Full wwPDB EM Validation Report

Sep 4, 2024 – 04:38 PM EDT

PDB ID	:	9C57
EMDB ID	:	EMD-45206
Title	:	Reconstituted P400 Subcomplex of the human TIP60 complex
Authors	:	Yang, Z.; Mameri, A.; Florez Ariza, A.J.; Cote, J.; Nogales, E.
Deposited on	:	2024-06-05
Resolution	:	2.75 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:

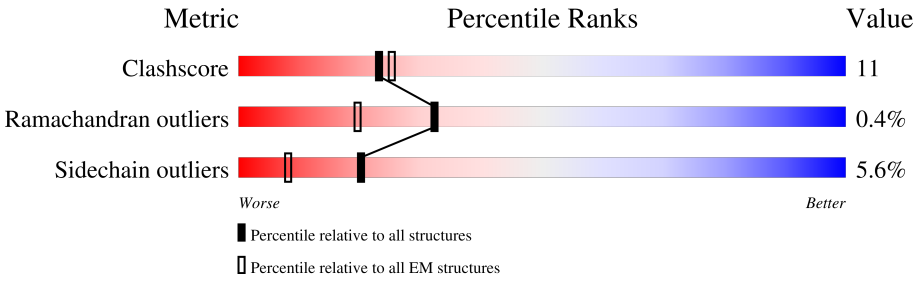
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 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	456	67% 22% 9%
1	C	456	80% 12% 7%
1	E	456	80% 14%
2	H	836	94%
3	L	429	63% 27% 6%
3	M	429	5% 52% 21% 24%
4	B	463	67% 16% 16%
4	D	463	77% 16% 7%

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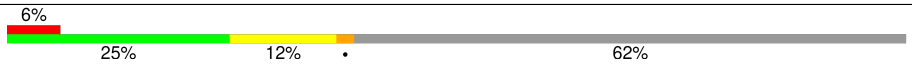
Mol	Chain	Length	Quality of chain
4	F	463	
5	G	3159	
6	I	467	
7	J	375	
8	K	364	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	AGS	D	501	-	-	X	-
9	AGS	F	501	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 77055 atoms, of which 38687 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 RuvB-like 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	E	437	Total	C	H	N	O	S	0	0
			6781	2111	3433	575	645	17		
1	C	425	Total	C	H	N	O	S	0	0
			6659	2064	3386	562	631	16		
1	A	416	Total	C	H	N	O	S	0	0
			6522	2017	3323	553	613	16		

- Molecule 2 is a protein called Enhancer of polycomb homolog 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	48	Total	C	H	N	O	S	0	0
			774	240	387	80	65	2		

- Molecule 3 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	M	324	Total	C	H	N	O	S	0	0
			5021	1608	2487	431	474	21		
3	L	404	Total	C	H	N	O	S	0	0
			6246	1990	3096	536	600	24		

- Molecule 4 is a protein called RuvB-like 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	B	389	Total	C	H	N	O	S	0	0
			6140	1899	3109	528	590	14		
4	D	431	Total	C	H	N	O	S	0	0
			6699	2082	3374	581	647	15		
4	F	431	Total	C	H	N	O	S	0	0
			6736	2085	3402	582	651	16		

- Molecule 5 is a protein called E1A-binding protein p400.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	G	878	14464	4555	7287	1291	1296	35	0	0

- Molecule 6 is a protein called DNA methyltransferase 1-associated protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	I	179	3012	972	1484	280	273	3	0	0

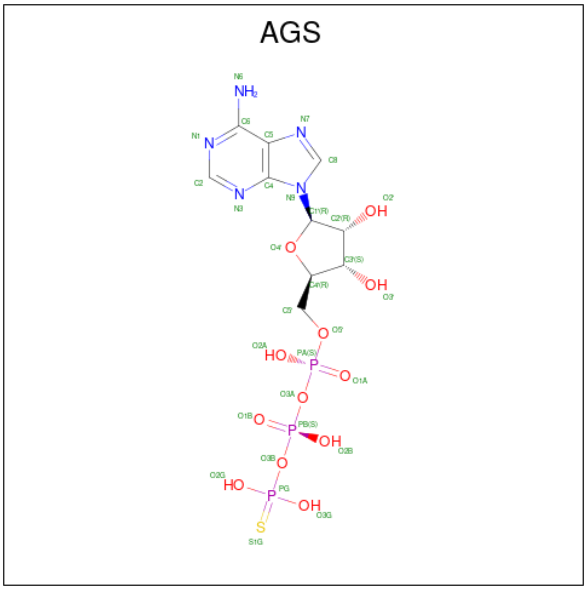
- Molecule 7 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	J	360	5602	1785	2788	471	538	20	0	0

- Molecule 8 is a protein called Vacuolar protein sorting-associated protein 72 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	K	123	2055	651	1035	183	183	3	0	0

- Molecule 9 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
			Total	C	H	N	O	P	S	
9	E	1	43	10	12	5	12	3	1	0

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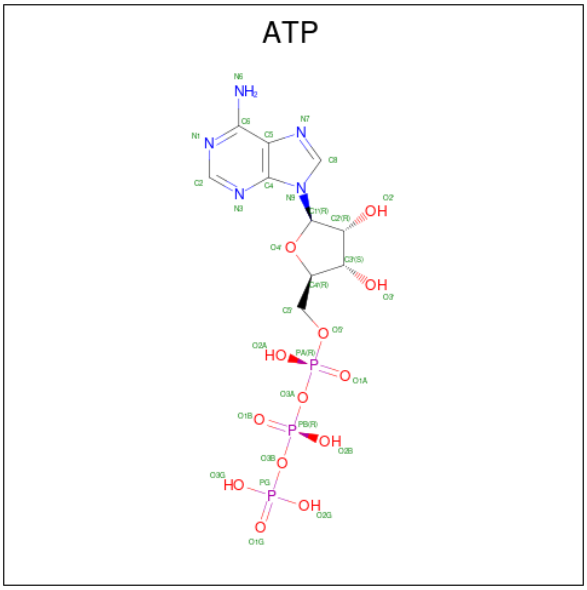
Mol	Chain	Residues	Atoms							AltConf
9	B	1	Total	C	H	N	O	P	S	0
			43	10	12	5	12	3	1	
9	C	1	Total	C	H	N	O	P	S	0
			43	10	12	5	12	3	1	
9	D	1	Total	C	H	N	O	P	S	0
			43	10	12	5	12	3	1	
9	F	1	Total	C	H	N	O	P	S	0
			43	10	12	5	12	3	1	
9	G	1	Total	C	H	N	O	P	S	0
			43	10	12	5	12	3	1	
9	A	1	Total	C	H	N	O	P	S	0
			43	10	12	5	12	3	1	

- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



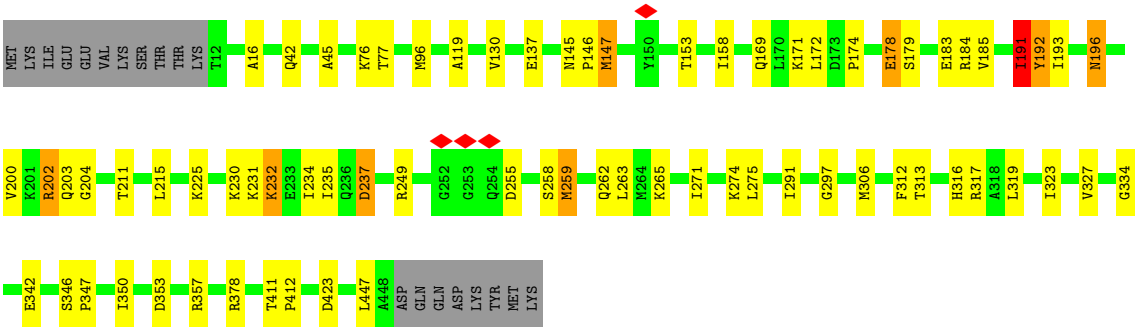
Mol	Chain	Residues	Atoms						AltConf
10	L	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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: RuvB-like 1

Chain E:

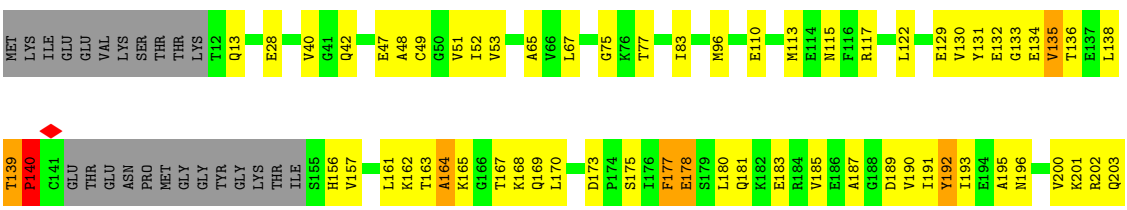


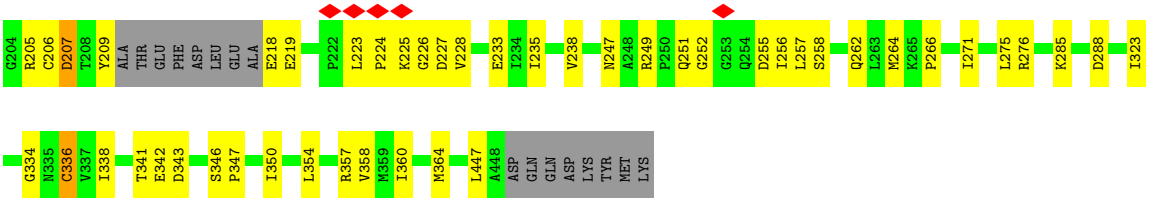
• Molecule 1: RuvB-like 1

Chain C:

• Molecule 1: RuvB-like 1

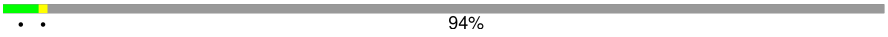
Chain A:

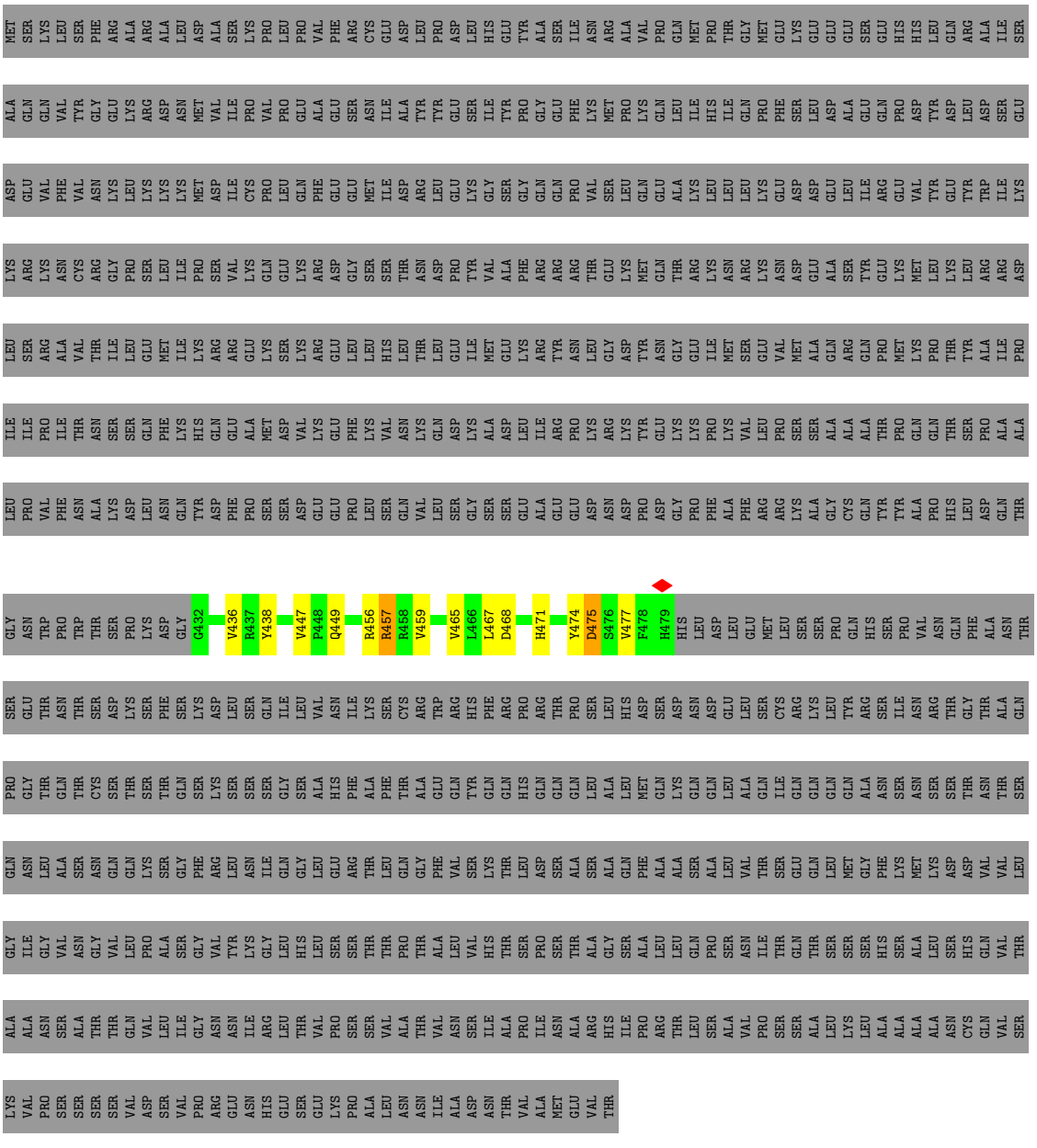




• Molecule 2: Enhancer of polycomb homolog 1

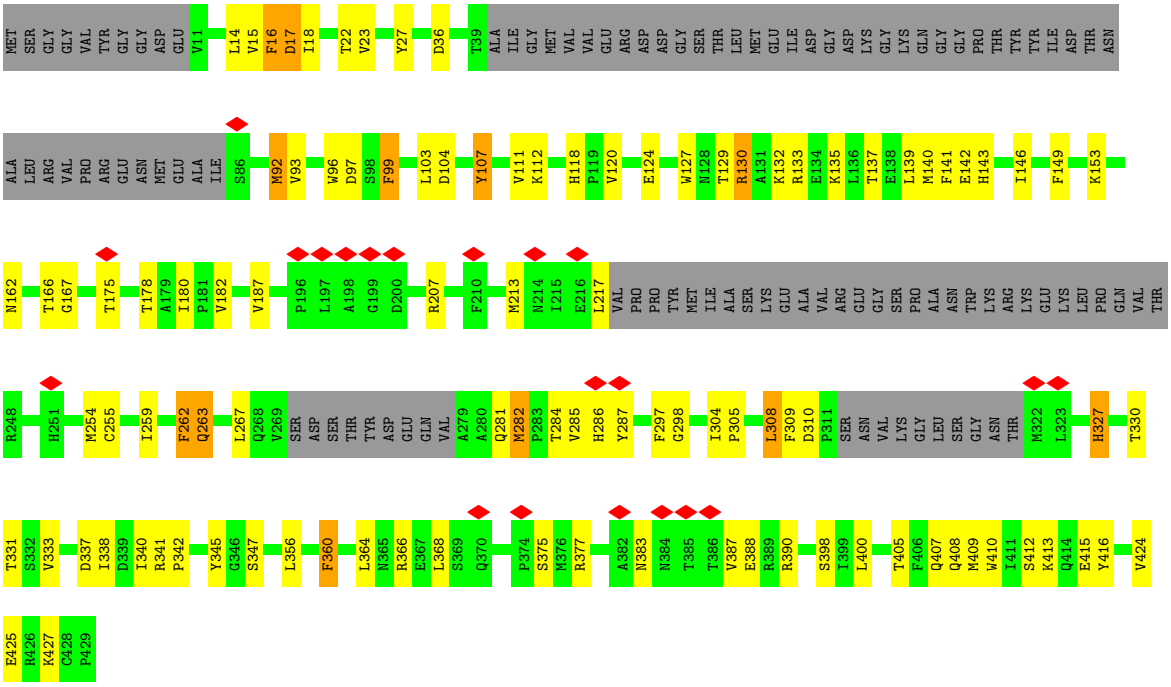
Chain H:





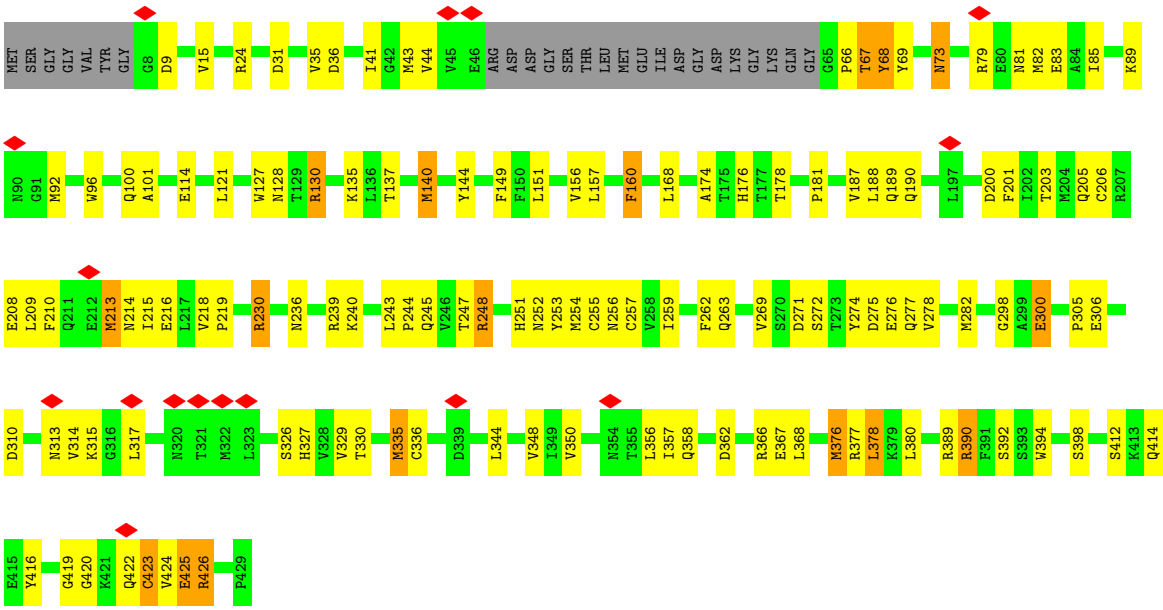
• Molecule 3: Actin-like protein 6A

Chain M:



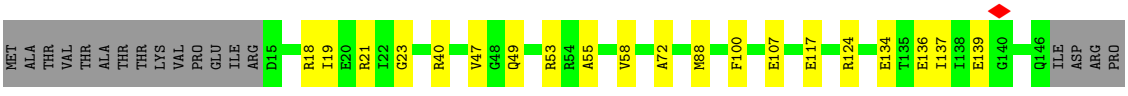
• Molecule 3: Actin-like protein 6A

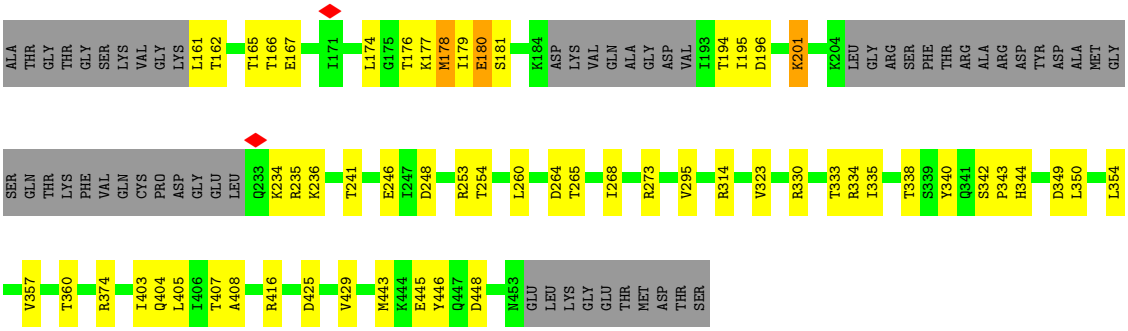
Chain L:



• Molecule 4: RuvB-like 2

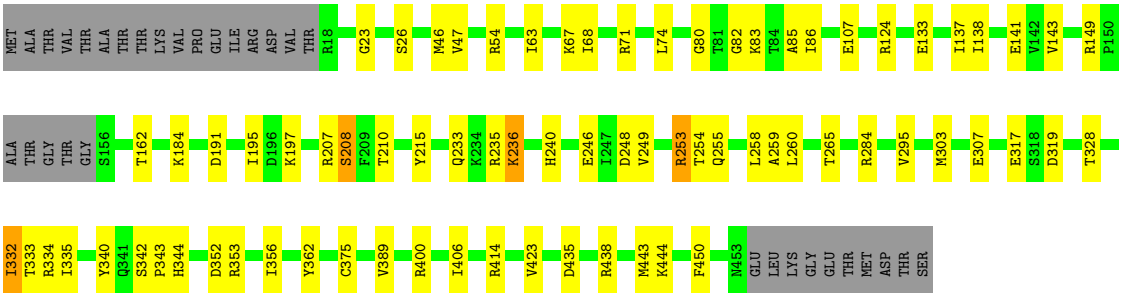
Chain B:





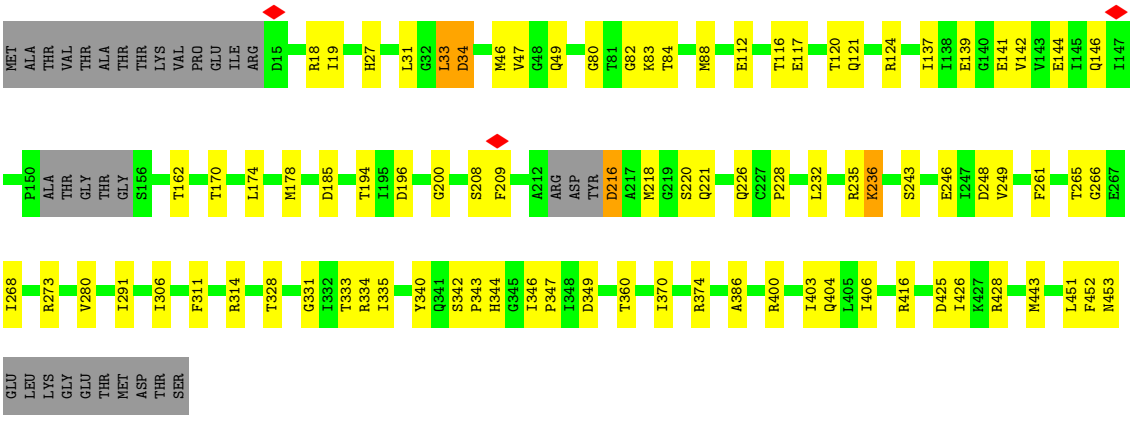
• Molecule 4: RuvB-like 2

Chain D:



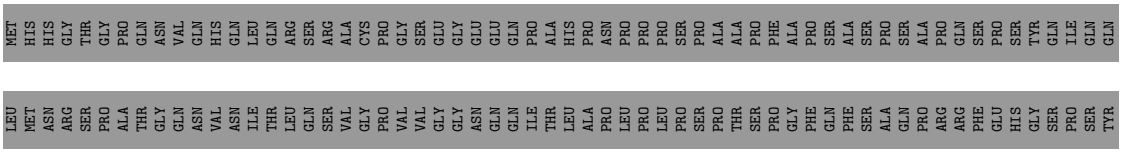
• Molecule 4: RuvB-like 2

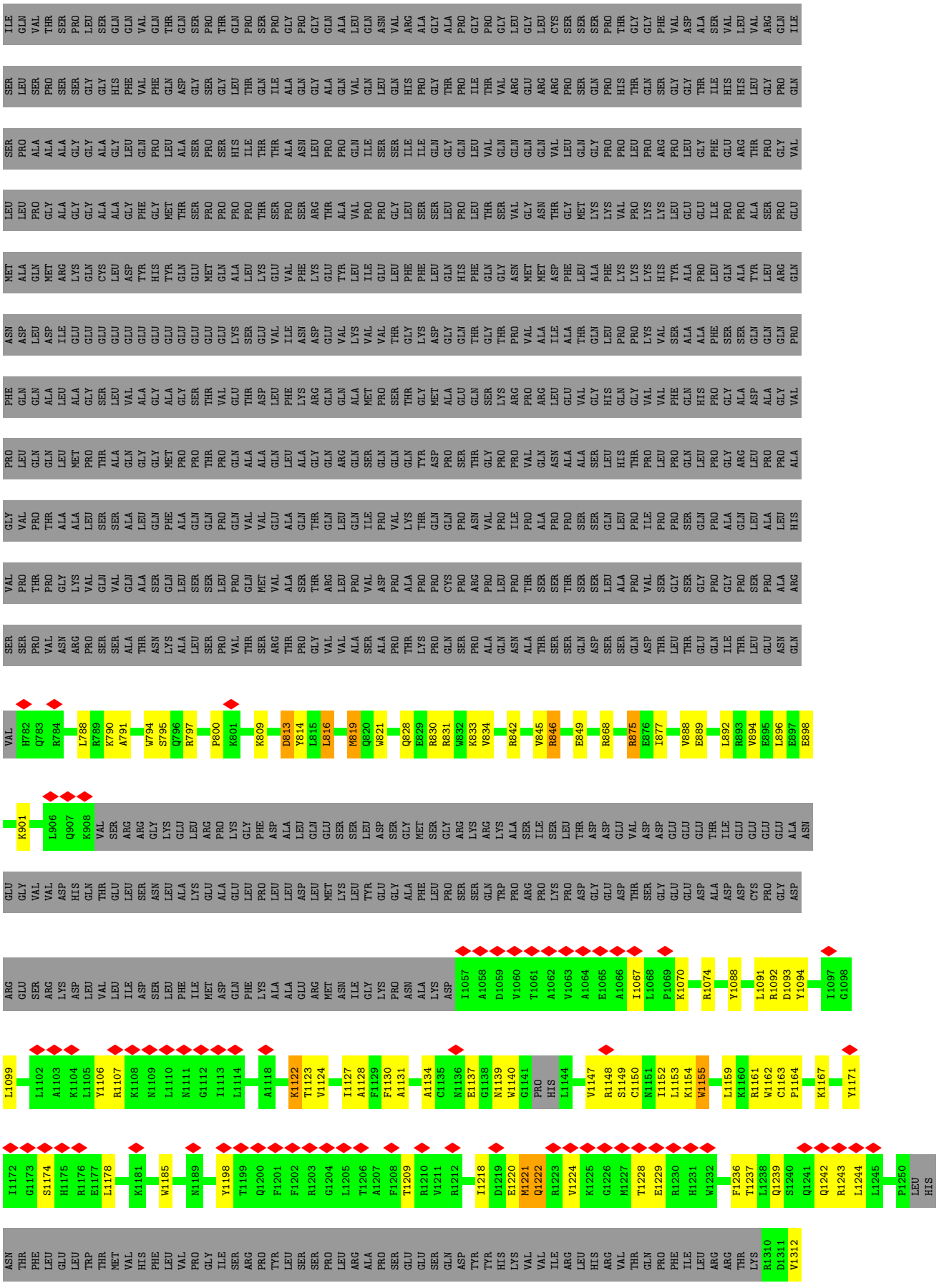
Chain F:

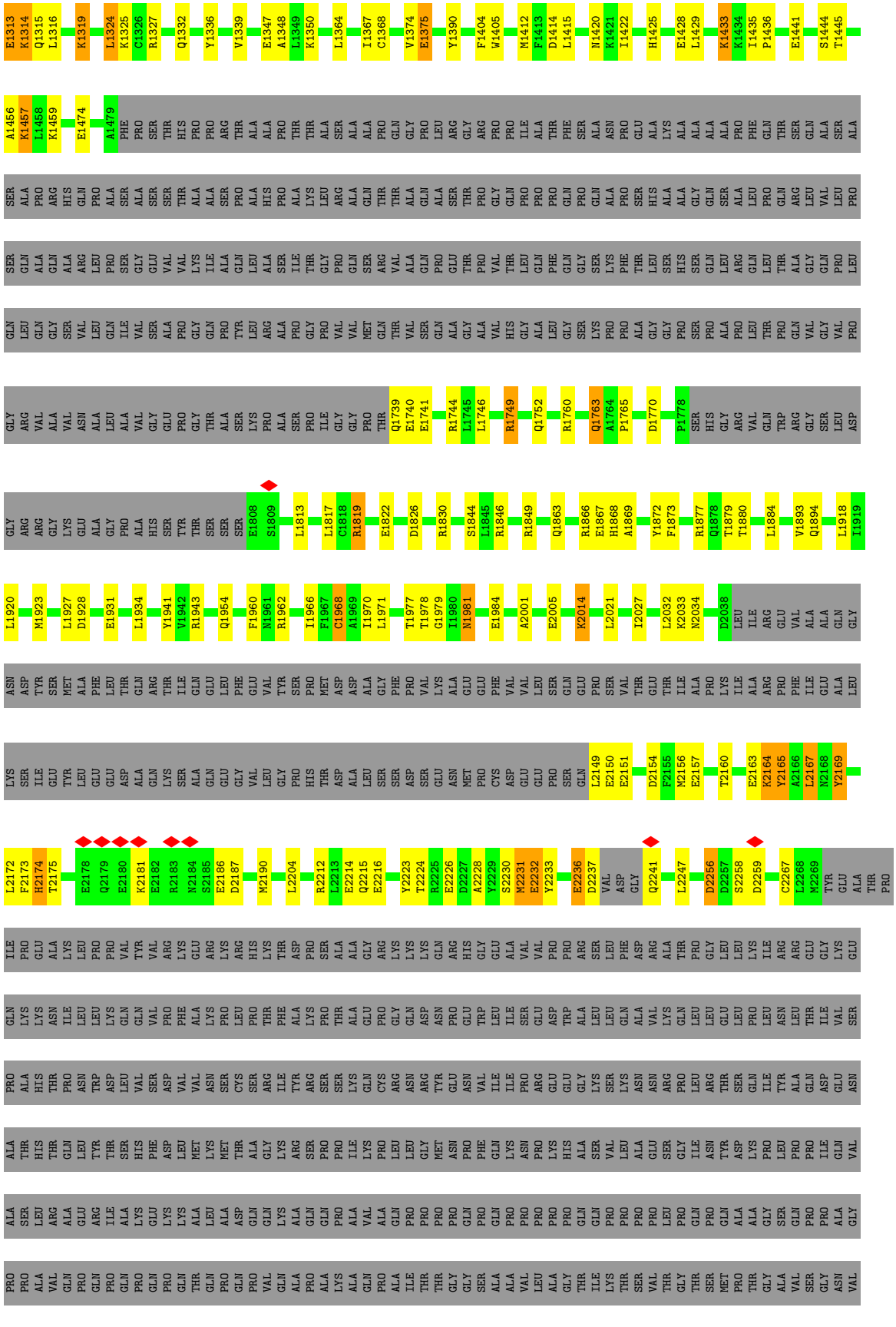


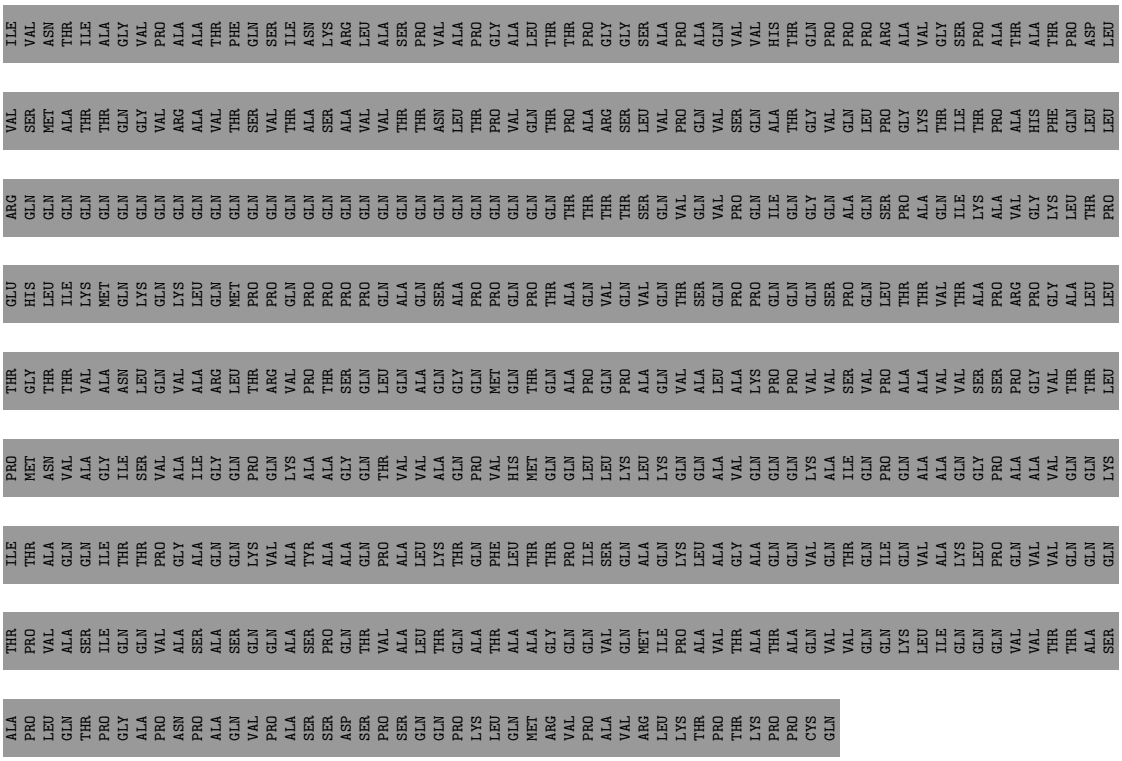
• Molecule 5: E1A-binding protein p400

Chain G:



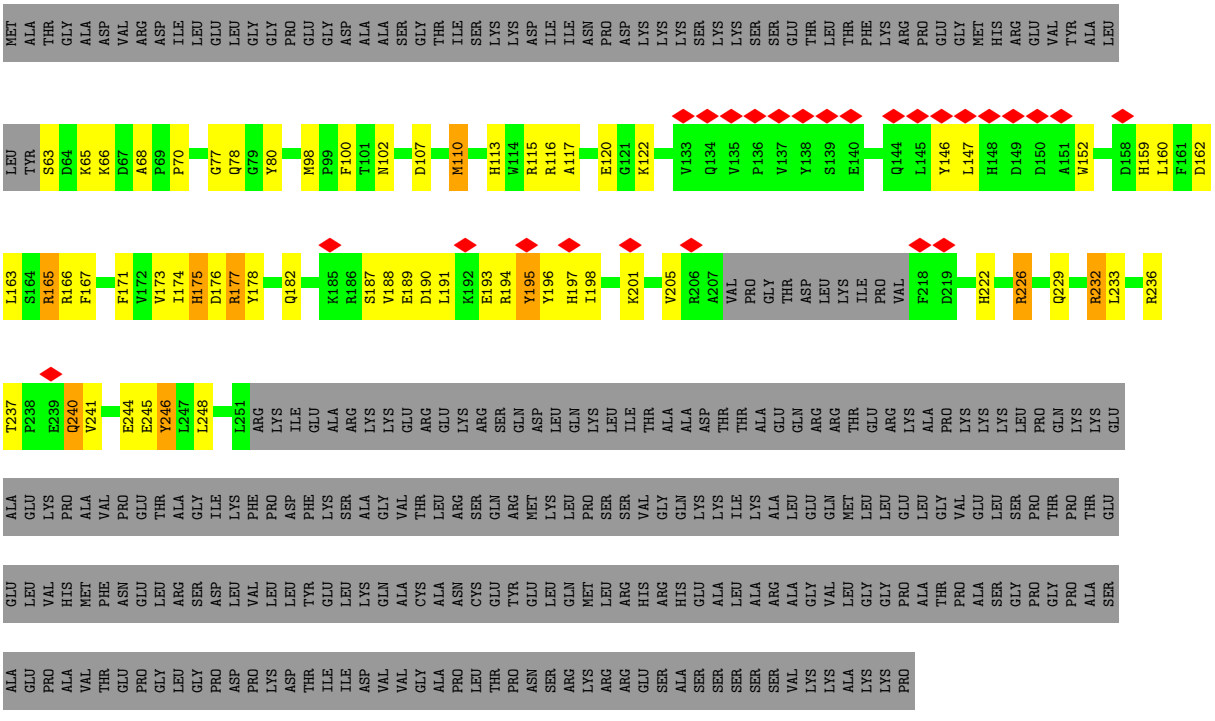



E1313 K1314 Q1315 L1316 K1319 L1324 K1325 C1326 R1327 Q1332 Y1336 V1339 E1347 A1348 L1349 K1350 L1364 I1367 C1368 V1374 E1375 Y1390 F1404 W1405 M1412 F1413 D1414 L1415 N1420 K1421 I1422 H1425 E1428 L1429 K1433 K1434 I1435 P1436 E1441 S1444 T1445
A1456 K1457 L1458 K1459 E1474 A1479
Q1739 E1740 E1741 R1744 L1745 L1746 R1749 Q1752 R1760 Q1763 A1764 P1765 D1770 P1778
E1808 S1809 L1813 L1817 C1818 R1819 E1822 D1826 R1830 S1844 L1845 R1846 R1849 Q1863 R1866 E1867 H1868 A1869 Y1872 F1873 R1877 Q1878 T1879 T1880 L1884 V1893 Q1894 L1918 I1919
L1920 M1923 L1927 D1928 E1931 L1934 Y1941 V1942 R1943 Q1954 F1960 N1961 R1962 I1966 F1967 C1968 A1969 I1970 L1971 T1977 T1978 G1979 I1980 N1981 E1984 A2001 E2005 K2014 L2021 I2027 L2032 K2033 N2034 D2038
L2149 E2150 E2151 D2154 F2155 M2156 E2157 T2160 E2163 K2164 Y2165 A2166 L2167 N2168 Y2169
L2172 F2173 H2174 T2175 E2178 Q2179 E2180 K2181 E2182 R2183 N2184 S2185 E2186 D2187 M2190 L2204 R2212 L2213 E2214 Q2215 E2216 Y2223 T2224 R2225 E2226 D2227 A2228 Y2229 S2230 M2231 E2232 Y2233 E2236 D2237 Q2241 L2247 D2256 D2257 S2258 D2259 C2267 L2268 M2269



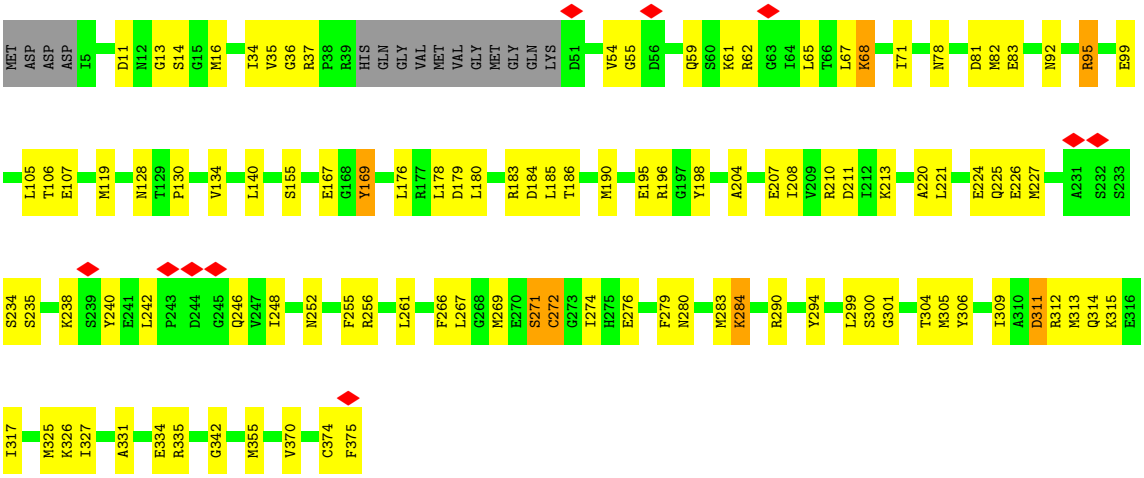
• Molecule 6: DNA methyltransferase 1-associated protein 1

Chain I:



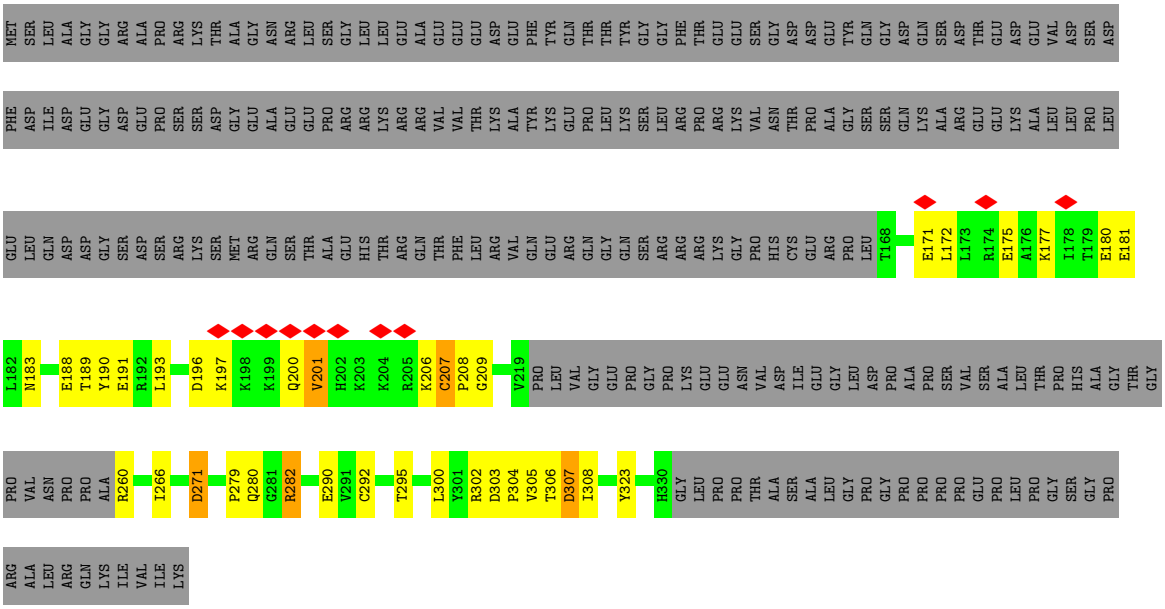
• Molecule 7: Actin, cytoplasmic 1

Chain J:



• Molecule 8: Vacuolar protein sorting-associated protein 72 homolog

Chain K:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	166442	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	21.007	Depositor
Minimum map value	-0.821	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.569	Depositor
Recommended contour level	2.4	Depositor
Map size (Å)	377.0, 377.0, 377.0	wwPDB
Map dimensions	377, 377, 377	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.32	1/3239 (0.0%)	0.59	3/4363 (0.1%)
1	C	0.28	0/3315	0.50	0/4468
1	E	0.54	5/3393 (0.1%)	0.57	2/4575 (0.0%)
2	H	0.27	0/394	0.67	0/529
3	L	0.29	0/3221	0.57	0/4367
3	M	0.27	0/2590	0.53	0/3504
4	B	0.27	0/3063	0.53	0/4121
4	D	0.29	0/3364	0.54	0/4531
4	F	0.28	0/3371	0.54	0/4538
5	G	0.28	0/7314	0.57	1/9868 (0.0%)
6	I	0.28	0/1570	0.61	0/2114
7	J	0.29	0/2875	0.57	0/3894
8	K	0.31	0/1045	0.58	0/1414
All	All	0.32	6/38754 (0.0%)	0.56	6/52286 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
3	L	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	204	GLY	C-O	-17.43	0.95	1.23
1	E	191	ILE	C-O	-11.96	1.00	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	204	GLY	CA-C	-8.00	1.39	1.51
1	A	140	PRO	CG-CD	-7.16	1.27	1.50
1	E	204	GLY	N-CA	-5.85	1.37	1.46
1	E	191	ILE	C-N	-5.30	1.21	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	140	PRO	N-CD-CG	-11.58	85.83	103.20
1	A	140	PRO	CA-CB-CG	-10.74	83.58	104.00
1	A	140	PRO	N-CA-CB	-8.05	93.64	103.30
1	E	192	TYR	CA-CB-CG	7.59	127.83	113.40
5	G	2027	ILE	CG1-CB-CG2	6.78	126.31	111.40
1	E	192	TYR	CA-C-O	5.56	131.78	120.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	THR	Peptide
1	E	202	ARG	Sidechain
3	L	67	THR	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	3199	3323	3317	91	0
1	C	3273	3386	3383	47	0
1	E	3348	3433	3447	60	0
2	H	387	387	386	13	0
3	L	3150	3096	3089	104	0
3	M	2534	2487	2482	74	0
4	B	3031	3109	3103	56	0
4	D	3325	3374	3370	65	0
4	F	3334	3402	3394	71	0
5	G	7177	7287	7306	187	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	1528	1484	1481	56	0
7	J	2814	2788	2785	82	0
8	K	1020	1035	1033	42	0
9	A	31	12	12	4	0
9	B	31	12	12	3	0
9	C	31	12	12	7	0
9	D	31	12	12	11	0
9	E	31	12	12	3	0
9	F	31	12	12	12	0
9	G	31	12	12	4	0
10	L	31	12	12	1	0
All	All	38368	38687	38672	842	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 11.

All (842) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:337:ASP:OD1	3:M:338:ILE:N	2.02	0.90
5:G:1984:GLU:OE1	5:G:1984:GLU:N	2.05	0.90
1:C:76:LYS:NZ	9:C:501:AGS:S1G	2.43	0.90
5:G:800:PRO:O	6:I:226:ARG:NH2	2.05	0.89
3:L:114:GLU:N	3:L:114:GLU:OE1	2.05	0.89
1:A:163:THR:O	1:A:165:LYS:N	2.06	0.89
3:M:207:ARG:NH1	3:M:255:CYS:SG	2.46	0.88
6:I:165:ARG:NE	6:I:165:ARG:O	2.06	0.87
1:A:135:VAL:HG23	1:A:161:LEU:CD2	2.05	0.86
7:J:155:SER:OG	7:J:304:THR:OG1	1.94	0.85
8:K:279:PRO:O	8:K:282:ARG:NH2	2.08	0.85
6:I:194:ARG:O	6:I:194:ARG:NH1	2.09	0.85
7:J:334:GLU:OE2	7:J:334:GLU:N	2.08	0.85
5:G:1752:GLN:NE2	1:A:196:ASN:OD1	2.10	0.84
5:G:1741:GLU:OE1	5:G:1741:GLU:N	2.10	0.84
7:J:235:SER:O	7:J:238:LYS:NZ	2.10	0.84
7:J:186:THR:OG1	7:J:213:LYS:NZ	2.13	0.82
4:D:400:ARG:NH1	9:D:501:AGS:O2A	2.11	0.82
5:G:2226:GLU:OE2	5:G:2226:GLU:N	2.10	0.82
5:G:1154:LYS:NZ	9:G:3201:AGS:O3G	2.13	0.81
5:G:1149:SER:O	5:G:1152:ILE:HG23	1.81	0.81
9:E:501:AGS:S1G	4:F:314:ARG:NH1	2.54	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:1315:GLN:N	5:G:1315:GLN:OE1	2.14	0.80
5:G:830:ARG:NH1	3:L:31:ASP:OD1	2.15	0.79
5:G:1819:ARG:NE	5:G:1822:GLU:OE1	2.16	0.78
7:J:224:GLU:OE1	7:J:224:GLU:N	2.14	0.78
1:C:401:THR:O	1:C:402:THR:HG23	1.86	0.76
9:D:501:AGS:O2A	9:D:501:AGS:O2G	2.04	0.76
4:F:84:THR:OG1	9:F:501:AGS:O2B	2.00	0.76
3:L:254:MET:SD	3:L:255:CYS:N	2.58	0.76
1:A:255:ASP:OD1	1:A:256:ILE:N	2.19	0.76
3:M:412:SER:N	3:M:415:GLU:OE1	2.18	0.76
4:D:124:ARG:NE	4:D:248:ASP:OD2	2.19	0.75
5:G:1221:MET:SD	5:G:1222:GLN:N	2.60	0.75
4:D:82:GLY:HA3	9:D:501:AGS:H2	1.68	0.74
1:E:76:LYS:NZ	9:E:501:AGS:O3G	2.21	0.74
5:G:846:ARG:NH1	5:G:2214:GLU:OE1	2.20	0.74
5:G:2163:GLU:OE2	5:G:2163:GLU:N	2.21	0.74
5:G:1164:PRO:O	8:K:183:ASN:ND2	2.21	0.74
1:C:189:ASP:OD2	1:C:202:ARG:NH1	2.20	0.74
6:I:78:GLN:N	6:I:78:GLN:OE1	2.21	0.73
3:L:206:CYS:HB2	3:L:259:ILE:HD11	1.70	0.73
5:G:1441:GLU:O	5:G:1445:THR:HG23	1.89	0.72
2:H:465:VAL:O	5:G:2223:TYR:OH	2.06	0.72
3:L:79:ARG:NH1	3:L:82:MET:SD	2.63	0.71
4:F:216:ASP:OD1	4:F:216:ASP:N	2.24	0.71
1:E:342:GLU:OE2	1:E:342:GLU:N	2.22	0.71
1:A:75:GLY:N	9:A:501:AGS:O1B	2.24	0.71
4:D:141:GLU:OE2	4:D:208:SER:OG	2.07	0.71
6:I:107:ASP:OD1	3:L:414:GLN:NE2	2.24	0.70
1:C:17:SER:O	9:C:501:AGS:O3'	2.08	0.70
1:A:135:VAL:HG23	1:A:161:LEU:HD22	1.73	0.70
1:C:20:HIS:HB3	1:C:381:THR:HG21	1.72	0.70
3:M:408:GLN:OE1	3:M:408:GLN:N	2.25	0.70
4:D:85:ALA:N	9:D:501:AGS:O2B	2.24	0.69
4:F:400:ARG:NH2	9:F:501:AGS:O3G	2.25	0.69
6:I:167:PHE:CD2	6:I:173:VAL:HG12	2.28	0.69
4:F:428:ARG:NH2	1:A:47:GLU:OE1	2.25	0.69
9:C:501:AGS:O2B	9:C:501:AGS:O1A	2.11	0.69
3:L:190:GLN:N	3:L:190:GLN:OE1	2.26	0.69
1:C:73:GLY:N	9:C:501:AGS:O1B	2.26	0.68
5:G:1147:VAL:HB	5:G:1152:ILE:HG22	1.75	0.68
7:J:313:MET:O	7:J:317:ILE:HG22	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:22:THR:OG1	3:M:390:ARG:NH2	2.26	0.68
1:E:262:GLN:HE22	1:A:257:LEU:HD21	1.59	0.68
4:B:23:GLY:O	4:B:374:ARG:NH2	2.25	0.68
1:A:136:THR:HG21	1:A:185:VAL:CG1	2.24	0.68
2:H:438:TYR:HH	6:I:63:SER:N	1.92	0.67
9:A:501:AGS:O2B	9:A:501:AGS:O1A	2.10	0.67
1:A:135:VAL:HG22	1:A:136:THR:HG23	1.77	0.67
1:E:171:LYS:NZ	5:G:2204:LEU:HD22	2.08	0.67
1:A:77:THR:N	9:A:501:AGS:O2B	2.28	0.67
4:F:400:ARG:NH2	9:F:501:AGS:O1B	2.27	0.67
3:M:16:PHE:HE1	3:M:120:VAL:HG13	1.60	0.67
5:G:819:MET:HE2	3:L:160:PHE:HA	1.77	0.66
1:E:137:GLU:OE2	1:E:169:GLN:NE2	2.27	0.66
3:M:127:TRP:CZ3	3:M:178:THR:HG21	2.31	0.66
6:I:165:ARG:C	6:I:165:ARG:HE	1.99	0.66
7:J:267:LEU:HD13	7:J:267:LEU:O	1.94	0.66
1:C:339:ARG:NH2	4:D:307:GLU:OE2	2.29	0.66
8:K:175:GLU:OE1	8:K:175:GLU:N	2.29	0.66
4:D:259:ALA:HB1	4:D:265:THR:HG23	1.77	0.66
4:B:314:ARG:NH2	9:A:501:AGS:S1G	2.69	0.65
1:E:265:LYS:NZ	4:F:112:GLU:OE2	2.29	0.65
4:B:166:THR:OG1	4:B:167:GLU:OE2	2.10	0.65
5:G:1122:LYS:NZ	9:G:3201:AGS:S1G	2.70	0.65
4:D:335:ILE:HD11	4:D:342:SER:HB3	1.79	0.65
1:E:263:LEU:HD11	1:A:264:MET:SD	2.37	0.64
5:G:1422:ILE:HG13	5:G:1765:PRO:HG3	1.79	0.64
5:G:1960:PHE:HA	5:G:1966:ILE:HD11	1.79	0.64
3:L:275:ASP:OD1	3:L:276:GLU:N	2.31	0.64
5:G:1236:PHE:O	5:G:1243:ARG:NH2	2.30	0.64
5:G:1740:GLU:N	5:G:1740:GLU:OE1	2.29	0.64
4:B:18:ARG:NH1	1:C:288:ASP:OD1	2.31	0.64
4:F:82:GLY:HA3	9:F:501:AGS:H2	1.80	0.64
5:G:1093:ASP:OD1	5:G:1094:TYR:N	2.31	0.64
1:E:271:ILE:HG23	1:E:275:LEU:HD23	1.79	0.64
7:J:59:GLN:O	7:J:62:ARG:NH1	2.30	0.64
7:J:211:ASP:OD2	7:J:240:TYR:OH	2.14	0.64
1:C:402:THR:HG21	4:D:352:ASP:OD2	1.98	0.63
1:C:353:ASP:OD1	1:C:353:ASP:N	2.32	0.63
7:J:92:ASN:O	7:J:95:ARG:NE	2.32	0.63
7:J:179:ASP:OD1	7:J:179:ASP:O	2.16	0.63
4:B:139:GLU:OE1	4:B:139:GLU:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:LEU:HD13	1:C:176:ILE:HG21	1.80	0.62
6:I:160:LEU:CD2	6:I:191:LEU:HD12	2.29	0.62
1:E:77:THR:OG1	4:F:314:ARG:NH2	2.31	0.62
3:M:162:ASN:OD1	5:G:2169:TYR:OH	2.15	0.62
1:A:169:GLN:OE1	1:A:169:GLN:N	2.31	0.62
7:J:283:MET:HA	7:J:283:MET:HE2	1.80	0.62
5:G:1107:ARG:NH1	5:G:1137:GLU:OE2	2.32	0.62
1:C:343:ASP:N	1:C:343:ASP:OD1	2.32	0.62
1:C:404:ARG:NH2	9:C:501:AGS:O3A	2.31	0.62
5:G:1457:LYS:HE2	5:G:1457:LYS:HA	1.82	0.62
6:I:240:GLN:OE1	6:I:240:GLN:O	2.17	0.62
5:G:2231:MET:O	5:G:2233:TYR:N	2.32	0.61
5:G:1934:LEU:HD11	5:G:1970:ILE:HD11	1.82	0.61
5:G:2230:SER:N	5:G:2232:GLU:OE2	2.28	0.61
1:E:237:ASP:N	1:E:237:ASP:OD1	2.33	0.61
5:G:1350:LYS:HE2	5:G:1350:LYS:HA	1.80	0.61
6:I:245:GLU:N	6:I:245:GLU:OE1	2.33	0.61
6:I:187:SER:N	6:I:190:ASP:OD2	2.32	0.61
9:E:501:AGS:O2B	9:E:501:AGS:O1A	2.17	0.61
3:L:213:MET:SD	3:L:215:ILE:HD12	2.41	0.61
7:J:71:ILE:HD11	7:J:82:MET:HE1	1.81	0.61
3:L:412:SER:O	3:L:416:TYR:N	2.30	0.61
4:D:80:GLY:N	9:D:501:AGS:S1G	2.73	0.61
1:A:110:GLU:OE2	1:A:117:ARG:NH2	2.34	0.61
1:A:96:MET:SD	1:A:115:ASN:ND2	2.69	0.61
3:L:15:VAL:HG22	3:L:121:LEU:HD21	1.82	0.61
3:M:282:MET:SD	3:M:282:MET:N	2.74	0.61
5:G:2236:GLU:N	5:G:2241:GLN:O	2.34	0.60
8:K:171:GLU:O	8:K:175:GLU:OE1	2.19	0.60
3:L:298:GLY:N	3:L:300:GLU:OE1	2.33	0.60
1:E:77:THR:HG21	4:F:314:ARG:HH21	1.65	0.60
4:D:47:VAL:N	9:D:501:AGS:HN61	1.99	0.60
3:L:24:ARG:NH1	3:L:390:ARG:O	2.34	0.60
1:E:178:GLU:OE2	4:D:149:ARG:NH2	2.34	0.60
5:G:1070:LYS:O	5:G:1074:ARG:N	2.33	0.60
3:L:245:GLN:N	3:L:245:GLN:OE1	2.35	0.60
3:M:141:PHE:O	3:M:413:LYS:NZ	2.35	0.60
5:G:1312:VAL:O	5:G:1312:VAL:HG13	2.02	0.59
3:L:358:GLN:N	3:L:358:GLN:OE1	2.34	0.59
1:A:140:PRO:O	1:A:140:PRO:HG2	2.02	0.59
1:A:168:LYS:HB2	1:A:228:VAL:HG11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:137:ILE:HG23	4:B:194:THR:HG21	1.85	0.59
2:H:447:VAL:HG21	5:G:2224:THR:HG21	1.84	0.59
4:D:389:VAL:HG21	4:D:423:VAL:HG23	1.84	0.59
5:G:1367:ILE:HG13	5:G:1374:VAL:HG11	1.84	0.59
2:H:459:VAL:HG23	5:G:2247:LEU:HD12	1.83	0.59
4:F:228:PRO:HA	5:G:1433:LYS:HE2	1.84	0.59
1:A:139:THR:HG22	1:A:140:PRO:CD	2.32	0.59
1:A:135:VAL:HG21	1:A:191:ILE:HG12	1.84	0.58
1:A:192:TYR:N	1:A:201:LYS:O	2.28	0.58
4:B:408:ALA:HB3	4:B:429:VAL:HG11	1.84	0.58
6:I:193:GLU:OE1	6:I:197:HIS:NE2	2.36	0.58
3:L:100:GLN:O	3:L:144:TYR:OH	2.19	0.58
4:F:331:GLY:O	4:F:343:PRO:O	2.21	0.58
7:J:299:LEU:HD12	7:J:304:THR:CG2	2.34	0.58
4:B:407:THR:HG21	1:C:61:MET:HG3	1.85	0.58
4:D:246:GLU:HA	4:D:260:LEU:HD21	1.85	0.58
2:H:475:ASP:N	2:H:475:ASP:OD1	2.35	0.58
4:B:265:THR:OG1	4:B:268:ILE:HD11	2.04	0.58
3:M:120:VAL:HG11	3:M:140:MET:CE	2.34	0.57
5:G:1174:SER:O	5:G:1178:LEU:N	2.35	0.57
6:I:175:HIS:CG	6:I:188:VAL:HG12	2.39	0.57
4:D:47:VAL:O	9:D:501:AGS:N6	2.37	0.57
4:D:259:ALA:CB	4:D:265:THR:HG23	2.33	0.57
1:E:158:ILE:HD13	1:E:171:LYS:HG3	1.87	0.57
4:D:83:LYS:NZ	9:D:501:AGS:S1G	2.77	0.57
5:G:819:MET:CE	3:L:160:PHE:HA	2.35	0.57
5:G:813:ASP:N	5:G:813:ASP:OD1	2.38	0.57
4:B:335:ILE:HD11	4:B:342:SER:HB2	1.86	0.56
4:F:280:VAL:HG11	4:F:291:ILE:HD11	1.86	0.56
5:G:1749:ARG:HH12	1:A:195:ALA:HB1	1.69	0.56
6:I:80:TYR:O	6:I:80:TYR:CD2	2.58	0.56
2:H:459:VAL:O	5:G:821:TRP:NE1	2.36	0.56
1:C:341:THR:O	1:C:342:GLU:HG2	2.04	0.56
3:M:137:THR:HG21	3:M:424:VAL:HB	1.88	0.56
4:D:137:ILE:HD12	4:D:137:ILE:O	2.05	0.56
8:K:207:CYS:O	8:K:209:GLY:N	2.38	0.56
5:G:1375:GLU:OE2	5:G:1375:GLU:O	2.23	0.56
3:L:259:ILE:HD12	3:L:262:PHE:HB3	1.87	0.56
5:G:2157:GLU:OE2	5:G:2157:GLU:HA	2.05	0.56
4:D:138:ILE:HG22	4:D:233:GLN:HG2	1.87	0.56
3:L:92:MET:SD	3:L:92:MET:N	2.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:133:ARG:O	3:M:137:THR:HG23	2.04	0.56
4:D:235:ARG:O	4:D:236:LYS:HG2	2.05	0.56
3:L:269:VAL:HG23	3:L:357:ILE:HG22	1.87	0.56
6:I:222:HIS:O	6:I:226:ARG:NH2	2.39	0.55
3:M:120:VAL:HG11	3:M:140:MET:HE1	1.88	0.55
3:M:124:GLU:N	3:M:124:GLU:OE1	2.38	0.55
1:C:334:GLY:O	1:C:347:PRO:O	2.24	0.55
4:D:249:VAL:HG22	4:D:265:THR:HG21	1.88	0.55
6:I:177:ARG:O	6:I:177:ARG:HD3	2.06	0.55
8:K:305:VAL:O	8:K:306:THR:OG1	2.22	0.55
1:E:171:LYS:HZ2	5:G:2204:LEU:HD22	1.70	0.55
1:A:136:THR:HG21	1:A:185:VAL:HG11	1.89	0.55
1:E:447:LEU:HD13	4:F:331:GLY:O	2.07	0.55
3:M:375:SER:O	3:M:377:ARG:NH1	2.39	0.55
4:D:332:ILE:N	4:D:343:PRO:O	2.40	0.55
3:L:41:ILE:HG13	3:L:69:TYR:O	2.07	0.55
7:J:59:GLN:OE1	7:J:59:GLN:HA	2.07	0.54
1:A:28:GLU:OE1	1:A:28:GLU:N	2.33	0.54
4:D:74:LEU:HD23	4:D:356:ILE:CD1	2.37	0.54
4:F:49:GLN:NE2	4:F:360:THR:O	2.40	0.54
5:G:834:VAL:HG12	7:J:169:TYR:CD2	2.42	0.54
5:G:1414:ASP:OD1	1:A:251:GLN:NE2	2.39	0.54
5:G:1161:ARG:NE	8:K:191:GLU:O	2.40	0.54
1:C:408:GLN:O	4:D:71:ARG:NH2	2.39	0.54
1:E:312:PHE:O	1:E:316:HIS:ND1	2.40	0.54
4:F:19:ILE:HG22	1:A:323:ILE:HG22	1.88	0.54
5:G:795:SER:HB2	6:I:232:ARG:HE	1.73	0.54
5:G:875:ARG:HH22	8:K:207:CYS:HA	1.72	0.54
5:G:1879:THR:O	5:G:1880:THR:OG1	2.18	0.54
1:A:334:GLY:O	1:A:347:PRO:O	2.26	0.54
3:L:83:GLU:N	3:L:83:GLU:OE1	2.40	0.54
4:F:116:THR:HG23	4:F:311:PHE:CE1	2.43	0.54
4:F:139:GLU:OE1	5:G:1429:LEU:HD11	2.08	0.54
3:M:327:HIS:O	3:M:331:THR:HG23	2.08	0.54
4:F:386:ALA:HB1	4:F:426:ILE:HD12	1.89	0.54
7:J:252:ASN:OD1	7:J:256:ARG:NH1	2.41	0.54
8:K:305:VAL:HG12	8:K:306:THR:HG23	1.89	0.54
1:A:52:ILE:HD11	1:A:83:ILE:HD13	1.90	0.54
1:E:146:PRO:HG3	1:E:153:THR:HG21	1.90	0.54
1:E:313:THR:HG21	4:D:303:MET:HG3	1.90	0.53
4:B:246:GLU:OE2	5:G:1390:TYR:OH	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:1209:THR:HG23	5:G:1239:GLN:HE22	1.73	0.53
7:J:13:GLY:O	7:J:71:ILE:HD13	2.08	0.53
1:E:346:SER:OG	1:E:350:ILE:O	2.21	0.53
4:D:47:VAL:H	9:D:501:AGS:HN61	1.55	0.53
4:F:82:GLY:CA	9:F:501:AGS:H2	2.37	0.53
4:B:21:ARG:NH2	1:C:324:ALA:O	2.42	0.53
7:J:34:ILE:CG2	7:J:67:LEU:HD12	2.39	0.53
2:H:465:VAL:HG11	5:G:2228:ALA:O	2.09	0.53
3:L:24:ARG:NH2	10:L:501:ATP:O2B	2.41	0.53
5:G:788:LEU:HD12	5:G:797:ARG:HD3	1.91	0.53
1:E:16:ALA:O	1:E:378:ARG:NH2	2.33	0.53
1:E:271:ILE:CG2	1:E:275:LEU:HD23	2.38	0.53
3:M:92:MET:N	3:M:92:MET:CE	2.72	0.53
7:J:68:LYS:N	7:J:68:LYS:HE2	2.24	0.53
8:K:206:LYS:O	8:K:207:CYS:HB3	2.07	0.53
2:H:474:TYR:O	2:H:477:VAL:HG22	2.09	0.53
4:B:344:HIS:CE1	1:A:447:LEU:HD21	2.44	0.53
1:C:194:GLU:OE1	1:C:197:SER:OG	2.27	0.53
7:J:107:GLU:OE1	7:J:107:GLU:N	2.40	0.53
3:L:206:CYS:CB	3:L:259:ILE:HD11	2.37	0.53
9:B:501:AGS:O2B	9:B:501:AGS:O5'	2.27	0.53
4:F:342:SER:OG	4:F:346:ILE:O	2.15	0.53
7:J:34:ILE:HG22	7:J:67:LEU:HD12	1.91	0.53
8:K:282:ARG:HD3	8:K:282:ARG:N	2.22	0.53
5:G:809:LYS:HE3	5:G:2258:SER:HG	1.74	0.53
1:E:317:ARG:NH1	4:D:107:GLU:OE2	2.41	0.52
5:G:831:ARG:NH2	6:I:68:ALA:O	2.42	0.52
5:G:868:ARG:NH1	8:K:271:ASP:OD1	2.38	0.52
5:G:1474:GLU:OE2	5:G:1474:GLU:HA	2.09	0.52
3:L:423:CYS:HA	3:L:426:ARG:CB	2.39	0.52
1:A:113:MET:O	1:A:117:ARG:HG3	2.09	0.52
1:E:234:ILE:HD12	1:E:234:ILE:N	2.24	0.52
4:B:40:ARG:O	4:B:53:ARG:NH2	2.32	0.52
1:E:130:VAL:HG22	1:E:231:LYS:HB2	1.91	0.52
4:F:141:GLU:OE2	4:F:208:SER:OG	2.16	0.52
5:G:819:MET:HE2	3:L:160:PHE:HD1	1.74	0.52
6:I:147:LEU:HD23	6:I:198:ILE:HD11	1.92	0.52
3:L:306:GLU:O	3:L:310:ASP:N	2.43	0.52
4:B:180:GLU:OE1	4:B:181:SER:N	2.42	0.52
5:G:2173:PHE:O	5:G:2174:HIS:ND1	2.42	0.52
5:G:1314:LYS:HD3	5:G:1314:LYS:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASP:OD2	1:A:202:ARG:NH2	2.41	0.52
4:F:236:LYS:HE3	5:G:1425:HIS:NE2	2.25	0.52
3:L:419:GLY:HA2	3:L:423:CYS:HB3	1.92	0.52
3:M:17:ASP:O	3:M:23:VAL:HG13	2.10	0.52
1:C:178:GLU:CG	5:G:1877:ARG:HH12	2.23	0.52
5:G:1127:ILE:HG21	5:G:1162:TRP:HB2	1.92	0.52
5:G:1749:ARG:NH2	1:A:129:GLU:OE1	2.42	0.52
1:E:274:LYS:NZ	5:G:1817:LEU:O	2.40	0.51
5:G:816:LEU:O	5:G:819:MET:HB3	2.10	0.51
5:G:1147:VAL:O	5:G:1198:TYR:N	2.41	0.51
5:G:1319:LYS:O	5:G:1319:LYS:HG3	2.10	0.51
4:F:249:VAL:HG12	4:F:268:ILE:HD11	1.91	0.51
5:G:1312:VAL:HG22	5:G:1315:GLN:NE2	2.25	0.51
7:J:176:LEU:HD21	7:J:284:LYS:CE	2.41	0.51
4:B:19:ILE:HD11	1:C:240:LEU:HD11	1.93	0.51
1:C:17:SER:OG	4:D:317:GLU:OE1	2.17	0.51
4:D:46:MET:HE2	4:D:86:ILE:HD13	1.93	0.51
4:D:138:ILE:HG12	4:D:195:ILE:HB	1.92	0.51
1:E:323:ILE:HG22	1:E:323:ILE:O	2.11	0.51
1:C:336:CYS:HG	4:D:340:TYR:HH	1.57	0.51
5:G:889:GLU:OE2	5:G:889:GLU:HA	2.10	0.51
5:G:1091:LEU:HD11	5:G:1128:ALA:CB	2.41	0.51
3:L:81:ASN:O	3:L:81:ASN:ND2	2.43	0.51
1:A:157:VAL:HG21	1:A:177:PHE:HB2	1.91	0.51
1:C:338:ILE:HD11	1:C:346:SER:HB2	1.92	0.51
5:G:2256:ASP:OD1	5:G:2256:ASP:C	2.49	0.51
3:L:127:TRP:CZ3	3:L:178:THR:HG21	2.46	0.51
1:A:223:LEU:HD22	1:A:226:GLY:HA3	1.91	0.51
5:G:800:PRO:O	6:I:226:ARG:CZ	2.59	0.51
3:L:168:LEU:HD21	3:L:329:VAL:HG23	1.93	0.51
5:G:833:LYS:HD3	7:J:375:PHE:HB2	1.93	0.51
5:G:834:VAL:HG12	7:J:169:TYR:CE2	2.46	0.51
8:K:306:THR:HG21	8:K:323:TYR:CG	2.46	0.51
3:L:81:ASN:OD1	3:L:245:GLN:NE2	2.43	0.51
3:M:16:PHE:CE1	3:M:120:VAL:HG13	2.42	0.51
5:G:842:ARG:HG2	5:G:842:ARG:HH11	1.76	0.50
5:G:898:GLU:OE2	5:G:898:GLU:HA	2.11	0.50
6:I:176:ASP:OD1	3:L:190:GLN:NE2	2.43	0.50
5:G:1123:THR:HG23	5:G:1155:TRP:CZ3	2.46	0.50
3:L:157:LEU:HA	3:L:160:PHE:HB2	1.93	0.50
3:L:376:MET:SD	3:L:377:ARG:NH1	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:243:SER:N	4:F:246:GLU:OE1	2.42	0.50
5:G:842:ARG:NH2	7:J:167:GLU:OE2	2.44	0.50
5:G:1314:LYS:HD3	5:G:1314:LYS:N	2.26	0.50
7:J:276:GLU:OE1	7:J:280:ASN:ND2	2.44	0.50
3:L:15:VAL:HG22	3:L:121:LEU:CD2	2.40	0.50
3:L:423:CYS:HA	3:L:426:ARG:HB3	1.92	0.50
4:B:343:PRO:O	1:A:447:LEU:HD23	2.11	0.50
1:C:177:PHE:HA	1:C:180:LEU:HD12	1.92	0.50
4:D:389:VAL:HG21	4:D:423:VAL:CG2	2.41	0.50
4:F:443:MET:CE	1:A:334:GLY:O	2.60	0.50
3:M:92:MET:N	3:M:92:MET:SD	2.85	0.50
1:C:184:ARG:HG3	1:C:184:ARG:HH11	1.76	0.50
7:J:207:GLU:OE2	7:J:207:GLU:HA	2.11	0.50
3:L:368:LEU:HD11	3:L:378:LEU:HD11	1.92	0.50
1:A:131:TYR:HB2	1:A:193:ILE:HG23	1.94	0.50
1:E:77:THR:HG21	4:F:314:ARG:NH2	2.26	0.50
3:M:175:THR:HG22	3:M:175:THR:O	2.12	0.50
4:B:334:ARG:NH1	4:B:338:THR:O	2.40	0.50
5:G:1763:GLN:OE1	1:A:285:LYS:NZ	2.36	0.50
8:K:181:GLU:OE1	8:K:181:GLU:C	2.50	0.50
1:E:334:GLY:O	4:D:443:MET:CE	2.60	0.50
9:F:501:AGS:O3G	9:F:501:AGS:O1B	2.30	0.50
4:F:404:GLN:NE2	1:A:357:ARG:O	2.44	0.50
3:M:146:ILE:HD11	3:M:149:PHE:HB2	1.94	0.50
6:I:244:GLU:O	6:I:248:LEU:N	2.45	0.50
7:J:242:LEU:HD23	7:J:246:GLN:CD	2.32	0.50
3:L:156:VAL:CG2	3:L:187:VAL:HG13	2.42	0.49
4:B:177:LYS:O	4:B:180:GLU:HG3	2.11	0.49
1:C:447:LEU:HD11	4:D:344:HIS:CE1	2.46	0.49
4:F:170:THR:HG22	4:F:232:LEU:HD13	1.93	0.49
5:G:791:ALA:O	5:G:795:SER:OG	2.13	0.49
5:G:1928:ASP:OD1	5:G:1943:ARG:NH1	2.38	0.49
6:I:195:TYR:O	6:I:198:ILE:HG22	2.12	0.49
1:A:130:VAL:HG11	1:A:192:TYR:CD1	2.47	0.49
1:A:223:LEU:HD13	1:A:223:LEU:O	2.12	0.49
7:J:178:LEU:HD21	7:J:274:ILE:HD13	1.94	0.49
1:E:147:MET:H	1:E:147:MET:CE	2.25	0.49
4:B:445:GLU:HG2	4:B:446:TYR:CD1	2.46	0.49
4:F:248:ASP:HB3	4:F:268:ILE:HD13	1.93	0.49
3:M:281:GLN:NE2	3:M:282:MET:O	2.45	0.49
4:D:332:ILE:HD13	4:D:343:PRO:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:78:ASN:ND2	7:J:81:ASP:OD2	2.40	0.49
3:L:216:GLU:OE2	3:L:216:GLU:O	2.31	0.49
1:E:196:ASN:N	1:E:196:ASN:HD22	2.11	0.49
2:H:465:VAL:O	2:H:465:VAL:HG13	2.12	0.49
2:H:467:LEU:HD23	5:G:2223:TYR:CZ	2.47	0.49
1:A:180:LEU:HD12	1:A:200:VAL:HG21	1.93	0.49
4:F:47:VAL:H	9:F:501:AGS:HN61	1.59	0.49
1:A:67:LEU:HD23	1:A:360:ILE:CD1	2.43	0.49
1:C:180:LEU:HD23	1:C:200:VAL:HG11	1.95	0.49
4:F:144:GLU:OE1	4:F:146:GLN:NE2	2.45	0.49
5:G:2172:LEU:HD23	5:G:2173:PHE:HE1	1.76	0.49
7:J:37:ARG:N	7:J:37:ARG:HD2	2.28	0.49
3:L:326:SER:HB3	3:L:367:GLU:HB3	1.95	0.49
5:G:1237:THR:O	5:G:1239:GLN:NE2	2.46	0.48
7:J:220:ALA:HB1	7:J:226:GLU:HG3	1.94	0.48
5:G:1822:GLU:HG3	5:G:1826:ASP:HB2	1.94	0.48
4:B:443:MET:CE	1:C:334:GLY:O	2.62	0.48
4:F:328:THR:HG21	4:F:344:HIS:HB3	1.95	0.48
3:L:203:THR:N	3:L:263:GLN:OE1	2.46	0.48
4:B:117:GLU:OE2	4:B:273:ARG:NH2	2.47	0.48
6:I:110:MET:SD	6:I:110:MET:O	2.71	0.48
7:J:269:MET:HA	7:J:269:MET:CE	2.43	0.48
1:A:135:VAL:HG11	1:A:189:ASP:O	2.13	0.48
1:A:177:PHE:O	1:A:181:GLN:OE1	2.30	0.48
6:I:80:TYR:O	6:I:80:TYR:CG	2.66	0.48
6:I:176:ASP:OD2	3:L:189:GLN:N	2.46	0.48
6:I:229:GLN:OE1	6:I:233:LEU:HD12	2.13	0.48
3:L:256:ASN:HA	3:L:259:ILE:HG22	1.96	0.48
1:A:48:ALA:O	1:A:51:VAL:HG22	2.13	0.48
1:C:21:VAL:HG23	1:C:21:VAL:O	2.13	0.48
5:G:1347:GLU:OE1	5:G:1348:ALA:N	2.47	0.48
7:J:62:ARG:HG3	7:J:62:ARG:HH11	1.78	0.48
1:A:132:GLU:OE1	1:A:192:TYR:CE1	2.67	0.48
4:B:161:LEU:HD23	4:B:162:THR:N	2.28	0.48
4:F:333:THR:HG22	4:F:334:ARG:N	2.29	0.48
5:G:1866:ARG:O	5:G:1867:GLU:HB2	2.13	0.48
6:I:107:ASP:OD1	6:I:107:ASP:C	2.52	0.48
1:E:334:GLY:O	4:D:443:MET:HE1	2.14	0.48
4:B:107:GLU:HG2	1:C:109:THR:HG21	1.95	0.48
5:G:1094:TYR:CG	5:G:1312:VAL:HG21	2.49	0.48
7:J:331:ALA:HB1	7:J:335:ARG:CZ	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:414:ARG:HG3	4:D:414:ARG:HH11	1.77	0.48
5:G:1122:LYS:HD3	5:G:1122:LYS:N	2.29	0.48
7:J:311:ASP:OD1	7:J:311:ASP:N	2.46	0.48
1:A:350:ILE:HG23	1:A:354:LEU:HD23	1.96	0.48
2:H:471:HIS:O	2:H:471:HIS:CG	2.67	0.47
4:D:74:LEU:HD23	4:D:356:ILE:HD13	1.94	0.47
5:G:2154:ASP:N	5:G:2154:ASP:OD1	2.47	0.47
7:J:198:TYR:CD1	7:J:198:TYR:N	2.81	0.47
5:G:2150:GLU:OE1	5:G:2150:GLU:N	2.45	0.47
6:I:122:LYS:HZ3	6:I:122:LYS:HB2	1.79	0.47
1:A:134:GLU:O	1:A:135:VAL:HG12	2.14	0.47
1:E:255:ASP:O	1:E:258:SER:N	2.46	0.47
3:M:99:PHE:CE1	3:M:103:LEU:HD22	2.49	0.47
4:F:370:ILE:HG23	9:F:501:AGS:C8	2.45	0.47
5:G:892:LEU:O	5:G:896:LEU:HD23	2.14	0.47
7:J:213:LYS:HD2	7:J:306:TYR:OH	2.14	0.47
3:L:378:LEU:HD13	3:L:378:LEU:O	2.15	0.47
3:M:285:VAL:HG22	3:M:286:HIS:N	2.30	0.47
4:B:246:GLU:HA	4:B:260:LEU:HD21	1.96	0.47
4:D:137:ILE:HD12	4:D:137:ILE:C	2.34	0.47
1:A:341:THR:O	1:A:342:GLU:HG2	2.15	0.47
3:M:143:HIS:C	3:M:143:HIS:CD2	2.88	0.47
4:B:340:TYR:HH	1:A:336:CYS:HG	1.59	0.47
1:E:158:ILE:HD13	1:E:171:LYS:CG	2.43	0.47
3:L:216:GLU:OE2	3:L:218:VAL:HG23	2.14	0.47
3:M:15:VAL:HG21	3:M:398:SER:HA	1.97	0.47
4:B:349:ASP:HB3	4:F:451:LEU:HD11	1.95	0.47
1:C:271:ILE:HG23	1:C:275:LEU:HD23	1.96	0.47
4:F:249:VAL:CG1	4:F:268:ILE:HD11	2.43	0.47
5:G:797:ARG:NH1	6:I:248:LEU:HD11	2.30	0.47
7:J:266:PHE:N	7:J:266:PHE:CD1	2.82	0.47
1:A:135:VAL:HG21	1:A:191:ILE:CG1	2.44	0.47
4:F:261:PHE:HD1	1:A:275:LEU:HD13	1.79	0.47
5:G:1324:LEU:O	5:G:1324:LEU:HD12	2.13	0.47
7:J:99:GLU:OE1	7:J:99:GLU:N	2.30	0.47
8:K:190:TYR:CD2	8:K:191:GLU:HG3	2.49	0.47
3:L:425:GLU:OE1	3:L:425:GLU:N	2.44	0.47
4:D:375:CYS:SG	4:D:406:ILE:HD12	2.55	0.47
4:F:416:ARG:NH2	4:F:425:ASP:OD2	2.46	0.47
5:G:1367:ILE:CG1	5:G:1374:VAL:HG11	2.44	0.47
1:A:135:VAL:HG11	1:A:191:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:137:ILE:O	4:B:234:LYS:N	2.47	0.47
1:C:323:ILE:HG22	1:C:323:ILE:O	2.15	0.47
4:D:210:THR:O	8:K:260:ARG:HA	2.15	0.47
5:G:1813:LEU:HD23	5:G:1813:LEU:O	2.15	0.47
7:J:176:LEU:HD21	7:J:284:LYS:HE3	1.97	0.47
3:L:376:MET:HA	3:L:376:MET:CE	2.45	0.47
4:F:452:PHE:O	4:F:453:ASN:HB2	2.15	0.46
8:K:306:THR:OG1	8:K:306:THR:O	2.32	0.46
4:F:117:GLU:OE2	4:F:273:ARG:NH2	2.48	0.46
4:F:265:THR:HG23	4:F:266:GLY:N	2.31	0.46
5:G:1218:ILE:HD12	5:G:1244:LEU:O	2.15	0.46
9:G:3201:AGS:H2'	9:G:3201:AGS:N3	2.30	0.46
7:J:54:VAL:HG12	7:J:55:GLY:N	2.31	0.46
8:K:180:GLU:OE1	8:K:180:GLU:HA	2.14	0.46
3:L:149:PHE:CE2	3:L:151:LEU:HD21	2.50	0.46
1:A:170:LEU:O	1:A:170:LEU:HD12	2.16	0.46
4:D:435:ASP:OD1	4:D:438:ARG:NH1	2.44	0.46
5:G:797:ARG:HA	5:G:797:ARG:CZ	2.46	0.46
1:A:164:ALA:HB3	1:A:223:LEU:HD23	1.97	0.46
3:M:213:MET:HE2	3:M:213:MET:N	2.31	0.46
4:B:134:GLU:OE1	4:B:235:ARG:NH1	2.48	0.46
4:D:23:GLY:N	4:D:26:SER:OG	2.47	0.46
8:K:303:ASP:O	8:K:307:ASP:HA	2.16	0.46
3:M:284:THR:OG1	3:M:297:PHE:O	2.33	0.46
4:B:333:THR:HG21	9:B:501:AGS:O1B	2.16	0.46
3:M:18:ILE:O	3:M:18:ILE:HG13	2.15	0.46
4:B:416:ARG:NH1	4:B:425:ASP:OD2	2.48	0.46
5:G:1150:CYS:O	5:G:1153:LEU:N	2.48	0.46
7:J:185:LEU:HD21	7:J:261:LEU:HG	1.98	0.46
1:A:122:LEU:N	1:A:238:VAL:O	2.44	0.46
1:E:262:GLN:NE2	1:A:257:LEU:HD21	2.30	0.46
3:M:327:HIS:HA	3:M:330:THR:HG22	1.98	0.46
4:B:349:ASP:OD1	4:B:350:LEU:N	2.49	0.46
1:C:432:GLU:OE1	4:D:54:ARG:NH1	2.43	0.46
1:E:334:GLY:O	1:E:347:PRO:O	2.34	0.46
4:B:195:ILE:HG22	4:B:196:ASP:N	2.31	0.46
4:D:46:MET:HG3	9:D:501:AGS:N6	2.31	0.46
4:D:191:ASP:OD1	4:D:207:ARG:NH1	2.49	0.46
4:D:328:THR:HG21	4:D:344:HIS:HB3	1.96	0.46
4:F:120:THR:O	4:F:124:ARG:HG2	2.16	0.46
6:I:177:ARG:O	6:I:178:TYR:C	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:335:ILE:HD11	4:F:342:SER:HB2	1.98	0.46
5:G:819:MET:CE	3:L:160:PHE:HD1	2.28	0.46
6:I:237:THR:O	6:I:241:VAL:HG23	2.15	0.46
7:J:11:ASP:OD1	7:J:106:THR:OG1	2.29	0.46
7:J:306:TYR:O	7:J:309:ILE:HG22	2.16	0.46
3:L:314:VAL:HG12	3:L:315:LYS:N	2.31	0.46
3:M:166:THR:HG23	3:M:166:THR:O	2.16	0.45
3:M:263:GLN:NE2	3:M:356:LEU:O	2.48	0.45
4:F:162:THR:HG23	8:K:304:PRO:CG	2.46	0.45
5:G:1067:ILE:O	5:G:1067:ILE:HG22	2.16	0.45
6:I:245:GLU:HA	6:I:248:LEU:HB2	1.98	0.45
1:E:42:GLN:HG3	1:E:45:ALA:HB3	1.98	0.45
1:E:447:LEU:HD11	4:F:344:HIS:CE1	2.52	0.45
3:M:405:THR:O	3:M:409:MET:HG3	2.16	0.45
4:D:253:ARG:O	4:D:253:ARG:HG2	2.16	0.45
7:J:186:THR:CB	7:J:213:LYS:HZ1	2.24	0.45
3:L:269:VAL:HG22	3:L:305:PRO:CB	2.46	0.45
4:B:405:LEU:CD2	4:B:429:VAL:HG12	2.46	0.45
1:C:18:HIS:O	1:C:21:VAL:HG22	2.16	0.45
4:D:74:LEU:HB3	4:D:356:ILE:HD13	1.99	0.45
7:J:300:SER:O	7:J:304:THR:OG1	2.24	0.45
3:L:248:ARG:O	3:L:248:ARG:HD3	2.16	0.45
5:G:1134:ALA:HB1	5:G:1140:TRP:CE3	2.51	0.45
7:J:225:GLN:C	7:J:225:GLN:OE1	2.55	0.45
1:E:258:SER:OG	1:E:259:MET:N	2.50	0.45
4:B:330:ARG:HA	9:B:501:AGS:H8	1.97	0.45
4:D:133:GLU:OE1	5:G:1830:ARG:NH1	2.50	0.45
5:G:875:ARG:HH22	8:K:207:CYS:N	2.14	0.45
5:G:1088:TYR:OH	8:K:180:GLU:OE2	2.24	0.45
5:G:1332:GLN:NE2	5:G:1368:CYS:O	2.47	0.45
7:J:195:GLU:OE1	7:J:196:ARG:N	2.49	0.45
7:J:204:ALA:O	7:J:208:ILE:HG12	2.16	0.45
1:A:207:ASP:N	1:A:207:ASP:OD1	2.49	0.45
3:M:182:VAL:HG12	3:M:187:VAL:HG22	1.99	0.45
1:C:286:TYR:CD1	1:C:291:ILE:HD11	2.51	0.45
6:I:163:LEU:HD12	6:I:174:ILE:HG23	1.98	0.45
6:I:167:PHE:N	6:I:167:PHE:CD1	2.84	0.45
7:J:35:VAL:HG11	7:J:81:ASP:OD1	2.17	0.45
3:L:378:LEU:HD13	3:L:378:LEU:C	2.36	0.45
3:M:93:VAL:HG11	3:M:96:TRP:CE3	2.52	0.45
4:B:374:ARG:HG2	4:B:403:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:GLU:CD	5:G:1877:ARG:HH12	2.20	0.45
4:D:143:VAL:HG13	4:D:162:THR:OG1	2.15	0.45
5:G:2186:GLU:O	5:G:2190:MET:HG3	2.16	0.45
6:I:77:GLY:O	6:I:78:GLN:HB2	2.17	0.45
1:C:142:GLU:OE1	1:C:142:GLU:C	2.55	0.45
4:F:34:ASP:OD1	4:F:34:ASP:N	2.49	0.45
4:F:314:ARG:HD2	4:F:314:ARG:N	2.31	0.45
5:G:845:VAL:O	5:G:849:GLU:HG3	2.16	0.45
5:G:1220:GLU:O	5:G:1224:VAL:HG23	2.17	0.45
5:G:1869:ALA:O	5:G:1873:PHE:N	2.50	0.45
7:J:272:CYS:SG	3:L:73:ASN:HA	2.57	0.45
7:J:283:MET:O	7:J:290:ARG:NH2	2.50	0.45
8:K:200:GLN:O	8:K:201:VAL:C	2.55	0.45
1:A:343:ASP:O	1:A:343:ASP:OD1	2.34	0.45
3:M:310:ASP:C	3:M:310:ASP:OD1	2.55	0.45
3:M:424:VAL:HG13	3:M:425:GLU:N	2.32	0.45
5:G:894:VAL:HG13	5:G:2149:LEU:HD12	1.98	0.45
5:G:1106:TYR:O	5:G:1242:GLN:NE2	2.50	0.45
5:G:1863:GLN:O	5:G:1866:ARG:O	2.35	0.45
3:L:68:TYR:HE2	3:L:101:ALA:HB3	1.81	0.45
3:M:407:GLN:OE1	3:M:407:GLN:N	2.44	0.45
4:D:67:LYS:HB3	4:D:68:ILE:HD12	1.99	0.45
5:G:1312:VAL:HG13	5:G:1316:LEU:HD13	1.99	0.45
6:I:116:ARG:O	6:I:117:ALA:HB3	2.17	0.45
7:J:180:LEU:HB2	7:J:184:ASP:OD1	2.17	0.45
3:L:310:ASP:OD1	3:L:310:ASP:C	2.55	0.45
1:A:134:GLU:O	1:A:134:GLU:OE2	2.35	0.45
5:G:1147:VAL:HG12	5:G:1148:ARG:H	1.82	0.44
5:G:1770:ASP:OD1	5:G:1770:ASP:N	2.50	0.44
3:L:66:PRO:HB3	3:L:68:TYR:CE1	2.52	0.44
1:C:42:GLN:NE2	1:C:364:MET:O	2.48	0.44
4:F:236:LYS:NZ	4:F:236:LYS:HB3	2.32	0.44
5:G:1415:LEU:N	1:A:247:ASN:OD1	2.45	0.44
3:L:362:ASP:OD1	3:L:362:ASP:N	2.48	0.44
3:M:139:LEU:HD23	3:M:140:MET:N	2.33	0.44
4:F:226:GLN:OE1	5:G:1436:PRO:HD3	2.17	0.44
4:F:443:MET:HE1	1:A:334:GLY:O	2.17	0.44
5:G:1155:TRP:O	5:G:1159:LEU:HD23	2.17	0.44
5:G:1313:GLU:OE2	5:G:1313:GLU:C	2.56	0.44
5:G:2165:TYR:CD1	5:G:2165:TYR:C	2.91	0.44
5:G:2237:ASP:OD2	5:G:2241:GLN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:201:LYS:O	6:I:205:VAL:HG12	2.17	0.44
1:C:13:GLN:OE1	4:D:284:ARG:NH2	2.51	0.44
5:G:1099:LEU:HD22	5:G:1128:ALA:HB1	1.98	0.44
5:G:1435:ILE:O	5:G:1435:ILE:HG23	2.16	0.44
5:G:2173:PHE:O	5:G:2174:HIS:CG	2.71	0.44
1:A:189:ASP:O	1:A:191:ILE:HG23	2.17	0.44
4:B:72:ALA:HB3	4:B:354:LEU:HD12	2.00	0.44
4:B:174:LEU:N	4:B:174:LEU:HD23	2.33	0.44
6:I:163:LEU:HD11	6:I:174:ILE:HA	1.99	0.44
6:I:166:ARG:HG2	6:I:167:PHE:CD1	2.53	0.44
7:J:61:LYS:O	7:J:65:LEU:HB2	2.18	0.44
7:J:82:MET:HE2	7:J:82:MET:HA	1.99	0.44
7:J:180:LEU:HD12	7:J:180:LEU:O	2.17	0.44
8:K:271:ASP:OD1	8:K:271:ASP:N	2.49	0.44
3:L:201:PHE:HZ	3:L:314:VAL:HG21	1.83	0.44
3:M:304:ILE:HB	3:M:305:PRO:HD3	2.00	0.44
3:M:377:ARG:NE	3:M:377:ARG:HA	2.33	0.44
4:F:386:ALA:HB1	4:F:426:ILE:CD1	2.47	0.44
5:G:1849:ARG:O	5:G:1849:ARG:HG3	2.17	0.44
5:G:1893:VAL:O	5:G:1894:GLN:HB3	2.17	0.44
5:G:1941:TYR:HA	5:G:1968:CYS:O	2.18	0.44
3:L:248:ARG:HA	3:L:248:ARG:NE	2.32	0.44
1:A:134:GLU:O	1:A:135:VAL:O	2.36	0.44
8:K:292:CYS:SG	8:K:295:THR:HG22	2.58	0.44
1:A:49:CYS:HA	1:A:52:ILE:HG12	2.00	0.44
3:M:400:LEU:HD23	5:G:877:ILE:HD11	2.00	0.44
4:F:80:GLY:N	9:F:501:AGS:O3G	2.40	0.44
4:F:220:SER:OG	4:F:221:GLN:N	2.51	0.44
5:G:1977:THR:O	5:G:1977:THR:OG1	2.35	0.44
1:A:338:ILE:HD11	1:A:346:SER:OG	2.18	0.44
3:M:14:LEU:HD11	3:M:27:TYR:CE1	2.53	0.44
1:C:207:ASP:OD2	5:G:1941:TYR:OH	2.20	0.43
4:F:221:GLN:HA	5:G:1760:ARG:NH1	2.33	0.43
7:J:271:SER:OG	7:J:272:CYS:N	2.51	0.43
8:K:177:LYS:HE2	8:K:177:LYS:N	2.33	0.43
1:E:183:GLU:HB2	1:E:185:VAL:HG23	1.99	0.43
3:M:285:VAL:HG22	3:M:286:HIS:H	1.84	0.43
4:F:137:ILE:HD13	4:F:194:THR:OG1	2.18	0.43
5:G:1336:TYR:CE1	5:G:1364:LEU:HD22	2.53	0.43
6:I:165:ARG:NE	6:I:165:ARG:C	2.67	0.43
6:I:193:GLU:O	6:I:197:HIS:ND1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:128:ASN:O	3:L:130:ARG:NH2	2.51	0.43
3:M:14:LEU:HD13	3:M:118:HIS:CG	2.53	0.43
3:M:92:MET:HG2	3:M:132:LYS:HE2	1.98	0.43
3:M:167:GLY:HA2	3:M:347:SER:OG	2.19	0.43
3:M:364:LEU:O	3:M:368:LEU:HG	2.17	0.43
4:B:253:ARG:HG2	1:A:266:PRO:HD3	2.00	0.43
4:D:254:THR:O	4:D:255:GLN:HB2	2.18	0.43
5:G:1088:TYR:CZ	8:K:180:GLU:OE2	2.70	0.43
6:I:177:ARG:O	6:I:177:ARG:NH1	2.49	0.43
8:K:172:LEU:O	8:K:175:GLU:OE1	2.37	0.43
3:L:181:PRO:HB3	3:L:344:LEU:HD21	1.99	0.43
1:E:334:GLY:CA	4:D:450:PHE:HB3	2.47	0.43
3:M:92:MET:HG3	3:M:132:LYS:HG3	2.01	0.43
4:D:414:ARG:HG3	4:D:414:ARG:NH1	2.33	0.43
3:L:85:ILE:C	3:L:85:ILE:HD12	2.38	0.43
3:L:335:MET:SD	3:L:336:CYS:N	2.91	0.43
3:L:390:ARG:HG2	3:L:390:ARG:HH11	1.82	0.43
1:E:191:ILE:HD11	1:E:193:ILE:HD11	2.00	0.43
3:M:14:LEU:HD23	3:M:16:PHE:CE2	2.54	0.43
4:B:295:VAL:HG23	4:B:323:VAL:O	2.18	0.43
4:F:334:ARG:HA	4:F:340:TYR:O	2.19	0.43
5:G:828:GLN:O	6:I:70:PRO:HG2	2.19	0.43
1:A:136:THR:HB	1:A:187:ALA:HA	2.01	0.43
1:A:164:ALA:HB3	1:A:223:LEU:CD2	2.48	0.43
1:E:119:ALA:O	1:E:297:GLY:N	2.50	0.43
3:M:107:TYR:HA	3:M:111:VAL:HG12	2.01	0.43
5:G:1124:VAL:HG23	5:G:1162:TRP:CD2	2.53	0.43
5:G:1978:THR:OG1	5:G:1979:GLY:N	2.51	0.43
1:A:135:VAL:HG21	1:A:191:ILE:CD1	2.48	0.43
1:A:190:VAL:HG23	1:A:203:GLN:HB2	2.00	0.43
5:G:846:ARG:HH11	5:G:846:ARG:HG2	1.83	0.43
5:G:1456:ALA:HB2	8:K:323:TYR:OH	2.17	0.43
7:J:252:ASN:OD1	7:J:252:ASN:C	2.56	0.43
5:G:1894:GLN:HG2	5:G:1894:GLN:O	2.19	0.43
7:J:16:MET:HE3	7:J:16:MET:HA	1.99	0.43
3:L:271:ASP:OD1	3:L:271:ASP:C	2.56	0.43
1:A:67:LEU:HD23	1:A:360:ILE:HD13	1.99	0.43
4:B:241:THR:HG23	4:B:241:THR:O	2.18	0.43
1:C:73:GLY:CA	9:C:501:AGS:O1B	2.67	0.43
5:G:2001:ALA:O	5:G:2005:GLU:HG2	2.19	0.43
5:G:2032:LEU:O	5:G:2033:LYS:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:243:LEU:HD23	3:L:244:PRO:HD2	2.00	0.43
3:L:275:ASP:HB3	3:L:278:VAL:HG22	2.00	0.43
1:A:190:VAL:O	1:A:203:GLN:N	2.51	0.43
1:A:205:ARG:NE	1:A:218:GLU:OE2	2.46	0.43
1:E:174:PRO:HB2	8:K:266:ILE:HG12	2.01	0.43
3:M:103:LEU:O	3:M:107:TYR:CD2	2.71	0.43
3:M:308:LEU:HD12	3:M:309:PHE:N	2.33	0.43
7:J:221:LEU:O	7:J:315:LYS:NZ	2.48	0.43
7:J:300:SER:OG	7:J:301:GLY:N	2.52	0.43
1:A:65:ALA:HB3	1:A:358:VAL:HG12	2.01	0.43
6:I:236:ARG:NH1	6:I:244:GLU:OE2	2.52	0.42
3:L:252:ASN:HA	3:L:255:CYS:SG	2.59	0.42
3:L:274:TYR:N	3:L:306:GLU:OE1	2.52	0.42
3:L:348:VAL:O	3:L:380:LEU:HD23	2.19	0.42
1:A:161:LEU:O	1:A:167:THR:HA	2.19	0.42
4:B:404:GLN:NE2	1:C:357:ARG:O	2.52	0.42
4:D:249:VAL:HG13	4:D:265:THR:HG21	2.01	0.42
5:G:2223:TYR:CE2	5:G:2228:ALA:HB2	2.54	0.42
7:J:210:ARG:HD2	7:J:213:LYS:HZ3	1.83	0.42
7:J:227:MET:SD	7:J:227:MET:N	2.92	0.42
3:L:43:MET:SD	3:L:85:ILE:HD11	2.59	0.42
1:E:172:LEU:N	1:E:172:LEU:HD22	2.34	0.42
4:B:176:THR:HG1	4:B:178:MET:CE	2.29	0.42
4:F:47:VAL:O	9:F:501:AGS:N6	2.52	0.42
4:F:162:THR:HG23	8:K:304:PRO:HG2	2.01	0.42
5:G:1962:ARG:NH1	8:K:188:GLU:OE2	2.52	0.42
3:L:15:VAL:O	3:L:394:TRP:NE1	2.49	0.42
1:A:134:GLU:HB3	1:A:162:LYS:HG2	2.01	0.42
3:M:140:MET:SD	3:M:146:ILE:HD13	2.59	0.42
5:G:1167:LYS:HE3	5:G:1167:LYS:HA	2.01	0.42
5:G:2032:LEU:O	5:G:2033:LYS:CG	2.67	0.42
6:I:98:MET:SD	6:I:120:GLU:HA	2.59	0.42
1:A:223:LEU:O	1:A:223:LEU:CD1	2.68	0.42
1:E:306:MET:HE1	4:F:306:ILE:HG12	2.01	0.42
3:M:130:ARG:NE	3:M:130:ARG:H	2.17	0.42
3:M:254:MET:O	3:M:254:MET:HE2	2.20	0.42
3:L:251:HIS:HA	3:L:254:MET:HG3	2.00	0.42
1:A:175:SER:O	1:A:178:GLU:HG3	2.18	0.42
1:C:157:VAL:HG13	1:C:157:VAL:O	2.20	0.42
9:C:501:AGS:S1G	9:C:501:AGS:O1B	2.76	0.42
7:J:210:ARG:HA	7:J:213:LYS:HZ3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:140:MET:HE3	3:L:144:TYR:CD2	2.54	0.42
1:E:171:LYS:HZ1	5:G:2204:LEU:HD22	1.81	0.42
1:E:411:THR:CG2	1:E:412:PRO:HD3	2.50	0.42
1:E:423:ASP:OD1	1:E:423:ASP:N	2.46	0.42
3:M:129:THR:OG1	3:M:132:LYS:HG2	2.19	0.42
3:M:337:ASP:OD1	3:M:337:ASP:C	2.56	0.42
4:B:165:THR:HG22	4:B:166:THR:N	2.35	0.42
5:G:2259:ASP:N	5:G:2259:ASP:OD1	2.53	0.42
3:L:239:ARG:HD3	3:L:240:LYS:O	2.20	0.42
1:A:205:ARG:O	1:A:206:CYS:C	2.58	0.42
3:M:180:ILE:CG2	3:M:187:VAL:HG13	2.50	0.42
3:M:360:PHE:O	3:M:364:LEU:HD23	2.20	0.42
4:B:254:THR:HG21	1:A:262:GLN:HB3	2.01	0.42
8:K:196:ASP:OD1	8:K:196:ASP:N	2.53	0.42
3:L:24:ARG:NH2	3:L:390:ARG:O	2.53	0.42
3:L:174:ALA:O	3:L:200:ASP:N	2.42	0.42
1:E:145:ASN:N	1:E:146:PRO:CD	2.82	0.42
1:E:185:VAL:HG22	1:E:202:ARG:HB2	2.00	0.42
3:M:17:ASP:N	3:M:17:ASP:OD1	2.53	0.42
3:M:36:ASP:C	3:M:36:ASP:OD1	2.58	0.42
3:M:383:ASN:OD1	3:M:383:ASN:N	2.41	0.42
4:F:374:ARG:HG3	4:F:403:ILE:HD12	2.02	0.42
5:G:1209:THR:HG23	5:G:1239:GLN:NE2	2.34	0.42
1:A:65:ALA:CB	1:A:358:VAL:HG12	2.50	0.42
1:E:145:ASN:N	1:E:146:PRO:HD3	2.35	0.42
2:H:457:ARG:NH1	5:G:2247:LEU:HD21	2.35	0.42
3:M:340:ILE:C	3:M:340:ILE:HD12	2.41	0.42
4:D:63:ILE:HD13	4:D:295:VAL:HG21	2.01	0.42
5:G:1324:LEU:HD11	5:G:2021:LEU:CD2	2.50	0.42
5:G:1844:SER:OG	5:G:1846:ARG:NH2	2.48	0.42
6:I:80:TYR:OH	7:J:130:PRO:HG3	2.20	0.42
3:M:309:PHE:HZ	3:M:364:LEU:HD22	1.85	0.41
3:M:341:ARG:N	3:M:342:PRO:HD2	2.34	0.41
4:B:55:ALA:O	4:B:58:VAL:HG12	2.19	0.41
4:B:100:PHE:CD2	4:B:295:VAL:CG1	3.03	0.41
4:F:403:ILE:HA	4:F:406:ILE:HD12	2.02	0.41
6:I:246:TYR:CD1	6:I:246:TYR:C	2.93	0.41
3:L:73:ASN:OD1	3:L:73:ASN:O	2.37	0.41
3:L:82:MET:O	3:L:247:THR:OG1	2.27	0.41
3:L:188:LEU:HD22	3:L:188:LEU:N	2.34	0.41
3:L:317:LEU:N	3:L:317:LEU:HD22	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:ASN:O	1:E:146:PRO:O	2.38	0.41
1:E:235:ILE:HG23	1:E:235:ILE:O	2.20	0.41
1:E:319:LEU:HD21	1:E:327:VAL:HG21	2.02	0.41
3:M:262:PHE:CZ	3:M:267:LEU:HD21	2.55	0.41
4:B:49:GLN:NE2	4:B:360:THR:O	2.51	0.41
4:B:405:LEU:HD22	4:B:429:VAL:HG12	2.02	0.41
4:D:362:TYR:OH	9:D:501:AGS:C2	2.67	0.41
4:F:196:ASP:O	4:F:200:GLY:N	2.52	0.41
5:G:892:LEU:HD22	5:G:896:LEU:CD2	2.50	0.41
5:G:1091:LEU:HD21	5:G:1124:VAL:HG22	2.02	0.41
5:G:2160:THR:OG1	5:G:2163:GLU:OE2	2.36	0.41
7:J:325:MET:HA	7:J:325:MET:CE	2.49	0.41
3:L:137:THR:OG1	3:L:424:VAL:HG21	2.19	0.41
1:A:133:GLY:HA2	1:A:163:THR:OG1	2.19	0.41
1:E:215:LEU:HA	1:E:215:LEU:HD23	1.80	0.41
3:M:217:LEU:HD21	3:M:259:ILE:CG2	2.51	0.41
4:F:83:LYS:NZ	9:F:501:AGS:S1G	2.82	0.41
5:G:1228:THR:HG22	5:G:1229:GLU:N	2.36	0.41
9:G:3201:AGS:N3	9:G:3201:AGS:C2'	2.83	0.41
7:J:198:TYR:CE2	7:J:248:ILE:HB	2.56	0.41
7:J:294:TYR:HD1	7:J:327:ILE:HD13	1.86	0.41
7:J:370:VAL:O	7:J:374:CYS:HB3	2.20	0.41
5:G:1931:GLU:OE2	5:G:1941:TYR:OH	2.38	0.41
6:I:166:ARG:NH2	3:L:425:GLU:O	2.50	0.41
6:I:188:VAL:HG23	6:I:189:GLU:N	2.35	0.41
8:K:290:GLU:OE1	8:K:290:GLU:HA	2.20	0.41
3:L:368:LEU:C	3:L:368:LEU:HD12	2.41	0.41
1:A:219:GLU:CD	1:A:219:GLU:N	2.74	0.41
1:E:258:SER:O	1:E:262:GLN:HG3	2.21	0.41
3:M:284:THR:HG21	3:M:298:GLY:HA2	2.02	0.41
5:G:1981:ASN:O	5:G:1981:ASN:ND2	2.50	0.41
7:J:105:LEU:O	7:J:134:VAL:HA	2.20	0.41
7:J:208:ILE:N	7:J:208:ILE:HD13	2.34	0.41
7:J:226:GLU:HB3	7:J:255:PHE:CZ	2.55	0.41
7:J:294:TYR:O	7:J:327:ILE:HD12	2.20	0.41
8:K:172:LEU:HD13	8:K:172:LEU:C	2.40	0.41
1:A:42:GLN:NE2	1:A:364:MET:O	2.53	0.41
1:C:26:LEU:HD23	1:C:32:ALA:HA	2.03	0.41
4:F:27:HIS:CE1	9:F:501:AGS:H8	2.55	0.41
5:G:1161:ARG:CD	8:K:191:GLU:O	2.69	0.41
3:L:96:TRP:CD1	3:L:135:LYS:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLY:O	1:A:258:SER:OG	2.36	0.41
1:A:276:ARG:HD2	1:A:276:ARG:HA	1.93	0.41
1:E:291:ILE:N	1:E:291:ILE:HD12	2.36	0.41
1:E:411:THR:N	1:E:412:PRO:HD2	2.36	0.41
2:H:436:VAL:HG12	2:H:436:VAL:O	2.21	0.41
3:M:387:VAL:HG13	3:M:388:GLU:N	2.36	0.41
4:B:136:GLU:O	4:B:137:ILE:HD13	2.20	0.41
5:G:1404:PHE:O	5:G:1405:TRP:HB2	2.21	0.41
5:G:2215:GLN:OE1	5:G:2215:GLN:C	2.58	0.41
7:J:36:GLY:C	7:J:65:LEU:HD11	2.41	0.41
3:L:35:VAL:HG22	3:L:36:ASP:N	2.36	0.41
3:L:140:MET:HE3	3:L:140:MET:HA	2.02	0.41
3:L:205:GLN:O	3:L:208:GLU:HG3	2.20	0.41
3:L:210:PHE:O	3:L:214:ASN:N	2.54	0.41
3:L:416:TYR:CE1	3:L:420:GLY:HA3	2.55	0.41
4:D:333:THR:HG22	4:D:334:ARG:N	2.36	0.41
5:G:809:LYS:HD2	5:G:814:TYR:CE1	2.56	0.41
5:G:2150:GLU:O	5:G:2154:ASP:OD1	2.39	0.41
6:I:162:ASP:OD1	6:I:162:ASP:C	2.58	0.41
1:A:183:GLU:OE2	1:A:201:LYS:HD2	2.21	0.41
1:E:313:THR:HG21	4:D:303:MET:CG	2.51	0.41
1:C:70:GLY:O	1:C:76:LYS:NZ	2.54	0.41
4:D:141:GLU:HG3	4:D:208:SER:CB	2.50	0.41
4:F:31:LEU:HD23	4:F:33:LEU:HD21	2.02	0.41
4:F:117:GLU:O	4:F:121:GLN:HG3	2.21	0.41
5:G:831:ARG:O	5:G:834:VAL:HG22	2.21	0.41
5:G:875:ARG:HH22	8:K:207:CYS:CA	2.34	0.41
6:I:167:PHE:HB2	6:I:174:ILE:HG13	2.02	0.41
7:J:105:LEU:HD13	7:J:119:MET:SD	2.61	0.41
7:J:140:LEU:O	7:J:342:GLY:HA3	2.21	0.41
7:J:314:GLN:OE1	7:J:327:ILE:HG23	2.20	0.41
7:J:317:ILE:O	7:J:317:ILE:CG1	2.69	0.41
3:L:44:VAL:HB	3:L:67:THR:OG1	2.21	0.41
3:L:68:TYR:CE2	3:L:101:ALA:HB3	2.56	0.41
3:L:230:ARG:H	3:L:230:ARG:NE	2.18	0.41
3:L:275:ASP:OD2	3:L:277:GLN:NE2	2.53	0.41
3:L:326:SER:HA	3:L:329:VAL:HG12	2.02	0.41
3:L:326:SER:O	3:L:329:VAL:HG12	2.21	0.41
3:M:333:VAL:HG11	3:M:345:TYR:CZ	2.56	0.41
4:B:124:ARG:NE	4:B:248:ASP:OD2	2.45	0.41
4:F:170:THR:HA	8:K:302:ARG:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:174:LEU:HD22	4:F:178:MET:HG2	2.03	0.41
5:G:888:VAL:HG22	5:G:2167:LEU:HD22	2.03	0.41
5:G:1131:ALA:HB2	5:G:1163:CYS:SG	2.61	0.41
8:K:188:GLU:C	8:K:189:THR:HG23	2.42	0.41
3:L:15:VAL:HG21	3:L:398:SER:HA	2.03	0.41
4:B:196:ASP:HB2	4:B:201:LYS:HE3	2.03	0.40
1:C:168:LYS:HB3	1:C:168:LYS:HE2	1.94	0.40
5:G:1336:TYR:O	5:G:1339:VAL:HG12	2.21	0.40
5:G:1923:MET:O	5:G:1927:LEU:HD13	2.21	0.40
5:G:2164:LYS:C	5:G:2164:LYS:HD2	2.42	0.40
6:I:163:LEU:HD13	6:I:163:LEU:C	2.42	0.40
3:L:356:LEU:HD11	3:L:389:ARG:HG3	2.02	0.40
4:B:178:MET:SD	4:B:178:MET:N	2.93	0.40
4:B:350:LEU:O	4:B:354:LEU:HD13	2.21	0.40
4:D:143:VAL:O	4:D:143:VAL:HG22	2.21	0.40
4:D:319:ASP:OD1	4:D:319:ASP:N	2.55	0.40
5:G:2174:HIS:CE1	8:K:181:GLU:OE2	2.74	0.40
3:M:112:LYS:N	3:M:112:LYS:HD3	2.36	0.40
4:B:268:ILE:H	4:B:268:ILE:HD12	1.85	0.40
5:G:1164:PRO:HG2	8:K:180:GLU:OE2	2.21	0.40
5:G:2173:PHE:N	5:G:2173:PHE:CD1	2.88	0.40
6:I:98:MET:CE	6:I:100:PHE:HB3	2.52	0.40
6:I:165:ARG:O	6:I:165:ARG:CZ	2.67	0.40
7:J:242:LEU:N	7:J:242:LEU:HD22	2.36	0.40
3:L:219:PRO:HA	3:L:254:MET:HE1	2.04	0.40
3:L:275:ASP:OD1	3:L:277:GLN:HG3	2.22	0.40
1:E:147:MET:H	1:E:147:MET:HE2	1.85	0.40
4:B:137:ILE:HD12	4:B:194:THR:CG2	2.51	0.40
4:F:18:ARG:NH1	1:A:288:ASP:OD1	2.47	0.40
5:G:2223:TYR:HE2	5:G:2228:ALA:CB	2.34	0.40
7:J:183:ARG:NE	7:J:183:ARG:HA	2.37	0.40
8:K:306:THR:O	8:K:308:ILE:N	2.54	0.40
3:L:310:ASP:O	3:L:313:ASN:OD1	2.40	0.40
1:A:271:ILE:HG23	1:A:275:LEU:HD23	2.04	0.40
4:D:240:HIS:HD1	5:G:1819:ARG:HD2	1.87	0.40
4:F:347:PRO:HB2	4:F:349:ASP:OD1	2.21	0.40
5:G:846:ARG:NE	5:G:2214:GLU:OE2	2.55	0.40
5:G:1920:LEU:HD21	5:G:1971:LEU:HD23	2.04	0.40
5:G:2173:PHE:N	5:G:2173:PHE:HD1	2.18	0.40
5:G:2174:HIS:O	5:G:2175:THR:HG23	2.21	0.40
1:A:53:VAL:HG22	1:A:83:ILE:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	410/456 (90%)	386 (94%)	21 (5%)	3 (1%)	19 32
1	C	421/456 (92%)	407 (97%)	14 (3%)	0	100 100
1	E	435/456 (95%)	412 (95%)	22 (5%)	1 (0%)	44 63
2	H	46/836 (6%)	44 (96%)	2 (4%)	0	100 100
3	L	400/429 (93%)	384 (96%)	15 (4%)	1 (0%)	37 55
3	M	314/429 (73%)	297 (95%)	16 (5%)	1 (0%)	37 55
4	B	381/463 (82%)	364 (96%)	16 (4%)	1 (0%)	37 55
4	D	427/463 (92%)	402 (94%)	24 (6%)	1 (0%)	44 63
4	F	425/463 (92%)	407 (96%)	18 (4%)	0	100 100
5	G	862/3159 (27%)	807 (94%)	50 (6%)	5 (1%)	22 36
6	I	175/467 (38%)	161 (92%)	14 (8%)	0	100 100
7	J	356/375 (95%)	334 (94%)	22 (6%)	0	100 100
8	K	119/364 (33%)	99 (83%)	15 (13%)	5 (4%)	2 2
All	All	4771/8816 (54%)	4504 (94%)	249 (5%)	18 (0%)	32 47

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	G	2014	LYS
8	K	201	VAL
8	K	207	CYS
8	K	208	PRO
8	K	280	GLN
3	L	73	ASN
1	A	135	VAL

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Mol	Chain	Res	Type
1	A	164	ALA
1	E	232	LYS
5	G	2034	ASN
5	G	2232	GLU
1	A	224	PRO
5	G	2174	HIS
8	K	307	ASP
4	B	236	LYS
5	G	2236	GLU
4	D	332	ILE
3	M	282	MET

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	352/387 (91%)	335 (95%)	17 (5%)	21 39
1	C	360/387 (93%)	350 (97%)	10 (3%)	38 60
1	E	365/387 (94%)	346 (95%)	19 (5%)	19 35
2	H	40/738 (5%)	35 (88%)	5 (12%)	3 6
3	L	346/364 (95%)	316 (91%)	30 (9%)	8 15
3	M	278/364 (76%)	257 (92%)	21 (8%)	11 19
4	B	330/390 (85%)	321 (97%)	9 (3%)	40 61
4	D	356/390 (91%)	347 (98%)	9 (2%)	42 64
4	F	361/390 (93%)	350 (97%)	11 (3%)	36 58
5	G	779/2663 (29%)	721 (93%)	58 (7%)	11 20
6	I	159/400 (40%)	139 (87%)	20 (13%)	3 5
7	J	306/318 (96%)	289 (94%)	17 (6%)	17 32
8	K	112/312 (36%)	107 (96%)	5 (4%)	23 42
All	All	4144/7490 (55%)	3913 (94%)	231 (6%)	20 32

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	96	MET
1	E	147	MET
1	E	178	GLU
1	E	179	SER
1	E	184	ARG
1	E	191	ILE
1	E	192	TYR
1	E	196	ASN
1	E	200	VAL
1	E	203	GLN
1	E	211	THR
1	E	225	LYS
1	E	230	LYS
1	E	232	LYS
1	E	237	ASP
1	E	249	ARG
1	E	259	MET
1	E	353	ASP
1	E	357	ARG
2	H	449	GLN
2	H	456	ARG
2	H	457	ARG
2	H	468	ASP
2	H	475	ASP
3	M	16	PHE
3	M	17	ASP
3	M	92	MET
3	M	97	ASP
3	M	99	PHE
3	M	104	ASP
3	M	107	TYR
3	M	130	ARG
3	M	135	LYS
3	M	142	GLU
3	M	153	LYS
3	M	262	PHE
3	M	263	GLN
3	M	287	TYR
3	M	308	LEU
3	M	327	HIS
3	M	360	PHE
3	M	366	ARG
3	M	410	TRP

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Mol	Chain	Res	Type
3	M	416	TYR
3	M	427	LYS
4	B	47	VAL
4	B	88	MET
4	B	178	MET
4	B	179	ILE
4	B	180	GLU
4	B	201	LYS
4	B	264	ASP
4	B	357	VAL
4	B	448	ASP
1	C	127	THR
1	C	168	LYS
1	C	173	ASP
1	C	185	VAL
1	C	230	LYS
1	C	262	GLN
1	C	316	HIS
1	C	336	CYS
1	C	343	ASP
1	C	353	ASP
4	D	184	LYS
4	D	197	LYS
4	D	208	SER
4	D	215	TYR
4	D	236	LYS
4	D	253	ARG
4	D	258	LEU
4	D	353	ARG
4	D	444	LYS
4	F	33	LEU
4	F	34	ASP
4	F	46	MET
4	F	88	MET
4	F	142	VAL
4	F	185	ASP
4	F	209	PHE
4	F	216	ASP
4	F	218	MET
4	F	235	ARG
4	F	236	LYS
5	G	790	LYS

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Mol	Chain	Res	Type
5	G	794	TRP
5	G	813	ASP
5	G	816	LEU
5	G	819	MET
5	G	846	ARG
5	G	875	ARG
5	G	901	LYS
5	G	1092	ARG
5	G	1122	LYS
5	G	1130	PHE
5	G	1139	ASN
5	G	1155	TRP
5	G	1171	TYR
5	G	1185	TRP
5	G	1221	MET
5	G	1222	GLN
5	G	1313	GLU
5	G	1314	LYS
5	G	1319	LYS
5	G	1324	LEU
5	G	1325	LYS
5	G	1327	ARG
5	G	1375	GLU
5	G	1412	MET
5	G	1420	ASN
5	G	1428	GLU
5	G	1433	LYS
5	G	1444	SER
5	G	1457	LYS
5	G	1459	LYS
5	G	1739	GLN
5	G	1744	ARG
5	G	1746	LEU
5	G	1749	ARG
5	G	1763	GLN
5	G	1819	ARG
5	G	1868	HIS
5	G	1872	TYR
5	G	1884	LEU
5	G	1918	LEU
5	G	1954	GLN
5	G	1968	CYS

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Mol	Chain	Res	Type
5	G	1981	ASN
5	G	2014	LYS
5	G	2151	GLU
5	G	2156	MET
5	G	2164	LYS
5	G	2165	TYR
5	G	2167	LEU
5	G	2169	TYR
5	G	2181	LYS
5	G	2187	ASP
5	G	2212	ARG
5	G	2216	GLU
5	G	2231	MET
5	G	2256	ASP
5	G	2267	CYS
6	I	65	LYS
6	I	66	LYS
6	I	102	ASN
6	I	110	MET
6	I	113	HIS
6	I	115	ARG
6	I	146	TYR
6	I	152	TRP
6	I	159	HIS
6	I	165	ARG
6	I	171	PHE
6	I	175	HIS
6	I	177	ARG
6	I	182	GLN
6	I	195	TYR
6	I	196	TYR
6	I	226	ARG
6	I	232	ARG
6	I	240	GLN
6	I	246	TYR
7	J	14	SER
7	J	68	LYS
7	J	83	GLU
7	J	95	ARG
7	J	128	ASN
7	J	169	TYR
7	J	190	MET

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Mol	Chain	Res	Type
7	J	234	SER
7	J	271	SER
7	J	272	CYS
7	J	279	PHE
7	J	284	LYS
7	J	305	MET
7	J	311	ASP
7	J	312	ARG
7	J	326	LYS
7	J	355	MET
8	K	193	LEU
8	K	197	LYS
8	K	271	ASP
8	K	282	ARG
8	K	300	LEU
3	L	9	ASP
3	L	68	TYR
3	L	89	LYS
3	L	130	ARG
3	L	140	MET
3	L	160	PHE
3	L	176	HIS
3	L	209	LEU
3	L	213	MET
3	L	230	ARG
3	L	236	ASN
3	L	248	ARG
3	L	253	TYR
3	L	257	CYS
3	L	272	SER
3	L	282	MET
3	L	300	GLU
3	L	327	HIS
3	L	330	THR
3	L	335	MET
3	L	350	VAL
3	L	366	ARG
3	L	376	MET
3	L	378	LEU
3	L	390	ARG
3	L	392	SER
3	L	422	GLN

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Mol	Chain	Res	Type
3	L	423	CYS
3	L	425	GLU
3	L	426	ARG
1	A	13	GLN
1	A	40	VAL
1	A	138	LEU
1	A	140	PRO
1	A	156	HIS
1	A	173	ASP
1	A	177	PHE
1	A	178	GLU
1	A	192	TYR
1	A	207	ASP
1	A	209	TYR
1	A	225	LYS
1	A	227	ASP
1	A	233	GLU
1	A	235	ILE
1	A	249	ARG
1	A	336	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	196	ASN
1	E	203	GLN
1	E	262	GLN
3	M	143	HIS
4	B	302	HIS
5	G	847	HIS
5	G	1192	HIS
5	G	1937	HIS
6	I	113	HIS
7	J	12	ASN
3	L	143	HIS
3	L	414	GLN
1	A	348	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	AGS	E	501	-	28,33,33	0.87	1 (3%)	31,52,52	1.00	2 (6%)
9	AGS	D	501	-	28,33,33	0.91	2 (7%)	31,52,52	1.20	3 (9%)
9	AGS	G	3201	-	28,33,33	0.72	1 (3%)	31,52,52	0.97	2 (6%)
9	AGS	F	501	-	28,33,33	0.79	1 (3%)	31,52,52	1.01	2 (6%)
9	AGS	C	501	-	28,33,33	0.98	3 (10%)	31,52,52	1.34	3 (9%)
10	ATP	L	501	-	28,33,33	0.67	0	34,52,52	0.95	2 (5%)
9	AGS	B	501	-	28,33,33	0.79	1 (3%)	31,52,52	0.89	2 (6%)
9	AGS	A	501	-	28,33,33	0.95	1 (3%)	31,52,52	1.07	2 (6%)

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
9	AGS	E	501	-	-	4/17/38/38	0/3/3/3
9	AGS	D	501	-	-	7/17/38/38	0/3/3/3
9	AGS	G	3201	-	-	9/17/38/38	0/3/3/3
9	AGS	F	501	-	-	4/17/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	AGS	C	501	-	-	4/17/38/38	0/3/3/3
10	ATP	L	501	-	-	7/18/38/38	0/3/3/3
9	AGS	B	501	-	-	4/17/38/38	0/3/3/3
9	AGS	A	501	-	-	5/17/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	501	AGS	PA-O3A	-2.33	1.57	1.59
9	E	501	AGS	PG-S1G	2.16	1.95	1.90
9	A	501	AGS	PG-S1G	2.15	1.95	1.90
9	B	501	AGS	PG-S1G	2.15	1.95	1.90
9	C	501	AGS	PB-O3A	-2.13	1.57	1.59
9	G	3201	AGS	PG-S1G	2.12	1.95	1.90
9	D	501	AGS	PA-O3A	-2.11	1.57	1.59
9	F	501	AGS	PG-S1G	2.08	1.95	1.90
9	C	501	AGS	PG-S1G	2.07	1.95	1.90
9	D	501	AGS	PG-S1G	2.03	1.95	1.90

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	501	AGS	PB-O3B-PG	-4.59	116.36	133.17
9	C	501	AGS	O4'-C1'-N9	4.29	114.43	108.75
9	C	501	AGS	PB-O3B-PG	-4.19	117.83	133.17
9	E	501	AGS	PB-O3B-PG	-4.10	118.15	133.17
9	F	501	AGS	PB-O3B-PG	-3.92	118.84	133.17
9	D	501	AGS	C4'-O4'-C1'	-3.78	106.46	109.92
9	D	501	AGS	PB-O3B-PG	-3.74	119.47	133.17
9	G	3201	AGS	PB-O3B-PG	-3.50	120.36	133.17
9	B	501	AGS	PB-O3B-PG	-2.93	122.45	133.17
9	F	501	AGS	C5-C6-N6	2.36	123.91	120.31
9	D	501	AGS	C5-C6-N6	2.34	123.88	120.31
10	L	501	ATP	C5-C6-N6	2.34	123.87	120.31
9	C	501	AGS	C5-C6-N6	2.33	123.87	120.31
9	A	501	AGS	C5-C6-N6	2.29	123.79	120.31
9	E	501	AGS	C5-C6-N6	2.28	123.79	120.31
9	B	501	AGS	C5-C6-N6	2.28	123.78	120.31
10	L	501	ATP	O3'-C3'-C2'	-2.28	104.52	111.82
9	G	3201	AGS	C5-C6-N6	2.20	123.66	120.31

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	E	501	AGS	PB-O3B-PG-O3G
9	B	501	AGS	PB-O3B-PG-O3G
9	C	501	AGS	PB-O3B-PG-O3G
9	D	501	AGS	PB-O3B-PG-O2G
9	D	501	AGS	PB-O3B-PG-O3G
9	D	501	AGS	C5'-O5'-PA-O1A
9	D	501	AGS	C4'-C5'-O5'-PA
9	D	501	AGS	C3'-C4'-C5'-O5'
9	G	3201	AGS	PB-O3B-PG-O2G
9	G	3201	AGS	C5'-O5'-PA-O2A
9	G	3201	AGS	C5'-O5'-PA-O3A
9	A	501	AGS	C5'-O5'-PA-O2A
10	L	501	ATP	PB-O3B-PG-O2G
10	L	501	ATP	C3'-C4'-C5'-O5'
9	F	501	AGS	O4'-C4'-C5'-O5'
9	F	501	AGS	C3'-C4'-C5'-O5'
9	G	3201	AGS	C3'-C4'-C5'-O5'
10	L	501	ATP	O4'-C4'-C5'-O5'
9	D	501	AGS	O4'-C4'-C5'-O5'
9	G	3201	AGS	O4'-C4'-C5'-O5'
9	G	3201	AGS	C4'-C5'-O5'-PA
10	L	501	ATP	C4'-C5'-O5'-PA
9	B	501	AGS	PB-O3A-PA-O5'
10	L	501	ATP	PB-O3B-PG-O3G
9	E	501	AGS	PA-O3A-PB-O2B
9	A	501	AGS	PB-O3A-PA-O1A
9	C	501	AGS	C4'-C5'-O5'-PA
9	A	501	AGS	C4'-C5'-O5'-PA
9	E	501	AGS	C4'-C5'-O5'-PA
9	B	501	AGS	PA-O3A-PB-O2B
9	C	501	AGS	PA-O3A-PB-O2B
9	A	501	AGS	PA-O3A-PB-O2B
9	E	501	AGS	PB-O3B-PG-O2G
9	F	501	AGS	PB-O3B-PG-O2G
9	F	501	AGS	PB-O3B-PG-O3G
9	G	3201	AGS	PB-O3B-PG-O3G
9	C	501	AGS	PA-O3A-PB-O1B
9	D	501	AGS	PA-O3A-PB-O2B
9	G	3201	AGS	PB-O3A-PA-O2A
10	L	501	ATP	PB-O3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
9	B	501	AGS	PA-O3A-PB-O1B
9	G	3201	AGS	PB-O3A-PA-O1A
9	A	501	AGS	PB-O3A-PA-O2A
10	L	501	ATP	PA-O3A-PB-O2B

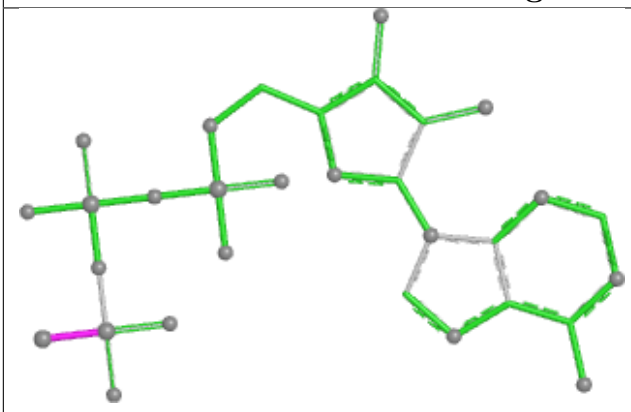
There are no ring outliers.

8 monomers are involved in 45 short contacts:

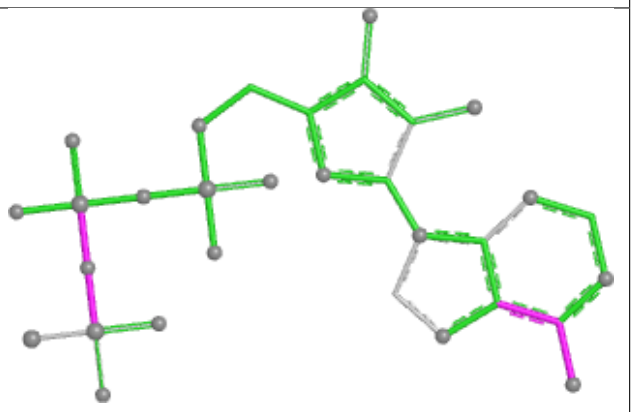
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	501	AGS	3	0
9	D	501	AGS	11	0
9	G	3201	AGS	4	0
9	F	501	AGS	12	0
9	C	501	AGS	7	0
10	L	501	ATP	1	0
9	B	501	AGS	3	0
9	A	501	AGS	4	0

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.

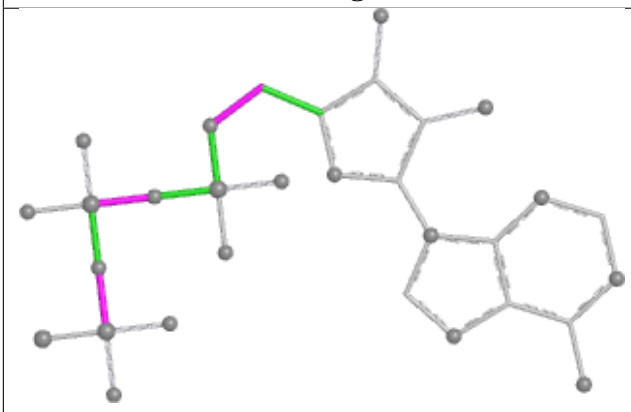
Ligand AGS E 501



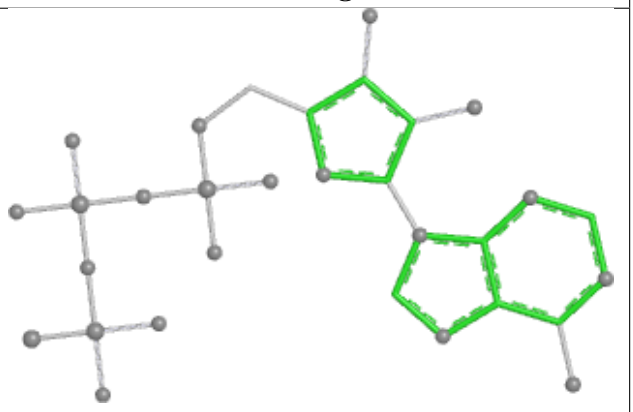
Bond lengths



Bond angles

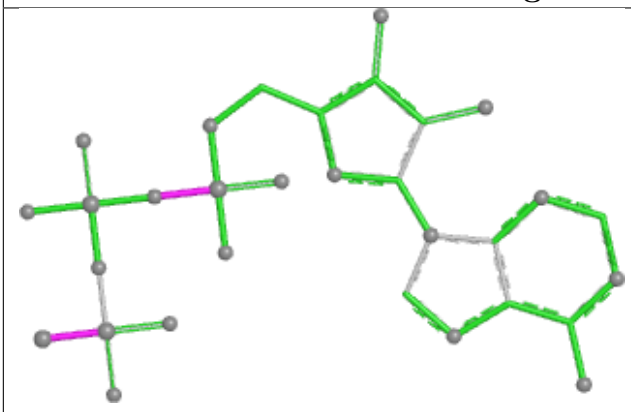


Torsions

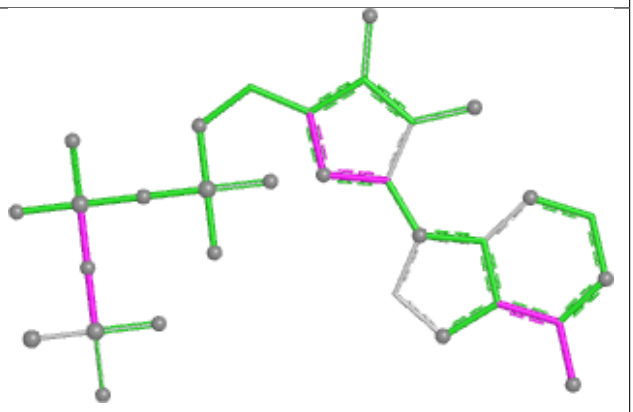


Rings

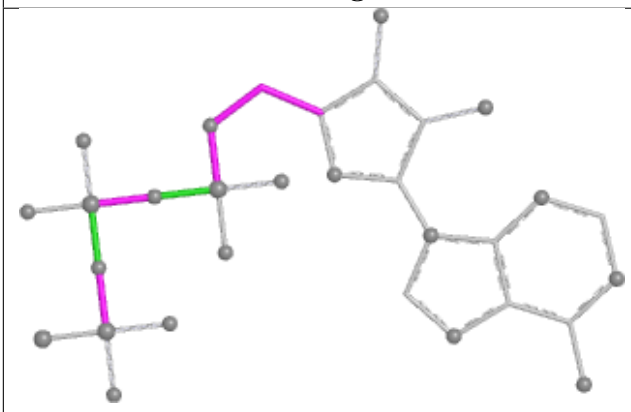
Ligand AGS D 501



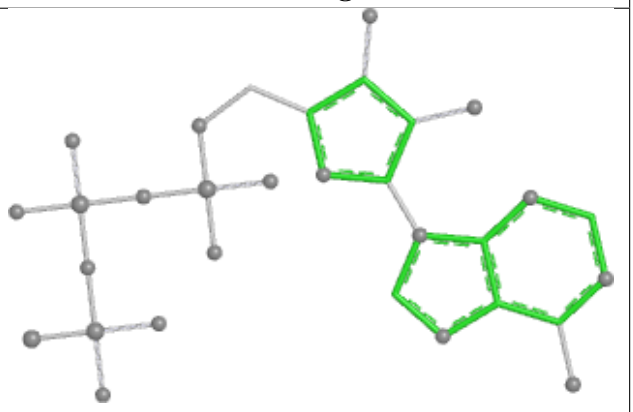
Bond lengths



Bond angles

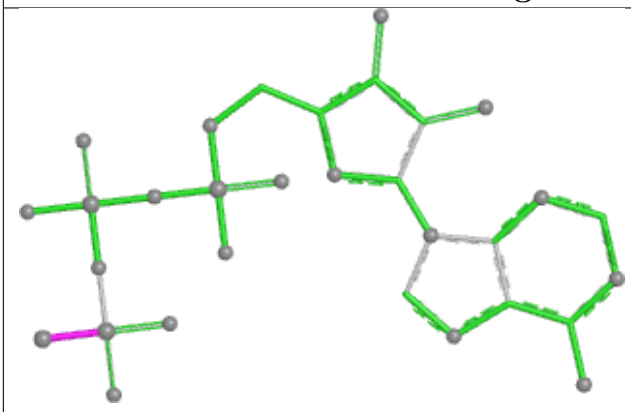


Torsions

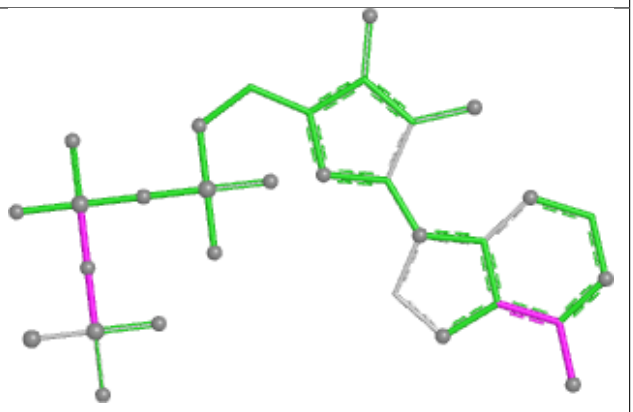


Rings

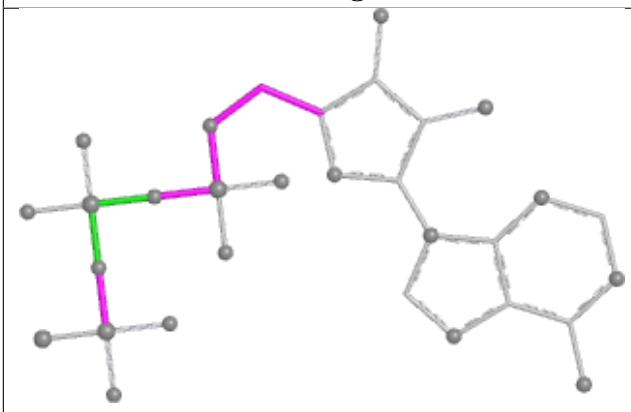
Ligand AGS G 3201



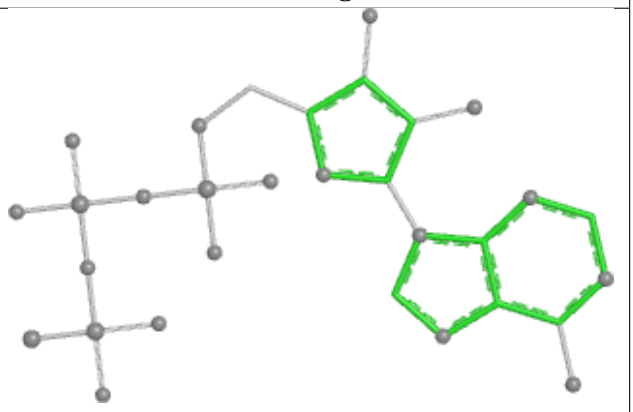
Bond lengths



Bond angles

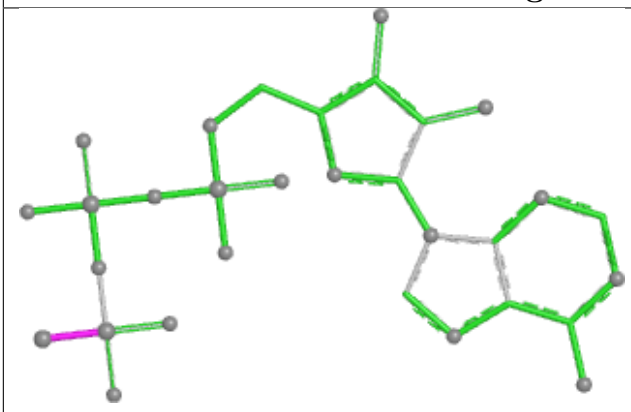


Torsions

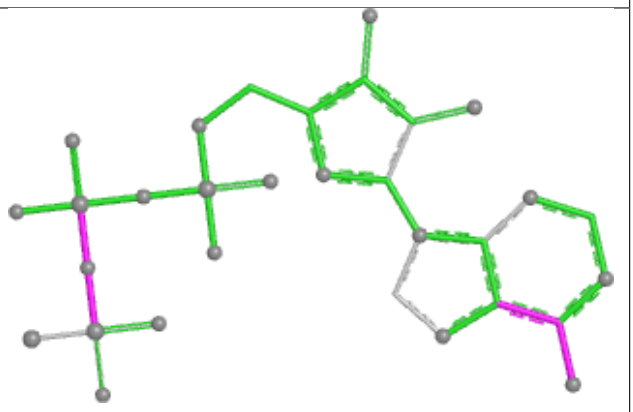


Rings

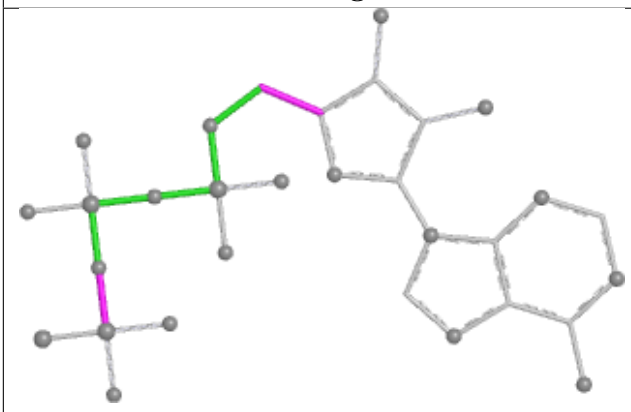
Ligand AGS F 501



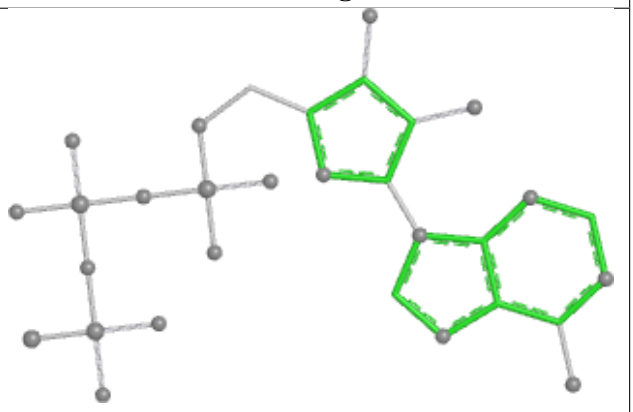
Bond lengths



Bond angles

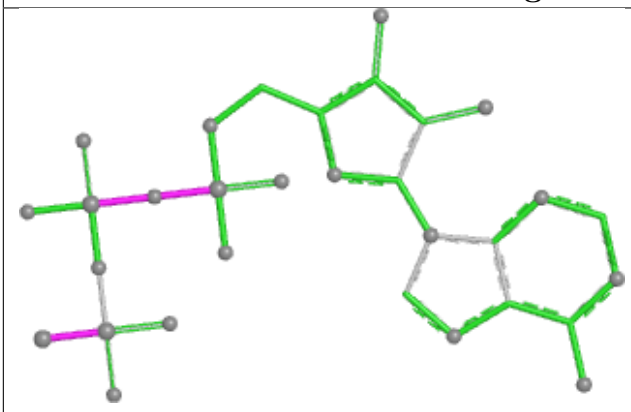


Torsions

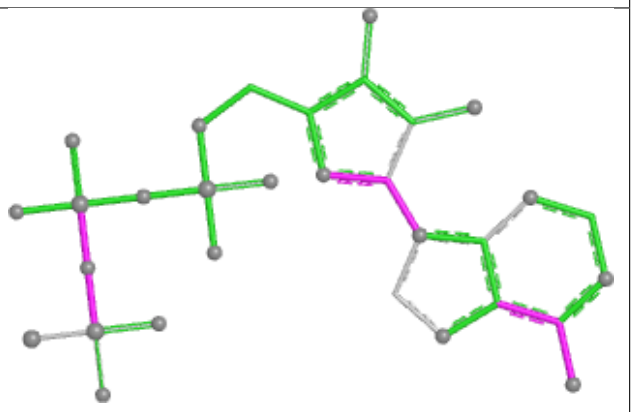


Rings

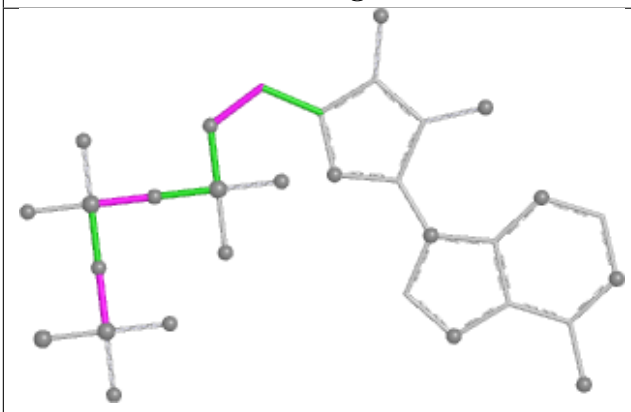
Ligand AGS C 501



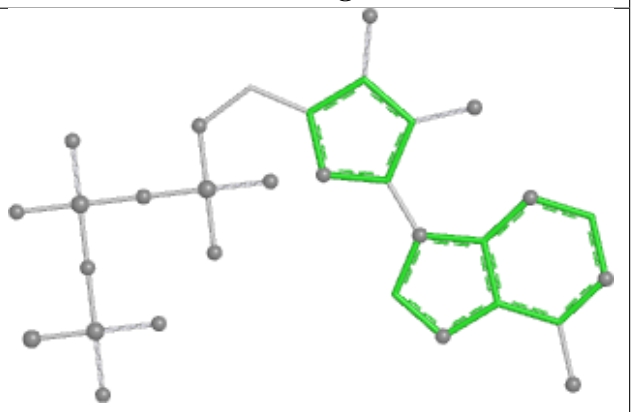
Bond lengths



Bond angles

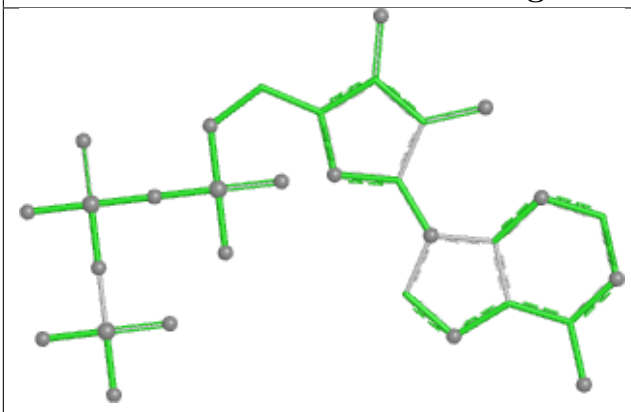


Torsions



Rings

Ligand ATP L 501



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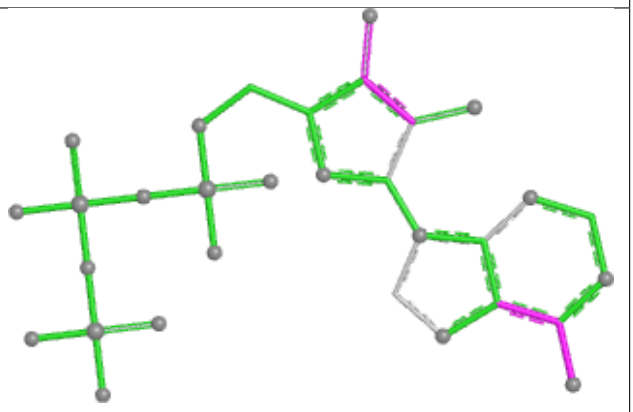
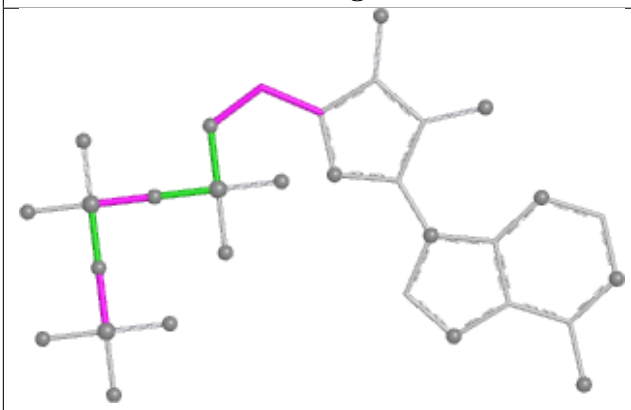
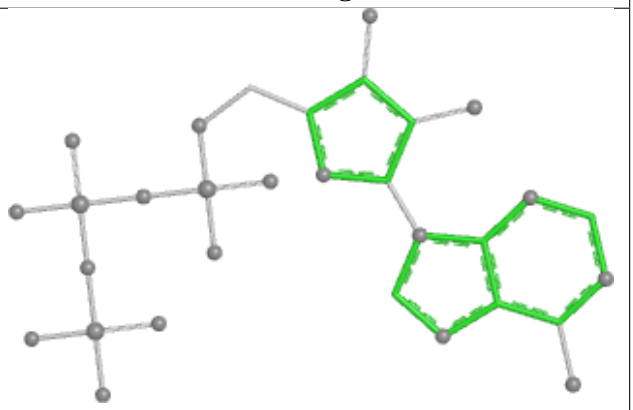


Bond angles

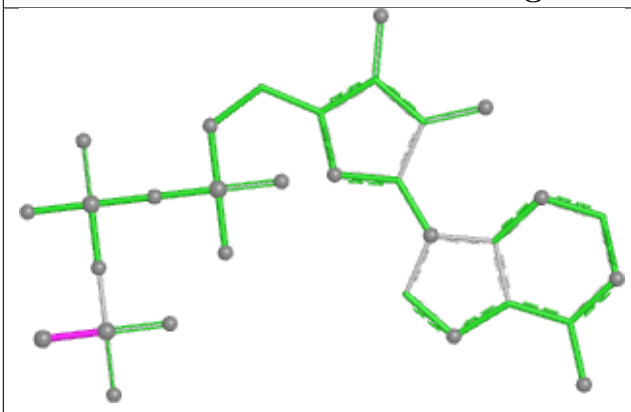


Torsions

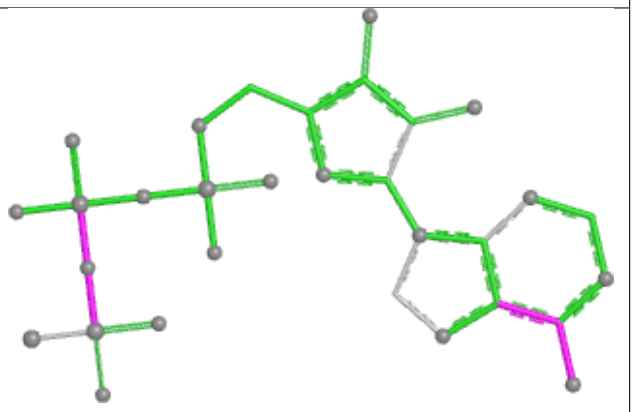


Rings

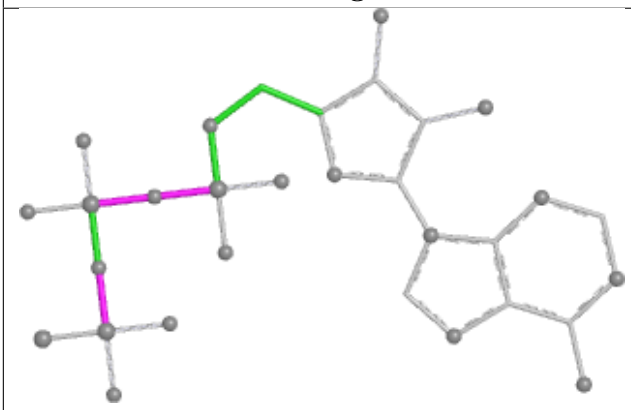
Ligand AGS B 501



Bond lengths



Bond angles



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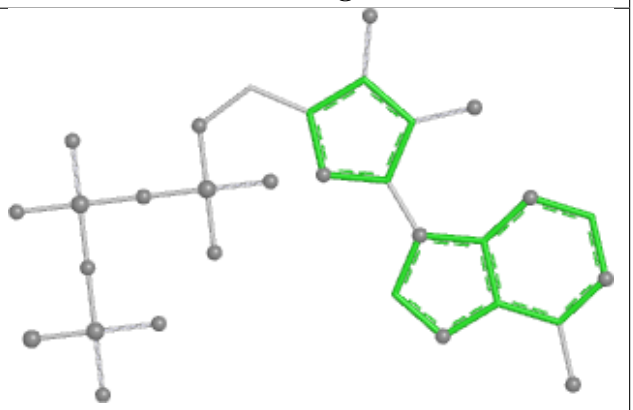
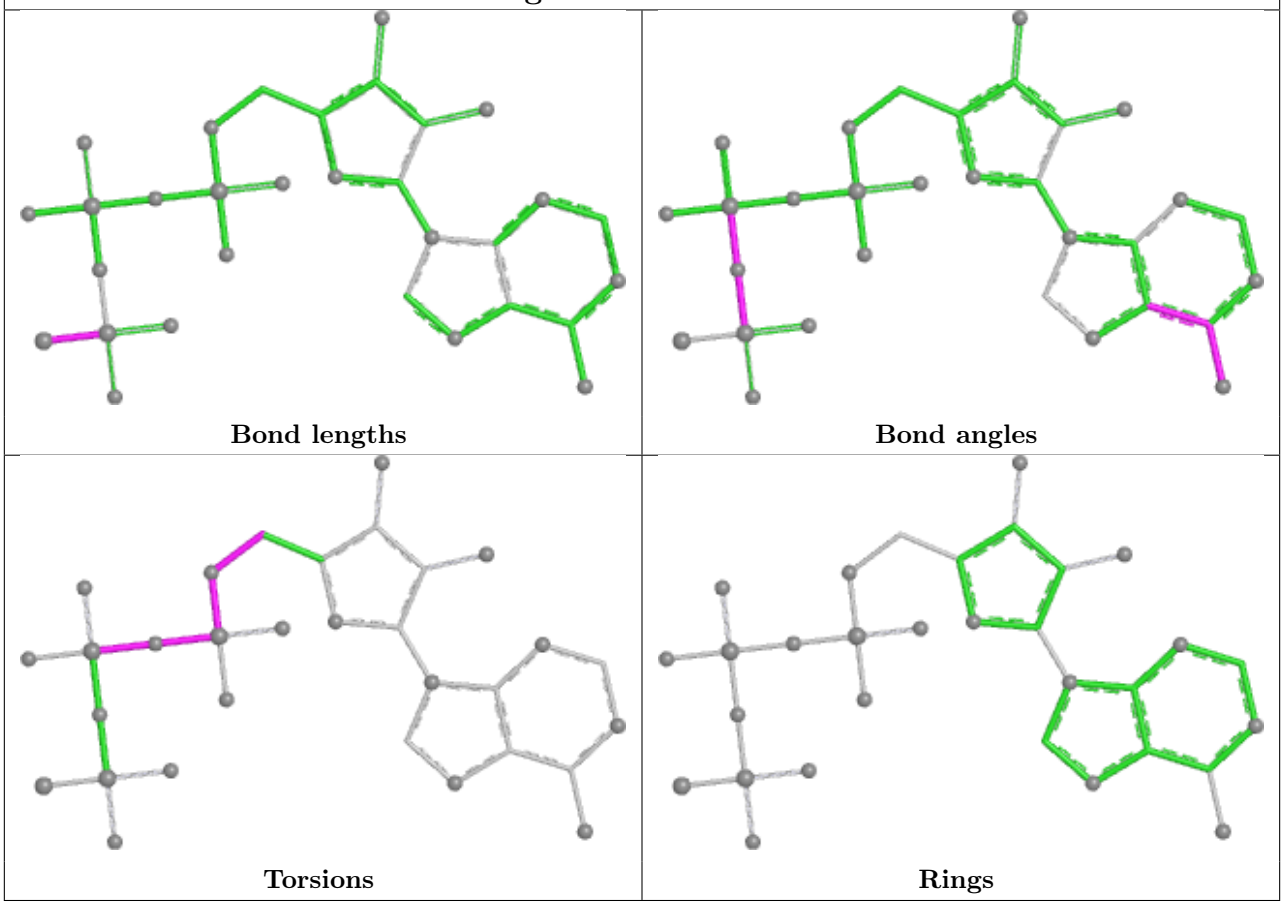


Rings

Ligand AGS A 501



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.

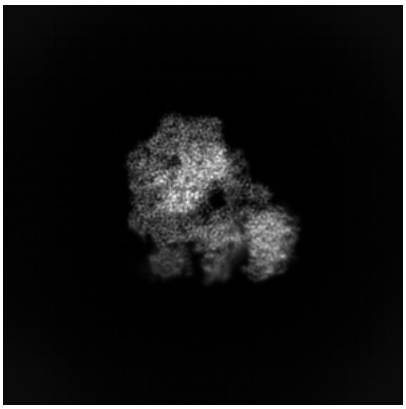
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45206. These allow visual inspection of the internal detail of the map and identification of artifacts.

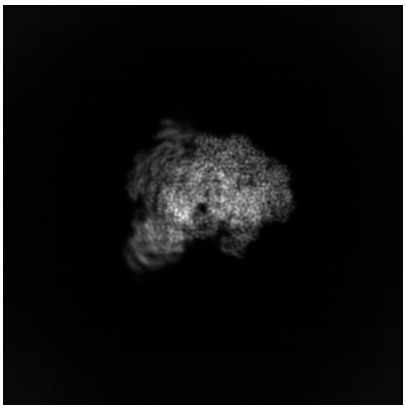
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

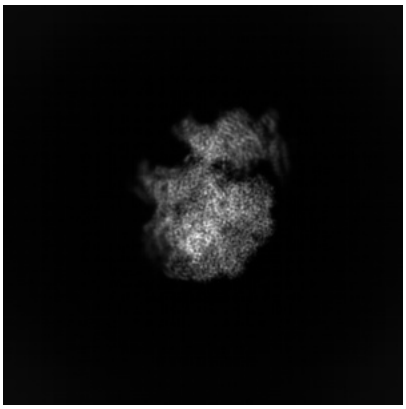
6.1.1 Primary map



X

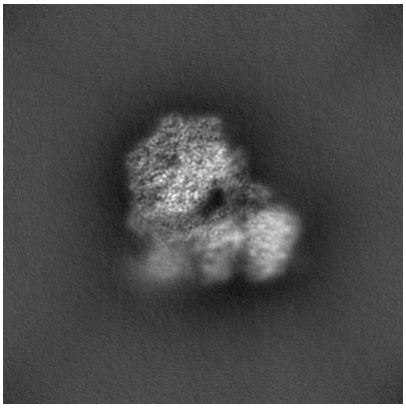


Y

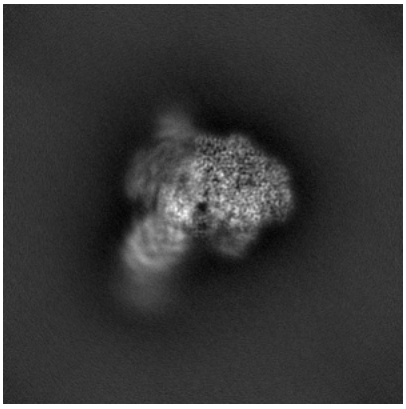


Z

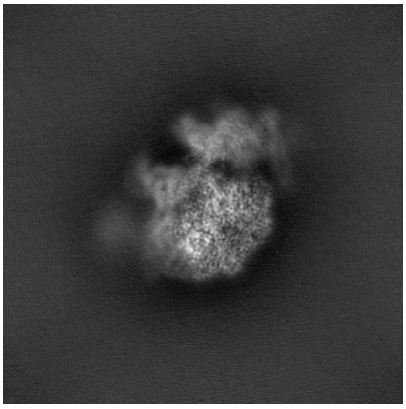
6.1.2 Raw map



X



Y

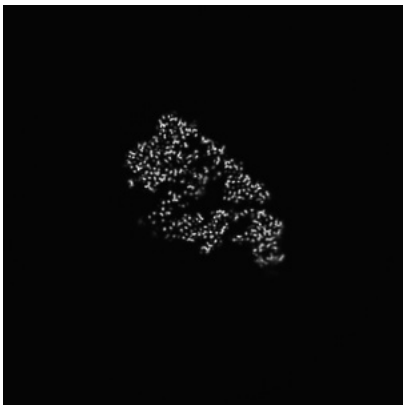


Z

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

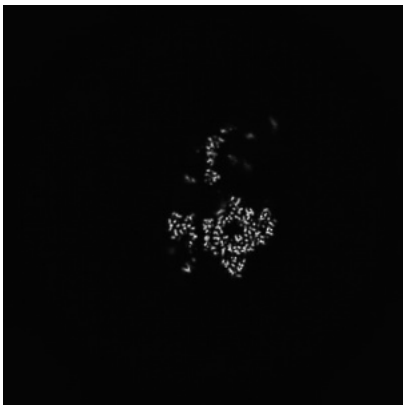
6.2 Central slices (i)

6.2.1 Primary map



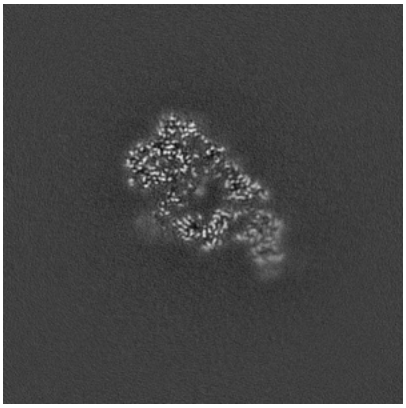
X Index: 188

Y Index: 188

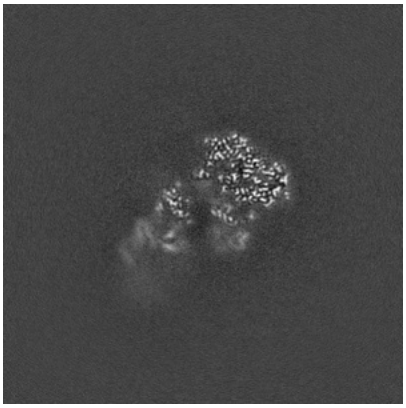


Z Index: 188

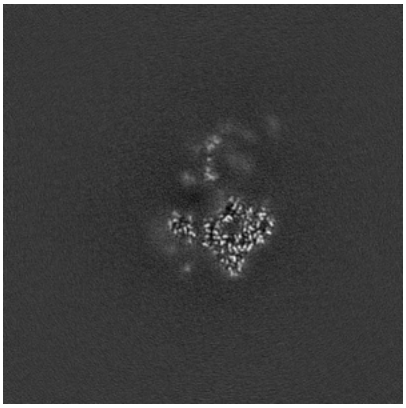
6.2.2 Raw map



X Index: 180



Y Index: 180

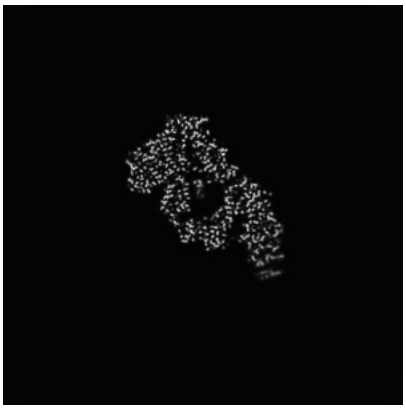


Z Index: 180

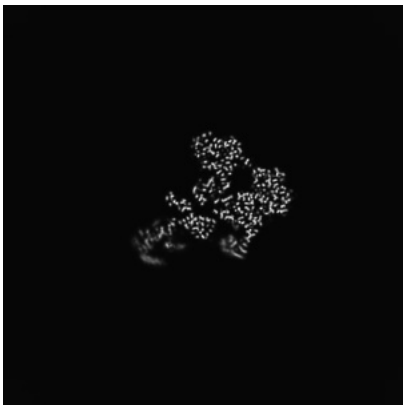
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



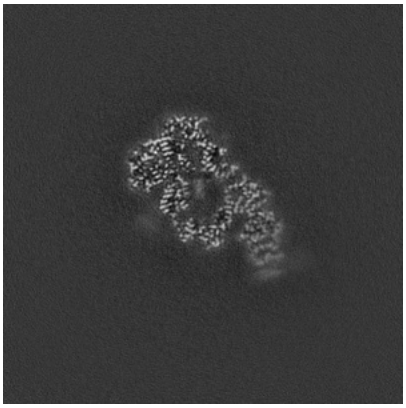
X Index: 194



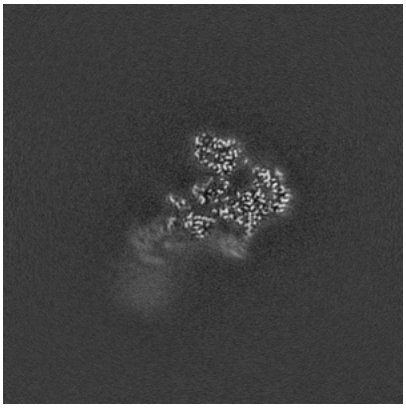
Y Index: 169

Z Index: 219

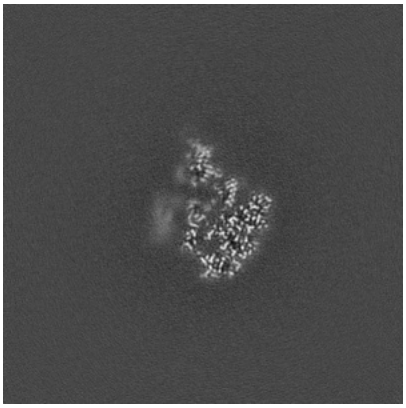
6.3.2 Raw map



X Index: 184



Y Index: 160

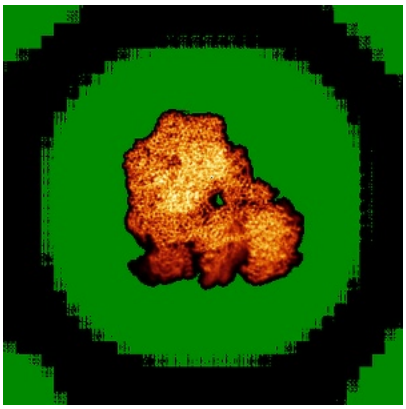


Z Index: 196

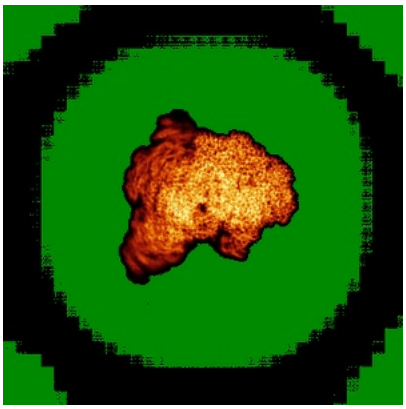
The images above show the largest variance slices of the map in three orthogonal directions.

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

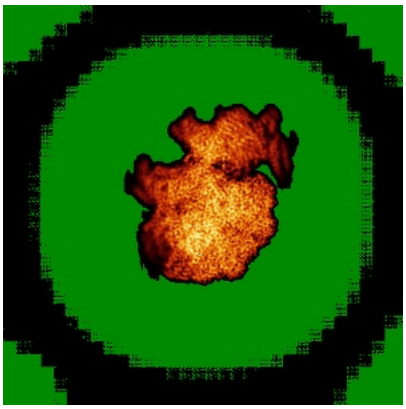
6.4.1 Primary map



X

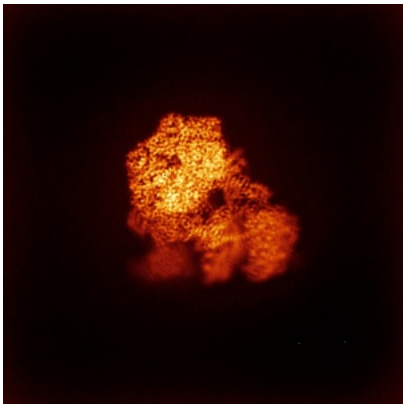


Y

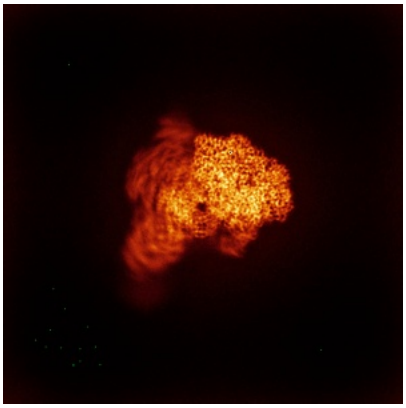


Z

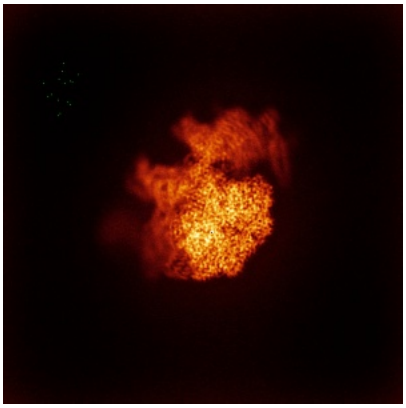
6.4.2 Raw map



X



Y

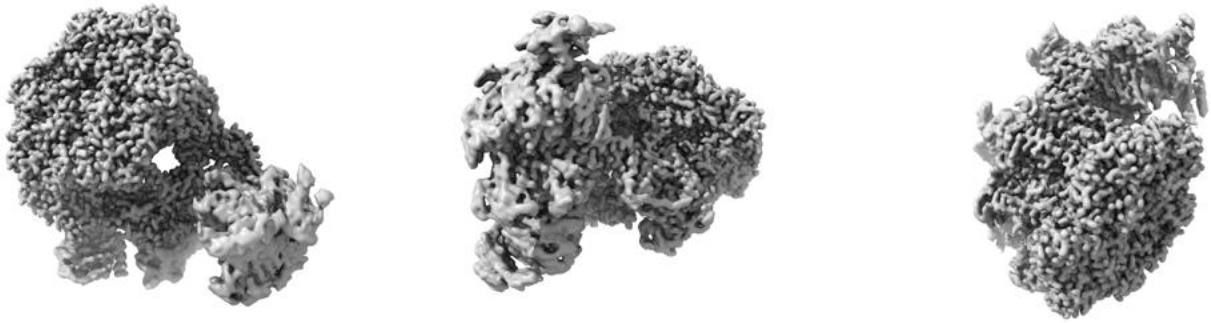


Z

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 2.4. 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.

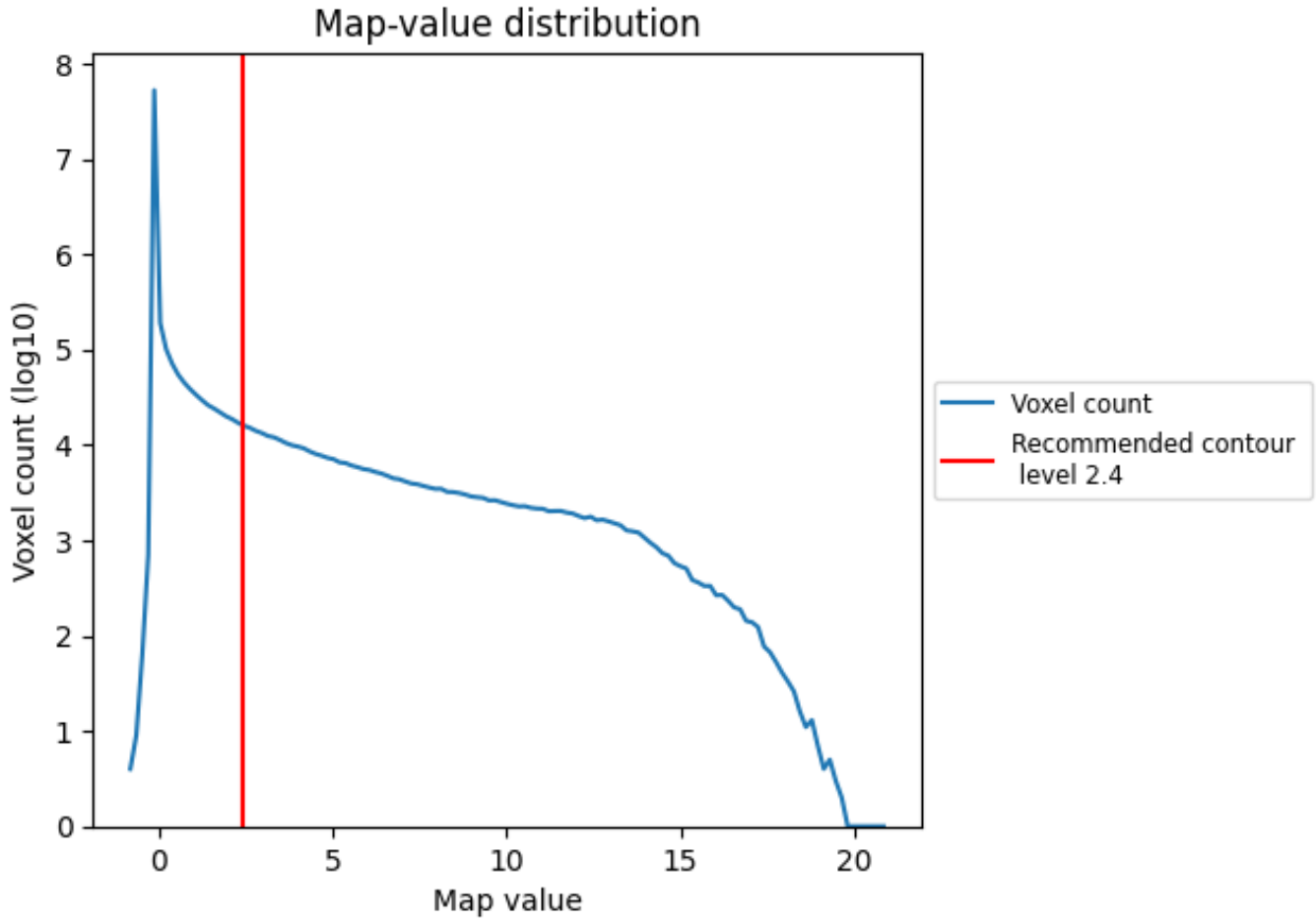
6.6 Mask visualisation (i)

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

7 Map analysis

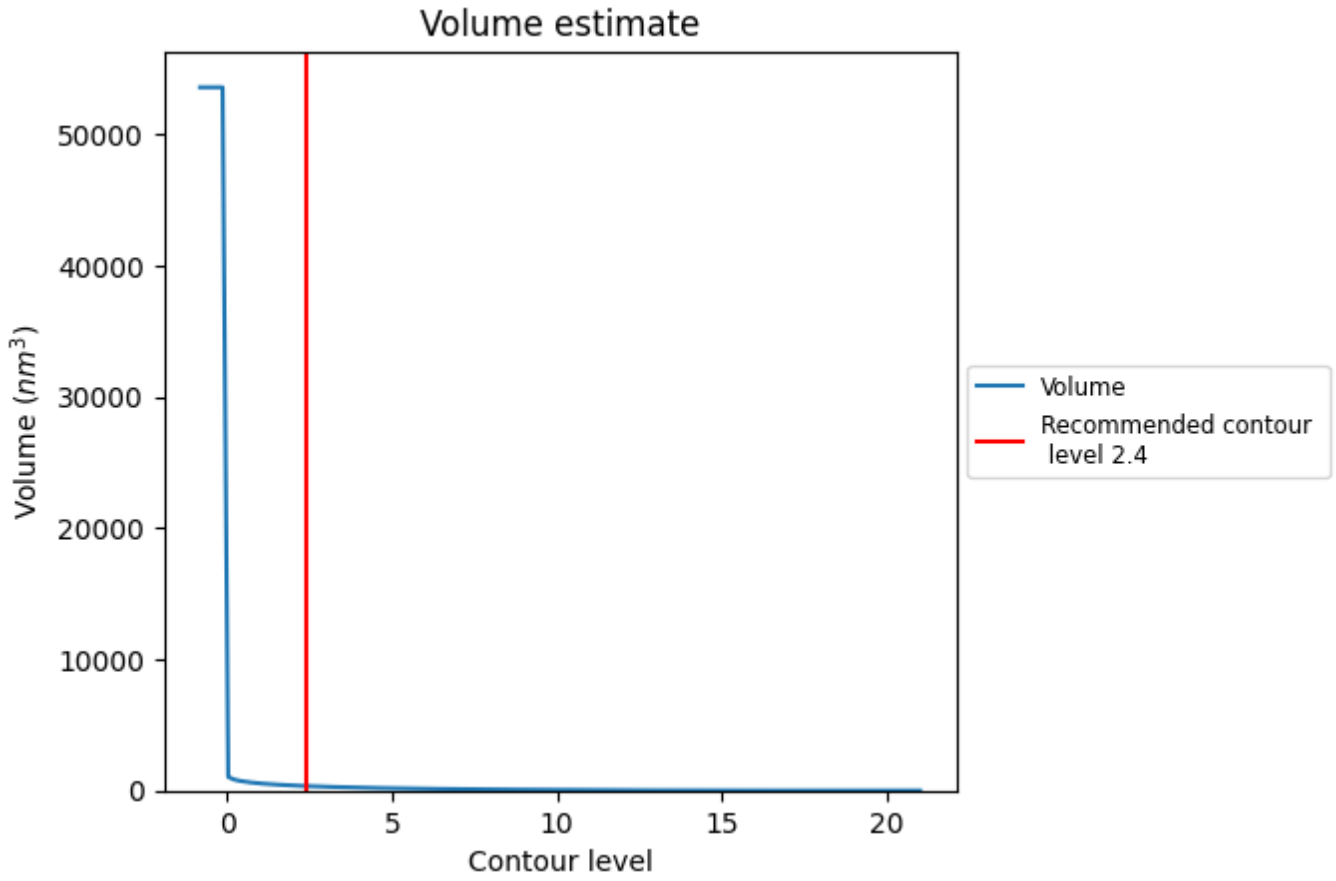
This section contains the results of statistical analysis of the map.

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.

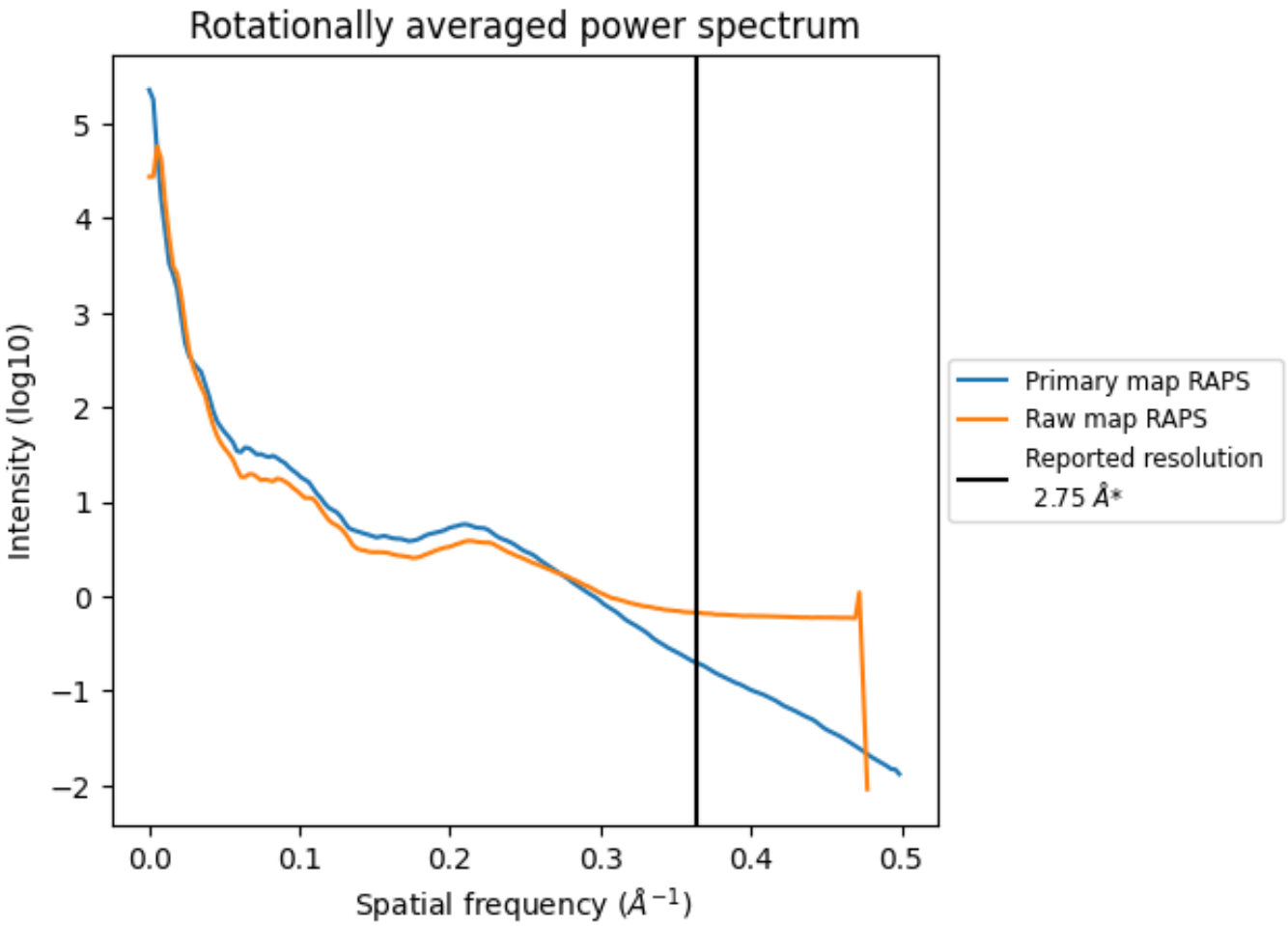
7.2 Volume estimate



The volume at the recommended contour level is 343 nm^3; this corresponds to an approximate mass of 310 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)

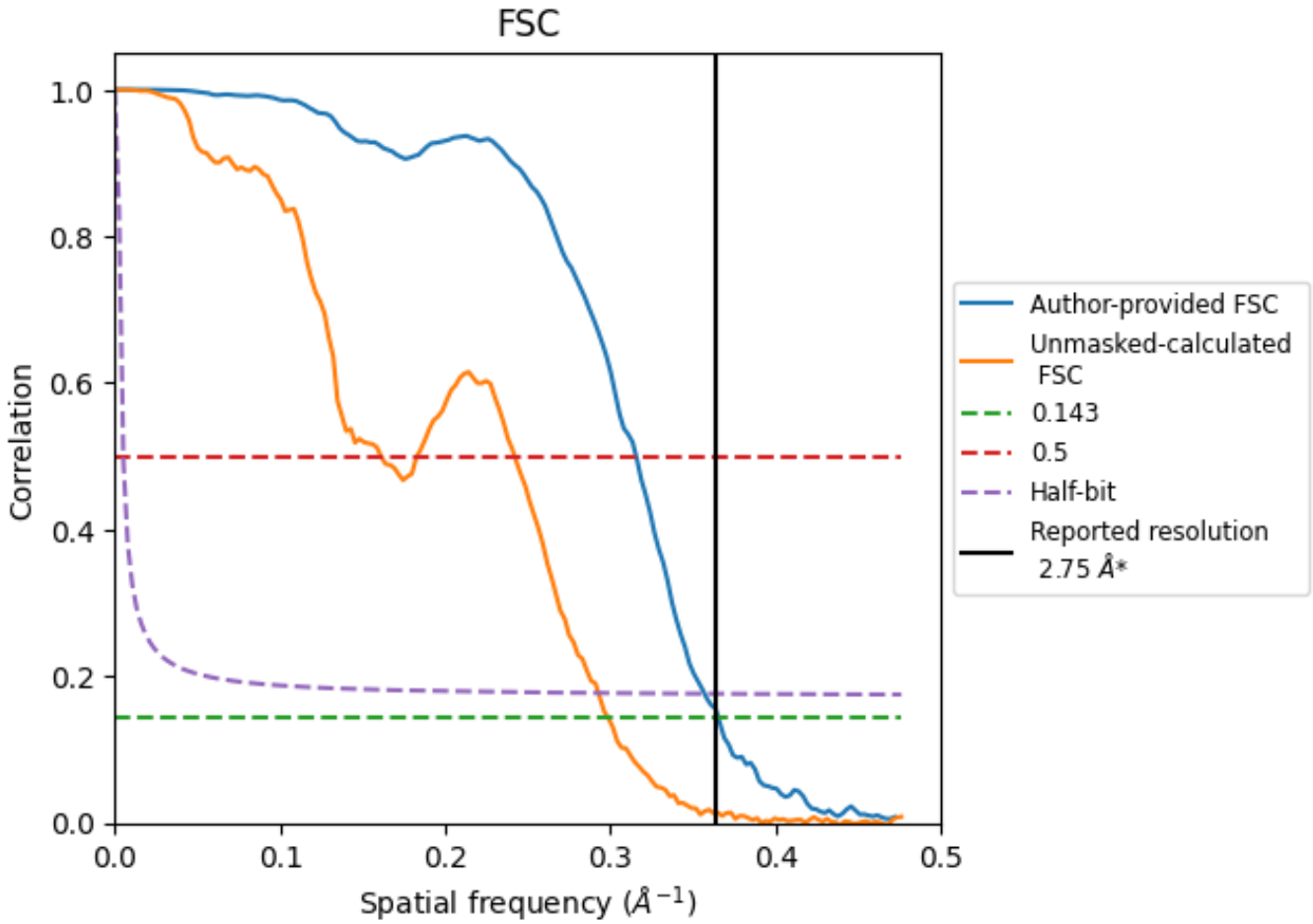


*Reported resolution corresponds to spatial frequency of 0.364 Å^{-1}

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 0.364 Å^{-1}

8.2 Resolution estimates (i)

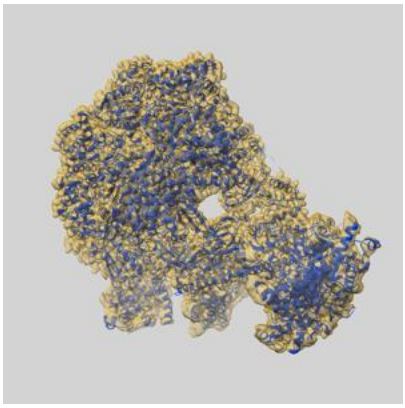
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.75	-	-
Author-provided FSC curve	2.74	3.17	2.80
Unmasked-calculated*	3.35	6.20	3.42

*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 3.35 differs from the reported value 2.75 by more than 10 %

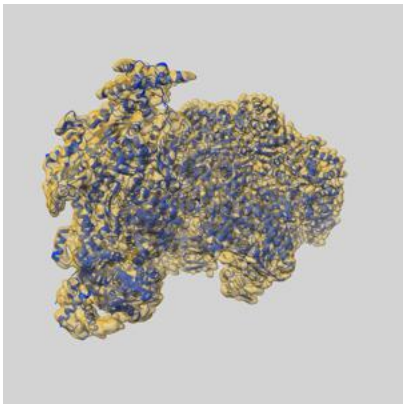
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45206 and PDB model 9C57. Per-residue inclusion information can be found in section 3 on page 7.

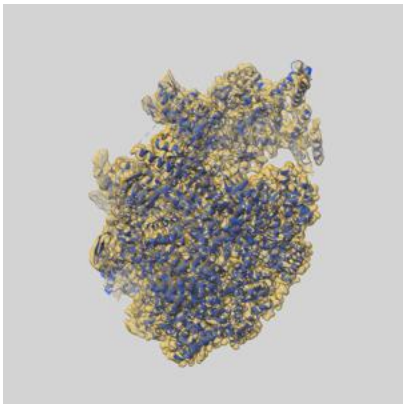
9.1 Map-model overlay



X



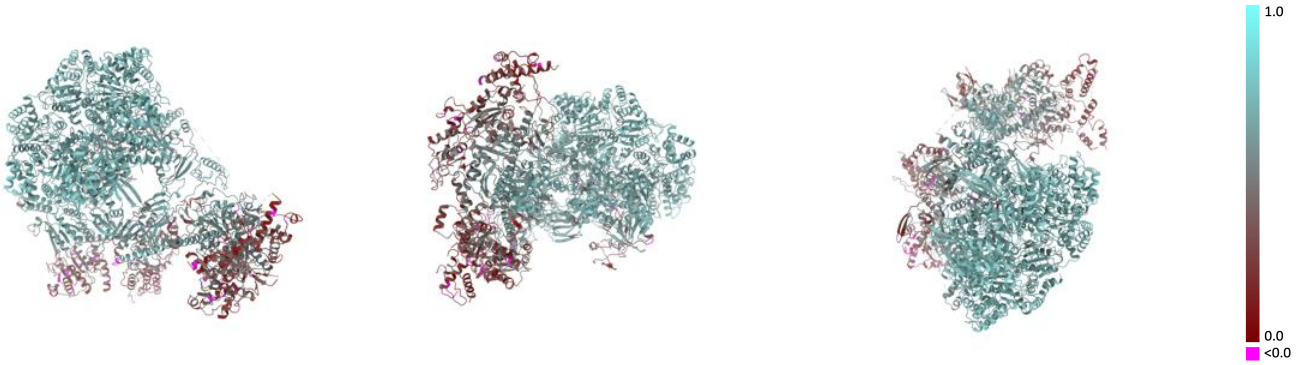
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.4 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.

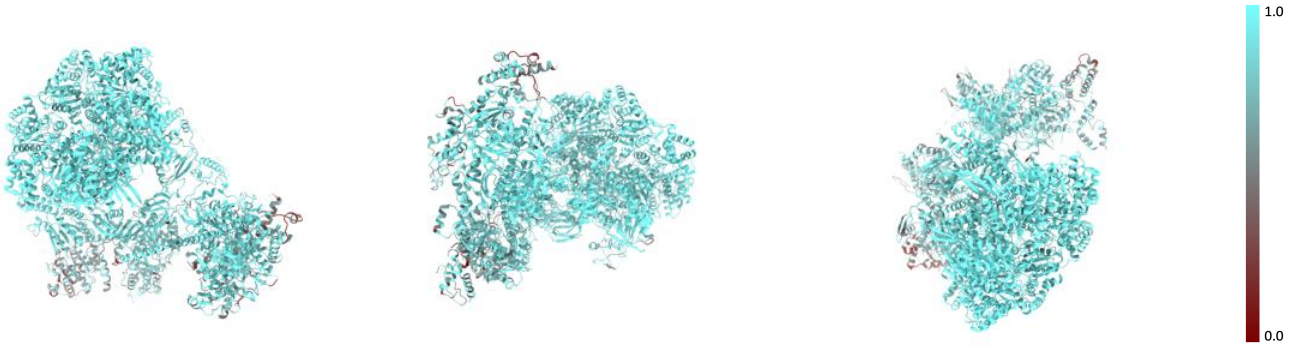
9.2 Q-score mapped to coordinate model (i)



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.

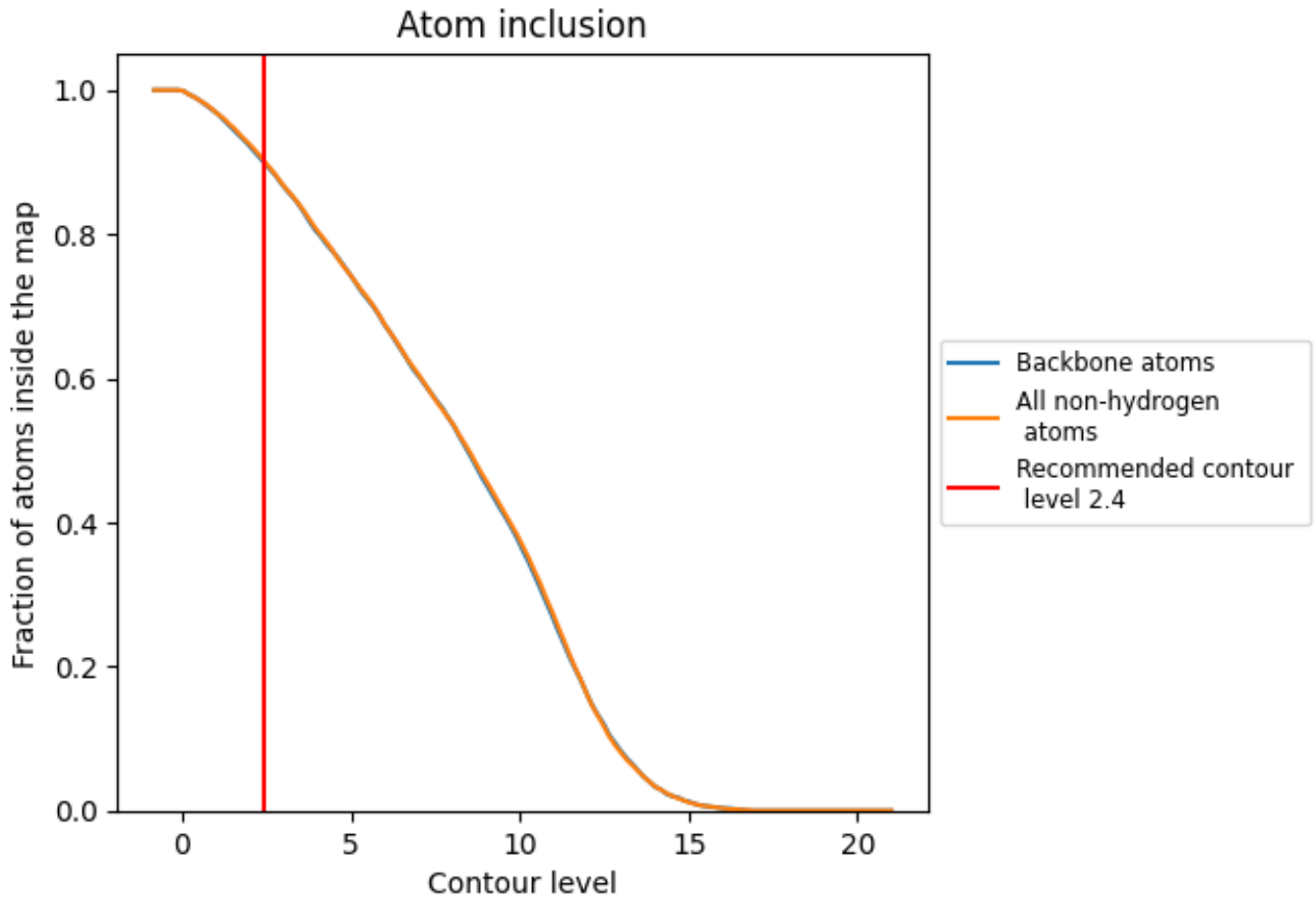
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.4).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9040	0.5440
A	0.9640	0.6300
B	0.9690	0.6320
C	0.9920	0.6730
D	0.9870	0.6710
E	0.9680	0.6490
F	0.9800	0.6550
G	0.8340	0.4810
H	0.8960	0.4590
I	0.7380	0.3360
J	0.8920	0.4850
K	0.8500	0.5190
L	0.8550	0.3810
M	0.7880	0.3070