Full wwPDB EM Validation Report ⓘ

Apr 30, 2024 – 07:49 PM JST

PDB ID	:	8I1U
EMDB ID	:	EMD-35122
Title	:	Human TRiC-PhLP2A complex in the closed state
Authors	:	Roh, S.H.; Park, J.; Kim, H.; Lim, S.
Deposited on	:	2023-01-13
Resolution	:	3.24 Å(reported)
Based on initial model	:	6NR8

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:

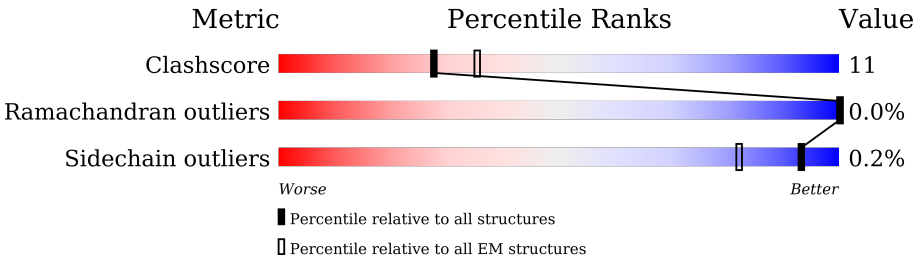
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.24 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	556	9% 70% 25% ·
1	I	556	11% 69% 27% ·
2	B	535	· 76% 21% ·
2	J	535	· 74% 23% ·
3	C	545	· 66% 29% ·
3	K	545	· 68% 28% ·
4	D	539	· 73% 23% ·
4	L	539	· 74% 23% ·

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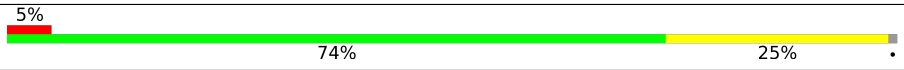
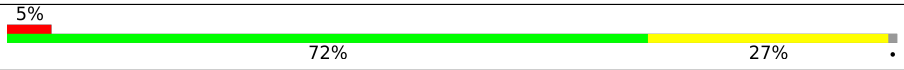
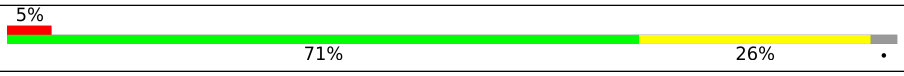
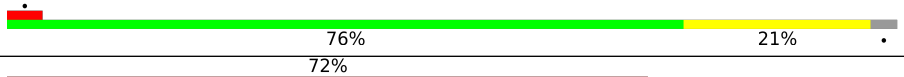
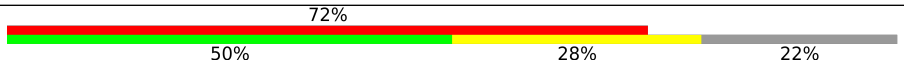
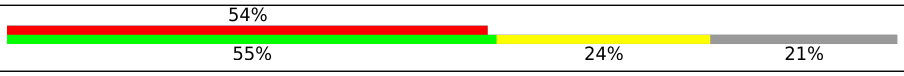
Mol	Chain	Length	Quality of chain
5	E	541	
5	M	541	
6	F	531	
6	N	531	
7	G	543	
7	O	543	
8	H	548	
8	P	548	
9	Q	239	
9	R	239	

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
12	AF3	E	603	-	-	X	-
12	AF3	F	603	-	-	X	-
12	AF3	H	603	-	-	X	-
12	AF3	K	603	-	-	X	-
12	AF3	L	603	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 67629 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	532	Total	C	N	O	S	0	0
			4041	2533	707	778	23		
1	I	532	Total	C	N	O	S	0	0
			4041	2533	707	778	23		

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	518	Total	C	N	O	S	0	0
			3898	2438	687	754	19		
2	J	522	Total	C	N	O	S	0	0
			3924	2455	691	759	19		

- Molecule 3 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	522	Total	C	N	O	S	0	0
			4055	2528	716	781	30		
3	K	524	Total	C	N	O	S	0	0
			4073	2540	720	783	30		

- Molecule 4 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	518	Total	C	N	O	S	0	0
			3908	2445	678	762	23		
4	L	519	Total	C	N	O	S	0	0
			3919	2451	682	763	23		

- Molecule 5 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	525	Total	C	N	O	S	0	0
			4050	2537	708	775	30		
5	M	525	Total	C	N	O	S	0	0
			4050	2537	708	775	30		

- Molecule 6 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	526	Total	C	N	O	S	0	0
			4028	2531	705	771	21		
6	N	525	Total	C	N	O	S	0	0
			4023	2528	704	770	21		

- Molecule 7 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	521	Total	C	N	O	S	0	0
			4002	2529	692	758	23		
7	O	520	Total	C	N	O	S	0	0
			3995	2524	691	757	23		

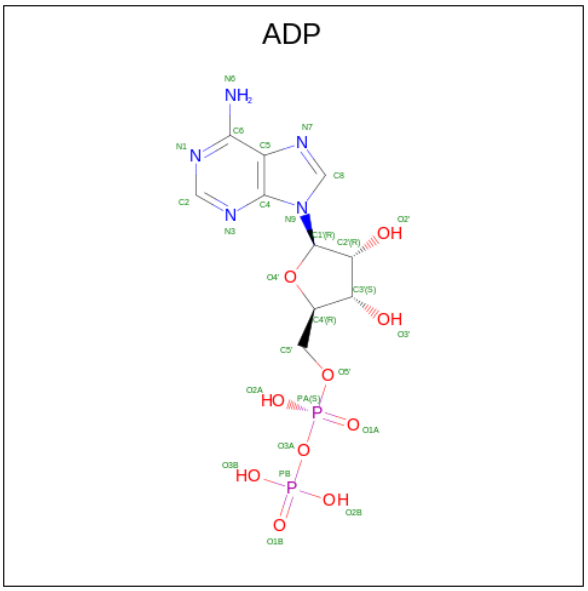
- Molecule 8 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	529	Total	C	N	O	S	0	0
			4029	2543	685	774	27		
8	P	529	Total	C	N	O	S	0	0
			4029	2543	685	774	27		

- Molecule 9 is a protein called Phosducin-like protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	187	Total	C	N	O	S	0	0
			1519	966	251	296	6		
9	R	189	Total	C	N	O	S	0	0
			1533	975	254	298	6		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	K	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	L	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	M	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	N	1	Total	C	N	O	P	0
			27	10	5	10	2	

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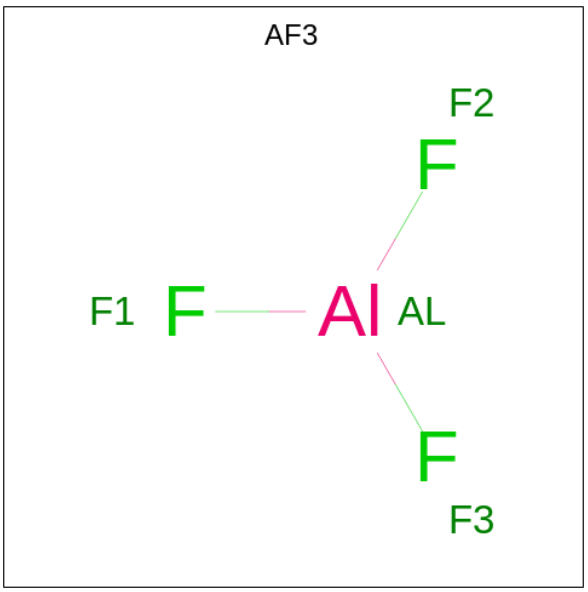
Mol	Chain	Residues	Atoms					AltConf
10	O	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	P	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Mg	0
			1	1	
11	B	1	Total	Mg	0
			1	1	
11	C	1	Total	Mg	0
			1	1	
11	D	1	Total	Mg	0
			1	1	
11	E	1	Total	Mg	0
			1	1	
11	F	1	Total	Mg	0
			1	1	
11	G	1	Total	Mg	0
			1	1	
11	H	1	Total	Mg	0
			1	1	
11	I	1	Total	Mg	0
			1	1	
11	J	1	Total	Mg	0
			1	1	
11	K	1	Total	Mg	0
			1	1	
11	L	1	Total	Mg	0
			1	1	
11	M	1	Total	Mg	0
			1	1	
11	N	1	Total	Mg	0
			1	1	
11	O	1	Total	Mg	0
			1	1	
11	P	1	Total	Mg	0
			1	1	

- Molecule 12 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3) (labeled

as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total Al F 4 1 3	0
12	B	1	Total Al F 4 1 3	0
12	C	1	Total Al F 4 1 3	0
12	D	1	Total Al F 4 1 3	0
12	E	1	Total Al F 4 1 3	0
12	F	1	Total Al F 4 1 3	0
12	G	1	Total Al F 4 1 3	0
12	H	1	Total Al F 4 1 3	0
12	I	1	Total Al F 4 1 3	0
12	J	1	Total Al F 4 1 3	0
12	K	1	Total Al F 4 1 3	0
12	L	1	Total Al F 4 1 3	0
12	M	1	Total Al F 4 1 3	0

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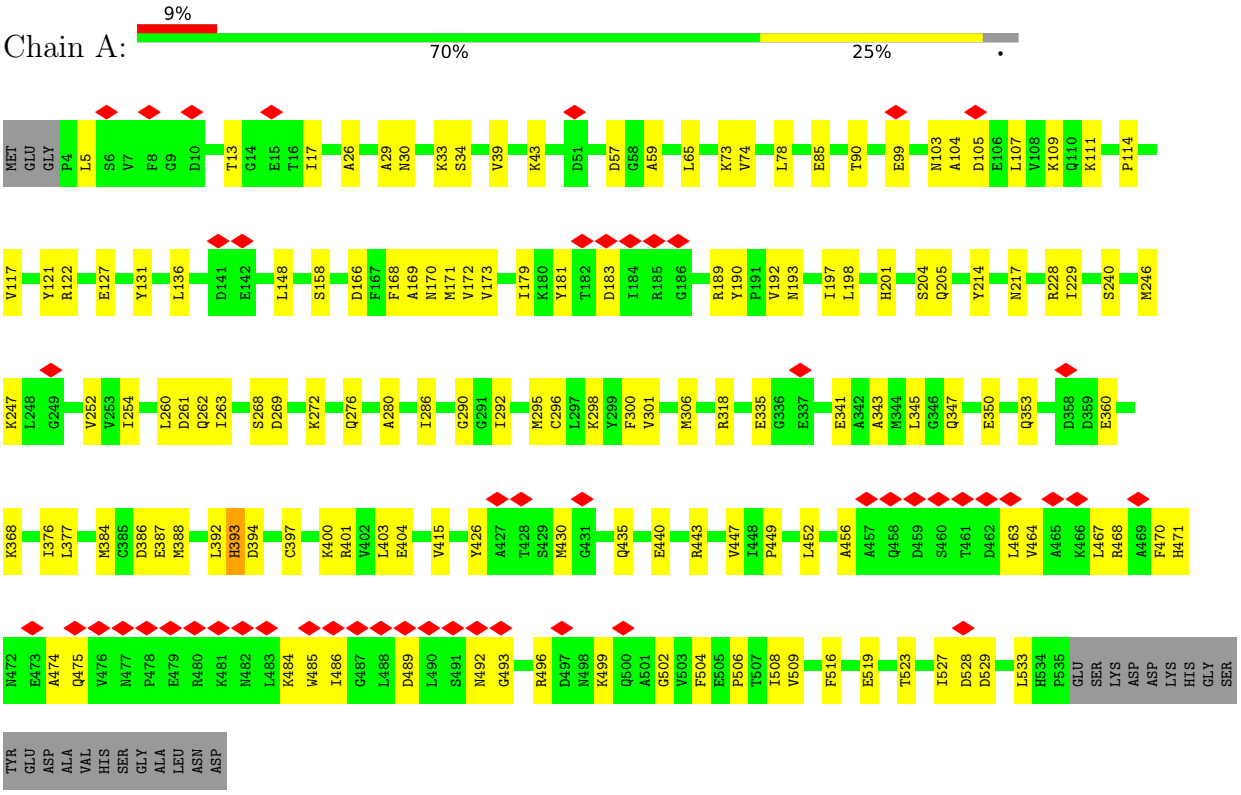
Mol	Chain	Residues	Atoms	AltConf
12	N	1	Total Al F 4 1 3	0
12	O	1	Total Al F 4 1 3	0
12	P	1	Total Al F 4 1 3	0

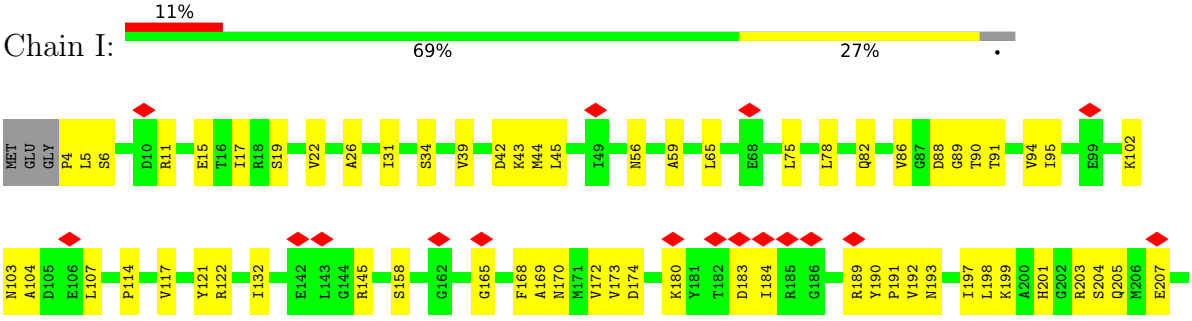
3 Residue-property plots (i)

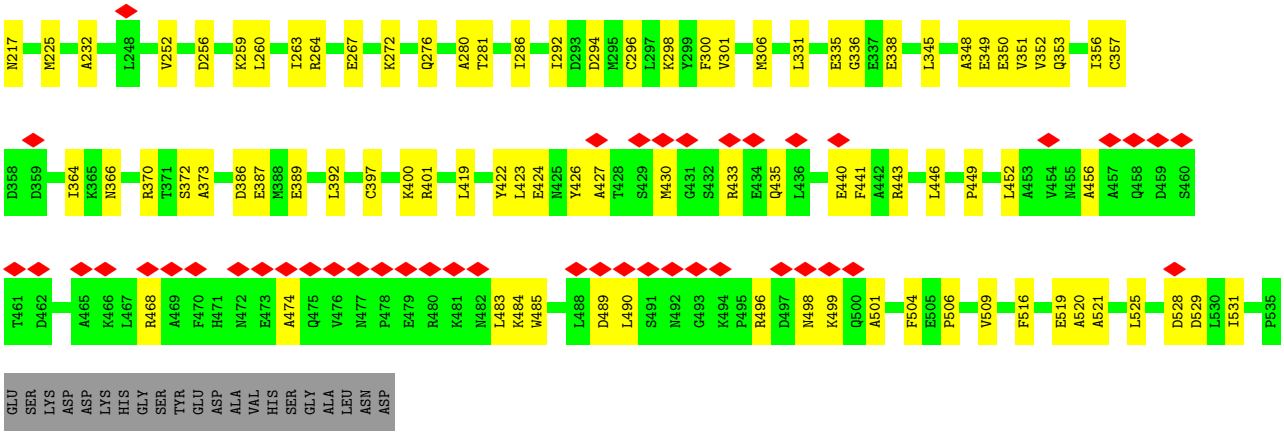
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: T-complex protein 1 subunit alpha



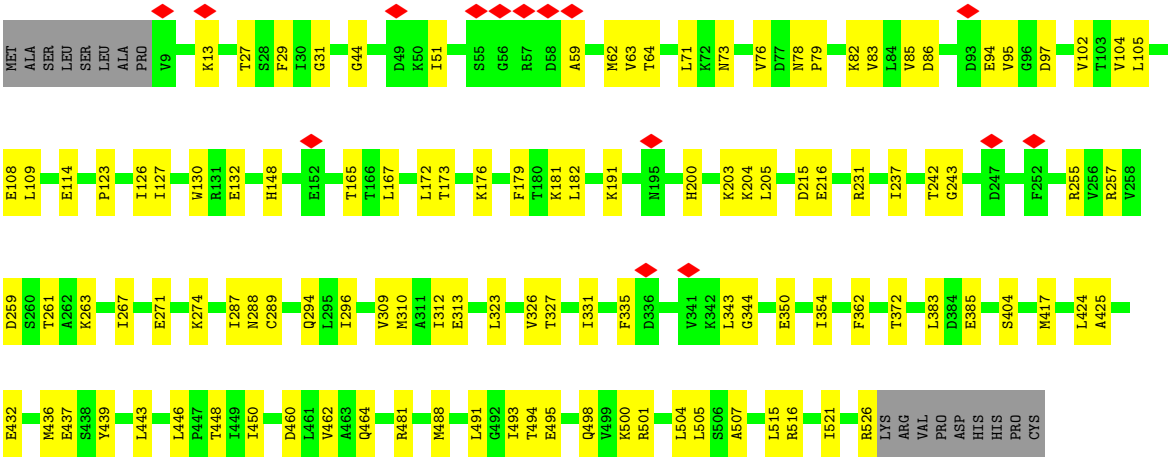
• Molecule 1: T-complex protein 1 subunit alpha





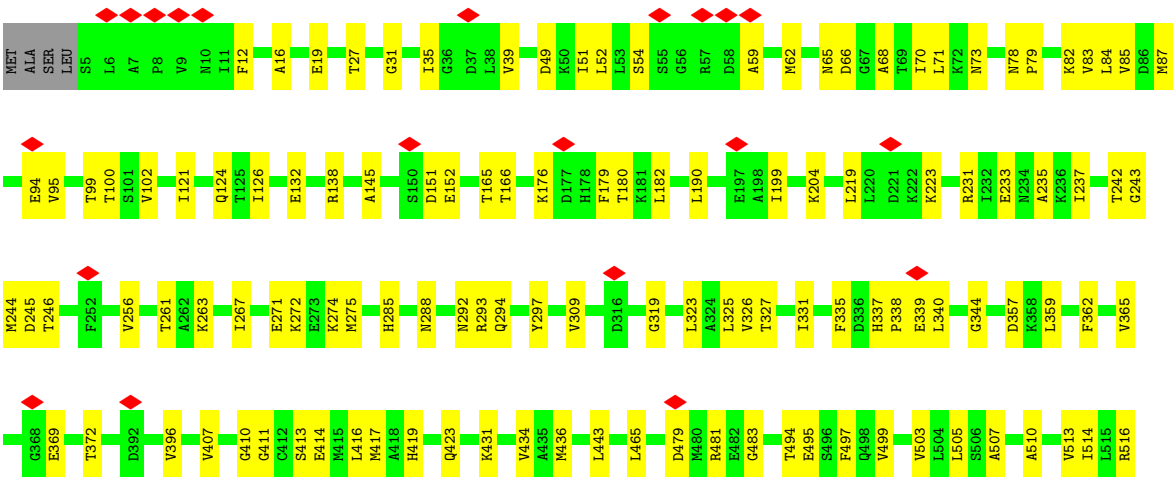
• Molecule 2: T-complex protein 1 subunit beta

Chain B:



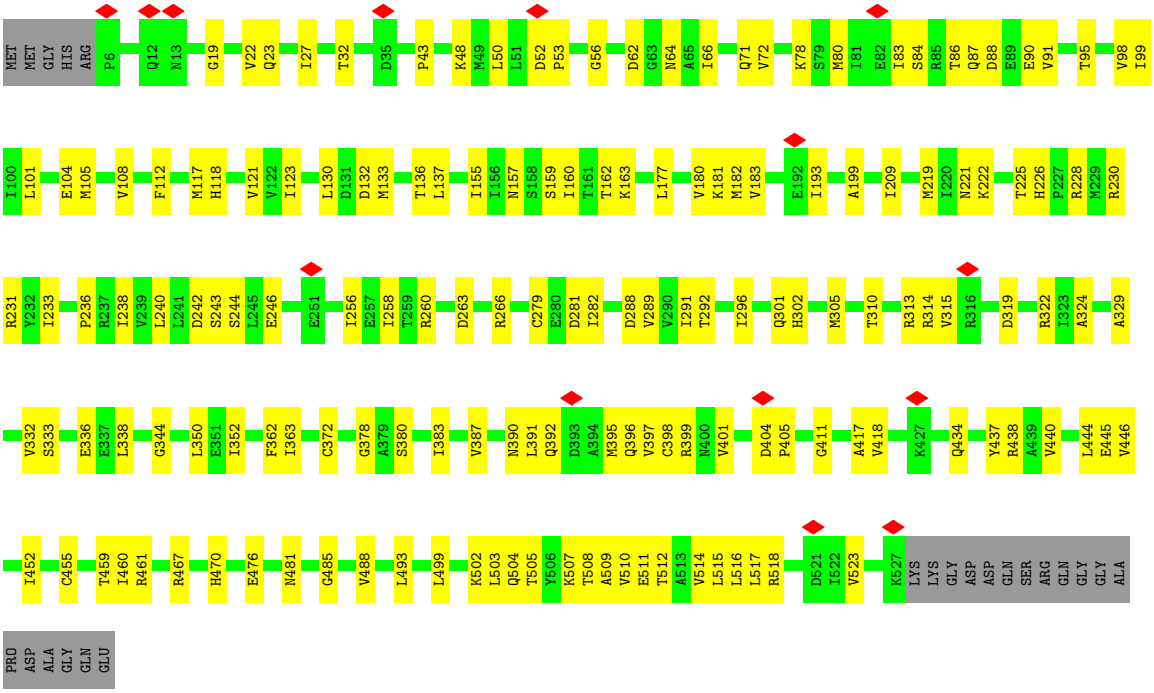
• Molecule 2: T-complex protein 1 subunit beta

Chain J:



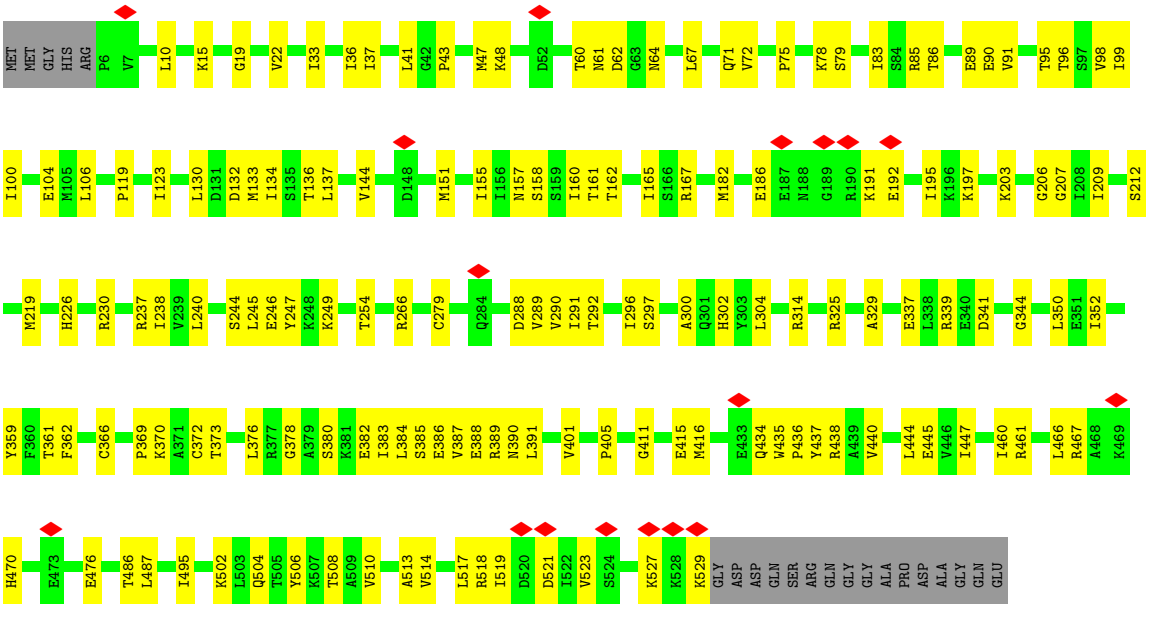
• Molecule 3: T-complex protein 1 subunit gamma

Chain C:



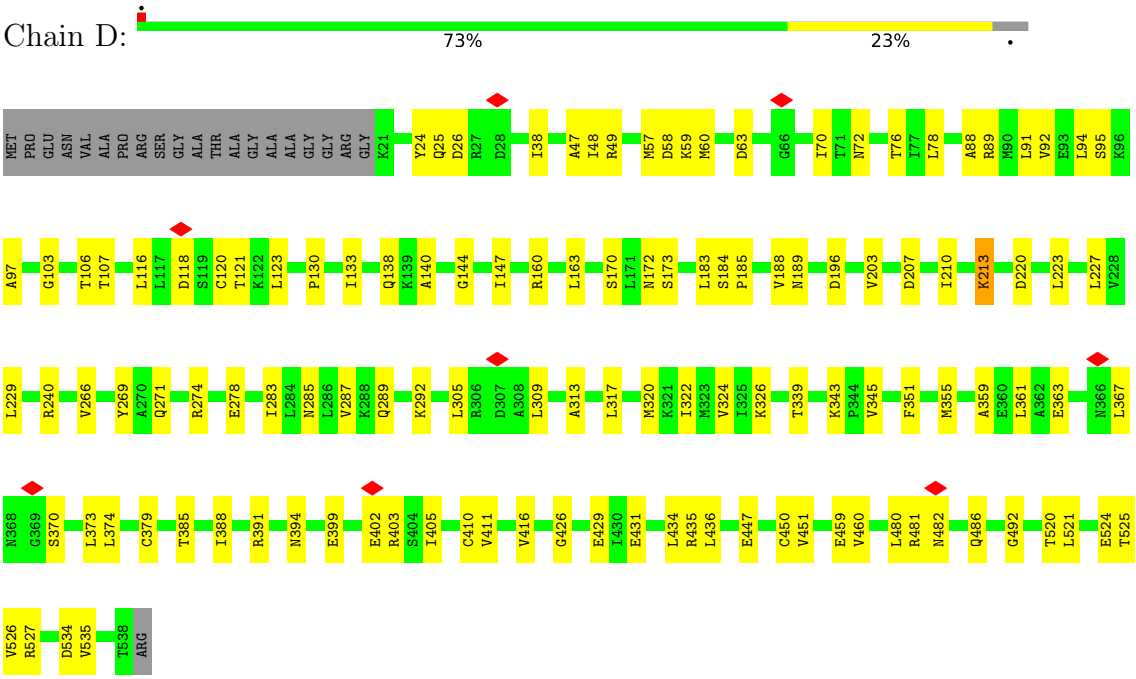
• Molecule 3: T-complex protein 1 subunit gamma

Chain K:



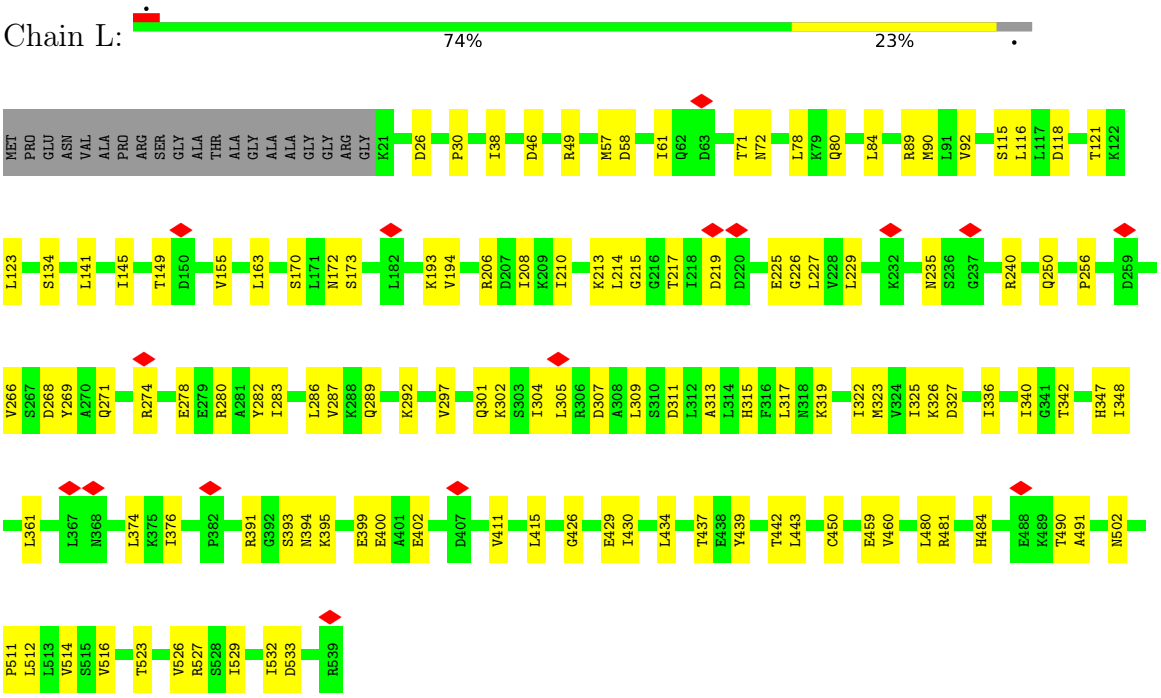
• Molecule 4: T-complex protein 1 subunit delta

Chain D:



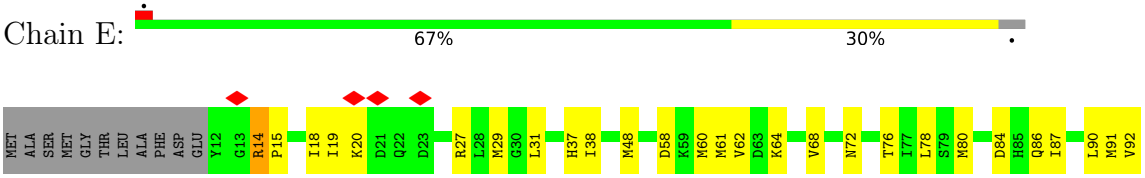
• Molecule 4: T-complex protein 1 subunit delta

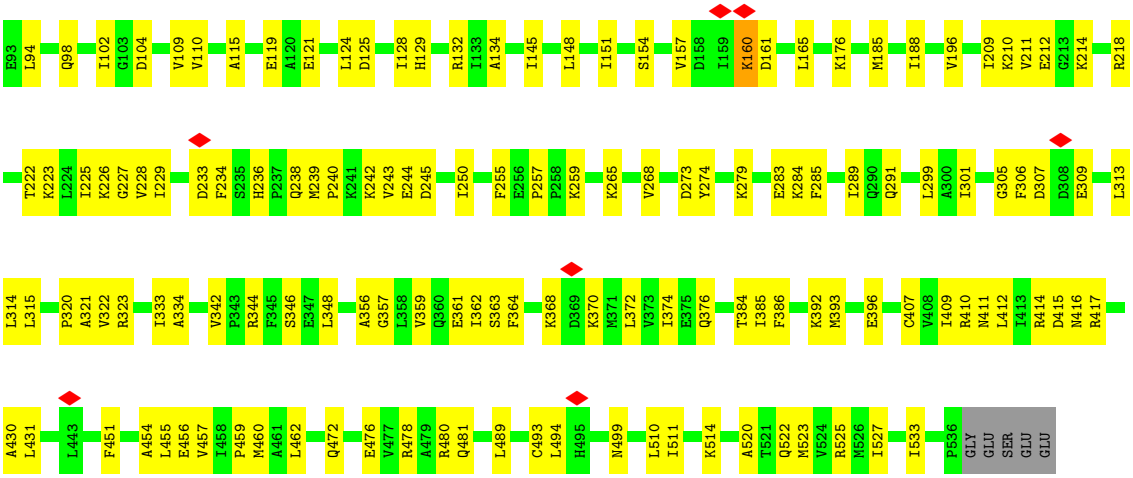
Chain L:



• Molecule 5: T-complex protein 1 subunit epsilon

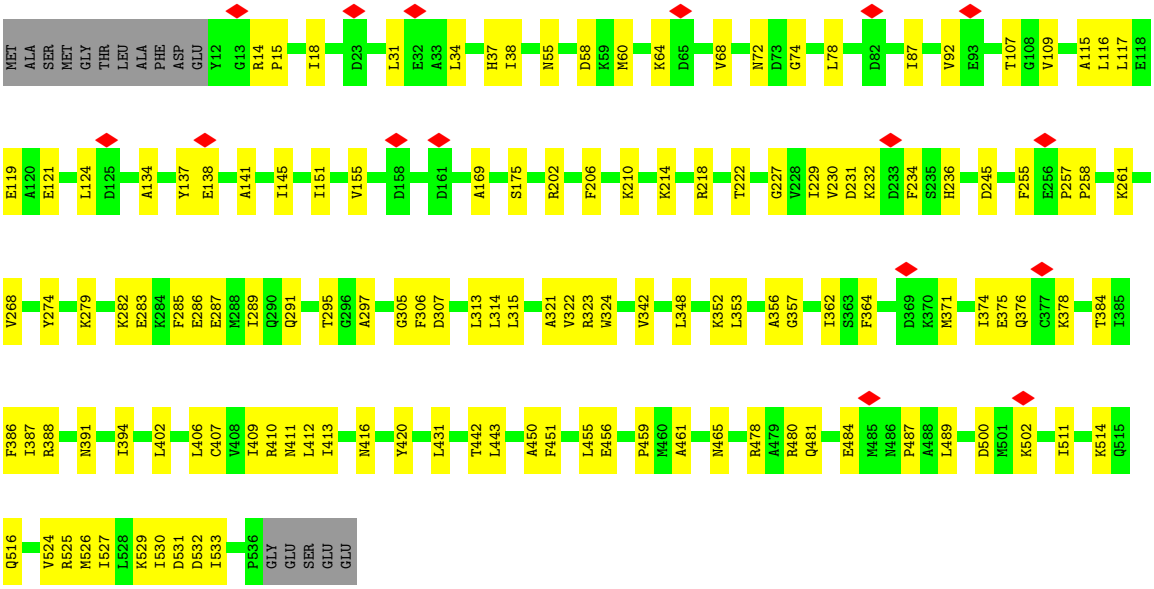
Chain E:





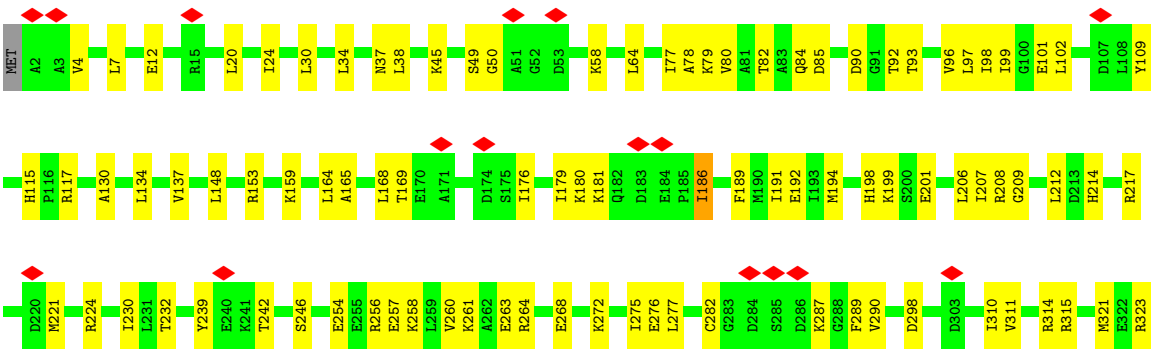
• Molecule 5: T-complex protein 1 subunit epsilon

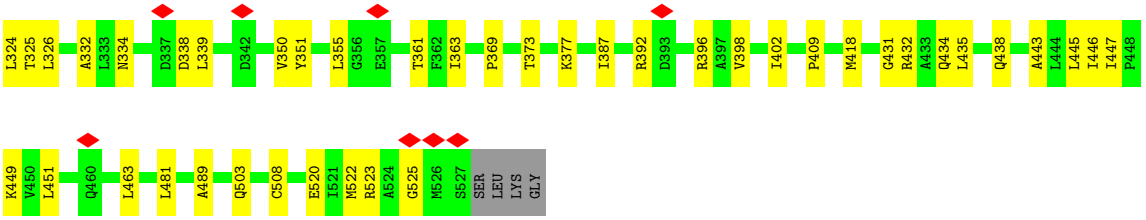
Chain M:



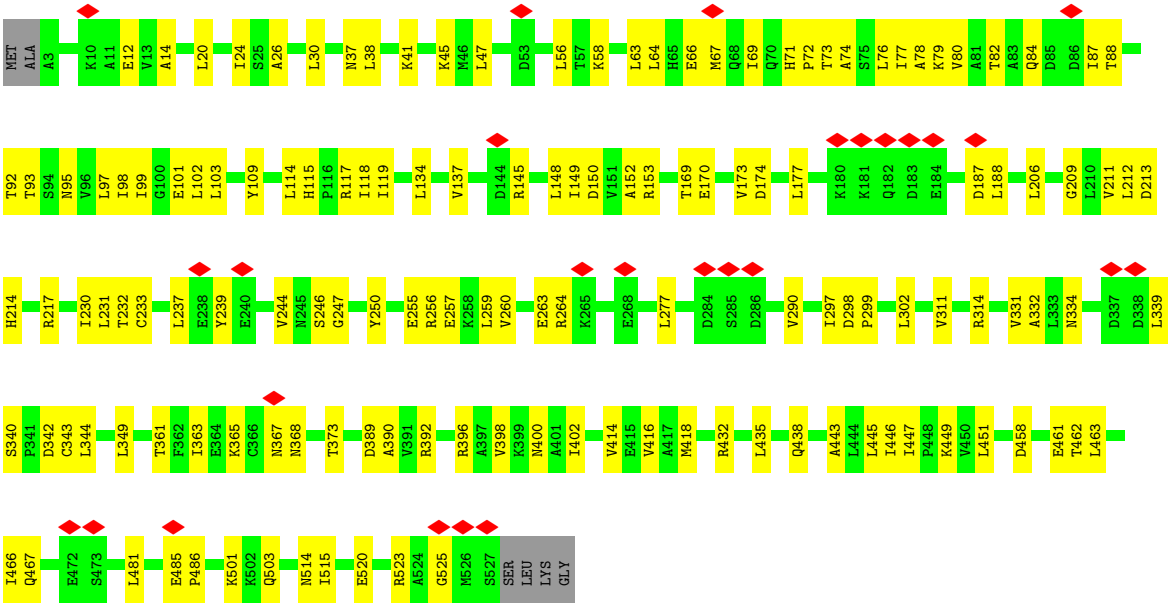
• Molecule 6: T-complex protein 1 subunit zeta

Chain F:

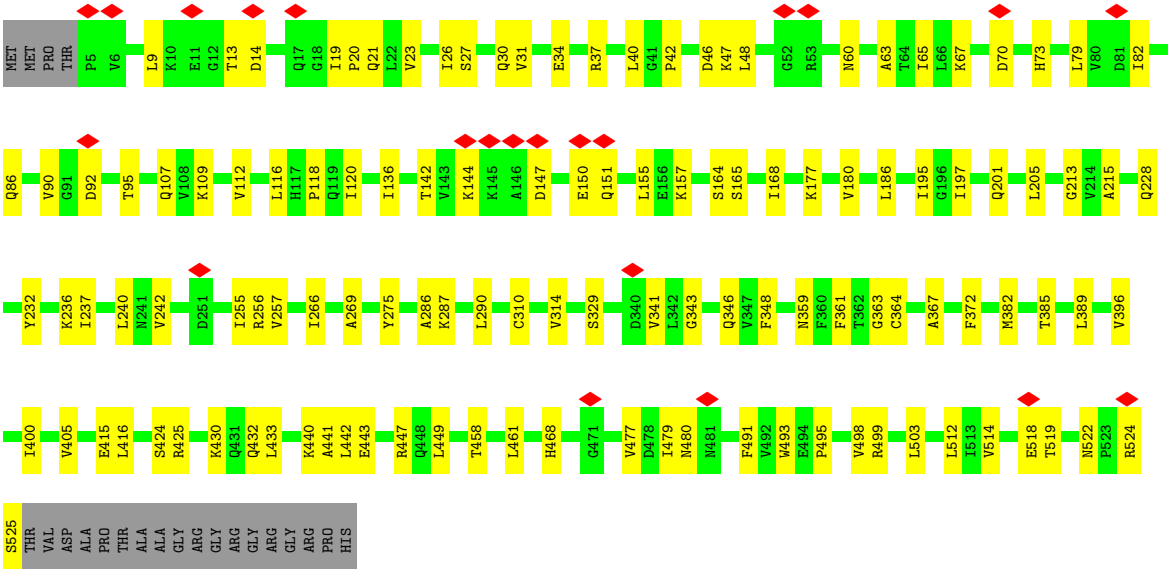




• Molecule 6: T-complex protein 1 subunit zeta

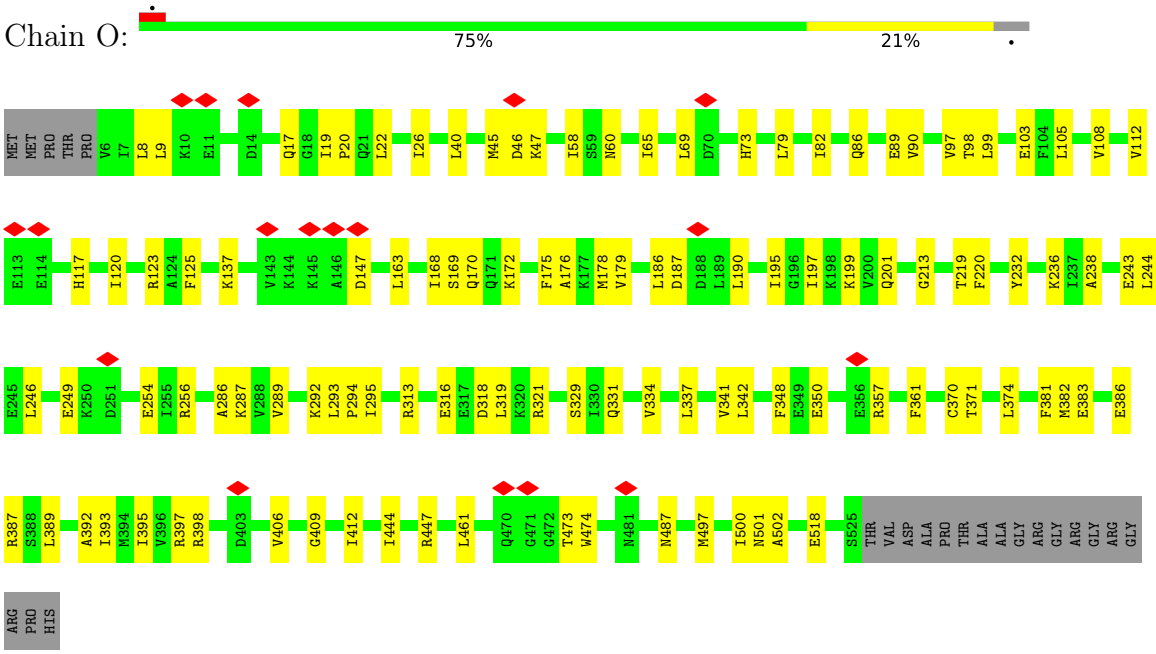


• Molecule 7: T-complex protein 1 subunit eta



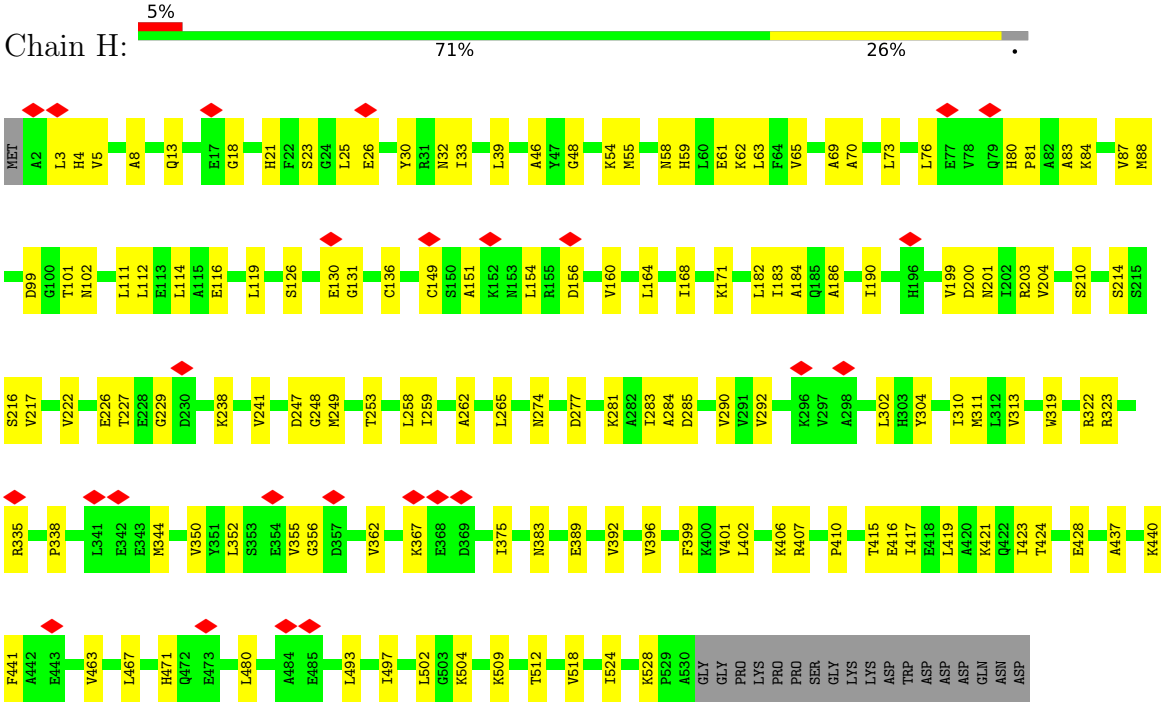
• Molecule 7: T-complex protein 1 subunit eta

Chain O:



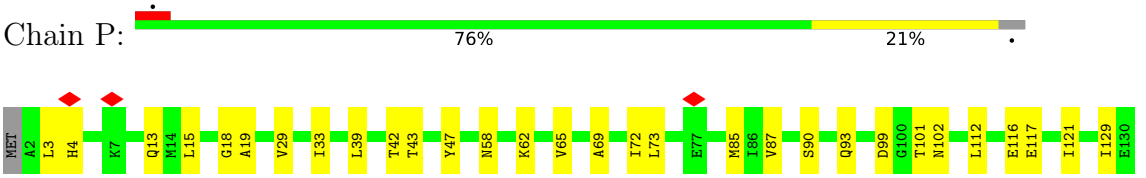
• Molecule 8: T-complex protein 1 subunit theta

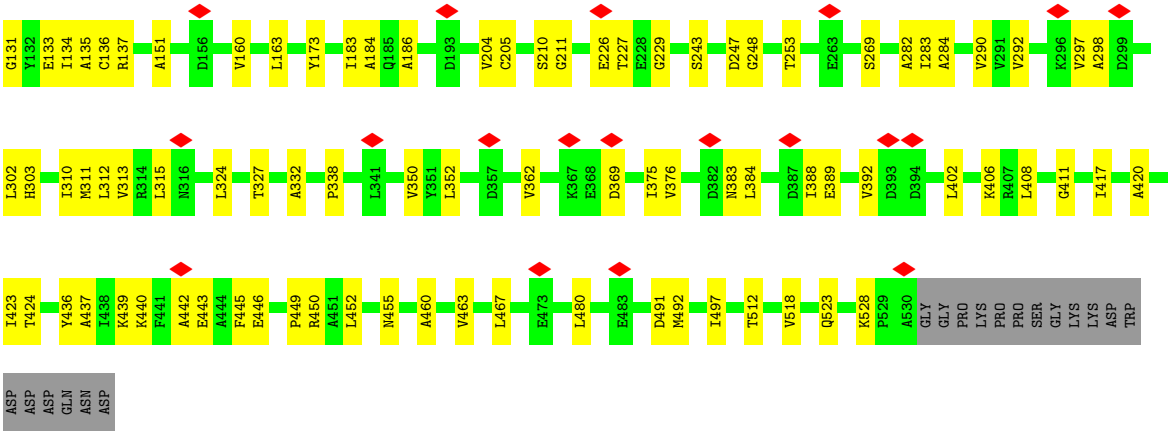
Chain H:



• Molecule 8: T-complex protein 1 subunit theta

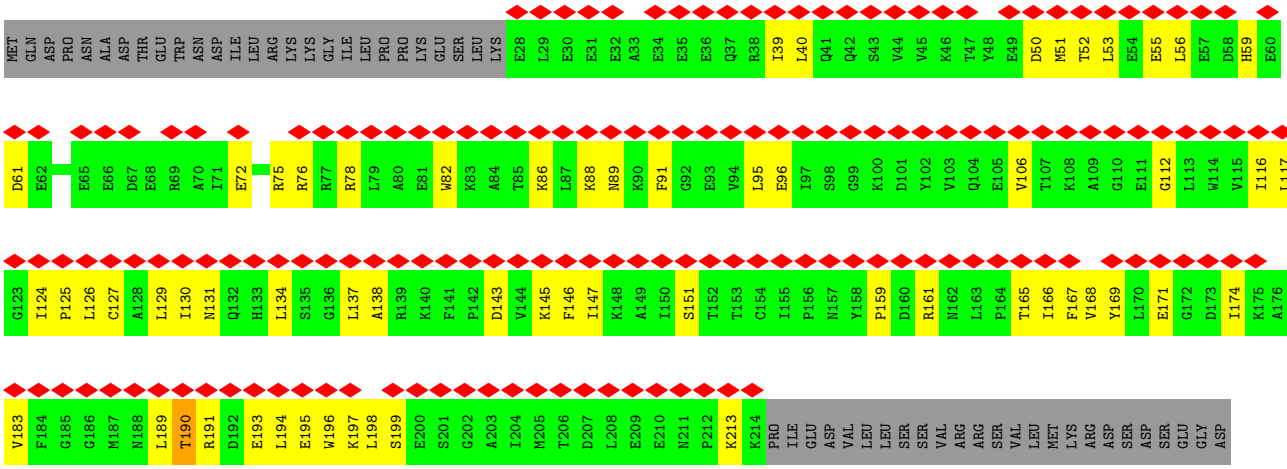
Chain P:





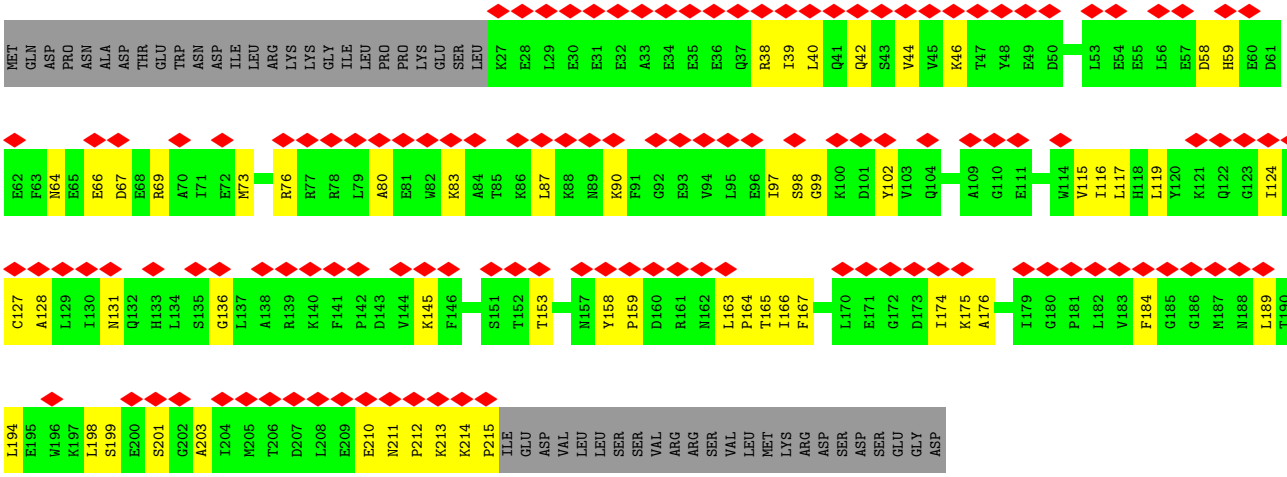
• Molecule 9: Phosducin-like protein 3

Chain Q:



• Molecule 9: Phosducin-like protein 3

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21028	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF correction was performed for every micrographs	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	6.576	Depositor
Minimum map value	-4.112	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.346	Depositor
Recommended contour level	1.23	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, AF3, 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	0.26	0/4081	0.51	0/5510
1	I	0.26	0/4081	0.51	0/5510
2	B	0.26	0/3940	0.51	0/5311
2	J	0.26	0/3967	0.50	0/5349
3	C	0.26	0/4101	0.52	0/5533
3	K	0.26	0/4119	0.51	0/5555
4	D	0.26	0/3940	0.51	0/5319
4	L	0.26	0/3951	0.51	0/5333
5	E	0.26	0/4099	0.50	0/5522
5	M	0.26	0/4099	0.50	0/5522
6	F	0.26	0/4075	0.49	0/5494
6	N	0.26	0/4070	0.51	0/5487
7	G	0.27	0/4058	0.50	0/5476
7	O	0.26	0/4050	0.49	0/5465
8	H	0.26	0/4087	0.48	0/5525
8	P	0.26	0/4087	0.48	0/5525
9	Q	0.25	0/1547	0.51	0/2087
9	R	0.25	0/1561	0.55	1/2105 (0.0%)
All	All	0.26	0/67913	0.50	1/91628 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	R	215	PRO	N-CA-CB	6.01	110.52	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4041	0	4205	106	0
1	I	4041	0	4205	95	0
2	B	3898	0	4008	77	0
2	J	3924	0	4036	87	0
3	C	4055	0	4189	113	0
3	K	4073	0	4215	113	0
4	D	3908	0	4115	87	0
4	L	3919	0	4128	86	0
5	E	4050	0	4174	114	0
5	M	4050	0	4174	90	0
6	F	4028	0	4166	94	0
6	N	4023	0	4161	104	0
7	G	4002	0	4106	77	0
7	O	3995	0	4098	79	0
8	H	4029	0	4099	94	0
8	P	4029	0	4099	76	0
9	Q	1519	0	1496	55	0
9	R	1533	0	1510	37	0
10	A	27	0	12	0	0
10	B	27	0	12	1	0
10	C	27	0	12	3	0
10	D	27	0	12	3	0
10	E	27	0	12	2	0
10	F	27	0	12	3	0
10	G	27	0	12	3	0
10	H	27	0	12	2	0
10	I	27	0	12	0	0
10	J	27	0	12	2	0
10	K	27	0	12	4	0
10	L	27	0	12	2	0
10	M	27	0	12	1	0
10	N	27	0	12	3	0
10	O	27	0	12	0	0
10	P	27	0	12	2	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	1	0	0	0	0
11	E	1	0	0	0	0
11	F	1	0	0	0	0
11	G	1	0	0	0	0
11	H	1	0	0	0	0
11	I	1	0	0	0	0
11	J	1	0	0	0	0
11	K	1	0	0	0	0
11	L	1	0	0	0	0
11	M	1	0	0	0	0
11	N	1	0	0	0	0
11	O	1	0	0	0	0
11	P	1	0	0	0	0
12	A	4	0	0	1	0
12	B	4	0	0	1	0
12	C	4	0	0	1	0
12	D	4	0	0	1	0
12	E	4	0	0	2	0
12	F	4	0	0	5	0
12	G	4	0	0	1	0
12	H	4	0	0	3	0
12	I	4	0	0	0	0
12	J	4	0	0	1	0
12	K	4	0	0	2	0
12	L	4	0	0	2	0
12	M	4	0	0	1	0
12	N	4	0	0	1	0
12	O	4	0	0	0	0
12	P	4	0	0	1	0
All	All	67629	0	69376	1470	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 (1470) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:209:GLY:HA3	6:F:363:ILE:O	1.70	0.91
3:C:302:HIS:HB2	6:F:334:ASN:HB2	1.57	0.87
4:L:78:LEU:HB3	4:L:92:VAL:HG12	1.57	0.85
5:M:529:LYS:HG3	7:O:46:ASP:HB2	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:213:GLY:HA3	7:G:361:PHE:O	1.80	0.82
6:N:209:GLY:HA3	6:N:363:ILE:O	1.82	0.80
1:A:347:GLN:HB3	1:A:368:LYS:HD3	1.65	0.79
3:K:36:ILE:O	3:K:48:LYS:NZ	2.16	0.78
2:B:417:MET:HG3	2:B:443:LEU:HD21	1.65	0.78
3:K:37:ILE:HD11	3:K:99:ILE:HG21	1.65	0.78
2:B:287:ILE:HG22	2:B:343:LEU:HD21	1.67	0.76
7:G:518:GLU:HB3	8:H:54:LYS:HD2	1.68	0.76
3:K:71:GLN:HB2	6:N:525:GLY:HA2	1.68	0.76
6:F:192:GLU:OE2	6:F:194:MET:HE2	1.86	0.76
3:K:302:HIS:HB2	6:N:334:ASN:HB2	1.71	0.73
2:J:84:LEU:HD13	2:J:87:MET:HE3	1.70	0.73
4:L:210:ILE:HG21	4:L:402:GLU:HG3	1.69	0.73
2:B:94:GLU:HG3	2:B:95:VAL:HG13	1.70	0.73
5:E:411:ASN:HB3	5:E:511:ILE:HD11	1.70	0.73
8:H:417:ILE:HG13	8:H:467:LEU:HD23	1.71	0.73
4:L:226:GLY:HA3	4:L:376:ILE:O	1.88	0.73
4:D:94:LEU:HD22	4:D:525:THR:HG21	1.71	0.73
4:D:78:LEU:HB3	4:D:92:VAL:HG12	1.71	0.72
4:D:220:ASP:HB3	4:D:391:ARG:HH11	1.55	0.72
8:H:204:VAL:HG21	8:H:389:GLU:HG3	1.72	0.72
6:F:242:THR:HB	6:F:246:SER:HB3	1.72	0.71
9:Q:130:ILE:HD12	9:Q:166:ILE:HD11	1.72	0.71
4:D:317:LEU:HD12	4:D:322:ILE:HG21	1.72	0.71
1:A:527:ILE:HD12	4:D:60:MET:HB2	1.72	0.71
4:L:229:LEU:HB2	4:L:374:LEU:HB3	1.72	0.71
9:Q:116:ILE:HG12	9:Q:168:VAL:HG12	1.73	0.71
6:F:176:ILE:HG21	6:F:398:VAL:HG11	1.73	0.71
1:A:527:ILE:HD11	4:D:70:ILE:HD12	1.73	0.71
2:B:27:THR:O	2:B:78:ASN:ND2	2.25	0.70
2:B:71:LEU:HB3	2:B:85:VAL:HG22	1.73	0.70
2:B:105:LEU:HD12	2:B:446:LEU:HD11	1.73	0.70
8:H:292:VAL:HG12	8:H:313:VAL:HB	1.73	0.70
5:M:229:ILE:HG22	5:M:384:THR:HG21	1.72	0.70
7:G:21:GLN:NE2	7:G:519:THR:OG1	2.25	0.70
1:A:298:LYS:NZ	3:C:242:ASP:OD2	2.24	0.70
3:K:41:LEU:HD21	3:K:447:ILE:HG23	1.74	0.70
1:A:254:ILE:HB	3:C:256:ILE:HG22	1.73	0.69
7:G:525:SER:HG	8:H:59:HIS:HD1	1.40	0.69
8:H:58:ASN:HD21	8:H:62:LYS:HB3	1.55	0.69
6:F:159:LYS:NZ	12:F:603:AF3:F2	2.15	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:79:LYS:HA	6:N:82:THR:HG22	1.73	0.69
5:E:134:ALA:HB1	5:E:525:ARG:HG3	1.75	0.69
5:E:357:GLY:HA3	5:E:376:GLN:HB2	1.74	0.69
3:K:90:GLU:HG3	3:K:91:VAL:HG13	1.74	0.69
5:M:376:GLN:HG3	5:M:378:LYS:H	1.56	0.69
3:C:313:ARG:HG2	3:C:314:ARG:H	1.57	0.69
7:G:499:ARG:NH2	10:G:601:ADP:O3'	2.26	0.69
1:A:384:MET:O	1:A:388:MET:HG3	1.93	0.69
4:L:305:LEU:HD21	9:R:128:ALA:HB1	1.74	0.69
5:E:229:ILE:HG22	5:E:384:THR:HG21	1.74	0.69
4:D:266:VAL:HG13	4:D:271:GLN:HB3	1.76	0.68
4:L:271:GLN:OE1	4:L:274:ARG:NH2	2.26	0.68
4:D:459:GLU:OE2	4:D:481:ARG:NH1	2.26	0.68
6:F:30:LEU:HG	6:F:77:ILE:HD11	1.74	0.68
5:E:305:GLY:HA2	5:E:323:ARG:HB2	1.76	0.68
9:Q:72:GLU:HA	9:Q:75:ARG:HG2	1.76	0.68
5:E:38:ILE:HG21	5:E:121:GLU:HB2	1.75	0.68
8:H:416:GLU:OE2	8:H:504:LYS:NZ	2.27	0.68
1:A:34:SER:OG	1:A:43:LYS:NZ	2.26	0.67
4:L:46:ASP:HA	4:L:49:ARG:HB2	1.76	0.67
4:L:134:SER:HB2	4:L:527:ARG:HG3	1.75	0.67
5:E:31:LEU:HD11	5:E:124:LEU:HD13	1.76	0.67
8:H:283:ILE:HA	8:H:338:PRO:HB3	1.76	0.67
1:A:99:GLU:HG2	1:A:447:VAL:HB	1.75	0.67
4:D:38:ILE:HG21	4:D:121:THR:HB	1.76	0.67
7:G:157:LYS:HD2	7:G:491:PHE:HB3	1.77	0.67
1:I:203:ARG:HD3	1:I:207:GLU:HG2	1.76	0.67
4:L:317:LEU:HD12	4:L:322:ILE:HG21	1.77	0.67
1:A:148:LEU:HD21	1:A:403:LEU:HD21	1.76	0.67
2:B:255:ARG:HH12	2:B:257:ARG:HH11	1.43	0.67
2:J:339:GLU:HG2	2:J:340:LEU:HD12	1.76	0.67
3:K:240:LEU:HD23	3:K:291:ILE:HB	1.76	0.67
8:H:46:ALA:HB2	8:H:54:LYS:HE3	1.78	0.66
2:J:62:MET:SD	2:J:73:ASN:ND2	2.68	0.66
3:C:160:ILE:HD11	3:C:390:ASN:HB3	1.76	0.66
1:I:26:ALA:HB2	1:I:102:LYS:HD3	1.77	0.66
6:F:79:LYS:HA	6:F:82:THR:HG22	1.78	0.66
1:I:103:ASN:OD1	1:I:443:ARG:NH2	2.28	0.66
5:E:18:ILE:HG13	5:E:19:ILE:HG12	1.76	0.66
5:M:305:GLY:HA2	5:M:323:ARG:HB2	1.77	0.66
3:K:123:ILE:HD11	3:K:517:LEU:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:274:ARG:O	4:L:278:GLU:HG2	1.96	0.66
7:O:447:ARG:HB2	7:O:461:LEU:HD11	1.78	0.66
8:P:463:VAL:HG21	8:P:480:LEU:HD13	1.77	0.66
5:M:117:LEU:HG	5:M:524:VAL:HG23	1.76	0.66
1:A:131:TYR:OH	1:A:475:GLN:NE2	2.29	0.66
5:E:20:LYS:HB3	7:G:70:ASP:HB3	1.77	0.65
5:M:31:LEU:HD11	5:M:124:LEU:HD13	1.77	0.65
5:E:494:LEU:HD11	10:E:601:ADP:HN62	1.60	0.65
1:I:39:VAL:HG23	1:I:490:LEU:HD22	1.78	0.65
5:E:165:LEU:HD13	5:E:412:LEU:HD23	1.77	0.65
1:I:59:ALA:HB2	1:I:90:THR:HG21	1.78	0.65
3:K:411:GLY:N	10:K:601:ADP:O2'	2.26	0.65
9:R:199:SER:HA	9:R:203:ALA:HB3	1.79	0.65
5:E:14:ARG:NH1	5:E:15:PRO:O	2.29	0.65
4:L:61:ILE:HG21	4:L:80:GLN:HB3	1.78	0.65
4:D:49:ARG:HH21	4:D:460:VAL:HG23	1.61	0.65
5:E:227:GLY:HA3	5:E:374:ILE:O	1.97	0.65
6:F:232:THR:OG1	6:F:321:MET:SD	2.54	0.65
8:P:69:ALA:HB3	8:P:101:THR:HG23	1.77	0.65
4:D:289:GLN:HA	4:D:292:LYS:HD3	1.79	0.64
3:C:332:VAL:HG11	3:C:338:LEU:HD13	1.79	0.64
6:F:192:GLU:OE2	6:F:194:MET:CE	2.46	0.64
6:N:47:LEU:HD13	6:N:66:GLU:HB2	1.79	0.64
1:I:43:LYS:HG2	3:K:521:ASP:HB2	1.80	0.64
5:M:431:LEU:HD21	5:M:478:ARG:HG3	1.78	0.64
7:O:22:LEU:HD22	7:O:112:VAL:HG11	1.80	0.64
9:R:211:ASN:HB2	9:R:212:PRO:HD3	1.80	0.64
8:H:171:LYS:NZ	12:H:603:AF3:F2	2.21	0.64
6:N:95:ASN:O	6:N:99:ILE:HG12	1.98	0.64
8:P:226:GLU:HG3	8:P:352:LEU:HD11	1.80	0.64
9:Q:88:LYS:NZ	9:Q:143:ASP:O	2.31	0.64
1:A:341:GLU:HG3	1:A:343:ALA:H	1.63	0.63
3:K:289:VAL:HG21	3:K:350:LEU:HD13	1.80	0.63
3:K:466:LEU:HD12	3:K:487:LEU:HD22	1.80	0.63
8:P:33:ILE:HD12	8:P:112:LEU:HB3	1.78	0.63
3:K:434:GLN:OE1	3:K:438:ARG:NH2	2.31	0.63
3:K:47:MET:SD	3:K:61:ASN:ND2	2.71	0.63
5:M:38:ILE:HG21	5:M:121:GLU:HB2	1.80	0.63
5:M:222:THR:HG22	5:M:388:ARG:H	1.63	0.63
1:A:214:TYR:OH	1:A:318:ARG:NH1	2.31	0.63
9:R:102:TYR:HE1	9:R:117:LEU:HD21	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:126:SER:O	8:H:130:GLU:HG2	1.98	0.63
6:N:102:LEU:HD22	6:N:443:ALA:HB1	1.81	0.63
3:C:499:LEU:HG	3:C:503:LEU:HD23	1.80	0.63
5:E:98:GLN:NE2	5:E:104:ASP:O	2.32	0.63
6:F:102:LEU:HD22	6:F:443:ALA:HB1	1.81	0.63
7:G:228:GLN:NE2	7:G:310:CYS:SG	2.67	0.63
4:L:266:VAL:HG13	4:L:271:GLN:HB2	1.80	0.63
6:F:92:THR:OG1	12:F:603:AF3:F3	2.06	0.63
3:K:527:LYS:HD3	3:K:529:LYS:H	1.64	0.63
9:Q:137:LEU:HD13	9:Q:194:LEU:HD11	1.81	0.63
6:F:99:ILE:HD11	6:F:508:CYS:HA	1.80	0.63
5:M:261:LYS:HG3	7:O:246:LEU:HB3	1.81	0.62
3:C:230:ARG:NH2	3:C:288:ASP:OD1	2.33	0.62
4:D:482:ASN:O	4:D:486:GLN:NE2	2.31	0.62
5:E:94:LEU:HB2	5:E:523:MET:SD	2.40	0.62
8:P:449:PRO:HA	8:P:452:LEU:HD12	1.82	0.62
4:D:480:LEU:HD11	4:D:492:GLY:HA2	1.81	0.62
7:O:213:GLY:HA3	7:O:361:PHE:O	2.00	0.62
2:B:331:ILE:HB	5:E:236:HIS:CE1	2.34	0.62
3:C:137:LEU:HD21	3:C:502:LYS:HB3	1.82	0.62
6:N:150:ASP:OD1	6:N:153:ARG:NH2	2.33	0.62
9:Q:95:LEU:HD21	9:Q:147:ILE:HG22	1.80	0.62
6:F:12:GLU:HB2	6:F:523:ARG:HB3	1.80	0.62
4:L:459:GLU:OE2	4:L:481:ARG:NH1	2.32	0.62
1:I:132:ILE:HD11	1:I:419:LEU:HD11	1.81	0.62
1:I:386:ASP:OD1	1:I:387:GLU:N	2.33	0.62
9:Q:119:LEU:HD12	9:Q:151:SER:HA	1.81	0.62
1:A:59:ALA:HB2	1:A:90:THR:HG21	1.82	0.62
5:E:430:ALA:HB2	5:E:455:LEU:HD11	1.82	0.62
4:L:30:PRO:HB3	4:L:533:ASP:HB2	1.82	0.62
8:H:55:MET:HG2	8:H:65:VAL:HG22	1.81	0.62
5:M:245:ASP:HA	5:M:356:ALA:O	2.00	0.62
3:C:396:GLN:OE1	3:C:399:ARG:NH1	2.33	0.62
7:G:13:THR:HG22	7:G:522:ASN:HA	1.82	0.62
7:O:329:SER:HB3	7:O:341:VAL:HG23	1.82	0.62
1:A:353:GLN:NE2	1:A:360:GLU:OE1	2.33	0.61
4:D:130:PRO:HA	4:D:133:ILE:HD12	1.81	0.61
1:I:11:ARG:HG2	1:I:531:ILE:HG12	1.82	0.61
5:M:14:ARG:NH1	5:M:15:PRO:O	2.32	0.61
5:M:391:ASN:HB2	5:M:394:ILE:HG12	1.83	0.61
7:G:237:ILE:N	7:G:343:GLY:O	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:530:ILE:HA	7:O:46:ASP:HB3	1.82	0.61
10:F:601:ADP:O3B	12:F:603:AF3:F2	2.08	0.61
2:J:39:VAL:HG12	2:J:100:THR:HG23	1.82	0.61
5:M:342:VAL:HG21	5:M:348:LEU:HD13	1.83	0.61
5:E:417:ARG:HD2	5:E:510:LEU:HD13	1.83	0.61
2:J:165:THR:HG21	2:J:494:THR:O	2.01	0.61
4:L:490:THR:O	4:L:502:ASN:ND2	2.34	0.61
3:C:231:ARG:HB3	3:C:352:ILE:HB	1.82	0.61
2:B:521:ILE:HD12	5:E:61:MET:HE2	1.82	0.61
4:D:72:ASN:ND2	4:D:173:SER:O	2.34	0.61
5:M:442:THR:HG23	5:M:443:LEU:HD12	1.81	0.61
6:N:41:LYS:NZ	6:N:481:LEU:O	2.31	0.61
6:N:239:TYR:N	6:N:298:ASP:OD2	2.33	0.61
6:N:392:ARG:O	6:N:396:ARG:HG2	2.00	0.61
5:E:431:LEU:HD21	5:E:478:ARG:HG3	1.82	0.61
2:J:124:GLN:HE21	5:M:55:ASN:HA	1.65	0.61
3:K:33:ILE:HG22	3:K:99:ILE:HD11	1.83	0.61
4:L:38:ILE:HG21	4:L:121:THR:HB	1.83	0.61
1:I:256:ASP:OD2	1:I:259:LYS:NZ	2.28	0.60
2:B:259:ASP:O	4:D:271:GLN:NE2	2.31	0.60
7:G:449:LEU:HD22	7:G:477:VAL:HG21	1.82	0.60
4:L:193:LYS:NZ	4:L:225:GLU:OE2	2.31	0.60
5:M:151:ILE:HD11	5:M:487:PRO:HB2	1.81	0.60
5:M:279:LYS:NZ	5:M:283:GLU:OE2	2.34	0.60
2:B:296:ILE:H	2:B:313:GLU:HG3	1.66	0.60
3:C:183:VAL:HG21	3:C:199:ALA:HB2	1.82	0.60
5:E:223:LYS:HE2	5:E:225:ILE:HD11	1.83	0.60
5:M:18:ILE:HA	7:O:73:HIS:HB2	1.82	0.60
6:N:148:LEU:HD11	6:N:402:ILE:HD11	1.84	0.60
6:N:38:LEU:HD12	6:N:93:THR:HG22	1.84	0.60
8:H:25:LEU:HD11	8:H:119:LEU:HD13	1.82	0.60
9:Q:86:LYS:HE2	9:Q:89:ASN:HD21	1.66	0.60
2:B:203:LYS:HB2	2:B:383:LEU:HD12	1.84	0.60
2:J:59:ALA:O	4:L:89:ARG:NH1	2.28	0.60
6:N:69:ILE:HD12	6:N:74:ALA:HB1	1.84	0.60
4:D:140:ALA:HB1	4:D:436:LEU:HD21	1.84	0.60
1:I:78:LEU:HD11	1:I:516:PHE:HB3	1.84	0.60
4:L:123:LEU:HD21	4:L:450:CYS:HA	1.82	0.60
9:R:175:LYS:O	9:R:201:SER:OG	2.20	0.60
2:B:310:MET:HE3	2:B:312:ILE:HD11	1.81	0.60
7:G:512:LEU:HD11	8:H:65:VAL:HG11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:34:SER:OG	1:I:43:LYS:NZ	2.29	0.60
1:I:427:ALA:HB1	1:I:435:GLN:HB2	1.83	0.60
3:K:209:ILE:HD12	3:K:209:ILE:H	1.67	0.60
4:L:297:VAL:HG12	4:L:323:MET:HB3	1.83	0.60
9:R:119:LEU:HB2	9:R:165:THR:HB	1.84	0.59
4:D:309:LEU:HD12	4:D:326:LYS:HD2	1.84	0.59
8:H:3:LEU:O	8:H:4:HIS:ND1	2.34	0.59
7:G:405:VAL:HG21	7:G:493:TRP:HB3	1.84	0.59
8:H:160:VAL:HG13	8:H:184:ALA:HB1	1.85	0.59
6:N:188:LEU:HD13	6:N:396:ARG:HH11	1.67	0.59
8:P:18:GLY:HA3	8:P:528:LYS:HD3	1.84	0.59
8:P:284:ALA:HB2	8:P:310:ILE:HD11	1.83	0.59
6:N:109:TYR:HD2	6:N:435:LEU:HD13	1.67	0.59
1:A:463:LEU:HD22	1:A:467:LEU:HD22	1.84	0.59
3:C:228:ARG:HB3	3:C:305:MET:HE3	1.84	0.59
5:E:268:VAL:HG23	5:E:273:ASP:HB3	1.82	0.59
6:F:198:HIS:CE1	6:F:199:LYS:HE2	2.38	0.59
7:G:236:LYS:HB2	7:G:286:ALA:HA	1.84	0.59
8:H:21:HIS:NE2	8:H:23:SER:OG	2.35	0.59
8:H:183:ILE:HD11	8:H:392:VAL:HG22	1.84	0.59
8:P:112:LEU:HD11	8:P:518:VAL:HG11	1.85	0.59
7:G:290:LEU:HD12	7:G:314:VAL:HG21	1.85	0.59
8:H:421:LYS:NZ	8:H:471:HIS:O	2.35	0.59
1:I:15:GLU:OE2	1:I:19:SER:OG	2.20	0.59
6:N:458:ASP:HB3	6:N:461:GLU:HG2	1.83	0.59
9:Q:124:ILE:HD12	9:Q:125:PRO:HD2	1.85	0.59
5:E:236:HIS:NE2	5:E:315:LEU:HD22	2.17	0.59
10:N:601:ADP:O1B	12:N:603:AF3:F3	2.11	0.59
9:R:64:ASN:ND2	9:R:66:GLU:OE2	2.35	0.59
3:K:359:TYR:OH	6:N:187:ASP:OD2	2.20	0.59
7:O:243:GLU:HB3	7:O:293:LEU:HB3	1.85	0.59
6:F:20:LEU:O	6:F:24:ILE:HG12	2.02	0.58
1:I:449:PRO:O	1:I:452:LEU:HB2	2.04	0.58
9:Q:159:PRO:HB2	9:Q:161:ARG:HG2	1.85	0.58
9:Q:189:LEU:HD21	9:Q:197:LYS:HZ1	1.68	0.58
2:B:494:THR:HG22	2:B:495:GLU:H	1.68	0.58
10:B:601:ADP:O2B	12:B:603:AF3:F3	2.12	0.58
4:D:309:LEU:HD11	4:D:324:VAL:HG11	1.85	0.58
8:H:99:ASP:OD1	12:H:603:AF3:F3	2.11	0.58
4:L:115:SER:HB2	4:L:460:VAL:HG21	1.85	0.58
2:B:481:ARG:HH12	2:B:491:LEU:HD22	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:292:LYS:HD2	7:O:316:GLU:HG3	1.83	0.58
8:P:204:VAL:HG21	8:P:389:GLU:HG3	1.85	0.58
3:C:289:VAL:HG22	3:C:310:THR:HB	1.85	0.58
8:H:406:LYS:HG3	8:H:407:ARG:H	1.67	0.58
1:I:272:LYS:NZ	3:K:337:GLU:OE2	2.36	0.58
4:D:343:LYS:HD2	4:D:355:MET:HB2	1.84	0.58
5:E:344:ARG:HH12	7:G:275:TYR:HE2	1.50	0.58
8:P:33:ILE:HG21	8:P:116:GLU:HB2	1.85	0.58
2:B:327:THR:HG22	2:B:344:GLY:HA3	1.85	0.58
3:C:319:ASP:OD1	3:C:322:ARG:NH2	2.35	0.58
5:E:157:VAL:HG12	5:E:165:LEU:HD21	1.85	0.58
9:Q:180:GLY:HA3	9:Q:183:VAL:HG12	1.84	0.58
1:A:246:MET:O	1:A:247:LYS:HG3	2.04	0.58
2:B:104:VAL:O	2:B:108:GLU:HG2	2.04	0.58
3:C:244:SER:OG	3:C:246:GLU:OE1	2.20	0.58
6:F:214:HIS:NE2	6:F:315:ARG:O	2.37	0.58
8:H:350:VAL:HA	8:H:362:VAL:O	2.04	0.58
6:N:63:LEU:O	6:N:67:MET:HG3	2.04	0.58
8:H:151:ALA:HB3	8:H:406:LYS:HD3	1.85	0.58
7:O:383:GLU:OE2	7:O:387:ARG:NH1	2.37	0.58
9:Q:39:ILE:HG13	9:Q:40:LEU:H	1.69	0.58
9:R:58:ASP:OD1	9:R:59:HIS:N	2.37	0.58
4:L:268:ASP:HB2	4:L:271:GLN:HG2	1.85	0.57
7:O:350:GLU:OE1	7:O:357:ARG:NH1	2.37	0.57
5:E:342:VAL:HG21	5:E:348:LEU:HD13	1.86	0.57
8:H:277:ASP:HB3	8:H:304:TYR:CZ	2.39	0.57
1:I:252:VAL:HG12	4:L:266:VAL:HB	1.86	0.57
6:N:145:ARG:NH2	6:N:170:GLU:OE1	2.37	0.57
9:R:127:CYS:O	9:R:131:ASN:ND2	2.36	0.57
7:G:116:LEU:HG	7:G:120:ILE:HD11	1.86	0.57
7:O:108:VAL:HG21	7:O:125:PHE:CZ	2.39	0.57
9:Q:119:LEU:HB2	9:Q:165:THR:HB	1.85	0.57
1:A:183:ASP:HB3	1:A:189:ARG:HE	1.69	0.57
1:A:529:ASP:OD1	4:D:59:LYS:HG3	2.05	0.57
2:B:200:HIS:HB3	2:B:372:THR:HG22	1.86	0.57
6:F:153:ARG:HA	6:F:169:THR:HG21	1.85	0.57
8:H:84:LYS:O	8:H:88:MET:HG3	2.04	0.57
3:C:123:ILE:HD12	3:C:514:VAL:HG13	1.86	0.57
5:M:78:LEU:HB3	5:M:92:VAL:HG22	1.86	0.57
6:N:20:LEU:O	6:N:24:ILE:HG12	2.04	0.57
2:J:166:THR:HG21	2:J:396:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:601:ADP:O1B	12:K:603:AF3:F1	2.13	0.57
7:O:175:PHE:HD2	7:O:389:LEU:HD21	1.70	0.57
3:C:98:VAL:HG21	3:C:508:THR:HG23	1.85	0.57
1:I:88:ASP:OD1	1:I:89:GLY:N	2.38	0.57
1:I:474:ALA:HB2	1:I:483:LEU:HB2	1.85	0.57
2:J:79:PRO:HB2	5:M:60:MET:SD	2.44	0.57
5:M:511:ILE:HA	5:M:514:LYS:HG2	1.87	0.57
1:A:114:PRO:HB2	4:D:57:MET:HE2	1.85	0.57
8:H:112:LEU:HD11	8:H:518:VAL:HG11	1.86	0.57
1:I:276:GLN:O	1:I:280:ALA:N	2.38	0.57
9:R:194:LEU:O	9:R:198:LEU:HG	2.05	0.57
8:H:168:ILE:HD11	8:H:183:ILE:HD12	1.87	0.57
1:I:44:MET:SD	3:K:519:ILE:HD13	2.44	0.57
1:A:114:PRO:HA	1:A:117:VAL:HG12	1.86	0.56
3:C:240:LEU:HD22	3:C:291:ILE:HB	1.86	0.56
4:D:305:LEU:HD21	9:Q:129:LEU:HD22	1.86	0.56
3:K:386:GLU:OE1	3:K:389:ARG:NH1	2.37	0.56
5:M:461:ALA:O	5:M:465:ASN:ND2	2.38	0.56
1:I:189:ARG:HG2	1:I:191:PRO:HD3	1.86	0.56
3:C:411:GLY:N	10:C:601:ADP:O2'	2.26	0.56
10:C:601:ADP:O3B	12:C:603:AF3:F1	2.14	0.56
6:F:4:VAL:HG21	6:F:522:MET:HE1	1.87	0.56
6:N:148:LEU:HD22	6:N:398:VAL:HG13	1.87	0.56
7:O:86:GLN:OE1	7:O:501:ASN:ND2	2.33	0.56
2:B:123:PRO:HA	2:B:126:ILE:HD12	1.86	0.56
2:B:425:ALA:HB2	2:B:436:MET:HB2	1.86	0.56
3:C:101:LEU:O	3:C:105:MET:HG3	2.06	0.56
7:G:151:GLN:O	7:G:155:LEU:HG	2.06	0.56
3:K:380:SER:HB3	3:K:383:ILE:HG12	1.88	0.56
7:O:195:ILE:HG22	7:O:370:CYS:HB3	1.87	0.56
8:P:424:THR:HB	8:P:442:ALA:HB2	1.88	0.56
6:N:389:ASP:OD1	6:N:390:ALA:N	2.38	0.56
9:Q:167:PHE:HB3	9:Q:177:GLN:HA	1.87	0.56
1:I:349:GLU:HB3	1:I:366:ASN:HB2	1.88	0.56
2:J:413:SER:O	2:J:417:MET:HG2	2.06	0.56
7:O:108:VAL:HG21	7:O:125:PHE:HZ	1.71	0.56
1:A:400:LYS:NZ	1:A:404:GLU:OE2	2.39	0.56
4:D:123:LEU:HD21	4:D:450:CYS:HA	1.87	0.56
2:J:325:LEU:HD22	2:J:369:GLU:HG2	1.87	0.56
5:M:155:VAL:O	5:M:416:ASN:ND2	2.34	0.56
5:E:124:LEU:HA	5:E:128:ILE:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:244:SER:HB3	3:K:246:GLU:OE1	2.06	0.55
4:D:210:ILE:HD13	4:D:388:ILE:HB	1.88	0.55
6:F:165:ALA:O	6:F:169:THR:HG23	2.06	0.55
7:G:256:ARG:HD3	8:H:258:LEU:HD11	1.88	0.55
1:I:198:LEU:HD11	1:I:217:ASN:HB2	1.87	0.55
2:J:272:LYS:HD3	4:L:347:HIS:ND1	2.21	0.55
4:L:72:ASN:ND2	4:L:173:SER:O	2.39	0.55
4:L:155:VAL:HG11	4:L:415:LEU:HD11	1.87	0.55
5:M:38:ILE:HD13	5:M:121:GLU:HB2	1.88	0.55
2:B:215:ASP:OD1	2:B:216:GLU:N	2.39	0.55
8:H:290:VAL:HG12	8:H:311:MET:HB3	1.89	0.55
7:G:42:PRO:HG2	7:G:479:ILE:HD13	1.88	0.55
8:H:186:ALA:HB2	8:H:375:ILE:HD11	1.89	0.55
2:J:479:ASP:OD1	2:J:481:ARG:NE	2.39	0.55
3:K:132:ASP:OD2	3:K:437:TYR:OH	2.25	0.55
6:N:277:LEU:HD22	6:N:339:LEU:HD22	1.88	0.55
7:O:331:GLN:NE2	7:O:341:VAL:HG21	2.22	0.55
8:P:417:ILE:HG13	8:P:467:LEU:HD13	1.89	0.55
10:M:601:ADP:O3B	12:M:603:AF3:F2	2.15	0.55
2:J:59:ALA:HB1	4:L:89:ARG:HH22	1.71	0.55
3:C:84:SER:HB2	3:C:99:ILE:HD11	1.89	0.55
5:E:27:ARG:NH1	5:E:29:MET:SD	2.80	0.55
8:H:73:LEU:HD13	8:H:87:VAL:HG12	1.88	0.55
1:I:45:LEU:HD23	3:K:523:VAL:HB	1.89	0.55
4:L:309:LEU:HD12	4:L:326:LYS:HD2	1.88	0.55
4:L:348:ILE:HD12	4:L:348:ILE:H	1.70	0.55
6:N:93:THR:N	10:N:601:ADP:O2B	2.40	0.55
6:N:114:LEU:HG	6:N:118:ILE:HD11	1.88	0.55
1:A:470:PHE:HD2	1:A:486:ILE:HD13	1.71	0.55
6:F:37:ASN:HB3	6:F:45:LYS:HZ3	1.72	0.55
2:J:31:GLY:HA3	2:J:78:ASN:HD22	1.72	0.55
2:J:204:LYS:NZ	2:J:357:ASP:OD2	2.35	0.55
3:C:470:HIS:CE1	3:C:476:GLU:HA	2.42	0.55
5:E:222:THR:HA	5:E:386:PHE:O	2.07	0.55
6:F:277:LEU:HD22	6:F:339:LEU:HD12	1.87	0.55
4:L:286:LEU:HD22	4:L:348:ILE:HG12	1.89	0.55
4:D:116:LEU:HD11	4:D:526:VAL:HG21	1.89	0.55
8:P:420:ALA:HB2	8:P:445:PHE:HB2	1.89	0.54
9:R:163:LEU:HB3	9:R:164:PRO:HD3	1.87	0.54
3:C:90:GLU:HG3	3:C:91:VAL:HG13	1.89	0.54
1:I:44:MET:HE2	3:K:75:PRO:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:92:THR:N	10:N:601:ADP:O2B	2.40	0.54
9:Q:52:THR:O	9:Q:78:ARG:NH2	2.40	0.54
4:D:103:GLY:HA3	4:D:410:CYS:HB3	1.89	0.54
4:D:431:GLU:OE2	4:D:435:ARG:NH1	2.38	0.54
1:A:260:LEU:O	1:A:263:ILE:HG12	2.08	0.54
1:A:529:ASP:OD2	4:D:59:LYS:NZ	2.40	0.54
3:C:71:GLN:HB2	6:F:525:GLY:HA2	1.90	0.54
3:C:440:VAL:O	3:C:444:LEU:HD12	2.07	0.54
5:E:62:VAL:HG12	5:E:68:VAL:HG22	1.90	0.54
4:L:26:ASP:N	4:L:26:ASP:OD1	2.40	0.54
3:C:130:LEU:HB2	3:C:510:VAL:HG11	1.88	0.54
5:M:282:LYS:NZ	5:M:286:GLU:OE2	2.33	0.54
3:C:434:GLN:OE1	3:C:438:ARG:NH1	2.31	0.54
5:E:102:ILE:HG22	5:E:104:ASP:H	1.72	0.54
8:H:70:ALA:HB2	8:H:101:THR:HG21	1.89	0.54
1:I:424:GLU:OE1	1:I:468:ARG:NH2	2.39	0.54
3:K:415:GLU:OE1	3:K:447:ILE:HB	2.07	0.54
1:A:489:ASP:O	1:A:493:GLY:HA2	2.08	0.54
2:B:498:GLN:OE1	2:B:501:ARG:NH2	2.40	0.54
4:D:138:GLN:OE1	4:D:527:ARG:NH1	2.41	0.54
5:E:86:GLN:HG3	7:G:48:LEU:HD21	1.89	0.54
1:I:260:LEU:O	1:I:263:ILE:HG12	2.07	0.54
3:K:195:ILE:HG12	3:K:197:LYS:H	1.72	0.54
1:A:78:LEU:HD11	1:A:516:PHE:HB3	1.88	0.54
1:A:377:LEU:HD22	1:A:388:MET:HE2	1.90	0.54
6:F:198:HIS:CD2	6:F:199:LYS:HG3	2.43	0.54
2:J:237:ILE:HD12	2:J:327:THR:HG21	1.90	0.54
5:M:480:ARG:NH2	5:M:484:GLU:OE2	2.37	0.54
5:M:531:ASP:HB2	7:O:45:MET:HB3	1.90	0.54
2:B:173:THR:HA	2:B:176:LYS:HB2	1.90	0.54
4:D:359:ALA:HA	4:D:379:CYS:HA	1.90	0.54
6:N:331:VAL:HG12	6:N:343:CYS:HA	1.88	0.54
9:Q:189:LEU:HG	9:Q:193:GLU:HB2	1.88	0.54
7:G:186:LEU:HD11	7:G:195:ILE:HD11	1.89	0.54
2:J:121:ILE:HG23	2:J:126:ILE:HD11	1.89	0.54
7:O:238:ALA:HB3	7:O:289:VAL:HG12	1.88	0.54
10:E:601:ADP:O1B	12:E:603:AF3:F2	2.15	0.53
6:F:232:THR:HG23	6:F:332:ALA:HA	1.89	0.53
8:H:200:ASP:O	8:H:203:ARG:NH1	2.41	0.53
3:K:79:SER:O	3:K:83:ILE:HG12	2.07	0.53
3:K:144:VAL:HG23	3:K:151:MET:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:LEU:HD11	2:B:172:LEU:HD13	1.91	0.53
4:D:240:ARG:HG2	4:D:363:GLU:HG3	1.89	0.53
2:J:138:ARG:HD2	2:J:505:LEU:HD21	1.90	0.53
4:L:118:ASP:O	4:L:121:THR:HG22	2.08	0.53
4:L:227:LEU:HD21	4:L:336:ILE:HG12	1.89	0.53
9:R:115:VAL:HG12	9:R:145:LYS:HD2	1.90	0.53
3:C:292:THR:HG21	3:C:296:ILE:HD11	1.91	0.53
5:E:76:THR:HG22	5:E:80:MET:HE1	1.90	0.53
7:G:424:SER:O	7:G:425:ARG:HD2	2.08	0.53
2:B:243:GLY:HA2	2:B:294:GLN:HE21	1.74	0.53
7:G:364:CYS:HB2	7:G:367:ALA:HB2	1.90	0.53
6:N:64:LEU:HD21	6:N:78:ALA:HA	1.89	0.53
8:P:160:VAL:HG13	8:P:184:ALA:HB1	1.90	0.53
1:A:489:ASP:O	1:A:493:GLY:CA	2.57	0.53
5:M:295:THR:HG22	5:M:353:LEU:HD11	1.90	0.53
6:F:451:LEU:HD12	6:F:481:LEU:HD21	1.91	0.53
7:G:257:VAL:HG11	7:G:266:ILE:HD11	1.88	0.53
3:K:106:LEU:HD11	3:K:513:ALA:HA	1.90	0.53
3:K:160:ILE:HD11	3:K:390:ASN:HB3	1.90	0.53
7:O:236:LYS:HB2	7:O:286:ALA:HA	1.90	0.53
3:C:157:ASN:HA	3:C:160:ILE:HG22	1.90	0.53
4:D:183:LEU:HD21	4:D:405:ILE:HG12	1.90	0.53
1:I:75:LEU:HD12	1:I:94:VAL:HG13	1.90	0.53
8:P:29:VAL:O	8:P:33:ILE:HG12	2.08	0.53
5:E:211:VAL:HG12	5:E:385:ILE:HB	1.91	0.53
9:Q:53:LEU:HD23	9:Q:78:ARG:HH22	1.73	0.53
3:C:64:ASN:ND2	3:C:88:ASP:OD2	2.42	0.53
6:F:180:LYS:NZ	6:F:181:LYS:O	2.40	0.53
2:J:179:PHE:O	2:J:182:LEU:HB3	2.09	0.53
7:O:199:LYS:HG2	7:O:374:LEU:HD21	1.90	0.53
1:A:26:ALA:O	1:A:30:ASN:ND2	2.33	0.53
1:A:489:ASP:HB2	1:A:496:ARG:HD3	1.90	0.53
5:E:185:MET:HA	5:E:188:ILE:HG12	1.90	0.53
5:E:322:VAL:HG11	5:E:372:LEU:HD22	1.90	0.53
8:P:384:LEU:O	8:P:388:ILE:HG12	2.09	0.53
4:L:149:THR:HA	4:L:512:LEU:HD11	1.91	0.52
8:P:402:LEU:HD11	8:P:408:LEU:HD21	1.91	0.52
2:B:165:THR:HG21	2:B:494:THR:O	2.09	0.52
5:E:359:VAL:HG12	5:E:374:ILE:HG12	1.91	0.52
6:F:445:LEU:HD12	6:F:463:LEU:HD11	1.90	0.52
4:L:214:LEU:HD12	4:L:215:GLY:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:289:ILE:HG13	5:M:313:LEU:HB3	1.90	0.52
7:O:97:VAL:HG12	7:O:502:ALA:HA	1.91	0.52
7:O:190:LEU:HB3	7:O:397:ARG:HD2	1.92	0.52
7:O:286:ALA:HB2	7:O:342:LEU:HD22	1.91	0.52
8:P:283:ILE:HA	8:P:338:PRO:HB3	1.91	0.52
4:L:213:LYS:O	4:L:391:ARG:NH1	2.43	0.52
5:M:119:GLU:HB3	5:M:450:ALA:HB1	1.90	0.52
1:A:276:GLN:O	1:A:280:ALA:N	2.42	0.52
5:E:125:ASP:OD1	4:L:49:ARG:NH2	2.38	0.52
7:G:9:LEU:HD11	8:H:76:LEU:HD13	1.91	0.52
1:I:103:ASN:HB3	1:I:440:GLU:HG3	1.91	0.52
9:R:87:LEU:O	9:R:90:LYS:NZ	2.38	0.52
2:B:516:ARG:O	5:E:58:ASP:N	2.41	0.52
7:G:458:THR:OG1	1:I:433:ARG:NH2	2.42	0.52
8:H:249:MET:SD	8:H:335:ARG:NE	2.83	0.52
5:M:532:ASP:HB3	7:O:47:LYS:HD2	1.91	0.52
2:B:417:MET:HE1	2:B:504:LEU:HD13	1.90	0.52
5:E:196:VAL:HG21	5:E:209:ILE:HG13	1.90	0.52
3:K:207:GLY:O	6:N:503:GLN:NE2	2.31	0.52
2:B:79:PRO:HA	2:B:82:LYS:HG3	1.92	0.52
6:F:290:VAL:HG13	6:F:311:VAL:HG13	1.91	0.52
8:H:18:GLY:HA3	8:H:528:LYS:HB3	1.91	0.52
2:J:288:ASN:HA	2:J:309:VAL:HG12	1.91	0.52
8:P:292:VAL:HG12	8:P:313:VAL:HB	1.91	0.52
9:Q:59:HIS:O	9:Q:61:ASP:N	2.43	0.52
1:A:401:ARG:HB3	1:A:508:ILE:HD12	1.90	0.52
6:N:445:LEU:HD12	6:N:463:LEU:HD21	1.91	0.52
1:A:272:LYS:HG2	1:A:276:GLN:HE22	1.75	0.52
3:C:132:ASP:OD2	3:C:437:TYR:OH	2.28	0.52
4:D:229:LEU:HB2	4:D:374:LEU:HB3	1.92	0.52
8:H:102:ASN:N	10:H:601:ADP:O2B	2.43	0.52
2:J:219:LEU:HB2	2:J:372:THR:HG21	1.91	0.52
6:N:246:SER:OG	6:N:247:GLY:N	2.43	0.52
7:O:195:ILE:HD11	7:O:393:ILE:HD12	1.91	0.52
5:E:279:LYS:O	5:E:283:GLU:HG2	2.10	0.52
6:F:239:TYR:OH	8:H:253:THR:OG1	2.28	0.52
7:G:19:ILE:HG13	7:G:20:PRO:HD3	1.92	0.52
6:N:149:ILE:HD13	6:N:173:VAL:HG21	1.91	0.52
3:C:104:GLU:HG2	3:C:446:VAL:HG11	1.91	0.51
6:F:445:LEU:HB3	6:F:449:LYS:HE2	1.90	0.51
1:I:204:SER:OG	1:I:205:GLN:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:243:GLY:HA2	2:J:294:GLN:HE21	1.75	0.51
3:K:445:GLU:OE2	3:K:467:ARG:NH1	2.42	0.51
8:P:65:VAL:HG12	8:P:383:ASN:HB3	1.92	0.51
8:P:93:GLN:NE2	8:P:99:ASP:O	2.33	0.51
3:C:19:GLY:O	3:C:22:VAL:HG22	2.10	0.51
3:C:130:LEU:HA	3:C:133:MET:SD	2.49	0.51
4:D:95:SER:OG	4:D:106:THR:OG1	2.23	0.51
5:E:228:VAL:HG11	5:E:333:ILE:HG12	1.92	0.51
6:F:217:ARG:HG3	6:F:314:ARG:HH21	1.75	0.51
1:I:356:ILE:HG13	1:I:357:CYS:H	1.75	0.51
2:J:517:VAL:HG11	5:M:60:MET:HE3	1.93	0.51
4:L:430:ILE:HG21	4:L:480:LEU:HG	1.92	0.51
5:M:236:HIS:CD2	5:M:315:LEU:HD22	2.45	0.51
1:A:57:ASP:OD1	1:A:57:ASP:N	2.44	0.51
1:A:198:LEU:HD11	1:A:217:ASN:HB2	1.92	0.51
5:E:18:ILE:HA	7:G:73:HIS:HB2	1.93	0.51
8:H:247:ASP:OD1	8:H:248:GLY:N	2.43	0.51
2:J:516:ARG:O	5:M:58:ASP:N	2.42	0.51
3:K:123:ILE:HG23	3:K:514:VAL:HG22	1.92	0.51
5:M:155:VAL:HG21	5:M:412:LEU:HD21	1.92	0.51
5:M:169:ALA:HB2	5:M:409:ILE:HD11	1.92	0.51
5:M:402:LEU:O	5:M:406:LEU:HG	2.09	0.51
6:N:145:ARG:O	6:N:149:ILE:HG12	2.10	0.51
7:O:331:GLN:OE1	8:P:303:HIS:NE2	2.43	0.51
4:D:160:ARG:NH1	4:D:189:ASN:OD1	2.44	0.51
6:F:34:LEU:HG	6:F:96:VAL:HG21	1.92	0.51
6:F:38:LEU:HD13	6:F:97:LEU:HD12	1.92	0.51
6:F:272:LYS:HA	6:F:275:ILE:HG22	1.92	0.51
2:J:94:GLU:HG3	2:J:95:VAL:HG13	1.93	0.51
3:K:182:MET:SD	3:K:372:CYS:HB3	2.51	0.51
7:O:249:GLU:OE2	8:P:269:SER:OG	2.26	0.51
1:A:39:VAL:HG21	1:A:456:ALA:HB2	1.91	0.51
3:C:130:LEU:O	3:C:133:MET:HG2	2.10	0.51
1:I:39:VAL:HG11	1:I:456:ALA:HA	1.93	0.51
6:N:152:ALA:HB3	6:N:169:THR:HG23	1.91	0.51
1:A:136:LEU:HD13	1:A:415:VAL:HG23	1.93	0.51
4:D:203:VAL:HG13	4:D:416:VAL:HG11	1.91	0.51
4:D:227:LEU:HB2	4:D:339:THR:HG21	1.91	0.51
6:F:230:ILE:HD13	6:F:290:VAL:HB	1.91	0.51
6:F:264:ARG:O	6:F:268:GLU:HG2	2.10	0.51
2:J:261:THR:HB	4:L:278:GLU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:14:ALA:O	6:N:520:GLU:HA	2.11	0.51
6:N:45:LYS:HG3	8:P:523:GLN:HB3	1.93	0.51
9:R:184:PHE:HB3	9:R:189:LEU:HD21	1.92	0.51
8:H:149:CYS:SG	8:H:493:LEU:HD11	2.51	0.51
2:J:35:ILE:O	2:J:39:VAL:HG23	2.11	0.51
3:K:366:CYS:SG	3:K:369:PRO:HB3	2.51	0.51
6:N:37:ASN:HB2	6:N:58:LYS:HG2	1.93	0.51
6:N:485:GLU:HG2	6:N:486:PRO:HD2	1.93	0.51
8:H:226:GLU:HG3	8:H:352:LEU:HD11	1.91	0.51
2:J:263:LYS:O	2:J:267:ILE:HG12	2.11	0.51
3:K:290:VAL:HG11	3:K:304:LEU:HD13	1.93	0.51
8:P:3:LEU:O	8:P:4:HIS:ND1	2.44	0.51
8:P:73:LEU:HG	8:P:87:VAL:HG22	1.93	0.51
8:P:210:SER:OG	8:P:211:GLY:N	2.44	0.51
3:C:159:SER:OG	3:C:397:VAL:HG21	2.11	0.51
7:G:168:ILE:HD13	7:G:385:THR:HG23	1.92	0.51
8:H:281:LYS:NZ	8:H:285:ASP:OD1	2.44	0.51
2:J:479:ASP:O	2:J:483:GLY:N	2.45	0.51
4:L:325:ILE:HD13	4:L:374:LEU:HD22	1.92	0.51
5:E:176:LYS:NZ	12:E:603:AF3:F1	2.34	0.50
8:H:190:ILE:HD11	8:H:201:ASN:HB3	1.91	0.50
8:H:222:VAL:HG22	8:H:362:VAL:HG22	1.94	0.50
3:K:19:GLY:O	3:K:22:VAL:HG12	2.11	0.50
3:K:137:LEU:HD21	3:K:502:LYS:HB3	1.92	0.50
3:K:314:ARG:NE	9:R:58:ASP:O	2.44	0.50
5:M:307:ASP:OD1	5:M:307:ASP:N	2.42	0.50
7:O:169:SER:O	7:O:172:LYS:HG3	2.11	0.50
7:O:175:PHE:CD2	7:O:389:LEU:HD21	2.46	0.50
9:Q:95:LEU:HD22	9:Q:145:LYS:HE2	1.93	0.50
9:R:166:ILE:HD13	9:R:184:PHE:HZ	1.76	0.50
1:A:17:ILE:HG21	1:A:529:ASP:HA	1.92	0.50
6:N:38:LEU:HD13	6:N:97:LEU:HD22	1.92	0.50
1:A:127:GLU:HG3	1:A:426:TYR:CZ	2.47	0.50
1:A:499:LYS:HD2	1:A:504:PHE:HE1	1.75	0.50
2:B:86:ASP:OD1	5:E:392:LYS:NZ	2.38	0.50
3:C:87:GLN:HE22	3:C:505:THR:HA	1.75	0.50
5:E:129:HIS:HB3	5:E:132:ARG:HG2	1.93	0.50
6:F:198:HIS:CG	6:F:199:LYS:H	2.28	0.50
2:J:79:PRO:HA	2:J:82:LYS:HG3	1.92	0.50
5:M:202:ARG:NH1	5:M:413:ILE:O	2.41	0.50
1:A:103:ASN:OD1	1:A:443:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:GLY:HA3	2:B:78:ASN:HD22	1.75	0.50
6:F:49:SER:OG	6:F:50:GLY:N	2.43	0.50
3:K:62:ASP:N	3:K:62:ASP:OD1	2.44	0.50
7:O:117:HIS:O	7:O:120:ILE:HG22	2.10	0.50
7:O:318:ASP:OD1	7:O:321:ARG:NH1	2.44	0.50
8:P:99:ASP:OD1	12:P:603:AF3:F3	2.19	0.50
7:G:495:PRO:O	7:G:498:VAL:HG12	2.12	0.50
2:J:271:GLU:HG2	5:M:274:TYR:CZ	2.47	0.50
2:J:417:MET:HG3	2:J:443:LEU:HD21	1.92	0.50
6:N:101:GLU:HG2	6:N:446:ILE:HB	1.93	0.50
7:O:40:LEU:HD11	7:O:99:LEU:HD12	1.93	0.50
1:A:105:ASP:O	1:A:109:LYS:HG2	2.11	0.50
3:C:182:MET:SD	3:C:372:CYS:HB3	2.51	0.50
5:E:480:ARG:HH12	5:E:499:ASN:HB2	1.76	0.50
10:G:601:ADP:O1B	12:G:603:AF3:F2	2.20	0.50
3:K:470:HIS:NE2	3:K:476:GLU:HA	2.27	0.50
7:O:197:ILE:HG21	7:O:386:GLU:HG3	1.93	0.50
8:P:39:LEU:O	8:P:42:THR:HG22	2.12	0.50
1:A:104:ALA:HB2	1:A:121:TYR:CE2	2.46	0.50
2:B:205:LEU:HD23	4:D:97:ALA:HB2	1.92	0.50
3:C:123:ILE:HD11	3:C:517:LEU:HB3	1.94	0.50
4:D:118:ASP:O	4:D:121:THR:HG22	2.11	0.50
5:E:38:ILE:HD13	5:E:121:GLU:HB2	1.92	0.50
6:F:90:ASP:OD1	12:F:603:AF3:F1	2.20	0.50
6:F:115:HIS:CE1	6:F:117:ARG:HG3	2.47	0.50
8:H:203:ARG:HD2	8:H:323:ARG:HD3	1.92	0.50
3:K:382:GLU:OE1	6:N:79:LYS:HD2	2.12	0.50
4:L:89:ARG:HA	4:L:92:VAL:HG22	1.93	0.50
5:E:289:ILE:HG13	5:E:313:LEU:HB3	1.94	0.50
6:F:409:PRO:HB3	6:F:489:ALA:HB3	1.93	0.50
1:I:42:ASP:OD2	3:K:518:ARG:NH1	2.44	0.50
3:K:206:GLY:HA3	6:N:87:ILE:HG13	1.94	0.50
4:L:307:ASP:OD1	4:L:307:ASP:N	2.44	0.50
2:B:102:VAL:HG23	2:B:507:ALA:HB2	1.93	0.50
6:F:134:LEU:HA	6:F:137:VAL:HG12	1.93	0.50
7:G:177:LYS:O	7:G:180:VAL:HG12	2.11	0.50
7:G:201:GLN:HA	7:G:382:MET:HE3	1.93	0.50
8:H:410:PRO:O	8:H:415:THR:OG1	2.23	0.50
4:L:141:LEU:O	4:L:145:ILE:HG12	2.11	0.50
6:N:237:LEU:HB2	6:N:297:ILE:HG23	1.94	0.50
3:C:50:LEU:HD11	3:C:66:ILE:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:367:LEU:HD11	4:D:373:LEU:HB2	1.95	0.49
5:E:454:ALA:O	5:E:457:VAL:HG22	2.11	0.49
7:G:447:ARG:HB2	7:G:461:LEU:HD22	1.93	0.49
8:H:497:ILE:HG13	8:H:497:ILE:O	2.11	0.49
5:M:230:VAL:HG22	5:M:232:LYS:HG2	1.93	0.49
6:N:217:ARG:HG3	6:N:314:ARG:NE	2.26	0.49
9:R:136:GLY:HA3	9:R:191:ARG:HH22	1.77	0.49
1:A:158:SER:O	3:C:518:ARG:NH2	2.45	0.49
1:A:181:TYR:HB3	1:A:189:ARG:HG3	1.94	0.49
1:A:489:ASP:HB2	1:A:496:ARG:HH11	1.77	0.49
3:C:105:MET:HA	3:C:108:VAL:HG12	1.93	0.49
5:E:306:PHE:CE2	5:E:323:ARG:HB3	2.47	0.49
3:K:416:MET:HB3	3:K:470:HIS:HD1	1.76	0.49
3:C:240:LEU:HD12	3:C:324:ALA:HB2	1.94	0.49
3:C:289:VAL:HG21	3:C:350:LEU:HD13	1.94	0.49
8:H:33:ILE:HG21	8:H:116:GLU:HB2	1.95	0.49
3:K:155:ILE:HD13	3:K:401:VAL:HG21	1.93	0.49
6:N:73:THR:HA	6:N:76:LEU:HD12	1.94	0.49
6:N:367:ASN:OD1	6:N:368:ASN:N	2.44	0.49
8:P:151:ALA:HB3	8:P:406:LYS:HB3	1.94	0.49
6:F:315:ARG:HH12	9:Q:76:ARG:HD3	1.77	0.49
5:M:530:ILE:HD11	7:O:58:ILE:HD13	1.95	0.49
6:N:114:LEU:HD23	6:N:119:ILE:HD11	1.93	0.49
2:B:231:ARG:NH1	2:B:350:GLU:OE1	2.45	0.49
7:G:136:ILE:HD11	7:G:416:LEU:HD11	1.95	0.49
7:G:142:THR:OG1	7:G:144:LYS:NZ	2.33	0.49
8:H:69:ALA:HB3	8:H:101:THR:OG1	2.12	0.49
1:I:114:PRO:HA	1:I:117:VAL:HG12	1.93	0.49
4:L:170:SER:HB3	4:L:411:VAL:HG21	1.94	0.49
7:O:370:CYS:SG	7:O:371:THR:N	2.85	0.49
2:B:263:LYS:O	2:B:267:ILE:HG12	2.12	0.49
4:L:250:GLN:NE2	4:L:301:GLN:OE1	2.34	0.49
9:Q:112:GLY:N	9:Q:171:GLU:OE2	2.45	0.49
2:B:79:PRO:O	2:B:83:VAL:HG23	2.13	0.49
3:C:225:THR:HG22	3:C:313:ARG:HB2	1.95	0.49
4:D:48:ILE:HD12	4:D:107:THR:HG23	1.95	0.49
7:G:34:GLU:HA	7:G:37:ARG:HD2	1.94	0.49
1:I:86:VAL:HG11	1:I:509:VAL:HG22	1.94	0.49
1:I:264:ARG:NH1	3:K:247:TYR:OH	2.46	0.49
2:J:235:ALA:HA	2:J:288:ASN:HD21	1.78	0.49
2:J:245:ASP:OD1	2:J:246:THR:N	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:499:VAL:O	2:J:503:VAL:HG23	2.12	0.49
3:K:130:LEU:HB2	3:K:510:VAL:HG11	1.93	0.49
4:L:116:LEU:HD11	4:L:526:VAL:HG21	1.94	0.49
6:N:12:GLU:HB2	6:N:523:ARG:HB3	1.95	0.49
2:B:432:GLU:O	2:B:436:MET:HG3	2.12	0.49
3:C:72:VAL:O	3:C:78:LYS:NZ	2.42	0.49
10:D:601:ADP:O1B	12:D:603:AF3:F3	2.20	0.49
5:M:387:ILE:HD11	5:M:402:LEU:HD12	1.95	0.49
7:O:79:LEU:O	7:O:82:ILE:HG22	2.13	0.49
7:O:147:ASP:OD1	7:O:147:ASP:N	2.46	0.49
8:P:102:ASN:N	10:P:601:ADP:O2B	2.46	0.49
4:D:399:GLU:O	4:D:402:GLU:HG3	2.12	0.49
5:E:233:ASP:N	5:E:233:ASP:OD1	2.45	0.49
5:E:407:CYS:O	5:E:410:ARG:HG3	2.13	0.49
1:I:252:VAL:HG23	3:K:254:THR:HA	1.93	0.49
4:L:340:ILE:HG13	4:L:342:THR:HG23	1.95	0.49
5:M:357:GLY:N	5:M:375:GLU:O	2.45	0.49
2:B:148:HIS:O	2:B:404:SER:OG	2.29	0.49
2:B:446:LEU:O	2:B:450:ILE:HG13	2.13	0.49
5:E:210:LYS:NZ	5:E:212:GLU:OE1	2.44	0.49
8:H:131:GLY:HA3	8:H:437:ALA:HB3	1.94	0.49
1:I:170:ASN:O	1:I:173:VAL:HG22	2.13	0.49
1:I:225:MET:HE2	1:I:306:MET:HA	1.95	0.49
10:J:601:ADP:O2B	12:J:603:AF3:F3	2.21	0.49
6:N:71:HIS:CD2	6:N:72:PRO:HD2	2.48	0.49
6:N:451:LEU:HD12	6:N:481:LEU:HD21	1.95	0.49
6:F:338:ASP:OD1	6:F:338:ASP:N	2.46	0.48
7:G:23:VAL:HG13	7:G:109:LYS:HD2	1.95	0.48
7:O:175:PHE:O	7:O:178:MET:HB3	2.13	0.48
9:Q:116:ILE:HB	9:Q:146:PHE:HB3	1.94	0.48
1:A:169:ALA:O	1:A:172:VAL:HB	2.13	0.48
3:C:219:MET:HG3	3:C:362:PHE:CE2	2.47	0.48
1:I:506:PRO:HG2	1:I:509:VAL:HG23	1.95	0.48
7:O:89:GLU:HG3	7:O:90:VAL:HG13	1.95	0.48
3:C:481:ASN:O	3:C:485:GLY:N	2.46	0.48
10:F:601:ADP:O1B	12:F:603:AF3:F1	2.21	0.48
7:G:107:GLN:HG3	7:G:441:ALA:HB2	1.96	0.48
2:J:256:VAL:HG12	5:M:268:VAL:HG23	1.95	0.48
3:K:219:MET:HB3	3:K:373:THR:HG21	1.94	0.48
4:L:58:ASP:HB3	4:L:72:ASN:HB2	1.94	0.48
4:L:434:LEU:O	4:L:437:THR:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:511:PRO:HG2	4:L:514:VAL:HG23	1.95	0.48
1:A:489:ASP:O	1:A:493:GLY:N	2.46	0.48
2:B:261:THR:HB	4:D:278:GLU:HB3	1.95	0.48
6:F:289:PHE:HB3	6:F:310:ILE:HD12	1.95	0.48
1:I:65:LEU:HD21	3:K:523:VAL:HG11	1.94	0.48
2:J:132:GLU:HB3	2:J:436:MET:HE2	1.96	0.48
5:M:74:GLY:HA3	5:M:107:THR:HG22	1.95	0.48
4:D:76:THR:HG21	4:D:403:ARG:HD3	1.94	0.48
6:F:435:LEU:O	6:F:438:GLN:HB3	2.14	0.48
7:G:47:LYS:HD2	7:G:65:ILE:HD13	1.94	0.48
7:G:116:LEU:HD11	7:G:430:LYS:HD2	1.96	0.48
8:H:5:VAL:HB	6:N:12:GLU:HB3	1.95	0.48
8:H:210:SER:HG	8:H:214:SER:HG	1.60	0.48
7:O:17:GLN:HG2	7:O:518:GLU:HG3	1.95	0.48
8:P:43:THR:HG23	8:P:72:ILE:HD11	1.95	0.48
8:P:324:LEU:HA	8:P:327:THR:HG22	1.96	0.48
6:F:130:ALA:HB1	6:F:418:MET:SD	2.53	0.48
7:G:79:LEU:O	7:G:82:ILE:HG22	2.13	0.48
1:I:281:THR:HG23	1:I:345:LEU:HD11	1.95	0.48
1:I:519:GLU:OE2	4:L:393:SER:HB3	2.14	0.48
2:B:62:MET:SD	2:B:73:ASN:ND2	2.86	0.48
3:C:504:GLN:O	3:C:508:THR:HG22	2.14	0.48
7:G:63:ALA:O	7:G:67:LYS:HG3	2.13	0.48
1:I:22:VAL:HG13	1:I:102:LYS:HG2	1.95	0.48
2:J:413:SER:O	2:J:416:LEU:HG	2.13	0.48
5:M:115:ALA:O	5:M:119:GLU:HG2	2.13	0.48
5:M:231:ASP:HA	5:M:371:MET:HG2	1.95	0.48
1:A:464:VAL:HG23	1:A:468:ARG:HH21	1.79	0.48
5:E:234:PHE:HA	5:E:322:VAL:HG12	1.96	0.48
8:H:424:THR:O	8:H:428:GLU:HG2	2.14	0.48
10:L:601:ADP:O3B	12:L:603:AF3:F1	2.21	0.48
6:N:212:LEU:HB2	6:N:361:THR:OG1	2.13	0.48
6:N:445:LEU:HD12	6:N:463:LEU:HD11	1.96	0.48
2:B:448:THR:OG1	2:B:462:VAL:HG21	2.13	0.48
8:H:48:GLY:HA2	10:H:601:ADP:H5'2	1.96	0.48
3:K:67:LEU:HD11	3:K:99:ILE:HD12	1.95	0.48
3:K:325:ARG:HG3	3:K:370:LYS:HB2	1.96	0.48
3:K:504:GLN:NE2	3:K:508:THR:OG1	2.43	0.48
7:G:524:ARG:HD3	8:H:61:GLU:HG3	1.96	0.48
1:I:31:ILE:HD11	3:K:10:LEU:HD11	1.96	0.48
2:J:410:GLY:HA2	10:J:601:ADP:N3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Q:82:TRP:O	9:Q:86:LYS:HG2	2.14	0.48
9:Q:91:PHE:CD1	9:Q:145:LYS:HD2	2.49	0.48
9:Q:118:HIS:NE2	9:Q:131:ASN:OD1	2.47	0.48
3:C:43:PRO:HA	3:C:162:THR:HA	1.95	0.47
2:B:51:ILE:HG12	2:B:63:VAL:HG22	1.96	0.47
4:D:172:ASN:HD22	10:D:601:ADP:HN61	1.62	0.47
4:D:213:LYS:HE3	4:D:391:ARG:HD3	1.96	0.47
5:E:314:LEU:HD23	5:E:321:ALA:HB3	1.96	0.47
2:J:231:ARG:NE	2:J:233:GLU:OE2	2.48	0.47
4:L:90:MET:SD	4:L:529:ILE:HG12	2.54	0.47
4:L:289:GLN:HA	4:L:292:LYS:HD2	1.96	0.47
1:A:192:VAL:HG12	1:A:193:ASN:H	1.79	0.47
3:C:281:ASP:OD2	3:C:336:GLU:HA	2.14	0.47
5:E:522:GLN:HE22	7:G:205:LEU:H	1.62	0.47
7:G:329:SER:HB2	7:G:341:VAL:HG23	1.95	0.47
2:J:292:ASN:OD1	2:J:293:ARG:N	2.46	0.47
4:L:235:ASN:ND2	4:L:322:ILE:O	2.42	0.47
7:O:331:GLN:HE21	7:O:341:VAL:HG11	1.80	0.47
8:P:247:ASP:OD1	8:P:248:GLY:N	2.47	0.47
9:Q:174:ILE:HD11	9:Q:177:GLN:HB3	1.96	0.47
6:N:88:THR:O	6:N:400:ASN:ND2	2.43	0.47
6:F:239:TYR:N	6:F:298:ASP:OD2	2.48	0.47
6:N:232:THR:HG23	6:N:332:ALA:HA	1.96	0.47
7:O:190:LEU:O	7:O:397:ARG:NH1	2.47	0.47
8:P:227:THR:HG22	8:P:352:LEU:HD13	1.96	0.47
8:P:436:TYR:HA	8:P:439:LYS:HE2	1.96	0.47
1:A:502:GLY:HA2	1:A:504:PHE:CZ	2.49	0.47
7:G:79:LEU:HA	7:G:82:ILE:HG22	1.97	0.47
1:I:145:ARG:NH2	1:I:174:ASP:OD1	2.47	0.47
5:M:37:HIS:NE2	5:M:533:ILE:HD11	2.29	0.47
6:N:211:VAL:HG23	6:N:373:THR:HG21	1.96	0.47
2:B:132:GLU:HG3	2:B:424:LEU:HD21	1.96	0.47
3:C:43:PRO:HG3	10:C:601:ADP:C6	2.49	0.47
3:C:266:ARG:HD2	3:C:266:ARG:HA	1.71	0.47
4:D:120:CYS:HA	4:D:123:LEU:HD13	1.96	0.47
4:D:170:SER:HB3	4:D:411:VAL:HG21	1.95	0.47
5:E:226:LYS:HB3	5:E:226:LYS:HE2	1.70	0.47
6:F:212:LEU:HB2	6:F:361:THR:OG1	2.15	0.47
7:G:90:VAL:HG11	7:G:498:VAL:HB	1.97	0.47
7:G:346:GLN:HB3	7:G:363:GLY:HA3	1.95	0.47
2:J:331:ILE:HB	5:M:236:HIS:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:186:GLU:OE1	3:K:192:GLU:HG3	2.14	0.47
2:B:181:LYS:HG3	2:B:182:LEU:N	2.30	0.47
5:E:78:LEU:HD13	5:E:92:VAL:HA	1.96	0.47
6:F:85:ASP:HB2	6:F:92:THR:HG21	1.97	0.47
6:F:148:LEU:HD11	6:F:402:ILE:HD11	1.97	0.47
3:K:203:LYS:HE3	3:K:388:GLU:HG2	1.96	0.47
7:O:60:ASN:HA	7:O:65:ILE:HD11	1.97	0.47
9:Q:169:TYR:HB3	9:Q:174:ILE:HA	1.97	0.47
1:A:263:ILE:HG22	4:D:269:TYR:HA	1.97	0.47
2:B:323:LEU:HD11	2:B:362:PHE:CE2	2.50	0.47
3:C:80:MET:O	3:C:83:ILE:HG22	2.15	0.47
4:D:184:SER:N	4:D:185:PRO:HD2	2.30	0.47
4:D:213:LYS:HE2	4:D:367:LEU:HD22	1.97	0.47
5:E:250:ILE:HD13	5:E:334:ALA:HA	1.96	0.47
2:J:145:ALA:HA	2:J:407:VAL:HG12	1.96	0.47
5:M:141:ALA:O	5:M:145:ILE:HG12	2.15	0.47
5:M:222:THR:HA	5:M:386:PHE:O	2.15	0.47
5:M:287:GLU:O	5:M:291:GLN:HG2	2.15	0.47
1:A:268:SER:HB3	1:A:295:MET:HE1	1.97	0.47
1:A:430:MET:O	1:A:435:GLN:HB3	2.14	0.47
4:D:283:ILE:O	4:D:287:VAL:HG23	2.14	0.47
6:F:189:PHE:O	6:F:323:ARG:NH2	2.46	0.47
3:K:98:VAL:HG21	3:K:508:THR:HB	1.96	0.47
8:P:467:LEU:HD23	8:P:467:LEU:HA	1.77	0.47
1:A:228:ARG:NE	1:A:350:GLU:OE2	2.37	0.46
6:F:168:LEU:HD11	6:F:387:ILE:HG23	1.97	0.46
3:K:385:SER:O	3:K:388:GLU:HG3	2.14	0.46
4:L:484:HIS:HE1	4:L:491:ALA:H	1.63	0.46
6:N:416:VAL:HG11	6:N:466:ILE:HG22	1.97	0.46
9:Q:91:PHE:CD2	9:Q:145:LYS:HB2	2.50	0.46
3:C:243:SER:OG	3:C:333:SER:O	2.21	0.46
6:F:101:GLU:HG2	6:F:446:ILE:HB	1.97	0.46
7:G:503:LEU:HD23	7:G:503:LEU:HA	1.75	0.46
2:J:54:SER:HB2	2:J:59:ALA:HA	1.96	0.46
2:J:494:THR:HG22	2:J:495:GLU:N	2.30	0.46
6:N:145:ARG:NH2	6:N:174:ASP:OD1	2.49	0.46
7:O:26:ILE:HG23	7:O:105:LEU:HB3	1.97	0.46
8:H:114:LEU:HB3	8:H:440:LYS:HD2	1.97	0.46
5:M:134:ALA:HB1	5:M:525:ARG:HG3	1.96	0.46
5:M:456:GLU:O	5:M:459:PRO:HD2	2.15	0.46
7:O:79:LEU:HD12	7:O:98:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:290:VAL:HG22	8:P:311:MET:HB3	1.96	0.46
9:Q:138:ALA:HB2	9:Q:146:PHE:CZ	2.50	0.46
2:J:79:PRO:HB3	5:M:68:VAL:HG21	1.98	0.46
9:Q:189:LEU:HD21	9:Q:197:LYS:NZ	2.30	0.46
1:A:471:HIS:O	1:A:475:GLN:HG2	2.16	0.46
3:C:313:ARG:O	3:C:315:VAL:HG23	2.15	0.46
5:E:392:LYS:O	5:E:396:GLU:HG2	2.16	0.46
6:F:350:VAL:HG22	6:F:363:ILE:HG12	1.98	0.46
8:H:39:LEU:HD22	8:H:83:ALA:HB1	1.96	0.46
8:H:284:ALA:HB2	8:H:310:ILE:HD11	1.95	0.46
6:N:449:LYS:HG3	6:N:463:LEU:HD22	1.96	0.46
1:A:198:LEU:HB2	1:A:376:ILE:HG12	1.97	0.46
1:A:205:GLN:N	3:C:511:GLU:OE2	2.48	0.46
2:B:271:GLU:O	2:B:274:LYS:HG2	2.15	0.46
3:C:226:HIS:CD2	6:F:334:ASN:HD21	2.33	0.46
4:D:24:TYR:O	4:D:25:GLN:HG3	2.15	0.46
6:F:206:LEU:HD12	6:F:373:THR:O	2.15	0.46
3:K:167:ARG:HA	3:K:167:ARG:NE	2.30	0.46
1:A:29:ALA:O	1:A:33:LYS:HB2	2.16	0.46
8:H:83:ALA:O	8:H:87:VAL:HG13	2.16	0.46
5:M:411:ASN:HB3	5:M:511:ILE:HD11	1.98	0.46
2:B:255:ARG:HH12	2:B:257:ARG:HD2	1.81	0.46
3:C:452:ILE:HG21	3:C:459:THR:HA	1.98	0.46
3:C:460:ILE:HG23	3:C:461:ARG:H	1.81	0.46
5:E:91:MET:HE3	5:E:110:VAL:HG13	1.98	0.46
6:F:239:TYR:HE2	6:F:263:GLU:HG2	1.81	0.46
6:F:256:ARG:O	6:F:260:VAL:HG13	2.16	0.46
1:I:168:PHE:O	1:I:172:VAL:HG23	2.16	0.46
2:J:285:HIS:CE1	2:J:338:PRO:HA	2.50	0.46
2:J:323:LEU:HA	2:J:326:VAL:HG12	1.98	0.46
5:M:87:ILE:HG23	5:M:527:ILE:HD12	1.97	0.46
6:N:290:VAL:HG13	6:N:311:VAL:HG13	1.98	0.46
6:N:414:VAL:O	6:N:418:MET:HG2	2.16	0.46
7:O:123:ARG:HH22	8:P:173:TYR:HE2	1.63	0.46
8:P:205:CYS:HB3	8:P:376:VAL:HG22	1.98	0.46
9:Q:127:CYS:HA	9:Q:130:ILE:HG12	1.97	0.46
3:C:32:THR:HG21	6:F:7:LEU:HG	1.97	0.46
3:C:313:ARG:HG2	3:C:314:ARG:HG3	1.98	0.46
3:C:363:ILE:HG22	3:C:363:ILE:O	2.16	0.46
6:F:109:TYR:CD1	6:F:435:LEU:HD13	2.51	0.46
7:G:442:LEU:HD11	7:G:503:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:6:SER:HB2	4:L:84:LEU:HB2	1.97	0.46
3:K:352:ILE:HD12	3:K:361:THR:HG22	1.97	0.46
5:M:451:PHE:CD1	5:M:455:LEU:HD23	2.50	0.46
6:N:264:ARG:HD2	6:N:264:ARG:HA	1.78	0.46
9:R:167:PHE:HZ	9:R:174:ILE:HG22	1.80	0.46
1:A:449:PRO:O	1:A:452:LEU:HB2	2.16	0.46
1:A:463:LEU:HB2	1:A:468:ARG:NH2	2.30	0.46
4:D:426:GLY:HA2	4:D:429:GLU:OE2	2.15	0.46
6:F:324:LEU:HD23	6:F:324:LEU:HA	1.81	0.46
7:G:164:SER:OG	10:G:601:ADP:N7	2.45	0.46
1:I:422:TYR:O	1:I:426:TYR:N	2.49	0.46
4:L:145:ILE:HD12	4:L:516:VAL:HG13	1.97	0.46
4:L:484:HIS:NE2	4:L:491:ALA:O	2.47	0.46
5:M:297:ALA:HB2	5:M:353:LEU:HD22	1.98	0.46
7:O:8:LEU:HG	7:O:9:LEU:HD23	1.97	0.46
2:B:242:THR:HG21	2:B:335:PHE:CE2	2.51	0.45
2:B:494:THR:HG22	2:B:495:GLU:N	2.29	0.45
3:C:233:ILE:HB	3:C:236:PRO:HG3	1.97	0.45
6:F:93:THR:N	10:F:601:ADP:O2B	2.49	0.45
8:H:355:VAL:HG23	8:H:356:GLY:H	1.80	0.45
6:N:256:ARG:O	6:N:260:VAL:HG13	2.16	0.45
6:N:463:LEU:O	6:N:466:ILE:N	2.49	0.45
8:P:90:SER:HB2	8:P:101:THR:OG1	2.15	0.45
5:E:255:PHE:HB2	5:E:306:PHE:CB	2.45	0.45
8:H:259:ILE:HG21	8:H:265:LEU:HB2	1.99	0.45
1:I:197:ILE:HD13	1:I:392:LEU:HD23	1.98	0.45
3:K:391:LEU:HD23	3:K:391:LEU:HA	1.83	0.45
6:N:134:LEU:HA	6:N:137:VAL:HG12	1.98	0.45
9:Q:50:ASP:OD1	9:Q:50:ASP:N	2.46	0.45
3:C:98:VAL:HB	3:C:505:THR:HG23	1.98	0.45
3:C:163:LYS:HD2	3:C:390:ASN:HD22	1.82	0.45
4:D:89:ARG:O	4:D:92:VAL:HG22	2.16	0.45
6:F:257:GLU:O	6:F:260:VAL:HG22	2.16	0.45
8:H:26:GLU:HA	8:H:30:TYR:HD2	1.81	0.45
8:H:274:ASN:HA	8:H:277:ASP:OD2	2.17	0.45
1:I:489:ASP:HB2	1:I:496:ARG:HD3	1.98	0.45
6:N:230:ILE:O	6:N:344:LEU:HA	2.16	0.45
3:C:515:LEU:HD23	3:C:516:LEU:HD23	1.98	0.45
5:E:87:ILE:HG23	5:E:527:ILE:HD12	1.98	0.45
1:I:201:HIS:O	3:K:86:THR:HG23	2.17	0.45
1:I:397:CYS:O	1:I:401:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:279:CYS:SG	3:K:300:ALA:HA	2.56	0.45
8:P:117:GLU:O	8:P:121:ILE:HG12	2.17	0.45
2:B:29:PHE:CD2	2:B:114:GLU:HB3	2.52	0.45
3:C:445:GLU:OE1	3:C:467:ARG:NH1	2.50	0.45
4:D:534:ASP:OD1	4:D:535:VAL:N	2.50	0.45
5:E:362:ILE:HD12	5:E:364:PHE:CE1	2.51	0.45
6:F:198:HIS:CD2	6:F:199:LYS:H	2.34	0.45
1:I:104:ALA:HB2	1:I:121:TYR:CE2	2.51	0.45
3:K:96:THR:HA	3:K:99:ILE:HG22	1.98	0.45
3:K:486:THR:HG22	3:K:487:LEU:N	2.31	0.45
5:M:222:THR:HG22	5:M:387:ILE:HA	1.98	0.45
6:N:26:ALA:HB2	6:N:71:HIS:CE1	2.52	0.45
4:D:26:ASP:OD1	4:D:26:ASP:N	2.49	0.45
5:E:214:LYS:HG2	5:E:364:PHE:CD2	2.51	0.45
8:H:111:LEU:HD21	8:H:441:PHE:CD1	2.52	0.45
2:J:526:ARG:HG3	5:M:64:LYS:HD2	1.99	0.45
3:K:119:PRO:O	3:K:123:ILE:HG12	2.17	0.45
3:K:237:ARG:H	3:K:288:ASP:HB3	1.82	0.45
5:M:342:VAL:HG11	5:M:352:LYS:HD3	1.97	0.45
7:O:334:VAL:O	7:O:337:LEU:HD23	2.17	0.45
8:P:135:ALA:HB1	8:P:423:ILE:HD11	1.98	0.45
9:Q:130:ILE:HG22	9:Q:189:LEU:HD13	1.98	0.45
3:C:226:HIS:HE1	6:F:332:ALA:HB3	1.81	0.45
5:E:368:LYS:HA	5:E:368:LYS:HD2	1.72	0.45
3:K:130:LEU:O	3:K:134:ILE:HG12	2.16	0.45
4:L:395:LYS:O	4:L:399:GLU:HG2	2.16	0.45
7:O:187:ASP:OD1	7:O:187:ASP:N	2.50	0.45
7:O:406:VAL:HG21	7:O:412:ILE:HD13	1.97	0.45
9:Q:106:VAL:HG12	9:Q:117:LEU:HD21	1.97	0.45
9:Q:182:LEU:H	9:Q:182:LEU:HD23	1.82	0.45
9:R:67:ASP:OD1	9:R:67:ASP:N	2.47	0.45
1:A:292:ILE:HG23	1:A:296:CYS:HB2	1.97	0.45
1:A:394:ASP:OD2	12:A:603:AF3:F2	2.25	0.45
6:F:272:LYS:O	6:F:276:GLU:HG2	2.17	0.45
1:I:351:VAL:HG22	1:I:364:ILE:HG12	1.97	0.45
1:I:423:LEU:HD13	1:I:441:PHE:HD2	1.82	0.45
2:J:151:ASP:OD1	2:J:152:GLU:N	2.50	0.45
3:K:64:ASN:N	3:K:95:THR:HG21	2.32	0.45
3:K:123:ILE:HD12	3:K:514:VAL:HA	1.99	0.45
8:P:131:GLY:HA3	8:P:437:ALA:HB3	1.98	0.45
2:B:172:LEU:HD23	2:B:179:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:460:ASP:OD1	2:B:464:GLN:NE2	2.45	0.45
4:D:520:THR:O	4:D:524:GLU:HG2	2.17	0.45
5:E:48:MET:HG3	5:E:110:VAL:HG11	1.98	0.45
6:F:224:ARG:HG3	6:F:351:TYR:HB3	1.99	0.45
8:H:13:GLN:NE2	8:P:13:GLN:HE22	2.14	0.45
10:L:601:ADP:O2B	12:L:603:AF3:F3	2.24	0.45
9:Q:177:GLN:O	9:Q:179:ILE:HG12	2.17	0.45
9:R:126:LEU:HB3	9:R:164:PRO:HG3	1.99	0.45
1:A:111:LYS:HA	1:A:111:LYS:HD3	1.76	0.45
6:F:164:LEU:HD12	6:F:201:GLU:HG3	1.98	0.45
8:H:419:LEU:O	8:H:423:ILE:HG12	2.17	0.45
1:I:286:ILE:HG13	1:I:300:PHE:CE1	2.52	0.45
3:K:158:SER:OG	3:K:495:ILE:HG23	2.16	0.45
3:K:292:THR:HG21	3:K:296:ILE:HD11	1.98	0.45
3:K:460:ILE:HG23	3:K:461:ARG:N	2.32	0.45
8:P:229:GLY:HA2	8:P:302:LEU:HD11	1.98	0.45
9:R:80:ALA:HA	9:R:83:LYS:HE3	2.00	0.45
1:A:74:VAL:HG13	4:D:394:ASN:HD22	1.82	0.44
1:A:533:LEU:HD12	4:D:63:ASP:HA	1.99	0.44
3:C:136:THR:HG23	3:C:418:VAL:HG12	1.99	0.44
3:C:180:VAL:HG21	3:C:398:CYS:HB3	2.00	0.44
4:D:144:GLY:HA2	4:D:147:ILE:HD12	1.98	0.44
5:E:165:LEU:HD12	5:E:409:ILE:HG23	1.99	0.44
2:J:242:THR:HG21	2:J:335:PHE:HE1	1.82	0.44
5:M:489:LEU:HD23	5:M:500:ASP:HA	1.99	0.44
6:N:56:LEU:HD11	8:P:85:MET:CE	2.47	0.44
6:N:501:LYS:HD3	6:N:501:LYS:HA	1.80	0.44
9:Q:39:ILE:HG13	9:Q:40:LEU:N	2.30	0.44
3:C:48:LYS:HB3	3:C:66:ILE:HD11	1.99	0.44
6:F:198:HIS:HB2	6:F:355:LEU:HD11	1.98	0.44
1:I:353:GLN:O	3:K:191:LYS:NZ	2.39	0.44
2:J:19:GLU:O	2:J:519:ASN:HA	2.17	0.44
3:K:157:ASN:HA	3:K:160:ILE:HG22	2.00	0.44
5:M:420:TYR:CZ	5:M:502:LYS:HE3	2.53	0.44
9:Q:195:GLU:O	9:Q:199:SER:OG	2.32	0.44
1:A:166:ASP:OD1	1:A:166:ASP:N	2.51	0.44
3:C:301:GLN:O	3:C:305:MET:HG3	2.17	0.44
5:E:307:ASP:OD1	5:E:307:ASP:N	2.42	0.44
5:E:462:LEU:HG	5:E:493:CYS:SG	2.57	0.44
6:F:221:MET:SD	6:F:311:VAL:HA	2.58	0.44
1:I:336:GLY:C	4:L:280:ARG:HH12	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:319:GLY:O	2:J:323:LEU:HD23	2.17	0.44
3:K:513:ALA:O	3:K:517:LEU:HB2	2.18	0.44
6:N:115:HIS:ND1	6:N:117:ARG:HG2	2.32	0.44
6:N:463:LEU:O	6:N:467:GLN:OE1	2.35	0.44
7:O:287:LYS:HD3	7:O:287:LYS:HA	1.70	0.44
7:O:406:VAL:HG23	7:O:474:TRP:HZ3	1.82	0.44
8:P:497:ILE:HD13	10:P:601:ADP:C6	2.52	0.44
9:R:213:LYS:HD3	9:R:213:LYS:HA	1.79	0.44
2:B:488:MET:SD	2:B:493:ILE:HB	2.58	0.44
3:C:391:LEU:O	3:C:395:MET:HG3	2.17	0.44
4:D:285:ASN:O	4:D:289:GLN:HG3	2.18	0.44
6:F:201:GLU:HA	6:F:377:LYS:O	2.18	0.44
7:G:240:LEU:HD12	7:G:242:VAL:HG12	2.00	0.44
8:H:319:TRP:HD1	8:H:322:ARG:HH21	1.65	0.44
1:I:263:ILE:HG22	4:L:269:TYR:HA	2.00	0.44
2:J:271:GLU:O	2:J:274:LYS:HG2	2.17	0.44
5:M:210:LYS:O	5:M:384:THR:HG23	2.18	0.44
5:M:227:GLY:HA3	5:M:374:ILE:O	2.17	0.44
5:M:306:PHE:CE2	5:M:323:ARG:HB3	2.53	0.44
7:O:137:LYS:HE3	7:O:500:ILE:HD13	2.00	0.44
9:R:73:MET:O	9:R:76:ARG:HG2	2.17	0.44
2:B:204:LYS:HG3	2:B:354:ILE:HD12	1.99	0.44
5:E:415:ASP:O	5:E:416:ASN:HB3	2.18	0.44
6:F:254:GLU:O	6:F:258:LYS:HG2	2.18	0.44
2:J:52:LEU:HD11	2:J:70:ILE:HG12	1.99	0.44
5:M:109:VAL:HG13	5:M:516:GLN:HG2	1.98	0.44
6:N:41:LYS:HZ2	6:N:41:LYS:HG3	1.62	0.44
1:A:471:HIS:HA	1:A:474:ALA:HB3	1.99	0.44
1:A:499:LYS:HD2	1:A:504:PHE:CE1	2.52	0.44
5:E:145:ILE:HG23	5:E:514:LYS:HD2	1.99	0.44
5:E:236:HIS:CD2	5:E:315:LEU:HD22	2.52	0.44
5:E:259:LYS:NZ	9:Q:96:GLU:O	2.45	0.44
5:E:291:GLN:NE2	5:E:346:SER:HA	2.32	0.44
7:G:197:ILE:HG22	7:G:372:PHE:HB2	2.00	0.44
7:G:255:ILE:HD13	8:H:259:ILE:HB	2.00	0.44
8:H:199:VAL:HG12	8:H:396:VAL:HG12	1.99	0.44
1:I:298:LYS:HA	1:I:301:VAL:HG12	1.99	0.44
3:K:230:ARG:NH2	3:K:288:ASP:OD1	2.51	0.44
3:K:245:LEU:HD23	3:K:245:LEU:HA	1.86	0.44
5:M:362:ILE:HG13	5:M:364:PHE:HE1	1.83	0.44
9:Q:193:GLU:HA	9:Q:196:TRP:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:124:ILE:O	9:R:128:ALA:CB	2.66	0.44
1:A:393:HIS:CE1	1:A:397:CYS:SG	3.11	0.44
4:D:91:LEU:HD23	4:D:91:LEU:HA	1.87	0.44
4:D:434:LEU:HG	4:D:481:ARG:HD2	1.99	0.44
5:E:284:LYS:HD2	5:E:284:LYS:HA	1.81	0.44
8:H:463:VAL:HG11	8:H:480:LEU:HD13	1.99	0.44
3:K:329:ALA:HB2	3:K:344:GLY:HA3	2.00	0.44
5:M:138:GLU:HG3	7:O:170:GLN:HG3	1.98	0.44
5:M:257:PRO:HD3	5:M:285:PHE:CE1	2.53	0.44
9:Q:53:LEU:HG	9:Q:78:ARG:HH12	1.82	0.44
1:A:229:ILE:HG12	1:A:306:MET:HE3	2.00	0.44
2:B:437:GLU:OE2	2:B:437:GLU:HA	2.18	0.44
3:C:64:ASN:N	3:C:95:THR:HG21	2.33	0.44
6:F:64:LEU:HD21	6:F:78:ALA:HA	2.00	0.44
7:G:40:LEU:HB2	7:G:95:THR:HG21	1.98	0.44
1:I:132:ILE:HG13	1:I:419:LEU:HD21	2.00	0.44
2:J:12:PHE:HB3	2:J:16:ALA:HB3	2.00	0.44
2:J:323:LEU:HD11	2:J:362:PHE:CE2	2.53	0.44
3:K:100:ILE:O	3:K:104:GLU:HG2	2.18	0.44
5:M:72:ASN:ND2	5:M:175:SER:O	2.50	0.44
9:Q:51:MET:HB3	9:Q:55:GLU:HG2	1.99	0.44
9:Q:116:ILE:HB	9:Q:146:PHE:CB	2.47	0.44
9:Q:134:LEU:HD12	9:Q:137:LEU:HD23	1.99	0.44
9:R:126:LEU:HB2	9:R:163:LEU:HD22	2.00	0.44
1:A:519:GLU:O	1:A:523:THR:HG23	2.18	0.44
2:B:13:LYS:HD2	5:E:84:ASP:OD2	2.18	0.44
3:C:112:PHE:O	3:C:117:MET:HB3	2.18	0.44
3:C:155:ILE:HG21	3:C:401:VAL:HG21	2.00	0.44
5:E:481:GLN:NE2	5:E:489:LEU:O	2.47	0.44
7:G:109:LYS:HA	7:G:112:VAL:HG12	1.99	0.44
3:K:352:ILE:HG23	3:K:361:THR:HG22	2.00	0.44
8:P:183:ILE:HD11	8:P:392:VAL:HA	1.99	0.44
6:F:257:GLU:O	6:F:261:LYS:HG2	2.18	0.43
7:G:215:ALA:HA	7:G:359:ASN:O	2.18	0.43
1:A:261:ASP:OD1	1:A:262:GLN:N	2.50	0.43
1:A:397:CYS:O	1:A:401:ARG:HG2	2.18	0.43
8:H:32:ASN:HD21	8:H:524:ILE:HD11	1.83	0.43
2:J:102:VAL:HG23	2:J:507:ALA:HB2	2.00	0.43
5:M:234:PHE:HA	5:M:322:VAL:HG12	2.00	0.43
6:N:37:ASN:O	6:N:58:LYS:HE3	2.18	0.43
6:N:101:GLU:HG3	6:N:443:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ILE:HD13	1:A:392:LEU:HD23	1.99	0.43
1:A:252:VAL:HG12	4:D:266:VAL:HB	2.01	0.43
1:A:386:ASP:OD1	1:A:387:GLU:N	2.51	0.43
2:B:79:PRO:HB2	5:E:60:MET:SD	2.58	0.43
2:B:130:TRP:CD1	2:B:439:TYR:HD2	2.36	0.43
3:C:52:ASP:OD1	3:C:53:PRO:HD2	2.18	0.43
3:C:52:ASP:HB3	3:C:56:GLY:H	1.83	0.43
5:E:154:SER:OG	5:E:416:ASN:OD1	2.24	0.43
5:E:451:PHE:O	5:E:454:ALA:HB3	2.18	0.43
8:H:154:LEU:HD23	8:H:154:LEU:HA	1.78	0.43
8:H:277:ASP:HB3	8:H:304:TYR:CE2	2.54	0.43
1:I:484:LYS:HG2	1:I:485:TRP:CE3	2.52	0.43
1:I:499:LYS:HA	1:I:504:PHE:HE1	1.83	0.43
2:J:244:MET:HA	2:J:275:MET:HE1	2.00	0.43
2:J:431:LYS:O	2:J:434:VAL:HG22	2.18	0.43
7:O:294:PRO:HB3	7:O:313:ARG:CZ	2.48	0.43
9:Q:126:LEU:O	9:Q:130:ILE:HG23	2.18	0.43
9:R:158:TYR:CG	9:R:159:PRO:HD2	2.53	0.43
1:A:170:ASN:O	1:A:173:VAL:HG22	2.18	0.43
1:A:201:HIS:O	3:C:86:THR:HG23	2.18	0.43
1:A:528:ASP:HB2	4:D:57:MET:HB2	1.99	0.43
3:C:62:ASP:OD1	3:C:62:ASP:N	2.52	0.43
5:E:265:LYS:NZ	9:Q:96:GLU:OE2	2.44	0.43
6:F:325:THR:HG23	6:F:326:LEU:HD12	2.00	0.43
1:I:446:LEU:HD11	1:I:468:ARG:HD2	2.00	0.43
8:P:369:ASP:OD1	8:P:369:ASP:N	2.47	0.43
2:B:323:LEU:HA	2:B:326:VAL:HG12	1.99	0.43
2:J:27:THR:O	2:J:78:ASN:ND2	2.48	0.43
4:L:240:ARG:HH21	4:L:361:LEU:HD11	1.83	0.43
6:N:214:HIS:HE1	9:R:69:ARG:CZ	2.31	0.43
6:N:299:PRO:HA	6:N:302:LEU:HB2	2.00	0.43
9:Q:116:ILE:HG23	9:Q:168:VAL:HG12	2.01	0.43
1:A:298:LYS:HD3	1:A:298:LYS:HA	1.77	0.43
4:D:313:ALA:O	4:D:317:LEU:HD23	2.18	0.43
5:E:102:ILE:HD13	5:E:102:ILE:HA	1.88	0.43
5:E:115:ALA:O	5:E:119:GLU:HG2	2.19	0.43
5:E:236:HIS:O	5:E:238:GLN:N	2.52	0.43
7:G:269:ALA:HB2	8:H:262:ALA:HB1	2.00	0.43
7:G:396:VAL:O	7:G:400:ILE:HG12	2.19	0.43
1:I:192:VAL:HG22	1:I:193:ASN:H	1.83	0.43
3:K:165:ILE:HG22	3:K:387:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:249:LYS:HA	6:N:244:VAL:HG22	2.00	0.43
6:N:297:ILE:HG22	6:N:302:LEU:HD22	2.00	0.43
8:P:134:ILE:HG12	8:P:137:ARG:HH21	1.83	0.43
8:P:247:ASP:OD2	8:P:298:ALA:HB2	2.19	0.43
8:P:450:ARG:HG2	8:P:460:ALA:HB1	2.00	0.43
9:Q:195:GLU:HA	9:Q:198:LEU:HB3	2.01	0.43
1:A:85:GLU:OE2	4:D:370:SER:OG	2.36	0.43
1:A:204:SER:HB3	3:C:507:LYS:HB3	1.99	0.43
2:B:501:ARG:O	2:B:505:LEU:HG	2.19	0.43
2:B:526:ARG:HH21	5:E:64:LYS:HD2	1.83	0.43
3:C:460:ILE:HD11	8:P:436:TYR:HE2	1.82	0.43
2:J:237:ILE:N	2:J:344:GLY:O	2.49	0.43
2:J:411:GLY:HA2	2:J:414:GLU:OE2	2.19	0.43
5:M:257:PRO:HA	5:M:258:PRO:HD3	1.92	0.43
6:N:103:LEU:HD21	6:N:515:ILE:HG21	1.99	0.43
6:N:250:TYR:HB2	6:N:255:GLU:HB2	2.00	0.43
7:O:176:ALA:O	7:O:179:VAL:HG22	2.18	0.43
3:C:50:LEU:HD11	3:C:66:ILE:HD13	2.01	0.43
3:C:177:LEU:HD11	3:C:181:LYS:HE3	2.00	0.43
5:E:37:HIS:NE2	5:E:533:ILE:HD11	2.34	0.43
5:E:301:ILE:HG12	5:E:322:VAL:HG22	2.00	0.43
1:I:259:LYS:HD3	4:L:268:ASP:OD1	2.18	0.43
2:J:327:THR:HG22	2:J:344:GLY:HA3	2.01	0.43
3:K:435:TRP:HB2	3:K:436:PRO:HD3	2.01	0.43
4:L:311:ASP:OD1	4:L:311:ASP:N	2.49	0.43
7:O:195:ILE:HG13	7:O:195:ILE:O	2.19	0.43
1:A:506:PRO:O	1:A:509:VAL:HG22	2.18	0.43
3:C:118:HIS:O	3:C:121:VAL:HG22	2.17	0.43
6:F:282:CYS:SG	6:F:287:LYS:HD2	2.59	0.43
8:H:164:LEU:HD21	8:H:399:PHE:HB2	2.01	0.43
8:H:229:GLY:HA2	8:H:302:LEU:HD11	1.99	0.43
3:K:72:VAL:O	3:K:78:LYS:NZ	2.40	0.43
7:O:69:LEU:HD23	7:O:69:LEU:HA	1.88	0.43
7:O:254:GLU:OE1	7:O:256:ARG:NH2	2.50	0.43
8:P:163:LEU:HD13	8:P:402:LEU:HD21	2.01	0.43
1:A:13:THR:HG23	1:A:529:ASP:HB3	2.00	0.43
1:A:168:PHE:O	1:A:171:MET:HG2	2.18	0.43
2:B:271:GLU:HG2	5:E:274:TYR:CE2	2.54	0.43
4:D:223:LEU:HD13	4:D:388:ILE:HG13	2.01	0.43
5:E:76:THR:HG22	5:E:80:MET:CE	2.49	0.43
5:E:257:PRO:HD3	5:E:285:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:472:GLN:O	5:E:476:GLU:HG3	2.19	0.43
8:H:63:LEU:HD23	8:H:383:ASN:OD1	2.19	0.43
5:M:34:LEU:HD12	5:M:34:LEU:HA	1.86	0.43
5:M:206:PHE:HZ	5:M:410:ARG:HG2	1.84	0.43
5:M:285:PHE:O	5:M:289:ILE:HG12	2.18	0.43
5:M:481:GLN:NE2	5:M:489:LEU:O	2.49	0.43
6:N:30:LEU:HG	6:N:77:ILE:HD11	2.00	0.43
6:N:177:LEU:HD12	6:N:177:LEU:HA	1.85	0.43
7:O:374:LEU:HD23	7:O:374:LEU:H	1.83	0.43
8:P:282:ALA:HB1	8:P:338:PRO:HG3	2.01	0.43
9:R:176:ALA:HB2	9:R:201:SER:HG	1.84	0.43
1:A:190:TYR:HE2	1:A:403:LEU:HB3	1.83	0.42
3:C:329:ALA:HB2	3:C:344:GLY:HA3	2.01	0.42
3:C:392:GLN:O	3:C:396:GLN:HG2	2.19	0.42
4:D:88:ALA:O	4:D:92:VAL:HG13	2.19	0.42
4:D:345:VAL:HG21	4:D:351:PHE:HD1	1.84	0.42
8:H:440:LYS:HD3	8:H:440:LYS:HA	1.63	0.42
3:K:380:SER:HB2	6:N:80:VAL:HG22	2.00	0.42
4:L:71:THR:HA	4:L:400:GLU:OE1	2.18	0.42
5:M:324:TRP:HZ2	9:R:153:THR:HA	1.84	0.42
7:O:398:ARG:HB3	7:O:497:MET:HE1	2.01	0.42
8:P:411:GLY:O	8:P:492:MET:HG3	2.19	0.42
2:B:255:ARG:HE	5:E:265:LYS:HB3	1.84	0.42
3:C:380:SER:HB3	3:C:383:ILE:HG12	2.01	0.42
7:G:14:ASP:OD1	7:G:14:ASP:N	2.52	0.42
8:H:8:ALA:O	8:H:13:GLN:HG3	2.19	0.42
8:H:156:ASP:O	8:H:160:VAL:HG12	2.19	0.42
8:H:227:THR:HG23	8:H:352:LEU:HD12	2.00	0.42
2:J:52:LEU:HB2	2:J:62:MET:HG3	2.00	0.42
2:J:407:VAL:HG13	2:J:497:PHE:HB2	2.01	0.42
2:J:465:LEU:HD23	2:J:465:LEU:HA	1.76	0.42
3:K:378:GLY:N	3:K:384:LEU:HD21	2.35	0.42
4:L:256:PRO:HD3	4:L:282:TYR:CD2	2.54	0.42
4:L:426:GLY:HA2	4:L:429:GLU:OE2	2.20	0.42
6:N:98:ILE:O	6:N:102:LEU:HD23	2.19	0.42
6:N:257:GLU:O	6:N:260:VAL:HG22	2.18	0.42
8:P:129:ILE:O	8:P:133:GLU:HG3	2.19	0.42
1:A:179:ILE:HG22	1:A:179:ILE:O	2.19	0.42
1:A:269:ASP:O	1:A:272:LYS:HB3	2.20	0.42
2:B:127:ILE:HG13	2:B:515:LEU:HD22	2.01	0.42
5:E:148:LEU:O	5:E:151:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:86:GLN:NE2	7:G:92:ASP:O	2.37	0.42
7:G:449:LEU:CD2	7:G:477:VAL:HG21	2.49	0.42
2:J:245:ASP:HB2	2:J:297:TYR:CE2	2.54	0.42
10:K:601:ADP:O3B	12:K:603:AF3:F2	2.27	0.42
4:L:214:LEU:HD11	4:L:393:SER:O	2.18	0.42
8:P:440:LYS:HA	8:P:440:LYS:HD2	1.85	0.42
1:A:73:LYS:HE3	1:A:73:LYS:HB3	1.63	0.42
1:A:484:LYS:HG2	1:A:485:TRP:CE3	2.54	0.42
5:E:58:ASP:OD1	5:E:72:ASN:HB2	2.20	0.42
6:F:261:LYS:HA	6:F:261:LYS:HD3	1.91	0.42
1:I:82:GLN:NE2	1:I:88:ASP:O	2.47	0.42
3:K:60:THR:OG1	3:K:62:ASP:OD1	2.34	0.42
3:K:133:MET:HA	3:K:136:THR:HG22	2.01	0.42
3:K:161:THR:HG23	3:K:162:THR:HG23	2.01	0.42
1:A:492:ASN:OD1	1:A:492:ASN:N	2.53	0.42
3:C:221:ASN:O	3:C:222:LYS:HD2	2.19	0.42
3:C:502:LYS:HD3	3:C:502:LYS:HA	1.94	0.42
5:E:18:ILE:HG13	5:E:19:ILE:N	2.34	0.42
6:F:37:ASN:HB2	6:F:58:LYS:HG2	2.00	0.42
7:G:60:ASN:ND2	7:G:165:SER:O	2.51	0.42
8:H:26:GLU:HA	8:H:30:TYR:CD2	2.55	0.42
1:I:521:ALA:O	1:I:525:LEU:HB2	2.20	0.42
5:M:116:LEU:O	5:M:137:TYR:OH	2.27	0.42
6:N:98:ILE:HD11	6:N:447:ILE:HG12	2.01	0.42
8:P:350:VAL:HA	8:P:362:VAL:O	2.19	0.42
1:A:34:SER:HG	1:A:43:LYS:HZ1	1.59	0.42
3:C:132:ASP:O	3:C:136:THR:HG22	2.20	0.42
5:E:239:MET:HB2	5:E:240:PRO:HD2	2.01	0.42
6:F:180:LYS:HG3	6:F:186:ILE:HD11	2.00	0.42
6:F:431:GLY:O	6:F:434:GLN:NE2	2.39	0.42
1:I:165:GLY:O	1:I:169:ALA:N	2.40	0.42
2:J:223:LYS:HD2	2:J:223:LYS:HA	1.78	0.42
4:L:163:LEU:HD13	4:L:415:LEU:HD23	2.01	0.42
4:L:194:VAL:HG21	4:L:208:ILE:HD11	2.01	0.42
4:L:484:HIS:CE1	4:L:491:ALA:H	2.37	0.42
2:B:44:GLY:HA3	2:B:450:ILE:HG23	2.01	0.42
3:C:133:MET:CE	3:C:444:LEU:HD21	2.49	0.42
4:D:287:VAL:HG12	4:D:320:MET:SD	2.60	0.42
5:E:109:VAL:HG23	5:E:520:ALA:HB2	2.02	0.42
6:F:84:GLN:HG2	6:F:503:GLN:HG2	2.02	0.42
1:I:498:ASN:HA	1:I:501:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:41:LEU:HB2	3:K:96:THR:HG21	2.02	0.42
3:K:466:LEU:O	3:K:470:HIS:HB2	2.20	0.42
4:L:302:LYS:HB2	4:L:327:ASP:HA	2.00	0.42
4:L:309:LEU:HD23	4:L:309:LEU:HA	1.87	0.42
8:P:112:LEU:HD23	8:P:112:LEU:HA	1.84	0.42
9:Q:190:THR:O	9:Q:194:LEU:HB2	2.20	0.42
9:Q:191:ARG:O	9:Q:195:GLU:HG3	2.20	0.42
2:B:64:THR:HA	2:B:385:GLU:OE1	2.20	0.42
2:B:237:ILE:HA	2:B:289:CYS:HB3	2.00	0.42
5:E:78:LEU:HB3	5:E:92:VAL:HG22	2.02	0.42
5:E:78:LEU:HD23	5:E:78:LEU:HA	1.89	0.42
2:J:51:ILE:HG13	4:L:532:ILE:HD12	2.02	0.42
2:J:83:VAL:HB	2:J:514:ILE:HD11	2.01	0.42
2:J:419:HIS:O	2:J:423:GLN:HG2	2.19	0.42
5:M:314:LEU:HD23	5:M:321:ALA:HB3	2.02	0.42
7:O:201:GLN:HA	7:O:382:MET:HE3	2.02	0.42
8:P:443:GLU:O	8:P:446:GLU:HB2	2.20	0.42
9:Q:51:MET:HB2	9:Q:56:LEU:HD13	2.02	0.42
1:A:286:ILE:HG13	1:A:300:PHE:CE1	2.54	0.42
2:B:500:LYS:HB3	2:B:500:LYS:HE3	1.84	0.42
4:D:207:ASP:O	4:D:385:THR:HG23	2.19	0.42
7:G:26:ILE:HG23	7:G:30:GLN:HE22	1.85	0.42
7:G:415:GLU:OE1	7:G:468:HIS:ND1	2.53	0.42
8:H:216:SER:OG	8:H:217:VAL:N	2.53	0.42
1:I:294:ASP:N	1:I:294:ASP:OD1	2.53	0.42
3:K:43:PRO:HG3	10:K:601:ADP:C6	2.54	0.42
4:L:442:THR:O	4:L:443:LEU:HD23	2.20	0.42
7:O:179:VAL:HB	7:O:393:ILE:HG22	2.01	0.42
8:P:186:ALA:HB2	8:P:375:ILE:HD11	2.02	0.42
3:C:23:GLN:O	3:C:27:ILE:HG12	2.20	0.42
3:C:48:LYS:HG3	6:F:520:GLU:HB3	2.01	0.42
4:D:363:GLU:O	4:D:374:LEU:HD12	2.20	0.42
5:E:363:SER:HA	5:E:370:LYS:HD3	2.01	0.42
6:F:264:ARG:HD2	6:F:264:ARG:HA	1.84	0.42
1:I:4:PRO:HB2	1:I:5:LEU:H	1.68	0.42
1:I:292:ILE:HG23	1:I:296:CYS:HB2	2.02	0.42
4:L:141:LEU:HB2	4:L:523:THR:HG21	2.02	0.42
5:M:407:CYS:O	5:M:410:ARG:HG3	2.20	0.42
7:O:232:TYR:HD2	7:O:348:PHE:HD2	1.68	0.42
8:P:243:SER:HB3	8:P:332:ALA:HB1	2.02	0.42
1:A:335:GLU:N	1:A:335:GLU:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:LEU:HB2	1:A:468:ARG:HH22	1.85	0.41
3:C:279:CYS:HA	3:C:282:ILE:HG22	2.02	0.41
3:C:383:ILE:O	3:C:387:VAL:HG23	2.20	0.41
7:G:385:THR:O	7:G:389:LEU:HD23	2.20	0.41
7:G:432:GLN:HG3	7:G:433:LEU:N	2.35	0.41
8:H:136:CYS:HB2	8:H:512:THR:HG21	2.02	0.41
8:H:437:ALA:O	8:H:440:LYS:HB2	2.19	0.41
1:I:350:GLU:HG2	1:I:352:VAL:HG13	2.02	0.41
7:O:219:THR:OG1	7:O:220:PHE:N	2.53	0.41
9:R:98:SER:OG	9:R:99:GLY:N	2.53	0.41
2:B:76:VAL:HG23	2:B:82:LYS:HG2	2.02	0.41
2:B:109:LEU:HD23	2:B:109:LEU:HA	1.89	0.41
3:C:238:ILE:HD13	3:C:289:VAL:HB	2.02	0.41
5:E:90:LEU:HD23	5:E:90:LEU:HA	1.83	0.41
5:E:243:VAL:HG22	5:E:359:VAL:HG22	2.02	0.41
6:F:208:ARG:HB3	6:F:369:PRO:HG2	2.02	0.41
1:I:180:LYS:O	1:I:370:ARG:NH2	2.53	0.41
6:N:239:TYR:OH	8:P:253:THR:OG1	2.38	0.41
7:O:244:LEU:HD12	7:O:295:ILE:HD12	2.02	0.41
1:A:298:LYS:HA	1:A:301:VAL:HG12	2.02	0.41
3:C:193:ILE:HG22	3:C:193:ILE:O	2.21	0.41
3:C:452:ILE:HA	3:C:455:CYS:SG	2.61	0.41
5:E:299:LEU:HD12	5:E:320:PRO:O	2.20	0.41
5:E:456:GLU:O	5:E:459:PRO:HD2	2.20	0.41
7:G:195:ILE:O	7:G:195:ILE:HG22	2.20	0.41
1:I:91:THR:O	1:I:95:ILE:HG12	2.20	0.41
1:I:331:LEU:O	1:I:338:GLU:HG2	2.21	0.41
3:K:226:HIS:HE1	6:N:332:ALA:HB3	1.85	0.41
6:N:435:LEU:O	6:N:438:GLN:HB3	2.20	0.41
6:N:445:LEU:HB3	6:N:449:LYS:HE2	2.03	0.41
7:O:382:MET:H	7:O:382:MET:HG2	1.72	0.41
8:P:15:LEU:HG	8:P:19:ALA:HB3	2.02	0.41
9:R:38:ARG:HD3	9:R:38:ARG:HA	1.76	0.41
1:A:114:PRO:HB2	4:D:57:MET:CE	2.47	0.41
1:A:506:PRO:HG2	1:A:509:VAL:HG13	2.03	0.41
2:B:191:LYS:HB3	2:B:191:LYS:HE3	1.85	0.41
2:B:288:ASN:HA	2:B:309:VAL:HG12	2.02	0.41
3:C:391:LEU:HD23	3:C:391:LEU:HA	1.94	0.41
4:D:59:LYS:HE2	4:D:59:LYS:HB2	1.83	0.41
4:D:163:LEU:HB3	4:D:188:VAL:HG21	2.02	0.41
4:D:172:ASN:ND2	10:D:601:ADP:HN61	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:414:ARG:HH21	5:E:511:ILE:HD12	1.86	0.41
6:F:179:ILE:HG13	6:F:191:ILE:HD11	2.02	0.41
8:H:101:THR:OG1	12:H:603:AF3:F1	2.24	0.41
1:I:17:ILE:HG21	1:I:529:ASP:HA	2.02	0.41
1:I:264:ARG:O	1:I:267:GLU:HB2	2.20	0.41
2:J:242:THR:HG21	2:J:335:PHE:CE1	2.55	0.41
2:J:271:GLU:HG2	5:M:274:TYR:OH	2.21	0.41
3:K:226:HIS:CD2	6:N:334:ASN:HD21	2.38	0.41
3:K:527:LYS:HZ3	3:K:529:LYS:HG3	1.85	0.41
4:L:439:TYR:CZ	4:L:443:LEU:HD11	2.56	0.41
6:N:213:ASP:OD1	6:N:214:HIS:ND1	2.53	0.41
6:N:396:ARG:O	6:N:400:ASN:ND2	2.54	0.41
8:P:492:MET:SD	8:P:497:ILE:HD12	2.61	0.41
1:A:65:LEU:HD21	3:C:523:VAL:HG11	2.02	0.41
4:D:447:GLU:O	4:D:451:VAL:HG23	2.21	0.41
1:I:56:ASN:ND2	1:I:158:SER:O	2.53	0.41
1:I:78:LEU:HD13	1:I:520:ALA:HB2	2.03	0.41
1:I:190:TYR:O	1:I:400:LYS:HE2	2.20	0.41
1:I:232:ALA:HB3	1:I:348:ALA:HB3	2.02	0.41
3:K:212:SER:HB2	3:K:376:LEU:HA	2.03	0.41
3:K:339:ARG:NH1	3:K:341:ASP:OD2	2.53	0.41
5:M:255:PHE:HB2	5:M:306:PHE:CB	2.51	0.41
6:N:231:LEU:HG	6:N:233:CYS:SG	2.61	0.41
6:N:340:SER:OG	6:N:342:ASP:OD1	2.31	0.41
8:P:47:TYR:O	8:P:455:ASN:ND2	2.44	0.41
8:P:69:ALA:O	8:P:73:LEU:HB2	2.21	0.41
9:Q:53:LEU:HG	9:Q:78:ARG:NH1	2.35	0.41
4:D:271:GLN:HE22	4:D:274:ARG:HH21	1.66	0.41
5:E:245:ASP:HA	5:E:356:ALA:O	2.20	0.41
6:F:398:VAL:O	6:F:402:ILE:HG12	2.21	0.41
6:F:432:ARG:O	6:F:435:LEU:HG	2.19	0.41
2:J:244:MET:SD	2:J:292:ASN:ND2	2.94	0.41
2:J:510:ALA:HA	2:J:513:VAL:HG12	2.01	0.41
7:O:473:THR:OG1	7:O:474:TRP:N	2.53	0.41
9:R:116:ILE:HD13	9:R:116:ILE:HA	1.93	0.41
2:B:83:VAL:HG22	5:E:393:MET:CE	2.50	0.41
2:B:95:VAL:HG23	2:B:97:ASP:H	1.85	0.41
3:C:83:ILE:HD12	3:C:512:THR:OG1	2.20	0.41
3:C:258:ILE:HG23	3:C:263:ASP:HB2	2.03	0.41
3:C:488:VAL:HG21	3:C:493:LEU:HD22	2.03	0.41
4:D:361:LEU:HD21	4:D:363:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:46:ASP:HA	7:G:60:ASN:HB3	2.03	0.41
7:G:147:ASP:HB3	7:G:150:GLU:HB3	2.03	0.41
8:H:241:VAL:HG13	8:H:292:VAL:HG23	2.03	0.41
2:J:71:LEU:HB3	2:J:85:VAL:HG22	2.02	0.41
3:K:15:LYS:HB3	3:K:15:LYS:HE3	1.80	0.41
3:K:440:VAL:O	3:K:444:LEU:HD12	2.20	0.41
4:L:283:ILE:O	4:L:287:VAL:HG23	2.21	0.41
4:L:304:ILE:HD12	4:L:304:ILE:H	1.84	0.41
6:N:260:VAL:O	6:N:263:GLU:HG2	2.21	0.41
6:N:349:LEU:HB2	6:N:365:LYS:HD3	2.03	0.41
9:R:97:ILE:HD12	9:R:102:TYR:HA	2.03	0.41
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.92	0.41
1:A:240:SER:HB3	1:A:290:GLY:HA3	2.03	0.41
3:C:350:LEU:HA	3:C:362:PHE:O	2.21	0.41
3:C:417:ALA:HA	3:C:470:HIS:CE1	2.56	0.41
6:F:447:ILE:O	6:F:451:LEU:HD23	2.20	0.41
7:G:440:LYS:O	7:G:443:GLU:HG2	2.21	0.41
1:I:199:LYS:NZ	1:I:389:GLU:OE1	2.41	0.41
1:I:372:SER:OG	1:I:373:ALA:N	2.54	0.41
3:K:33:ILE:CG2	3:K:99:ILE:HD11	2.48	0.41
3:K:144:VAL:HG12	3:K:405:PRO:O	2.21	0.41
4:L:313:ALA:O	4:L:317:LEU:HD23	2.20	0.41
6:N:84:GLN:HG2	6:N:503:GLN:HG2	2.02	0.41
6:N:255:GLU:O	6:N:259:LEU:HD23	2.20	0.41
6:N:432:ARG:O	6:N:435:LEU:HG	2.20	0.41
7:O:319:LEU:HD12	7:O:319:LEU:HA	1.77	0.41
8:P:58:ASN:OD1	8:P:62:LYS:N	2.40	0.41
9:R:40:LEU:HA	9:R:44:VAL:O	2.20	0.41
1:A:107:LEU:HD11	1:A:440:GLU:HG3	2.02	0.41
3:C:209:ILE:HD13	3:C:378:GLY:HA2	2.02	0.41
3:C:380:SER:HB2	6:F:80:VAL:HG22	2.02	0.41
6:F:98:ILE:O	6:F:102:LEU:HD23	2.20	0.41
6:F:207:ILE:HB	6:F:373:THR:CG2	2.51	0.41
7:G:479:ILE:HG13	7:G:480:ASN:N	2.36	0.41
8:H:154:LEU:HD21	8:H:402:LEU:HD23	2.02	0.41
8:H:182:LEU:HD21	8:H:375:ILE:HD12	2.02	0.41
8:H:509:LYS:HE2	8:H:509:LYS:HB2	1.65	0.41
2:J:190:LEU:HD11	2:J:199:ILE:HD11	2.03	0.41
3:K:460:ILE:HG23	3:K:461:ARG:H	1.85	0.41
4:L:217:THR:O	4:L:391:ARG:HB2	2.21	0.41
4:L:315:HIS:CE1	4:L:319:LYS:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:214:LYS:HG2	5:M:364:PHE:CD2	2.56	0.41
7:O:19:ILE:N	7:O:20:PRO:HD2	2.35	0.41
7:O:197:ILE:HD13	7:O:386:GLU:HG3	2.02	0.41
8:P:417:ILE:HD13	8:P:417:ILE:HA	1.93	0.41
9:Q:213:LYS:HA	9:Q:213:LYS:HD2	1.95	0.41
9:R:166:ILE:HD13	9:R:184:PHE:CZ	2.55	0.41
1:A:345:LEU:HD23	1:A:345:LEU:HA	1.93	0.41
5:E:160:LYS:HD2	5:E:161:ASP:N	2.36	0.41
7:G:27:SER:O	7:G:31:VAL:HG23	2.21	0.41
7:G:118:PRO:HB3	7:G:514:VAL:HG12	2.03	0.41
7:G:232:TYR:HD2	7:G:348:PHE:HD2	1.67	0.41
8:H:111:LEU:HD23	8:H:111:LEU:HA	1.68	0.41
8:H:401:VAL:HG13	8:H:502:LEU:HD23	2.02	0.41
1:I:183:ASP:OD1	1:I:184:ILE:N	2.52	0.41
1:I:335:GLU:N	1:I:335:GLU:OE1	2.53	0.41
2:J:176:LYS:O	2:J:180:THR:HG23	2.21	0.41
3:K:219:MET:HG3	3:K:362:PHE:CE2	2.56	0.41
6:N:206:LEU:HD12	6:N:373:THR:O	2.21	0.41
5:E:242:LYS:NZ	5:E:244:GLU:OE2	2.39	0.40
5:E:456:GLU:O	5:E:460:MET:HG3	2.20	0.40
1:I:107:LEU:HD23	1:I:107:LEU:HA	1.92	0.40
1:I:122:ARG:NH2	4:L:219:ASP:OD1	2.55	0.40
3:K:85:ARG:NH1	3:K:89:GLU:OE2	2.52	0.40
3:K:238:ILE:HA	3:K:289:VAL:O	2.21	0.40
3:K:436:PRO:O	3:K:440:VAL:HG23	2.20	0.40
4:L:490:THR:OG1	4:L:502:ASN:ND2	2.42	0.40
7:O:186:LEU:HD23	7:O:186:LEU:HA	1.94	0.40
1:A:5:LEU:HD11	4:D:47:ALA:HB2	2.03	0.40
4:D:58:ASP:HB3	4:D:72:ASN:HB2	2.04	0.40
8:H:80:HIS:HA	8:H:81:PRO:HD3	1.91	0.40
2:J:337:HIS:HB3	2:J:340:LEU:HD13	2.04	0.40
6:N:462:THR:O	6:N:466:ILE:HG12	2.21	0.40
7:O:163:LEU:HD12	7:O:168:ILE:HB	2.02	0.40
8:P:136:CYS:HB2	8:P:512:THR:HG21	2.03	0.40
8:P:315:LEU:HD23	8:P:315:LEU:HA	1.90	0.40
2:B:172:LEU:H	2:B:172:LEU:HD12	1.87	0.40
5:E:309:GLU:O	5:E:313:LEU:HD23	2.21	0.40
8:H:238:LYS:HB3	8:H:344:MET:CE	2.52	0.40
2:J:66:ASP:N	2:J:66:ASP:OD1	2.54	0.40
2:J:219:LEU:HB3	2:J:359:LEU:HD23	2.02	0.40
2:J:326:VAL:O	2:J:365:VAL:HB	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:266:ARG:HD2	3:K:266:ARG:HA	1.91	0.40
3:K:415:GLU:HG2	3:K:506:TYR:OH	2.22	0.40
4:L:393:SER:OG	4:L:394:ASN:N	2.54	0.40
5:M:202:ARG:HD3	5:M:202:ARG:HA	1.75	0.40
8:P:297:VAL:HG21	8:P:312:LEU:HD21	2.03	0.40
9:R:38:ARG:O	9:R:42:GLN:HG3	2.21	0.40
1:A:183:ASP:OD2	1:A:189:ARG:NH2	2.54	0.40
3:C:48:LYS:HE2	3:C:48:LYS:HB2	1.93	0.40
3:C:98:VAL:HG23	3:C:509:ALA:HB2	2.03	0.40
3:C:404:ASP:HA	3:C:405:PRO:HD3	1.89	0.40
2:J:219:LEU:HD23	2:J:219:LEU:HA	1.92	0.40
7:O:103:GLU:HG2	7:O:444:ILE:HB	2.02	0.40
7:O:392:ALA:O	7:O:395:ILE:HG22	2.20	0.40
8:P:39:LEU:HD11	8:P:73:LEU:HD11	2.04	0.40
9:R:39:ILE:HD11	9:R:46:LYS:HG2	2.03	0.40
2:B:59:ALA:O	4:D:89:ARG:NH1	2.54	0.40
4:D:94:LEU:HD11	4:D:521:LEU:HB3	2.04	0.40
4:D:196:ASP:OD1	4:D:196:ASP:N	2.50	0.40
5:E:361:GLU:HG2	5:E:370:LYS:HD2	2.03	0.40
6:F:392:ARG:O	6:F:396:ARG:HG2	2.21	0.40
7:G:287:LYS:HD3	7:G:287:LYS:HA	1.90	0.40
1:I:452:LEU:HD23	1:I:452:LEU:HA	1.93	0.40
1:I:528:ASP:HB2	4:L:57:MET:HB2	2.02	0.40
1:I:529:ASP:OD1	1:I:529:ASP:N	2.55	0.40
2:J:49:ASP:HB3	2:J:65:ASN:HB2	2.03	0.40
2:J:68:ALA:HB2	2:J:99:THR:HG21	2.02	0.40
3:K:246:GLU:HB3	3:K:297:SER:HB2	2.03	0.40
5:M:526:MET:HE2	7:O:381:PHE:HD2	1.86	0.40
6:N:447:ILE:O	6:N:451:LEU:HD23	2.21	0.40
7:O:409:GLY:HA3	7:O:487:ASN:ND2	2.36	0.40
8:P:491:ASP:OD1	8:P:492:MET:N	2.55	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	530/556 (95%)	496 (94%)	34 (6%)	0	100	100
1	I	530/556 (95%)	498 (94%)	32 (6%)	0	100	100
2	B	516/535 (96%)	484 (94%)	32 (6%)	0	100	100
2	J	520/535 (97%)	495 (95%)	25 (5%)	0	100	100
3	C	520/545 (95%)	490 (94%)	30 (6%)	0	100	100
3	K	522/545 (96%)	490 (94%)	32 (6%)	0	100	100
4	D	516/539 (96%)	495 (96%)	21 (4%)	0	100	100
4	L	517/539 (96%)	493 (95%)	24 (5%)	0	100	100
5	E	523/541 (97%)	494 (94%)	29 (6%)	0	100	100
5	M	523/541 (97%)	501 (96%)	22 (4%)	0	100	100
6	F	524/531 (99%)	493 (94%)	30 (6%)	1 (0%)	47	78
6	N	523/531 (98%)	490 (94%)	33 (6%)	0	100	100
7	G	519/543 (96%)	487 (94%)	32 (6%)	0	100	100
7	O	518/543 (95%)	496 (96%)	22 (4%)	0	100	100
8	H	527/548 (96%)	491 (93%)	36 (7%)	0	100	100
8	P	527/548 (96%)	500 (95%)	27 (5%)	0	100	100
9	Q	185/239 (77%)	166 (90%)	18 (10%)	1 (0%)	29	64
9	R	187/239 (78%)	156 (83%)	29 (16%)	2 (1%)	14	48
All	All	8727/9154 (95%)	8215 (94%)	508 (6%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	186	ILE
9	R	214	LYS
9	Q	190	THR
9	R	210	GLU

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	444/463 (96%)	442 (100%)	2 (0%)	88 94
1	I	444/463 (96%)	443 (100%)	1 (0%)	93 97
2	B	412/427 (96%)	412 (100%)	0	100 100
2	J	415/427 (97%)	415 (100%)	0	100 100
3	C	453/469 (97%)	452 (100%)	1 (0%)	93 97
3	K	455/469 (97%)	455 (100%)	0	100 100
4	D	441/452 (98%)	440 (100%)	1 (0%)	93 97
4	L	442/452 (98%)	440 (100%)	2 (0%)	88 94
5	E	444/456 (97%)	441 (99%)	3 (1%)	84 92
5	M	444/456 (97%)	443 (100%)	1 (0%)	93 97
6	F	438/442 (99%)	438 (100%)	0	100 100
6	N	438/442 (99%)	437 (100%)	1 (0%)	93 97
7	G	428/443 (97%)	428 (100%)	0	100 100
7	O	427/443 (96%)	427 (100%)	0	100 100
8	H	436/452 (96%)	435 (100%)	1 (0%)	93 97
8	P	436/452 (96%)	436 (100%)	0	100 100
9	Q	164/215 (76%)	164 (100%)	0	100 100
9	R	165/215 (77%)	165 (100%)	0	100 100
All	All	7326/7638 (96%)	7313 (100%)	13 (0%)	93 97

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ARG
1	A	393	HIS
3	C	260	ARG
4	D	213	LYS
5	E	14	ARG
5	E	160	LYS
5	E	218	ARG
8	H	367	LYS
1	I	430	MET
4	L	172	ASN
4	L	206	ARG

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Mol	Chain	Res	Type
5	M	218	ARG
6	N	514	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	475	GLN
3	C	87	GLN
3	C	226	HIS
3	C	470	HIS
5	E	236	HIS
7	G	21	GLN
2	J	124	GLN
3	K	226	HIS
6	N	71	HIS
6	N	214	HIS
8	P	13	GLN
8	P	32	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 48 ligands modelled in this entry, 16 are monoatomic - leaving 32 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	ADP	K	601	11	24,29,29	0.94	1 (4%)	29,45,45	1.46	4 (13%)
12	AF3	C	603	-	0,3,3	-	-	-		
10	ADP	H	601	11	24,29,29	0.91	1 (4%)	29,45,45	1.47	4 (13%)
10	ADP	J	601	11	24,29,29	0.94	1 (4%)	29,45,45	1.42	4 (13%)
12	AF3	K	603	-	0,3,3	-	-	-		
12	AF3	I	603	-	0,3,3	-	-	-		
12	AF3	L	603	-	0,3,3	-	-	-		
10	ADP	C	601	11	24,29,29	0.94	1 (4%)	29,45,45	1.45	4 (13%)
12	AF3	G	603	-	0,3,3	-	-	-		
10	ADP	I	601	11	24,29,29	0.92	1 (4%)	29,45,45	1.43	4 (13%)
10	ADP	N	601	11	24,29,29	0.94	1 (4%)	29,45,45	1.49	4 (13%)
12	AF3	P	603	-	0,3,3	-	-	-		
10	ADP	E	601	11	24,29,29	0.94	1 (4%)	29,45,45	1.34	4 (13%)
12	AF3	F	603	-	0,3,3	-	-	-		
12	AF3	A	603	-	0,3,3	-	-	-		
12	AF3	O	603	-	0,3,3	-	-	-		
12	AF3	H	603	-	0,3,3	-	-	-		
10	ADP	M	601	11	24,29,29	0.94	1 (4%)	29,45,45	1.36	4 (13%)
12	AF3	M	603	-	0,3,3	-	-	-		
10	ADP	A	601	11	24,29,29	0.94	1 (4%)	29,45,45	1.51	4 (13%)
12	AF3	B	603	-	0,3,3	-	-	-		
12	AF3	J	603	-	0,3,3	-	-	-		
10	ADP	B	601	11	24,29,29	0.92	1 (4%)	29,45,45	1.51	4 (13%)
10	ADP	L	601	11	24,29,29	0.92	1 (4%)	29,45,45	1.33	4 (13%)
12	AF3	N	603	-	0,3,3	-	-	-		
10	ADP	P	601	11	24,29,29	0.91	1 (4%)	29,45,45	1.47	4 (13%)
10	ADP	D	601	11	24,29,29	0.94	1 (4%)	29,45,45	1.39	4 (13%)
10	ADP	G	601	11	24,29,29	0.92	1 (4%)	29,45,45	1.39	4 (13%)
10	ADP	O	601	11	24,29,29	0.94	1 (4%)	29,45,45	1.37	4 (13%)
12	AF3	D	603	-	0,3,3	-	-	-		
10	ADP	F	601	11	24,29,29	0.94	1 (4%)	29,45,45	1.51	4 (13%)
12	AF3	E	603	-	0,3,3	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ADP	K	601	11	-	5/12/32/32	0/3/3/3
10	ADP	C	601	11	-	0/12/32/32	0/3/3/3
10	ADP	M	601	11	-	2/12/32/32	0/3/3/3
10	ADP	H	601	11	-	2/12/32/32	0/3/3/3
10	ADP	J	601	11	-	1/12/32/32	0/3/3/3
10	ADP	A	601	11	-	1/12/32/32	0/3/3/3
10	ADP	L	601	11	-	0/12/32/32	0/3/3/3
10	ADP	I	601	11	-	4/12/32/32	0/3/3/3
10	ADP	D	601	11	-	4/12/32/32	0/3/3/3
10	ADP	N	601	11	-	1/12/32/32	0/3/3/3
10	ADP	P	601	11	-	2/12/32/32	0/3/3/3
10	ADP	G	601	11	-	4/12/32/32	0/3/3/3
10	ADP	B	601	11	-	0/12/32/32	0/3/3/3
10	ADP	O	601	11	-	4/12/32/32	0/3/3/3
10	ADP	E	601	11	-	0/12/32/32	0/3/3/3
10	ADP	F	601	11	-	2/12/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	601	ADP	C5-C4	2.41	1.47	1.40
10	F	601	ADP	C5-C4	2.41	1.47	1.40
10	K	601	ADP	C5-C4	2.40	1.47	1.40
10	I	601	ADP	C5-C4	2.39	1.47	1.40
10	J	601	ADP	C5-C4	2.39	1.47	1.40
10	A	601	ADP	C5-C4	2.38	1.47	1.40
10	N	601	ADP	C5-C4	2.38	1.47	1.40
10	D	601	ADP	C5-C4	2.37	1.47	1.40
10	C	601	ADP	C5-C4	2.36	1.47	1.40
10	O	601	ADP	C5-C4	2.36	1.47	1.40
10	B	601	ADP	C5-C4	2.35	1.47	1.40
10	E	601	ADP	C5-C4	2.33	1.47	1.40
10	L	601	ADP	C5-C4	2.33	1.47	1.40
10	P	601	ADP	C5-C4	2.32	1.47	1.40
10	G	601	ADP	C5-C4	2.31	1.47	1.40
10	H	601	ADP	C5-C4	2.31	1.47	1.40

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	601	ADP	PA-O3A-PB	-4.16	118.56	132.83
10	F	601	ADP	PA-O3A-PB	-4.00	119.10	132.83
10	A	601	ADP	PA-O3A-PB	-3.88	119.50	132.83
10	N	601	ADP	PA-O3A-PB	-3.78	119.86	132.83
10	I	601	ADP	PA-O3A-PB	-3.72	120.08	132.83
10	P	601	ADP	PA-O3A-PB	-3.71	120.08	132.83
10	H	601	ADP	PA-O3A-PB	-3.63	120.36	132.83
10	A	601	ADP	C3'-C2'-C1'	3.40	106.10	100.98
10	L	601	ADP	N3-C2-N1	-3.30	123.51	128.68
10	G	601	ADP	N3-C2-N1	-3.29	123.53	128.68
10	J	601	ADP	PA-O3A-PB	-3.29	121.55	132.83
10	I	601	ADP	N3-C2-N1	-3.25	123.60	128.68
10	K	601	ADP	PA-O3A-PB	-3.25	121.68	132.83
10	M	601	ADP	N3-C2-N1	-3.23	123.62	128.68
10	P	601	ADP	N3-C2-N1	-3.23	123.63	128.68
10	J	601	ADP	N3-C2-N1	-3.23	123.64	128.68
10	B	601	ADP	N3-C2-N1	-3.21	123.66	128.68
10	D	601	ADP	N3-C2-N1	-3.21	123.66	128.68
10	O	601	ADP	N3-C2-N1	-3.20	123.67	128.68
10	H	601	ADP	N3-C2-N1	-3.20	123.68	128.68
10	A	601	ADP	N3-C2-N1	-3.19	123.70	128.68
10	C	601	ADP	PA-O3A-PB	-3.18	121.92	132.83
10	F	601	ADP	N3-C2-N1	-3.15	123.76	128.68
10	E	601	ADP	N3-C2-N1	-3.14	123.77	128.68
10	N	601	ADP	N3-C2-N1	-3.09	123.84	128.68
10	B	601	ADP	C3'-C2'-C1'	3.09	105.64	100.98
10	C	601	ADP	N3-C2-N1	-3.05	123.91	128.68
10	G	601	ADP	PA-O3A-PB	-3.04	122.40	132.83
10	F	601	ADP	C3'-C2'-C1'	3.01	105.51	100.98
10	O	601	ADP	C3'-C2'-C1'	3.00	105.49	100.98
10	K	601	ADP	C4-C5-N7	-2.99	106.28	109.40
10	D	601	ADP	PA-O3A-PB	-2.99	122.57	132.83
10	N	601	ADP	C3'-C2'-C1'	2.98	105.46	100.98
10	K	601	ADP	C3'-C2'-C1'	2.96	105.44	100.98
10	D	601	ADP	C3'-C2'-C1'	2.88	105.32	100.98
10	C	601	ADP	C4-C5-N7	-2.87	106.40	109.40
10	H	601	ADP	C4-C5-N7	-2.86	106.42	109.40
10	L	601	ADP	C3'-C2'-C1'	2.85	105.27	100.98
10	L	601	ADP	C4-C5-N7	-2.81	106.47	109.40
10	M	601	ADP	C3'-C2'-C1'	2.79	105.18	100.98
10	P	601	ADP	C3'-C2'-C1'	2.79	105.17	100.98
10	I	601	ADP	C3'-C2'-C1'	2.78	105.17	100.98
10	J	601	ADP	C3'-C2'-C1'	2.78	105.17	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	H	601	ADP	C3'-C2'-C1'	2.77	105.15	100.98
10	D	601	ADP	C4-C5-N7	-2.77	106.52	109.40
10	K	601	ADP	N3-C2-N1	-2.76	124.36	128.68
10	E	601	ADP	C3'-C2'-C1'	2.76	105.13	100.98
10	C	601	ADP	C3'-C2'-C1'	2.75	105.11	100.98
10	M	601	ADP	PA-O3A-PB	-2.74	123.41	132.83
10	E	601	ADP	PA-O3A-PB	-2.74	123.43	132.83
10	F	601	ADP	C4-C5-N7	-2.74	106.55	109.40
10	J	601	ADP	C4-C5-N7	-2.74	106.55	109.40
10	P	601	ADP	C4-C5-N7	-2.70	106.59	109.40
10	M	601	ADP	C4-C5-N7	-2.69	106.59	109.40
10	N	601	ADP	C4-C5-N7	-2.69	106.60	109.40
10	O	601	ADP	C4-C5-N7	-2.69	106.60	109.40
10	I	601	ADP	C4-C5-N7	-2.68	106.60	109.40
10	G	601	ADP	C3'-C2'-C1'	2.68	105.02	100.98
10	A	601	ADP	C4-C5-N7	-2.63	106.65	109.40
10	G	601	ADP	C4-C5-N7	-2.62	106.67	109.40
10	O	601	ADP	PA-O3A-PB	-2.60	123.89	132.83
10	B	601	ADP	C4-C5-N7	-2.58	106.71	109.40
10	E	601	ADP	C4-C5-N7	-2.54	106.75	109.40
10	L	601	ADP	PA-O3A-PB	-2.52	124.19	132.83

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	F	601	ADP	C5'-O5'-PA-O1A
10	G	601	ADP	PB-O3A-PA-O5'
10	G	601	ADP	C5'-O5'-PA-O2A
10	H	601	ADP	O4'-C4'-C5'-O5'
10	I	601	ADP	C5'-O5'-PA-O1A
10	I	601	ADP	C5'-O5'-PA-O2A
10	J	601	ADP	PB-O3A-PA-O5'
10	K	601	ADP	C5'-O5'-PA-O1A
10	K	601	ADP	C5'-O5'-PA-O2A
10	O	601	ADP	PA-O3A-PB-O3B
10	O	601	ADP	C5'-O5'-PA-O3A
10	K	601	ADP	C3'-C4'-C5'-O5'
10	H	601	ADP	C3'-C4'-C5'-O5'
10	K	601	ADP	O4'-C4'-C5'-O5'
10	D	601	ADP	PB-O3A-PA-O5'
10	M	601	ADP	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
10	D	601	ADP	C5'-O5'-PA-O3A
10	G	601	ADP	C5'-O5'-PA-O3A
10	K	601	ADP	C5'-O5'-PA-O3A
10	M	601	ADP	C5'-O5'-PA-O3A
10	O	601	ADP	C5'-O5'-PA-O1A
10	P	601	ADP	O4'-C4'-C5'-O5'
10	I	601	ADP	C5'-O5'-PA-O3A
10	A	601	ADP	O4'-C4'-C5'-O5'
10	F	601	ADP	O4'-C4'-C5'-O5'
10	N	601	ADP	O4'-C4'-C5'-O5'
10	I	601	ADP	PB-O3A-PA-O2A
10	D	601	ADP	C5'-O5'-PA-O1A
10	D	601	ADP	C5'-O5'-PA-O2A
10	G	601	ADP	C5'-O5'-PA-O1A
10	O	601	ADP	C5'-O5'-PA-O2A
10	P	601	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

27 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	K	601	ADP	4	0
12	C	603	AF3	1	0
10	H	601	ADP	2	0
10	J	601	ADP	2	0
12	K	603	AF3	2	0
12	L	603	AF3	2	0
10	C	601	ADP	3	0
12	G	603	AF3	1	0
10	N	601	ADP	3	0
12	P	603	AF3	1	0
10	E	601	ADP	2	0
12	F	603	AF3	5	0
12	A	603	AF3	1	0
12	H	603	AF3	3	0
10	M	601	ADP	1	0
12	M	603	AF3	1	0
12	B	603	AF3	1	0
12	J	603	AF3	1	0
10	B	601	ADP	1	0
10	L	601	ADP	2	0
12	N	603	AF3	1	0

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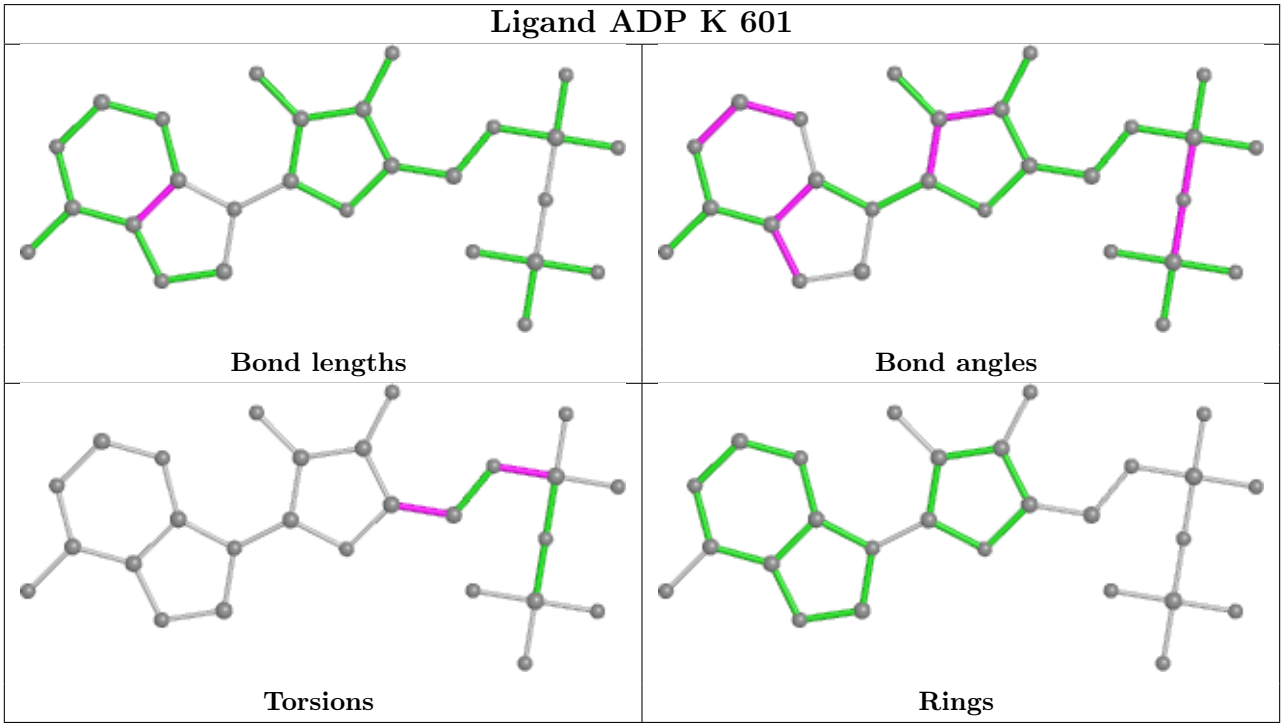
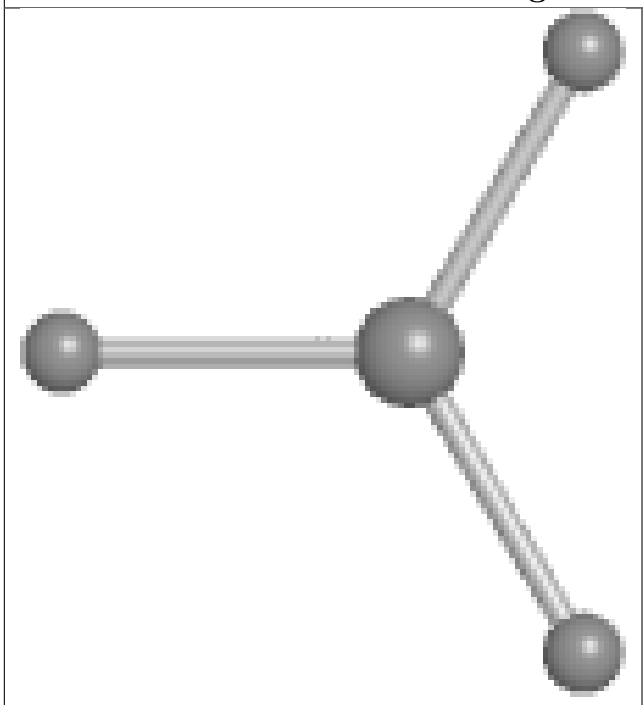
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	P	601	ADP	2	0
10	D	601	ADP	3	0
10	G	601	ADP	3	0
12	D	603	AF3	1	0
10	F	601	ADP	3	0
12	E	603	AF3	2	0

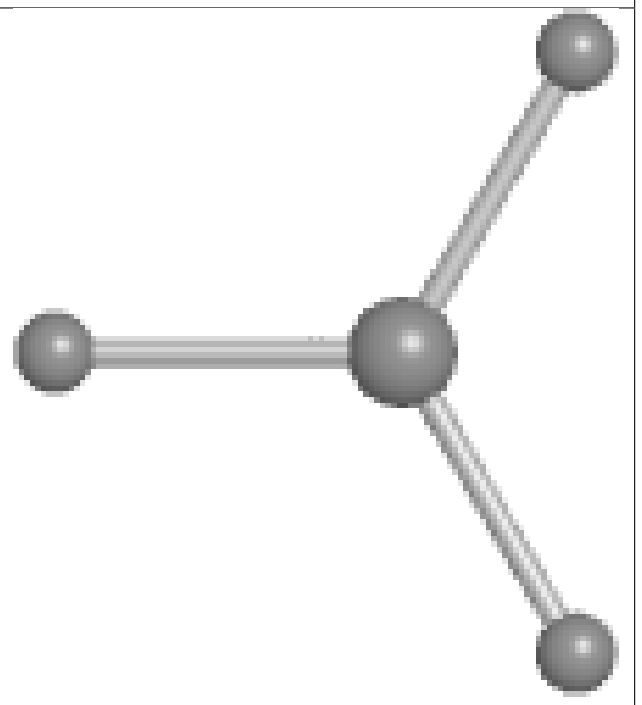
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



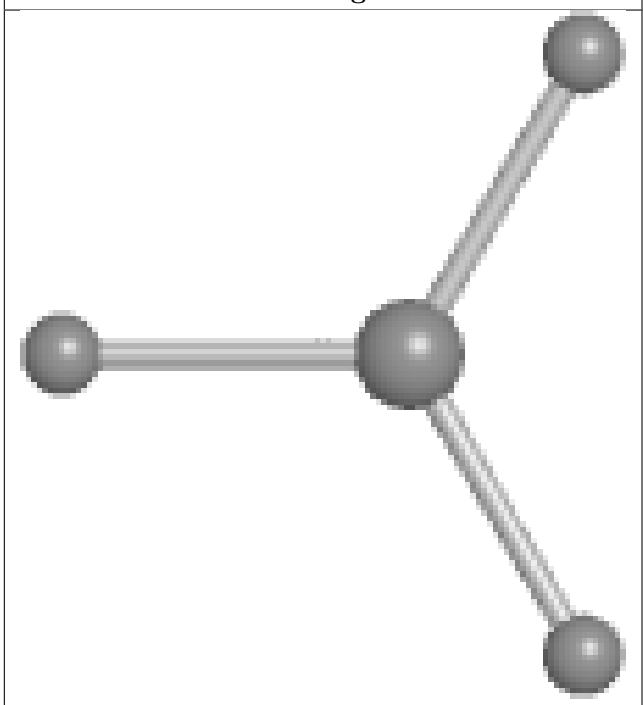
Ligand AF3 C 603



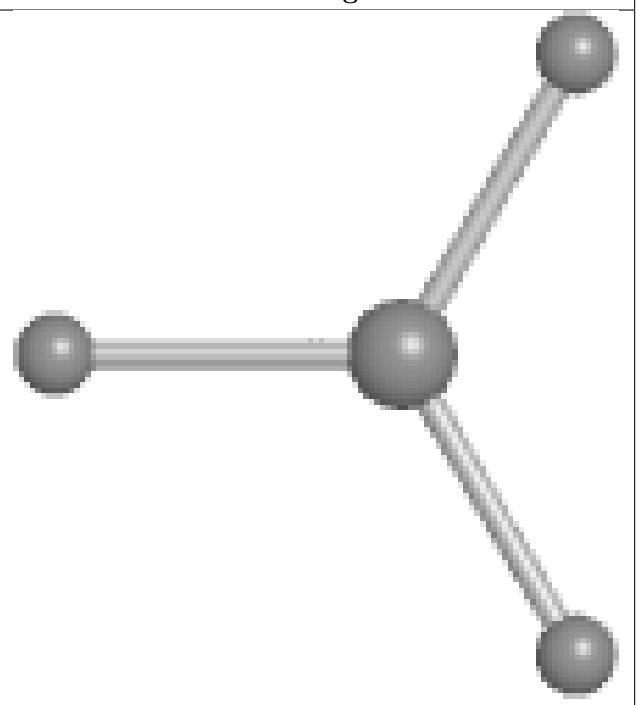
Bond lengths



Bond angles

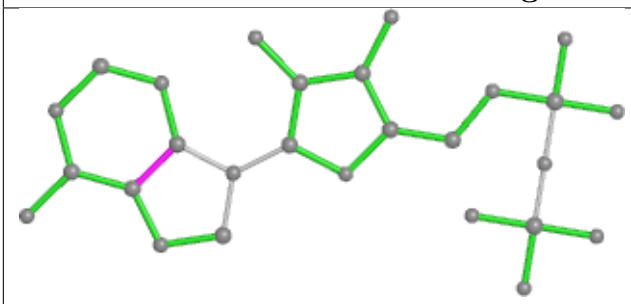


Torsions



Rings

Ligand ADP H 601



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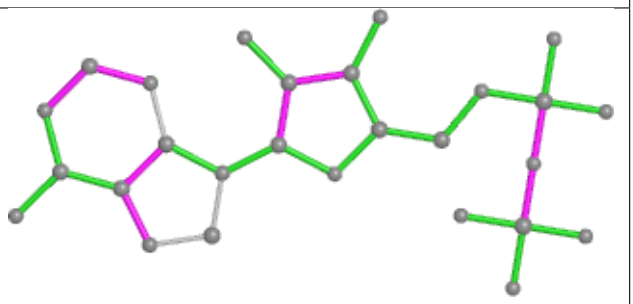
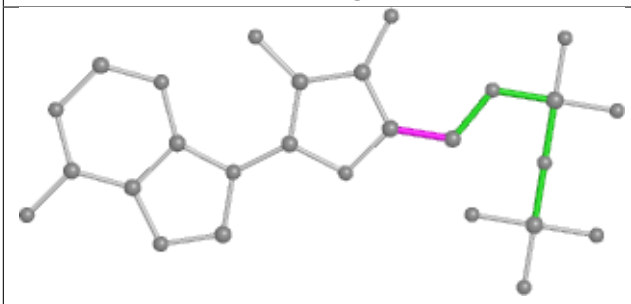
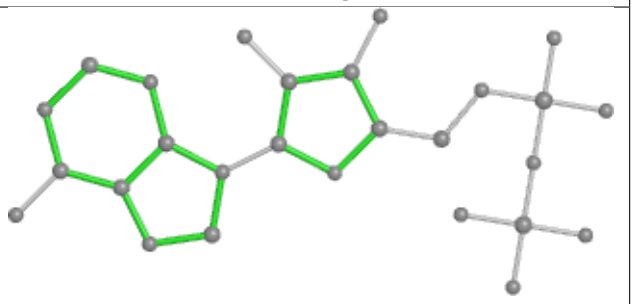


Bond angles

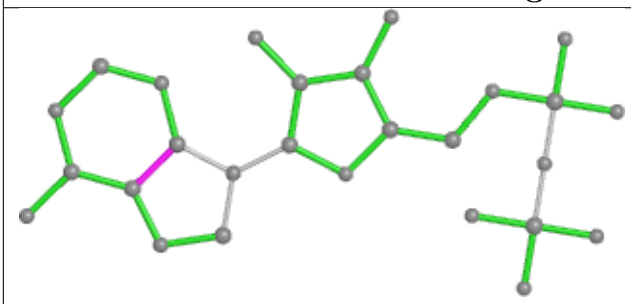


Torsions



Rings

Ligand ADP J 601



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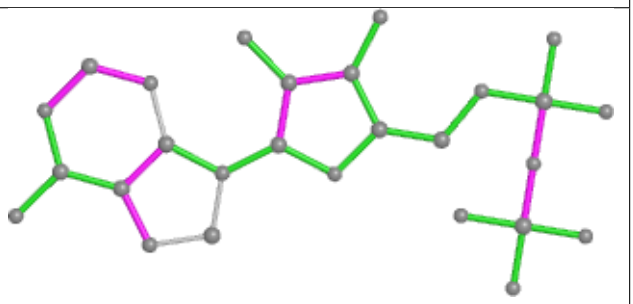
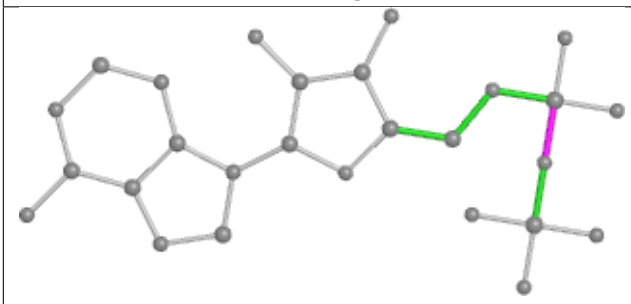


Bond angles



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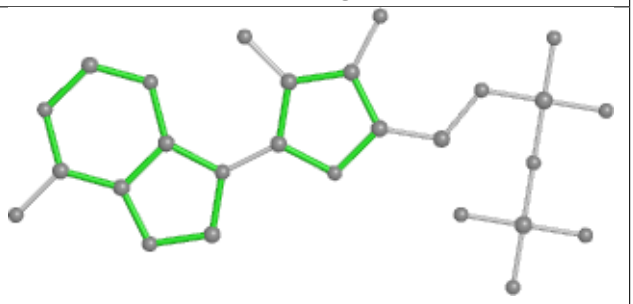
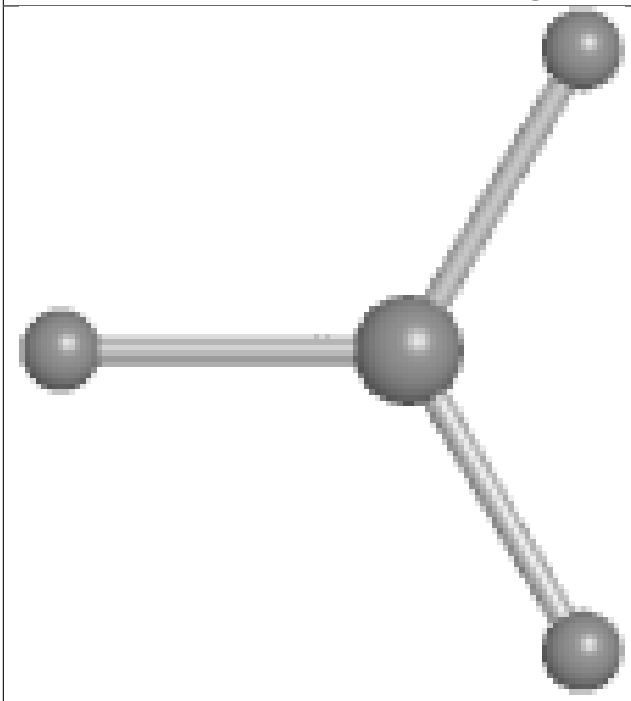


Rings

Ligand AF3 K 603



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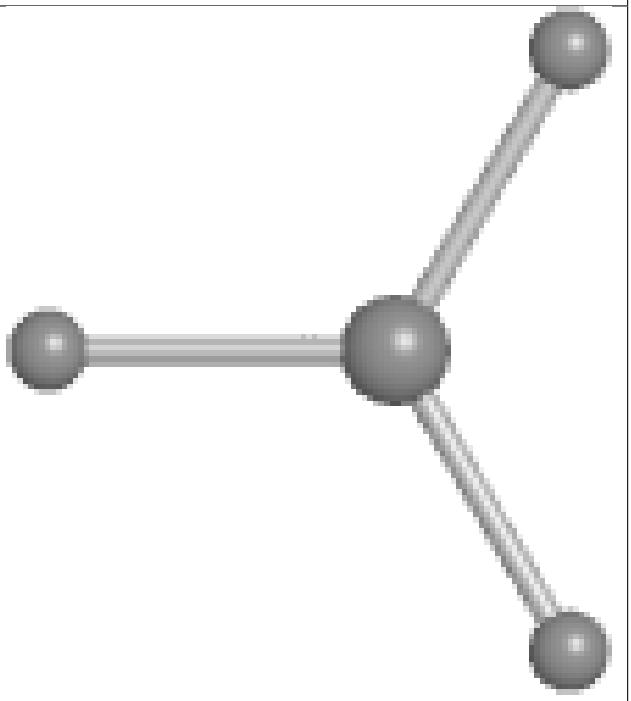

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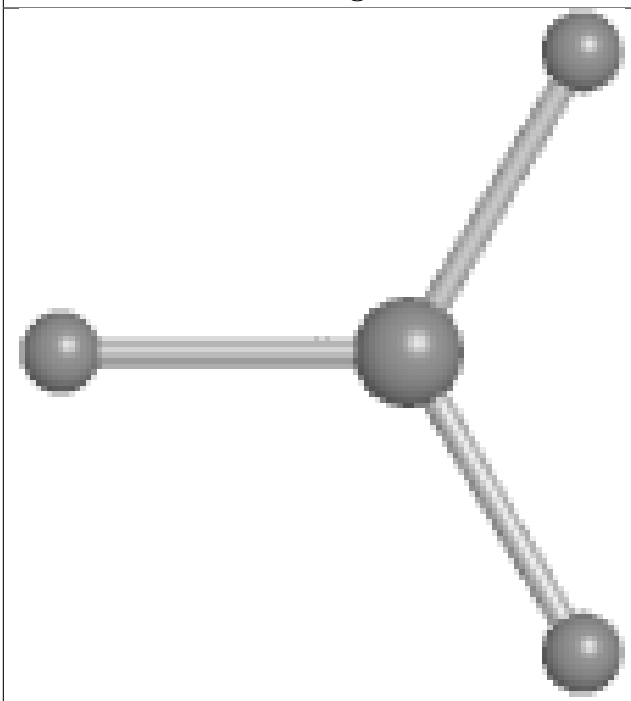

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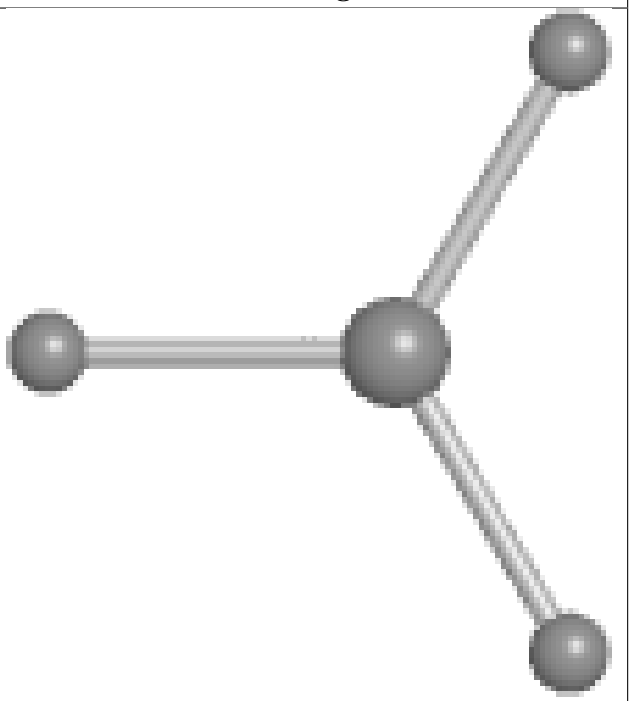
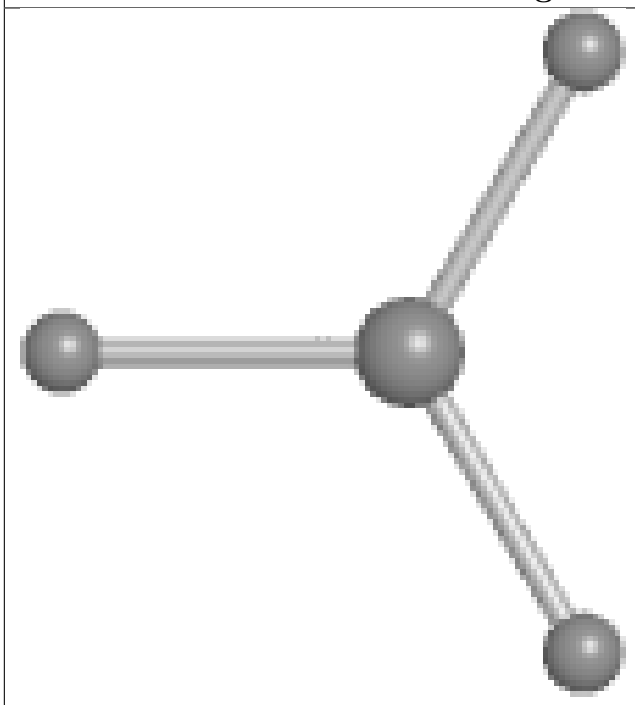


Rings

Ligand AF3 I 603



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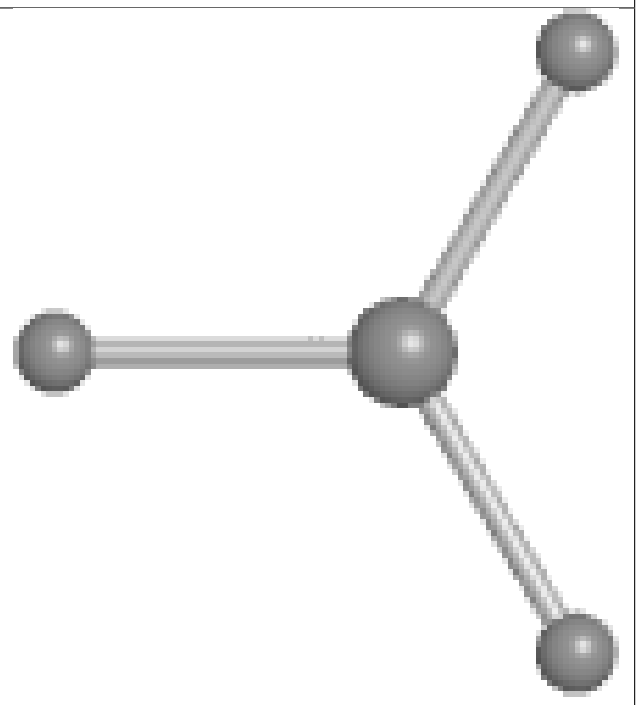

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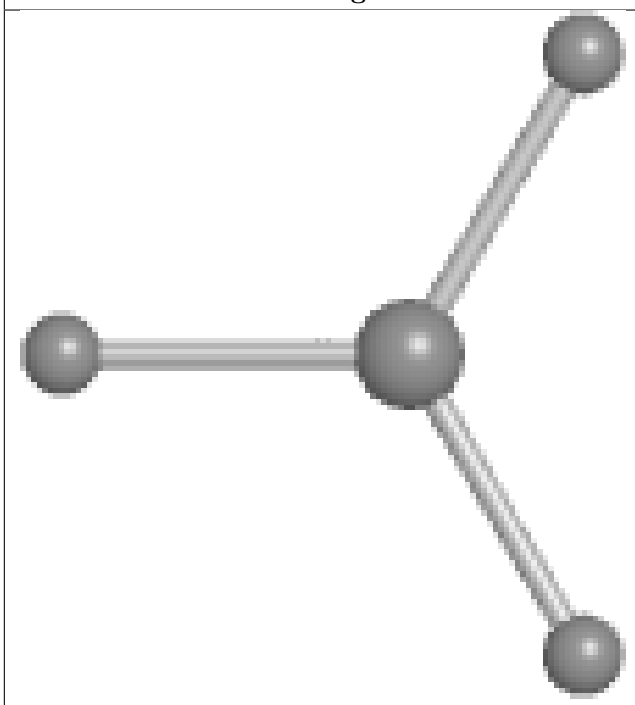

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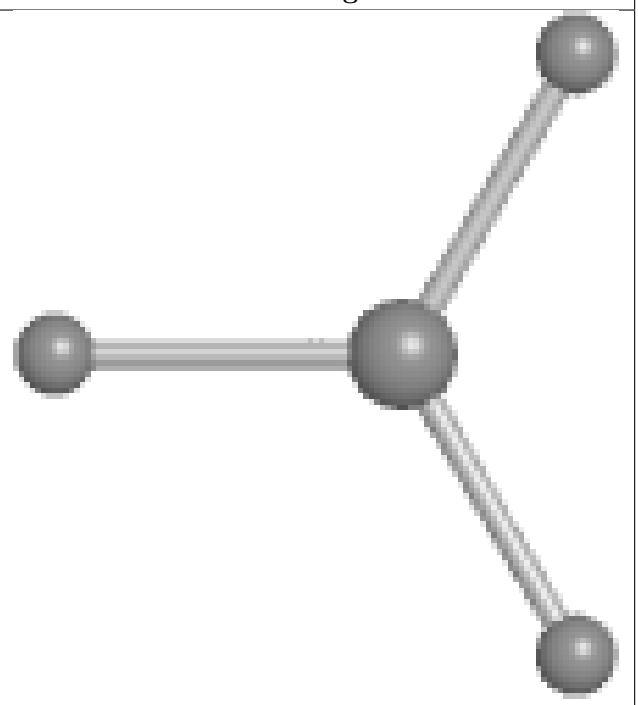
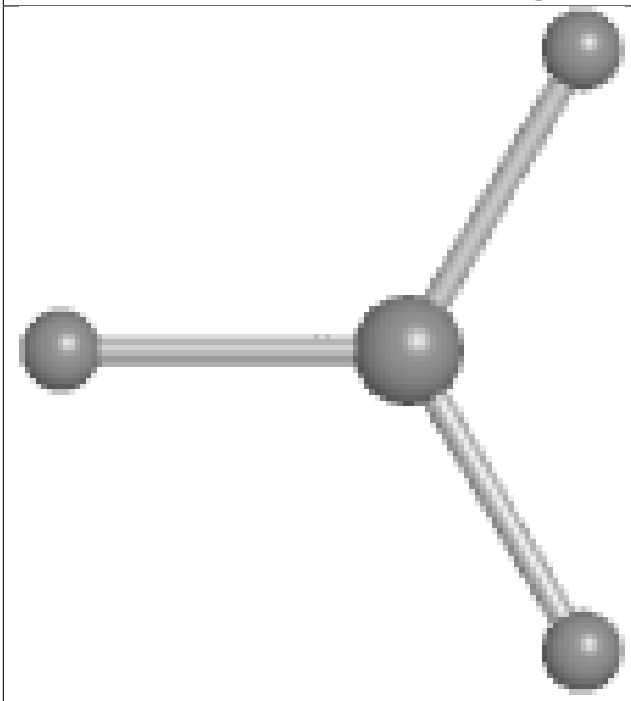


Rings

Ligand AF3 L 603



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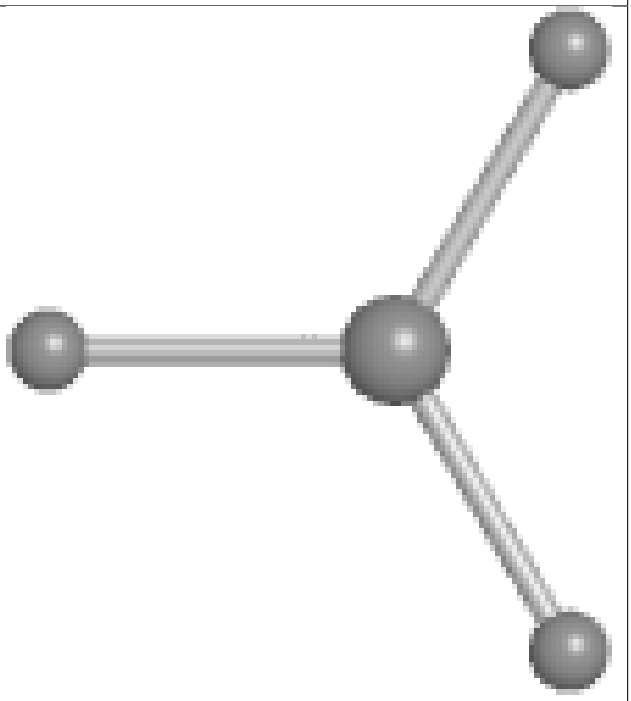

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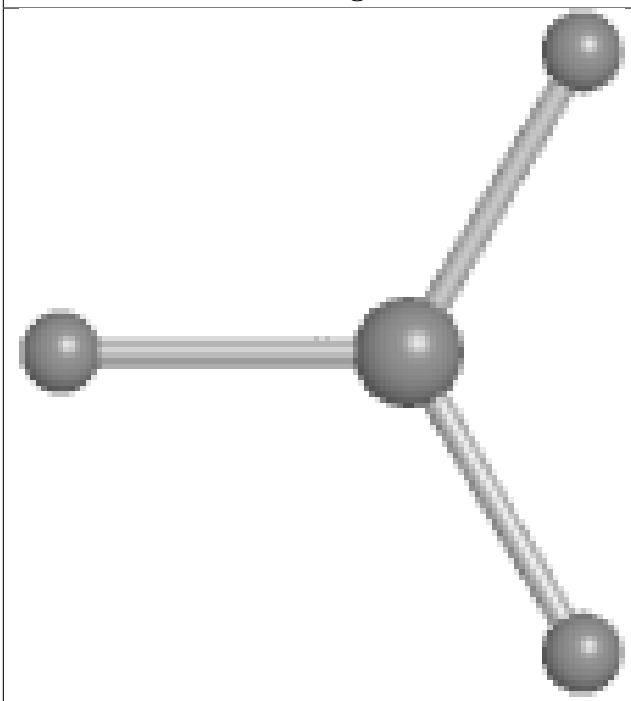

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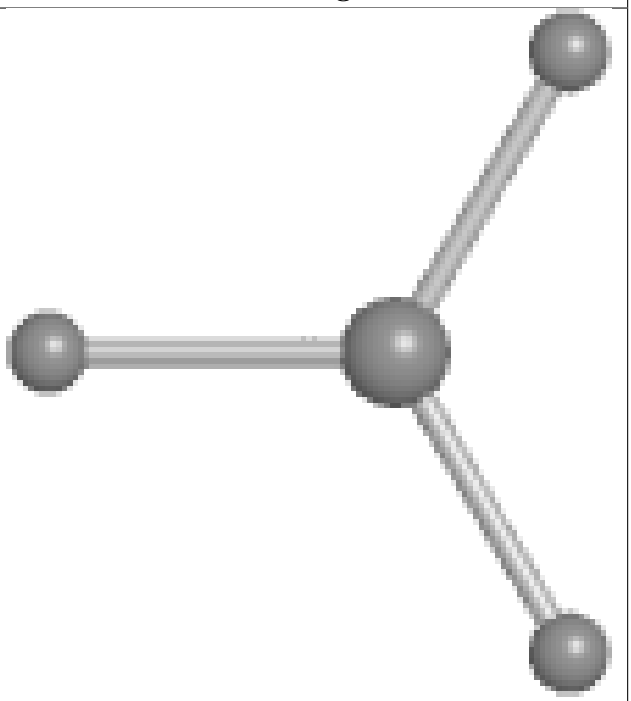
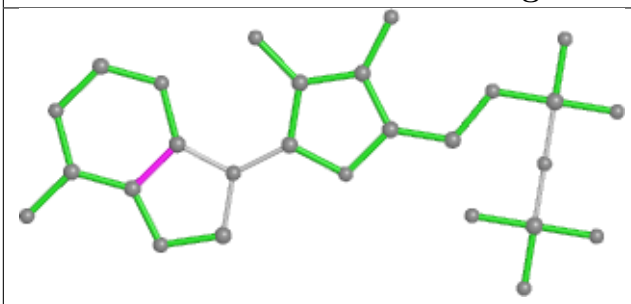


Rings

Ligand ADP C 601



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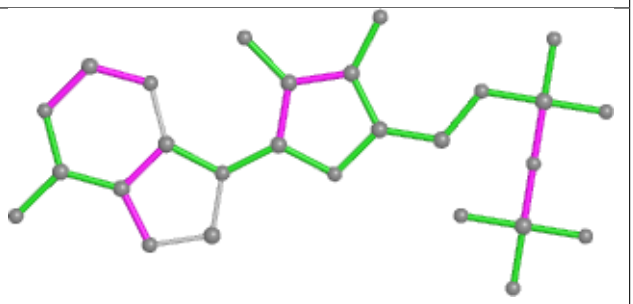

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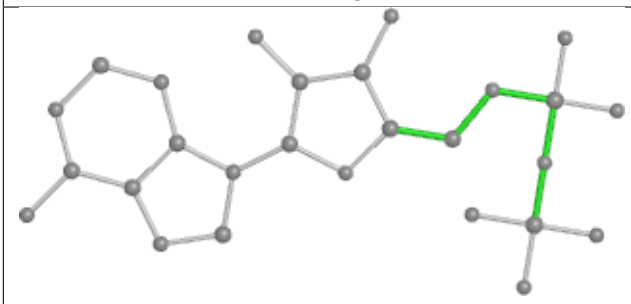

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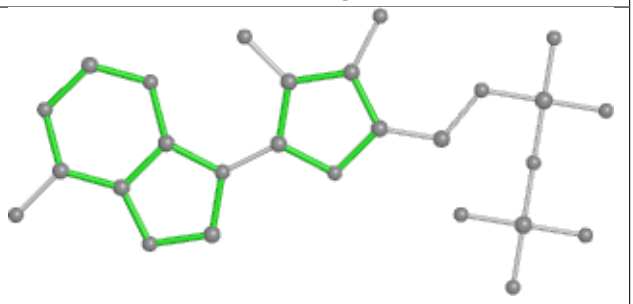
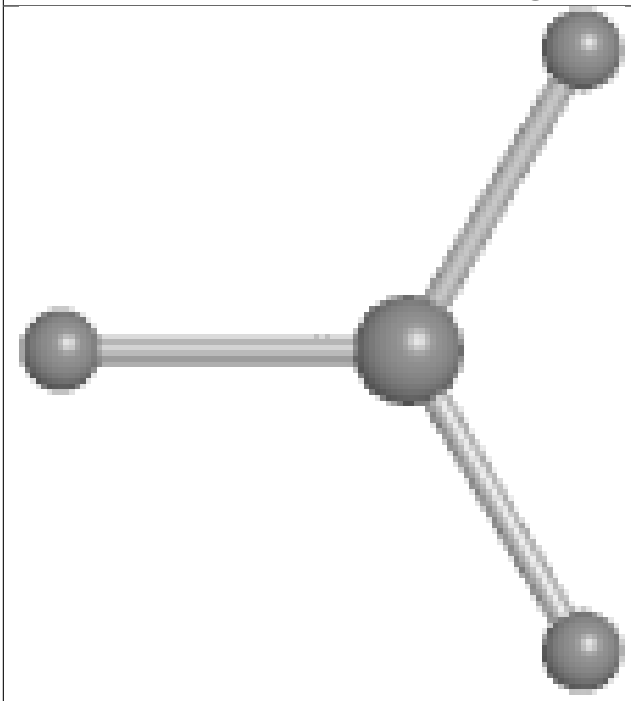


Rings

Ligand AF3 G 603



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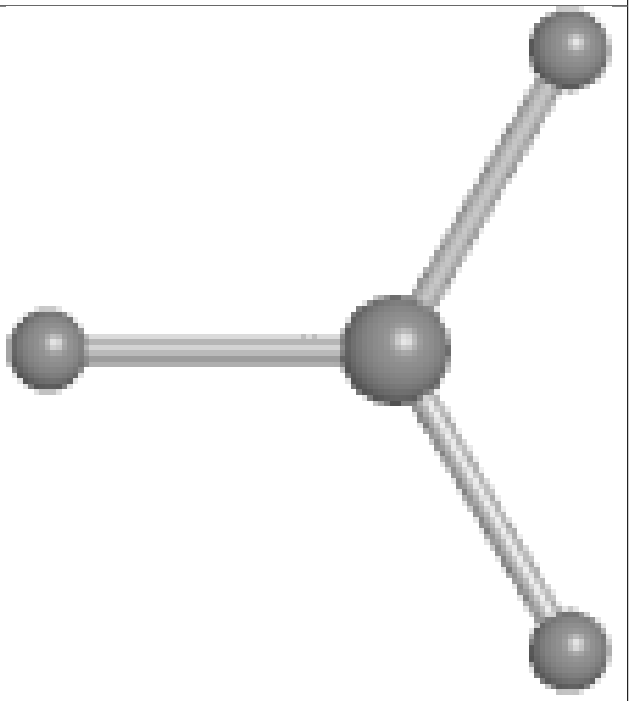

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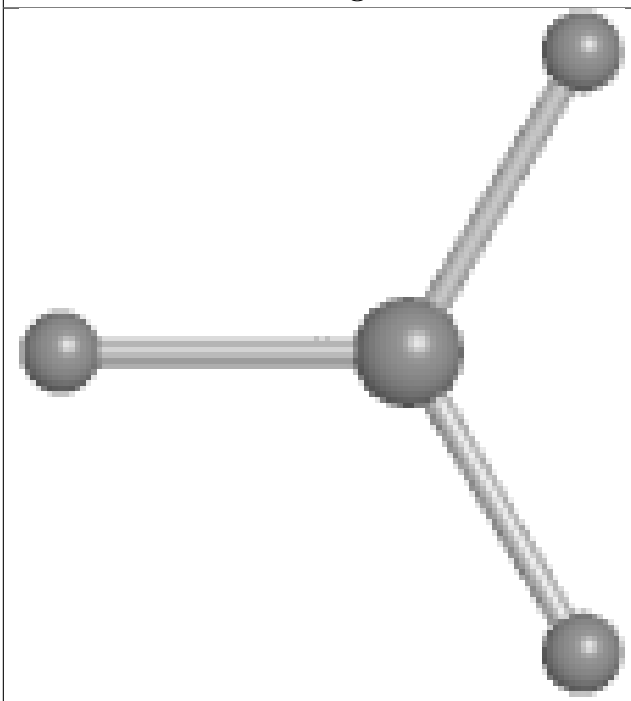

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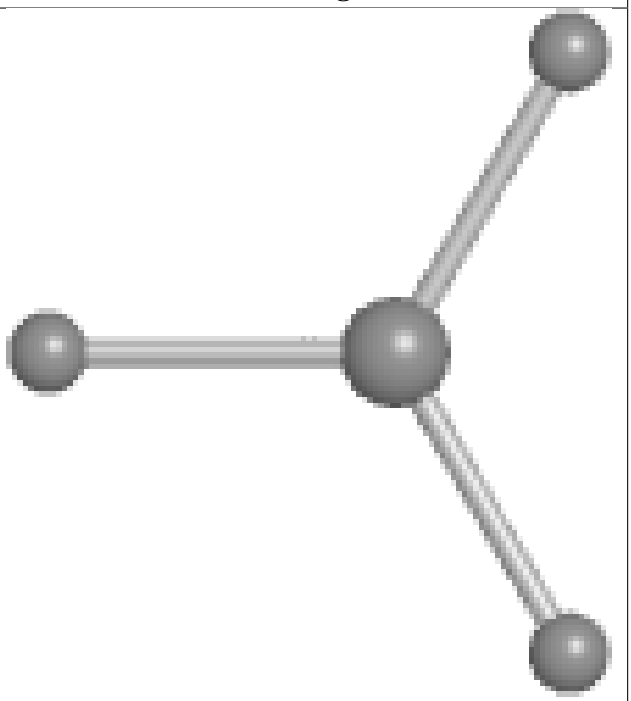
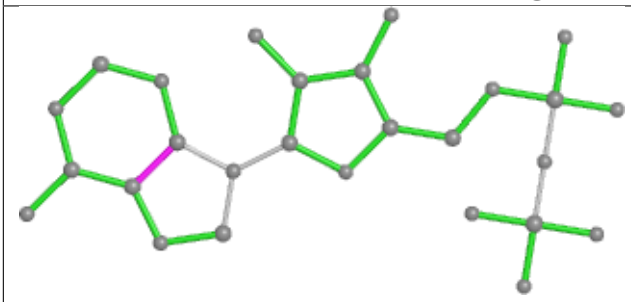
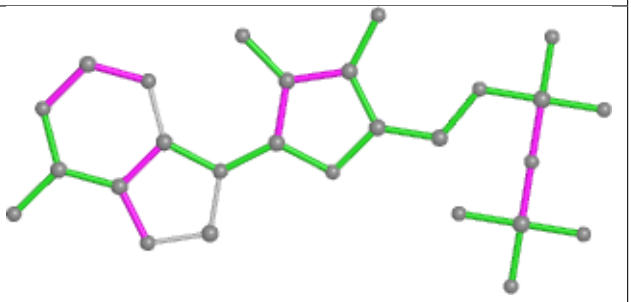
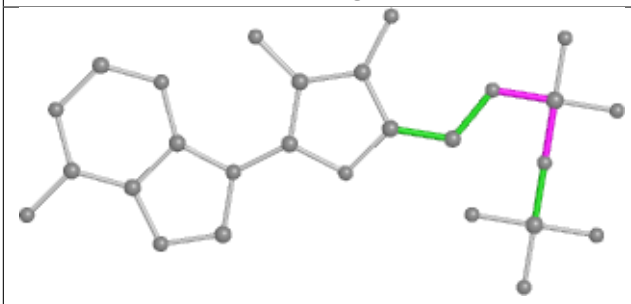
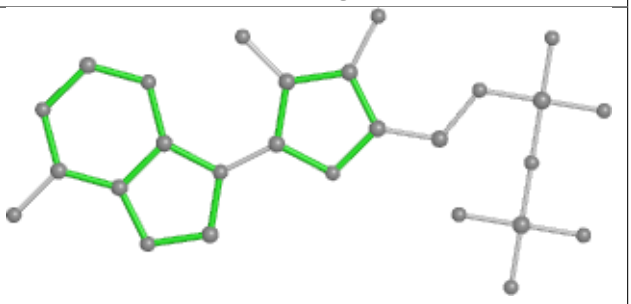
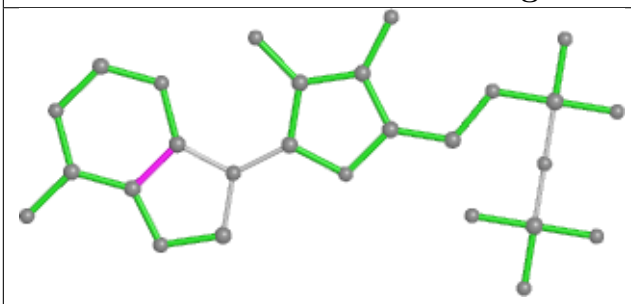
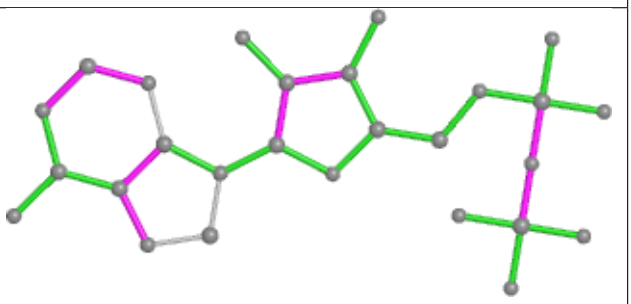
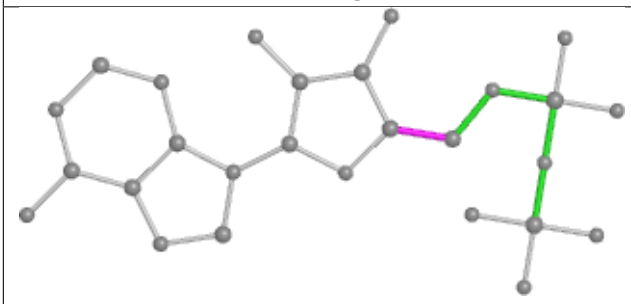
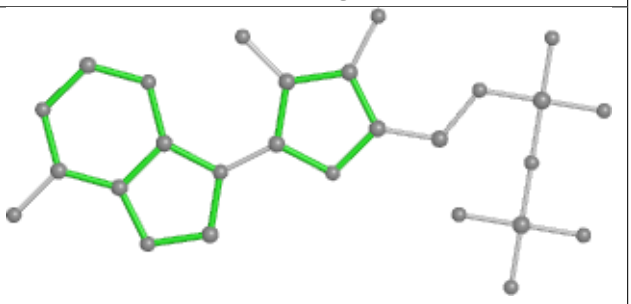
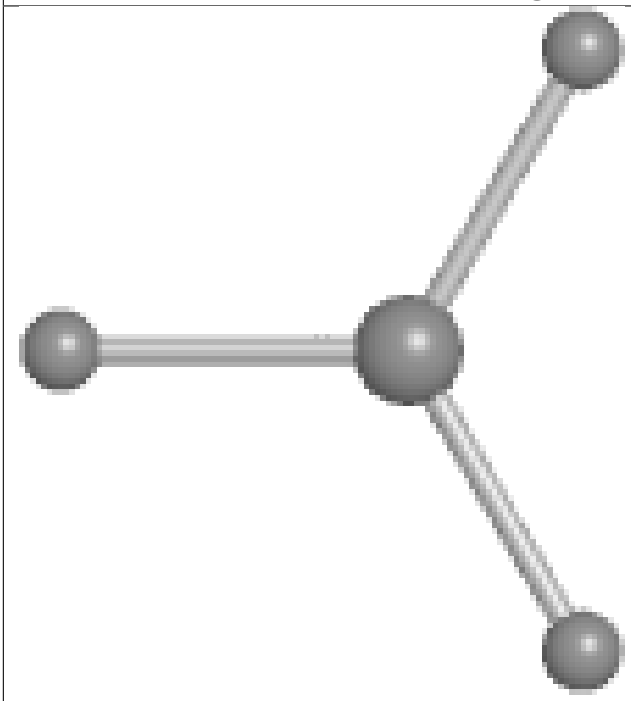


Rings

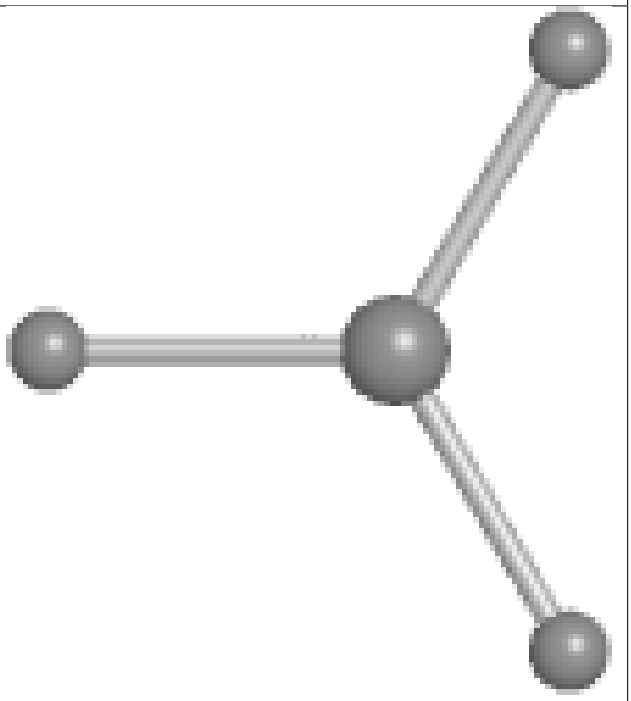
Ligand ADP I 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP N 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

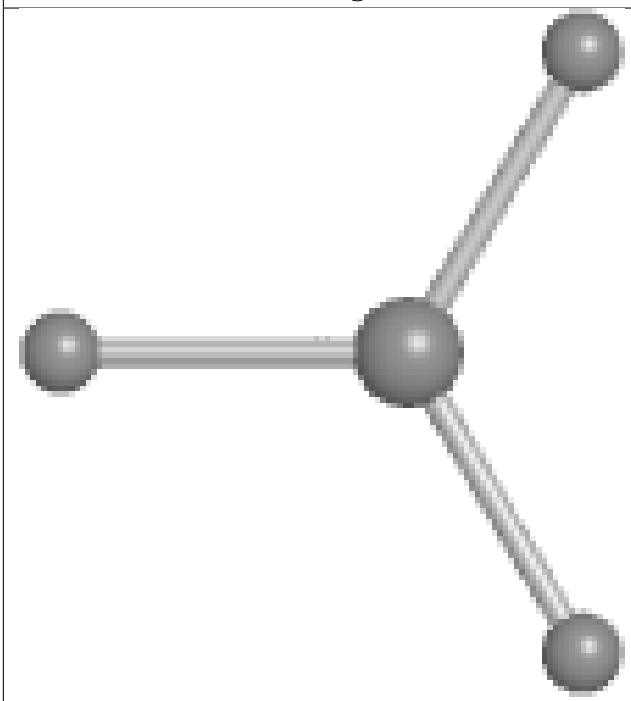
Ligand AF3 P 603



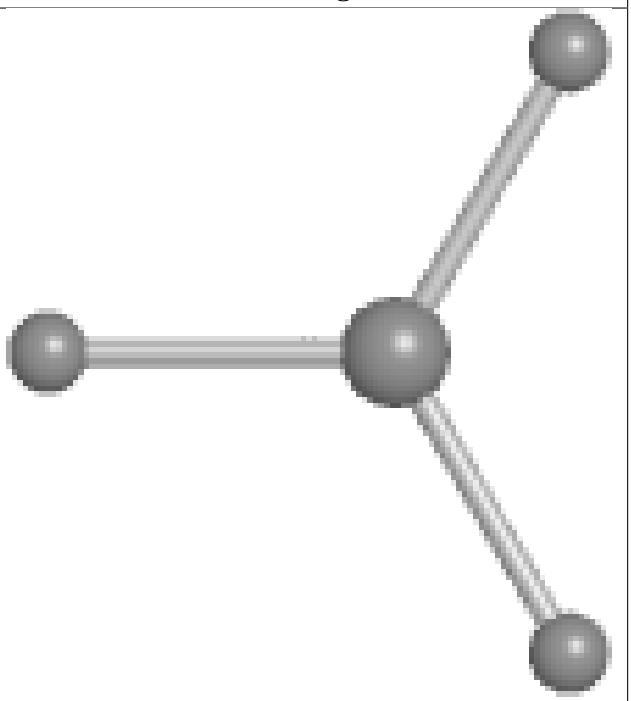
Bond lengths



Bond angles

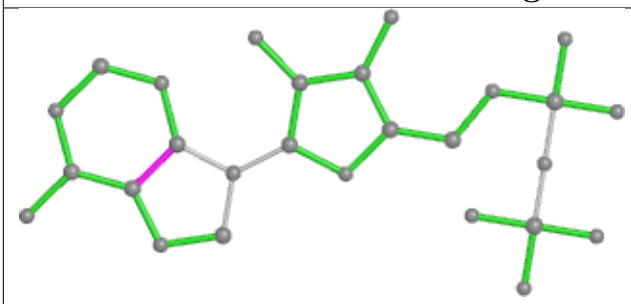


Torsions

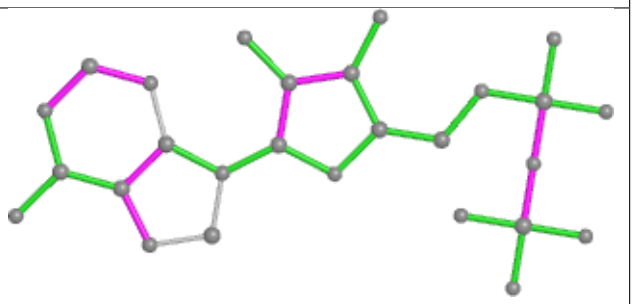


Rings

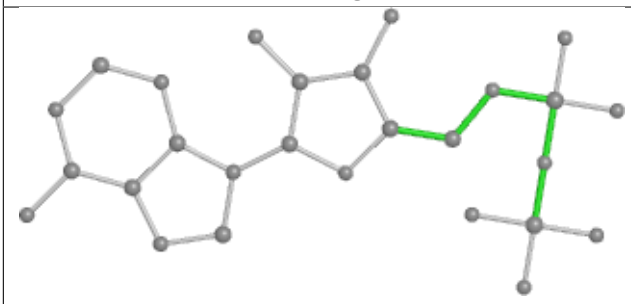
Ligand ADP E 601



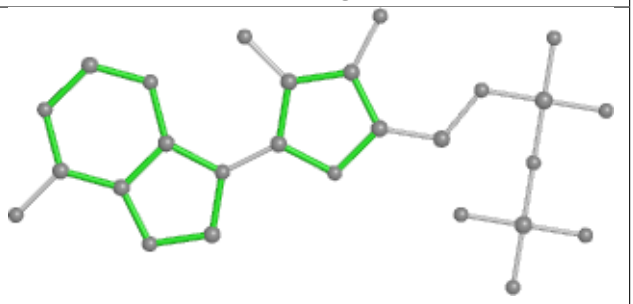
Bond lengths



Bond angles

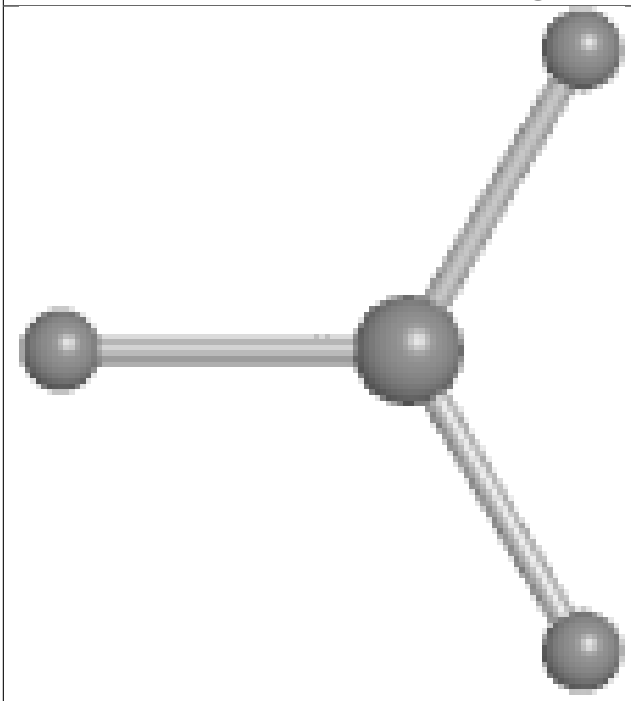


Torsions



Rings

Ligand AF3 F 603



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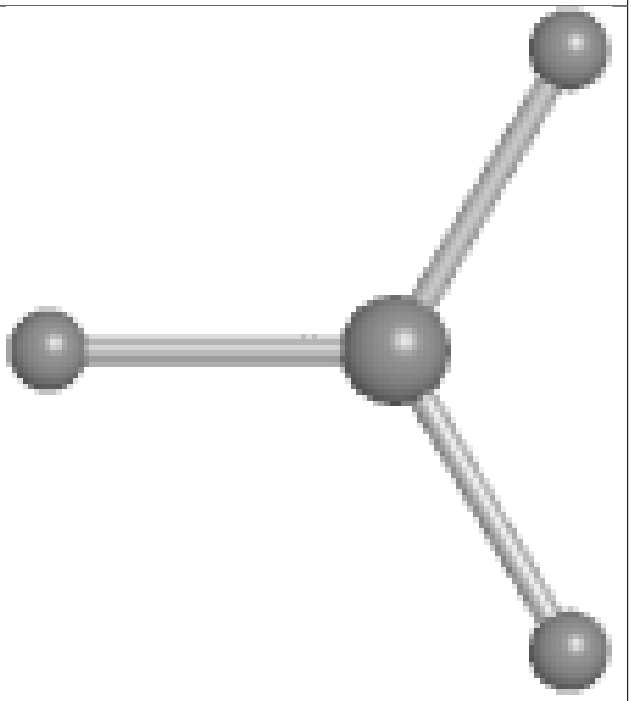
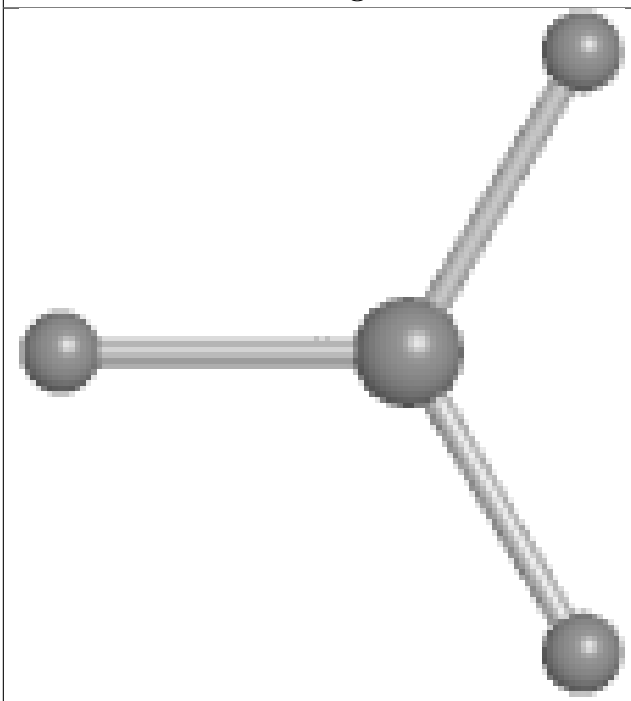
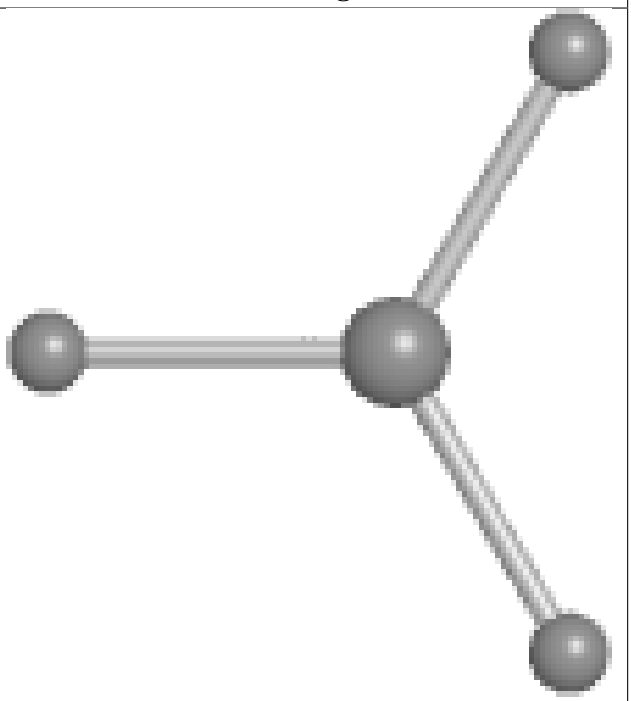


Bond angles

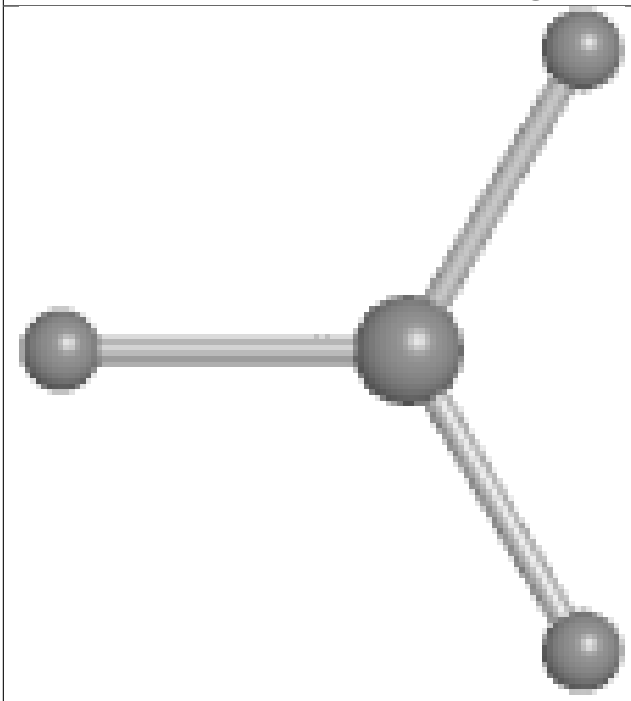


Torsions



Rings

Ligand AF3 A 603



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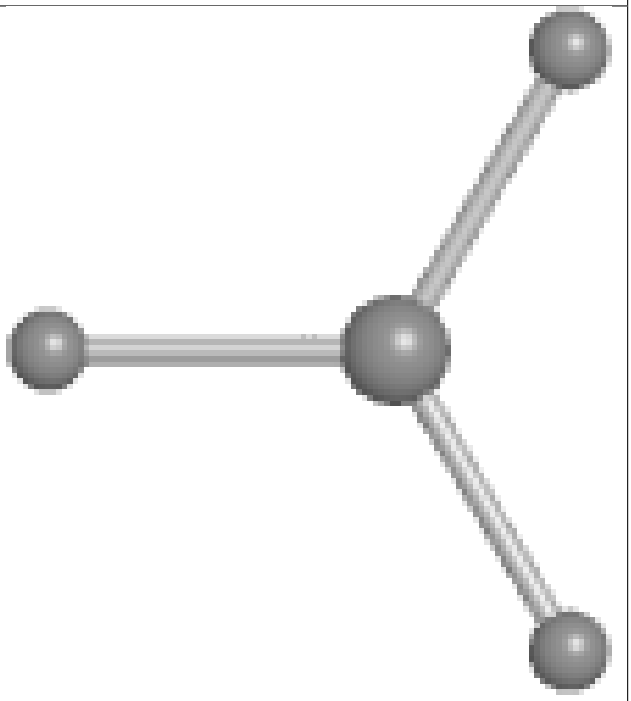

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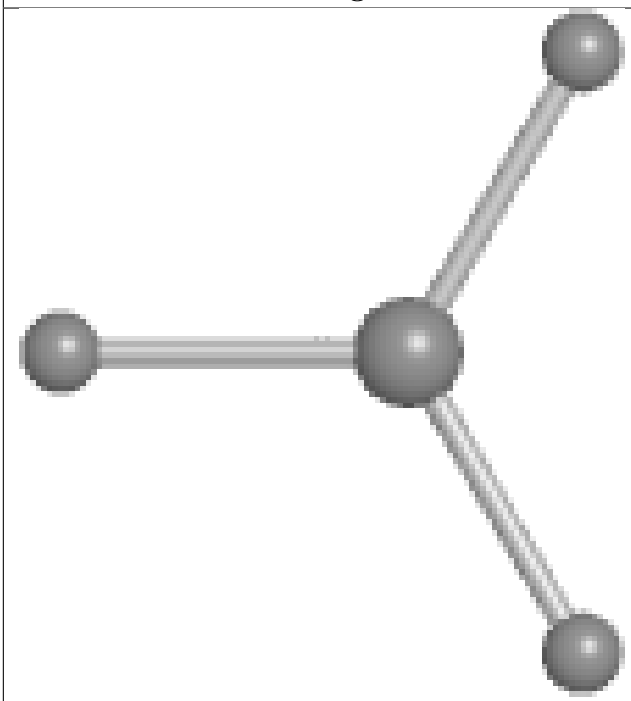

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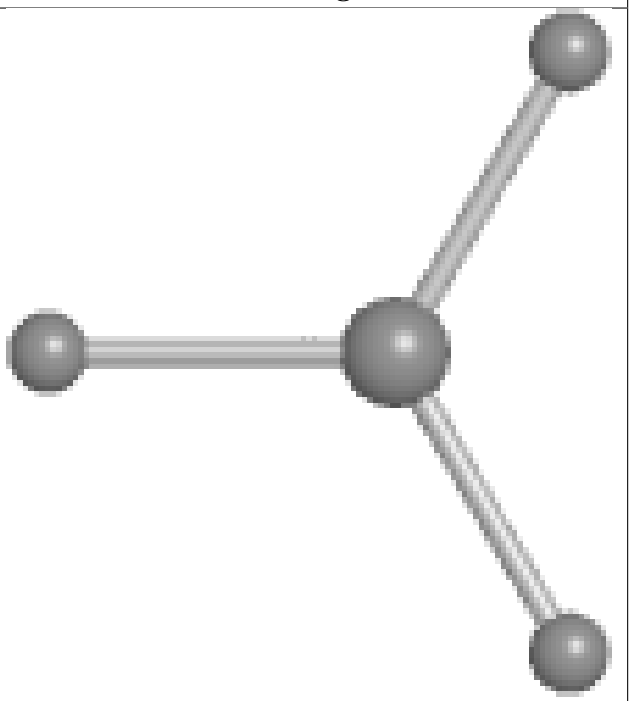
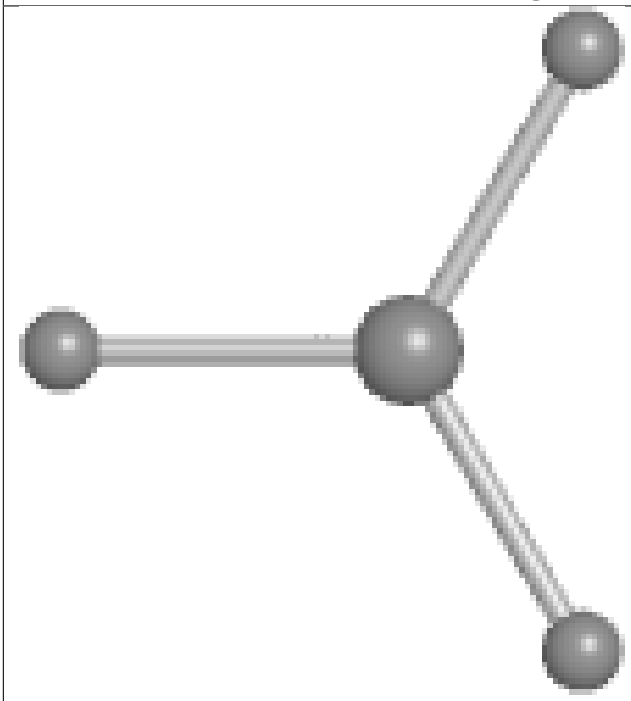


Rings

Ligand AF3 O 603



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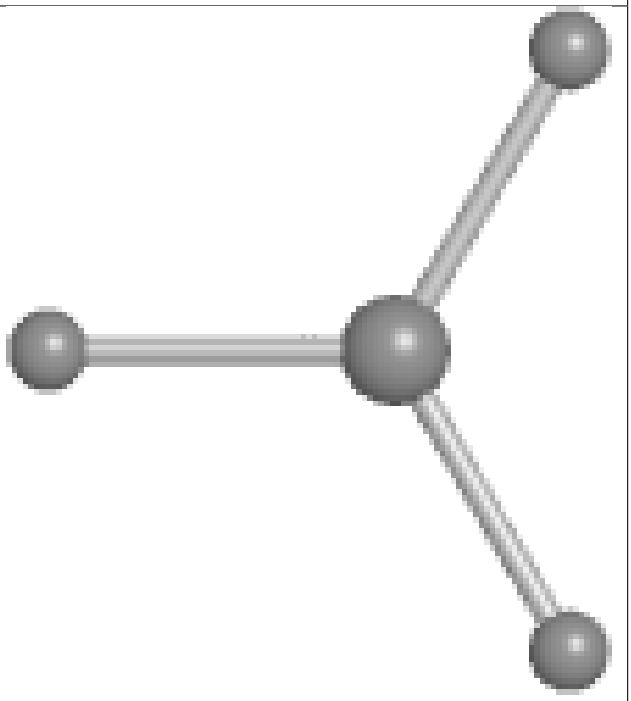

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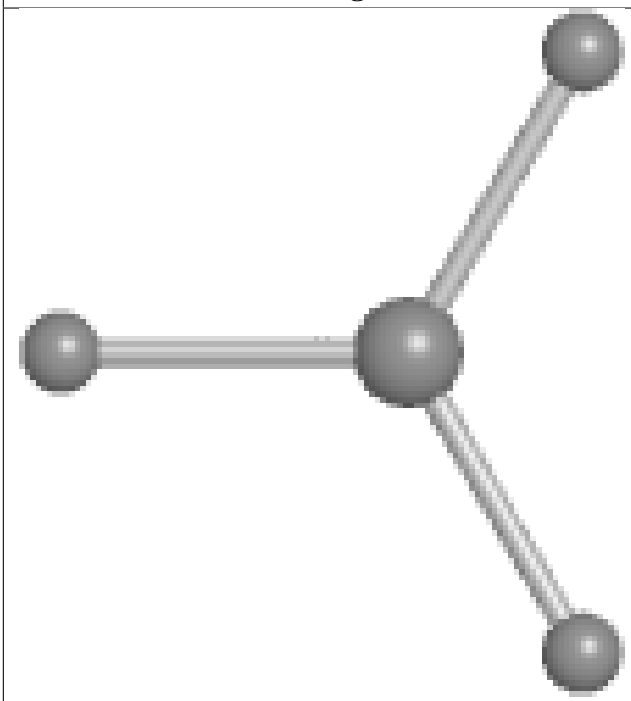

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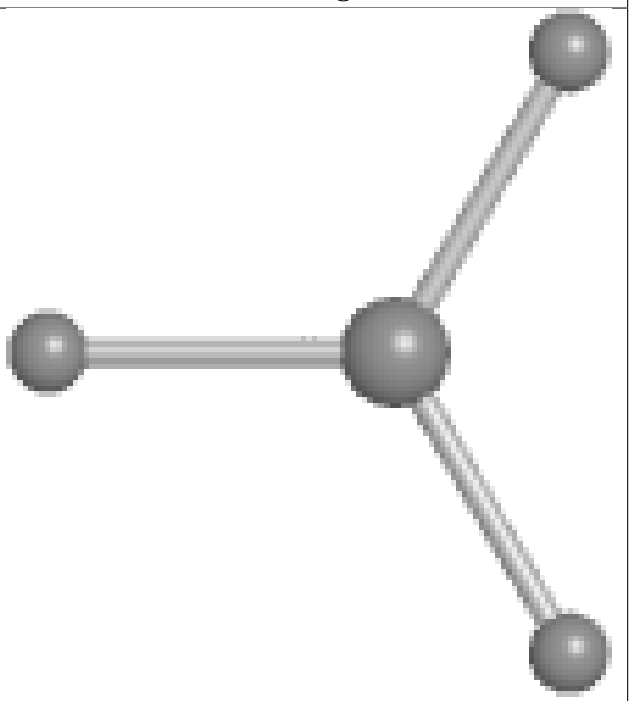
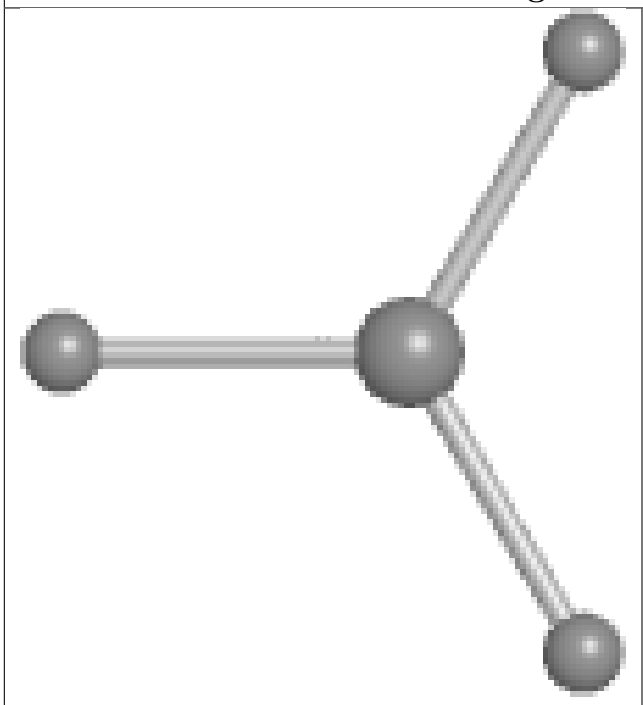


Rings

Ligand AF3 H 603



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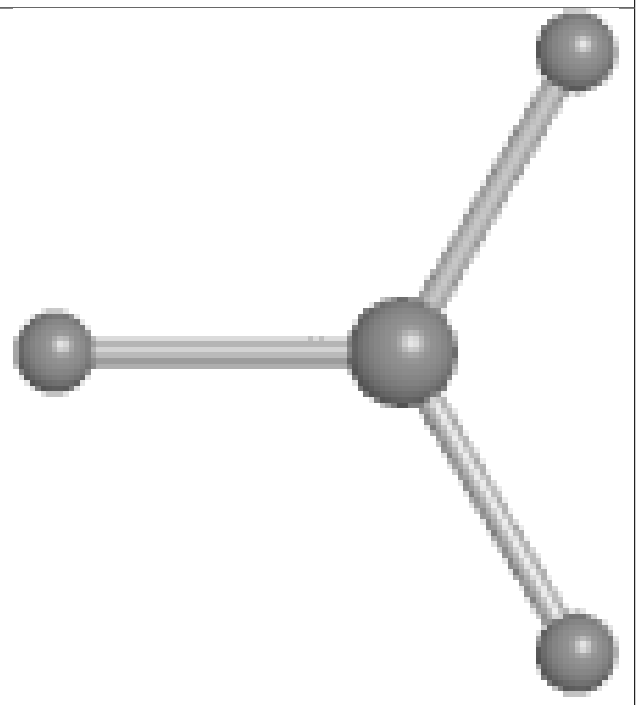

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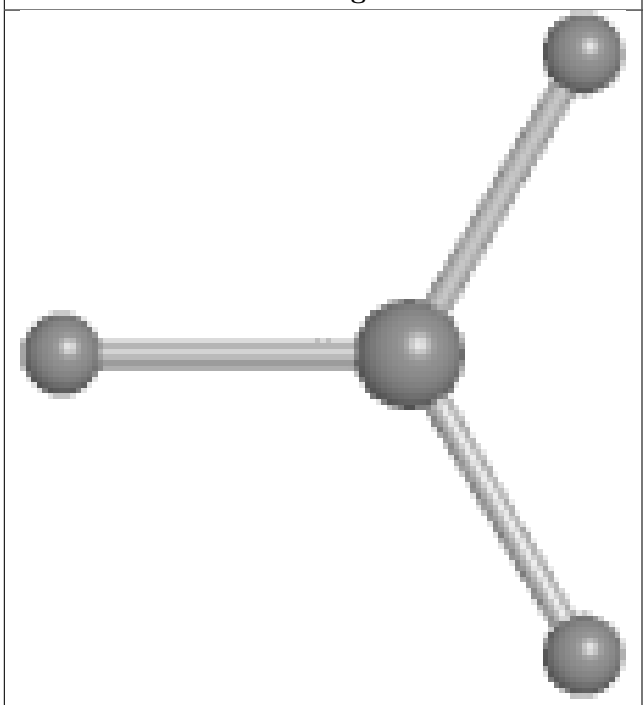

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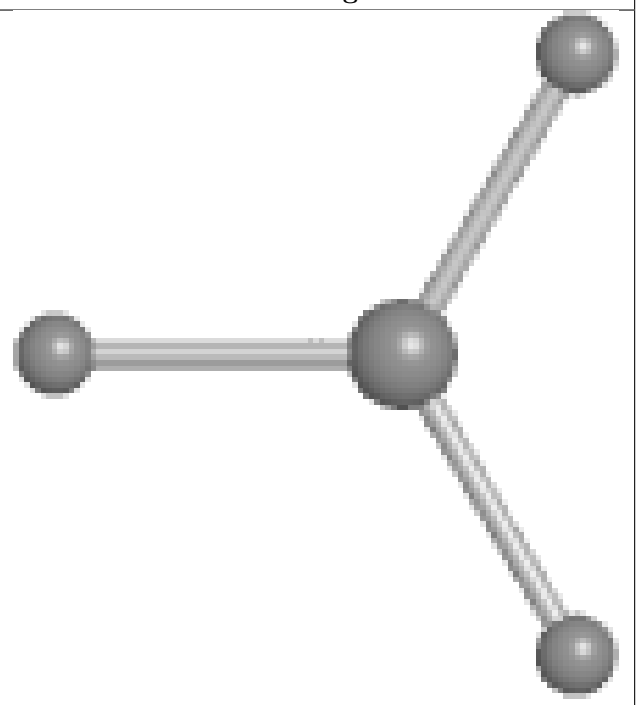
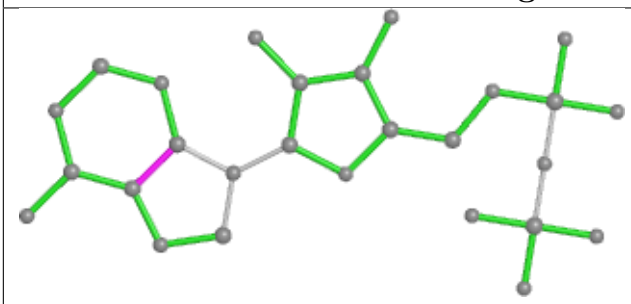


Rings

Ligand ADP M 601



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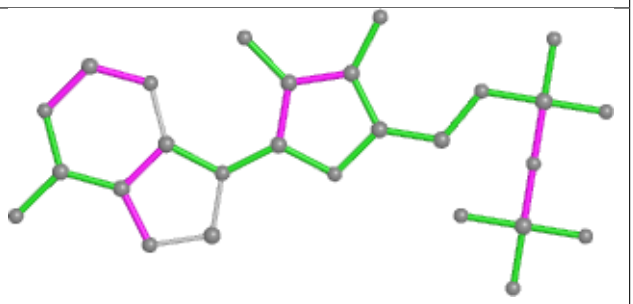

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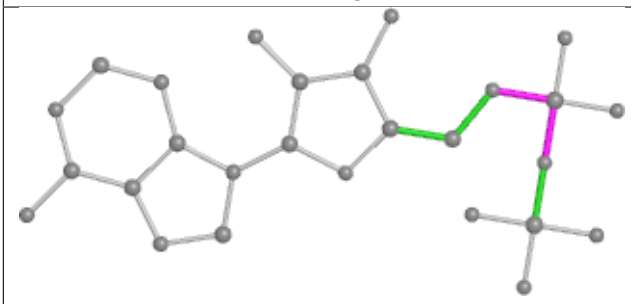

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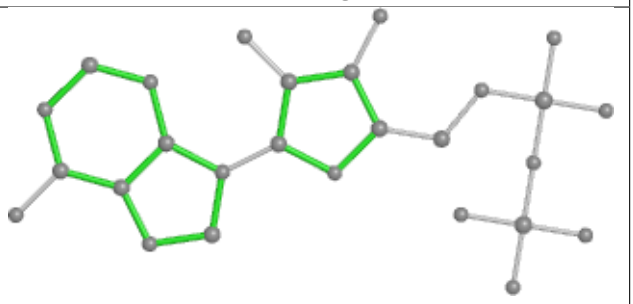
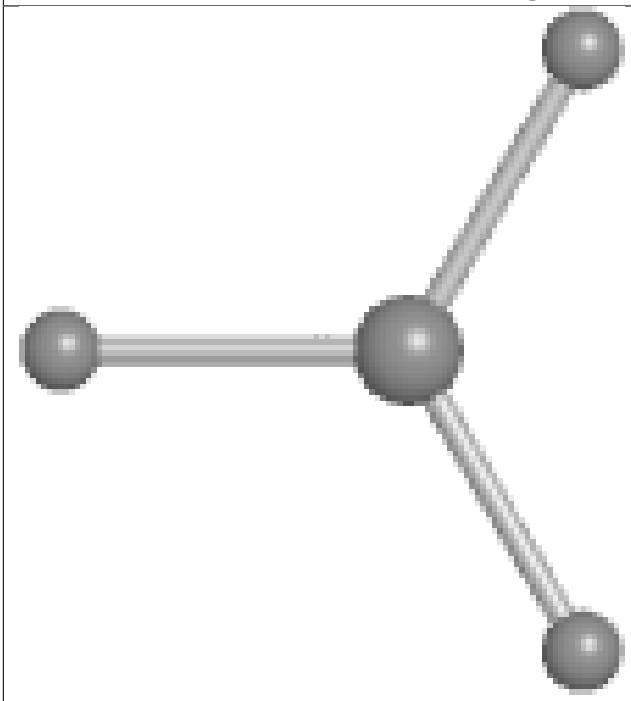


Rings

Ligand AF3 M 603



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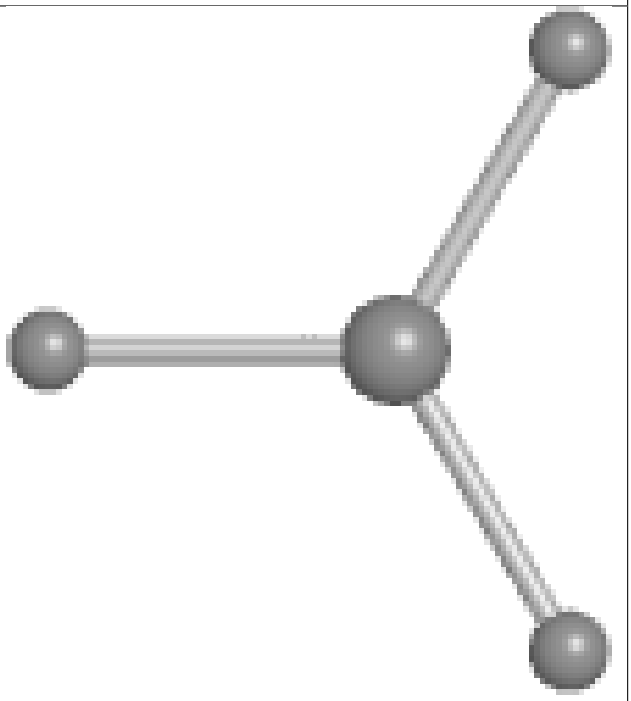

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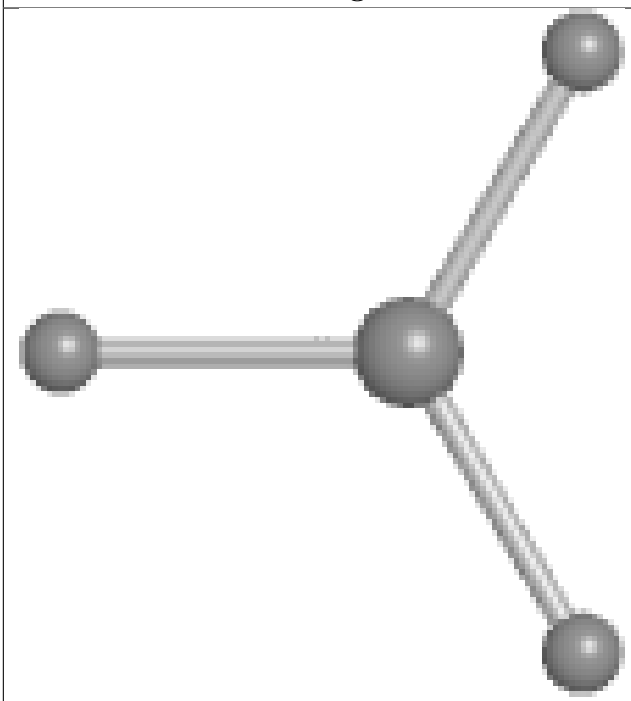

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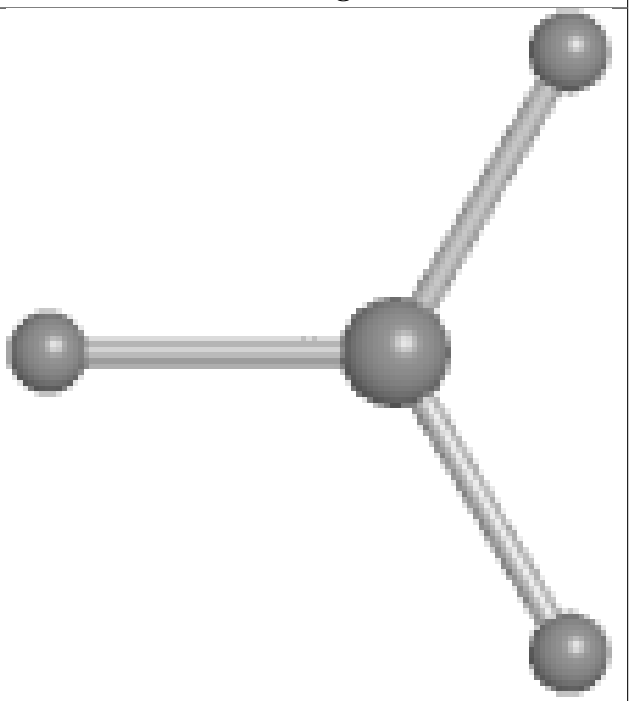
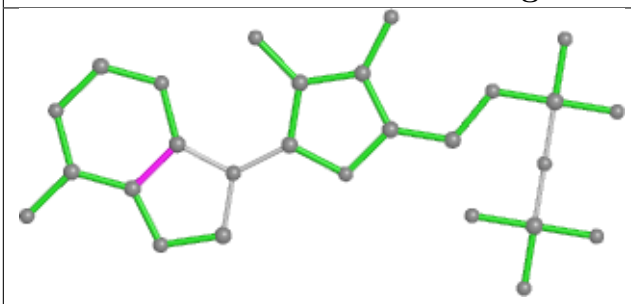


Rings

Ligand ADP A 601



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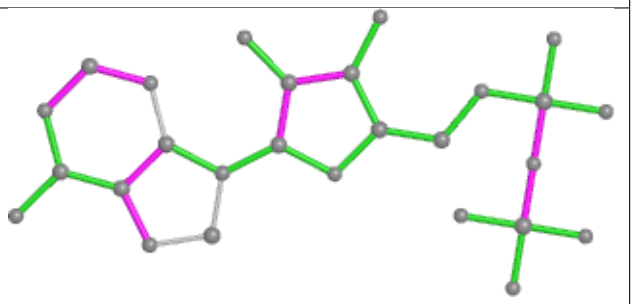

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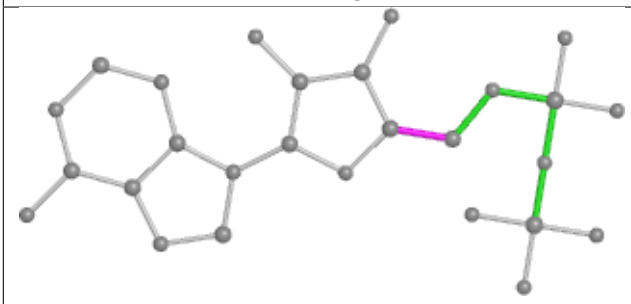

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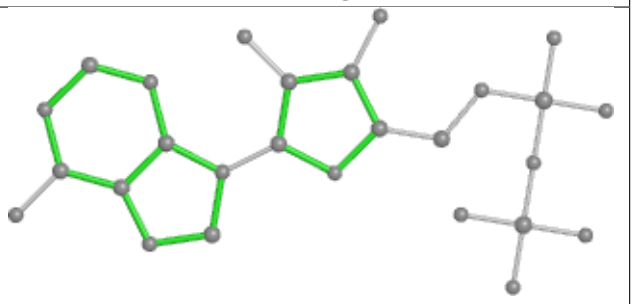
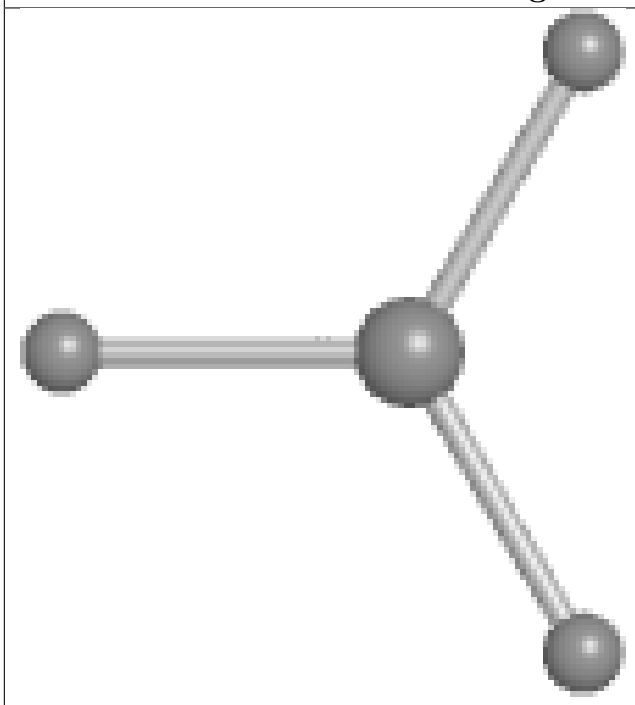


Rings

Ligand AF3 B 603



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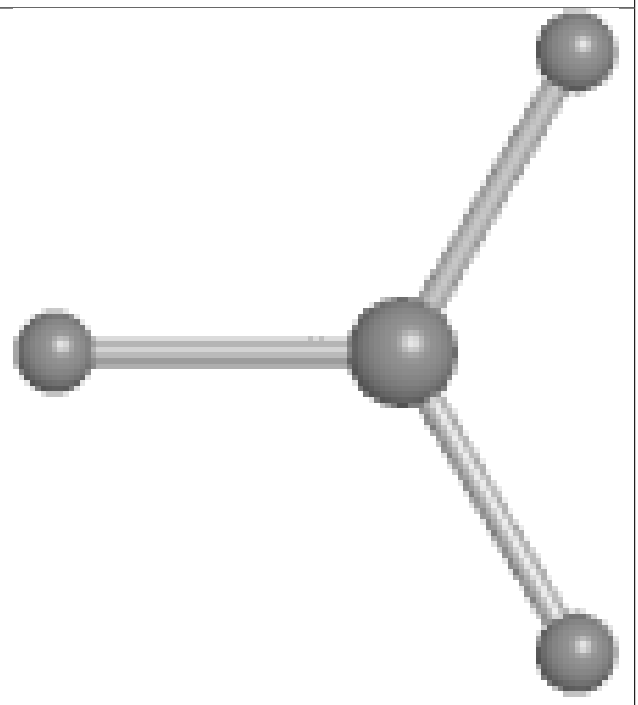

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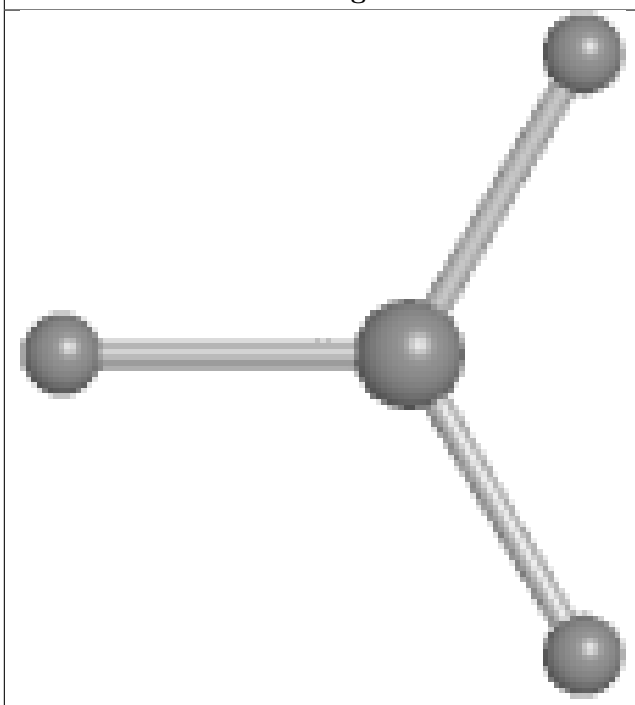

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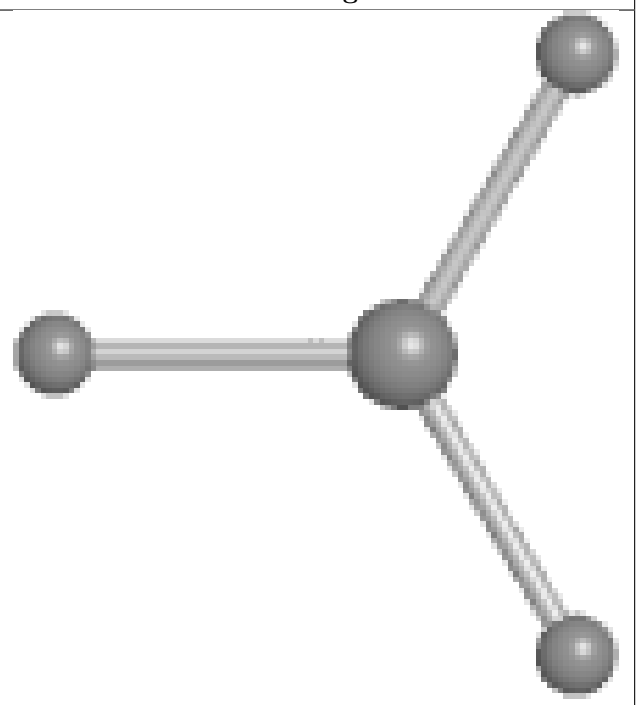
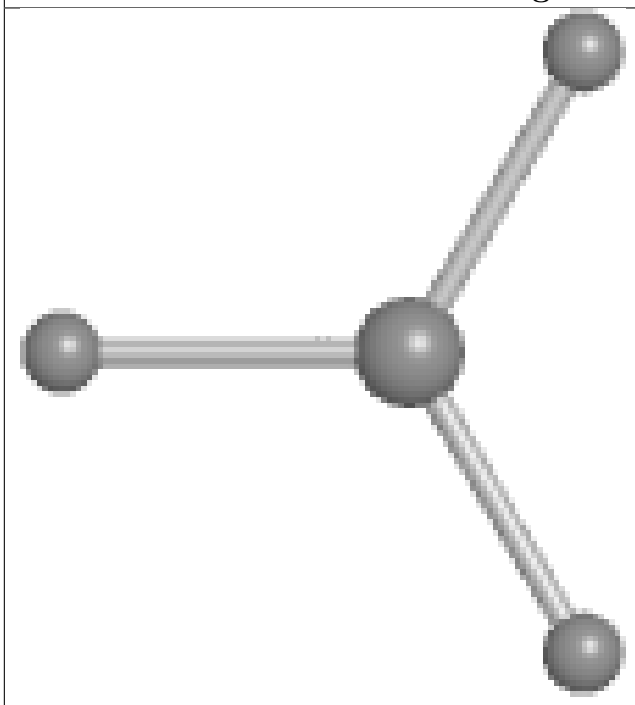


Rings

Ligand AF3 J 603



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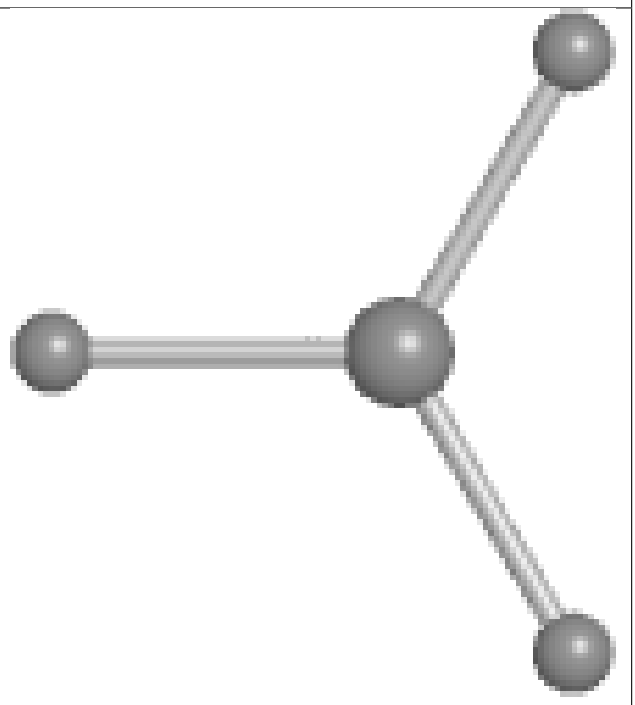

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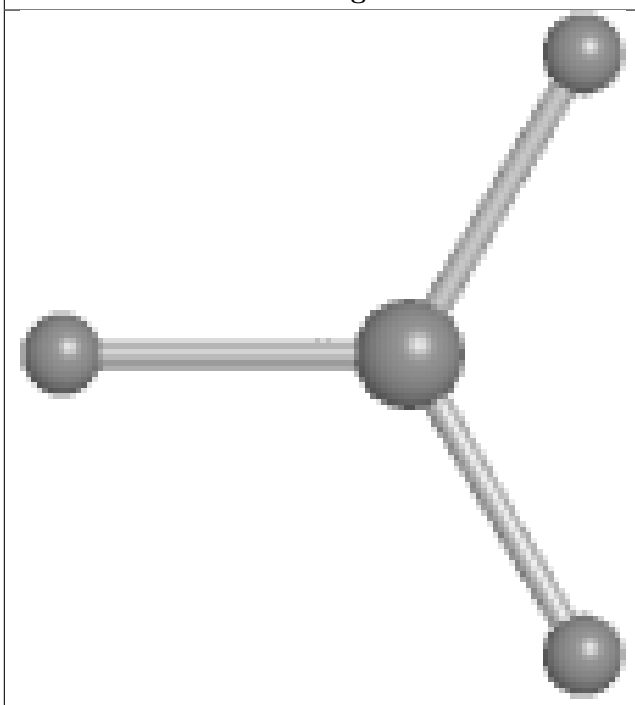

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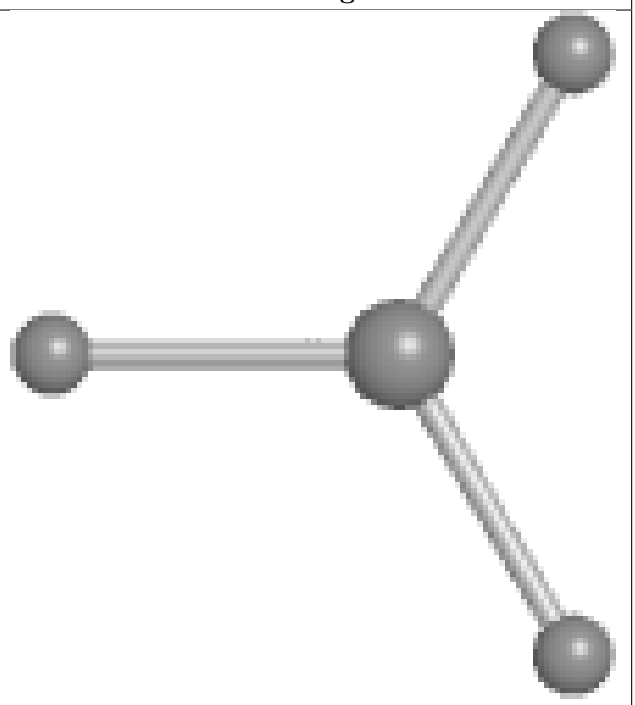
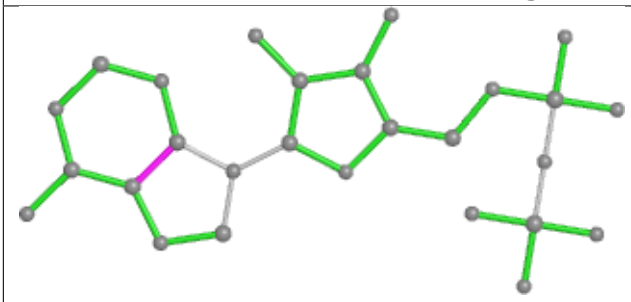
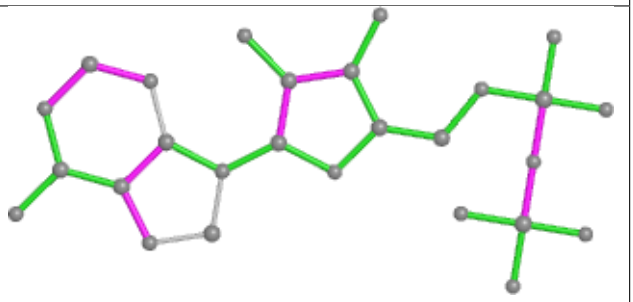
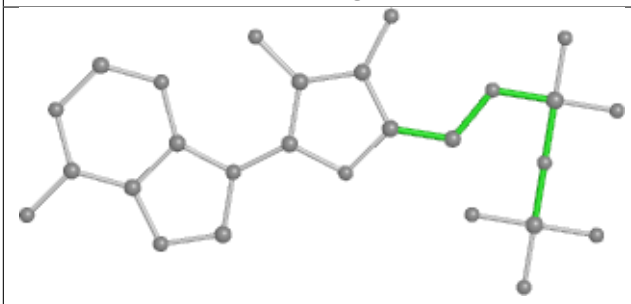
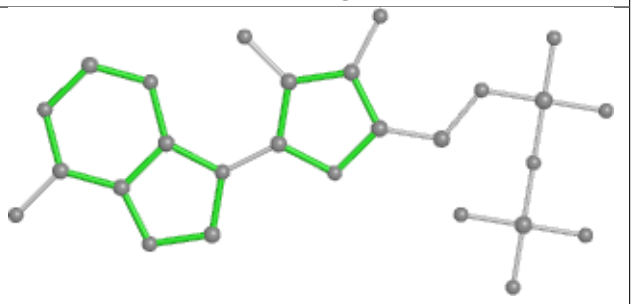
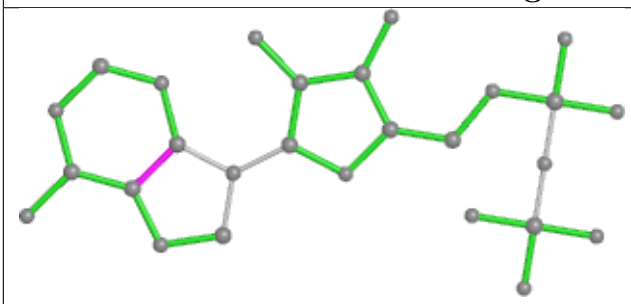
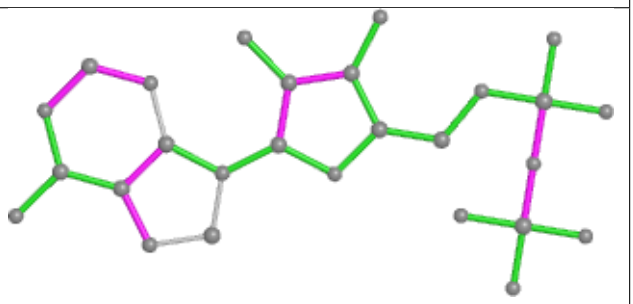
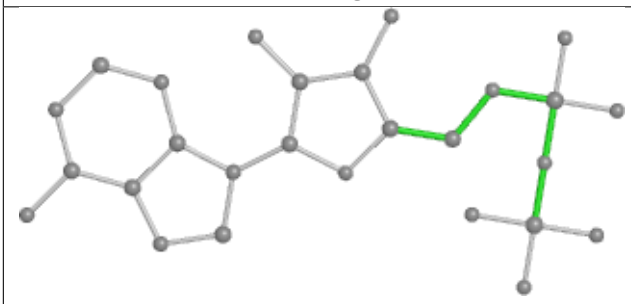
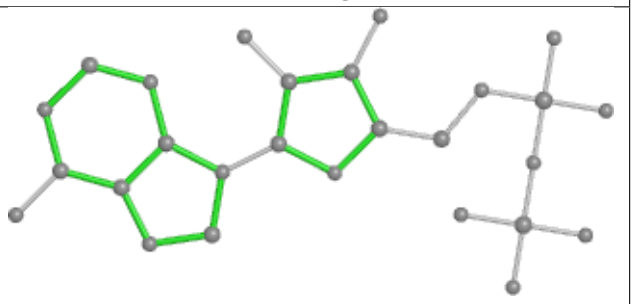
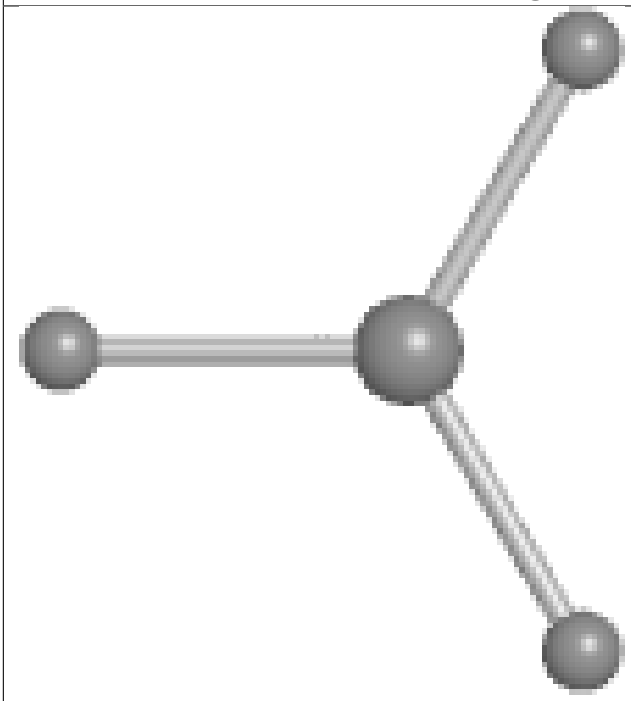


Rings

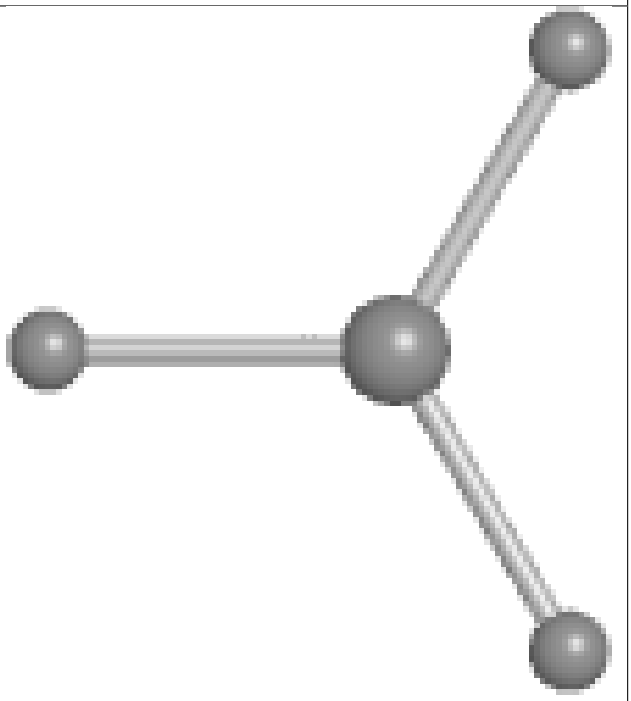
Ligand ADP B 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP L 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

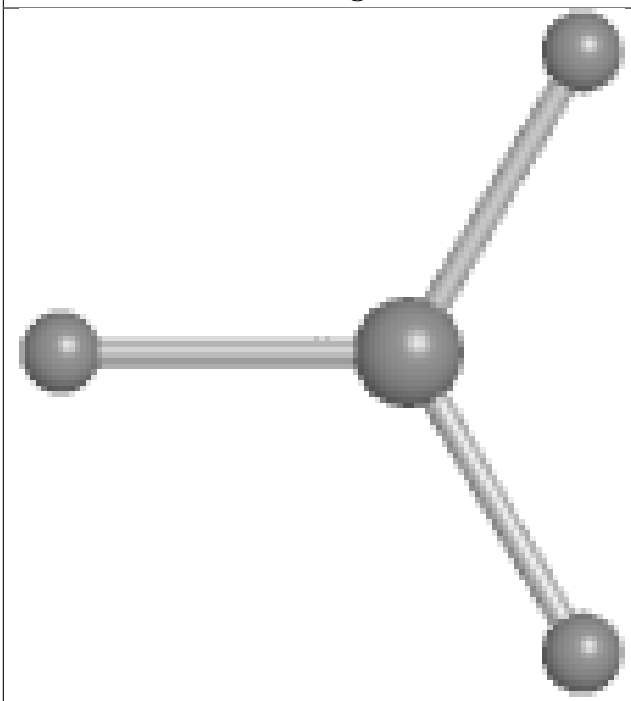
Ligand AF3 N 603



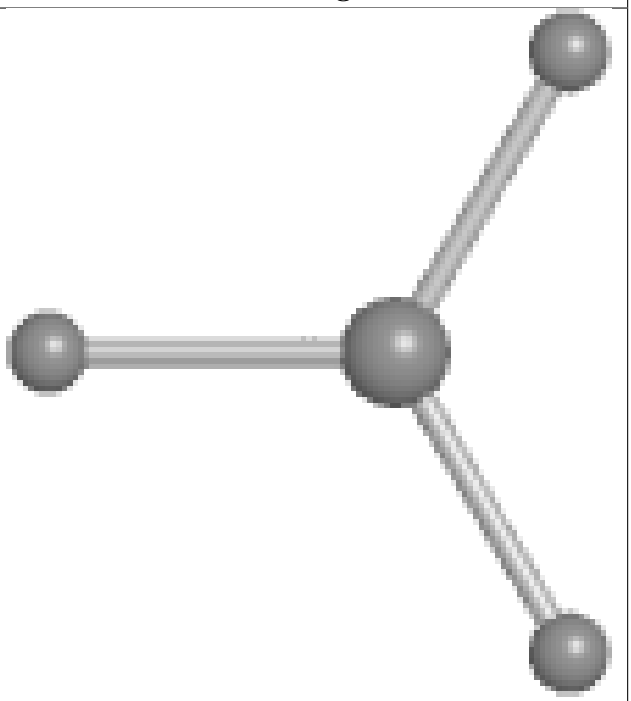
Bond lengths



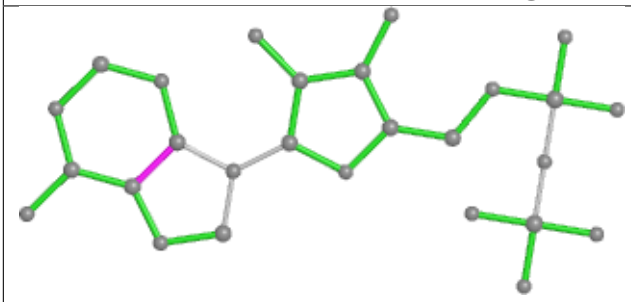
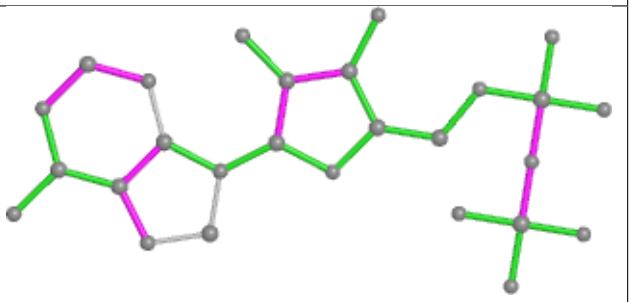
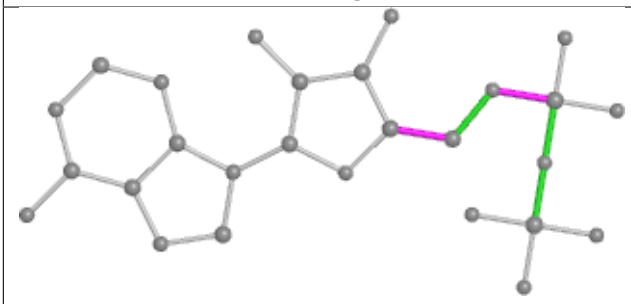
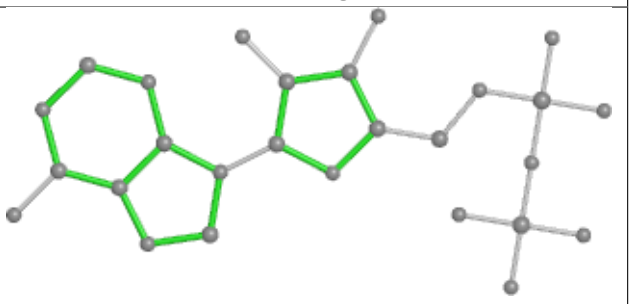
Bond angles

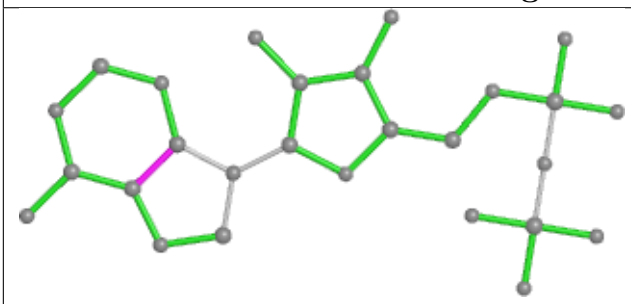
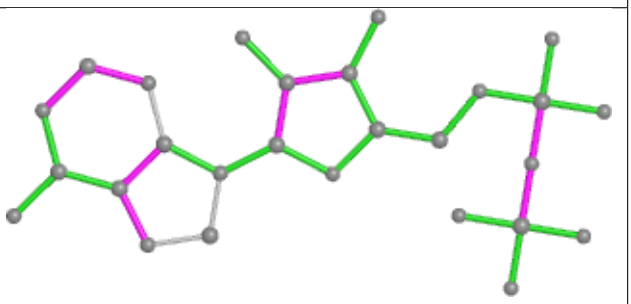
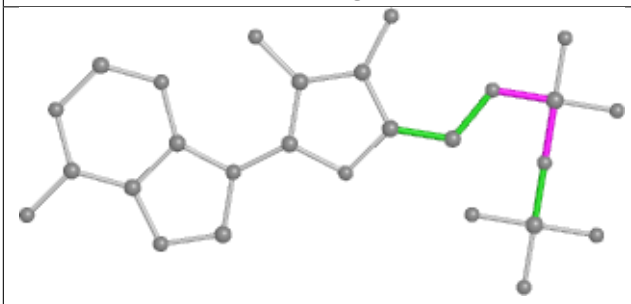
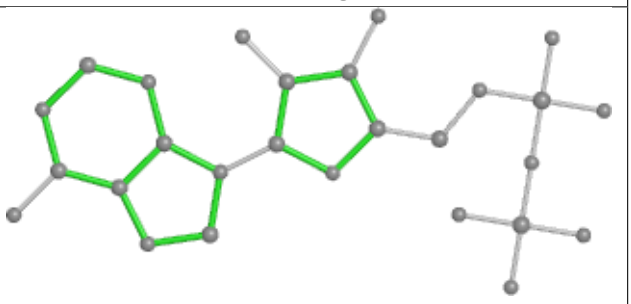


Torsions

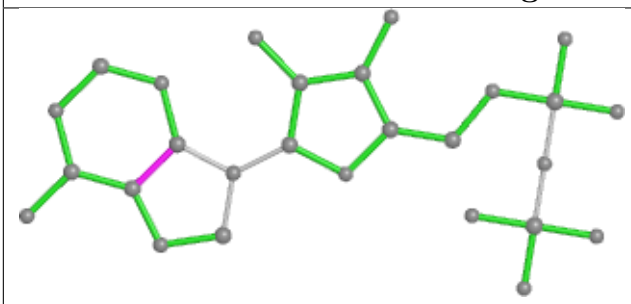


Rings

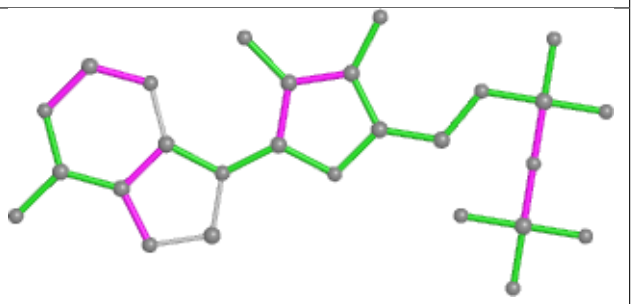
Ligand ADP P 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP D 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

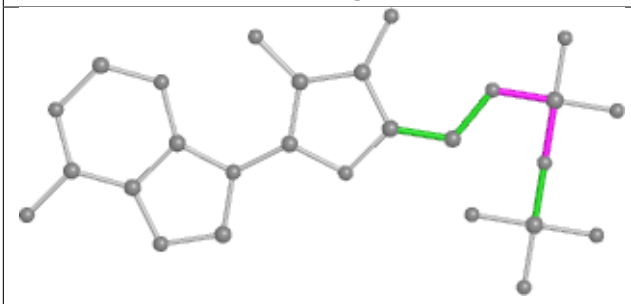
Ligand ADP G 601



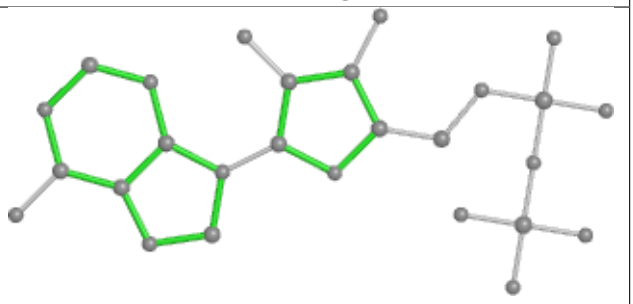
Bond lengths



Bond angles

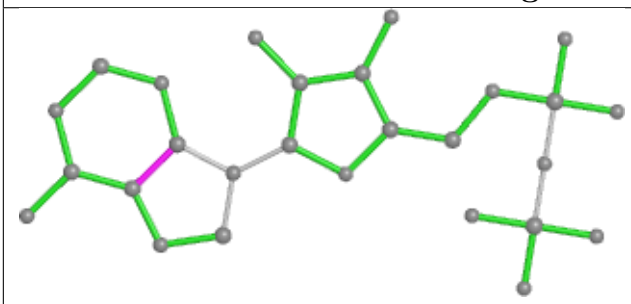


Torsions

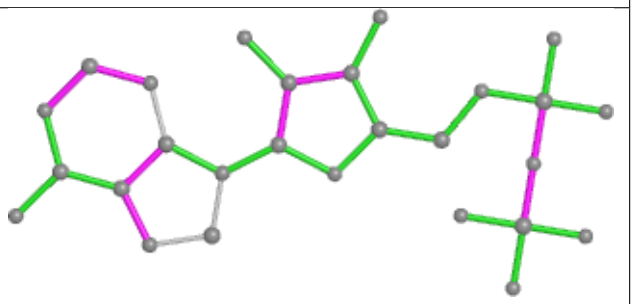


Rings

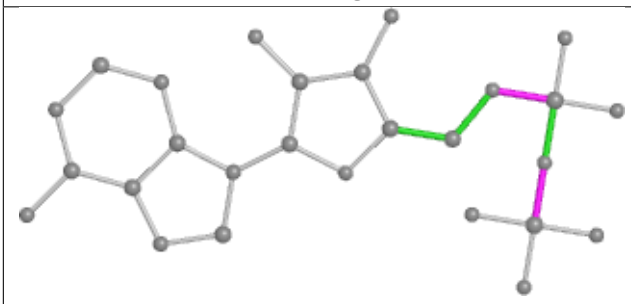
Ligand ADP O 601



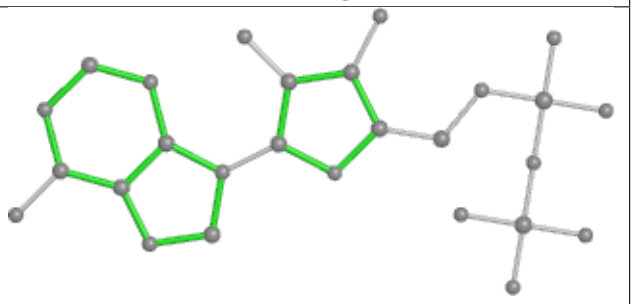
Bond lengths



Bond angles

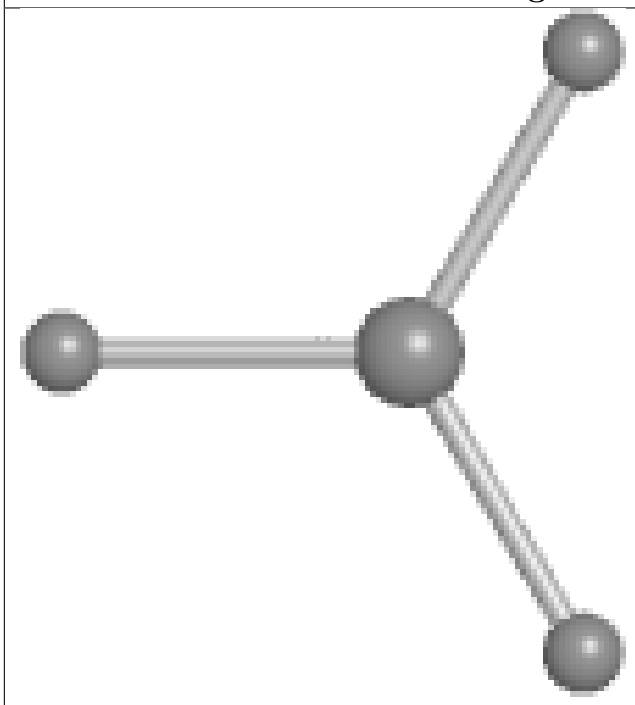


Torsions

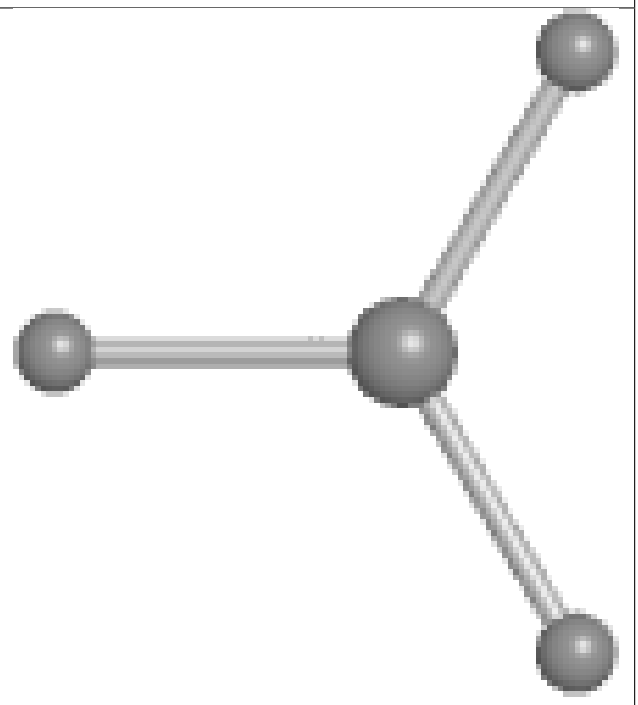


Rings

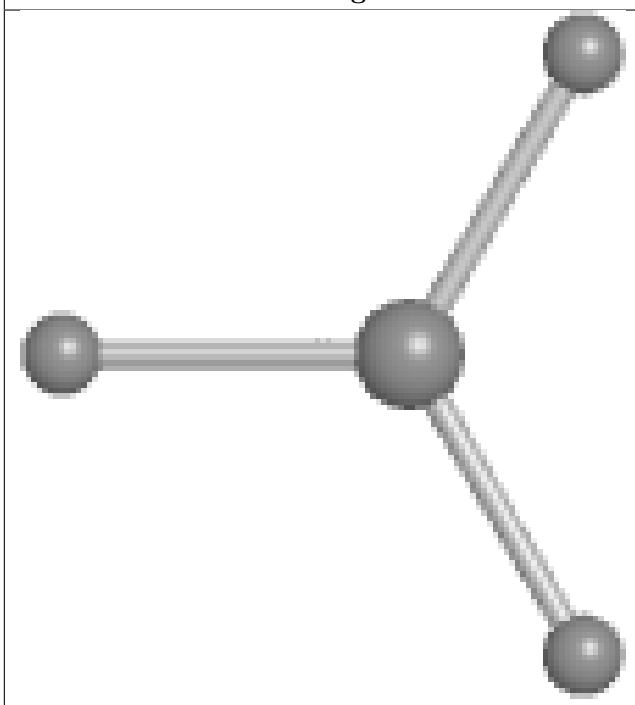
Ligand AF3 D 603



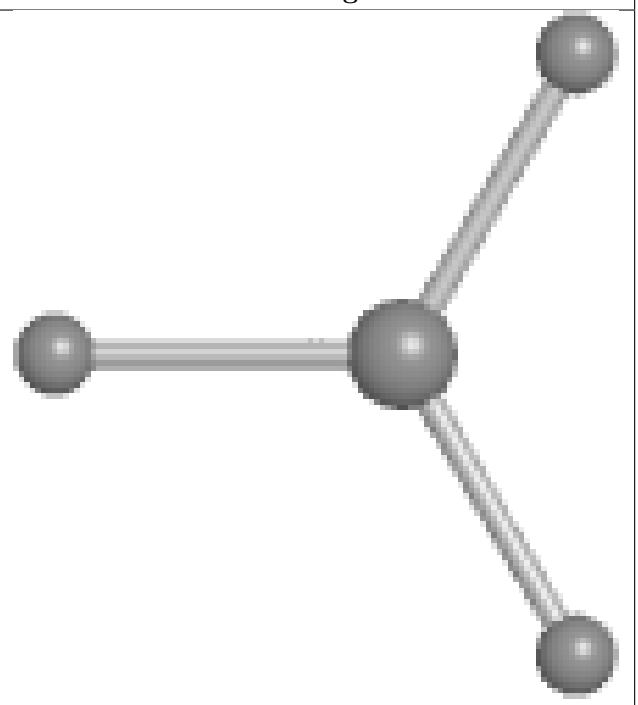
Bond lengths



Bond angles

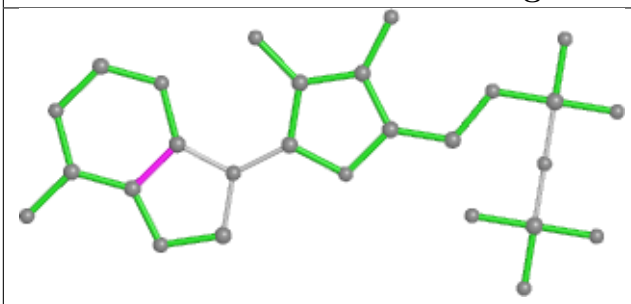


Torsions

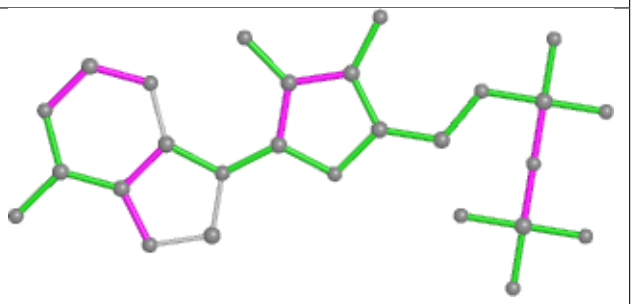


Rings

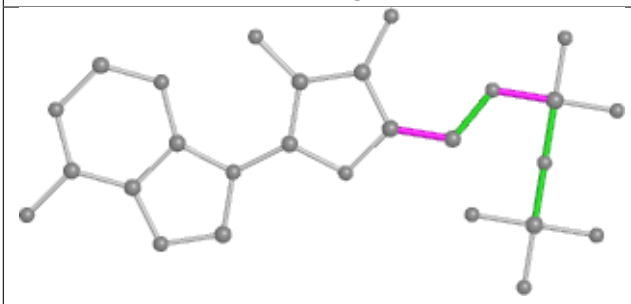
Ligand ADP F 601



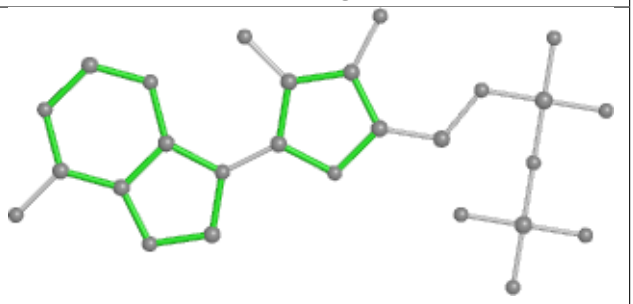
Bond lengths



Bond angles

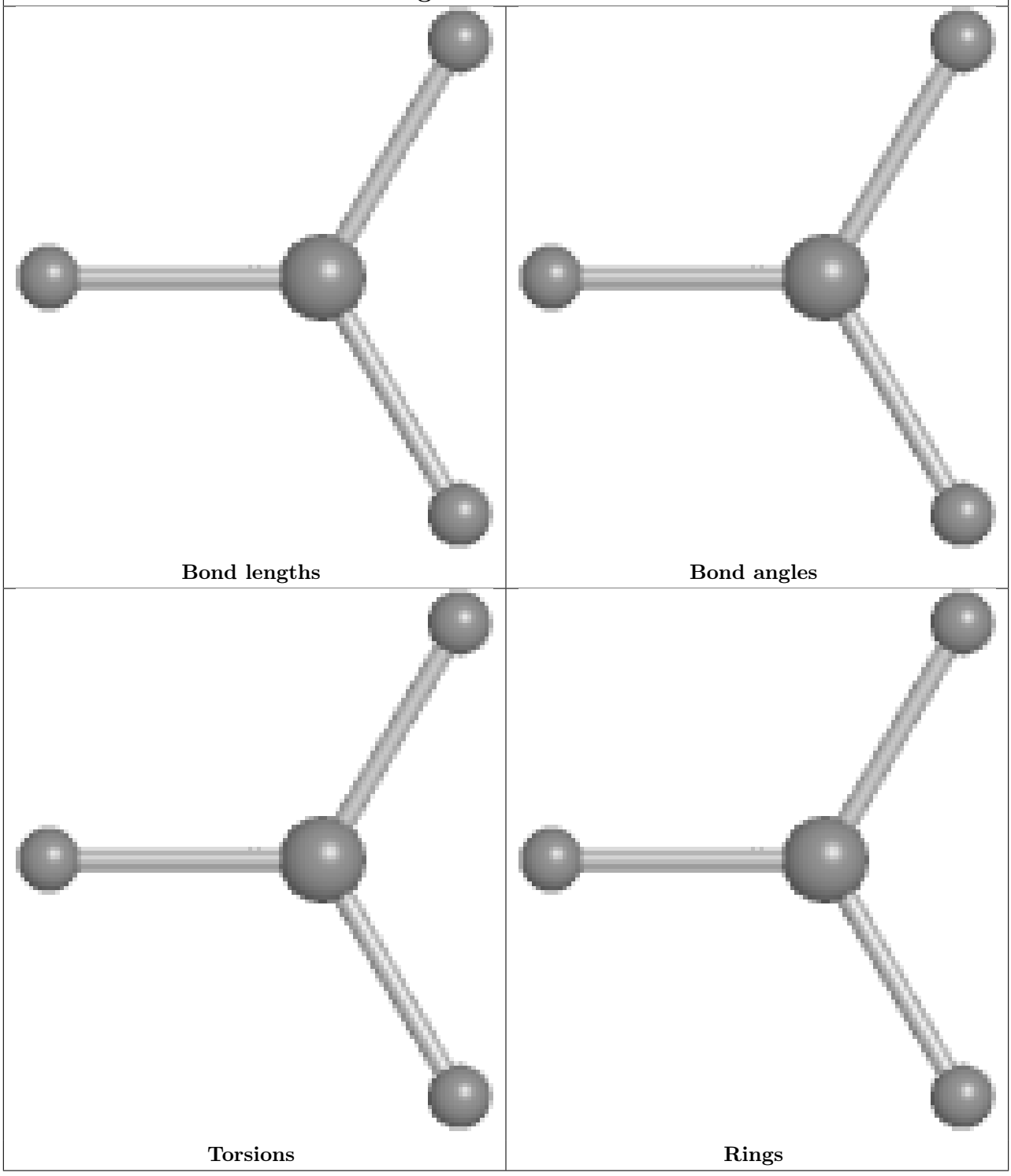


Torsions



Rings

Ligand AF3 E 603



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.

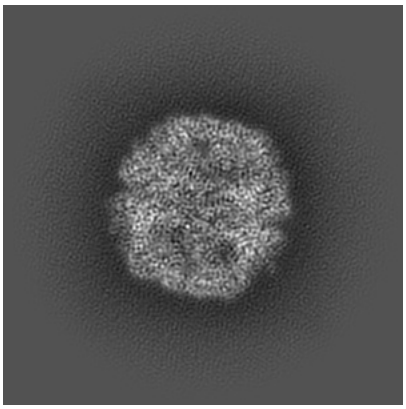
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35122. These allow visual inspection of the internal detail of the map and identification of artifacts.

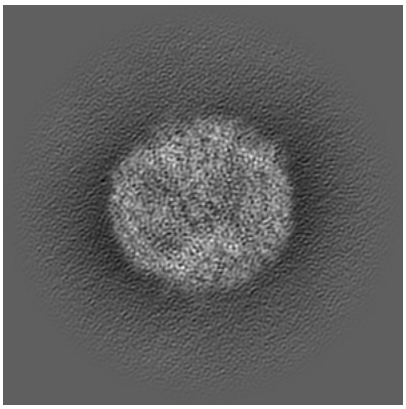
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

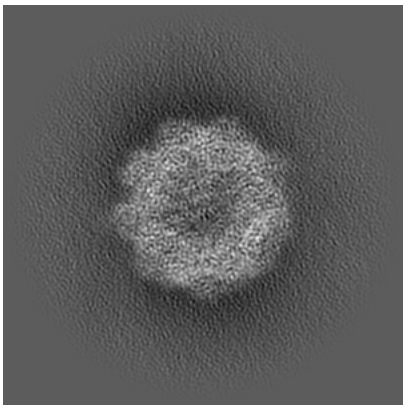
6.1.1 Primary map



X

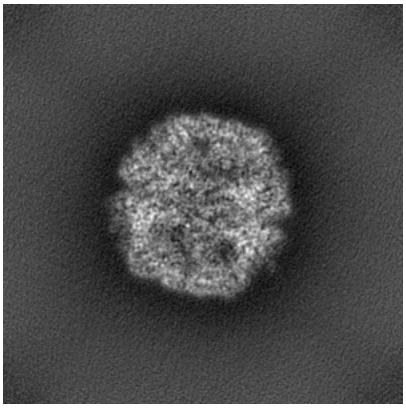


Y

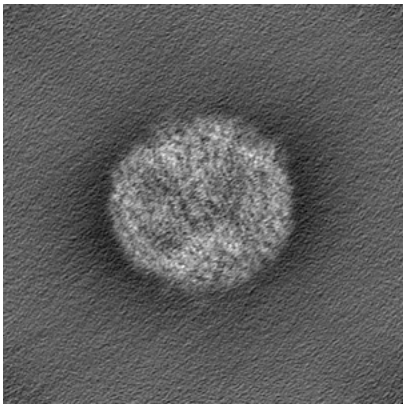


Z

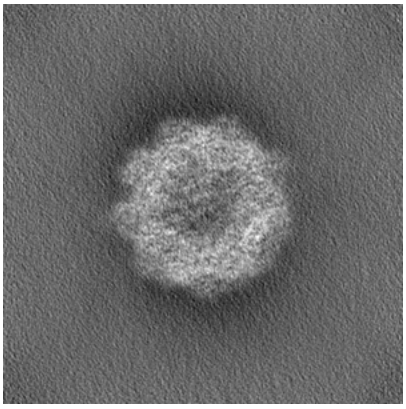
6.1.2 Raw map



X



Y

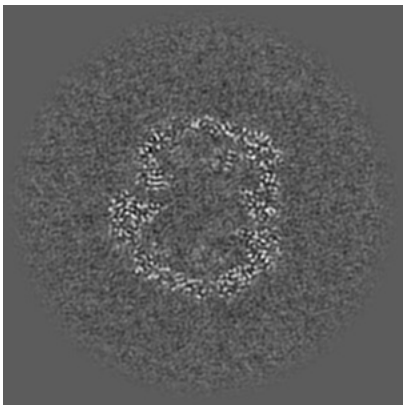


Z

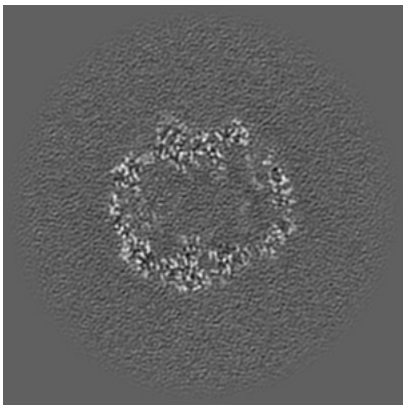
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

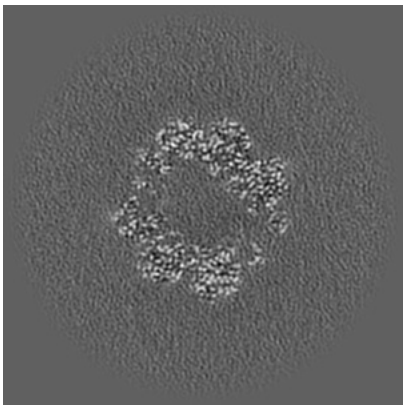
6.2.1 Primary map



X Index: 160

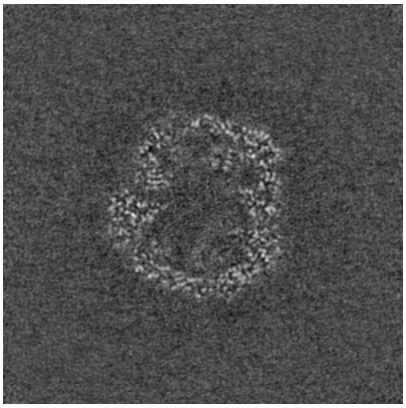


Y Index: 160

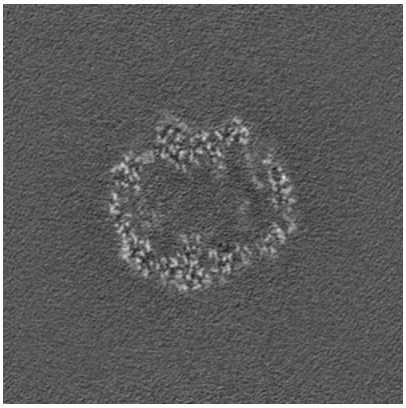


Z Index: 160

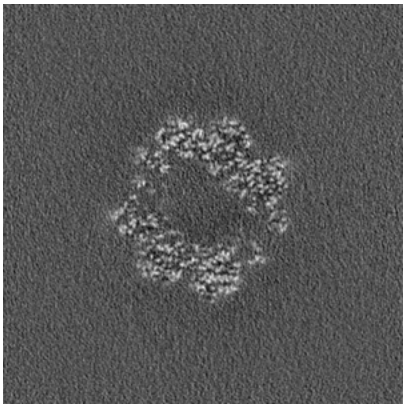
6.2.2 Raw map



X Index: 160



Y Index: 160

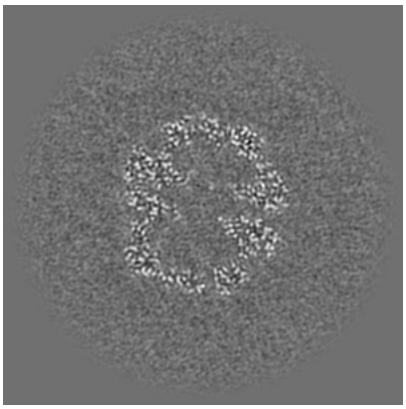


Z Index: 160

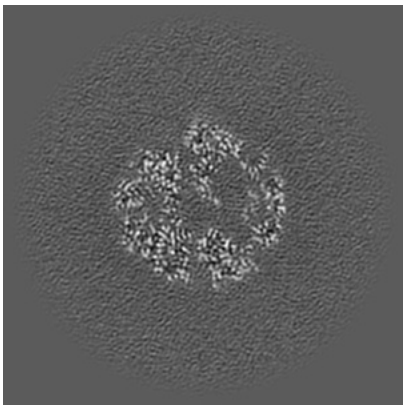
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

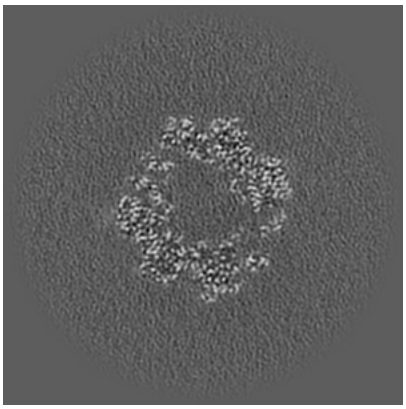
6.3.1 Primary map



X Index: 140

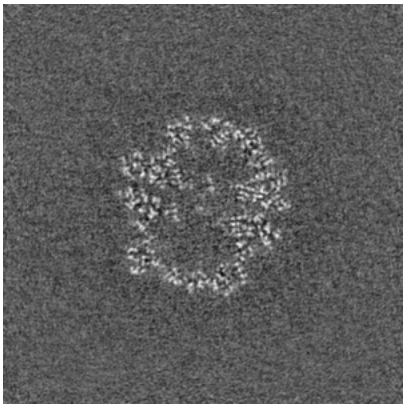


Y Index: 189

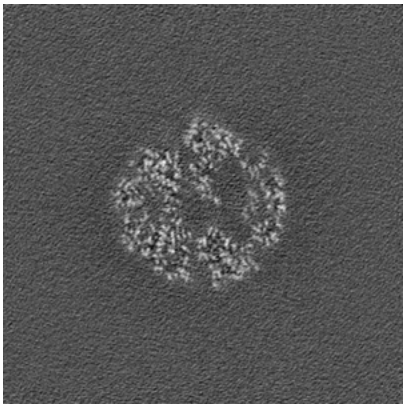


Z Index: 157

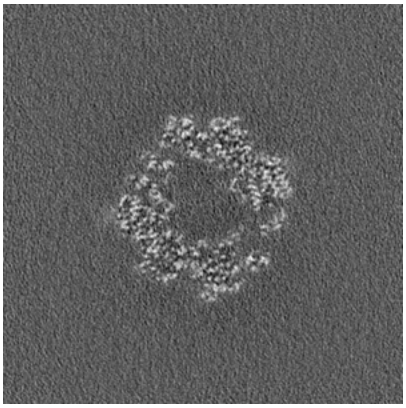
6.3.2 Raw map



X Index: 136



Y Index: 189

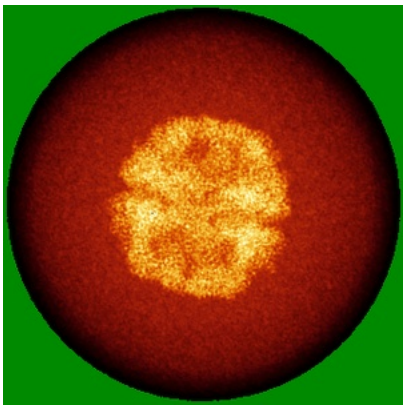


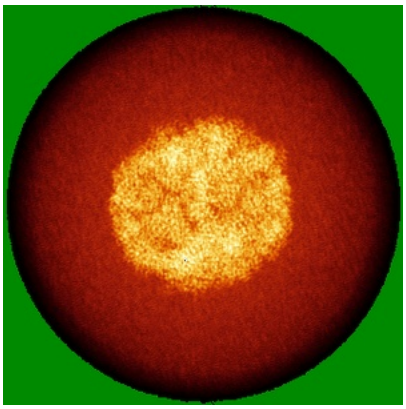
Z Index: 157

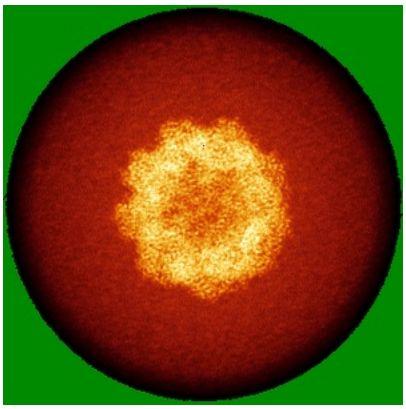
The images above show the largest variance slices of the map in three orthogonal directions.

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

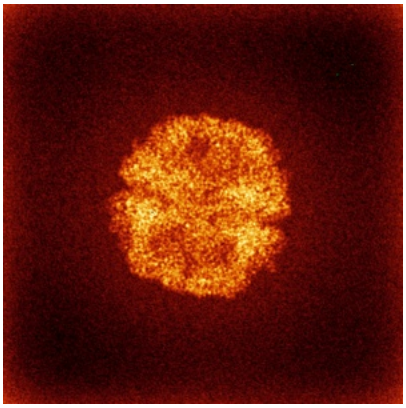
6.4.1 Primary map

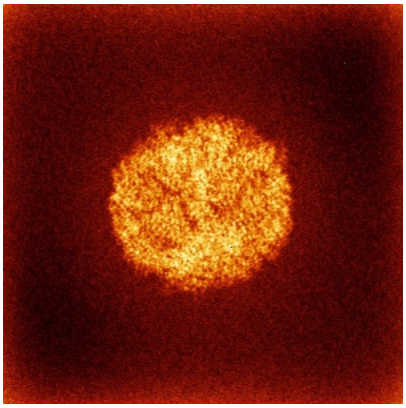

X

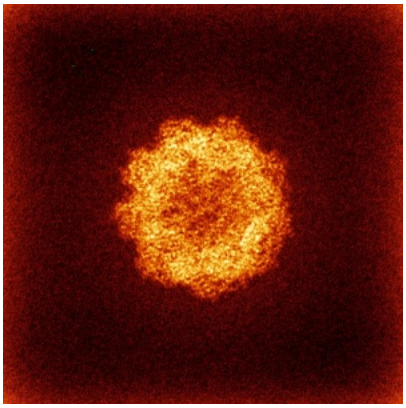

Y


Z

6.4.2 Raw map


X

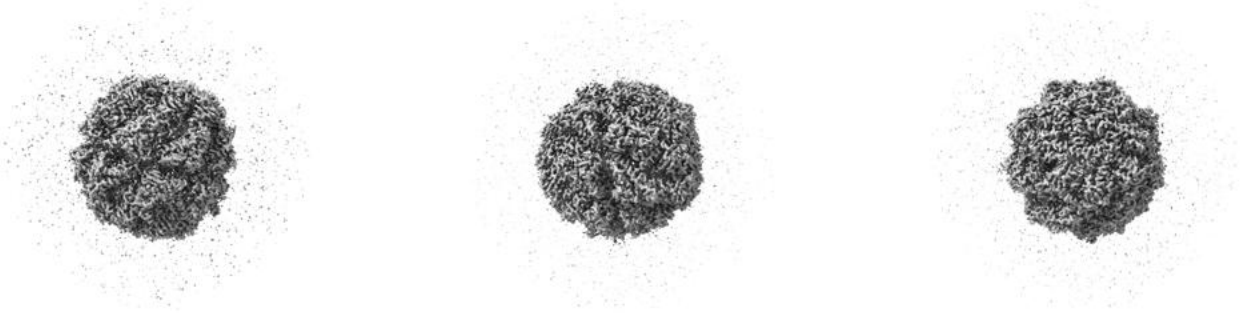

Y


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)

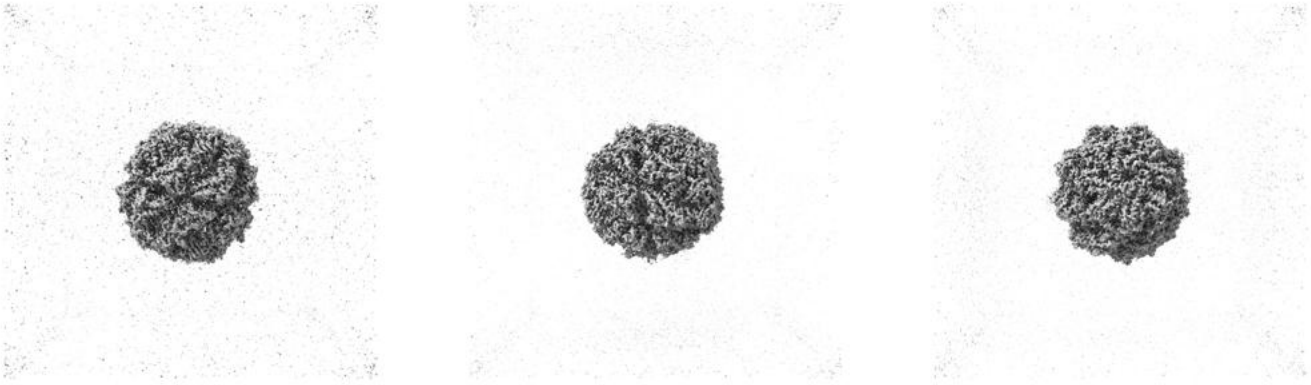
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.23. 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.

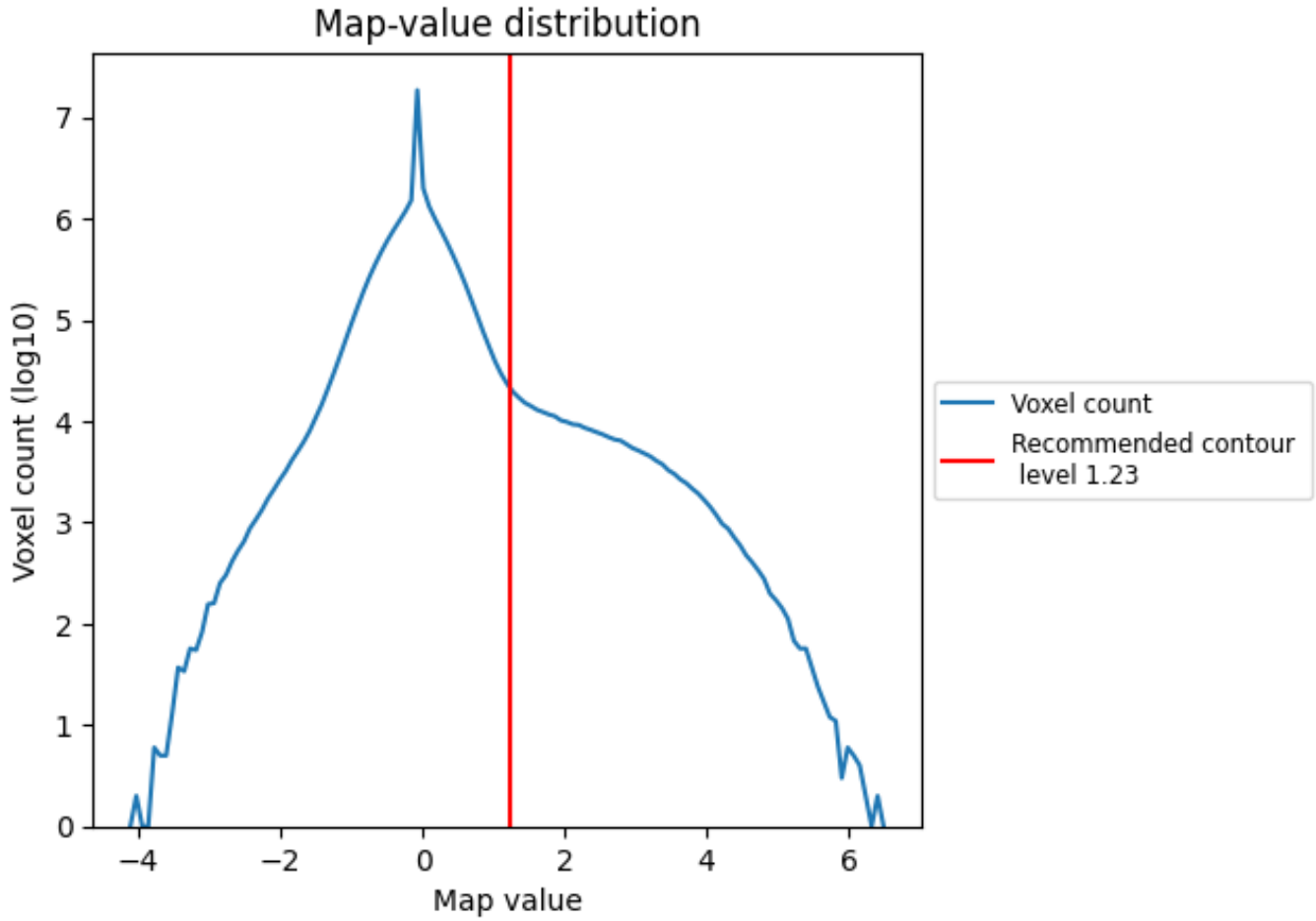
6.6 Mask visualisation (i)

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

7 Map analysis

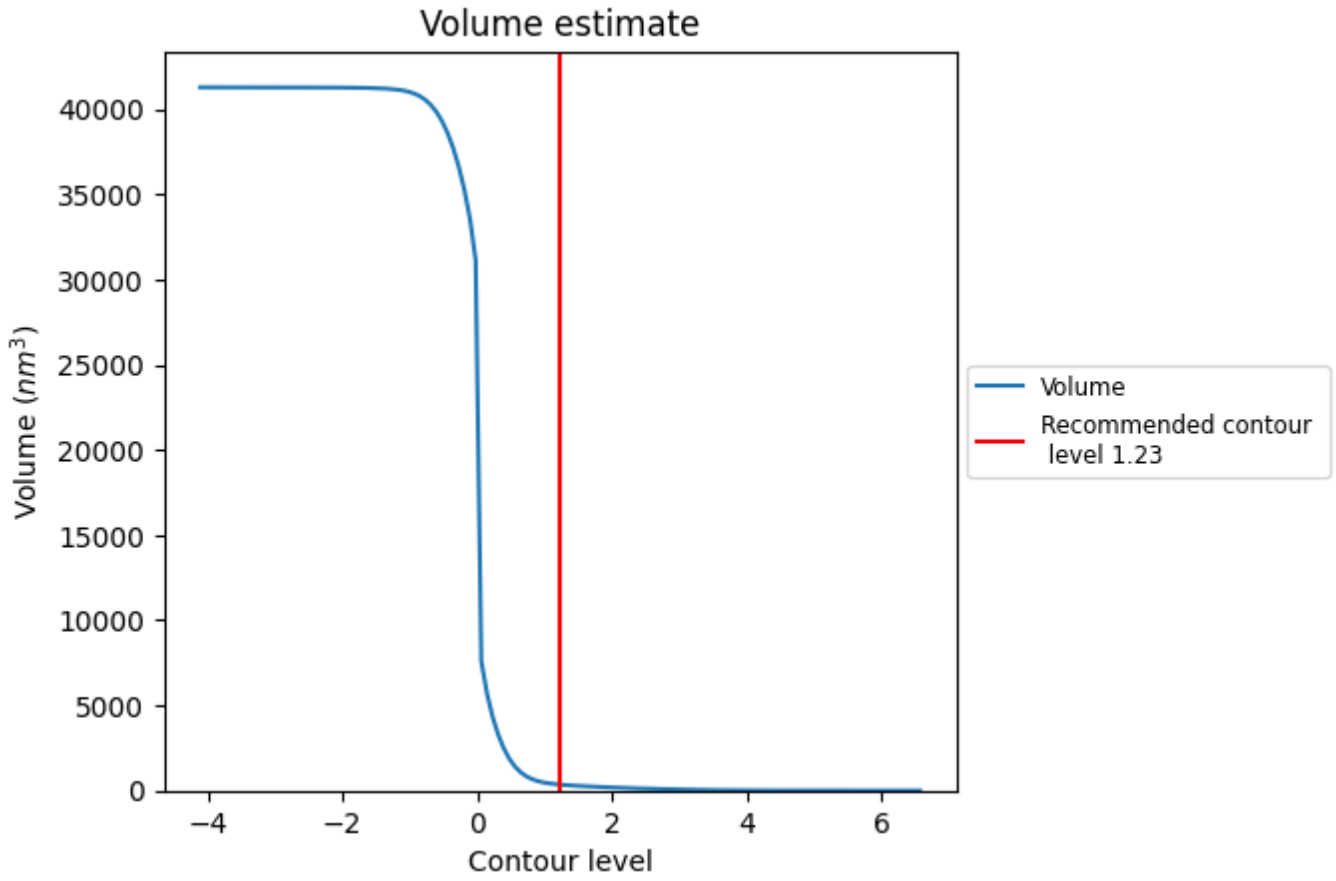
This section contains the results of statistical analysis of the map.

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.

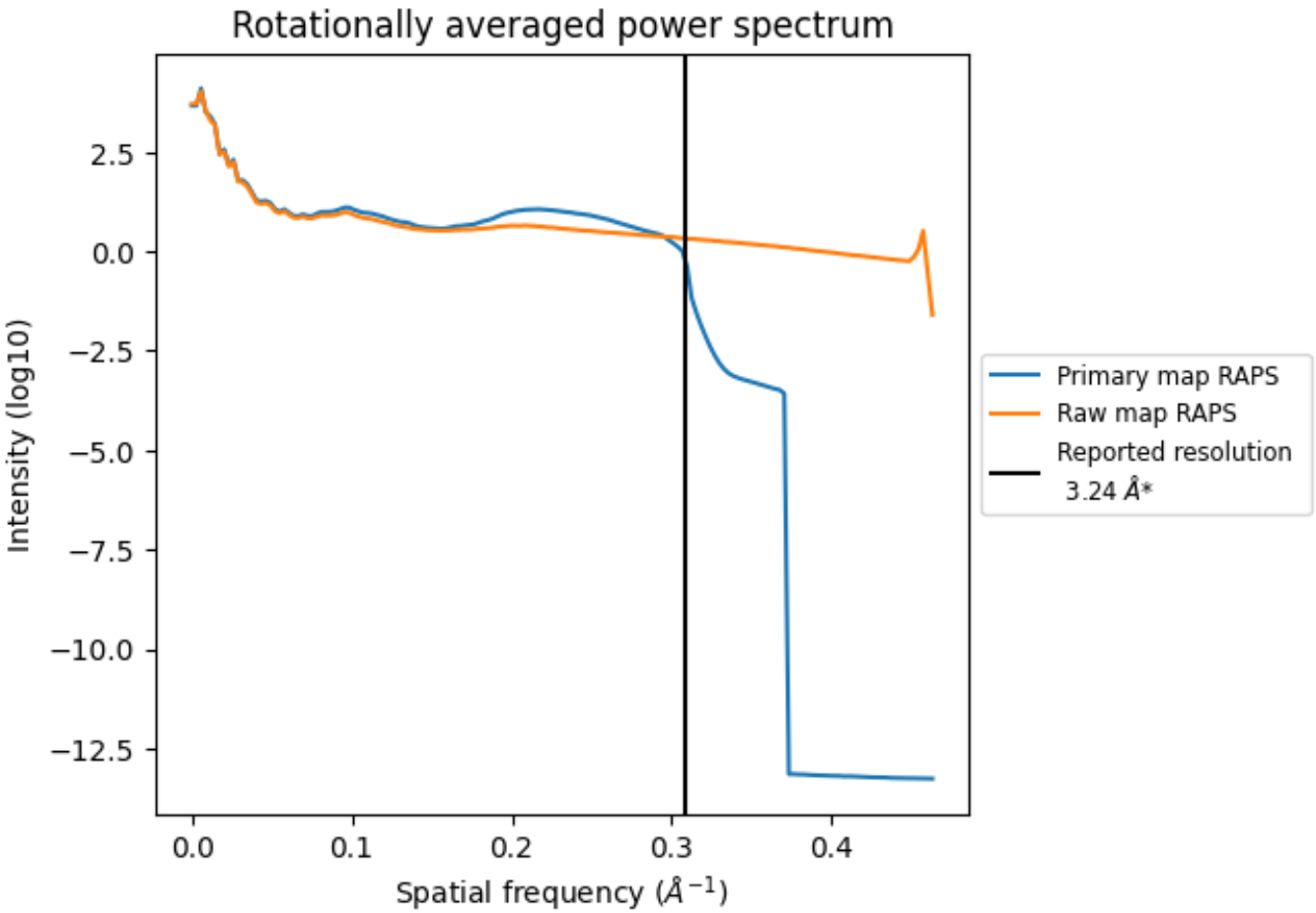
7.2 Volume estimate



The volume at the recommended contour level is 348 nm^3; this corresponds to an approximate mass of 314 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)

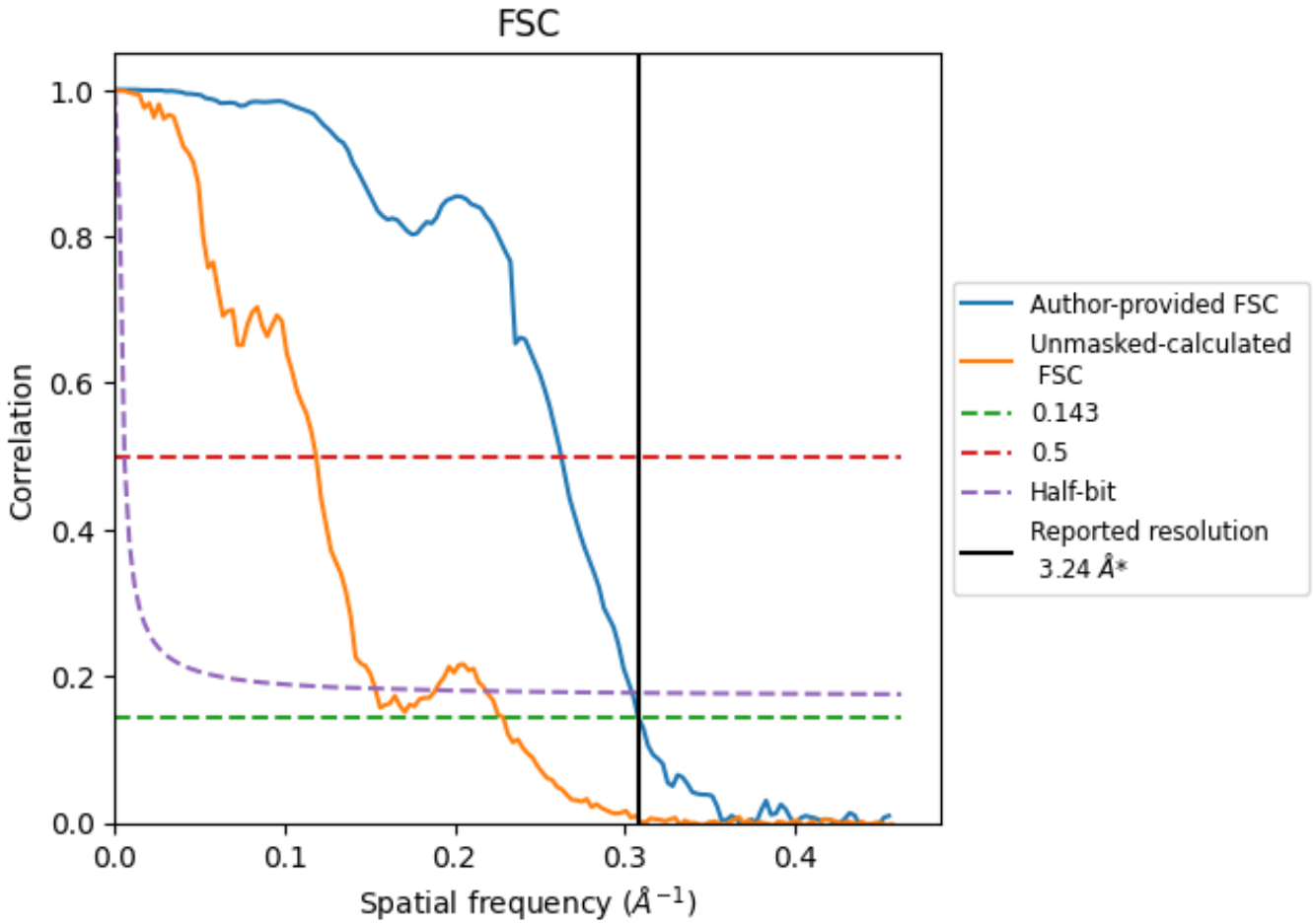


*Reported resolution corresponds to spatial frequency of 0.309 Å^{-1}

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 0.309 Å^{-1}

8.2 Resolution estimates (i)

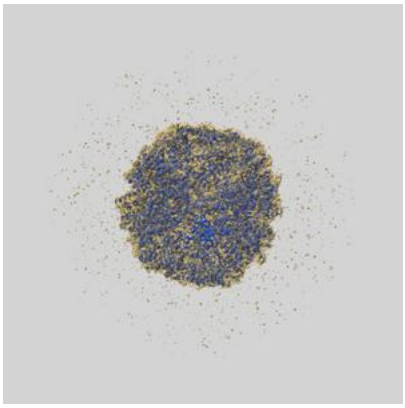
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	3.24	3.81	3.28
Unmasked-calculated*	4.37	8.43	6.52

*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 4.37 differs from the reported value 3.24 by more than 10 %

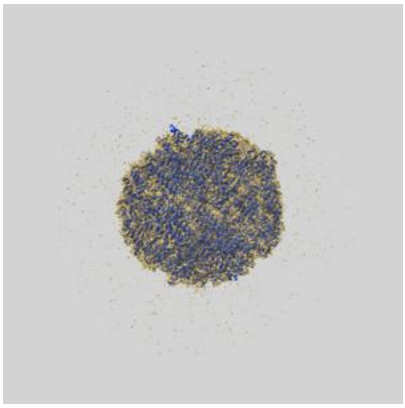
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35122 and PDB model 8I1U. Per-residue inclusion information can be found in section 3 on page 10.

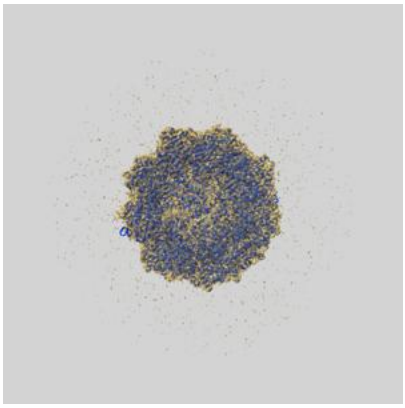
9.1 Map-model overlay



X



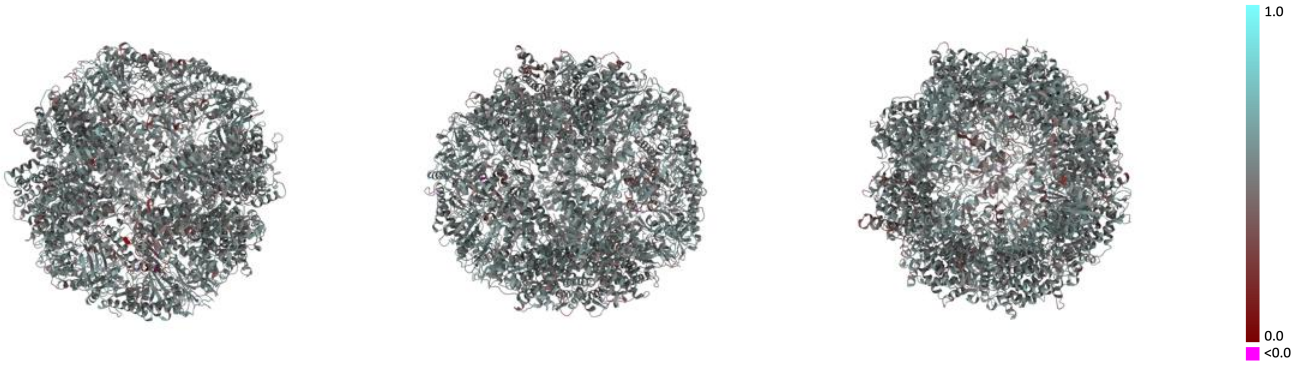
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.23 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.

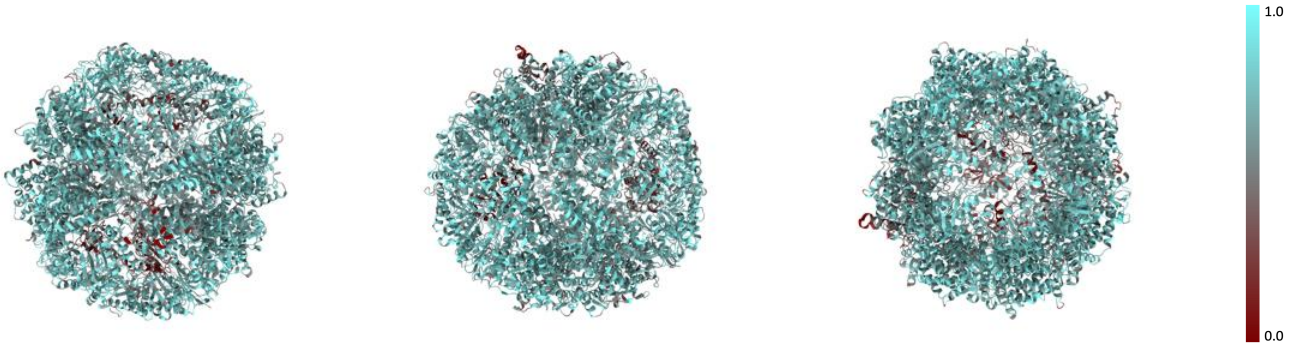
9.2 Q-score mapped to coordinate model (i)



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.

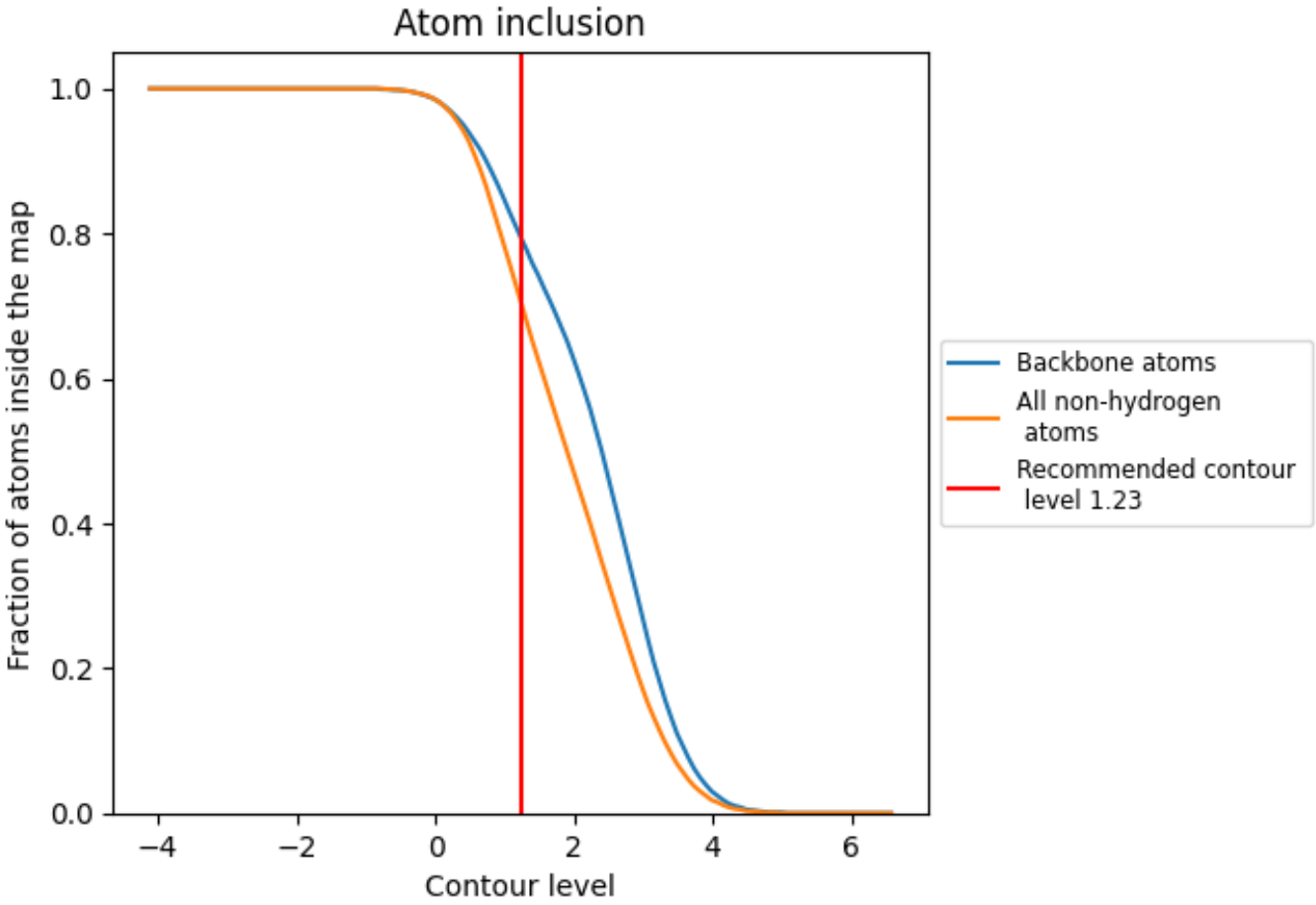
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.23).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 71% 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 (1.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7070	0.5060
A	0.6750	0.4990
B	0.7600	0.5190
C	0.7510	0.5170
D	0.7300	0.5130
E	0.7500	0.5150
F	0.7340	0.5160
G	0.7350	0.5150
H	0.7240	0.5180
I	0.6610	0.4910
J	0.7480	0.5190
K	0.7490	0.5130
L	0.7230	0.5150
M	0.7460	0.5150
N	0.7240	0.5050
O	0.7380	0.5170
P	0.7350	0.5140
Q	0.1210	0.3430
R	0.3170	0.3830