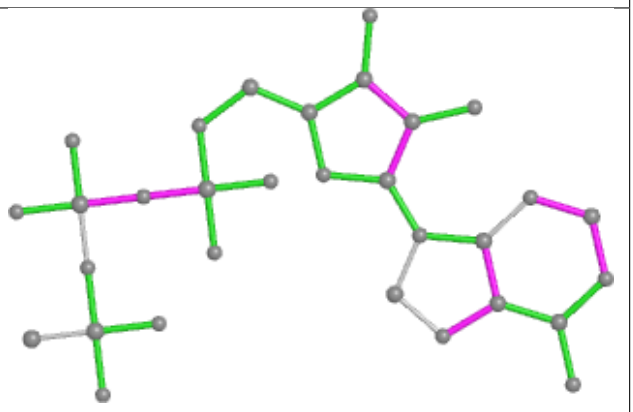


Rings

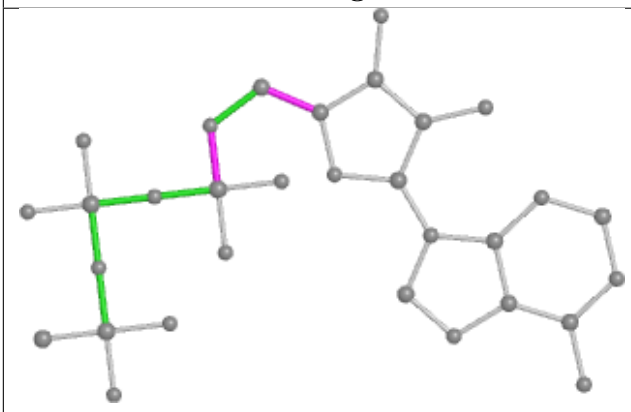
Ligand AGS M 701



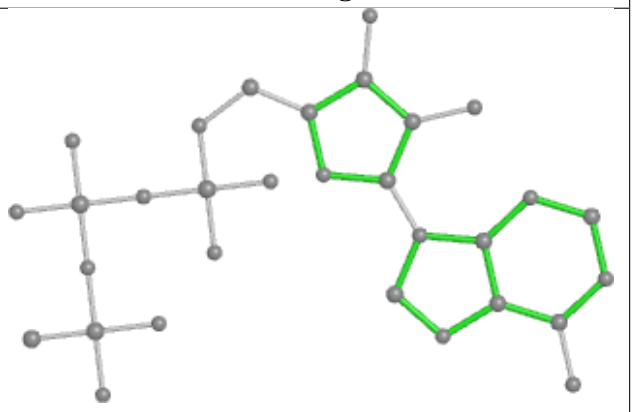
Bond lengths



Bond angles

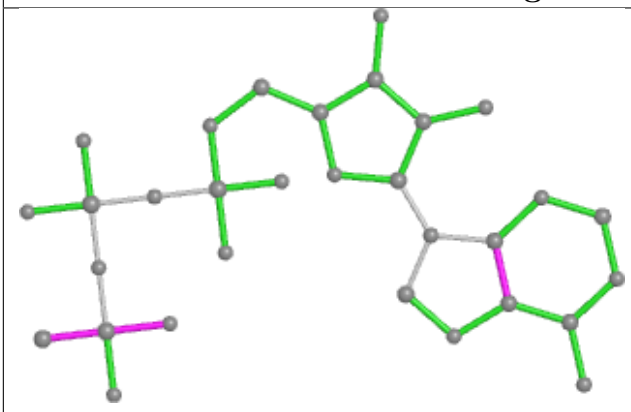


Torsions

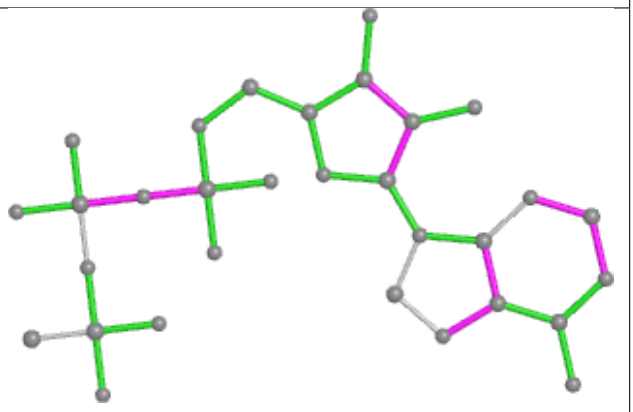


Rings

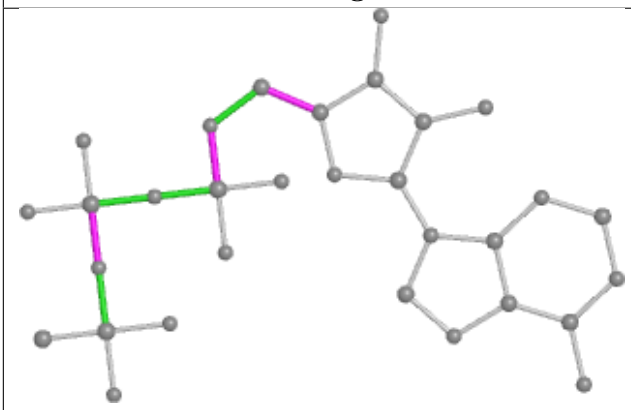
Ligand AGS O 701



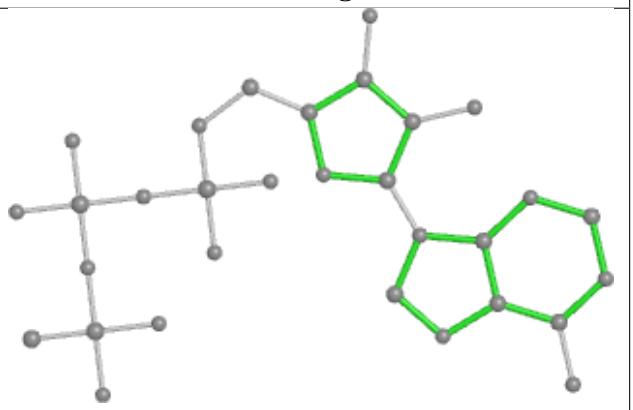
Bond lengths



Bond angles

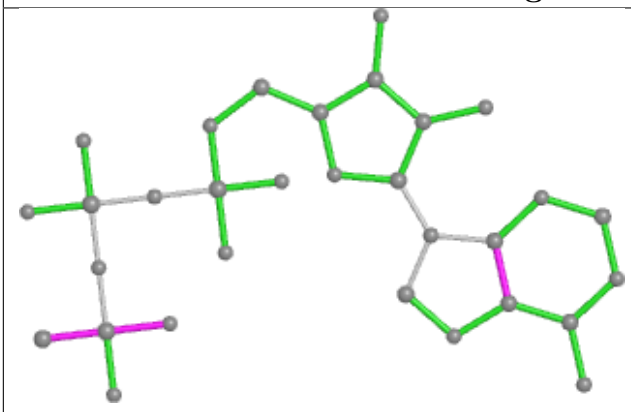


Torsions

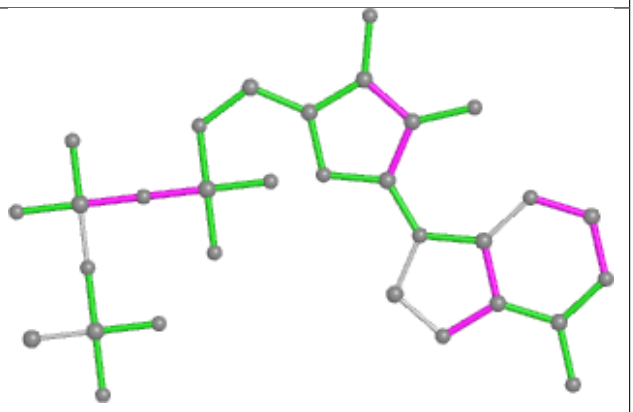


Rings

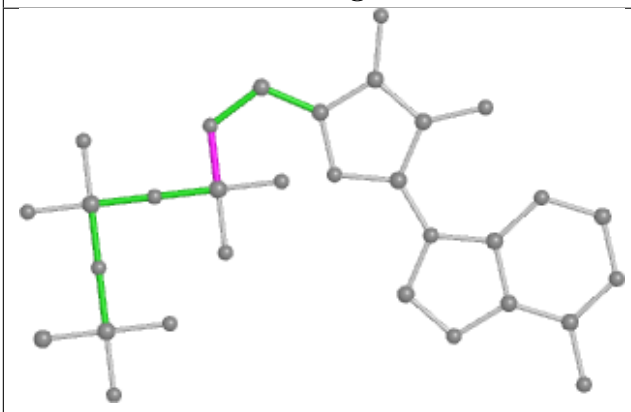
Ligand AGS P 701



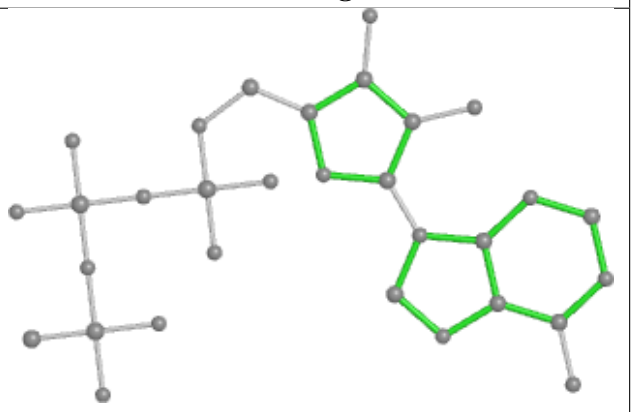
Bond lengths



Bond angles

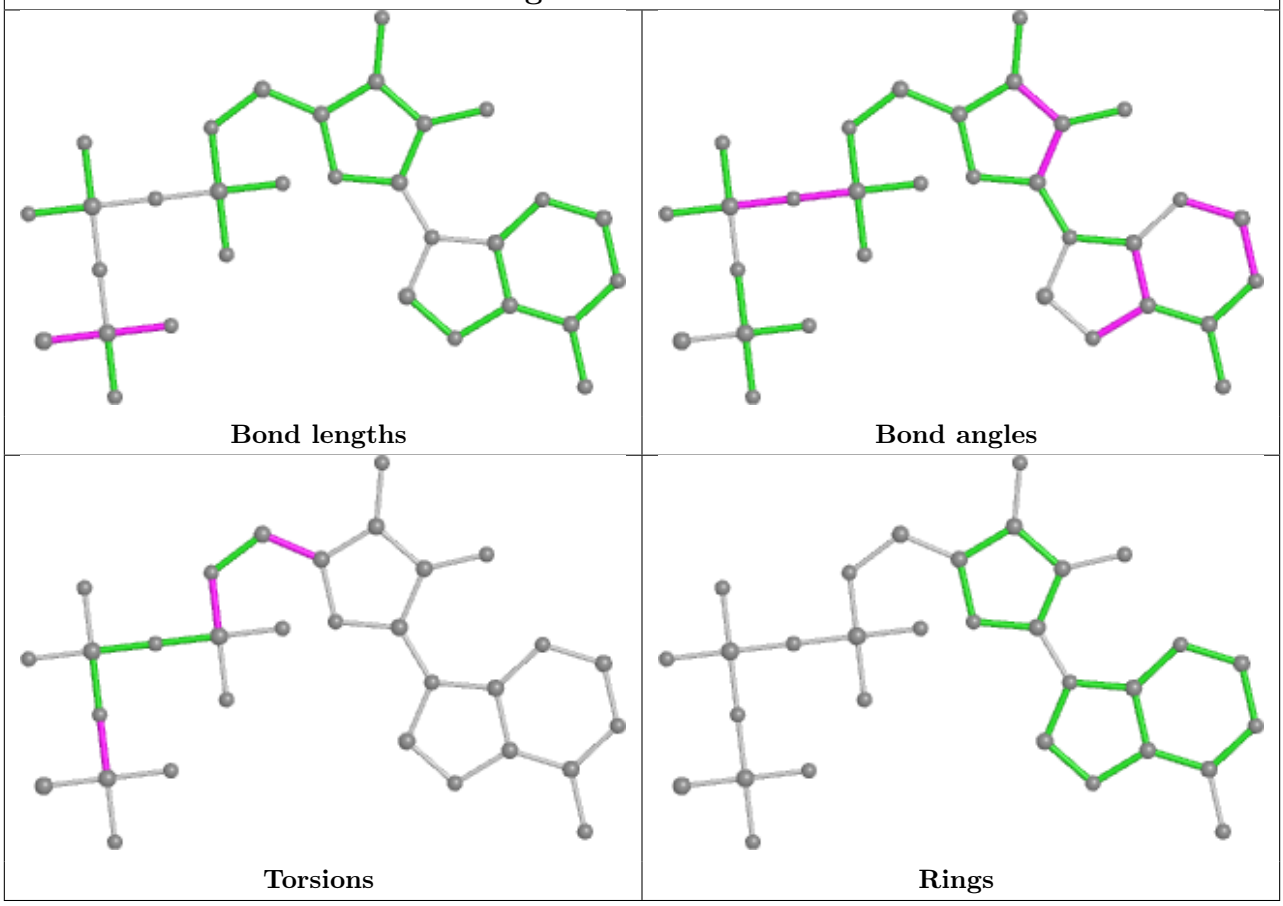


Torsions



Rings

Ligand AGS R 701



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.

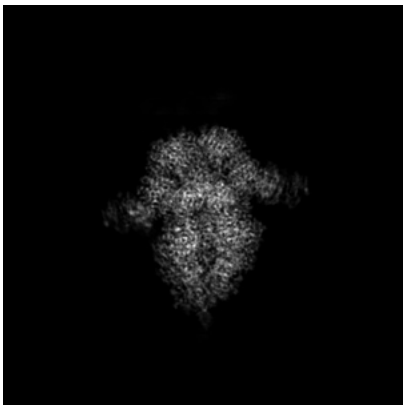
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60129. These allow visual inspection of the internal detail of the map and identification of artifacts.

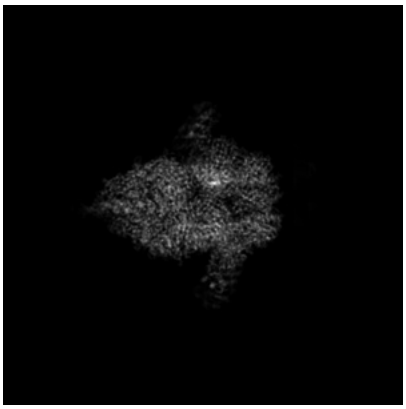
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

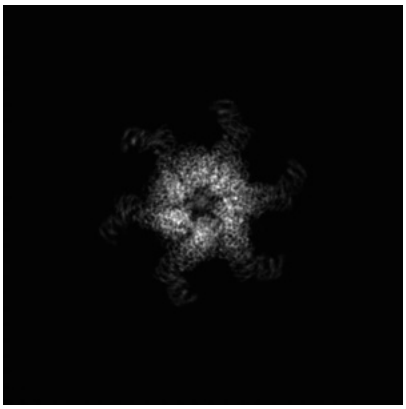
6.1.1 Primary map



X

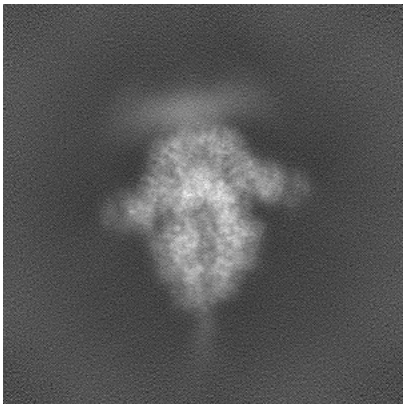


Y

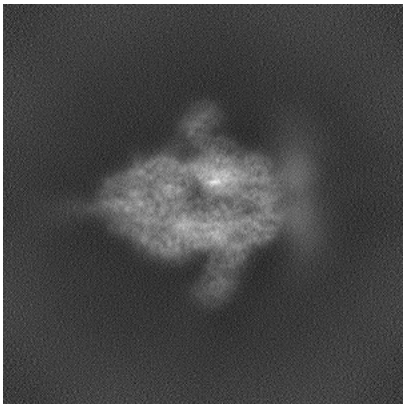


Z

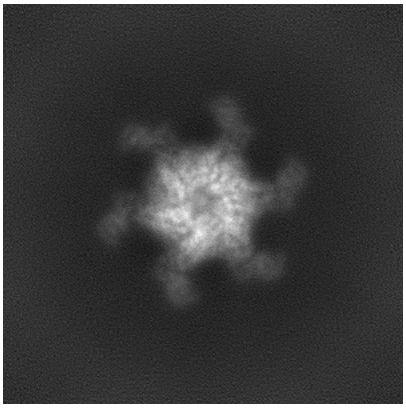
6.1.2 Raw map



X



Y



Z

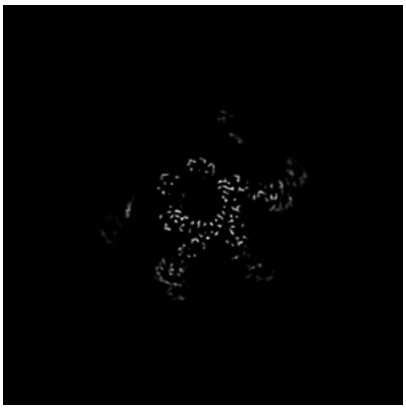
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

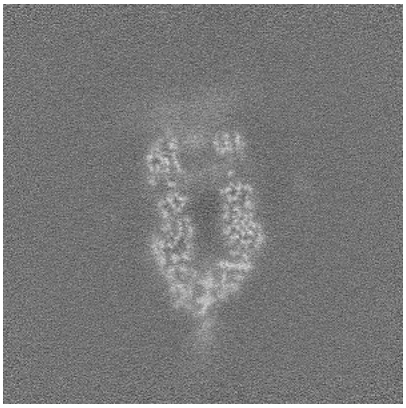
X Index: 240

Y Index: 240

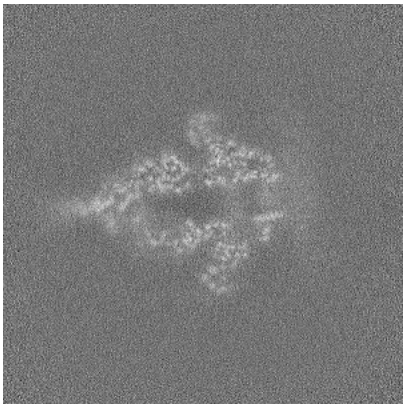


Z Index: 240

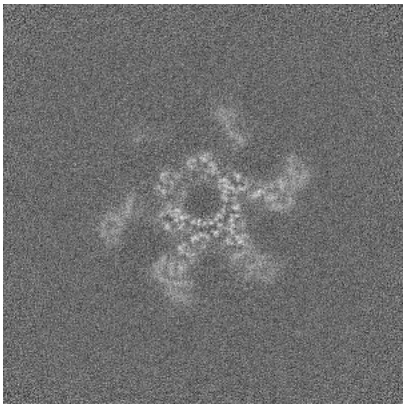
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

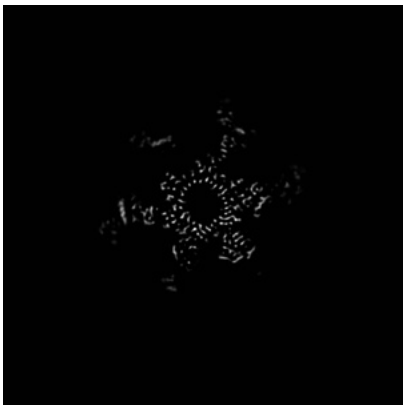
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

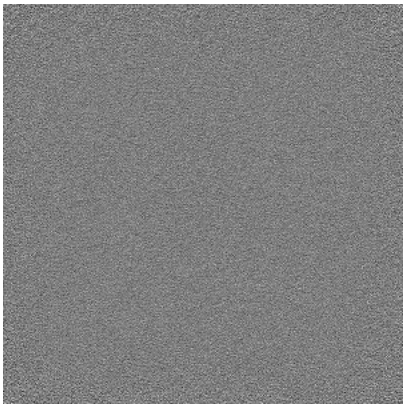
X Index: 267

Y Index: 222

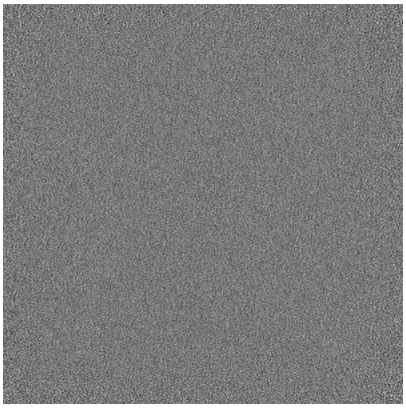


Z Index: 251

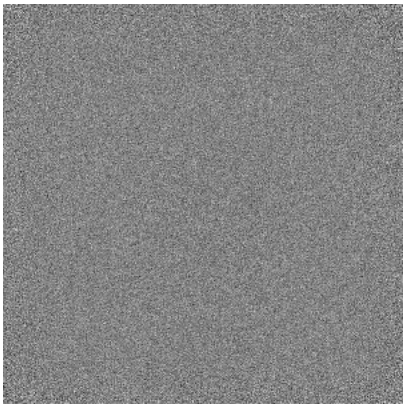
6.3.2 Raw map



X Index: 0



Y Index: 0

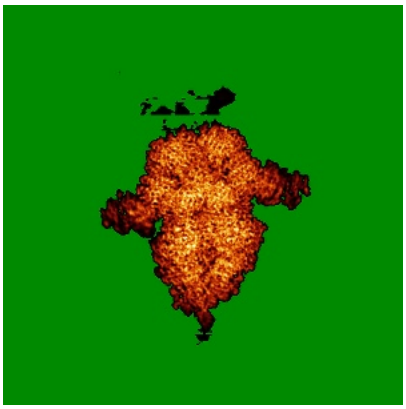


Z Index: 479

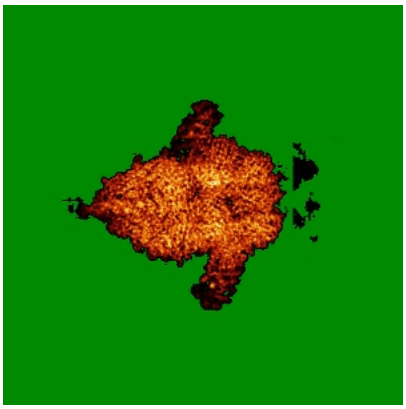
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

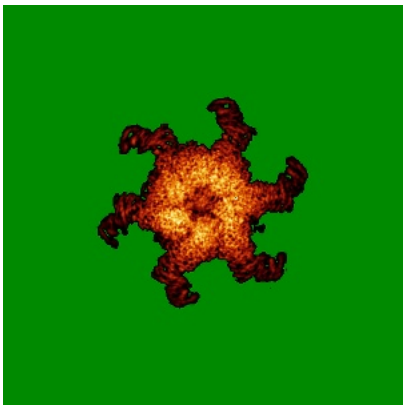
6.4.1 Primary map



X

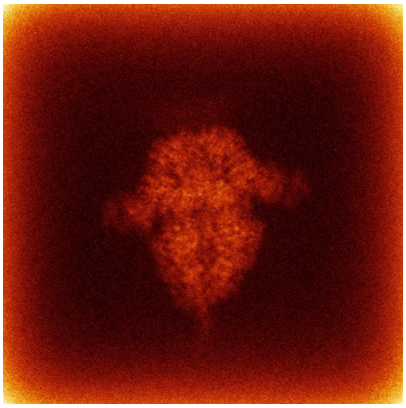


Y

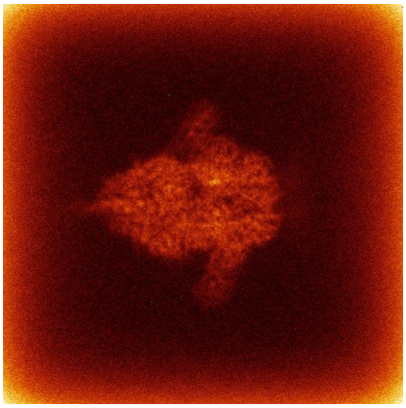


Z

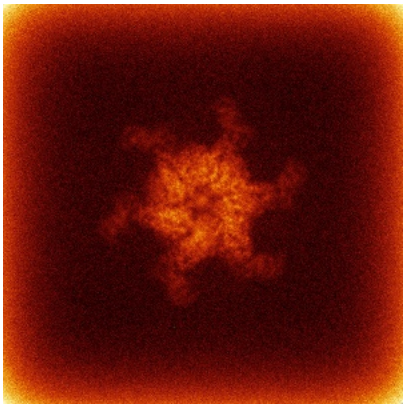
6.4.2 Raw map



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.

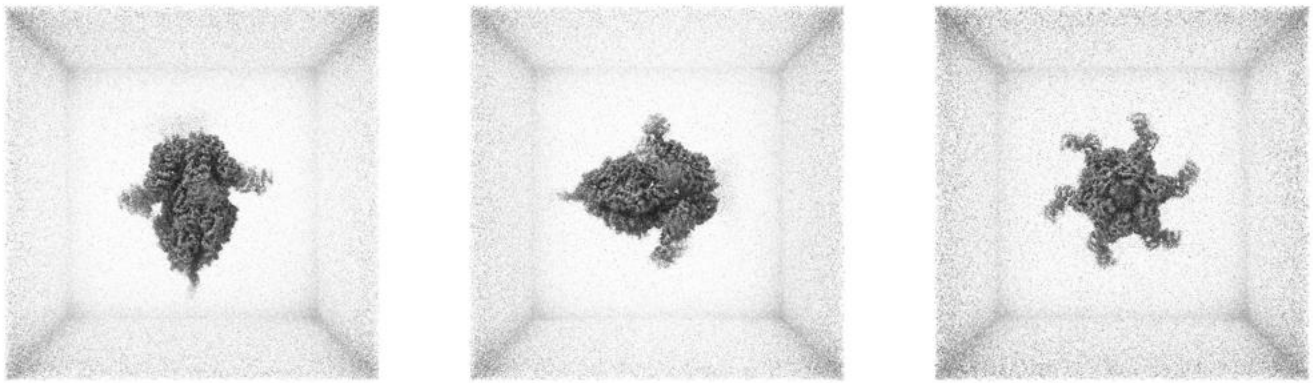
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0121. 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.

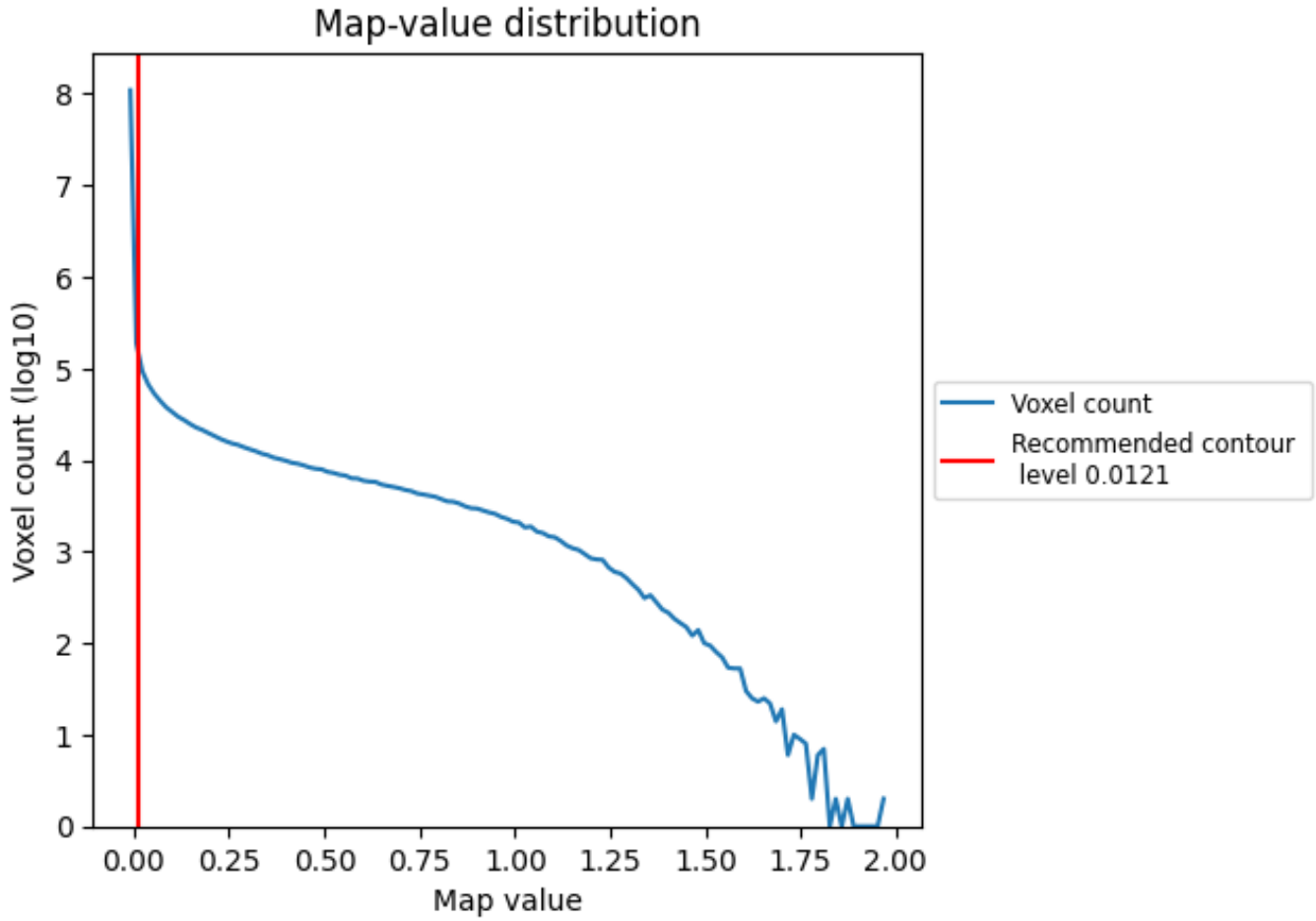
6.6 Mask visualisation (i)

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

7 Map analysis

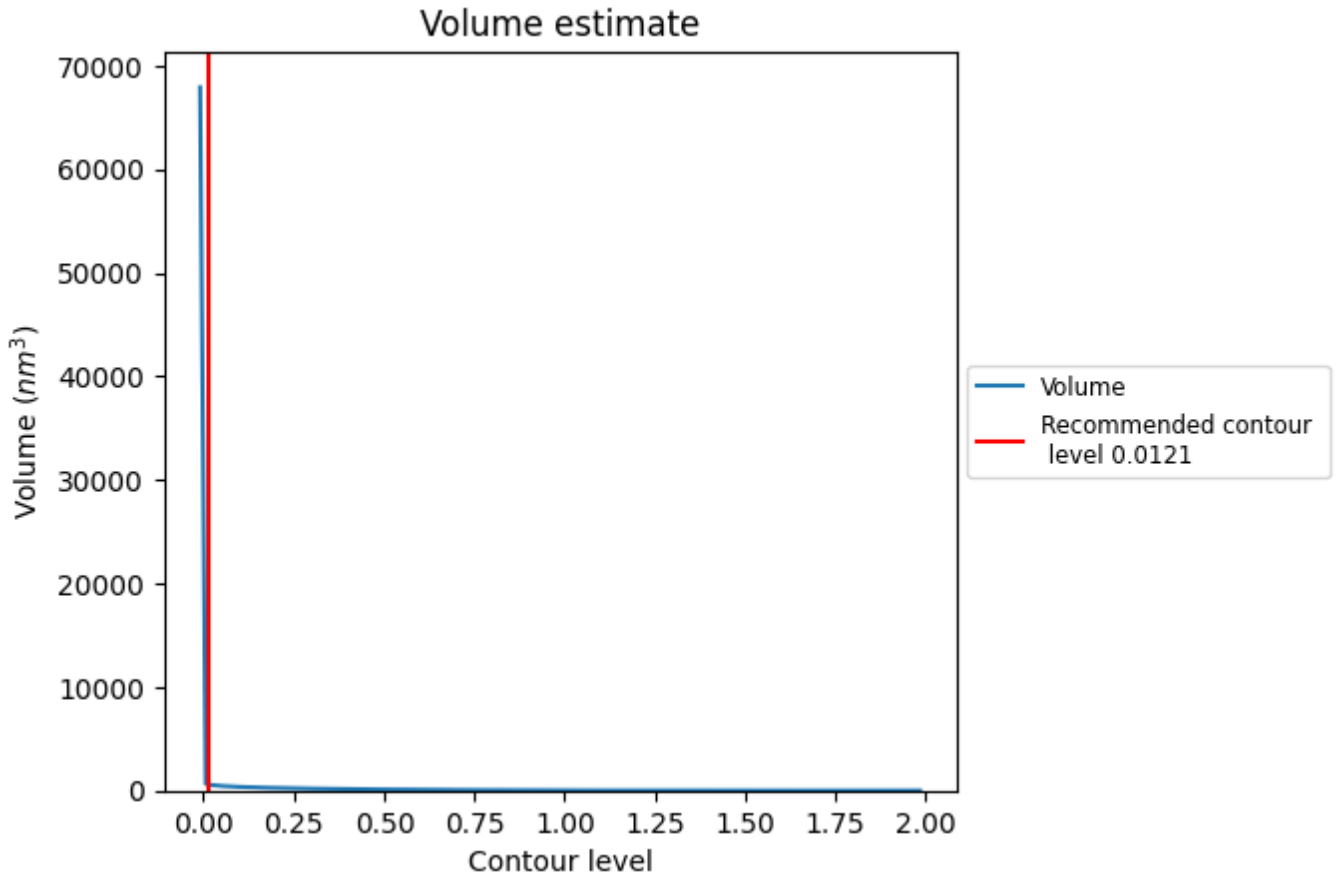
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

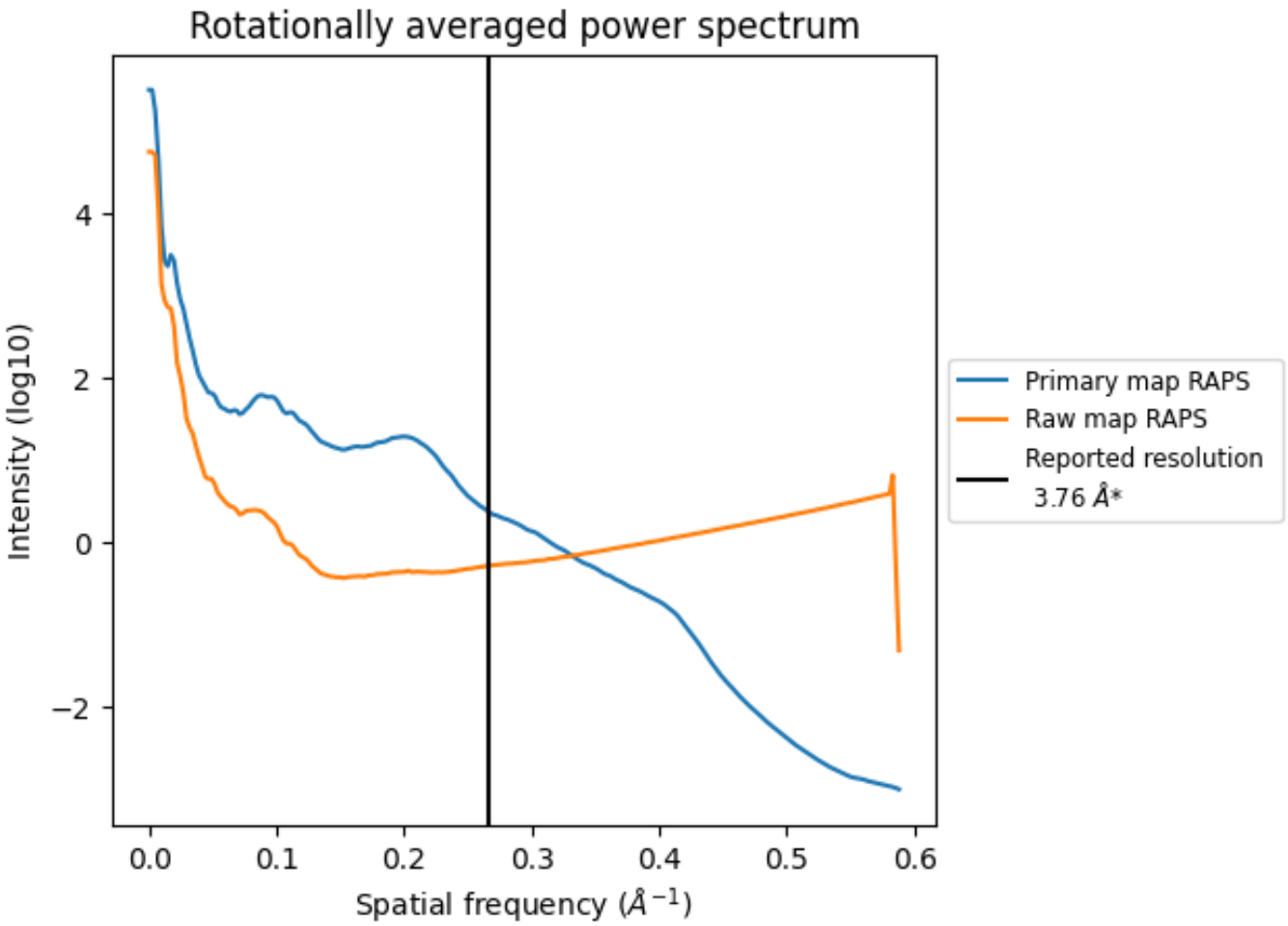
7.2 Volume estimate (i)



The volume at the recommended contour level is 610 nm^3; this corresponds to an approximate mass of 551 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 (i)

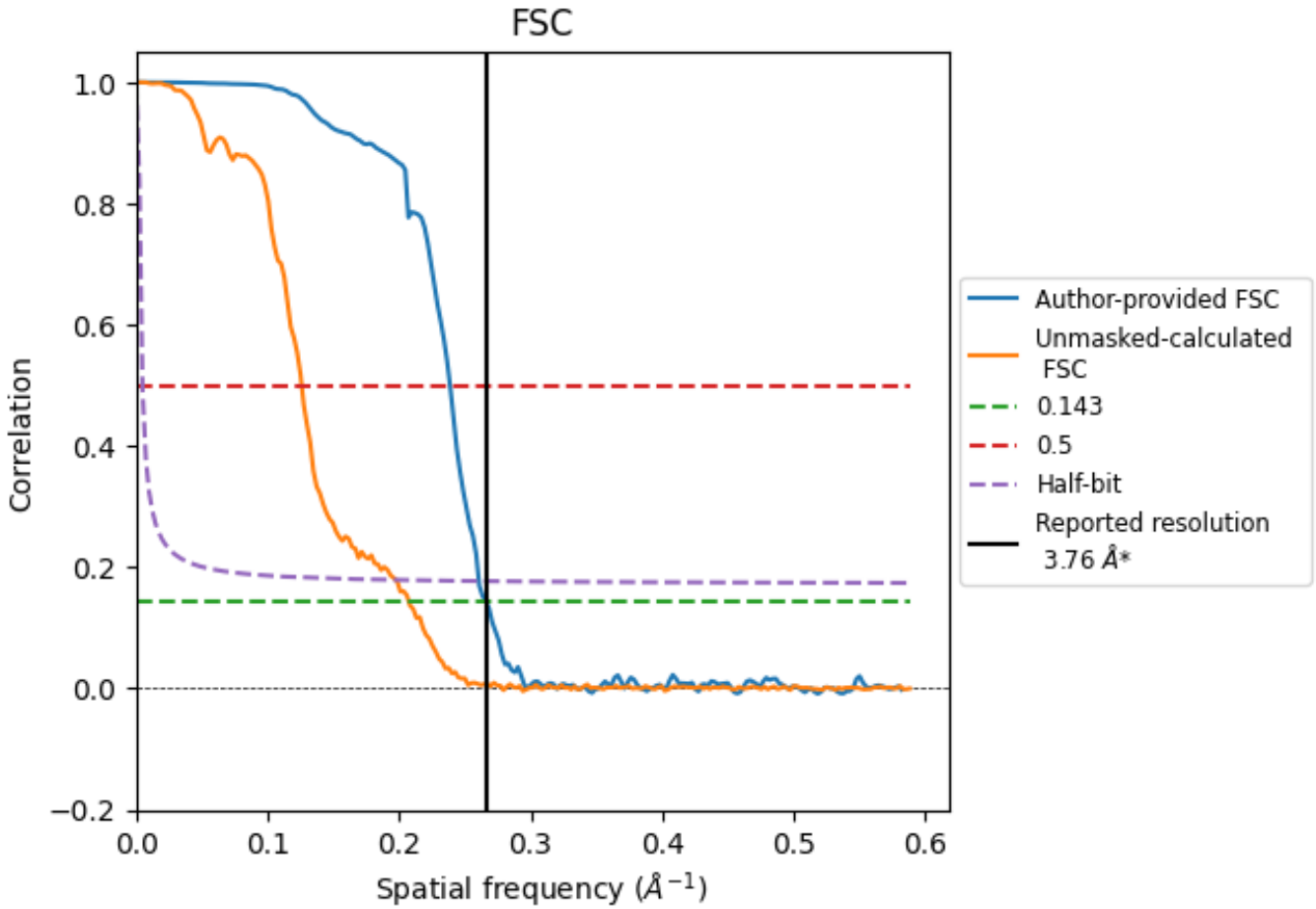


*Reported resolution corresponds to spatial frequency of 0.266 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.266 $Å^{-1}$

8.2 Resolution estimates (i)

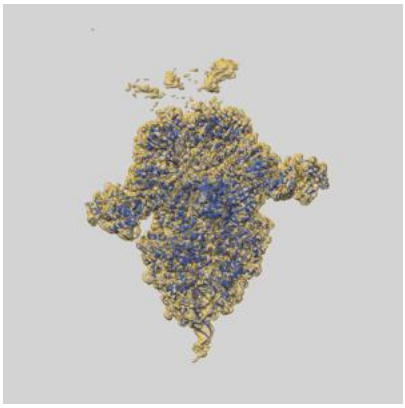
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.76	-	-
Author-provided FSC curve	3.76	4.19	3.84
Unmasked-calculated*	4.82	7.94	5.06

*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 4.82 differs from the reported value 3.76 by more than 10 %

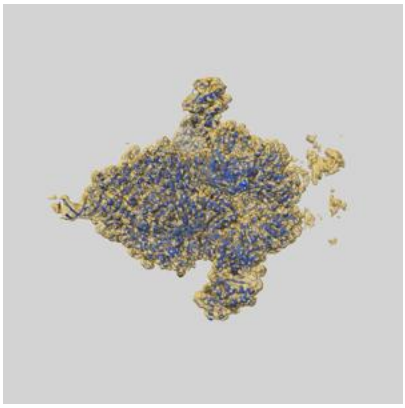
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-60129 and PDB model 8ZIT. Per-residue inclusion information can be found in section 3 on page 7.

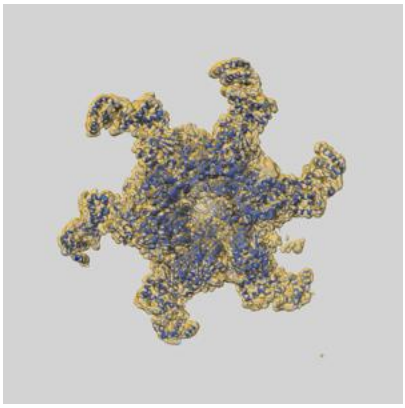
9.1 Map-model overlay



X



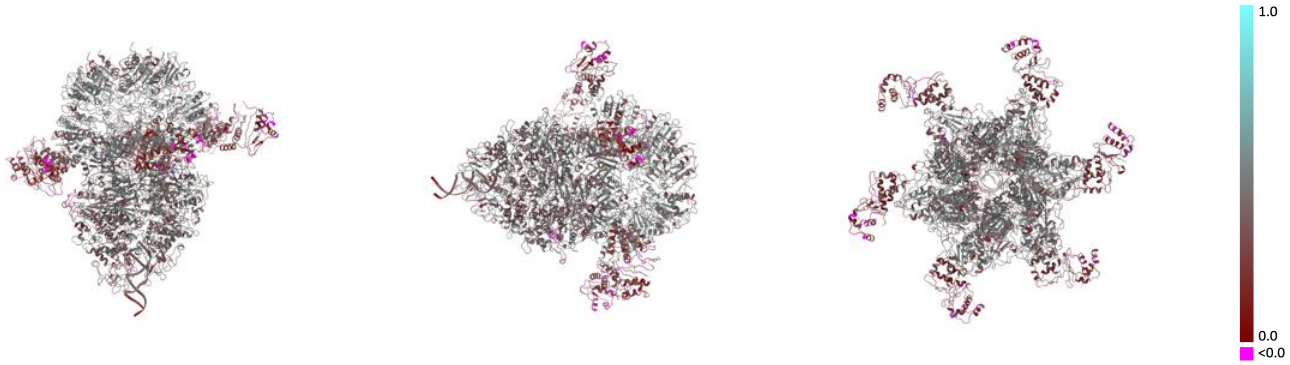
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0121 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.

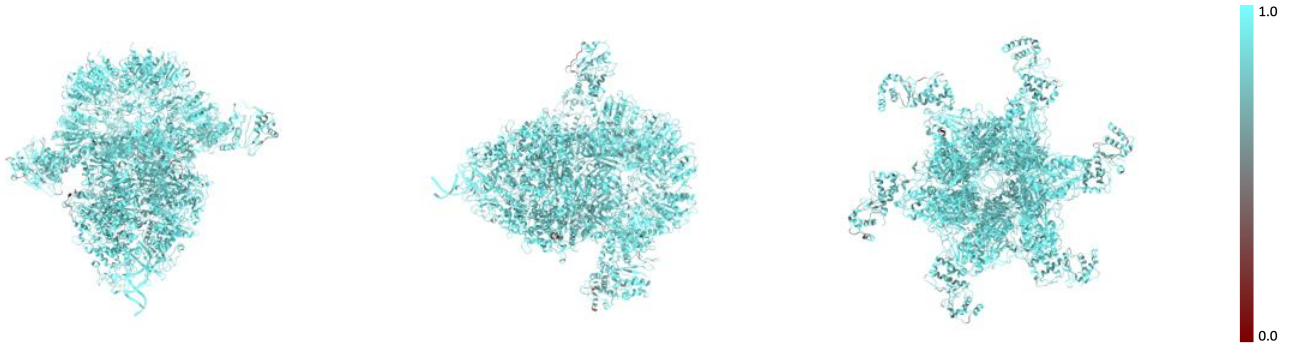
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

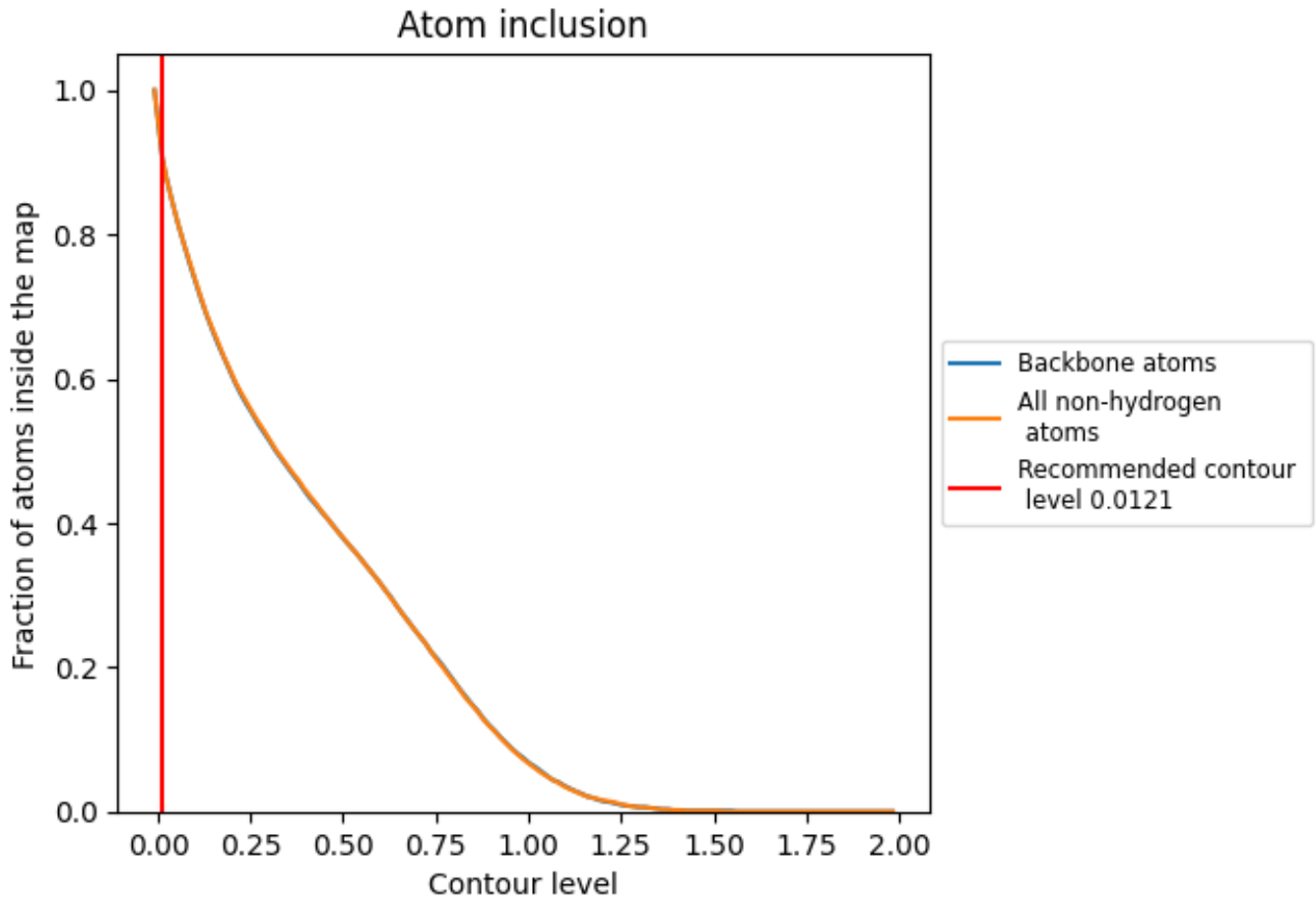
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0121).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.0121) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9070	0.3940
A	0.8730	0.3320
B	0.9440	0.4440
C	0.8870	0.3490
D	0.9310	0.4410
E	0.8830	0.3440
F	0.9340	0.4390
G	0.8710	0.3360
H	0.9390	0.4360
I	0.8740	0.3400
J	0.9280	0.4370
K	0.8920	0.3530
L	0.9370	0.4420
M	0.9500	0.4420
N	0.9360	0.4270
O	0.9170	0.4040
P	0.9220	0.4040
Q	0.9160	0.3990
R	0.9310	0.4270
U	0.9760	0.3410
V	0.9540	0.3340