Full wwPDB EM Validation Report ⓘ

May 30, 2022 – 07:58 pm BST

PDB ID	:	7PT7
EMDB ID	:	EMD-13620
Title	:	Structure of MCM2-7 DH complexed with Cdc7-Dbf4 in the presence of ADP:BeF3, state I
Authors	:	Saleh, A.; Noguchi, Y.; Aramayo, R.; Ivanova, M.E.; Speck, C.
Deposited on	:	2021-09-26
Resolution	:	3.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

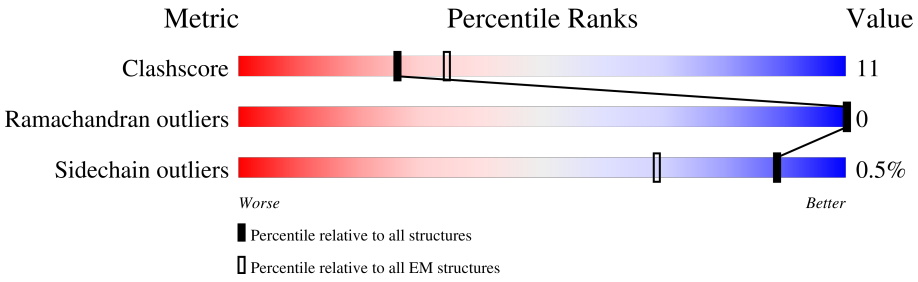
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 3.80 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	1	4	100% 100%
2	2	868	7% 52% 20% 28%
2	B	868	8% 51% 21% 28%
3	3	971	50% 15% 35%
3	C	971	52% 13% 35%
4	4	933	53% 18% 28%
4	D	933	53% 18% 28%
5	5	775	61% 20% 19%

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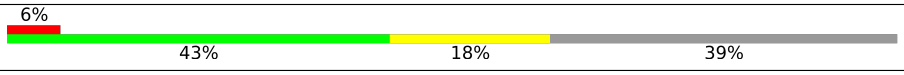
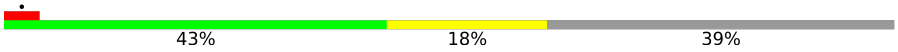
Mol	Chain	Length	Quality of chain
5	E	775	
6	6	1017	
6	F	1017	
7	7	845	
7	G	845	
8	8	507	
9	9	704	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 67420 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 Undefined Mcm4 flexible N-terminal tail.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	4	Total	C	N	O	0	0
			20	12	4	4		

- Molecule 2 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	626	Total	C	N	O	S	0	0
			4960	3124	880	937	19		
2	B	626	Total	C	N	O	S	0	0
			4960	3124	880	937	19		

- Molecule 3 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	635	Total	C	N	O	S	0	0
			4986	3152	885	936	13		
3	C	633	Total	C	N	O	S	0	0
			4966	3141	880	932	13		

- Molecule 4 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	668	Total	C	N	O	S	0	0
			5323	3341	920	1033	29		
4	D	668	Total	C	N	O	S	0	0
			5323	3341	920	1033	29		

- Molecule 5 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	628	Total	C	N	O	S	0	0
			4927	3098	844	962	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	628	Total	C	N	O	S	0	0
			4927	3098	844	962	23		

- Molecule 6 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	617	Total	C	N	O	S	0	0
			4889	3083	850	931	25		
6	F	617	Total	C	N	O	S	0	0
			4889	3083	850	931	25		

- Molecule 7 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	683	Total	C	N	O	S	0	0
			5370	3382	924	1034	30		
7	G	683	Total	C	N	O	S	0	0
			5370	3382	924	1034	30		

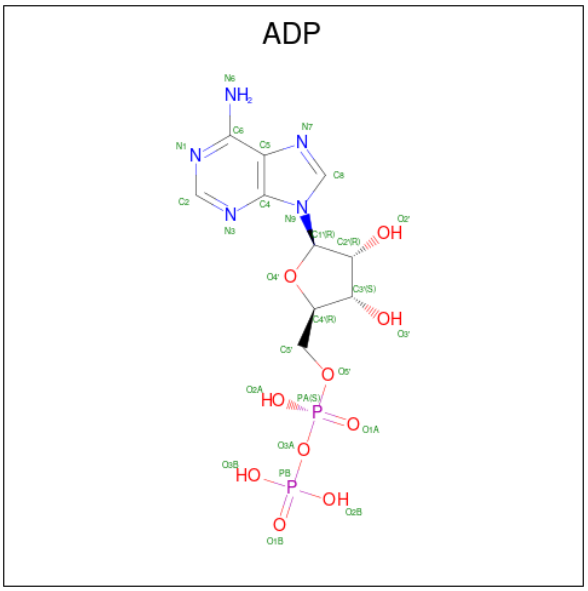
- Molecule 8 is a protein called Cell division control protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	402	Total	C	N	O	S	0	0
			3292	2126	551	599	16		

- Molecule 9 is a protein called DDK kinase regulatory subunit DBF4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	337	Total	C	N	O	S	0	0
			2813	1793	494	514	12		

- 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	2	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	3	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	4	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	5	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	6	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	7	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	8	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	

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Lig-

and of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
11	2	1	Total Mg 1 1	0
11	3	1	Total Mg 1 1	0
11	4	1	Total Mg 1 1	0
11	5	1	Total Mg 1 1	0
11	6	1	Total Mg 1 1	0
11	7	1	Total Mg 1 1	0
11	8	2	Total Mg 2 2	0
11	B	1	Total Mg 1 1	0
11	C	1	Total Mg 1 1	0
11	D	1	Total Mg 1 1	0
11	E	1	Total Mg 1 1	0
11	F	1	Total Mg 1 1	0
11	G	1	Total Mg 1 1	0

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
12	2	1	Total Zn 1 1	0
12	4	1	Total Zn 1 1	0
12	5	1	Total Zn 1 1	0
12	6	1	Total Zn 1 1	0
12	7	1	Total Zn 1 1	0

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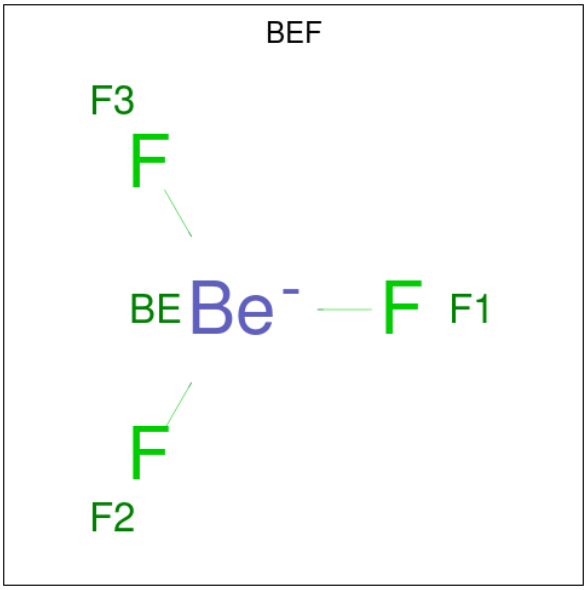
Mol	Chain	Residues	Atoms	AltConf
12	8	1	Total Zn 1 1	0
12	9	1	Total Zn 1 1	0
12	B	1	Total Zn 1 1	0
12	D	1	Total Zn 1 1	0
12	E	1	Total Zn 1 1	0
12	F	1	Total Zn 1 1	0
12	G	1	Total Zn 1 1	0

- Molecule 13 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
13	3	1	Total Be F 8 2 6	0
13	3	1	Total Be F 8 2 6	0
13	4	1	Total Be F 4 1 3	0
13	8	1	Total Be F 4 1 3	0

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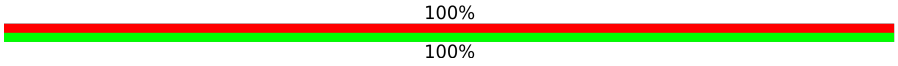
Mol	Chain	Residues	Atoms			AltConf
13	D	1	Total 4	Be 1	F 3	0
13	E	1	Total 4	Be 1	F 3	0
13	G	1	Total 4	Be 1	F 3	0

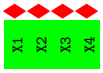
3 Residue-property plots (i)

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: Undefined Mcm4 flexible N-terminal tail

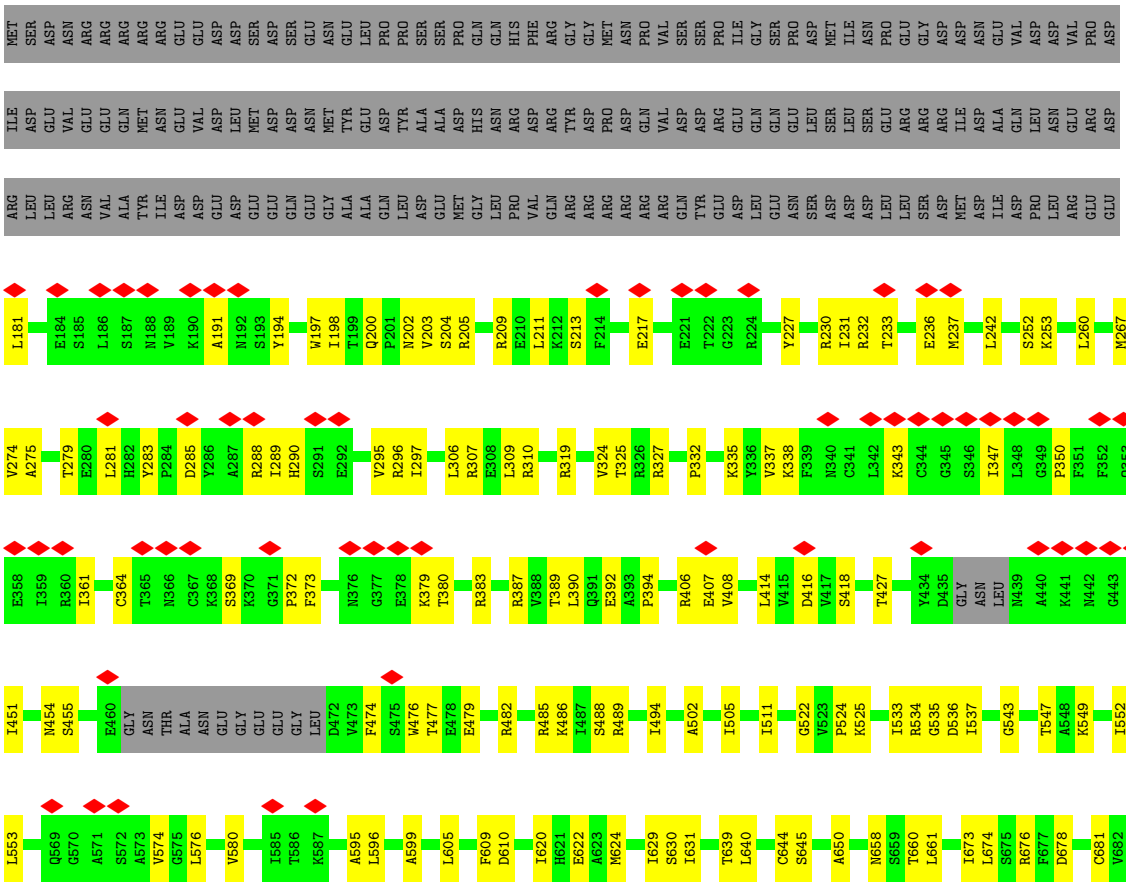
Chain 1:

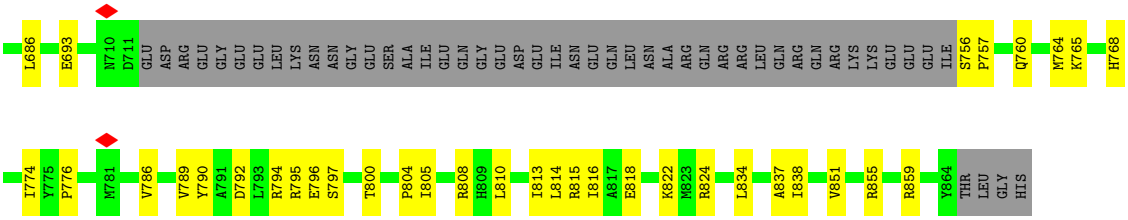




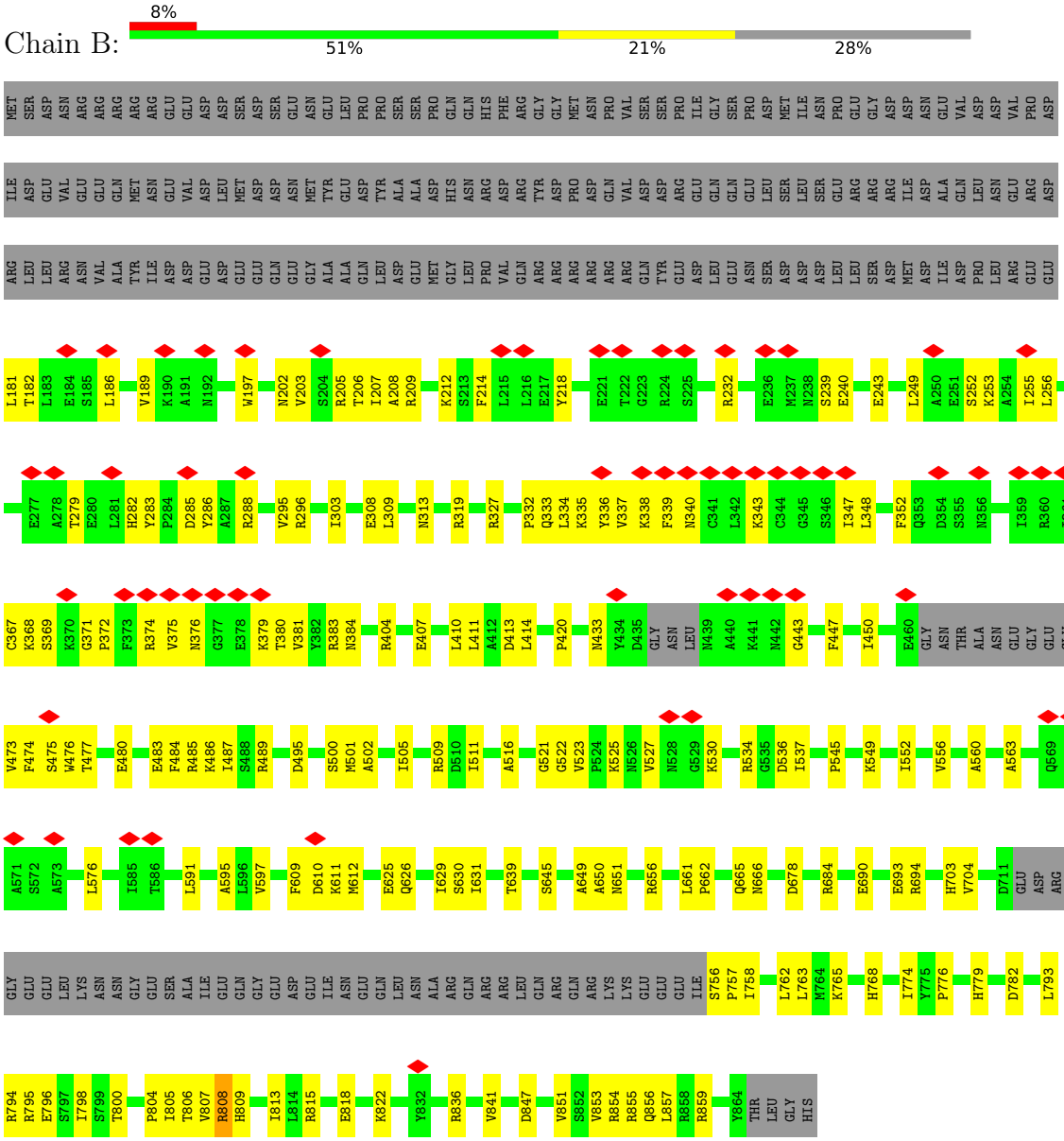
• Molecule 2: DNA replication licensing factor MCM2

Chain 2:

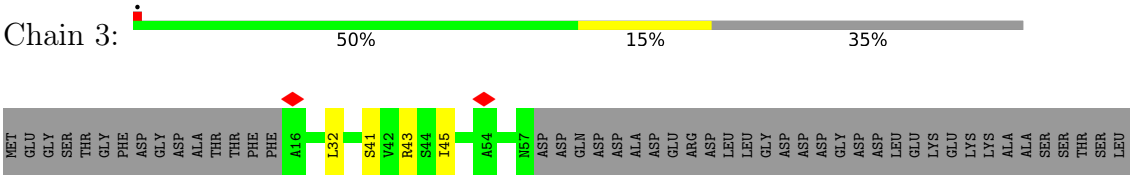


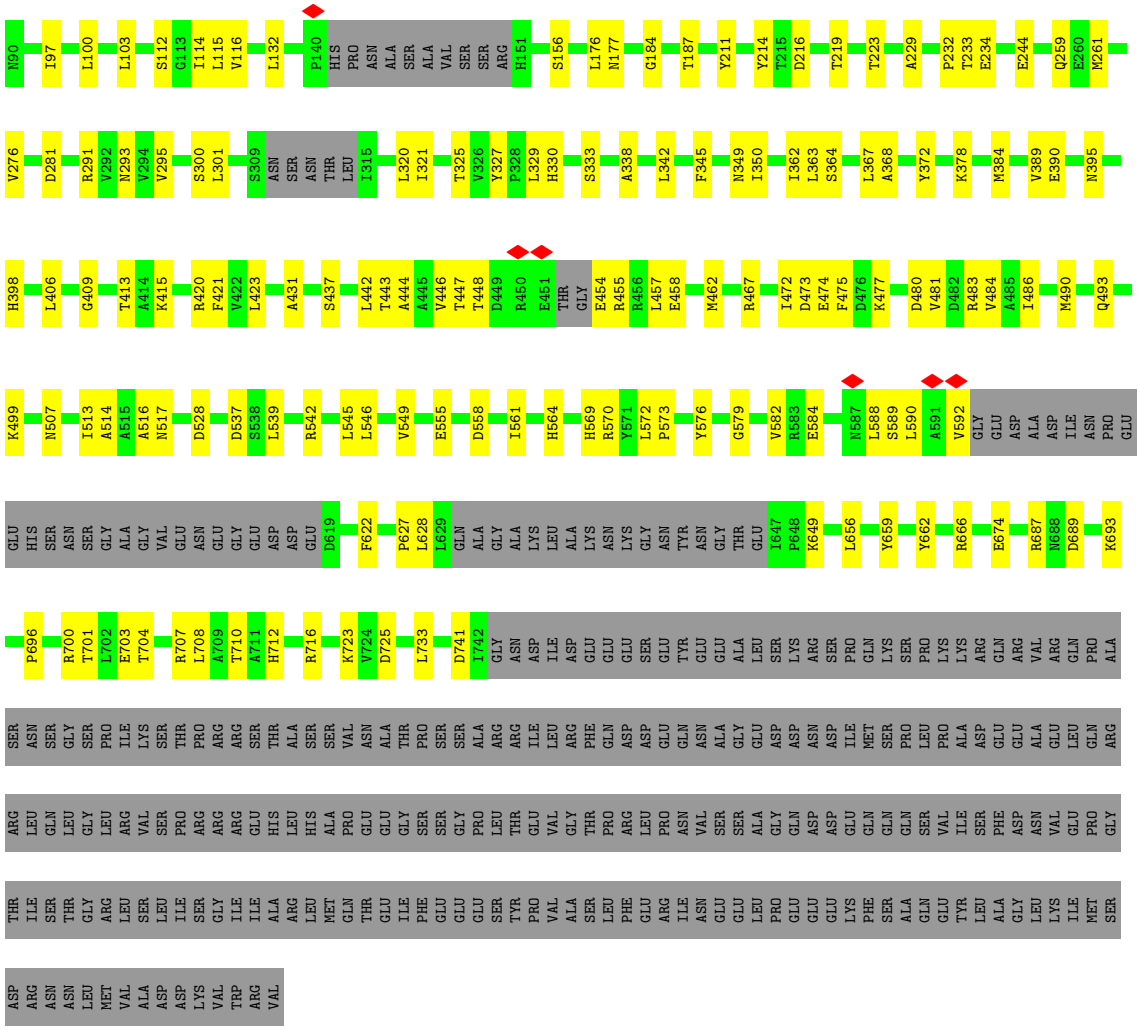


• Molecule 2: DNA replication licensing factor MCM2



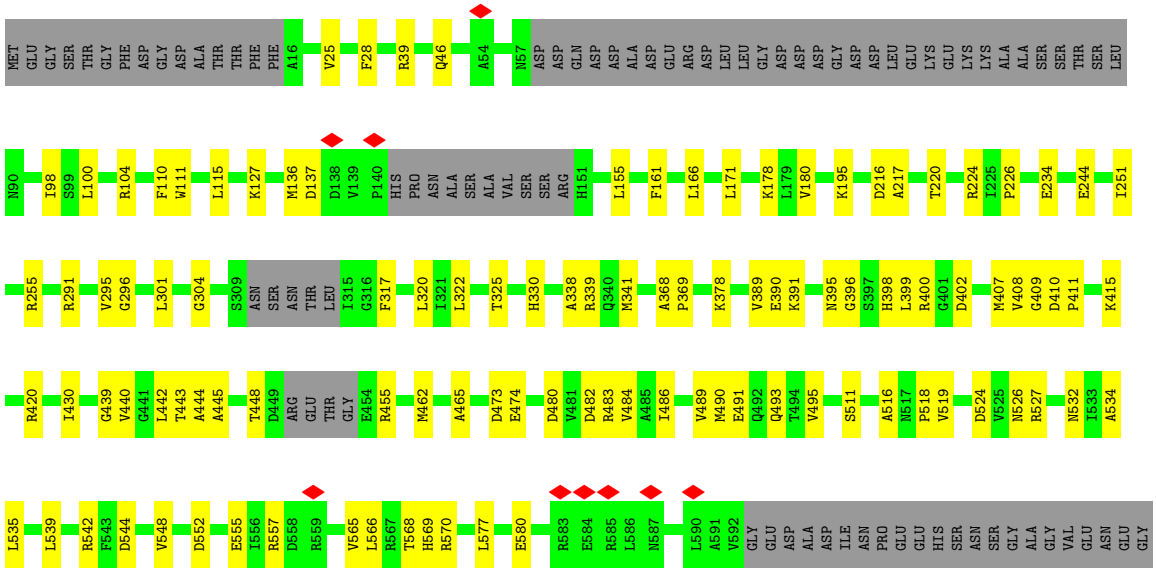
• Molecule 3: DNA replication licensing factor MCM3

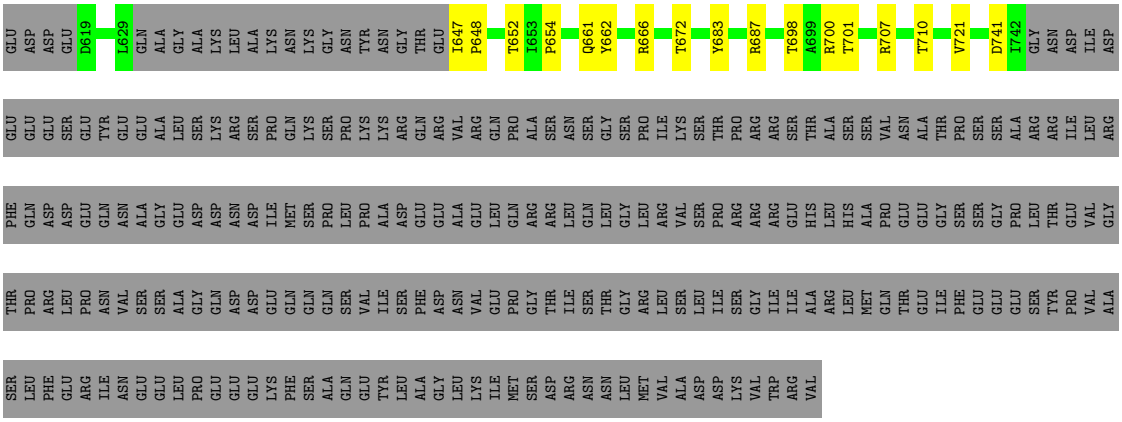




• Molecule 3: DNA replication licensing factor MCM3

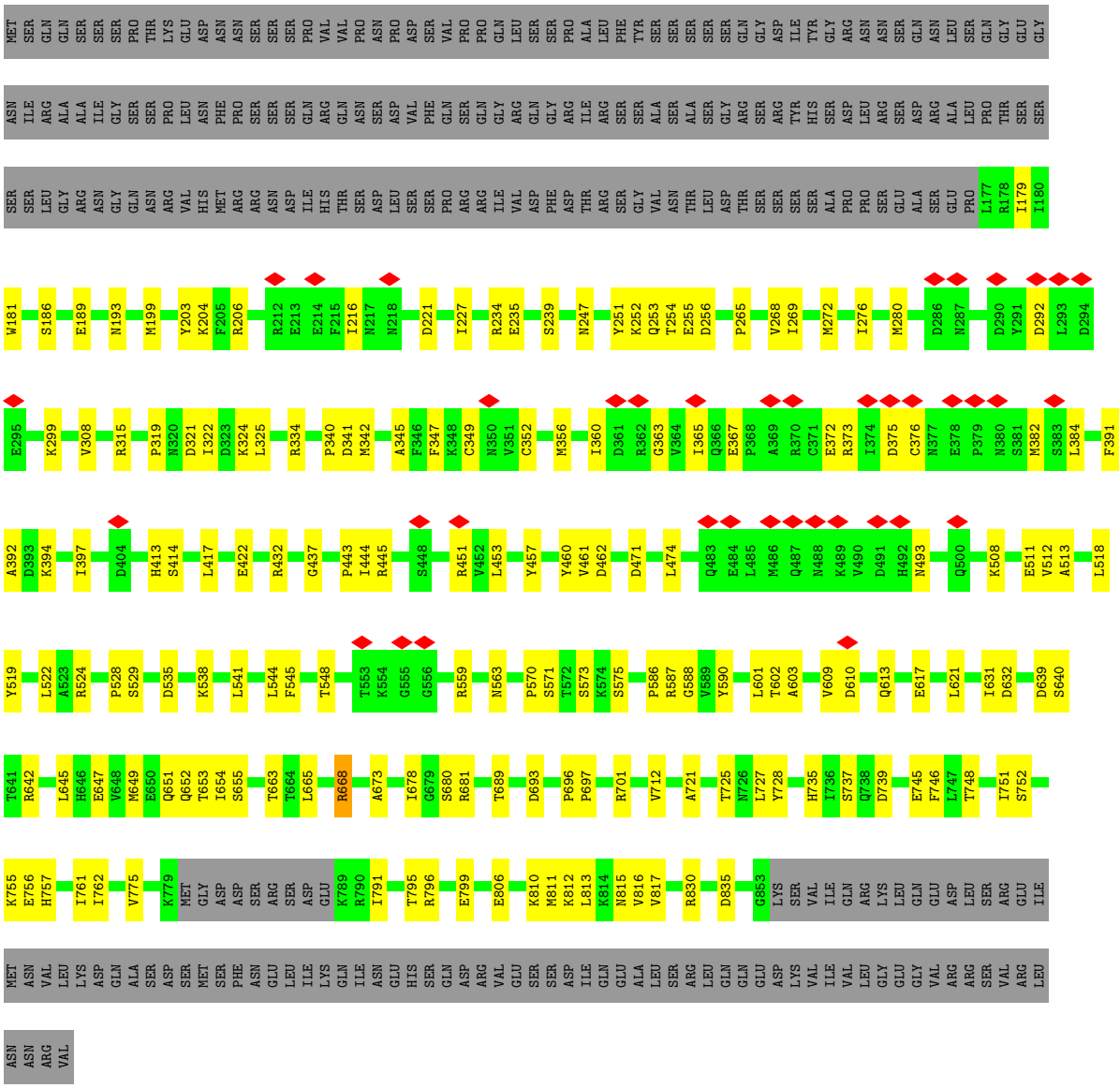
Chain C:





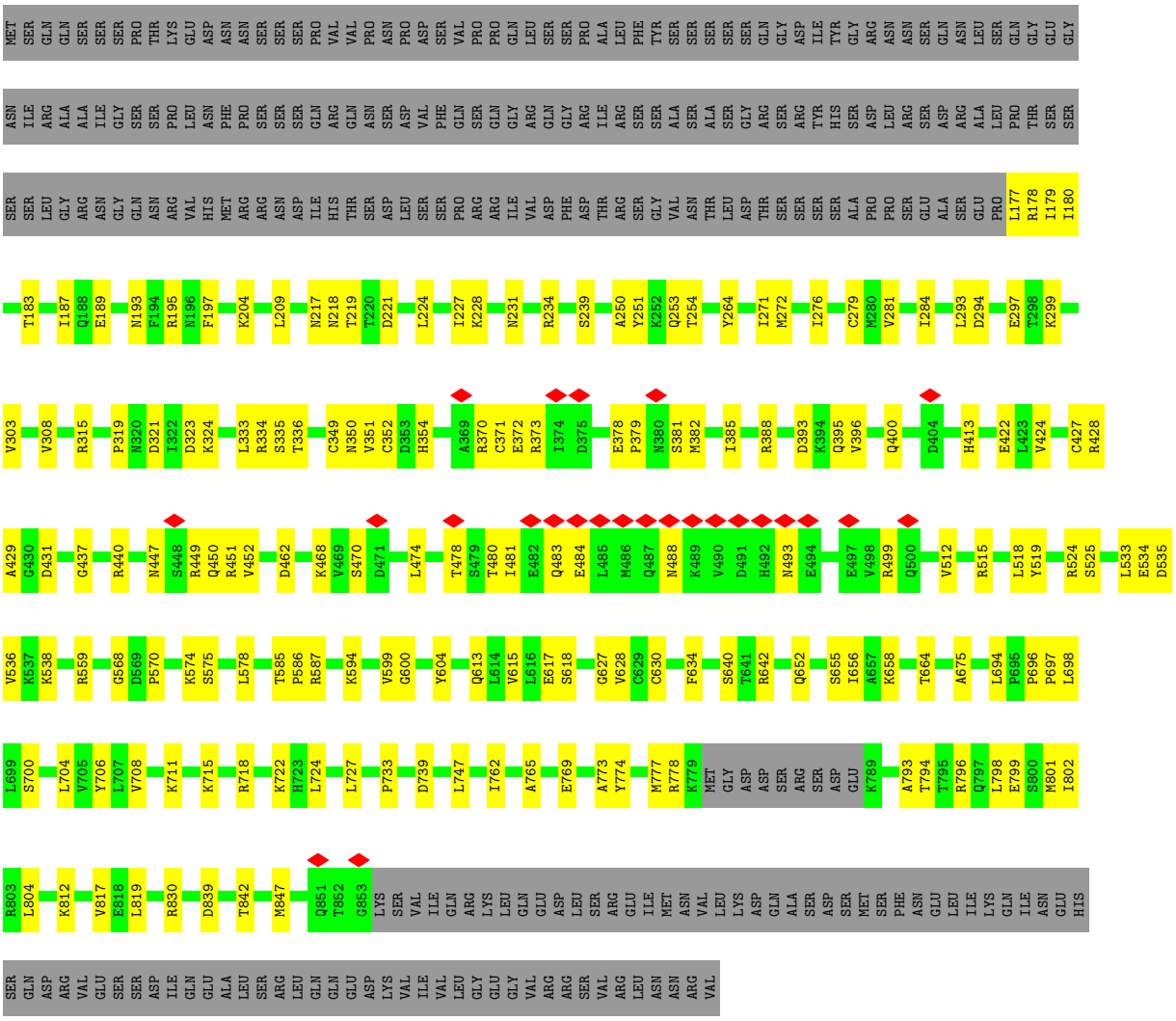
• Molecule 4: DNA replication licensing factor MCM4

Chain 4:



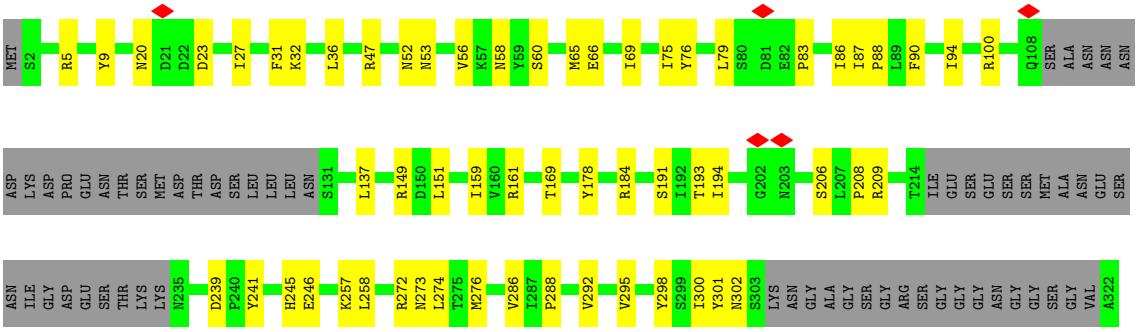
• Molecule 4: DNA replication licensing factor MCM4

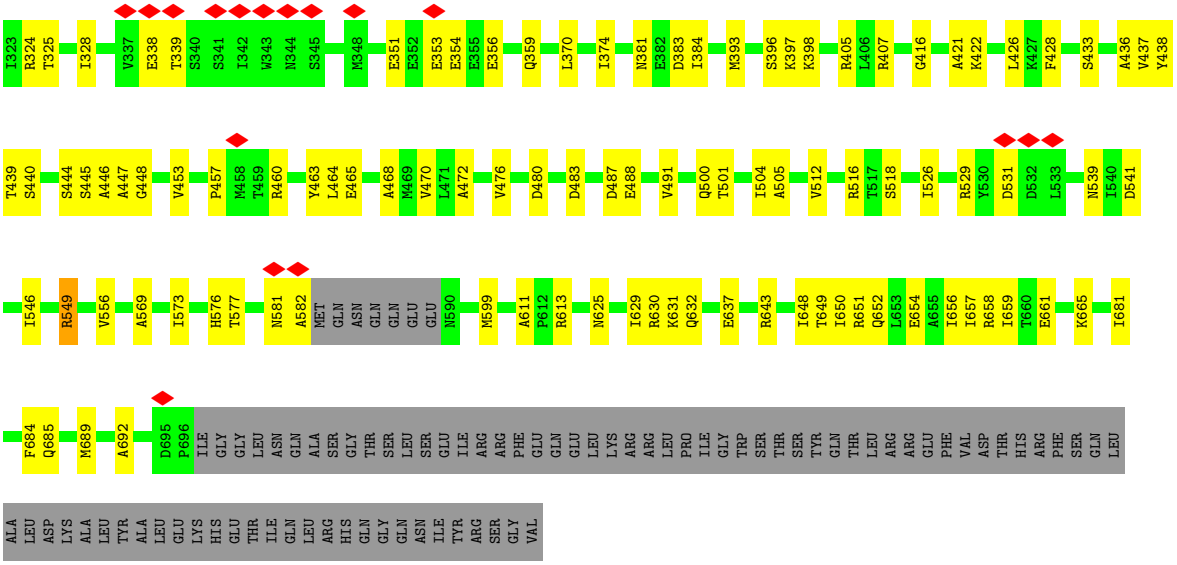
Chain D:



• Molecule 5: Minichromosome maintenance protein 5

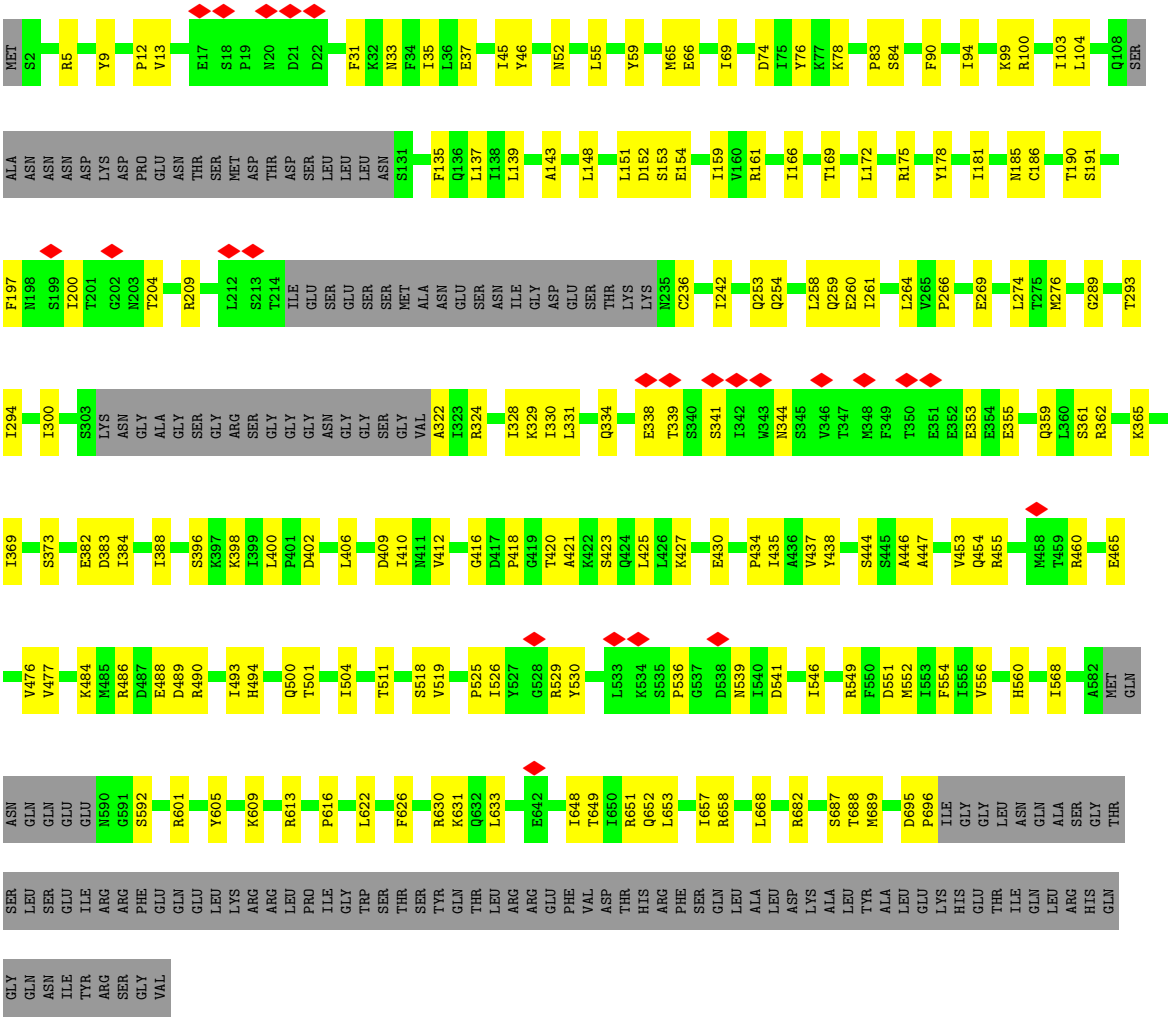
Chain 5:





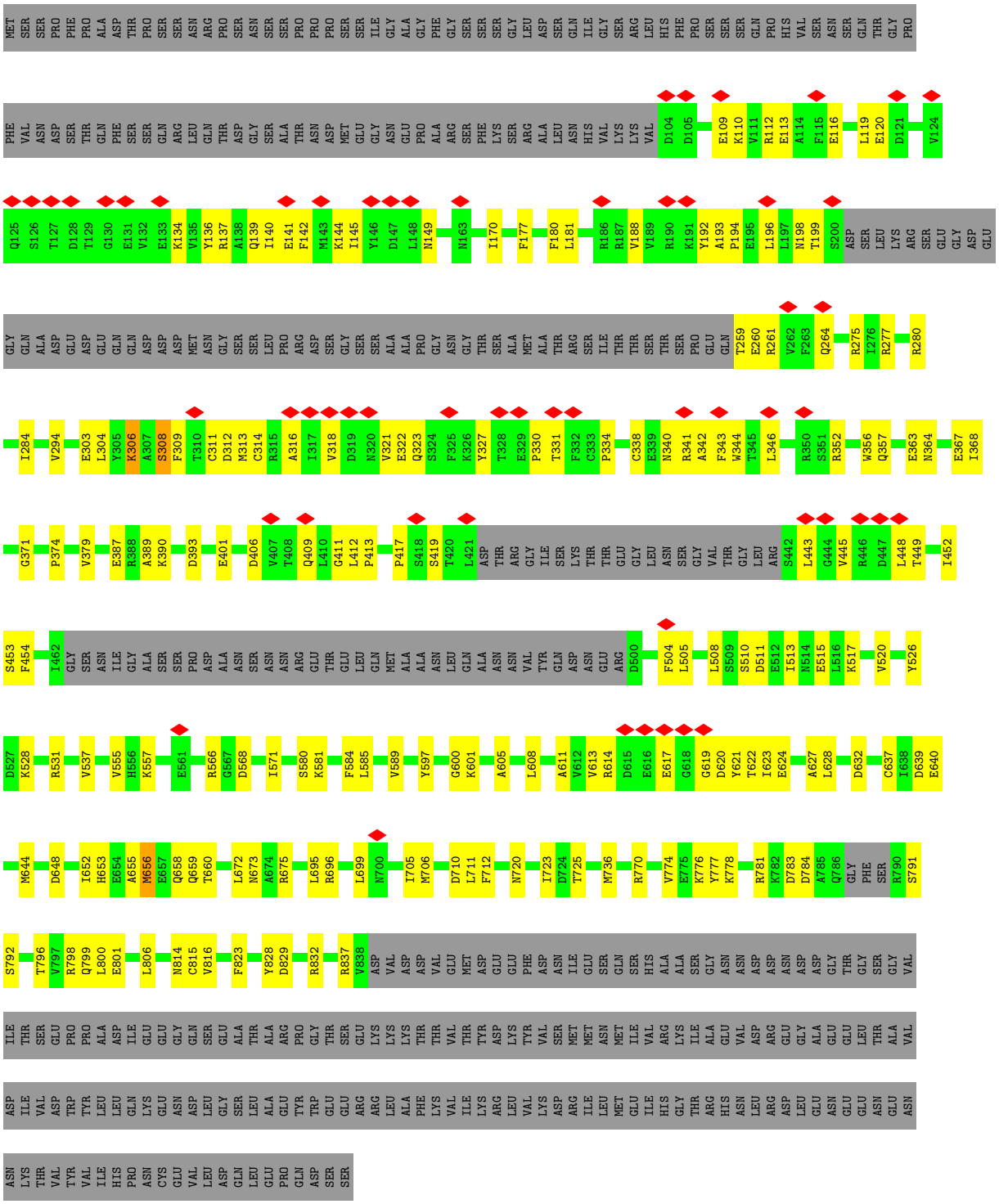
• Molecule 5: Minichromosome maintenance protein 5

Chain E:



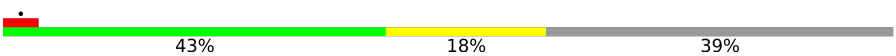
• Molecule 6: DNA replication licensing factor MCM6

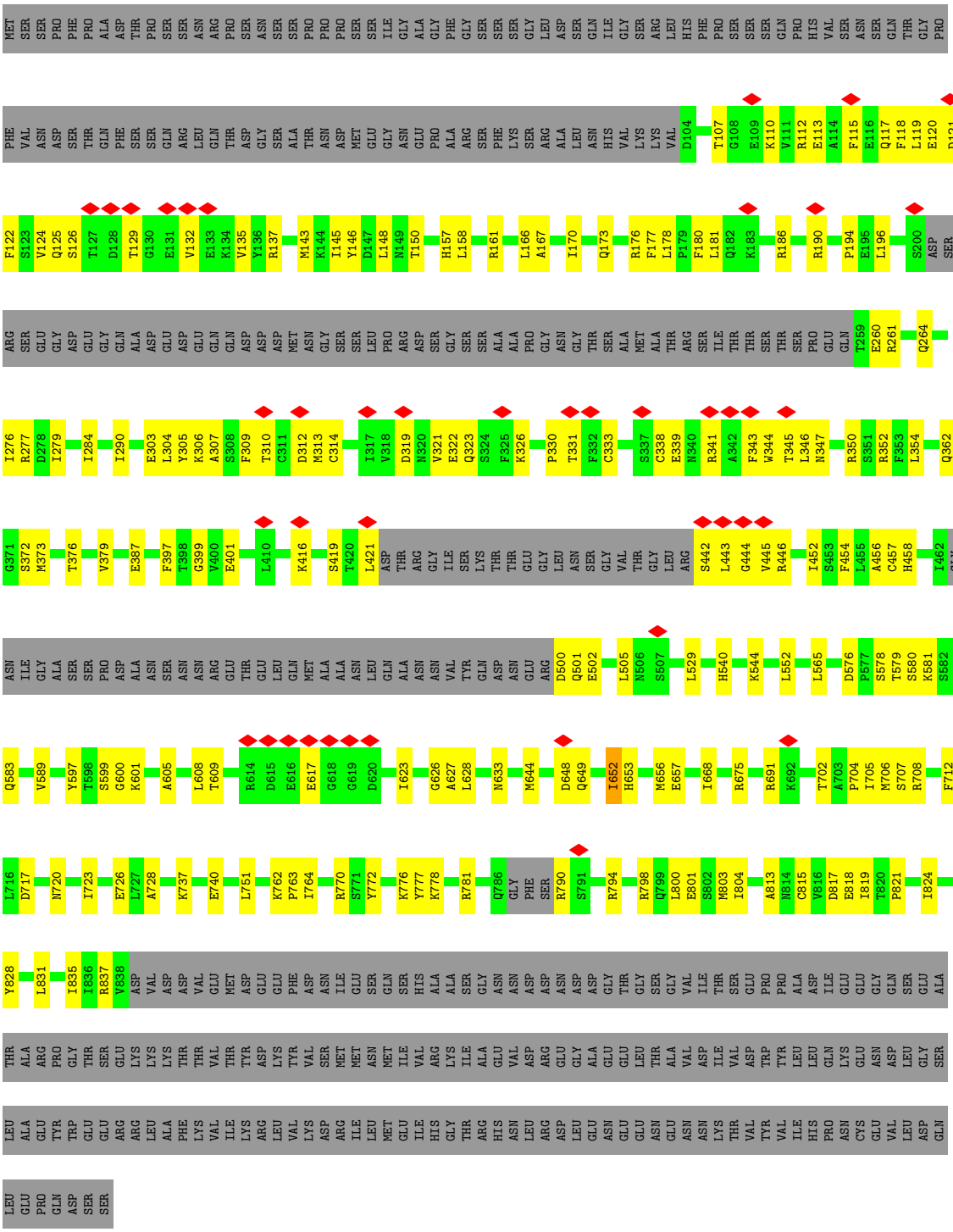
Chain 6:



• Molecule 6: DNA replication licensing factor MCM6

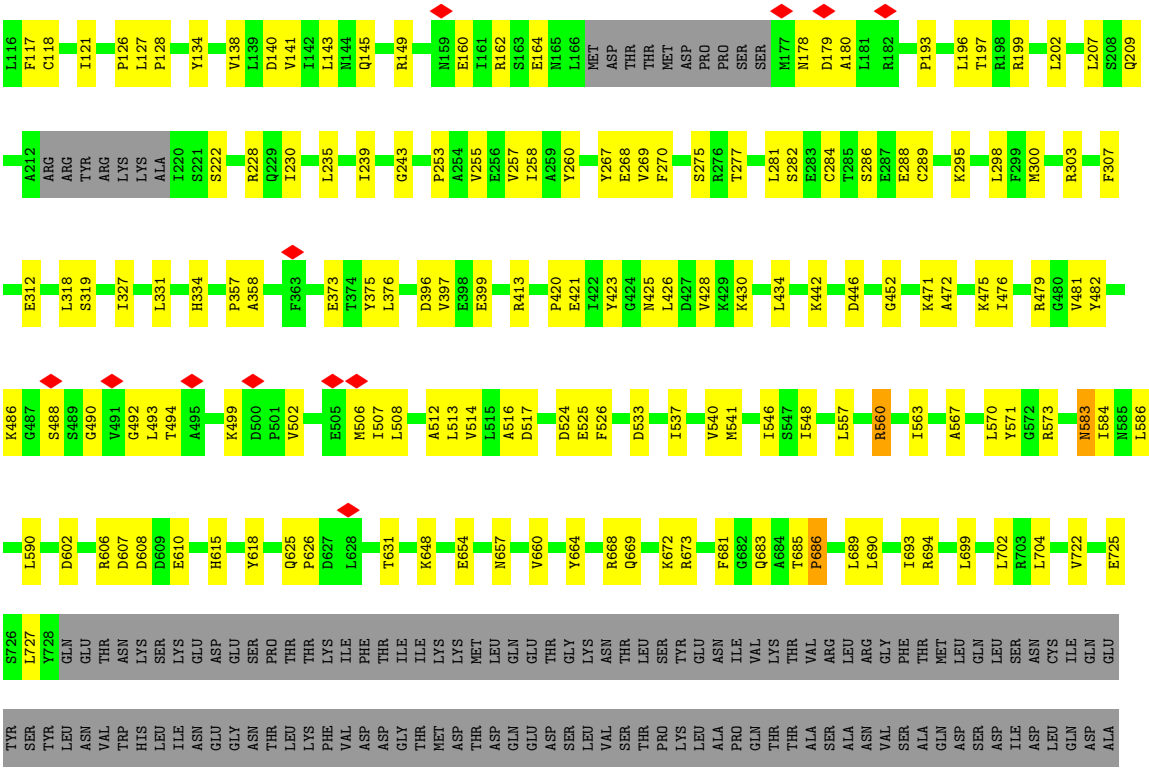
Chain F:





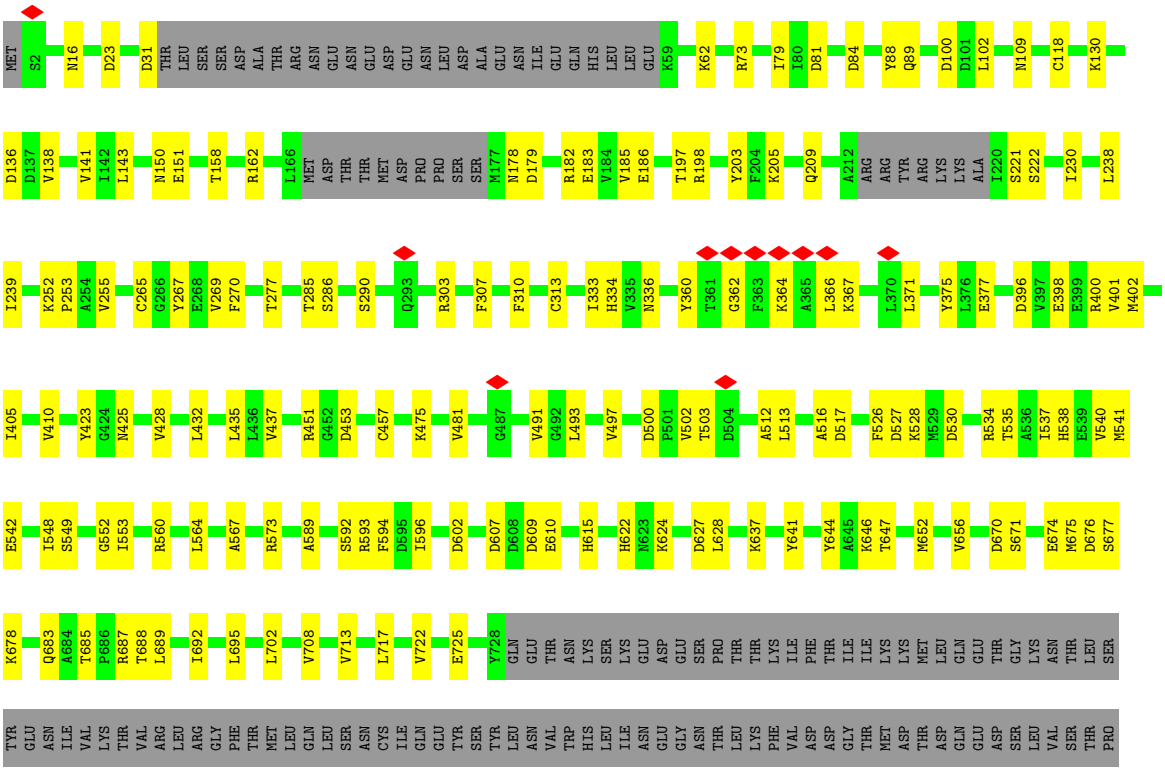
• Molecule 7: DNA replication licensing factor MCM7

Chain 7:



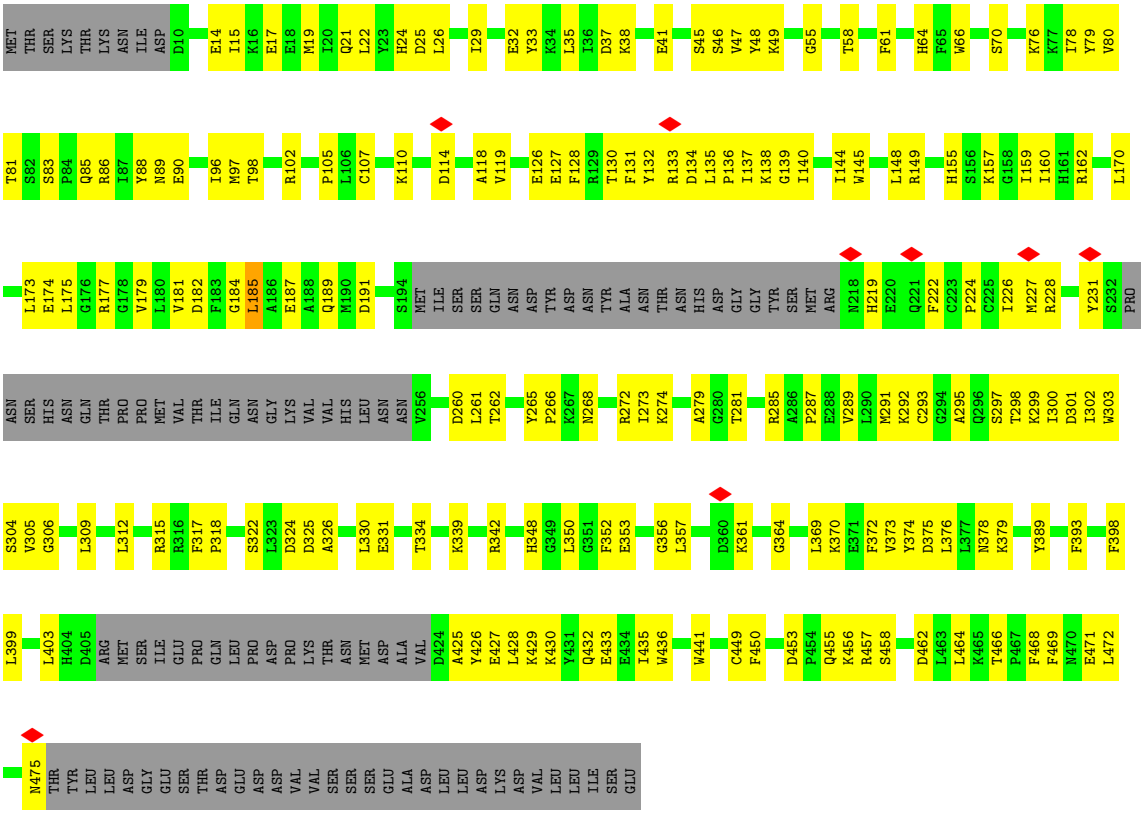
• Molecule 7: DNA replication licensing factor MCM7

Chain G:



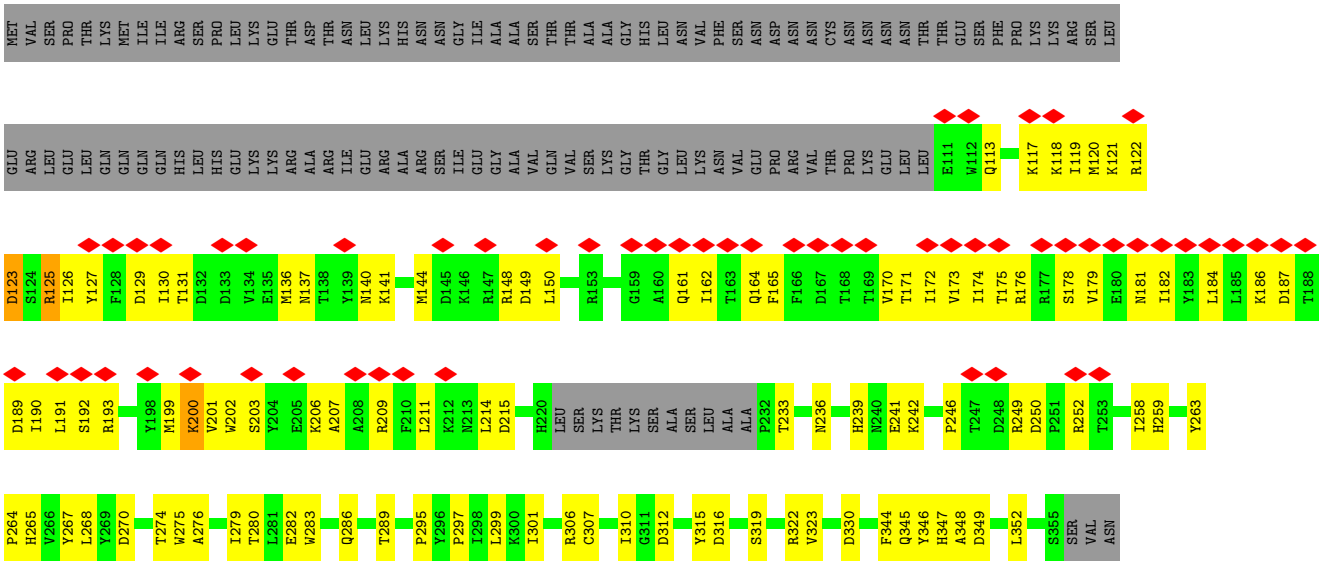
• Molecule 8: Cell division control protein 7

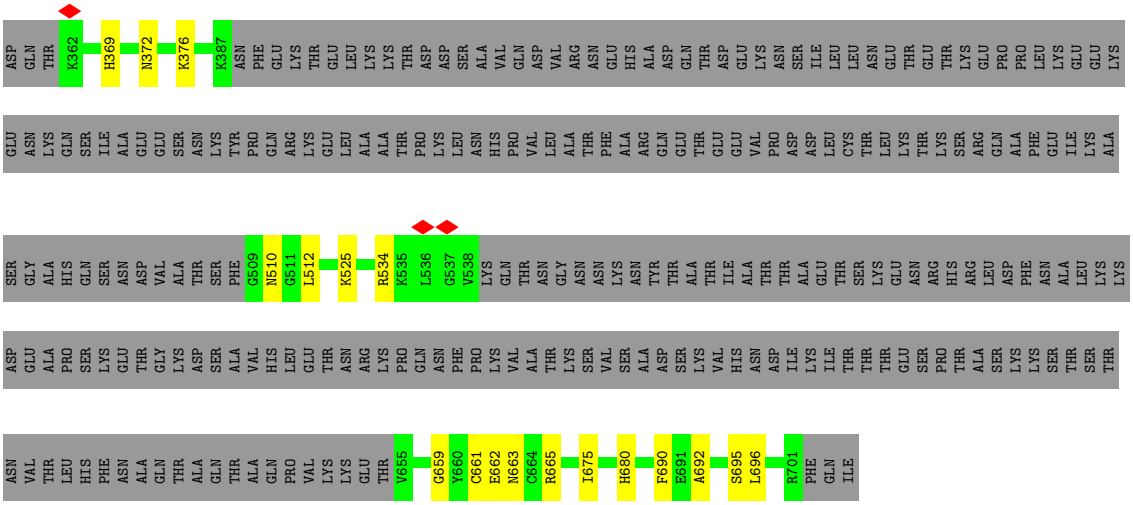
Chain 8:



• Molecule 9: DDK kinase regulatory subunit DBF4

Chain 9:




ASP GLN THR K362 H369 N372 K376 K387 ASN PHE GLU LYS THR GLU LEU LYS LYS THR ASP ASP SER ALA VAL GLN ASP VAL ARG ASN GLU HIS ALA ASP GLN THR ASP GLU LYS ASN SER ILE LEU LEU ASN GLU THR GLU THR LYS GLU PRO PRO LEU LYS GLU GLU LYS
GLU ASN LYS GLN SER ILE ALA GLU GLU SER ASN LYS TYR PRO GLN ARG LYS GLU LEU ALA ALA THR PRO LYS LEU ASN HIS PRO VAL LEU ALA THR PHE ALA ARG GLN GLU THR GLU GLU VAL PRO ASP ASP LEU CYS THR LEU LYS THR LYS SER ARG GLN ALA PHE GLU ILE LYS ALA
SER GLY ALA HIS GLN SER ASN ASP VAL ALA THR SER PHE G509 N510 G511 L512 K525 R534 K535 L536 G537 V538 LYS GLN THR ASN GLY ASN ASN LYS ASN TYR THR ALA THR ILE ALA THR THR ALA GLU THR SER LYS GLU ASN ARG HIS ARG LEU ASP PHE ASN ALA LEU LYS LYS
ASP GLU ALA PRO SER LYS GLU THR GLY LYS ASP SER ALA VAL HIS LEU GLU THR ASN ARG LYS PRO GLN ASN PHE PRO LYS VAL ALA THR LYS SER VAL SER ALA ASP SER LYS VAL HIS ASN ASP ILE LYS ILE THR THR THR GLU SER PRO THR ALA SER LYS LYS SER THR SER THR
ASN VAL THR LEU HIS PHE ASN ALA GLN THR ALA GLN THR ALA GLN PRO VAL LYS LYS GLU THR V655 G659 Y660 C661 E662 N663 C664 R665 I675 H680 F690 E691 A692 S695 L696 R701 PHE GLN ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30807	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.033	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	385.92, 385.92, 385.92	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ADP, BEF, 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
2	2	0.27	0/5046	0.51	0/6817
2	B	0.27	0/5046	0.52	0/6817
3	3	0.30	0/5073	0.51	0/6878
3	C	0.32	0/5053	0.51	0/6852
4	4	0.30	0/5401	0.51	0/7302
4	D	0.29	0/5401	0.49	0/7302
5	5	0.29	0/5000	0.49	0/6766
5	E	0.28	0/5000	0.50	0/6766
6	6	0.32	0/4968	0.54	0/6704
6	F	0.31	0/4968	0.54	0/6704
7	7	0.32	0/5451	0.52	0/7368
7	G	0.31	0/5451	0.49	0/7368
8	8	0.29	0/3373	0.51	0/4549
9	9	0.27	0/2872	0.49	0/3864
All	All	0.30	0/68103	0.51	0/92057

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1	20	0	6	0	0
2	2	4960	0	5001	116	0
2	B	4960	0	5002	138	0
3	3	4986	0	5053	106	0
3	C	4966	0	5034	94	0
4	4	5323	0	5387	130	0
4	D	5323	0	5387	117	0
5	5	4927	0	4982	117	0
5	E	4927	0	4982	140	0
6	6	4889	0	4913	128	0
6	F	4889	0	4913	128	0
7	7	5370	0	5426	129	0
7	G	5370	0	5426	95	0
8	8	3292	0	3249	148	0
9	9	2813	0	2821	102	0
10	2	27	0	12	0	0
10	3	27	0	12	3	0
10	4	27	0	12	1	0
10	5	27	0	12	3	0
10	6	27	0	12	3	0
10	7	27	0	12	1	0
10	8	27	0	12	6	0
10	B	27	0	12	3	0
10	C	27	0	12	1	0
10	D	27	0	12	1	0
10	E	27	0	12	2	0
10	F	27	0	12	2	0
10	G	27	0	12	0	0
11	2	1	0	0	0	0
11	3	1	0	0	0	0
11	4	1	0	0	0	0
11	5	1	0	0	0	0
11	6	1	0	0	0	0
11	7	1	0	0	0	0
11	8	2	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
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
12	2	1	0	0	0	0
12	4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	5	1	0	0	0	0
12	6	1	0	0	0	0
12	7	1	0	0	0	0
12	8	1	0	0	0	0
12	9	1	0	0	0	0
12	B	1	0	0	0	0
12	D	1	0	0	0	0
12	E	1	0	0	0	0
12	F	1	0	0	0	0
12	G	1	0	0	0	0
13	3	8	0	0	1	0
13	4	4	0	0	0	0
13	8	4	0	0	0	0
13	D	4	0	0	1	0
13	E	4	0	0	1	0
13	G	4	0	0	0	0
All	All	67420	0	67738	1511	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 (1511) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:519:VAL:HG21	3:C:534:ALA:CB	1.72	1.16
3:C:519:VAL:HG21	3:C:534:ALA:HB2	1.34	1.09
4:4:609:VAL:CG1	7:7:506:MET:HG2	1.88	1.03
2:B:181:LEU:N	2:B:206:THR:HG1	1.56	1.01
3:C:519:VAL:CG2	3:C:534:ALA:HB3	1.95	0.94
10:3:1001:ADP:H5'2	5:5:651:ARG:HH21	1.31	0.94
4:D:642:ARG:HD3	4:D:698:LEU:HD22	1.50	0.91
2:B:794:ARG:HG2	2:B:805:ILE:HD11	1.52	0.90
3:C:519:VAL:HG21	3:C:534:ALA:HB3	1.53	0.90
3:C:519:VAL:CG2	3:C:534:ALA:CB	2.49	0.90
4:4:519:TYR:HD1	4:4:811:MET:CE	1.86	0.88
3:3:384:MET:HE1	3:3:513:ILE:HB	1.54	0.87
4:4:609:VAL:HG11	7:7:506:MET:HG2	1.55	0.86
6:F:362:GLN:HG3	6:F:376:THR:HG22	1.59	0.84
3:C:652:THR:HG22	3:C:654:PRO:HD2	1.61	0.82
4:4:349:CYS:HB3	4:4:352:CYS:SG	2.19	0.82
8:8:398:PHE:HA	8:8:436:TRP:HZ3	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:120:MET:HA	9:9:123:ASP:HB3	1.61	0.81
7:G:118:CYS:SG	7:G:198:ARG:NH1	2.53	0.81
2:B:327:ARG:HE	2:B:420:PRO:HD3	1.45	0.81
2:B:794:ARG:CD	2:B:805:ILE:HD11	2.10	0.80
2:B:794:ARG:CG	2:B:805:ILE:HD11	2.11	0.80
9:9:172:ILE:HA	9:9:200:LYS:HE3	1.63	0.79
6:6:312:ASP:HB2	6:6:343:PHE:HB2	1.65	0.79
3:C:216:ASP:OD1	3:C:217:ALA:N	2.16	0.77
6:6:504:PHE:O	6:6:508:LEU:HG	1.81	0.77
7:7:722:VAL:HA	7:7:725:GLU:HG3	1.67	0.77
4:D:474:LEU:HB2	4:D:586:PRO:HD3	1.67	0.76
4:4:609:VAL:HG13	7:7:506:MET:HG2	1.67	0.76
6:6:331:THR:HA	6:6:341:ARG:HD2	1.68	0.76
6:6:505:LEU:HD23	6:6:508:LEU:HD12	1.68	0.76
2:2:693:GLU:HB2	6:6:778:LYS:HD3	1.67	0.75
4:4:422:GLU:HB2	4:4:493:ASN:HA	1.68	0.74
4:4:762:ILE:HB	6:6:736:MET:HE1	1.69	0.74
2:2:227:TYR:HA	2:2:230:ARG:HE	1.52	0.74
6:6:313:MET:HE1	6:F:313:MET:HA	1.68	0.74
4:D:351:VAL:HG21	4:D:378:GLU:HG3	1.70	0.74
5:E:185:ASN:ND2	5:E:236:CYS:O	2.21	0.74
3:3:368:ALA:HB3	3:3:378:LYS:HE2	1.70	0.73
7:7:67:LEU:HD11	7:7:121:ILE:HD12	1.71	0.73
4:D:422:GLU:HB2	4:D:493:ASN:HA	1.71	0.73
5:5:630:ARG:NH1	5:5:648:ILE:O	2.21	0.73
6:F:341:ARG:HB3	6:F:344:TRP:HE1	1.54	0.73
2:B:376:ASN:HB3	2:B:379:LYS:HD3	1.69	0.72
8:8:138:LYS:HE3	9:9:348:ALA:N	2.04	0.72
9:9:127:TYR:HD1	9:9:173:VAL:HG22	1.55	0.72
2:2:794:ARG:HG2	2:2:805:ILE:HD11	1.72	0.72
8:8:133:ARG:HA	8:8:315:ARG:HG3	1.72	0.72
6:6:513:ILE:O	6:6:517:LYS:HG2	1.89	0.72
8:8:224:PRO:HG2	8:8:226:ILE:HG22	1.72	0.72
7:7:228:ARG:NH2	7:7:327:ILE:O	2.23	0.71
3:C:569:HIS:O	5:E:613:ARG:NH1	2.22	0.71
4:4:519:TYR:HD1	4:4:811:MET:HE3	1.54	0.71
6:6:614:ARG:HA	6:6:621:TYR:HA	1.71	0.71
6:F:576:ASP:O	6:F:581:LYS:NZ	2.24	0.71
4:4:519:TYR:CD1	4:4:811:MET:CE	2.74	0.71
8:8:441:TRP:HB3	8:8:468:PHE:HB2	1.73	0.71
2:B:338:LYS:HD2	2:B:379:LYS:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:389:VAL:HG22	3:3:710:THR:HG21	1.73	0.70
5:E:536:PRO:HB2	5:E:695:ASP:HA	1.74	0.70
8:8:293:CYS:SG	8:8:348:HIS:CE1	2.77	0.70
4:4:639:ASP:OD1	4:4:642:ARG:NH2	2.25	0.70
4:4:471:ASP:HB3	4:4:745:GLU:HG3	1.74	0.69
6:F:600:GLY:HA2	6:F:644:MET:HB2	1.74	0.69
2:2:792:ASP:OD1	2:2:795:ARG:NH1	2.25	0.69
5:5:79:LEU:HA	5:5:86:ILE:HG21	1.75	0.69
5:5:87:ILE:HD11	5:5:137:LEU:HD23	1.74	0.69
3:C:420:ARG:HH22	5:E:501:THR:HG21	1.58	0.69
4:4:609:VAL:CG1	7:7:506:MET:CG	2.69	0.69
5:5:405:ARG:NH2	5:5:500:GLN:OE1	2.25	0.69
8:8:433:GLU:HA	8:8:436:TRP:HD1	1.58	0.69
2:B:800:THR:HG21	2:B:856:GLN:HB2	1.75	0.69
4:D:335:SER:OG	4:D:395:GLN:NE2	2.26	0.68
6:F:178:LEU:HA	6:F:181:LEU:HD12	1.74	0.68
9:9:203:SER:O	9:9:207:ALA:N	2.24	0.68
8:8:64:HIS:HD2	8:8:105:PRO:HG2	1.59	0.68
6:6:620:ASP:OD1	6:6:621:TYR:N	2.26	0.68
9:9:239:HIS:HA	9:9:242:LYS:HG3	1.74	0.68
7:G:513:LEU:HD13	7:G:540:VAL:HG21	1.76	0.68
6:6:341:ARG:HG3	6:6:344:TRP:HE1	1.58	0.68
9:9:186:LYS:HB3	9:9:192:SER:HB3	1.76	0.68
2:2:485:ARG:NH1	2:2:488:SER:OG	2.27	0.68
7:G:230:ILE:HD12	7:G:239:ILE:HD12	1.74	0.68
2:2:387:ARG:NH2	2:2:407:GLU:OE1	2.27	0.68
8:8:432:GLN:OE1	8:8:436:TRP:NE1	2.23	0.68
6:F:170:ILE:HD11	6:F:181:LEU:HD11	1.76	0.67
2:2:268:LEU:HD21	2:2:297:ILE:HD11	1.75	0.67
4:4:762:ILE:HA	4:4:817:VAL:HG12	1.76	0.67
3:3:689:ASP:OD1	7:7:606:ARG:NH2	2.27	0.67
2:B:271:PHE:HB3	2:B:295:VAL:HG21	1.76	0.67
9:9:161:GLN:NE2	9:9:162:ILE:O	2.28	0.67
3:3:584:GLU:OE1	5:5:397:LYS:NZ	2.27	0.67
3:C:480:ASP:OD1	3:C:483:ARG:NH2	2.26	0.67
7:G:73:ARG:NH2	7:G:130:LYS:O	2.28	0.67
2:2:620:ILE:O	2:2:624:MET:HG2	1.95	0.67
4:4:334:ARG:HD3	4:4:617:GLU:HG2	1.76	0.67
2:B:443:GLY:O	6:F:326:LYS:NZ	2.28	0.67
6:6:109:GLU:HB3	6:6:112:ARG:HH21	1.60	0.66
6:F:421:LEU:HB3	6:F:444:GLY:HA3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:206:ARG:NH1	4:4:247:ASN:OD1	2.29	0.66
8:8:35:LEU:HD11	8:8:48:TYR:HB3	1.76	0.66
8:8:37:ASP:O	8:8:49:LYS:N	2.28	0.66
4:D:429:ALA:O	4:D:587:ARG:NH2	2.28	0.66
3:C:448:THR:HG23	3:C:455:ARG:HH12	1.61	0.66
3:C:430:ILE:HD12	3:C:465:ALA:HB2	1.76	0.66
8:8:80:VAL:O	9:9:663:ASN:ND2	2.29	0.66
8:8:181:VAL:HG21	10:8:1001:ADP:N7	2.11	0.66
6:F:644:MET:O	6:F:649:GLN:NE2	2.28	0.66
9:9:126:ILE:HB	9:9:162:ILE:HA	1.78	0.66
7:7:270:PHE:HB2	5:E:9:TYR:HB2	1.77	0.65
3:C:577:LEU:HB2	3:C:580:GLU:HB2	1.77	0.65
2:2:525:LYS:NZ	5:5:577:THR:OG1	2.28	0.65
6:F:173:GLN:OE1	6:F:176:ARG:NH2	2.29	0.65
2:2:181:LEU:N	2:2:209:ARG:HH21	1.95	0.65
2:B:384:ASN:ND2	5:E:152:ASP:OD1	2.27	0.65
2:B:475:SER:O	2:B:765:LYS:NZ	2.30	0.65
4:D:440:ARG:NH1	4:D:462:ASP:OD2	2.30	0.65
4:4:613:GLN:HB2	6:6:617:GLU:HG3	1.77	0.65
4:D:478:THR:HA	4:D:481:ILE:HG22	1.77	0.65
7:G:336:ASN:ND2	7:G:377:GLU:OE2	2.24	0.65
8:8:144:ILE:HG13	8:8:309:LEU:HD13	1.79	0.65
2:B:495:ASP:OD1	2:B:836:ARG:NH2	2.30	0.65
8:8:272:ARG:NH2	4:D:294:ASP:OD1	2.27	0.65
8:8:375:ASP:HA	8:8:378:ASN:HB2	1.79	0.65
2:2:543:GLY:HA3	2:2:683:VAL:HG23	1.78	0.64
7:G:396:ASP:OD2	7:G:400:ARG:NH2	2.30	0.64
2:2:364:CYS:HB3	2:2:369:SER:H	1.62	0.64
6:6:504:PHE:CZ	6:6:508:LEU:HD21	2.33	0.64
4:4:559:ARG:HG3	4:4:668:ARG:HG2	1.78	0.64
5:E:526:ILE:HB	5:E:541:ASP:HB3	1.78	0.64
6:F:190:ARG:HA	6:F:194:PRO:HB3	1.79	0.64
8:8:472:LEU:O	8:8:475:ASN:ND2	2.30	0.64
3:3:689:ASP:O	3:3:693:LYS:NZ	2.31	0.64
7:7:514:VAL:HG21	7:7:557:LEU:HD23	1.80	0.64
2:B:285:ASP:OD2	2:B:288:ARG:NH2	2.30	0.64
5:E:649:THR:H	5:E:652:GLN:HG2	1.63	0.64
5:5:689:MET:HA	5:5:692:ALA:HB3	1.79	0.64
7:7:235:LEU:HD22	7:7:357:PRO:HG3	1.80	0.64
6:F:580:SER:N	10:F:1101:ADP:O2A	2.30	0.64
9:9:236:ASN:HA	9:9:239:HIS:CD2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:260:GLU:O	6:F:352:ARG:NH1	2.30	0.64
7:G:502:VAL:HG23	7:G:503:THR:HG23	1.80	0.64
6:6:314:CYS:SG	6:6:338:CYS:HB2	2.37	0.64
6:6:528:LYS:HG2	6:6:531:ARG:HH21	1.63	0.63
6:F:186:ARG:NH2	6:F:261:ARG:O	2.29	0.63
2:2:232:ARG:NH1	2:2:283:TYR:OH	2.30	0.63
3:3:481:VAL:HG13	7:7:486:LYS:HD3	1.79	0.63
5:E:409:ASP:O	5:E:658:ARG:NH1	2.31	0.63
6:6:112:ARG:HB2	6:6:180:PHE:HB3	1.81	0.63
2:B:249:LEU:HD11	2:B:256:LEU:HD22	1.80	0.63
5:E:494:HIS:HB3	5:E:549:ARG:HH21	1.62	0.63
2:B:545:PRO:HG3	2:B:651:ASN:HD21	1.63	0.63
2:2:816:ILE:HG23	2:2:837:ALA:HB1	1.80	0.63
3:3:211:TYR:HB3	7:7:8:ILE:HD11	1.79	0.63
7:G:89:GLN:OE1	7:G:102:LEU:N	2.32	0.63
6:6:608:LEU:HD23	6:6:652:ILE:HD13	1.79	0.63
4:D:634:PHE:HB3	4:D:675:ALA:HB2	1.80	0.63
9:9:307:CYS:HB3	9:9:310:ILE:HG22	1.80	0.63
6:F:777:TYR:OH	6:F:781:ARG:NH1	2.30	0.63
3:3:712:HIS:ND1	3:3:725:ASP:OD1	2.32	0.63
8:8:86:ARG:HH12	9:9:512:LEU:HD21	1.64	0.63
2:2:394:PRO:O	6:6:673:ASN:ND2	2.31	0.63
6:6:605:ALA:N	6:6:648:ASP:OD1	2.31	0.63
8:8:350:LEU:HD21	9:9:268:LEU:HD21	1.81	0.63
7:G:542:GLU:OE2	7:G:687:ARG:NE	2.32	0.62
8:8:432:GLN:HA	8:8:435:ILE:HG12	1.81	0.62
9:9:137:ASN:O	9:9:141:LYS:N	2.30	0.62
4:4:522:LEU:HB3	4:4:541:LEU:HD11	1.81	0.62
7:7:526:PHE:HB3	7:7:567:ALA:HB2	1.81	0.62
3:3:395:ASN:ND2	7:7:421:GLU:OE1	2.31	0.62
9:9:265:HIS:HB3	9:9:282:GLU:HG3	1.81	0.62
2:B:774:ILE:HG22	2:B:776:PRO:HD3	1.81	0.62
5:E:31:PHE:CG	5:E:90:PHE:HD1	2.18	0.62
2:2:327:ARG:NH2	2:2:416:ASP:OD1	2.31	0.62
3:3:443:THR:OG1	3:3:444:ALA:N	2.31	0.62
7:7:16:ASN:ND2	7:7:100:ASP:OD2	2.33	0.62
2:B:813:ILE:HG13	2:B:841:VAL:HG21	1.81	0.62
7:G:526:PHE:HB3	7:G:567:ALA:HB2	1.79	0.62
6:6:409:GLN:HB2	6:6:412:LEU:HD12	1.80	0.62
9:9:306:ARG:NH1	9:9:312:ASP:OD1	2.32	0.62
5:5:649:THR:H	5:5:652:GLN:HG2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:368:ALA:HB3	3:C:378:LYS:HE2	1.81	0.62
4:4:529:SER:HA	4:4:735:HIS:CD2	2.35	0.62
6:6:580:SER:N	10:6:1101:ADP:O2A	2.31	0.62
7:7:499:LYS:HB2	7:7:506:MET:SD	2.39	0.62
8:8:219:HIS:HA	8:8:222:PHE:HB2	1.82	0.62
4:4:587:ARG:HH22	6:6:371:GLY:HA3	1.64	0.61
3:C:244:GLU:OE1	7:G:109:ASN:ND2	2.32	0.61
3:C:647:ILE:HD12	3:C:648:PRO:HD2	1.82	0.61
5:E:90:PHE:HE2	5:E:137:LEU:HD13	1.65	0.61
5:E:409:ASP:HB3	5:E:518:SER:HB3	1.80	0.61
6:F:457:CYS:SG	6:F:458:HIS:ND1	2.69	0.61
4:4:727:LEU:O	7:7:442:LYS:NZ	2.33	0.61
5:5:31:PHE:CG	5:5:90:PHE:HD1	2.19	0.61
9:9:510:ASN:HB2	9:9:659:GLY:HA3	1.83	0.61
5:E:359:GLN:OE1	5:E:362:ARG:NH2	2.33	0.61
4:4:508:LYS:HA	4:4:511:GLU:HG2	1.82	0.61
6:6:608:LEU:HA	6:6:627:ALA:HB3	1.82	0.61
5:5:656:ILE:HD11	5:5:684:PHE:CG	2.36	0.61
2:2:230:ARG:HB3	2:2:242:LEU:HD11	1.81	0.61
2:2:306:LEU:HD23	2:2:406:ARG:HG3	1.83	0.61
5:5:53:ASN:ND2	5:5:60:SER:O	2.27	0.61
9:9:118:LYS:O	9:9:121:LYS:NZ	2.32	0.61
2:2:307:ARG:O	2:2:310:ARG:NH1	2.33	0.61
2:B:243:GLU:HA	2:B:296:ARG:HB2	1.82	0.61
2:B:806:THR:OG1	2:B:808:ARG:HB3	2.01	0.61
2:2:335:LYS:HG3	2:2:383:ARG:HH21	1.65	0.61
6:6:304:LEU:HD23	6:6:323:GLN:HE21	1.66	0.61
6:6:695:LEU:HD23	6:6:792:SER:HB2	1.83	0.61
2:B:335:LYS:HE3	2:B:383:ARG:HD2	1.82	0.61
3:3:409:GLY:HA3	3:3:549:VAL:HG23	1.81	0.61
8:8:398:PHE:HD2	8:8:399:LEU:HD12	1.64	0.61
2:B:796:GLU:HB3	2:B:856:GLN:NE2	2.16	0.61
7:7:426:LEU:HG	7:7:430:LYS:HE3	1.83	0.60
8:8:334:THR:HB	9:9:299:LEU:HD11	1.82	0.60
2:B:855:ARG:HD3	2:B:859:ARG:HH21	1.66	0.60
10:3:1001:ADP:C5'	5:5:651:ARG:HH21	2.10	0.60
5:5:178:TYR:HD1	5:5:193:THR:HG22	1.66	0.60
6:6:828:TYR:OH	6:6:832:ARG:NH1	2.34	0.60
2:B:678:ASP:OD2	2:B:815:ARG:NH2	2.34	0.60
8:8:312:LEU:O	8:8:315:ARG:NH1	2.35	0.60
4:4:609:VAL:HG13	7:7:506:MET:CG	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:396:SER:O	5:5:398:LYS:NZ	2.33	0.60
2:B:404:ARG:NH2	6:F:387:GLU:OE2	2.35	0.60
9:9:174:ILE:HD12	9:9:202:TRP:HB2	1.84	0.60
8:8:191:ASP:O	8:8:228:ARG:NH2	2.35	0.60
8:8:361:LYS:HB3	8:8:364:GLY:HA3	1.82	0.60
8:8:398:PHE:HA	8:8:436:TRP:CZ3	2.32	0.60
5:5:476:VAL:HG12	5:5:518:SER:HB2	1.84	0.60
6:6:277:ARG:NH2	6:6:363:GLU:OE1	2.34	0.60
2:B:807:VAL:HG21	5:E:568:ILE:HG21	1.83	0.60
6:F:117:GLN:NE2	6:F:121:ASP:OD2	2.34	0.60
6:6:505:LEU:HA	6:6:508:LEU:HD12	1.82	0.60
4:D:600:GLY:HA3	7:G:549:SER:O	2.02	0.60
7:G:437:VAL:O	7:G:646:LYS:NZ	2.27	0.60
4:D:349:CYS:HB3	4:D:354:HIS:H	1.67	0.60
4:4:601:LEU:HB3	4:4:621:LEU:HD23	1.83	0.59
7:7:76:ASN:OD1	7:7:199:ARG:NH2	2.35	0.59
2:B:343:LYS:HD3	2:B:367:CYS:HB3	1.84	0.59
2:B:776:PRO:HG2	2:B:818:GLU:HB2	1.84	0.59
2:2:537:ILE:HG23	2:2:678:ASP:HB2	1.84	0.59
4:4:445:ARG:HH21	4:4:451:ARG:H	1.50	0.59
8:8:293:CYS:SG	8:8:348:HIS:CG	2.87	0.59
2:B:340:ASN:HB3	2:B:347:ILE:HA	1.84	0.59
5:E:388:ILE:HG13	5:E:425:LEU:HD21	1.82	0.59
5:E:536:PRO:HB2	5:E:696:PRO:HD3	1.85	0.59
7:7:258:ILE:HD11	7:7:300:MET:HG2	1.85	0.59
4:D:323:ASP:O	7:G:303:ARG:NH2	2.34	0.59
7:G:209:GLN:HG2	7:G:222:SER:HB2	1.84	0.59
4:4:268:VAL:O	4:4:272:MET:HG3	2.00	0.59
7:7:584:ILE:HG22	7:7:586:LEU:H	1.68	0.59
5:5:65:MET:SD	5:5:161:ARG:NH1	2.74	0.59
5:5:569:ALA:O	5:5:573:ILE:HG12	2.03	0.59
9:9:171:THR:HA	9:9:199:MET:HE3	1.85	0.59
8:8:265:TYR:O	9:9:259:HIS:N	2.34	0.59
8:8:273:ILE:HD13	9:9:276:ALA:HB3	1.85	0.59
9:9:211:LEU:HD12	9:9:214:LEU:HB2	1.85	0.59
3:C:100:LEU:HD13	3:C:115:LEU:HD11	1.84	0.59
5:5:32:LYS:HZ2	5:5:100:ARG:HH22	1.49	0.59
6:6:294:VAL:HG21	6:6:389:ALA:HB1	1.85	0.59
8:8:433:GLU:HA	8:8:436:TRP:CD1	2.36	0.59
8:8:464:LEU:HA	8:8:469:PHE:HD2	1.68	0.59
2:B:794:ARG:CD	2:B:805:ILE:CD1	2.79	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:231:ILE:HD13	2:2:279:THR:HG22	1.83	0.58
3:3:490:MET:HB3	3:3:542:ARG:HD3	1.84	0.58
3:3:537:ASP:OD2	7:7:573:ARG:NH1	2.36	0.58
6:6:139:GLN:HA	6:6:142:PHE:HB3	1.85	0.58
6:6:783:ASP:OD1	6:6:784:ASP:N	2.36	0.58
9:9:534:ARG:HA	4:D:179:ILE:HG12	1.84	0.58
2:B:549:LYS:HD3	2:B:649:ALA:HB1	1.85	0.58
5:E:274:LEU:HD21	5:E:328:ILE:HG13	1.84	0.58
6:6:571:ILE:HG12	6:6:711:LEU:HB2	1.83	0.58
2:2:324:VAL:HG21	2:2:418:SER:HB2	1.85	0.58
6:F:309:PHE:HB3	6:F:344:TRP:HB3	1.86	0.58
5:5:90:PHE:CD2	5:5:137:LEU:HD22	2.39	0.58
7:7:281:LEU:HB2	7:7:298:LEU:HD11	1.86	0.58
7:G:537:ILE:O	7:G:541:MET:HG3	2.04	0.58
5:5:625:ASN:HD22	5:5:681:ILE:HG12	1.69	0.58
7:G:400:ARG:HH11	7:G:637:LYS:HE3	1.69	0.58
5:5:464:LEU:HD21	5:5:470:VAL:HG21	1.85	0.58
7:7:413:ARG:HH21	7:7:631:THR:HG23	1.67	0.58
8:8:76:LYS:HB3	8:8:118:ALA:HB3	1.85	0.58
4:D:794:THR:HG22	4:D:796:ARG:H	1.68	0.58
6:F:702:THR:HG22	6:F:705:ILE:HD12	1.86	0.58
6:6:119:LEU:HB3	6:6:136:TYR:CE2	2.37	0.58
4:D:228:LYS:HA	4:D:231:ASN:HD22	1.68	0.58
4:D:578:LEU:HD12	4:D:630:CYS:HB3	1.85	0.58
2:2:319:ARG:HG3	2:2:427:THR:HG22	1.86	0.58
6:6:706:MET:HA	6:6:712:PHE:HZ	1.69	0.58
7:7:275:SER:OG	7:7:277:THR:O	2.22	0.58
7:7:452:GLY:H	7:7:694:ARG:HH11	1.51	0.58
3:C:409:GLY:O	3:C:518:PRO:HD3	2.03	0.58
5:E:412:VAL:HG13	5:E:552:MET:HG3	1.86	0.58
3:3:244:GLU:OE1	7:7:109:ASN:ND2	2.37	0.57
7:7:267:TYR:CE2	7:7:288:GLU:HG2	2.39	0.57
9:9:125:ARG:HB3	9:9:170:VAL:HA	1.85	0.57
5:E:434:PRO:HB2	5:E:435:ILE:HD12	1.86	0.57
2:2:338:LYS:HD2	2:2:379:LYS:HB3	1.85	0.57
2:2:445:PRO:HB3	6:6:327:TYR:HE1	1.70	0.57
3:3:701:THR:HG23	3:3:733:LEU:HD21	1.86	0.57
7:7:162:ARG:NH2	7:7:178:ASN:OD1	2.37	0.57
7:7:179:ASP:OD1	7:7:180:ALA:N	2.35	0.57
2:B:477:THR:O	2:B:480:GLU:HG3	2.03	0.57
2:B:609:PHE:HB3	2:B:650:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:626:PHE:CZ	5:E:630:ARG:HD2	2.38	0.57
6:F:310:THR:HB	6:F:345:THR:HB	1.86	0.57
10:3:1001:ADP:H5'2	5:5:651:ARG:NH2	2.11	0.57
4:4:519:TYR:CD1	4:4:811:MET:HE3	2.37	0.57
4:4:735:HIS:CE1	4:4:737:SER:HB2	2.39	0.57
6:6:306:LYS:HA	6:6:322:GLU:HA	1.84	0.57
6:F:800:LEU:HA	6:F:803:MET:HE2	1.87	0.57
4:4:602:THR:OG1	4:4:603:ALA:N	2.38	0.57
9:9:345:GLN:HG2	9:9:346:TYR:CD1	2.39	0.57
2:B:336:TYR:HB2	2:B:381:VAL:HB	1.86	0.57
3:C:440:VAL:HG13	3:C:445:ALA:HB2	1.85	0.57
2:2:343:LYS:HZ3	2:2:372:PRO:HD3	1.68	0.57
9:9:182:ILE:HG22	9:9:184:LEU:H	1.69	0.57
2:B:279:THR:O	2:B:283:TYR:N	2.35	0.57
4:D:519:TYR:CE1	4:D:538:LYS:HE2	2.39	0.57
3:C:442:LEU:HD13	3:C:486:ILE:HD13	1.87	0.57
5:5:276:MET:HG2	5:5:328:ILE:HB	1.86	0.57
5:E:486:ARG:HG2	5:E:488:GLU:HG2	1.85	0.57
6:F:312:ASP:HB2	6:F:343:PHE:HB3	1.87	0.57
4:4:367:GLU:HG3	6:6:419:SER:HB3	1.85	0.57
10:B:901:ADP:O3B	6:F:798:ARG:NH2	2.37	0.57
5:E:90:PHE:CE2	5:E:137:LEU:HD13	2.40	0.57
5:E:369:ILE:HD12	5:E:592:SER:HA	1.85	0.57
3:3:390:GLU:OE1	3:3:467:ARG:NH1	2.33	0.57
7:7:86:LEU:HD22	7:7:207:LEU:HD11	1.86	0.56
9:9:129:ASP:O	9:9:148:ARG:NH1	2.38	0.56
3:C:39:ARG:HE	3:C:136:MET:HE1	1.70	0.56
2:2:202:ASN:OD1	2:2:205:ARG:NH1	2.38	0.56
4:4:179:ILE:HG22	4:4:186:SER:HB3	1.87	0.56
5:E:276:MET:HE3	5:E:294:ILE:HG21	1.87	0.56
7:7:479:ARG:NH1	7:7:517:ASP:O	2.38	0.56
2:B:552:ILE:O	2:B:556:VAL:HG23	2.05	0.56
6:F:306:LYS:HG2	6:F:322:GLU:HA	1.86	0.56
2:2:797:SER:HB2	2:2:804:PRO:HA	1.87	0.56
4:4:474:LEU:HD23	4:4:748:THR:HG22	1.88	0.56
5:E:455:ARG:NH1	5:E:460:ARG:O	2.36	0.56
6:F:158:LEU:HD11	6:F:166:LEU:HD23	1.86	0.56
2:2:285:ASP:OD2	2:2:288:ARG:NH1	2.37	0.56
8:8:127:GLU:HB2	8:8:130:THR:HG23	1.88	0.56
5:E:353:GLU:HG3	5:E:601:ARG:HH21	1.71	0.56
2:2:289:ILE:O	2:2:290:HIS:ND1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:622:GLU:OE1	5:5:445:SER:N	2.38	0.56
4:D:195:ARG:HH22	4:D:279:CYS:HA	1.71	0.56
5:E:490:ARG:HD3	5:E:546:ILE:HD11	1.88	0.56
3:3:293:ASN:HB3	3:3:327:TYR:HB2	1.88	0.56
4:4:640:SER:O	6:6:601:LYS:NZ	2.39	0.56
7:7:140:ASP:OD1	7:7:199:ARG:NE	2.37	0.56
2:2:260:LEU:HD21	2:2:297:ILE:HD13	1.88	0.56
5:5:657:ILE:O	5:5:661:GLU:HG2	2.06	0.56
2:B:340:ASN:HA	2:B:348:LEU:HG	1.86	0.56
4:D:239:SER:OG	4:D:299:LYS:NZ	2.39	0.56
3:3:367:LEU:HD12	3:3:421:PHE:HE2	1.72	0.55
7:7:209:GLN:HG3	7:7:222:SER:HB2	1.88	0.55
7:7:396:ASP:O	7:7:399:GLU:HG3	2.06	0.55
8:8:373:VAL:HG23	8:8:399:LEU:HD21	1.88	0.55
3:C:473:ASP:OD1	3:C:474:GLU:N	2.40	0.55
2:2:236:GLU:HG3	2:2:237:MET:SD	2.46	0.55
3:3:364:SER:HA	3:3:367:LEU:HD23	1.87	0.55
8:8:170:LEU:CD1	10:8:1001:ADP:C2	2.89	0.55
8:8:353:GLU:N	9:9:267:TYR:O	2.38	0.55
3:C:526:ASN:OD1	3:C:527:ARG:N	2.39	0.55
4:4:204:LYS:HB3	4:4:221:ASP:HB3	1.87	0.55
3:C:226:PRO:HD3	5:E:242:ILE:HD13	1.88	0.55
7:7:334:HIS:HD2	7:7:375:TYR:CG	2.25	0.55
9:9:113:GLN:O	9:9:117:LYS:N	2.39	0.55
2:B:795:ARG:HA	5:E:560:HIS:CE1	2.42	0.55
4:D:762:ILE:HA	4:D:817:VAL:HB	1.88	0.55
5:5:302:ASN:HA	5:5:324:ARG:HG3	1.87	0.55
6:6:510:SER:HA	6:6:513:ILE:HB	1.87	0.55
3:C:389:VAL:HG22	3:C:710:THR:HG21	1.89	0.55
5:E:90:PHE:CE2	5:E:94:ILE:HD11	2.42	0.55
5:5:151:LEU:HD13	5:5:298:TYR:HE2	1.72	0.55
7:7:193:PRO:HG2	5:E:9:TYR:CD2	2.42	0.55
2:B:384:ASN:HD21	5:E:153:SER:H	1.54	0.55
4:D:470:SER:O	4:D:499:ARG:NH2	2.38	0.55
5:E:169:THR:HB	5:E:254:GLN:HE21	1.71	0.55
8:8:83:SER:N	9:9:662:GLU:OE2	2.39	0.55
8:8:175:LEU:HD13	8:8:177:ARG:HE	1.71	0.55
8:8:398:PHE:HD1	8:8:436:TRP:HE3	1.54	0.55
9:9:149:ASP:OD1	9:9:150:LEU:N	2.40	0.55
2:B:239:SER:O	2:B:286:TYR:OH	2.25	0.55
6:F:276:ILE:HD13	6:F:363:GLU:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:406:ARG:NH2	2:2:449:THR:OG1	2.34	0.55
6:6:303:GLU:HB2	6:6:356:TRP:HB2	1.89	0.55
9:9:179:VAL:HG13	9:9:201:VAL:HG22	1.88	0.55
4:D:778:ARG:HG3	4:D:793:ALA:HB3	1.88	0.55
6:F:540:HIS:O	6:F:544:LYS:NZ	2.29	0.55
3:3:97:ILE:HD13	3:3:156:SER:HB2	1.89	0.54
7:7:664:TYR:OH	7:7:668:ARG:NH1	2.40	0.54
6:F:112:ARG:HB2	6:F:180:PHE:HB3	1.89	0.54
6:F:331:THR:HA	6:F:341:ARG:HD3	1.89	0.54
5:5:405:ARG:HH21	5:5:516:ARG:HG2	1.73	0.54
7:G:150:ASN:OD1	7:G:151:GLU:N	2.40	0.54
3:3:233:THR:HG23	3:3:234:GLU:HG2	1.89	0.54
8:8:317:PHE:HB3	8:8:318:PRO:HD3	1.89	0.54
2:B:693:GLU:HB2	6:F:778:LYS:HD3	1.88	0.54
6:F:126:SER:OG	6:F:129:THR:O	2.22	0.54
4:4:647:GLU:OE1	4:4:655:SER:N	2.39	0.54
8:8:322:SER:OG	8:8:324:ASP:O	2.26	0.54
4:D:618:SER:HB3	6:F:373:MET:HG2	1.90	0.54
5:E:175:ARG:NH1	5:E:253:GLN:OE1	2.40	0.54
6:F:319:ASP:HB3	6:F:350:ARG:HD3	1.88	0.54
2:2:271:PHE:HD2	2:2:295:VAL:HG21	1.73	0.54
4:4:756:GLU:OE2	4:4:757:HIS:ND1	2.41	0.54
5:5:407:ARG:NH2	5:5:658:ARG:HH22	2.06	0.54
6:6:777:TYR:HB2	6:6:800:LEU:HD13	1.90	0.54
2:2:855:ARG:O	2:2:859:ARG:N	2.40	0.54
6:F:347:ASN:HD21	6:F:350:ARG:HB2	1.73	0.54
2:2:789:VAL:HG11	2:2:838:ILE:HD13	1.89	0.54
3:C:443:THR:OG1	3:C:444:ALA:N	2.41	0.54
3:C:555:GLU:HB2	5:E:631:LYS:HE2	1.90	0.54
4:D:197:PHE:HB2	4:D:254:THR:HG21	1.90	0.54
6:F:115:PHE:HA	6:F:118:PHE:CE1	2.43	0.54
8:8:175:LEU:HB3	8:8:177:ARG:HG2	1.90	0.54
3:C:439:GLY:N	3:C:482:ASP:OD1	2.41	0.54
6:F:362:GLN:HG3	6:F:376:THR:CG2	2.36	0.54
6:F:702:THR:HG23	6:F:704:PRO:HD2	1.90	0.54
7:7:334:HIS:HD2	7:7:375:TYR:CD1	2.26	0.53
7:7:660:VAL:HG11	7:7:693:ILE:HD11	1.91	0.53
8:8:226:ILE:HG12	8:8:231:TYR:HD1	1.72	0.53
5:E:66:GLU:HA	5:E:69:ILE:HD13	1.88	0.53
5:E:172:LEU:HD23	5:E:254:GLN:HB2	1.90	0.53
6:F:737:LYS:HB2	6:F:740:GLU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:790:ARG:O	6:F:837:ARG:NH1	2.41	0.53
4:4:570:PRO:HD3	4:4:680:SER:O	2.07	0.53
5:5:66:GLU:O	5:5:69:ILE:HG12	2.09	0.53
7:7:127:LEU:HD12	7:7:128:PRO:HD2	1.90	0.53
7:7:513:LEU:HD23	7:7:540:VAL:HG21	1.91	0.53
9:9:203:SER:H	9:9:206:LYS:HB2	1.72	0.53
3:C:687:ARG:NH2	7:G:602:ASP:OD1	2.42	0.53
2:2:482:ARG:O	2:2:486:LYS:HG2	2.09	0.53
3:3:475:PHE:HB3	3:3:516:ALA:HB2	1.89	0.53
6:6:379:VAL:HG22	6:6:454:PHE:HB3	1.90	0.53
3:C:339:ARG:NE	3:C:661:GLN:OE1	2.41	0.53
4:D:656:ILE:HD11	4:D:658:LYS:HD2	1.90	0.53
5:E:530:TYR:HB2	5:E:539:ASN:HB2	1.90	0.53
6:F:589:VAL:HG11	6:F:597:TYR:HB2	1.89	0.53
4:4:725:THR:HB	7:7:657:ASN:HB2	1.91	0.53
7:7:284:CYS:SG	7:7:286:SER:OG	2.56	0.53
8:8:331:GLU:O	8:8:334:THR:OG1	2.22	0.53
8:8:372:PHE:O	8:8:376:LEU:HD23	2.07	0.53
5:E:266:PRO:HB2	5:E:269:GLU:HB2	1.89	0.53
5:5:381:ASN:HB3	5:5:384:ILE:HB	1.90	0.53
6:6:137:ARG:HA	6:6:140:ILE:HD12	1.90	0.53
4:D:449:ARG:HD2	4:D:450:GLN:N	2.24	0.53
5:E:551:ASP:OD2	5:E:658:ARG:NH1	2.42	0.53
3:3:507:ASN:ND2	7:7:319:SER:O	2.42	0.53
5:5:374:ILE:HD13	5:5:428:PHE:HE2	1.73	0.53
8:8:97:MET:HG3	8:8:157:LYS:HG3	1.91	0.53
4:D:217:ASN:ND2	4:D:219:THR:OG1	2.42	0.53
4:D:224:LEU:HD13	4:D:227:ILE:HD12	1.91	0.53
4:D:272:MET:HB3	4:D:303:VAL:HG21	1.90	0.53
4:D:354:HIS:CE1	4:D:372:GLU:HB3	2.44	0.53
2:B:309:LEU:O	2:B:313:ASN:ND2	2.41	0.53
2:B:794:ARG:HD3	2:B:805:ILE:HD11	1.89	0.53
4:D:483:GLN:HG3	4:D:484:GLU:HG2	1.89	0.53
4:D:640:SER:O	6:F:601:LYS:NZ	2.42	0.53
7:G:23:ASP:OD2	7:G:88:TYR:OH	2.26	0.53
4:4:321:ASP:HA	4:4:324:LYS:HD3	1.91	0.53
4:4:535:ASP:HA	4:4:538:LYS:HD2	1.90	0.53
9:9:349:ASP:HB3	9:9:352:LEU:HB3	1.91	0.53
2:B:253:LYS:HB3	2:B:256:LEU:HB3	1.91	0.53
6:F:801:GLU:HA	6:F:804:ILE:HD12	1.91	0.53
2:2:599:ALA:O	2:2:644:CYS:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:537:VAL:HG11	6:6:584:PHE:CZ	2.44	0.53
8:8:287:PRO:O	8:8:291:MET:HG2	2.09	0.53
2:B:794:ARG:HD3	2:B:805:ILE:CD1	2.38	0.53
3:C:195:LYS:N	3:C:251:ILE:O	2.41	0.53
3:C:402:ASP:HB3	3:C:511:SER:HB3	1.91	0.53
3:C:552:ASP:O	3:C:557:ARG:NH2	2.42	0.53
6:F:720:ASN:HB3	6:F:723:ILE:HG12	1.90	0.53
2:2:477:THR:HG22	2:2:479:GLU:H	1.73	0.53
3:3:480:ASP:O	3:3:484:VAL:HG23	2.09	0.53
5:5:356:GLU:O	5:5:359:GLN:HG3	2.09	0.53
6:6:275:ARG:HD2	6:6:367:GLU:HB2	1.89	0.53
9:9:270:ASP:OD2	9:9:274:THR:N	2.41	0.53
2:B:536:ASP:HB3	2:B:645:SER:HB3	1.89	0.53
3:C:535:LEU:HD22	3:C:539:LEU:HD23	1.91	0.53
5:E:65:MET:O	5:E:69:ILE:HD12	2.09	0.53
6:F:310:THR:N	6:F:345:THR:O	2.42	0.53
6:F:379:VAL:HG22	6:F:454:PHE:HB3	1.91	0.53
7:G:451:ARG:NH1	7:G:453:ASP:O	2.42	0.53
2:2:296:ARG:HD2	2:2:454:ASN:O	2.08	0.52
2:2:485:ARG:NH2	2:2:489:ARG:HE	2.06	0.52
4:4:571:SER:OG	7:7:686:PRO:HD2	2.08	0.52
5:5:149:ARG:NH1	5:5:272:ARG:HD3	2.23	0.52
8:8:88:TYR:HE1	9:9:696:LEU:HD13	1.72	0.52
2:B:800:THR:HG23	2:B:856:GLN:HE21	1.74	0.52
2:2:233:THR:HG23	2:2:237:MET:HE2	1.91	0.52
2:2:332:PRO:HG2	5:5:300:ILE:HD11	1.91	0.52
5:E:261:ILE:HD13	5:E:264:LEU:HD12	1.91	0.52
5:E:418:PRO:HA	10:E:802:ADP:O3B	2.09	0.52
2:2:631:ILE:HA	5:5:446:ALA:HB3	1.92	0.52
3:3:579:GLY:O	5:5:611:ALA:N	2.42	0.52
4:4:513:ALA:HA	4:4:518:LEU:HD22	1.92	0.52
4:4:689:THR:HG22	4:4:791:ILE:HG23	1.90	0.52
9:9:136:MET:HG3	9:9:140:ASN:HB3	1.91	0.52
3:C:570:ARG:HA	5:E:613:ARG:HH11	1.75	0.52
6:F:442:SER:OG	6:F:443:LEU:N	2.42	0.52
6:6:526:TYR:HB2	6:6:814:ASN:HD21	1.73	0.52
8:8:281:THR:N	8:8:285:ARG:HH21	2.07	0.52
4:D:187:ILE:HG12	4:D:271:ILE:HD11	1.91	0.52
4:4:347:PHE:HE1	4:4:384:LEU:HD12	1.74	0.52
5:5:422:LYS:HB2	10:5:801:ADP:O2B	2.08	0.52
2:B:332:PRO:HG2	5:E:300:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:566:LEU:O	3:C:570:ARG:HG2	2.10	0.52
2:2:522:GLY:O	2:2:822:LYS:NZ	2.42	0.52
3:3:590:LEU:HG	3:3:592:VAL:HG13	1.92	0.52
6:6:613:VAL:O	6:6:622:THR:N	2.40	0.52
2:B:239:SER:OG	2:B:240:GLU:N	2.43	0.52
2:B:703:HIS:CD2	6:F:565:LEU:HD13	2.45	0.52
7:G:596:ILE:HD11	7:G:695:LEU:HD21	1.91	0.52
3:3:558:ASP:OD2	5:5:630:ARG:HG3	2.10	0.52
3:3:696:PRO:HB3	7:7:573:ARG:HH22	1.75	0.52
4:4:654:ILE:HG23	4:4:665:LEU:HB2	1.91	0.52
8:8:138:LYS:HG2	9:9:344:PHE:CD2	2.45	0.52
4:D:281:VAL:HA	4:D:284:ILE:HD12	1.92	0.52
7:G:143:LEU:HD22	7:G:197:THR:HA	1.92	0.52
3:3:398:HIS:NE2	3:3:493:GLN:OE1	2.32	0.52
6:6:136:TYR:CZ	6:6:140:ILE:HD11	2.45	0.52
4:D:204:LYS:HB3	4:D:221:ASP:HB3	1.91	0.52
3:3:561:ILE:HG21	5:5:650:ILE:HG12	1.92	0.52
4:4:349:CYS:HA	4:4:382:MET:HA	1.92	0.52
4:4:559:ARG:HB2	4:4:652:GLN:HG3	1.90	0.52
4:4:645:LEU:O	4:4:649:MET:HB2	2.09	0.52
6:6:198:ASN:O	6:6:261:ARG:NH1	2.43	0.52
7:7:255:VAL:HG22	7:7:307:PHE:HE1	1.75	0.52
8:8:32:GLU:OE1	8:8:32:GLU:N	2.43	0.52
2:B:447:PHE:CE2	6:F:304:LEU:HD21	2.44	0.52
6:6:614:ARG:NE	6:6:619:GLY:O	2.32	0.52
2:B:181:LEU:N	2:B:206:THR:OG1	2.34	0.52
2:B:856:GLN:HE22	2:B:859:ARG:HD2	1.75	0.52
2:2:260:LEU:HB2	2:2:267:MET:HE2	1.92	0.51
4:4:795:THR:OG1	10:6:1101:ADP:O4'	2.28	0.51
7:7:423:TYR:HB2	7:7:615:HIS:CD2	2.45	0.51
8:8:138:LYS:HZ1	9:9:347:HIS:HB2	1.74	0.51
2:B:656:ARG:NE	6:F:794:ARG:HG3	2.25	0.51
3:C:489:VAL:HG22	3:C:495:VAL:HG22	1.92	0.51
3:C:683:TYR:OH	3:C:687:ARG:NH1	2.43	0.51
5:5:83:PRO:HG3	5:5:159:ILE:HG13	1.91	0.51
3:C:672:THR:OG1	3:C:721:VAL:O	2.28	0.51
4:D:604:TYR:CE1	4:D:617:GLU:HG2	2.46	0.51
7:G:607:ASP:O	7:G:610:GLU:HG3	2.09	0.51
9:9:246:PRO:O	9:9:249:ARG:NH1	2.43	0.51
4:D:447:ASN:OD1	4:D:450:GLN:NE2	2.28	0.51
5:E:605:TYR:CZ	5:E:609:LYS:HG3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:399:GLY:HA3	6:F:456:ALA:HA	1.92	0.51
2:2:525:LYS:HD2	2:2:533:ILE:HD12	1.92	0.51
3:3:700:ARG:HE	10:7:1102:ADP:H5'2	1.76	0.51
6:F:277:ARG:NH2	6:F:372:SER:HB2	2.25	0.51
6:F:290:ILE:HG13	6:F:397:PHE:HB2	1.93	0.51
7:7:607:ASP:OD1	7:7:608:ASP:N	2.42	0.51
4:D:799:GLU:HA	4:D:802:ILE:HD12	1.91	0.51
4:4:334:ARG:NH1	4:4:617:GLU:OE2	2.43	0.51
6:F:120:GLU:OE2	6:F:137:ARG:NH2	2.28	0.51
3:3:330:HIS:CG	3:3:338:ALA:HB2	2.46	0.51
4:4:342:MET:HE3	6:6:448:LEU:HD21	1.93	0.51
4:4:373:ARG:HD2	4:4:375:ASP:HB3	1.92	0.51
5:5:581:ASN:OD1	5:5:582:ALA:N	2.43	0.51
8:8:61:PHE:HB3	8:8:64:HIS:HB2	1.93	0.51
8:8:145:TRP:HE1	8:8:472:LEU:HB3	1.76	0.51
9:9:130:ILE:O	9:9:176:ARG:NH2	2.29	0.51
10:C:1001:ADP:O1B	5:E:651:ARG:NH2	2.43	0.51
6:F:122:PHE:HE1	6:F:161:ARG:HB2	1.76	0.51
7:G:62:LYS:NZ	7:G:84:ASP:OD2	2.32	0.51
4:4:649:MET:HG2	4:4:701:ARG:HD3	1.92	0.51
7:7:149:ARG:NH2	5:E:13:VAL:O	2.41	0.51
2:B:505:ILE:HD11	10:B:901:ADP:C5	2.46	0.51
2:B:661:LEU:HD22	2:B:665:GLN:HG3	1.93	0.51
3:C:687:ARG:NH1	7:G:609:ASP:OD2	2.44	0.51
3:3:545:LEU:HD11	3:3:708:LEU:HD11	1.93	0.51
5:E:152:ASP:OD1	5:E:153:SER:N	2.44	0.51
5:E:341:SER:H	5:E:344:ASN:HB3	1.76	0.51
3:3:261:MET:HE1	3:3:588:LEU:HD11	1.93	0.51
5:5:32:LYS:HZ2	5:5:100:ARG:NH2	2.08	0.51
4:D:599:VAL:HG12	4:D:604:TYR:HB3	1.92	0.51
5:E:139:LEU:HD12	5:E:331:LEU:HD13	1.93	0.51
2:2:338:LYS:HE2	2:2:350:PRO:HG3	1.92	0.50
8:8:155:HIS:CD2	8:8:298:THR:HB	2.46	0.50
2:B:296:ARG:NH2	2:B:413:ASP:OD1	2.44	0.50
2:B:796:GLU:HB3	2:B:856:GLN:HE22	1.74	0.50
4:D:534:GLU:OE2	4:D:538:LYS:HD2	2.11	0.50
2:2:474:PHE:O	2:2:768:HIS:ND1	2.40	0.50
2:2:630:SER:HB3	2:2:639:THR:HG22	1.92	0.50
3:3:214:TYR:CD1	3:3:229:ALA:HB1	2.46	0.50
4:4:308:VAL:HG11	4:4:325:LEU:HD23	1.93	0.50
5:5:453:VAL:HG21	5:5:504:ILE:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:170:LEU:HD11	10:8:1001:ADP:C4	2.46	0.50
3:C:255:ARG:NH1	7:G:366:LEU:HA	2.27	0.50
4:D:334:ARG:HD3	4:D:615:VAL:HG11	1.92	0.50
5:E:99:LYS:O	5:E:103:ILE:HG12	2.11	0.50
9:9:187:ASP:O	9:9:193:ARG:NH2	2.44	0.50
4:D:189:GLU:OE2	4:D:193:ASN:ND2	2.45	0.50
5:E:383:ASP:OD1	5:E:682:ARG:NH2	2.27	0.50
6:F:628:LEU:HD11	6:F:652:ILE:HD13	1.93	0.50
7:G:162:ARG:NH2	7:G:178:ASN:OD1	2.44	0.50
7:7:517:ASP:OD1	7:7:560:ARG:N	2.44	0.50
9:9:319:SER:O	9:9:323:VAL:HG23	2.12	0.50
3:C:565:VAL:O	3:C:568:THR:OG1	2.27	0.50
4:D:724:LEU:HD12	7:G:689:LEU:HD23	1.93	0.50
5:E:178:TYR:CE1	5:E:191:SER:HB3	2.46	0.50
6:F:821:PRO:HA	6:F:824:ILE:HD12	1.93	0.50
7:7:524:ASP:OD2	7:7:525:GLU:N	2.44	0.50
2:B:854:ARG:HH11	2:B:857:LEU:HD22	1.76	0.50
3:C:570:ARG:HH21	5:E:616:PRO:HG3	1.77	0.50
2:2:275:ALA:O	2:2:279:THR:HG23	2.11	0.50
2:2:534:ARG:O	2:2:815:ARG:HD3	2.12	0.50
5:5:69:ILE:HG22	5:5:76:TYR:CG	2.46	0.50
4:D:773:ALA:O	4:D:777:MET:HG3	2.11	0.50
4:4:545:PHE:HE1	4:4:751:ILE:HA	1.76	0.50
5:5:444:SER:HB2	5:5:447:ALA:HB3	1.93	0.50
4:D:352:CYS:SG	4:D:354:HIS:HB2	2.52	0.50
7:7:230:ILE:HD12	7:7:239:ILE:HD12	1.93	0.50
2:2:200:GLN:O	2:2:204:SER:N	2.36	0.50
2:2:390:LEU:HD23	2:2:408:VAL:HB	1.94	0.50
4:4:451:ARG:CZ	6:6:445:VAL:HG13	2.41	0.50
3:C:402:ASP:OD2	3:C:493:GLN:NE2	2.45	0.50
6:F:307:ALA:N	6:F:321:VAL:O	2.45	0.50
7:G:221:SER:OG	7:G:238:LEU:O	2.30	0.50
7:G:481:VAL:HG21	7:G:512:ALA:HB1	1.94	0.50
7:G:692:ILE:HD12	7:G:717:LEU:HD22	1.94	0.50
4:4:548:THR:N	4:4:806:GLU:OE1	2.41	0.49
6:6:357:GLN:NE2	6:6:387:GLU:OE1	2.40	0.49
8:8:266:PRO:HA	9:9:258:ILE:HA	1.93	0.49
9:9:241:GLU:OE2	6:F:107:THR:OG1	2.20	0.49
7:G:534:ARG:O	7:G:537:ILE:HG22	2.12	0.49
4:4:647:GLU:HG2	4:4:653:THR:O	2.13	0.49
4:D:700:SER:OG	4:D:794:THR:HG21	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:453:VAL:HG23	5:E:504:ILE:HD13	1.92	0.49
6:F:599:SER:OG	6:F:600:GLY:N	2.45	0.49
2:2:296:ARG:HB3	2:2:455:SER:HB2	1.93	0.49
2:2:361:ILE:HB	2:2:373:PHE:HB3	1.93	0.49
2:2:610:ASP:OD1	2:2:610:ASP:N	2.44	0.49
3:3:214:TYR:HD1	3:3:229:ALA:HB1	1.76	0.49
8:8:393:PHE:HB3	9:9:369:HIS:CD2	2.46	0.49
9:9:178:SER:HA	9:9:181:ASN:HB2	1.94	0.49
3:C:407:MET:HE2	3:C:415:LYS:HA	1.94	0.49
2:2:814:LEU:O	2:2:818:GLU:HG2	2.12	0.49
8:8:301:ASP:O	8:8:305:VAL:HG23	2.12	0.49
3:C:98:ILE:HG13	3:C:155:LEU:HD11	1.94	0.49
4:D:385:ILE:HG21	4:D:388:ARG:HD3	1.94	0.49
4:D:428:ARG:HH12	4:D:481:ILE:HD11	1.77	0.49
5:E:185:ASN:OD1	5:E:186:CYS:N	2.44	0.49
2:2:309:LEU:HD21	2:2:451:ILE:HD11	1.94	0.49
2:2:524:PRO:HA	2:2:535:GLY:HA3	1.94	0.49
4:4:812:LYS:O	4:4:813:LEU:HB2	2.11	0.49
4:D:293:LEU:HD23	4:D:293:LEU:H	1.77	0.49
5:E:355:GLU:O	5:E:359:GLN:HG2	2.11	0.49
6:F:115:PHE:HD2	6:F:118:PHE:CE1	2.30	0.49
6:F:579:THR:HB	6:F:715:ILE:HG21	1.94	0.49
2:2:194:TYR:O	2:2:198:ILE:HG12	2.12	0.49
3:3:447:THR:HB	3:3:458:GLU:HG3	1.95	0.49
4:4:721:ALA:HB2	7:7:664:TYR:HD2	1.77	0.49
5:5:90:PHE:HD2	5:5:137:LEU:HD22	1.75	0.49
5:5:656:ILE:HD13	5:5:659:ILE:HD12	1.94	0.49
6:6:696:ARG:NH1	6:6:791:SER:O	2.45	0.49
7:7:117:PHE:O	7:7:121:ILE:HG12	2.11	0.49
7:7:499:LYS:CB	7:7:506:MET:SD	3.01	0.49
9:9:534:ARG:HG2	4:D:177:LEU:HD23	1.94	0.49
7:7:267:TYR:HE2	7:7:288:GLU:HG2	1.78	0.49
4:D:718:ARG:HG2	4:D:722:LYS:HE2	1.94	0.49
7:7:607:ASP:O	7:7:610:GLU:HG3	2.12	0.49
8:8:136:PRO:O	8:8:139:GLY:N	2.44	0.49
9:9:250:ASP:OD1	9:9:250:ASP:N	2.45	0.49
2:B:626:GLN:NE2	5:E:430:GLU:OE2	2.46	0.49
5:E:622:LEU:HD13	5:E:657:ILE:HG12	1.94	0.49
3:3:499:LYS:HD3	7:7:488:SER:HA	1.95	0.49
2:B:364:CYS:HB3	2:B:369:SER:H	1.77	0.49
4:D:512:VAL:HA	4:D:515:ARG:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:74:ASP:N	5:E:74:ASP:OD1	2.45	0.49
4:4:444:ILE:HD11	6:6:411:GLY:HA2	1.94	0.49
6:6:443:LEU:HD23	7:7:282:SER:HB3	1.93	0.49
8:8:134:ASP:OD1	8:8:134:ASP:N	2.46	0.49
9:9:206:LYS:HA	9:9:209:ARG:HD2	1.95	0.49
3:C:524:ASP:OD2	3:C:527:ARG:NH2	2.45	0.49
7:G:286:SER:O	7:G:290:SER:N	2.44	0.49
4:4:319:PRO:HB3	7:7:253:PRO:HB3	1.95	0.48
6:6:453:SER:OG	6:6:454:PHE:N	2.46	0.48
8:8:268:ASN:HA	9:9:525:LYS:HZ1	1.77	0.48
2:B:534:ARG:HG2	2:B:536:ASP:H	1.78	0.48
3:C:25:VAL:HG21	3:C:127:LYS:HD3	1.94	0.48
4:D:765:ALA:HB1	4:D:819:LEU:HD21	1.95	0.48
5:E:152:ASP:HB3	5:E:154:GLU:HG2	1.95	0.48
2:2:271:PHE:HA	2:2:274:VAL:HG22	1.94	0.48
4:4:681:ARG:HH12	7:7:683:GLN:HB3	1.78	0.48
5:5:629:ILE:O	5:5:632:GLN:HG3	2.12	0.48
9:9:144:MET:HE1	9:9:176:ARG:HD2	1.94	0.48
9:9:192:SER:OG	9:9:193:ARG:NH1	2.45	0.48
2:B:335:LYS:HB2	2:B:383:ARG:HD2	1.94	0.48
6:F:309:PHE:HA	6:F:346:LEU:HA	1.95	0.48
2:2:494:ILE:HD11	2:2:824:ARG:HD3	1.95	0.48
6:6:112:ARG:O	6:6:116:GLU:HG3	2.13	0.48
9:9:372:ASN:HA	9:9:376:LYS:HE2	1.94	0.48
3:C:304:GLY:HA3	3:C:317:PHE:CD1	2.48	0.48
4:D:272:MET:O	4:D:276:ILE:HG12	2.13	0.48
6:F:115:PHE:CD1	6:F:181:LEU:HA	2.48	0.48
5:5:90:PHE:HE2	5:5:137:LEU:HD13	1.79	0.48
5:5:654:GLU:O	5:5:658:ARG:NE	2.39	0.48
6:6:280:ARG:HD3	6:6:280:ARG:HA	1.68	0.48
2:B:383:ARG:HH22	2:B:411:LEU:HD13	1.78	0.48
4:4:272:MET:O	4:4:276:ILE:HG12	2.14	0.48
5:5:53:ASN:HB3	5:5:58:ASN:O	2.13	0.48
6:6:309:PHE:HB3	6:6:344:TRP:CE3	2.48	0.48
8:8:96:ILE:HG13	8:8:97:MET:SD	2.53	0.48
8:8:182:ASP:HB2	10:8:1001:ADP:O2A	2.13	0.48
3:3:233:THR:OG1	5:E:5:ARG:HB2	2.14	0.48
3:3:437:SER:HB3	5:5:505:ALA:HB3	1.96	0.48
7:7:654:GLU:HA	7:7:657:ASN:HD21	1.78	0.48
8:8:162:ARG:HE	8:8:279:ALA:HB3	1.78	0.48
2:B:630:SER:HA	2:B:639:THR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:79:ILE:HD13	7:G:203:TYR:HB2	1.95	0.48
2:2:800:THR:HA	2:2:855:ARG:HH21	1.79	0.48
4:4:199:MET:SD	4:4:227:ILE:HD11	2.54	0.48
4:4:340:PRO:HB2	4:4:391:PHE:CD1	2.48	0.48
8:8:426:TYR:CE1	8:8:429:LYS:HE2	2.49	0.48
6:F:110:LYS:O	6:F:113:GLU:HG3	2.13	0.48
3:3:295:VAL:HG12	3:3:325:THR:HB	1.96	0.48
4:4:204:LYS:HB2	4:4:216:ILE:HD11	1.95	0.48
5:5:90:PHE:CE2	5:5:94:ILE:HD11	2.48	0.48
8:8:227:MET:HE2	8:8:295:ALA:HB2	1.96	0.48
9:9:202:TRP:HE3	9:9:206:LYS:HB3	1.79	0.48
4:D:525:SER:HB3	4:D:747:LEU:HD22	1.96	0.48
3:3:687:ARG:NH2	7:7:602:ASP:OD2	2.47	0.48
8:8:274:LYS:HB2	8:8:292:LYS:HE3	1.96	0.48
3:C:28:PHE:HD1	3:C:110:PHE:CE2	2.32	0.48
4:D:350:ASN:N	4:D:381:SER:O	2.42	0.48
4:D:431:ASP:OD2	4:D:468:LYS:NZ	2.47	0.48
5:E:178:TYR:HE1	5:E:191:SER:HB3	1.79	0.48
6:F:279:ILE:HG21	6:F:452:ILE:HG21	1.95	0.48
6:F:657:GLU:HG3	6:F:708:ARG:NE	2.29	0.48
7:G:497:VAL:HG13	7:G:497:VAL:O	2.14	0.48
3:3:187:THR:HG21	3:3:259:GLN:OE1	2.14	0.48
3:3:564:HIS:CE1	3:3:628:LEU:HB2	2.49	0.48
3:C:220:THR:HG21	3:C:224:ARG:HG3	1.94	0.48
4:D:727:LEU:O	4:D:733:PRO:HG2	2.14	0.48
4:4:341:ASP:N	4:4:392:ALA:O	2.46	0.47
5:5:457:PRO:HA	5:5:460:ARG:HH11	1.78	0.47
8:8:466:THR:HG23	8:8:469:PHE:H	1.79	0.47
9:9:250:ASP:OD2	9:9:252:ARG:NH2	2.44	0.47
2:B:202:ASN:HA	2:B:205:ARG:HD3	1.96	0.47
5:E:69:ILE:HG13	5:E:76:TYR:CD2	2.49	0.47
5:E:630:ARG:HH12	5:E:649:THR:HA	1.79	0.47
7:G:481:VAL:HG22	7:G:516:ALA:HB2	1.96	0.47
6:6:711:LEU:HD21	6:6:806:LEU:HD11	1.95	0.47
8:8:135:LEU:HD11	8:8:139:GLY:HA3	1.94	0.47
8:8:330:LEU:HD11	9:9:297:PRO:HD2	1.96	0.47
9:9:119:ILE:O	9:9:123:ASP:N	2.47	0.47
5:E:444:SER:HB2	5:E:447:ALA:HB3	1.96	0.47
6:F:803:MET:HG3	6:F:831:LEU:HD12	1.95	0.47
3:3:454:GLU:HG3	3:3:455:ARG:HG3	1.96	0.47
2:B:809:HIS:O	2:B:813:ILE:HD12	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:35:ILE:HD11	5:E:90:PHE:CZ	2.49	0.47
6:F:143:MET:SD	6:F:148:LEU:HB2	2.54	0.47
3:3:420:ARG:NH2	5:5:501:THR:OG1	2.47	0.47
5:5:353:GLU:O	5:5:356:GLU:HG2	2.14	0.47
6:6:144:LYS:HG3	6:6:196:LEU:HB3	1.96	0.47
3:C:687:ARG:HG2	7:G:609:ASP:OD2	2.15	0.47
4:D:559:ARG:HB2	4:D:652:GLN:HG3	1.95	0.47
5:E:300:ILE:HG23	5:E:324:ARG:HB3	1.96	0.47
2:2:536:ASP:HB3	2:2:645:SER:HB3	1.95	0.47
2:2:804:PRO:HD3	5:5:529:ARG:NH2	2.30	0.47
3:3:32:LEU:HD13	3:3:132:LEU:HD13	1.96	0.47
6:6:311:CYS:HB2	6:6:344:TRP:CH2	2.49	0.47
6:6:316:ALA:HB3	6:6:334:PRO:HG3	1.96	0.47
6:6:406:ASP:O	6:6:449:THR:OG1	2.21	0.47
6:6:816:VAL:HG21	6:6:823:PHE:HZ	1.79	0.47
7:7:289:CYS:O	7:7:295:LYS:NZ	2.39	0.47
8:8:45:SER:HB2	8:8:78:ILE:HA	1.96	0.47
8:8:138:LYS:HE3	9:9:348:ALA:H	1.79	0.47
2:B:202:ASN:HA	2:B:205:ARG:HH11	1.80	0.47
2:B:433:ASN:HB2	2:B:450:ILE:HG12	1.96	0.47
5:E:200:ILE:HG13	5:E:329:LYS:HZ1	1.80	0.47
5:E:477:VAL:HG13	5:E:519:VAL:HG23	1.96	0.47
3:3:177:ASN:ND2	5:5:245:HIS:O	2.48	0.47
3:3:211:TYR:CD1	7:7:8:ILE:HD11	2.50	0.47
4:4:256:ASP:HB3	7:7:134:TYR:CD2	2.49	0.47
4:4:443:PRO:HB2	4:4:453:LEU:HD13	1.96	0.47
6:6:199:THR:O	6:6:261:ARG:NH2	2.47	0.47
6:6:313:MET:HB3	6:6:338:CYS:SG	2.55	0.47
2:2:814:LEU:HD11	5:5:573:ILE:HG22	1.97	0.47
3:3:223:THR:N	5:5:246:GLU:OE2	2.38	0.47
5:5:169:THR:HG23	5:5:288:PRO:HG3	1.95	0.47
5:5:531:ASP:N	5:5:531:ASP:OD1	2.47	0.47
6:6:720:ASN:HB3	6:6:723:ILE:HG22	1.97	0.47
6:6:776:LYS:HD2	6:6:828:TYR:CG	2.50	0.47
6:6:829:ASP:HA	6:6:832:ARG:HG2	1.96	0.47
7:7:499:LYS:HG3	7:7:506:MET:SD	2.55	0.47
7:7:669:GLN:O	7:7:673:ARG:HG3	2.14	0.47
8:8:21:GLN:NE2	8:8:25:ASP:OD2	2.47	0.47
8:8:85:GLN:NE2	8:8:89:ASN:OD1	2.48	0.47
8:8:170:LEU:HD11	10:8:1001:ADP:C2	2.50	0.47
9:9:661:CYS:O	9:9:665:ARG:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:TYR:HE2	2:B:352:PHE:HD2	1.62	0.47
3:C:415:LYS:NZ	13:E:801:BEF:F2	2.35	0.47
7:G:367:LYS:HA	7:G:371:LEU:HD12	1.96	0.47
3:3:442:LEU:HD13	3:3:462:MET:HE3	1.96	0.47
6:6:144:LYS:HA	6:6:196:LEU:HD13	1.96	0.47
7:7:648:LYS:NZ	7:7:704:LEU:HB3	2.30	0.47
8:8:139:GLY:HA2	9:9:344:PHE:CE2	2.50	0.47
2:B:334:LEU:HB3	2:B:337:VAL:HG22	1.97	0.47
3:C:544:ASP:OD1	3:C:707:ARG:NH2	2.36	0.47
4:D:315:ARG:CZ	4:D:413:HIS:HB2	2.45	0.47
4:D:393:ASP:HB3	4:D:424:VAL:HG21	1.97	0.47
2:2:808:ARG:HG3	10:5:801:ADP:H4'	1.97	0.47
3:3:569:HIS:HA	5:5:398:LYS:HD3	1.96	0.47
4:4:234:ARG:HG3	4:4:280:MET:HE3	1.97	0.47
5:5:20:ASN:N	5:5:23:ASP:OD2	2.48	0.47
5:5:448:GLY:O	5:5:468:ALA:N	2.47	0.47
5:5:483:ASP:N	5:5:483:ASP:OD1	2.46	0.47
6:6:611:ALA:HB3	6:6:624:GLU:HB3	1.97	0.47
2:B:189:VAL:HG22	2:B:197:TRP:CG	2.49	0.47
2:B:502:ALA:O	2:B:505:ILE:HG22	2.15	0.47
3:C:462:MET:HE2	3:C:486:ILE:HD11	1.97	0.47
3:C:519:VAL:HG23	3:C:532:ASN:O	2.15	0.47
5:E:100:ARG:O	5:E:104:LEU:HD23	2.15	0.47
6:F:303:GLU:OE2	6:F:354:LEU:HB2	2.14	0.47
6:F:623:ILE:HD11	6:F:668:ILE:HG21	1.97	0.47
7:G:530:ASP:N	7:G:530:ASP:OD1	2.48	0.47
2:2:553:LEU:HD22	2:2:605:LEU:HD22	1.96	0.47
4:4:356:MET:CE	4:4:372:GLU:H	2.27	0.47
6:6:589:VAL:HG11	6:6:597:TYR:HB2	1.97	0.47
5:E:181:ILE:HG13	5:E:190:THR:HB	1.97	0.47
5:E:338:GLU:HG3	5:E:339:THR:H	1.80	0.47
5:E:486:ARG:HB2	5:E:486:ARG:NH1	2.29	0.47
6:F:500:ASP:HB3	6:F:502:GLU:HG2	1.97	0.47
6:F:529:LEU:HD23	6:F:751:LEU:HD22	1.97	0.47
6:F:580:SER:HB2	6:F:583:GLN:HB2	1.97	0.47
7:G:644:TYR:O	7:G:647:THR:OG1	2.21	0.47
4:4:193:ASN:ND2	4:4:253:GLN:O	2.34	0.46
5:5:258:LEU:HB2	5:5:276:MET:CE	2.45	0.46
7:7:472:ALA:O	7:7:476:ILE:HD12	2.15	0.46
8:8:370:LYS:O	8:8:374:TYR:HB2	2.15	0.46
8:8:471:GLU:HG3	9:9:348:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:330:HIS:CG	3:C:338:ALA:HB2	2.50	0.46
3:C:491:GLU:HG2	3:C:700:ARG:HH21	1.80	0.46
4:D:694:LEU:HD13	4:D:698:LEU:HD23	1.96	0.46
7:G:81:ASP:OD1	7:G:205:LYS:HD2	2.15	0.46
2:2:660:THR:HA	2:2:851:VAL:HG22	1.97	0.46
5:5:87:ILE:HG22	5:5:88:PRO:HD3	1.97	0.46
5:5:637:GLU:OE1	5:5:643:ARG:HA	2.15	0.46
9:9:189:ASP:O	9:9:192:SER:OG	2.25	0.46
7:G:410:VAL:HG21	7:G:641:TYR:CZ	2.50	0.46
7:G:671:SER:HB3	7:G:683:GLN:HA	1.97	0.46
4:4:356:MET:HE3	4:4:372:GLU:H	1.80	0.46
5:5:5:ARG:NH1	3:C:234:GLU:OE2	2.48	0.46
7:7:583:ASN:O	7:7:583:ASN:ND2	2.46	0.46
8:8:379:LYS:NZ	9:9:301:ILE:HB	2.30	0.46
2:B:505:ILE:HD11	10:B:901:ADP:C6	2.50	0.46
2:B:560:ALA:HB3	2:B:563:ALA:HB2	1.97	0.46
5:E:554:PHE:CZ	5:E:687:SER:HB3	2.50	0.46
2:2:760:GLN:O	2:2:764:MET:HG3	2.15	0.46
3:3:415:LYS:HE2	3:3:415:LYS:HB2	1.74	0.46
4:4:575:SER:HB2	10:4:1102:ADP:O1A	2.15	0.46
5:5:625:ASN:ND2	5:5:681:ILE:HG12	2.30	0.46
8:8:98:THR:HA	8:8:105:PRO:HB3	1.98	0.46
2:B:591:LEU:O	5:E:259:GLN:NE2	2.41	0.46
5:E:382:GLU:OE1	5:E:382:GLU:N	2.47	0.46
2:2:810:LEU:HA	2:2:813:ILE:HD12	1.97	0.46
3:3:216:ASP:OD1	3:3:219:THR:OG1	2.23	0.46
4:4:315:ARG:CZ	4:4:413:HIS:HB2	2.45	0.46
4:4:340:PRO:HG3	6:6:452:ILE:HG13	1.97	0.46
2:B:303:ILE:HG13	2:B:319:ARG:HD3	1.96	0.46
3:C:698:THR:CG2	7:G:573:ARG:HH22	2.29	0.46
5:E:484:LYS:HD2	5:E:484:LYS:HA	1.79	0.46
7:G:656:VAL:HG13	7:G:713:VAL:HG21	1.98	0.46
3:3:43:ARG:HA	3:3:43:ARG:HD2	1.73	0.46
5:5:338:GLU:HG3	5:5:339:THR:H	1.80	0.46
7:7:618:TYR:HB3	7:7:626:PRO:HG3	1.97	0.46
2:B:690:GLU:HG3	2:B:694:ARG:NH1	2.30	0.46
3:C:341:MET:SD	3:C:341:MET:N	2.88	0.46
3:3:291:ARG:O	3:3:329:LEU:N	2.34	0.46
4:4:460:TYR:CG	6:6:413:PRO:HB3	2.51	0.46
4:4:761:ILE:HG22	4:4:816:VAL:HG12	1.98	0.46
5:5:439:THR:HG22	5:5:440:SER:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:243:GLY:HA2	7:7:318:LEU:HG	1.97	0.46
7:7:471:LYS:O	7:7:475:LYS:HG2	2.16	0.46
4:4:519:TYR:CD1	4:4:811:MET:HE1	2.48	0.46
5:5:27:ILE:HG23	5:5:75:ILE:HD11	1.97	0.46
8:8:138:LYS:HZ2	9:9:347:HIS:H	1.63	0.46
8:8:170:LEU:HD11	10:8:1001:ADP:N3	2.31	0.46
8:8:325:ASP:OD1	8:8:326:ALA:N	2.49	0.46
8:8:453:ASP:HB3	8:8:456:LYS:HB3	1.98	0.46
9:9:675:ILE:HA	9:9:680:HIS:CD2	2.51	0.46
2:B:208:ALA:O	2:B:212:LYS:HG3	2.16	0.46
2:B:521:GLY:HA2	2:B:537:ILE:HD12	1.98	0.46
2:B:662:PRO:O	2:B:666:ASN:ND2	2.47	0.46
5:E:552:MET:HB2	5:E:687:SER:HB2	1.98	0.46
2:2:233:THR:HG23	2:2:237:MET:CE	2.45	0.46
2:2:252:SER:OG	2:2:253:LYS:N	2.49	0.46
2:2:271:PHE:CD2	2:2:295:VAL:HG21	2.50	0.46
8:8:265:TYR:C	9:9:258:ILE:HG13	2.36	0.46
2:B:793:LEU:HD12	2:B:805:ILE:HG21	1.98	0.46
2:2:596:LEU:HD11	2:2:620:ILE:HD13	1.98	0.46
3:3:184:GLY:HA2	3:3:261:MET:HG3	1.97	0.46
3:3:363:LEU:HD22	3:3:656:LEU:HD13	1.98	0.46
4:4:437:GLY:HA3	4:4:462:ASP:O	2.15	0.46
6:6:390:LYS:HB2	6:6:393:ASP:HB2	1.98	0.46
4:D:308:VAL:HG13	4:D:308:VAL:O	2.16	0.46
7:G:360:TYR:CZ	7:G:362:GLY:HA3	2.51	0.46
4:4:413:HIS:CG	4:4:414:SER:H	2.33	0.45
5:5:351:GLU:HA	5:5:354:GLU:OE2	2.15	0.45
5:5:681:ILE:O	5:5:685:GLN:HG2	2.16	0.45
6:6:791:SER:OG	6:6:837:ARG:NH2	2.32	0.45
7:7:492:GLY:O	7:7:512:ALA:N	2.41	0.45
3:C:104:ARG:HD3	3:C:111:TRP:CE2	2.51	0.45
3:C:408:VAL:O	3:C:548:VAL:HA	2.16	0.45
4:D:655:SER:HA	4:D:664:THR:HA	1.98	0.45
5:E:369:ILE:O	5:E:373:SER:N	2.49	0.45
2:2:337:VAL:HA	2:2:380:THR:HG23	1.98	0.45
7:7:358:ALA:N	7:7:373:GLU:O	2.45	0.45
7:7:482:TYR:OH	7:7:524:ASP:OD1	2.26	0.45
8:8:126:GLU:OE2	8:8:173:LEU:N	2.50	0.45
2:B:684:ARG:NH2	2:B:847:ASP:OD1	2.48	0.45
4:D:319:PRO:HB3	7:G:253:PRO:HB3	1.99	0.45
3:3:103:LEU:HD21	3:3:114:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:292:ASP:OD1	4:4:292:ASP:N	2.47	0.45
9:9:175:THR:O	9:9:203:SER:HA	2.17	0.45
3:C:301:LEU:HD12	3:C:320:LEU:HD21	1.97	0.45
3:C:462:MET:HE3	3:C:462:MET:HB3	1.76	0.45
4:D:427:CYS:HA	4:D:468:LYS:NZ	2.32	0.45
4:D:570:PRO:HB3	13:D:1103:BEF:F3	2.07	0.45
5:E:148:LEU:HA	5:E:151:LEU:HD23	1.98	0.45
5:5:194:ILE:O	5:5:194:ILE:HG22	2.16	0.45
5:5:257:LYS:HD3	5:5:273:ASN:HD22	1.80	0.45
5:5:487:ASP:OD1	5:5:488:GLU:N	2.50	0.45
6:6:504:PHE:CE2	6:6:508:LEU:HD21	2.50	0.45
7:7:89:GLN:OE1	7:7:102:LEU:N	2.47	0.45
2:B:484:PHE:HZ	2:B:765:LYS:HB3	1.80	0.45
2:B:486:LYS:HA	2:B:486:LYS:HD3	1.79	0.45
5:E:84:SER:HA	5:E:197:PHE:HE2	1.81	0.45
5:E:276:MET:HE1	5:E:330:ILE:HD11	1.98	0.45
2:2:549:LYS:HA	2:2:552:ILE:HD12	1.98	0.45
2:2:686:LEU:O	6:6:781:ARG:NH2	2.46	0.45
4:4:432:ARG:HH21	4:4:588:GLY:H	1.64	0.45
5:5:69:ILE:HG22	5:5:76:TYR:CD2	2.52	0.45
5:5:383:ASP:OD1	5:5:383:ASP:N	2.48	0.45
5:5:421:ALA:HB2	10:5:801:ADP:C8	2.51	0.45
7:7:193:PRO:HG2	5:E:9:TYR:CE2	2.52	0.45
2:B:853:VAL:HG13	2:B:853:VAL:O	2.16	0.45
3:C:420:ARG:NH1	5:E:501:THR:OG1	2.42	0.45
5:E:83:PRO:HG3	5:E:159:ILE:HG13	1.99	0.45
6:F:326:LYS:HA	6:F:326:LYS:HD3	1.79	0.45
7:G:31:ASP:HB2	7:G:62:LYS:HD3	1.98	0.45
7:G:425:ASN:HB3	7:G:428:VAL:CG2	2.47	0.45
6:6:170:ILE:HD12	6:6:181:LEU:HD11	1.98	0.45
8:8:132:TYR:CE2	8:8:133:ARG:HG2	2.51	0.45
8:8:426:TYR:CD1	8:8:429:LYS:HE2	2.52	0.45
9:9:345:GLN:HG2	9:9:346:TYR:HD1	1.81	0.45
2:B:756:SER:HB3	2:B:757:PRO:HD3	1.99	0.45
3:C:662:TYR:CE1	3:C:666:ARG:HG3	2.52	0.45
4:D:696:PRO:N	4:D:697:PRO:HD2	2.30	0.45
2:2:576:LEU:HD23	2:2:595:ALA:HB3	1.97	0.45
4:4:474:LEU:HB2	4:4:586:PRO:HD3	1.98	0.45
4:4:712:VAL:HG21	7:7:672:LYS:HB2	1.99	0.45
5:5:208:PRO:HB2	5:5:241:TYR:CE2	2.52	0.45
6:6:568:ASP:N	6:6:568:ASP:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:303:GLU:N	6:F:303:GLU:OE1	2.50	0.45
6:F:313:MET:HE1	6:F:338:CYS:HA	1.98	0.45
7:G:158:THR:HA	7:G:185:VAL:HG11	1.97	0.45
2:2:408:VAL:HG22	2:2:451:ILE:HB	1.99	0.45
4:4:799:GLU:OE2	10:6:1101:ADP:O3'	2.31	0.45
6:6:141:GLU:O	6:6:145:ILE:HG13	2.16	0.45
6:6:177:PHE:O	6:6:181:LEU:HG	2.16	0.45
7:7:434:LEU:HD11	7:7:699:LEU:HG	1.98	0.45
8:8:128:PHE:HA	8:8:131:PHE:CE1	2.52	0.45
2:B:527:VAL:O	2:B:530:LYS:N	2.49	0.45
7:G:310:PHE:HE1	7:G:334:HIS:HD1	1.65	0.45
7:G:535:THR:O	7:G:538:HIS:HB2	2.17	0.45
7:G:627:ASP:OD1	7:G:628:LEU:N	2.50	0.45
4:4:181:TRP:CZ3	7:7:145:GLN:HB3	2.51	0.45
8:8:274:LYS:HE2	9:9:275:TRP:CE3	2.52	0.45
4:D:774:TYR:HD2	6:F:728:ALA:HB2	1.81	0.45
4:D:778:ARG:HH22	6:F:717:ASP:CG	2.20	0.45
4:4:775:VAL:HG21	6:6:725:THR:HG22	1.98	0.45
5:5:286:VAL:HG11	5:5:292:VAL:HG11	1.97	0.45
6:6:193:ALA:N	6:6:194:PRO:HD3	2.32	0.45
8:8:356:GLY:HA3	9:9:264:PRO:HB3	1.98	0.45
8:8:425:ALA:HA	8:8:428:LEU:HD12	1.99	0.45
4:D:480:THR:HB	6:F:370:THR:HG21	1.99	0.45
4:D:488:ASN:HB3	4:D:493:ASN:HD21	1.82	0.45
6:F:122:PHE:CE2	6:F:157:HIS:HB3	2.52	0.45
7:G:527:ASP:OD1	7:G:527:ASP:N	2.48	0.45
3:3:372:TYR:HB2	3:3:564:HIS:HD1	1.81	0.44
3:3:457:LEU:HA	3:3:457:LEU:HD23	1.84	0.44
3:3:701:THR:HA	3:3:704:THR:HG22	2.00	0.44
4:4:345:ALA:HB3	4:4:365:ILE:HG21	1.97	0.44
6:6:284:ILE:HA	6:6:401:GLU:HB2	1.97	0.44
7:7:533:ASP:O	7:7:537:ILE:HG12	2.17	0.44
2:B:214:PHE:O	2:B:218:TYR:HB2	2.17	0.44
2:B:597:VAL:HG23	2:B:629:ILE:HD12	1.99	0.44
2:B:815:ARG:HA	2:B:818:GLU:OE2	2.17	0.44
4:D:251:TYR:CE2	4:D:253:GLN:HB2	2.51	0.44
7:G:702:LEU:HD23	7:G:702:LEU:HA	1.84	0.44
2:2:347:ILE:HD13	2:2:379:LYS:HD2	1.98	0.44
5:5:549:ARG:HA	5:5:651:ARG:HD3	1.99	0.44
6:6:196:LEU:HD23	6:6:196:LEU:H	1.82	0.44
8:8:301:ASP:O	8:8:304:SER:OG	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:LEU:HD22	2:B:207:ILE:HG13	2.00	0.44
2:B:511:ILE:HG21	2:B:552:ILE:HD13	1.99	0.44
3:C:166:LEU:HD12	3:C:171:LEU:HD23	1.98	0.44
4:D:568:GLY:HA3	4:D:708:VAL:O	2.17	0.44
5:E:688:THR:HG22	5:E:689:MET:N	2.33	0.44
2:2:191:ALA:HB3	2:2:197:TRP:HB2	1.98	0.44
2:2:502:ALA:HB1	2:2:505:ILE:HB	1.99	0.44
4:4:610:ASP:HB3	6:6:412:LEU:HD23	1.99	0.44
4:4:696:PRO:N	4:4:697:PRO:HD2	2.31	0.44
5:5:426:LEU:HB3	5:5:438:TYR:HE2	1.82	0.44
6:6:417:PRO:HB2	6:6:448:LEU:HB3	1.99	0.44
6:6:796:THR:O	6:6:799:GLN:HB2	2.17	0.44
7:7:268:GLU:HG3	5:E:13:VAL:HG21	1.99	0.44
8:8:21:GLN:HA	8:8:24:HIS:CD2	2.52	0.44
8:8:219:HIS:CE1	8:8:455:GLN:HB2	2.53	0.44
5:E:31:PHE:O	5:E:35:ILE:HG12	2.17	0.44
5:E:384:ILE:HD12	5:E:384:ILE:H	1.82	0.44
6:F:339:GLU:O	6:F:341:ARG:NH1	2.49	0.44
6:F:605:ALA:N	6:F:648:ASP:OD1	2.50	0.44
2:2:200:GLN:HB2	2:2:203:VAL:HB	2.00	0.44
2:2:213:SER:HB3	9:9:131:THR:HG21	1.99	0.44
6:6:600:GLY:HA3	6:6:640:GLU:O	2.18	0.44
7:7:541:MET:HG3	7:7:563:ILE:HD12	1.99	0.44
9:9:252:ARG:NE	4:D:373:ARG:HG3	2.33	0.44
2:B:347:ILE:HD13	2:B:379:LYS:HG2	1.98	0.44
2:B:476:TRP:HZ3	2:B:768:HIS:CE1	2.36	0.44
3:3:223:THR:OG1	5:5:246:GLU:OE1	2.31	0.44
3:3:345:PHE:O	3:3:349:ASN:ND2	2.51	0.44
3:3:446:VAL:HG22	3:3:448:THR:H	1.82	0.44
3:3:472:ILE:O	3:3:514:ALA:HA	2.18	0.44
6:6:770:ARG:O	6:6:774:VAL:HG23	2.17	0.44
7:7:117:PHE:HB3	7:7:202:LEU:HD11	2.00	0.44
2:B:500:SER:OG	2:B:758:ILE:N	2.43	0.44
6:F:776:LYS:HD2	6:F:828:TYR:CD2	2.52	0.44
7:G:269:VAL:HG21	7:G:285:THR:HB	2.00	0.44
5:5:161:ARG:HG2	5:5:295:VAL:HG22	1.99	0.44
7:7:255:VAL:HG22	7:7:307:PHE:CE1	2.53	0.44
7:7:570:LEU:HD23	7:7:571:TYR:CG	2.53	0.44
8:8:159:ILE:HA	8:8:189:GLN:H	1.83	0.44
7:G:73:ARG:NE	7:G:136:ASP:OD2	2.51	0.44
7:G:183:GLU:O	7:G:186:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:425:ASN:HB3	7:G:428:VAL:HG22	1.99	0.44
2:2:547:THR:HG22	2:2:547:THR:O	2.18	0.44
3:3:517:ASN:ND2	13:3:1002:BEF:F2	2.41	0.44
8:8:260:ASP:HB3	8:8:262:THR:HG23	2.00	0.44
8:8:352:PHE:HD1	9:9:268:LEU:HB2	1.82	0.44
3:C:291:ARG:HH22	5:E:511:THR:HB	1.83	0.44
4:D:437:GLY:HA3	4:D:462:ASP:O	2.18	0.44
4:D:518:LEU:HD23	4:D:812:LYS:HD3	2.00	0.44
5:E:166:ILE:O	5:E:289:GLY:N	2.30	0.44
5:E:453:VAL:HG21	5:E:504:ILE:HG21	2.00	0.44
6:F:125:GLN:HA	6:F:132:VAL:HG23	1.98	0.44
6:F:552:LEU:HD13	6:F:813:ALA:HB2	1.98	0.44
6:F:609:THR:O	6:F:626:GLY:HA3	2.17	0.44
7:G:364:LYS:HD3	7:G:364:LYS:HA	1.79	0.44
7:G:423:TYR:HB2	7:G:615:HIS:CG	2.53	0.44
3:3:662:TYR:CE1	3:3:666:ARG:HG3	2.53	0.44
7:7:481:VAL:HG22	7:7:516:ALA:HB2	1.99	0.44
9:9:233:THR:HB	9:9:236:ASN:HB3	1.98	0.44
3:C:369:PRO:HD2	5:E:402:ASP:OD2	2.17	0.44
3:C:741:ASP:N	3:C:741:ASP:OD1	2.51	0.44
7:G:252:LYS:HA	7:G:252:LYS:HD3	1.73	0.44
4:4:512:VAL:HG21	4:4:746:PHE:CE2	2.53	0.44
4:4:728:TYR:HA	7:7:442:LYS:NZ	2.33	0.44
8:8:297:SER:OG	8:8:298:THR:N	2.51	0.44
2:B:181:LEU:HB3	2:B:182:THR:H	1.61	0.44
2:B:202:ASN:OD1	2:B:203:VAL:N	2.51	0.44
5:E:410:ILE:O	5:E:518:SER:HB2	2.17	0.44
6:F:330:PRO:HD2	6:F:344:TRP:CE2	2.53	0.44
6:F:764:ILE:N	6:F:817:ASP:O	2.43	0.44
2:2:774:ILE:HG22	2:2:776:PRO:HD3	1.99	0.43
3:3:115:LEU:HD23	3:3:115:LEU:HA	1.76	0.43
4:4:752:SER:O	4:4:756:GLU:HG3	2.19	0.43
5:5:52:ASN:O	5:5:56:VAL:HG23	2.18	0.43
7:7:690:LEU:HD23	7:7:690:LEU:HA	1.81	0.43
8:8:137:ILE:HA	8:8:140:ILE:HD13	1.99	0.43
8:8:287:PRO:HD3	8:8:303:TRP:CE2	2.53	0.43
2:B:473:VAL:HG23	2:B:474:PHE:CD1	2.53	0.43
2:B:851:VAL:O	2:B:854:ARG:HG2	2.18	0.43
3:C:552:ASP:HB2	3:C:557:ARG:HH22	1.83	0.43
4:D:533:LEU:HD12	4:D:536:VAL:HG21	2.00	0.43
4:4:701:ARG:HA	4:4:796:ARG:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:36:LEU:HB3	5:5:47:ARG:HH21	1.83	0.43
5:5:301:TYR:O	5:5:325:THR:N	2.41	0.43
6:6:644:MET:SD	6:6:648:ASP:HB2	2.58	0.43
9:9:315:TYR:HB3	9:9:322:ARG:NH1	2.34	0.43
2:B:255:ILE:HG13	2:B:259:PHE:CZ	2.53	0.43
2:B:483:GLU:O	2:B:487:ILE:HD12	2.17	0.43
5:E:396:SER:OG	5:E:398:LYS:NZ	2.42	0.43
6:F:284:ILE:HA	6:F:401:GLU:HG3	1.99	0.43
6:F:608:LEU:HD13	6:F:652:ILE:CG1	2.48	0.43
6:6:585:LEU:HB3	6:6:637:CYS:HB3	2.00	0.43
6:6:623:ILE:HG21	6:6:672:LEU:HD21	1.98	0.43
8:8:265:TYR:CD1	9:9:280:THR:HG21	2.53	0.43
2:B:485:ARG:O	2:B:489:ARG:HG3	2.19	0.43
4:D:715:LYS:HB3	4:D:715:LYS:HE2	1.70	0.43
7:G:398:GLU:O	7:G:402:MET:HG2	2.18	0.43
7:G:401:VAL:O	7:G:405:ILE:HG12	2.18	0.43
2:2:306:LEU:HD13	2:2:392:GLU:HG2	2.00	0.43
2:2:325:THR:OG1	2:2:389:THR:O	2.30	0.43
2:2:485:ARG:HD2	2:2:485:ARG:HA	1.90	0.43
5:5:209:ARG:HD2	5:5:209:ARG:N	2.34	0.43
7:7:702:LEU:HD23	7:7:702:LEU:HA	1.70	0.43
8:8:38:LYS:HB2	8:8:48:TYR:CE1	2.53	0.43
8:8:107:CYS:HB2	8:8:119:VAL:HG12	2.00	0.43
8:8:140:ILE:H	8:8:140:ILE:HD12	1.84	0.43
8:8:299:LYS:HA	8:8:302:ILE:HG12	2.00	0.43
2:B:339:PHE:CE1	2:B:375:VAL:HG22	2.53	0.43
4:D:209:LEU:HG	4:D:250:ALA:HA	2.00	0.43
4:D:839:ASP:HB3	4:D:842:THR:O	2.19	0.43
7:G:313:CYS:HB2	7:G:333:ILE:HB	2.01	0.43
4:4:234:ARG:HH21	4:4:235:GLU:HG2	1.84	0.43
4:4:461:VAL:HG12	4:4:462:ASP:O	2.18	0.43
4:4:512:VAL:HG21	4:4:746:PHE:HE2	1.83	0.43
5:5:383:ASP:OD1	5:5:384:ILE:HD12	2.18	0.43
7:7:546:ILE:O	7:7:557:LEU:N	2.52	0.43
8:8:29:ILE:HD11	8:8:110:LYS:HD3	2.00	0.43
8:8:261:LEU:HD23	9:9:258:ILE:HD12	2.01	0.43
8:8:297:SER:O	8:8:300:ILE:HG12	2.17	0.43
8:8:330:LEU:O	8:8:334:THR:HG23	2.18	0.43
8:8:458:SER:HB2	8:8:462:ASP:HB2	2.00	0.43
2:B:252:SER:OG	2:B:253:LYS:N	2.51	0.43
4:D:613:GLN:HA	6:F:617:GLU:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:365:LYS:O	5:E:369:ILE:HG12	2.18	0.43
6:F:145:ILE:HG22	6:F:146:TYR:CD1	2.53	0.43
7:G:138:VAL:HG21	7:G:303:ARG:NH1	2.34	0.43
7:G:675:MET:SD	7:G:676:ASP:HB2	2.58	0.43
3:3:112:SER:O	3:3:116:VAL:HG12	2.18	0.43
3:3:301:LEU:HD12	3:3:320:LEU:HD21	1.99	0.43
4:4:315:ARG:NH1	4:4:413:HIS:HB2	2.33	0.43
4:4:721:ALA:HB2	7:7:664:TYR:CD2	2.53	0.43
6:6:313:MET:HE3	6:F:314:CYS:H	1.82	0.43
6:6:632:ASP:OD1	6:6:675:ARG:N	2.52	0.43
8:8:45:SER:OG	8:8:46:SER:N	2.52	0.43
9:9:263:TYR:HB3	9:9:264:PRO:HD2	1.99	0.43
9:9:534:ARG:HD3	4:D:177:LEU:HA	2.01	0.43
2:B:333:GLN:O	2:B:383:ARG:HG2	2.18	0.43
3:C:570:ARG:NH2	5:E:616:PRO:HG3	2.33	0.43
5:E:74:ASP:HB2	5:E:78:LYS:NZ	2.33	0.43
6:F:306:LYS:HA	6:F:323:GLN:H	1.84	0.43
7:G:179:ASP:O	7:G:182:ARG:NH2	2.52	0.43
3:3:528:ASP:OD1	3:3:528:ASP:N	2.51	0.43
4:4:252:LYS:HA	4:4:255:GLU:HG3	1.99	0.43
4:4:631:ILE:O	4:4:673:ALA:HA	2.19	0.43
5:5:184:ARG:NH1	5:5:239:ASP:O	2.52	0.43
7:7:143:LEU:HD22	7:7:197:THR:HA	2.01	0.43
8:8:47:VAL:HG22	8:8:76:LYS:HE2	2.00	0.43
8:8:81:THR:OG1	9:9:661:CYS:HA	2.19	0.43
8:8:185:LEU:HG	8:8:279:ALA:HB1	2.00	0.43
3:C:104:ARG:HB2	3:C:111:TRP:CD1	2.53	0.43
3:C:484:VAL:HG22	7:G:528:LYS:HD3	2.00	0.43
4:D:178:ARG:HA	4:D:178:ARG:HD2	1.89	0.43
5:E:259:GLN:HG2	5:E:260:GLU:O	2.19	0.43
5:E:489:ASP:O	5:E:493:ILE:HG12	2.19	0.43
6:F:118:PHE:O	6:F:122:PHE:HB2	2.19	0.43
3:3:696:PRO:HB3	7:7:573:ARG:NH2	2.33	0.43
6:6:318:VAL:HG21	6:6:334:PRO:HD3	2.01	0.43
6:6:338:CYS:SG	6:6:340:ASN:HB2	2.59	0.43
8:8:352:PHE:HA	9:9:268:LEU:HA	2.01	0.43
2:B:523:VAL:H	2:B:818:GLU:HG3	1.84	0.43
4:D:524:ARG:HD2	4:D:739:ASP:OD2	2.19	0.43
4:D:777:MET:HG2	4:D:830:ARG:NH2	2.34	0.43
5:E:190:THR:HG22	5:E:191:SER:N	2.33	0.43
6:F:608:LEU:HA	6:F:627:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:790:TYR:HB2	2:2:810:LEU:HD13	2.01	0.43
4:4:375:ASP:OD1	4:4:376:CYS:N	2.52	0.43
4:4:451:ARG:NH1	6:6:445:VAL:HG13	2.33	0.43
6:6:308:SER:O	6:6:346:LEU:HA	2.19	0.43
9:9:268:LEU:HB3	9:9:279:ILE:HG22	2.01	0.43
9:9:316:ASP:O	9:9:322:ARG:HD3	2.18	0.43
3:C:395:ASN:OD1	3:C:396:GLY:N	2.52	0.43
3:C:491:GLU:HB2	3:C:542:ARG:HD2	2.00	0.43
5:E:59:TYR:HA	5:E:135:PHE:CZ	2.54	0.43
2:2:227:TYR:HB3	9:9:165:PHE:HE2	1.82	0.43
2:2:580:VAL:HG23	2:2:631:ILE:HD11	2.01	0.43
3:3:413:THR:O	3:3:413:THR:HG22	2.19	0.43
5:5:178:TYR:CE1	5:5:191:SER:HB3	2.53	0.43
5:5:206:SER:HB2	5:5:209:ARG:NH2	2.34	0.43
6:6:656:MET:HE2	6:6:656:MET:HB2	1.90	0.43
7:7:29:LYS:HB3	7:7:61:PRO:HA	2.01	0.43
7:7:654:GLU:HA	7:7:657:ASN:ND2	2.33	0.43
8:8:285:ARG:HG2	8:8:289:VAL:HG13	2.00	0.43
2:B:522:GLY:O	2:B:822:LYS:NZ	2.50	0.43
4:D:704:LEU:HD11	4:D:804:LEU:HD21	2.00	0.43
4:D:711:LYS:HE2	4:D:847:MET:O	2.19	0.43
5:E:622:LEU:HD23	5:E:622:LEU:HA	1.90	0.43
2:2:609:PHE:HB3	2:2:650:ALA:HB2	2.00	0.42
3:3:214:TYR:OH	3:3:232:PRO:HD3	2.19	0.42
3:3:474:GLU:HB3	3:3:477:LYS:HD3	2.01	0.42
7:7:312:GLU:HB3	7:7:502:VAL:HG21	2.01	0.42
8:8:369:LEU:O	8:8:373:VAL:HG22	2.19	0.42
9:9:190:ILE:HG13	9:9:191:LEU:N	2.34	0.42
9:9:283:TRP:CD1	9:9:295:PRO:HG2	2.54	0.42
9:9:316:ASP:OD2	9:9:319:SER:N	2.52	0.42
3:C:698:THR:H	3:C:701:THR:HG23	1.83	0.42
4:D:739:ASP:OD1	4:D:739:ASP:N	2.51	0.42
6:F:706:MET:HA	6:F:712:PHE:HZ	1.84	0.42
3:3:741:ASP:OD1	3:3:741:ASP:N	2.51	0.42
6:6:341:ARG:HG3	6:6:344:TRP:NE1	2.30	0.42
7:7:267:TYR:CE1	5:E:12:PRO:HB3	2.53	0.42
8:8:90:GLU:OE1	8:8:184:GLY:HA2	2.18	0.42
8:8:102:ARG:NH1	8:8:149:ARG:HG2	2.34	0.42
8:8:429:LYS:HA	8:8:432:GLN:HG3	2.01	0.42
2:B:186:LEU:HD11	2:B:206:THR:HG22	2.01	0.42
2:B:206:THR:O	2:B:209:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:PHE:CB	2:B:295:VAL:HG21	2.46	0.42
2:B:371:GLY:N	2:B:372:PRO:HD3	2.34	0.42
2:B:501:MET:HG3	2:B:516:ALA:HB2	2.00	0.42
3:C:483:ARG:O	3:C:486:ILE:HG22	2.19	0.42
4:D:336:THR:HG22	4:D:396:VAL:H	1.85	0.42
5:E:31:PHE:CE2	5:E:90:PHE:HB2	2.54	0.42
5:E:200:ILE:HD13	5:E:204:THR:HG21	2.01	0.42
2:2:537:ILE:HD11	2:2:815:ARG:HB3	2.01	0.42
3:3:342:LEU:HD21	3:3:662:TYR:HB2	2.01	0.42
3:3:473:ASP:OD1	3:3:474:GLU:N	2.52	0.42
5:5:437:VAL:HG23	5:5:472:ALA:HB2	2.00	0.42
7:7:260:TYR:HB2	7:7:269:VAL:HG23	2.01	0.42
7:7:425:ASN:HB3	7:7:428:VAL:CG2	2.49	0.42
8:8:144:ILE:O	8:8:148:LEU:HD23	2.19	0.42
3:C:390:GLU:OE2	3:C:398:HIS:HE1	2.02	0.42
6:F:150:THR:HG23	6:F:264:GLN:HB3	2.00	0.42
6:F:347:ASN:ND2	6:F:350:ARG:HB2	2.34	0.42
6:F:772:TYR:HD2	6:F:824:ILE:HB	1.84	0.42
6:F:777:TYR:HB2	6:F:800:LEU:HD13	2.01	0.42
7:G:722:VAL:HA	7:G:725:GLU:HB2	2.01	0.42
4:4:360:ILE:HD11	4:4:363:GLY:HA2	2.02	0.42
4:4:544:LEU:HD23	4:4:544:LEU:HA	1.81	0.42
5:5:393:MET:O	5:5:665:LYS:NZ	2.41	0.42
5:5:463:TYR:OH	5:5:465:GLU:HG2	2.20	0.42
6:6:581:LYS:HB2	6:6:581:LYS:HE2	1.80	0.42
7:7:493:LEU:HG	7:7:513:LEU:HD13	2.00	0.42
2:B:704:VAL:HG11	6:F:770:ARG:HH21	1.84	0.42
2:B:779:HIS:HB3	2:B:782:ASP:OD1	2.18	0.42
2:B:800:THR:CG2	2:B:856:GLN:HE21	2.32	0.42
3:C:400:ARG:HH21	3:C:707:ARG:HH22	1.68	0.42
4:D:568:GLY:HA3	4:D:708:VAL:HG23	2.01	0.42
5:E:52:ASN:HA	5:E:55:LEU:HD12	2.01	0.42
5:E:525:PRO:HG2	5:E:530:TYR:HD1	1.83	0.42
6:F:723:ILE:O	6:F:726:GLU:HG2	2.20	0.42
6:6:566:ARG:NH2	6:6:710:ASP:OD1	2.52	0.42
6:6:600:GLY:N	6:6:639:ASP:O	2.52	0.42
2:B:804:PRO:HD3	5:E:529:ARG:NH2	2.33	0.42
3:C:296:GLY:HA3	3:C:322:LEU:O	2.20	0.42
5:E:409:ASP:HB2	5:E:500:GLN:HE22	1.84	0.42
6:F:800:LEU:HA	6:F:803:MET:CE	2.50	0.42
7:G:265:CYS:SG	7:G:267:TYR:HB2	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:334:HIS:HD2	7:G:375:TYR:CG	2.37	0.42
7:G:552:GLY:O	7:G:553:ILE:HD13	2.19	0.42
2:2:476:TRP:HA	2:2:765:LYS:HD2	2.01	0.42
2:2:658:ASN:ND2	2:2:661:LEU:HG	2.34	0.42
3:3:362:ILE:HD13	3:3:362:ILE:HA	1.94	0.42
3:3:448:THR:HG22	3:3:455:ARG:NH2	2.34	0.42
4:4:563:ASN:HB2	4:4:649:MET:HE1	2.01	0.42
5:5:440:SER:HA	5:5:480:ASP:OD1	2.20	0.42
6:6:136:TYR:O	6:6:139:GLN:HG2	2.20	0.42
7:7:115:GLU:HA	7:7:118:CYS:SG	2.60	0.42
7:7:586:LEU:HD22	7:7:590:LEU:HD23	2.01	0.42
8:8:15:ILE:O	8:8:19:MET:HG3	2.19	0.42
8:8:55:GLY:O	8:8:58:THR:OG1	2.24	0.42
8:8:228:ARG:HA	8:8:228:ARG:HD3	1.78	0.42
3:C:396:GLY:O	7:G:475:LYS:HE3	2.20	0.42
6:F:401:GLU:OE2	6:F:452:ILE:HG23	2.20	0.42
7:G:622:HIS:HB3	7:G:624:LYS:HZ3	1.84	0.42
2:2:756:SER:HB2	2:2:757:PRO:HD3	2.02	0.42
2:2:786:VAL:HG12	2:2:834:LEU:HD21	2.01	0.42
3:3:211:TYR:CE1	7:7:6:PRO:HB2	2.55	0.42
3:3:423:LEU:HD13	3:3:431:ALA:HB2	2.02	0.42
3:3:716:ARG:NH2	3:3:725:ASP:OD2	2.39	0.42
6:6:364:ASN:O	6:6:368:ILE:HG13	2.20	0.42
7:7:196:LEU:HD21	7:7:257:VAL:HG21	2.02	0.42
8:8:14:GLU:HA	8:8:17:GLU:OE1	2.19	0.42
8:8:41:GLU:OE2	8:8:79:TYR:OH	2.36	0.42
8:8:102:ARG:HA	8:8:179:VAL:HG12	2.02	0.42
2:B:576:LEU:HD23	2:B:595:ALA:HB3	2.01	0.42
4:D:585:THR:HG21	4:D:628:VAL:HB	2.02	0.42
4:D:587:ARG:O	4:D:627:GLY:HA3	2.19	0.42
4:D:613:GLN:O	4:D:615:VAL:HG23	2.20	0.42
5:E:476:VAL:HG12	5:E:518:SER:OG	2.19	0.42
7:G:16:ASN:ND2	7:G:100:ASP:OD2	2.53	0.42
8:8:389:TYR:OH	9:9:330:ASP:OD1	2.27	0.42
8:8:464:LEU:HA	8:8:469:PHE:CD2	2.53	0.42
9:9:692:ALA:O	9:9:695:SER:OG	2.28	0.42
2:B:366:ASN:O	2:B:368:LYS:NZ	2.53	0.42
4:D:711:LYS:NZ	4:D:847:MET:SD	2.72	0.42
6:F:764:ILE:O	6:F:818:GLU:HA	2.19	0.42
2:2:211:LEU:HD22	2:2:271:PHE:CD1	2.54	0.42
3:3:406:LEU:HD23	3:3:546:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:251:TYR:HB3	4:4:254:THR:HG22	2.01	0.42
4:4:678:ILE:HD13	4:4:693:ASP:OD2	2.19	0.42
5:5:460:ARG:HA	5:5:460:ARG:HD2	1.81	0.42
8:8:22:LEU:HD12	8:8:26:LEU:HD23	2.01	0.42
2:B:485:ARG:HD3	2:B:485:ARG:HA	1.87	0.42
3:C:400:ARG:HG3	3:C:493:GLN:NE2	2.35	0.42
4:D:451:ARG:HD2	6:F:445:VAL:HG21	2.01	0.42
4:D:452:VAL:HG12	7:G:277:THR:HG22	2.01	0.42
4:D:642:ARG:HD3	4:D:698:LEU:CD2	2.36	0.42
5:E:400:LEU:HD23	5:E:406:LEU:HD23	2.00	0.42
6:F:416:LYS:HD3	6:F:416:LYS:HA	1.85	0.42
7:G:589:ALA:O	7:G:593:ARG:NH1	2.53	0.42
2:2:574:VAL:HB	2:2:595:ALA:HB2	2.02	0.42
4:4:522:LEU:HB3	4:4:541:LEU:CD1	2.50	0.42
4:4:590:TYR:OH	4:4:632:ASP:OD2	2.34	0.42
4:4:712:VAL:HB	7:7:672:LYS:HD3	2.01	0.42
5:5:258:LEU:HB2	5:5:276:MET:HE1	2.02	0.42
5:5:370:LEU:HD22	5:5:599:MET:HE3	2.01	0.42
6:6:120:GLU:OE2	6:6:188:VAL:HG13	2.19	0.42
6:6:655:ALA:O	6:6:659:GLN:N	2.50	0.42
7:7:138:VAL:O	7:7:141:VAL:HG22	2.20	0.42
8:8:29:ILE:HG23	8:8:33:TYR:HD2	1.85	0.42
2:B:407:GLU:HB3	2:B:450:ILE:HG22	2.01	0.42
4:D:575:SER:HB2	10:D:1102:ADP:O1A	2.20	0.42
4:D:769:GLU:OE1	4:D:819:LEU:HB3	2.20	0.42
5:E:633:LEU:HD22	5:E:648:ILE:HG12	2.01	0.42
6:F:158:LEU:HG	6:F:167:ALA:HB2	2.01	0.42
6:F:330:PRO:HD2	6:F:344:TRP:NE1	2.34	0.42
7:G:457:CYS:HB2	7:G:594:PHE:CD1	2.55	0.42
7:G:685:THR:O	7:G:688:THR:OG1	2.27	0.42
2:2:281:LEU:HB3	9:9:164:GLN:HG2	2.01	0.41
3:3:555:GLU:HG3	5:5:631:LYS:HD3	2.01	0.41
4:4:397:ILE:O	4:4:417:LEU:N	2.46	0.41
7:7:396:ASP:OD1	7:7:397:VAL:N	2.52	0.41
8:8:299:LYS:HD3	8:8:457:ARG:HB3	2.03	0.41
2:B:333:GLN:HE22	5:E:322:ALA:HB1	1.84	0.41
3:C:486:ILE:HG13	3:C:490:MET:HG3	2.02	0.41
5:E:258:LEU:HB2	5:E:276:MET:SD	2.59	0.41
6:F:505:LEU:HD23	6:F:505:LEU:HA	1.82	0.41
7:G:428:VAL:O	7:G:432:LEU:HG	2.20	0.41
4:4:528:PRO:HD2	7:7:446:ASP:CG	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:653:HIS:CG	6:6:705:ILE:HD12	2.55	0.41
8:8:339:LYS:HZ1	8:8:342:ARG:HH22	1.68	0.41
3:C:161:PHE:CZ	3:C:295:VAL:HG21	2.55	0.41
3:C:391:LYS:HB2	3:C:399:LEU:HD12	2.01	0.41
2:2:511:ILE:HD13	2:2:681:CYS:HB3	2.02	0.41
2:2:534:ARG:HG2	2:2:536:ASP:H	1.85	0.41
3:3:576:TYR:CE2	3:3:582:VAL:HA	2.55	0.41
4:4:755:LYS:HA	4:4:810:LYS:HD3	2.02	0.41
5:5:416:GLY:HA2	5:5:556:VAL:O	2.20	0.41
7:7:442:LYS:HD2	7:7:442:LYS:HA	1.85	0.41
8:8:374:TYR:HB2	8:8:399:LEU:HD23	2.02	0.41
8:8:449:CYS:SG	8:8:450:PHE:N	2.93	0.41
2:B:410:LEU:HD23	2:B:414:LEU:O	2.20	0.41
3:C:46:GLN:HE22	3:C:137:ASP:HB2	1.85	0.41
3:C:98:ILE:CG1	3:C:155:LEU:HD11	2.50	0.41
4:D:217:ASN:OD1	4:D:218:ASN:N	2.54	0.41
4:D:231:ASN:HA	4:D:234:ARG:NH1	2.35	0.41
6:F:633:ASN:N	6:F:675:ARG:O	2.46	0.41
7:G:435:LEU:HD21	7:G:564:LEU:HB2	2.02	0.41
3:3:472:ILE:HG21	3:3:475:PHE:HD1	1.85	0.41
4:4:203:TYR:CZ	4:4:206:ARG:HD3	2.55	0.41
6:6:137:ARG:HD2	6:6:192:TYR:CD2	2.55	0.41
6:6:141:GLU:HA	6:6:144:LYS:HB3	2.01	0.41
7:7:681:PHE:HZ	7:7:727:LEU:HD21	1.85	0.41
8:8:306:GLY:HA3	8:8:449:CYS:SG	2.61	0.41
5:E:33:ASN:O	5:E:37:GLU:HB2	2.19	0.41
5:E:143:ALA:HB3	5:E:161:ARG:HE	1.86	0.41
7:G:677:SER:OG	7:G:678:LYS:N	2.53	0.41
3:3:41:SER:O	3:3:45:ILE:HG12	2.20	0.41
3:3:276:VAL:HG22	3:3:321:ILE:HB	2.02	0.41
5:5:9:TYR:HB2	7:G:270:PHE:HB2	2.03	0.41
6:6:312:ASP:HB3	6:6:342:ALA:HB3	2.01	0.41
6:6:321:VAL:HG11	6:6:330:PRO:HD3	2.02	0.41
7:7:631:THR:HG23	7:7:631:THR:O	2.20	0.41
2:B:625:GLU:OE2	5:E:438:TYR:OH	2.36	0.41
2:B:758:ILE:HG23	2:B:762:LEU:HD23	2.02	0.41
5:E:688:THR:HG22	5:E:689:MET:H	1.85	0.41
3:3:100:LEU:HD23	3:3:100:LEU:HA	1.88	0.41
4:4:394:LYS:HB3	4:4:394:LYS:HE2	1.77	0.41
4:4:830:ARG:NH1	4:4:835:ASP:OD2	2.47	0.41
6:6:134:LYS:HG3	6:6:137:ARG:HH12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:658:GLN:HG3	6:6:660:THR:H	1.85	0.41
7:7:490:GLY:O	7:7:494:THR:HG23	2.20	0.41
9:9:137:ASN:H	9:9:140:ASN:HB3	1.86	0.41
9:9:286:GLN:O	9:9:289:THR:OG1	2.31	0.41
2:B:308:GLU:N	2:B:308:GLU:OE1	2.54	0.41
2:B:500:SER:HB3	2:B:763:LEU:HD22	2.03	0.41
3:C:178:LYS:O	3:C:180:VAL:HG13	2.21	0.41
3:C:295:VAL:CG1	3:C:325:THR:HB	2.51	0.41
4:D:321:ASP:HA	4:D:324:LYS:HD3	2.02	0.41
4:D:371:CYS:HA	4:D:382:MET:CE	2.50	0.41
4:D:594:LYS:HD2	4:D:594:LYS:HA	1.63	0.41
5:E:536:PRO:HA	5:E:539:ASN:ND2	2.35	0.41
5:E:626:PHE:CG	5:E:653:LEU:HD12	2.56	0.41
6:F:305:TYR:HB2	6:F:354:LEU:HG	2.02	0.41
6:F:763:PRO:HB2	6:F:819:ILE:HD11	2.02	0.41
2:2:525:LYS:HZ1	5:5:576:HIS:CD2	2.38	0.41
2:2:629:ILE:O	2:2:640:LEU:N	2.50	0.41
4:4:256:ASP:HB3	7:7:134:TYR:HD2	1.84	0.41
4:4:457:TYR:HB2	7:7:253:PRO:HG2	2.03	0.41
5:5:526:ILE:HG22	5:5:539:ASN:O	2.20	0.41
9:9:125:ARG:HB3	9:9:170:VAL:HG13	2.02	0.41
4:D:180:ILE:HB	4:D:183:THR:OG1	2.21	0.41
4:D:798:LEU:HA	4:D:801:MET:CE	2.50	0.41
5:E:69:ILE:HG13	5:E:76:TYR:CG	2.56	0.41
5:E:293:THR:HB	5:E:334:GLN:HB3	2.02	0.41
6:F:115:PHE:CE2	6:F:119:LEU:HD21	2.56	0.41
6:F:122:PHE:CE1	6:F:161:ARG:HB2	2.55	0.41
6:F:419:SER:OG	6:F:446:ARG:NH1	2.54	0.41
7:G:255:VAL:HA	7:G:307:PHE:HD1	1.86	0.41
2:2:674:LEU:HD12	2:2:674:LEU:HA	1.92	0.41
3:3:483:ARG:O	3:3:486:ILE:HG22	2.21	0.41
3:3:703:GLU:HB3	3:3:707:ARG:HH12	1.86	0.41
4:4:545:PHE:CE1	4:4:751:ILE:HA	2.54	0.41
4:4:663:THR:HG21	6:6:374:PRO:HG3	2.03	0.41
5:5:75:ILE:HD12	5:5:75:ILE:HA	1.94	0.41
6:6:110:LYS:O	6:6:113:GLU:HG3	2.20	0.41
6:6:149:ASN:O	6:6:264:GLN:N	2.34	0.41
6:6:277:ARG:HE	6:6:277:ARG:HB2	1.75	0.41
6:6:306:LYS:HB3	6:6:352:ARG:HB2	2.03	0.41
6:6:555:VAL:HG12	6:6:557:LYS:HG3	2.03	0.41
7:7:420:PRO:HB2	7:7:625:GLN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:272:ARG:NE	4:D:297:GLU:OE2	2.53	0.41
2:B:232:ARG:HD3	2:B:282:HIS:CE1	2.56	0.41
2:B:609:PHE:O	2:B:612:MET:HG3	2.20	0.41
5:E:361:SER:HB2	5:E:668:LEU:HD13	2.03	0.41
5:E:423:SER:O	5:E:427:LYS:HG3	2.20	0.41
6:F:170:ILE:HD12	6:F:170:ILE:HA	1.91	0.41
6:F:177:PHE:O	6:F:181:LEU:HG	2.20	0.41
6:F:831:LEU:O	6:F:835:ILE:HG22	2.20	0.41
7:G:517:ASP:OD1	7:G:560:ARG:HG2	2.20	0.41
7:G:670:ASP:O	7:G:674:GLU:HG2	2.21	0.41
2:2:279:THR:O	2:2:283:TYR:N	2.39	0.41
2:2:414:LEU:HD11	2:2:454:ASN:O	2.21	0.41
2:2:673:ILE:HA	2:2:676:ARG:HG2	2.03	0.41
3:3:330:HIS:N	3:3:589:SER:O	2.51	0.41
3:3:570:ARG:HB3	5:5:613:ARG:HH21	1.85	0.41
4:4:265:PRO:O	4:4:269:ILE:HB	2.21	0.41
4:4:524:ARG:HD2	4:4:739:ASP:OD2	2.21	0.41
5:5:274:LEU:HD12	5:5:274:LEU:HA	1.89	0.41
5:5:526:ILE:HB	5:5:541:ASP:HB2	2.03	0.41
7:7:160:GLU:O	7:7:164:GLU:HG2	2.20	0.41
7:7:298:LEU:H	7:7:298:LEU:HD23	1.86	0.41
8:8:66:TRP:HZ2	8:8:179:VAL:HG13	1.86	0.41
8:8:114:ASP:HA	9:9:690:PHE:CE2	2.56	0.41
8:8:427:GLU:HA	8:8:430:LYS:HD3	2.02	0.41
2:B:337:VAL:HA	2:B:380:THR:HG23	2.03	0.41
2:B:340:ASN:OD1	2:B:374:ARG:HB3	2.21	0.41
2:B:525:LYS:HD2	2:B:525:LYS:HA	1.96	0.41
4:D:183:THR:HG22	4:D:264:TYR:CD1	2.56	0.41
4:D:218:ASN:OD1	4:D:219:THR:HG23	2.21	0.41
4:D:535:ASP:O	4:D:706:TYR:OH	2.29	0.41
5:E:45:ILE:HG13	5:E:46:TYR:N	2.36	0.41
5:E:416:GLY:HA3	5:E:556:VAL:HG23	2.03	0.41
5:E:420:THR:HG22	5:E:420:THR:O	2.21	0.41
5:E:437:VAL:HG23	5:E:477:VAL:HG23	2.02	0.41
6:F:707:SER:HB3	6:F:798:ARG:NH1	2.36	0.41
7:G:138:VAL:HA	7:G:141:VAL:HG12	2.03	0.41
7:G:491:VAL:HB	7:G:493:LEU:O	2.20	0.41
7:G:500:ASP:HB3	7:G:503:THR:O	2.21	0.41
2:2:217:GLU:OE1	9:9:190:ILE:HD13	2.20	0.41
3:3:350:ILE:HG23	3:3:659:TYR:CD2	2.56	0.41
3:3:564:HIS:NE2	3:3:627:PRO:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:628:LEU:HD11	6:6:652:ILE:HD12	2.02	0.41
7:7:548:ILE:HD12	7:7:557:LEU:HD13	2.03	0.41
7:7:668:ARG:HA	7:7:668:ARG:HD2	1.94	0.41
8:8:148:LEU:HD21	8:8:305:VAL:HG11	2.02	0.41
2:B:610:ASP:OD1	2:B:611:LYS:N	2.54	0.41
2:B:631:ILE:HD12	5:E:446:ALA:HB3	2.03	0.41
2:B:798:ILE:HD12	2:B:798:ILE:HA	1.92	0.41
5:E:74:ASP:HB2	5:E:78:LYS:HZ1	1.86	0.41
5:E:454:GLN:HB2	5:E:465:GLU:HG3	2.03	0.41
3:3:176:LEU:HD22	3:3:300:SER:HB3	2.03	0.40
3:3:477:LYS:HG2	5:5:491:VAL:HG12	2.03	0.40
4:4:186:SER:OG	4:4:189:GLU:HB2	2.20	0.40
7:7:138:VAL:HG11	7:7:303:ARG:NH1	2.36	0.40
8:8:160:ILE:N	8:8:187:GLU:O	2.42	0.40
4:D:370:ARG:HA	4:D:379:PRO:HA	2.04	0.40
5:E:605:TYR:CE1	5:E:609:LYS:HG3	2.56	0.40
6:F:578:SER:O	10:F:1101:ADP:H8	2.05	0.40
7:G:360:TYR:HB2	7:G:371:LEU:O	2.21	0.40
2:2:343:LYS:NZ	2:2:372:PRO:HD3	2.34	0.40
4:4:239:SER:OG	4:4:299:LYS:HD3	2.21	0.40
4:4:651:GLN:HG2	4:4:653:THR:HG22	2.03	0.40
7:7:67:LEU:HB3	7:7:126:PRO:CD	2.51	0.40
8:8:357:LEU:HD12	8:8:357:LEU:H	1.85	0.40
9:9:211:LEU:O	9:9:215:ASP:N	2.25	0.40
2:B:384:ASN:ND2	5:E:153:SER:H	2.19	0.40
6:F:143:MET:HG3	6:F:196:LEU:HD23	2.03	0.40
3:3:572:LEU:HD23	3:3:573:PRO:O	2.22	0.40
3:3:674:GLU:CD	3:3:723:LYS:HB2	2.42	0.40
3:C:408:VAL:HA	3:C:516:ALA:O	2.22	0.40
4:D:333:LEU:HD11	4:D:400:GLN:HB2	2.03	0.40
6:F:122:PHE:HD1	6:F:161:ARG:HH11	1.69	0.40
6:F:124:VAL:HB	6:F:135:VAL:HG11	2.04	0.40
7:G:652:MET:HA	7:G:708:VAL:HB	2.03	0.40
2:2:796:GLU:OE2	2:2:859:ARG:HB3	2.21	0.40
3:3:333:SER:OG	5:5:512:VAL:HG23	2.21	0.40
3:3:483:ARG:HB3	3:3:539:LEU:HD11	2.03	0.40
3:3:733:LEU:HD12	3:3:733:LEU:HA	1.82	0.40
4:4:319:PRO:O	4:4:322:ILE:HG12	2.21	0.40
4:4:529:SER:HA	4:4:735:HIS:NE2	2.35	0.40
6:6:259:THR:HG22	6:6:260:GLU:HG3	2.03	0.40
6:6:699:LEU:HD23	6:6:699:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:138:LYS:HG2	9:9:344:PHE:HD2	1.85	0.40
2:B:509:ARG:NH1	2:B:509:ARG:HB3	2.37	0.40
3:C:410:ASP:HB3	3:C:411:PRO:HD2	2.04	0.40
4:D:336:THR:CG2	4:D:396:VAL:H	2.34	0.40
6:F:333:CYS:SG	6:F:338:CYS:HB3	2.61	0.40
7:G:493:LEU:HD21	7:G:548:ILE:HD11	2.03	0.40
3:3:622:PHE:CE2	3:3:649:LYS:HD3	2.57	0.40
5:5:433:SER:OG	5:5:436:ALA:HB2	2.21	0.40
7:7:331:LEU:HD21	7:7:376:LEU:HB2	2.02	0.40
8:8:399:LEU:O	8:8:403:LEU:HB2	2.22	0.40
9:9:239:HIS:HB2	9:9:242:LYS:NZ	2.36	0.40
2:B:855:ARG:HD3	2:B:859:ARG:NH2	2.34	0.40
3:C:226:PRO:HG2	5:E:242:ILE:HG21	2.03	0.40
4:D:349:CYS:HB3	4:D:354:HIS:N	2.33	0.40
4:D:574:LYS:O	4:D:578:LEU:HD23	2.22	0.40
5:E:421:ALA:HA	10:E:802:ADP:H5'2	2.04	0.40
5:E:631:LYS:HD3	5:E:631:LYS:HA	1.75	0.40
7:G:592:SER:OG	7:G:687:ARG:NH1	2.54	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	
2	2	618/868 (71%)	596 (96%)	22 (4%)	0	100	100
2	B	618/868 (71%)	594 (96%)	24 (4%)	0	100	100
3	3	621/971 (64%)	601 (97%)	20 (3%)	0	100	100
3	C	619/971 (64%)	595 (96%)	24 (4%)	0	100	100
4	4	664/933 (71%)	639 (96%)	25 (4%)	0	100	100
4	D	664/933 (71%)	645 (97%)	19 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	5	618/775 (80%)	604 (98%)	14 (2%)	0	100	100
5	E	618/775 (80%)	598 (97%)	20 (3%)	0	100	100
6	6	607/1017 (60%)	589 (97%)	18 (3%)	0	100	100
6	F	607/1017 (60%)	588 (97%)	19 (3%)	0	100	100
7	7	675/845 (80%)	655 (97%)	20 (3%)	0	100	100
7	G	675/845 (80%)	652 (97%)	23 (3%)	0	100	100
8	8	394/507 (78%)	381 (97%)	13 (3%)	0	100	100
9	9	327/704 (46%)	312 (95%)	15 (5%)	0	100	100
All	All	8325/12029 (69%)	8049 (97%)	276 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	551/770 (72%)	551 (100%)	0	100	100
2	B	551/770 (72%)	550 (100%)	1 (0%)	93	97
3	3	550/835 (66%)	549 (100%)	1 (0%)	93	97
3	C	548/835 (66%)	548 (100%)	0	100	100
4	4	607/848 (72%)	604 (100%)	3 (0%)	88	94
4	D	607/848 (72%)	607 (100%)	0	100	100
5	5	564/688 (82%)	562 (100%)	2 (0%)	91	95
5	E	564/688 (82%)	563 (100%)	1 (0%)	93	97
6	6	541/886 (61%)	532 (98%)	9 (2%)	60	78
6	F	541/886 (61%)	534 (99%)	7 (1%)	69	82
7	7	603/753 (80%)	595 (99%)	8 (1%)	69	82
7	G	603/753 (80%)	603 (100%)	0	100	100
8	8	356/454 (78%)	353 (99%)	3 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	9	313/639 (49%)	309 (99%)	4 (1%)	69 82
All	All	7499/10653 (70%)	7460 (100%)	39 (0%)	89 94

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	281	ASP
4	4	573	SER
4	4	668	ARG
4	4	815	ASN
5	5	546	ILE
5	5	549	ARG
6	6	306	LYS
6	6	308	SER
6	6	511	ASP
6	6	515	GLU
6	6	520	VAL
6	6	656	MET
6	6	798	ARG
6	6	801	GLU
6	6	815	CYS
7	7	73	ARG
7	7	507	ILE
7	7	508	LEU
7	7	560	ARG
7	7	583	ASN
7	7	685	THR
7	7	686	PRO
7	7	689	LEU
8	8	70	SER
8	8	174	GLU
8	8	185	LEU
9	9	122	ARG
9	9	123	ASP
9	9	125	ARG
9	9	200	LYS
2	B	808	ARG
5	E	209	ARG
6	F	501	GLN
6	F	652	ILE
6	F	653	HIS
6	F	656	MET

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Mol	Chain	Res	Type
6	F	691	ARG
6	F	762	LYS
6	F	815	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
4	4	676	ASN
4	4	685	ASN
5	5	576	HIS
5	5	625	ASN
6	6	814	ASN
7	7	334	HIS
8	8	85	GLN
8	8	89	ASN
8	8	168	ASN
8	8	475	ASN
9	9	369	HIS
9	9	510	ASN
2	B	376	ASN
2	B	856	GLN
4	D	676	ASN
5	E	499	GLN

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 46 ligands modelled in this entry, 26 are monoatomic - leaving 20 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	2	901	11	24,29,29	0.68	0	29,45,45	0.78	1 (3%)
10	ADP	D	1102	13,11	24,29,29	0.72	0	29,45,45	0.79	1 (3%)
10	ADP	7	1102	13,11	24,29,29	0.72	0	29,45,45	0.73	1 (3%)
10	ADP	E	802	11	24,29,29	0.71	0	29,45,45	0.81	1 (3%)
13	BEF	3	1002	10	0,3,3	-	-	-		
10	ADP	3	1001	13,11	24,29,29	0.75	0	29,45,45	0.73	1 (3%)
13	BEF	3	1004	10	0,3,3	-	-	-		
13	BEF	G	1103	10	0,3,3	-	-	-		
10	ADP	8	1001	13,11	24,29,29	0.70	0	29,45,45	0.73	1 (3%)
10	ADP	6	1101	11	24,29,29	3.61	15 (62%)	29,45,45	2.52	6 (20%)
13	BEF	4	1103	10	0,3,3	-	-	-		
10	ADP	5	801	11	24,29,29	0.72	0	29,45,45	0.71	1 (3%)
10	ADP	G	1102	13,11	24,29,29	0.72	0	29,45,45	0.73	1 (3%)
10	ADP	B	901	11	24,29,29	0.73	0	29,45,45	0.73	1 (3%)
10	ADP	4	1102	13,11	24,29,29	0.72	0	29,45,45	0.79	1 (3%)
13	BEF	8	1003	10	0,3,3	-	-	-		
10	ADP	C	1001	13,11	24,29,29	0.75	0	29,45,45	0.73	1 (3%)
13	BEF	D	1103	10	0,3,3	-	-	-		
13	BEF	E	801	10	0,3,3	-	-	-		
10	ADP	F	1101	11	24,29,29	3.60	14 (58%)	29,45,45	2.51	6 (20%)

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	2	901	11	-	4/12/32/32	0/3/3/3
10	ADP	D	1102	13,11	-	2/12/32/32	0/3/3/3
10	ADP	7	1102	13,11	-	8/12/32/32	0/3/3/3
10	ADP	G	1102	13,11	-	8/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ADP	B	901	11	-	6/12/32/32	0/3/3/3
10	ADP	4	1102	13,11	-	2/12/32/32	0/3/3/3
10	ADP	E	802	11	-	3/12/32/32	0/3/3/3
10	ADP	8	1001	13,11	-	1/12/32/32	0/3/3/3
10	ADP	6	1101	11	-	4/12/32/32	0/3/3/3
10	ADP	3	1001	13,11	-	4/12/32/32	0/3/3/3
10	ADP	F	1101	11	-	4/12/32/32	0/3/3/3
10	ADP	C	1001	13,11	-	4/12/32/32	0/3/3/3
10	ADP	5	801	11	-	4/12/32/32	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	6	1101	ADP	C2'-C3'	-9.93	1.26	1.53
10	F	1101	ADP	C2'-C3'	-9.91	1.26	1.53
10	F	1101	ADP	C2'-C1'	8.41	1.66	1.53
10	6	1101	ADP	C2'-C1'	8.40	1.66	1.53
10	6	1101	ADP	O4'-C1'	-5.51	1.33	1.41
10	F	1101	ADP	O4'-C1'	-5.49	1.33	1.41
10	F	1101	ADP	C5'-C4'	-4.51	1.37	1.51
10	F	1101	ADP	C6-N6	4.50	1.50	1.34
10	6	1101	ADP	C6-N6	4.49	1.50	1.34
10	6	1101	ADP	C5'-C4'	-4.48	1.37	1.51
10	6	1101	ADP	C3'-C4'	3.23	1.61	1.53
10	F	1101	ADP	C3'-C4'	3.23	1.61	1.53
10	6	1101	ADP	O4'-C4'	2.98	1.51	1.45
10	F	1101	ADP	O4'-C4'	2.95	1.51	1.45
10	6	1101	ADP	C6-C5	-2.72	1.33	1.43
10	F	1101	ADP	C6-C5	-2.71	1.33	1.43
10	F	1101	ADP	O2'-C2'	2.40	1.48	1.43
10	6	1101	ADP	O2'-C2'	2.40	1.48	1.43
10	F	1101	ADP	C5-C4	-2.39	1.34	1.40
10	6	1101	ADP	C5-C4	-2.38	1.34	1.40
10	6	1101	ADP	PA-O5'	2.37	1.68	1.59
10	F	1101	ADP	PA-O5'	2.35	1.68	1.59
10	6	1101	ADP	PA-O1A	2.31	1.59	1.50
10	F	1101	ADP	PA-O1A	2.29	1.59	1.50
10	6	1101	ADP	O5'-C5'	-2.12	1.36	1.44
10	F	1101	ADP	O5'-C5'	-2.12	1.36	1.44
10	6	1101	ADP	C2-N3	2.04	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	1101	ADP	C2-N3	2.02	1.35	1.32
10	6	1101	ADP	O3'-C3'	2.01	1.47	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	6	1101	ADP	C5-C6-N6	8.32	132.99	120.35
10	F	1101	ADP	C5-C6-N6	8.30	132.97	120.35
10	F	1101	ADP	N6-C6-N1	-5.68	106.78	118.57
10	6	1101	ADP	N6-C6-N1	-5.68	106.79	118.57
10	6	1101	ADP	N3-C2-N1	-5.54	120.02	128.68
10	F	1101	ADP	N3-C2-N1	-5.52	120.05	128.68
10	F	1101	ADP	C1'-N9-C4	-4.04	119.54	126.64
10	6	1101	ADP	C1'-N9-C4	-4.04	119.55	126.64
10	F	1101	ADP	C3'-C2'-C1'	3.57	106.35	100.98
10	6	1101	ADP	C3'-C2'-C1'	3.57	106.35	100.98
10	6	1101	ADP	PA-O3A-PB	-3.41	121.14	132.83
10	F	1101	ADP	PA-O3A-PB	-3.40	121.18	132.83
10	4	1102	ADP	C5-C6-N6	2.27	123.80	120.35
10	D	1102	ADP	C5-C6-N6	2.26	123.79	120.35
10	3	1001	ADP	C5-C6-N6	2.24	123.75	120.35
10	C	1001	ADP	C5-C6-N6	2.22	123.72	120.35
10	G	1102	ADP	C5-C6-N6	2.21	123.72	120.35
10	7	1102	ADP	C5-C6-N6	2.20	123.69	120.35
10	E	802	ADP	C5-C6-N6	2.19	123.68	120.35
10	2	901	ADP	C5-C6-N6	2.17	123.64	120.35
10	B	901	ADP	C5-C6-N6	2.13	123.59	120.35
10	8	1001	ADP	C5-C6-N6	2.10	123.54	120.35
10	5	801	ADP	C5-C6-N6	2.07	123.49	120.35

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	2	901	ADP	PA-O3A-PB-O2B
10	2	901	ADP	PA-O3A-PB-O3B
10	2	901	ADP	C5'-O5'-PA-O2A
10	2	901	ADP	C5'-O5'-PA-O3A
10	3	1001	ADP	PA-O3A-PB-O2B
10	4	1102	ADP	O4'-C4'-C5'-O5'
10	5	801	ADP	PA-O3A-PB-O2B
10	6	1101	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
10	6	1101	ADP	C5'-O5'-PA-O2A
10	7	1102	ADP	C5'-O5'-PA-O3A
10	7	1102	ADP	O4'-C4'-C5'-O5'
10	B	901	ADP	C5'-O5'-PA-O1A
10	C	1001	ADP	PA-O3A-PB-O2B
10	D	1102	ADP	O4'-C4'-C5'-O5'
10	E	802	ADP	C5'-O5'-PA-O3A
10	F	1101	ADP	C5'-O5'-PA-O1A
10	F	1101	ADP	C5'-O5'-PA-O2A
10	G	1102	ADP	C5'-O5'-PA-O3A
10	G	1102	ADP	O4'-C4'-C5'-O5'
10	4	1102	ADP	C3'-C4'-C5'-O5'
10	D	1102	ADP	C3'-C4'-C5'-O5'
10	7	1102	ADP	C3'-C4'-C5'-O5'
10	B	901	ADP	O4'-C4'-C5'-O5'
10	B	901	ADP	C3'-C4'-C5'-O5'
10	G	1102	ADP	C3'-C4'-C5'-O5'
10	5	801	ADP	O4'-C4'-C5'-O5'
10	5	801	ADP	C3'-C4'-C5'-O5'
10	7	1102	ADP	PA-O3A-PB-O1B
10	G	1102	ADP	PA-O3A-PB-O1B
10	B	901	ADP	C4'-C5'-O5'-PA
10	B	901	ADP	C5'-O5'-PA-O3A
10	3	1001	ADP	O4'-C4'-C5'-O5'
10	C	1001	ADP	O4'-C4'-C5'-O5'
10	7	1102	ADP	C5'-O5'-PA-O1A
10	7	1102	ADP	C5'-O5'-PA-O2A
10	B	901	ADP	C5'-O5'-PA-O2A
10	E	802	ADP	C5'-O5'-PA-O1A
10	G	1102	ADP	C5'-O5'-PA-O1A
10	G	1102	ADP	C5'-O5'-PA-O2A
10	6	1101	ADP	O4'-C4'-C5'-O5'
10	F	1101	ADP	O4'-C4'-C5'-O5'
10	5	801	ADP	C4'-C5'-O5'-PA
10	3	1001	ADP	PA-O3A-PB-O1B
10	C	1001	ADP	PA-O3A-PB-O1B
10	3	1001	ADP	C3'-C4'-C5'-O5'
10	C	1001	ADP	C3'-C4'-C5'-O5'
10	7	1102	ADP	PA-O3A-PB-O2B
10	7	1102	ADP	PA-O3A-PB-O3B
10	G	1102	ADP	PA-O3A-PB-O2B
10	G	1102	ADP	PA-O3A-PB-O3B

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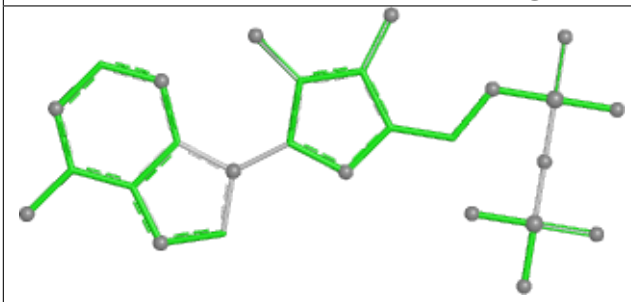
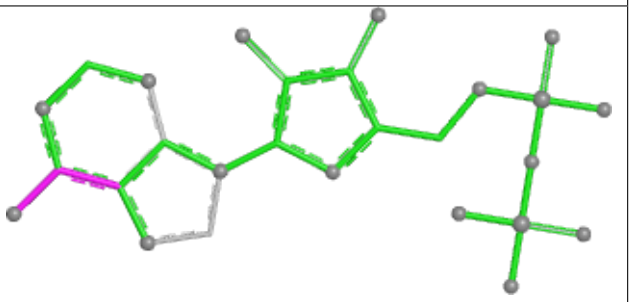
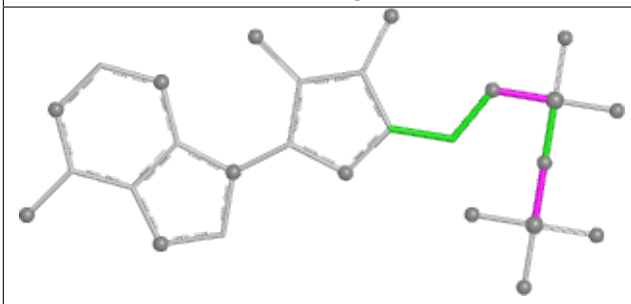
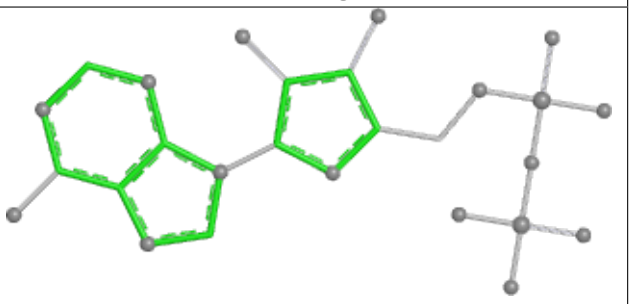
Mol	Chain	Res	Type	Atoms
10	6	1101	ADP	C5'-O5'-PA-O3A
10	F	1101	ADP	C5'-O5'-PA-O3A
10	E	802	ADP	C4'-C5'-O5'-PA
10	8	1001	ADP	PB-O3A-PA-O1A

There are no ring outliers.

14 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	1102	ADP	1	0
10	7	1102	ADP	1	0
10	E	802	ADP	2	0
13	3	1002	BEF	1	0
10	3	1001	ADP	3	0
10	8	1001	ADP	6	0
10	6	1101	ADP	3	0
10	5	801	ADP	3	0
10	B	901	ADP	3	0
10	4	1102	ADP	1	0
10	C	1001	ADP	1	0
13	D	1103	BEF	1	0
13	E	801	BEF	1	0
10	F	1101	ADP	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 ADP 2 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

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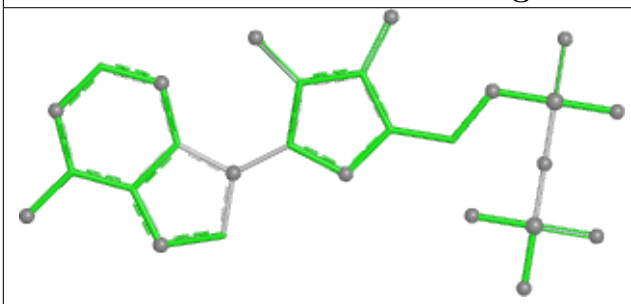
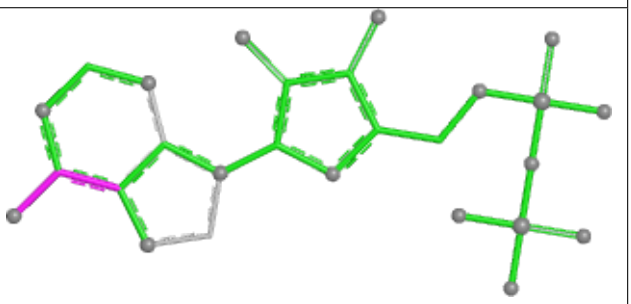
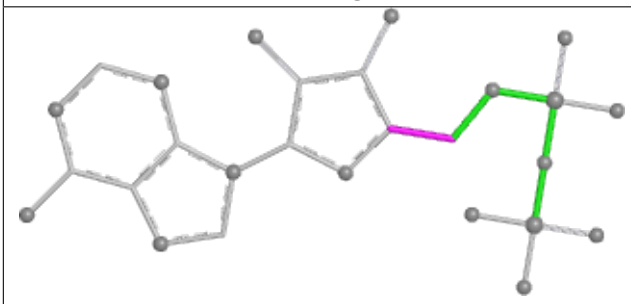
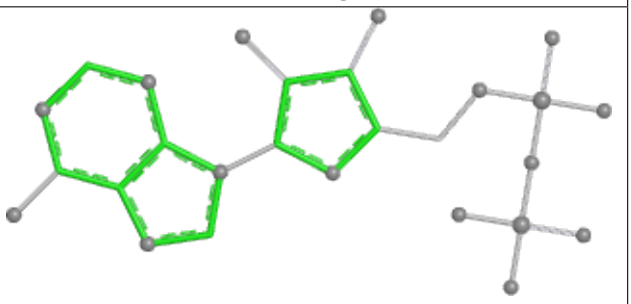
 Bond lengths	 Bond angles
 Torsions	 Rings

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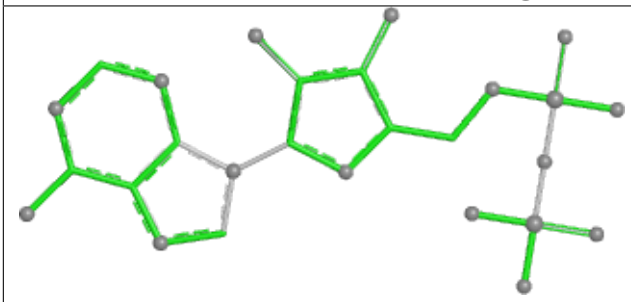
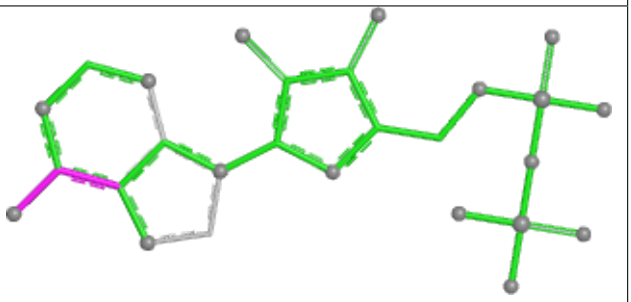
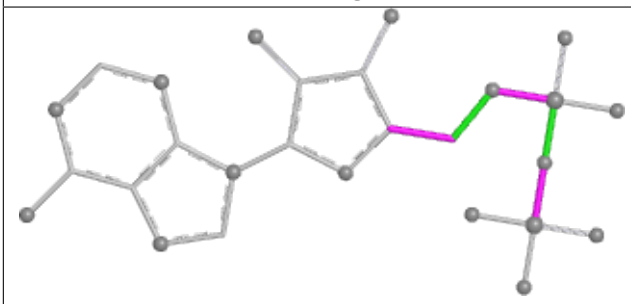
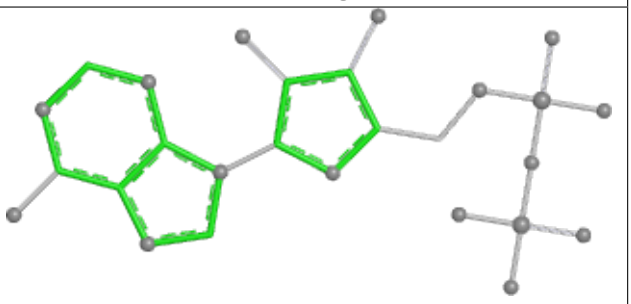
 Bond lengths	 Bond angles
 Torsions	 Rings

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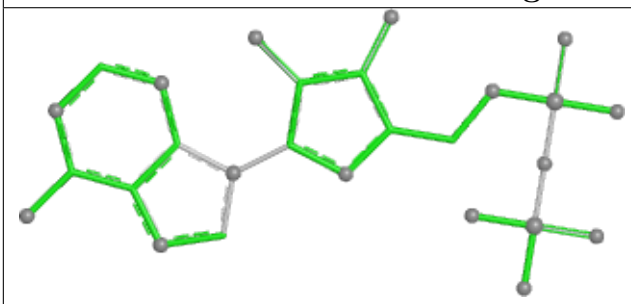
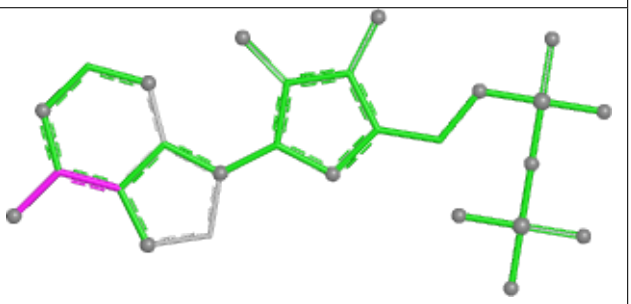
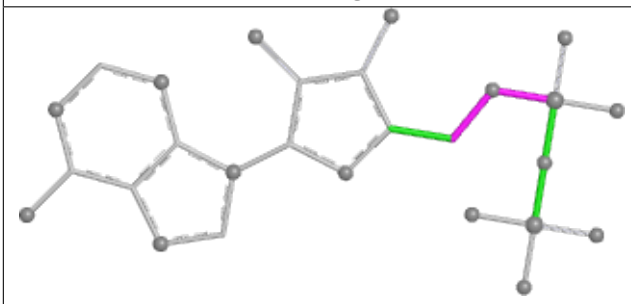
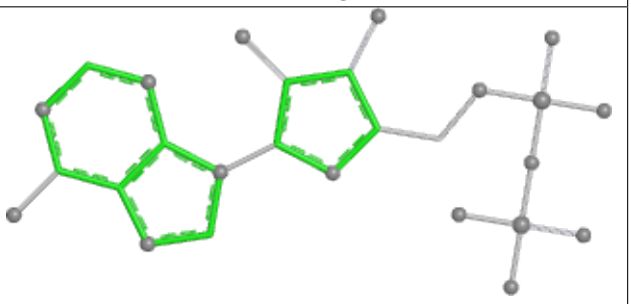
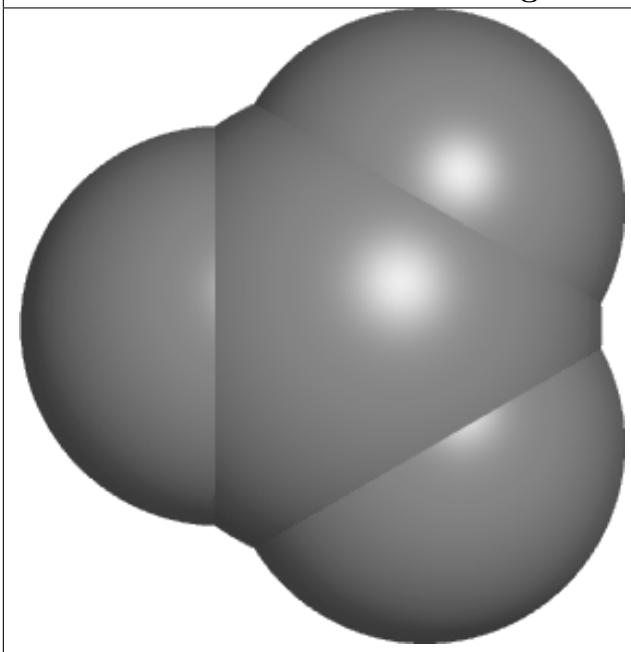
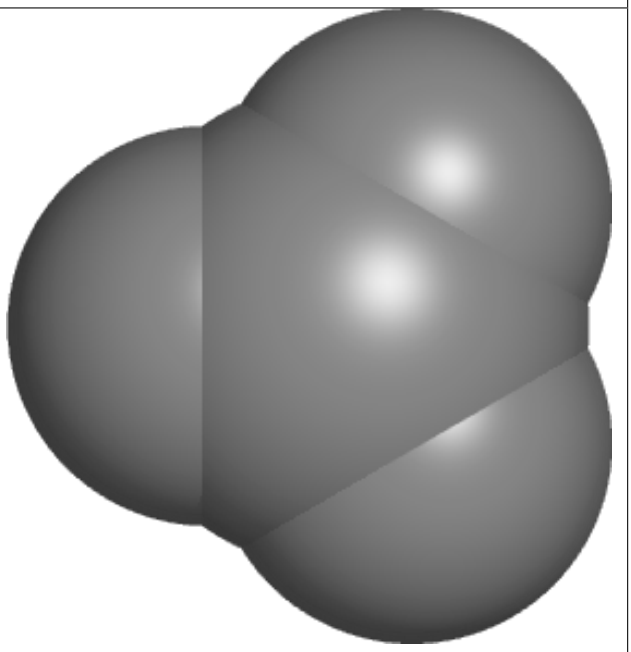
 Bond lengths	 Bond angles
 Torsions	 Rings

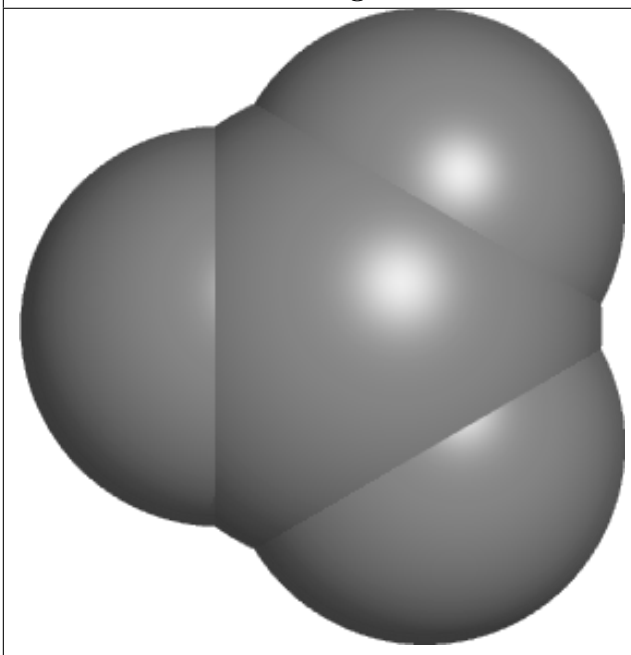
Ligand BEF 3 1002



Bond lengths



Bond angles



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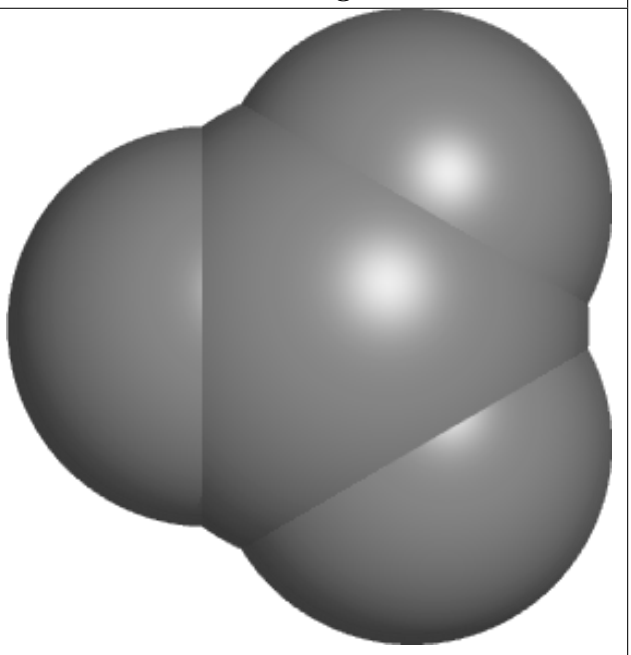

Rings

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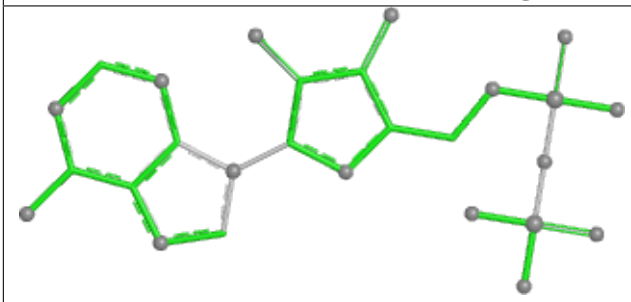
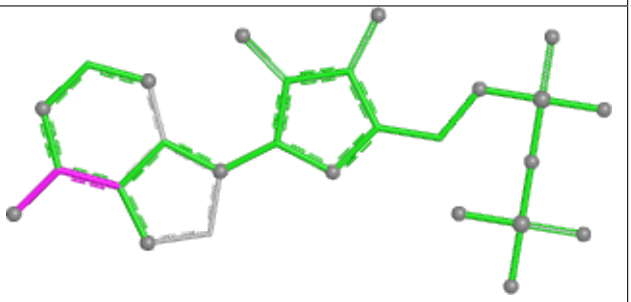
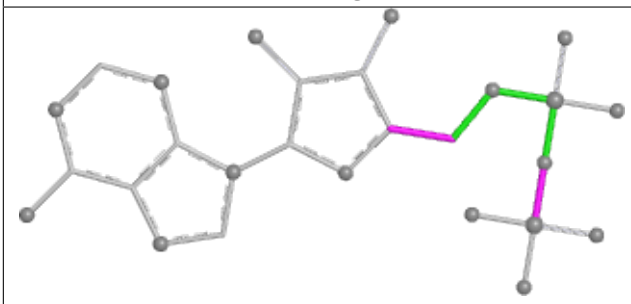
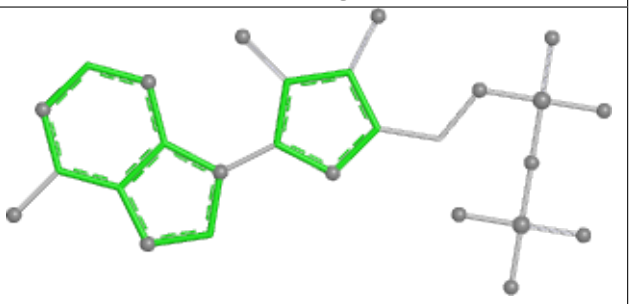
 Bond lengths	 Bond angles
 Torsions	 Rings

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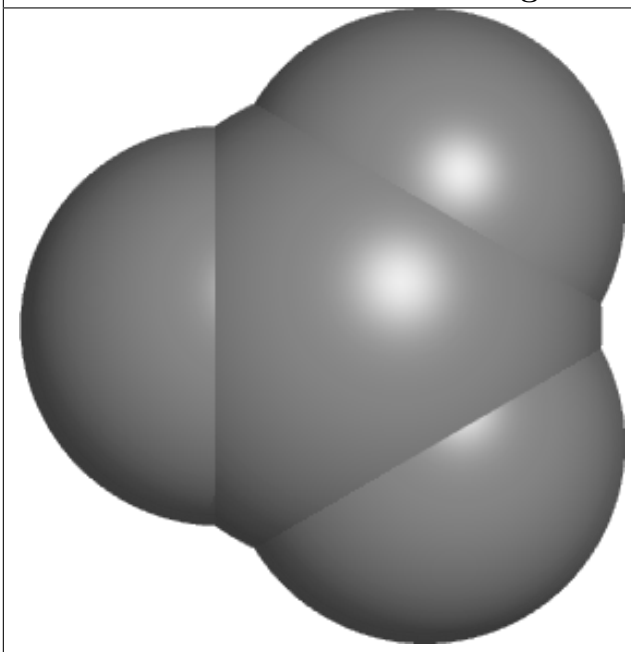
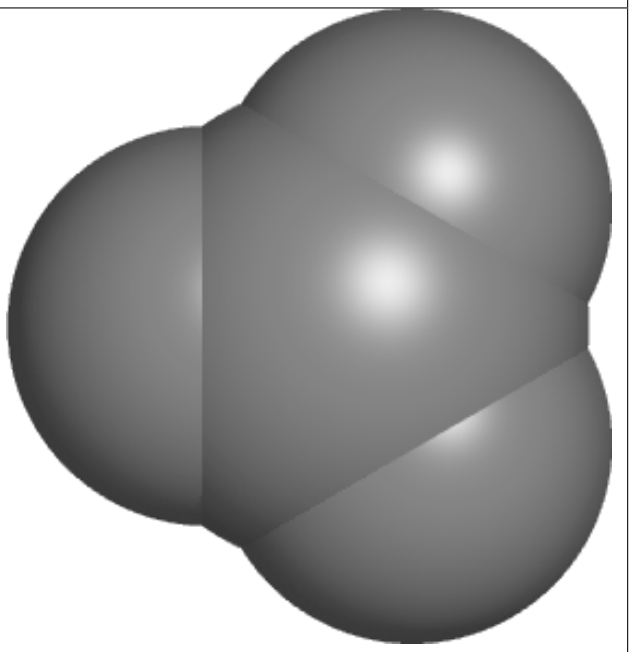


Bond lengths



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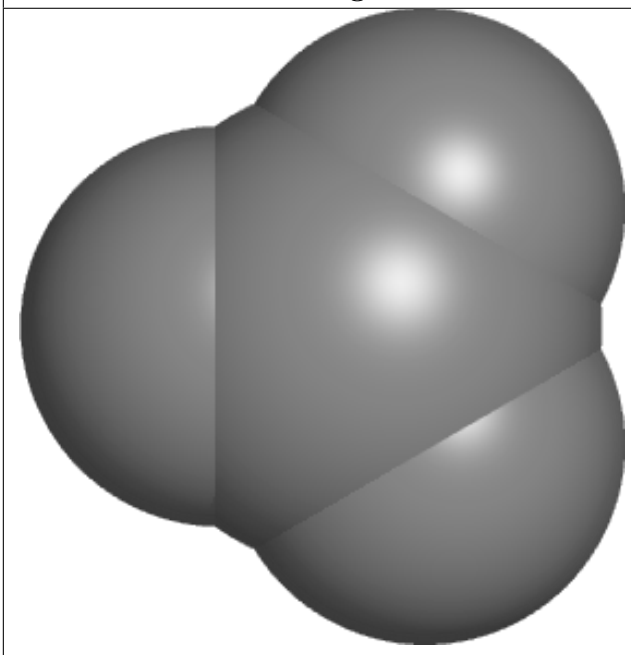
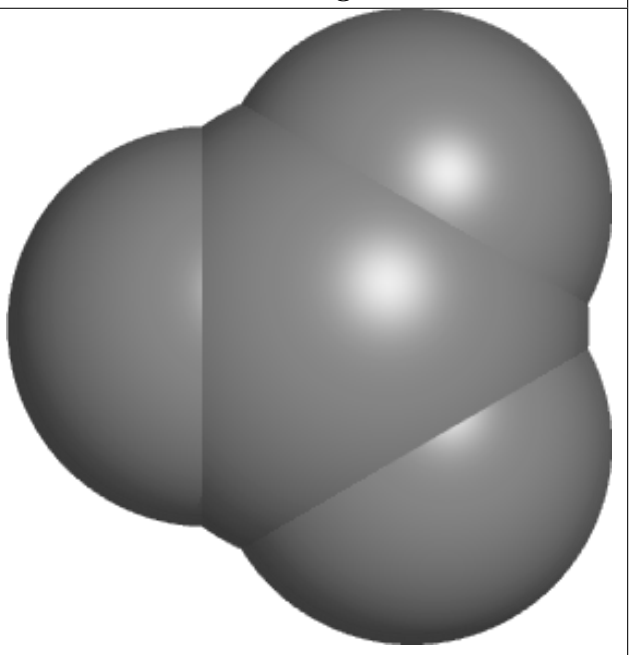


Torsions



Rings

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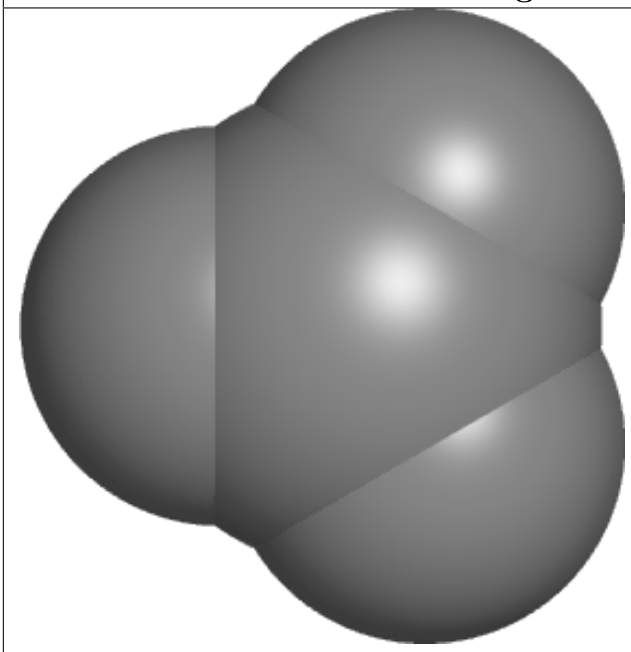

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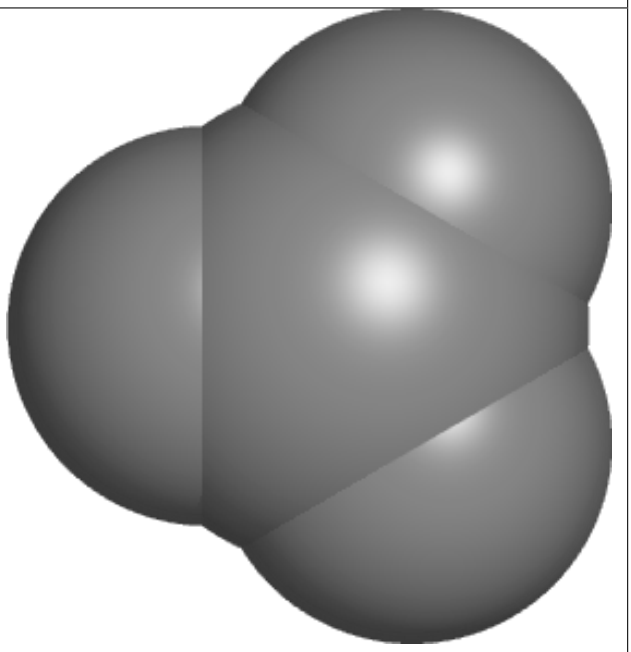

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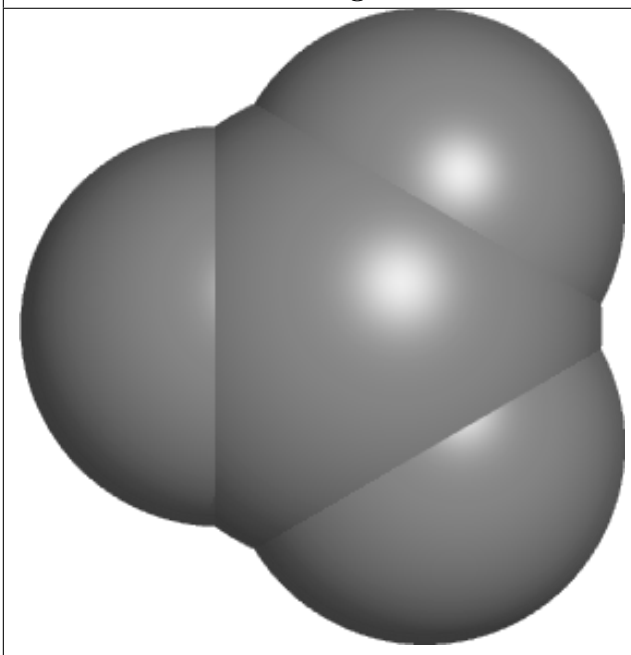

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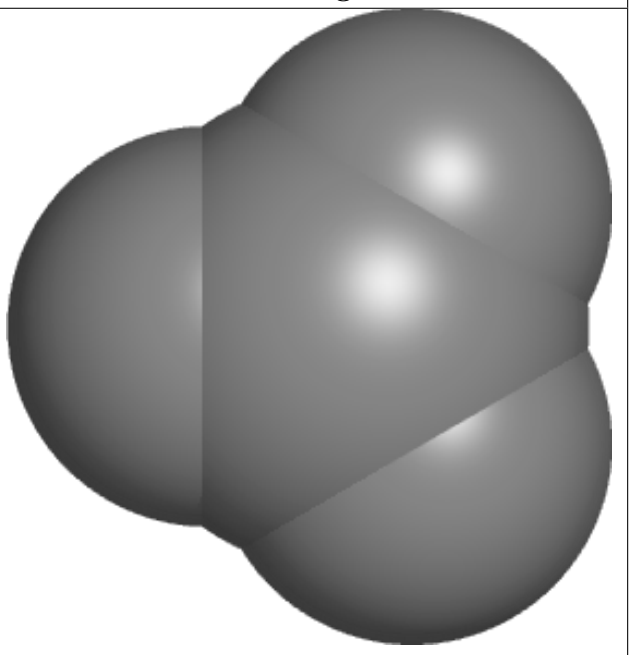
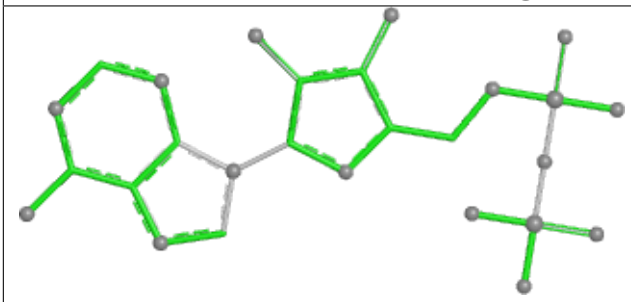
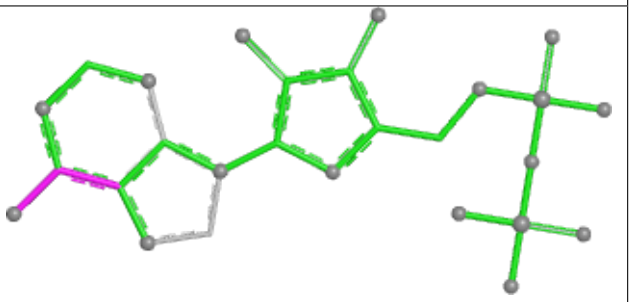
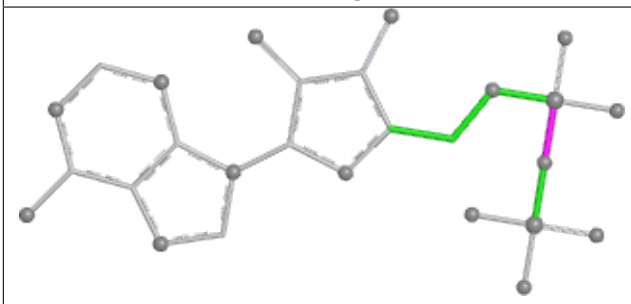
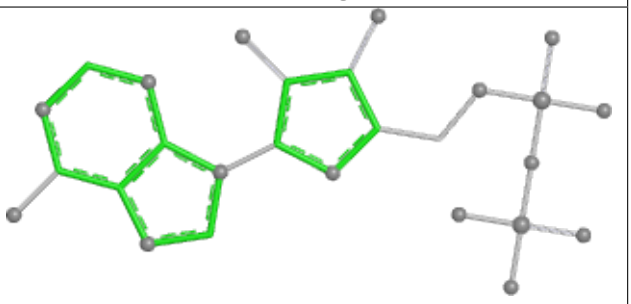


Rings

Ligand ADP 8 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

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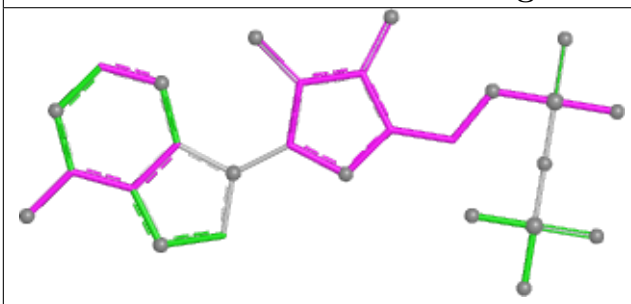
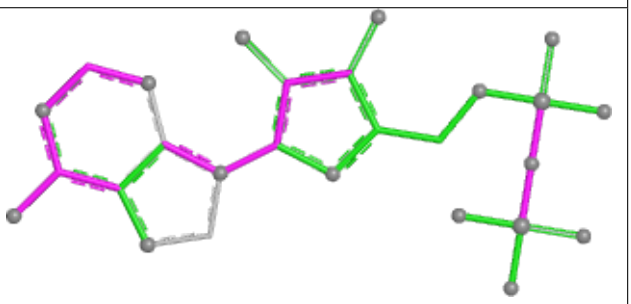
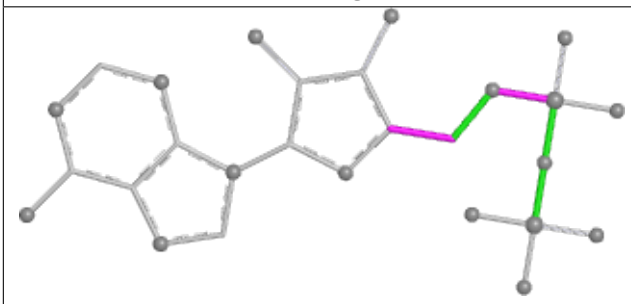
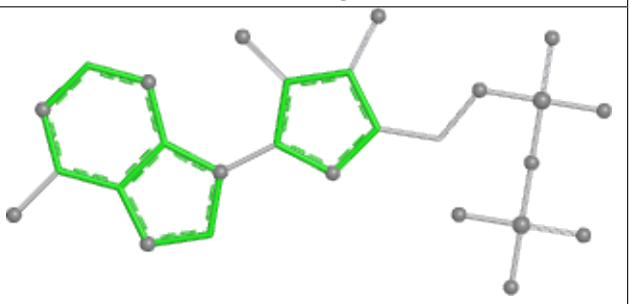
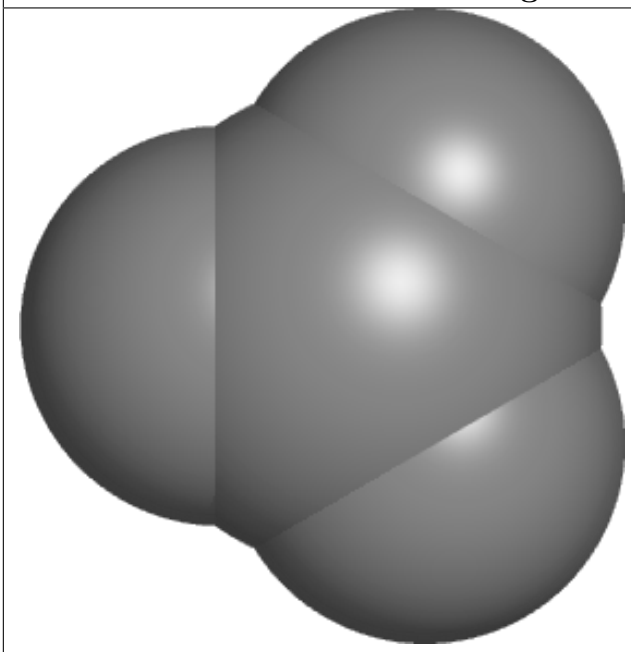
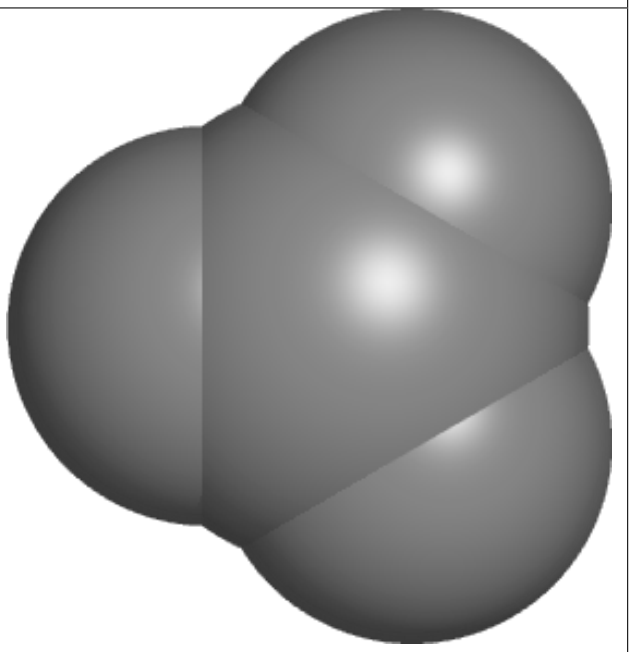
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BEF 4 1103



Bond lengths



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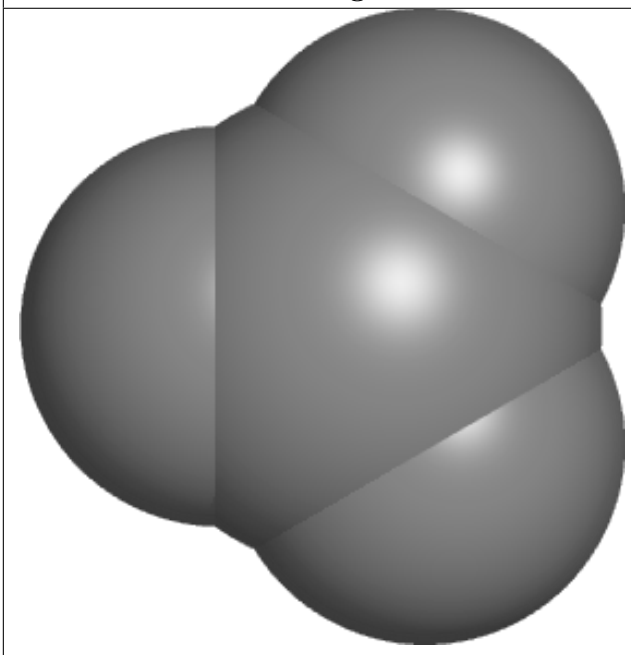
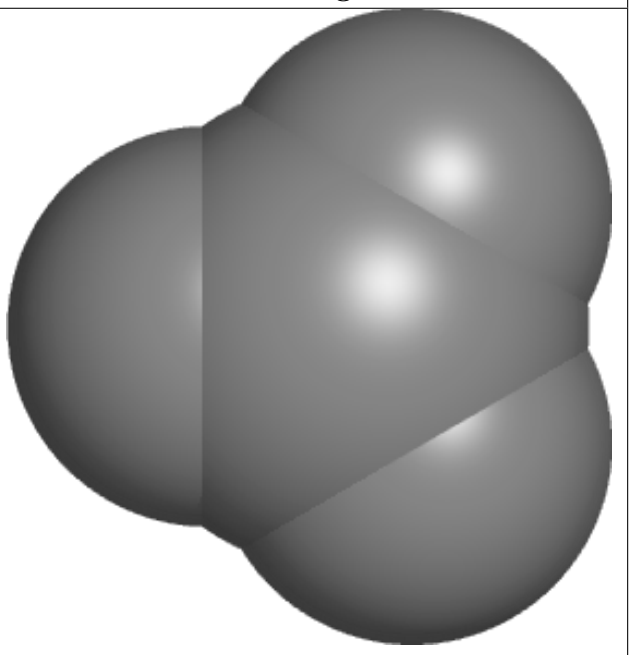


Torsions



Rings

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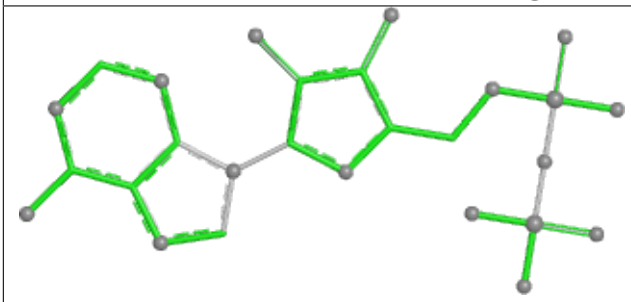
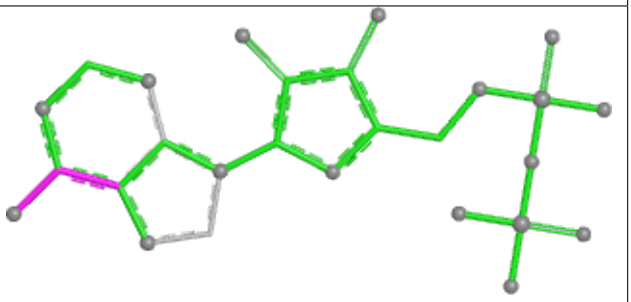
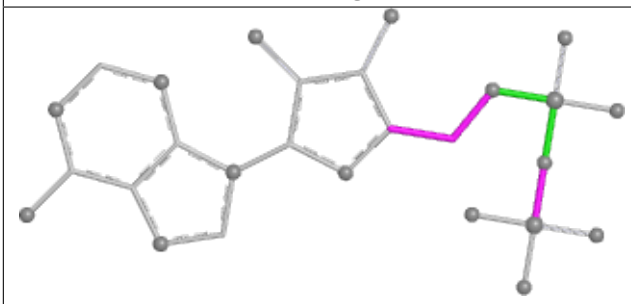
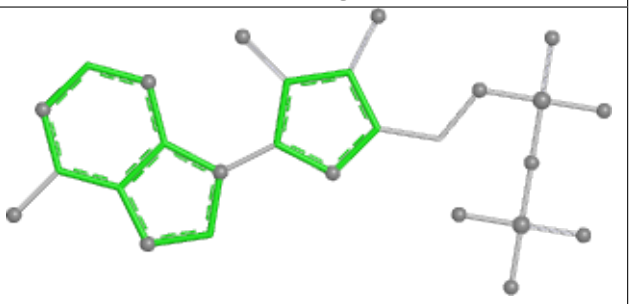
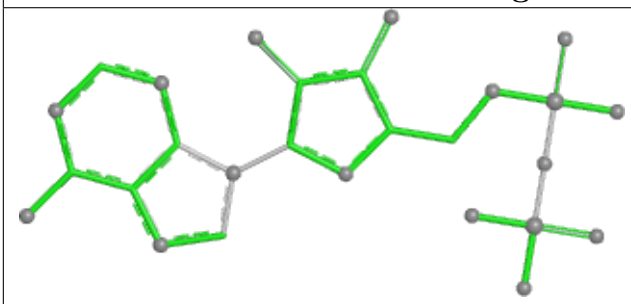
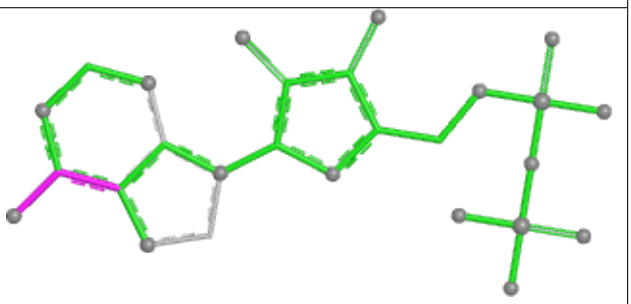
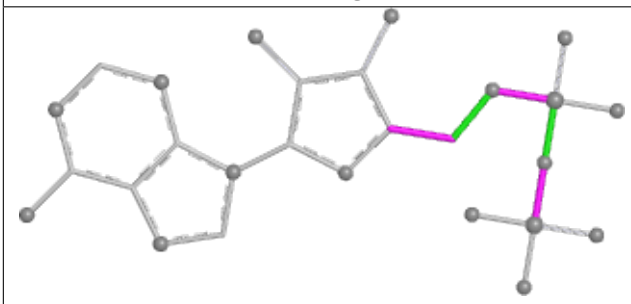
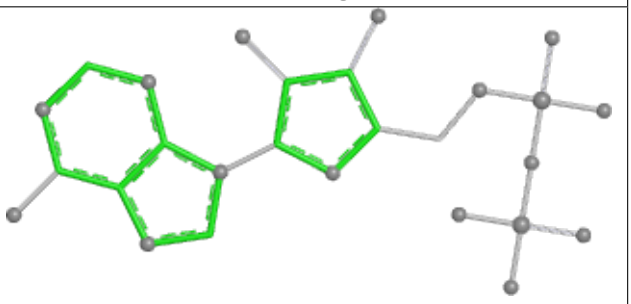
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP G 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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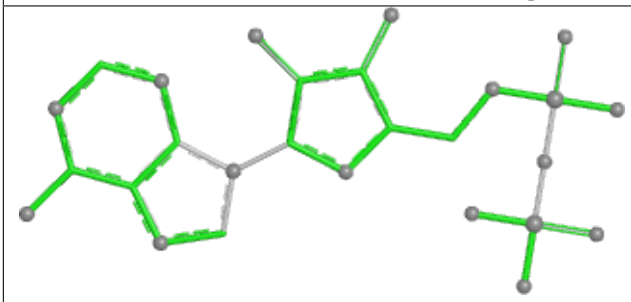
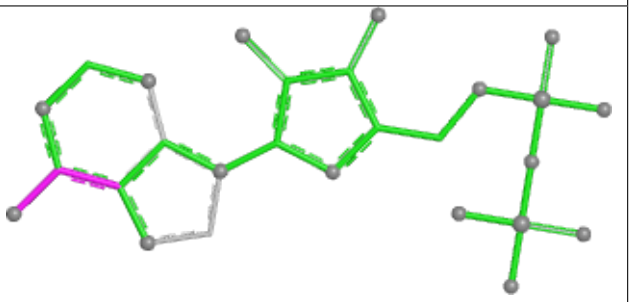
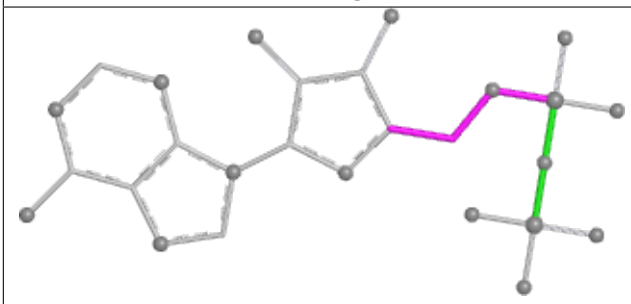
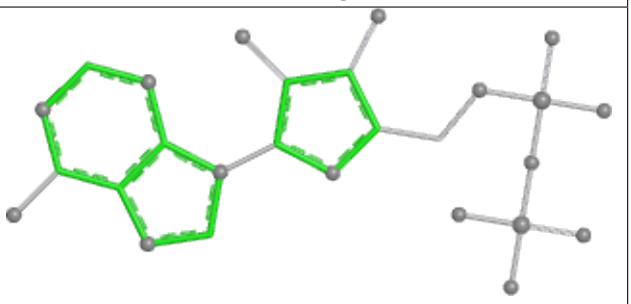
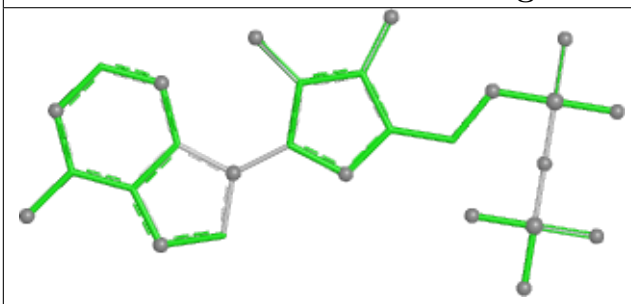
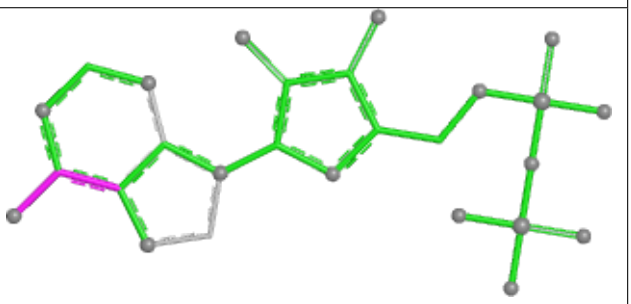
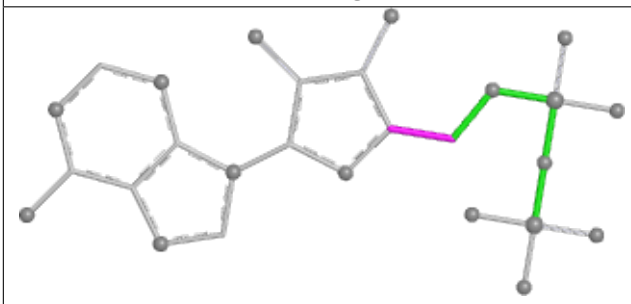
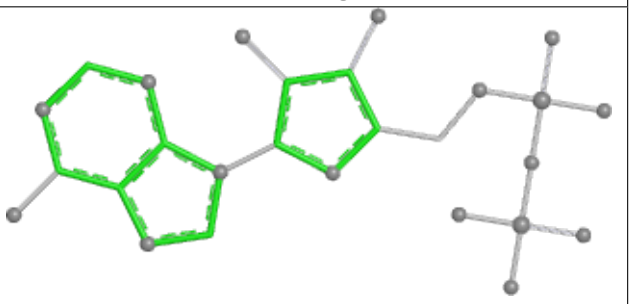
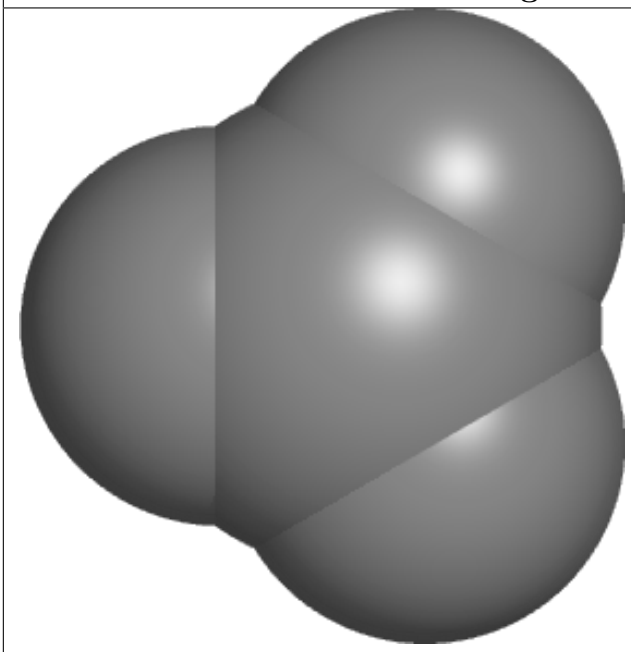
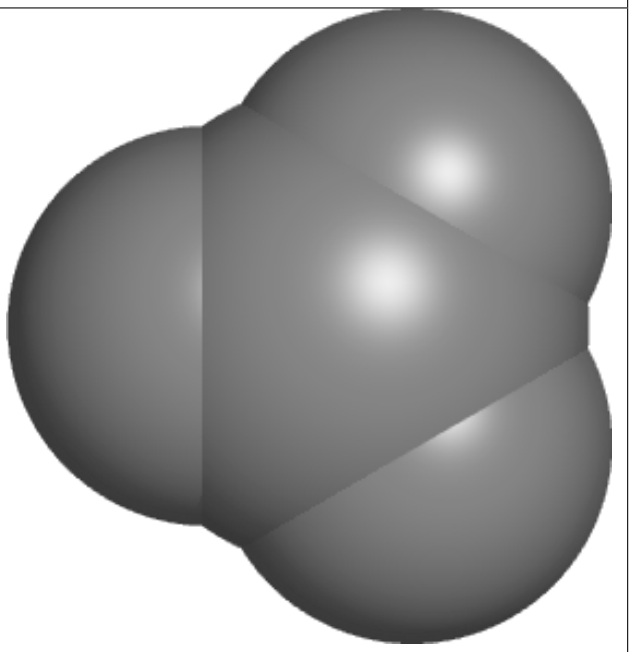
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP 4 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

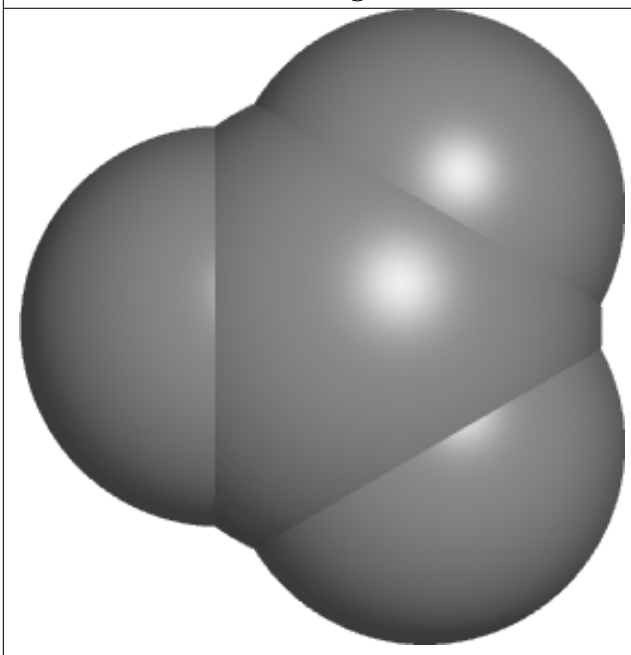
Ligand BEF 8 1003



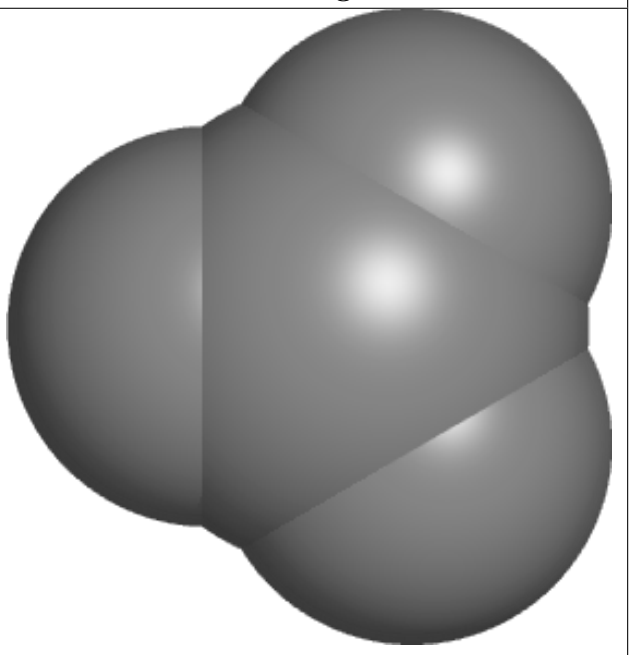
Bond lengths



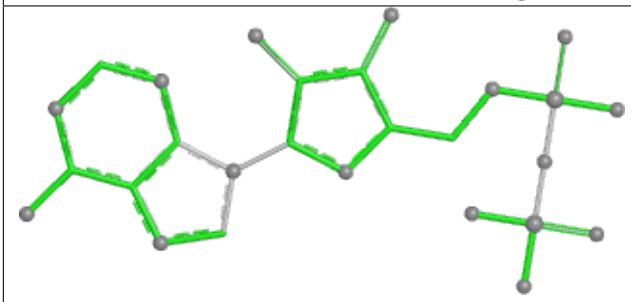
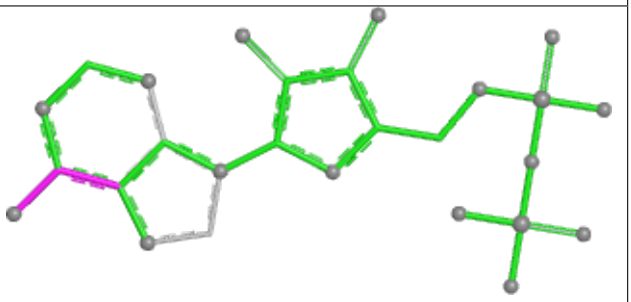
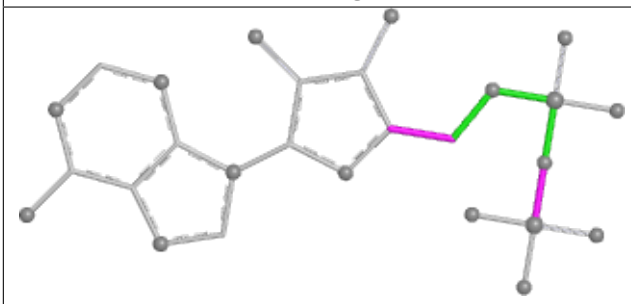
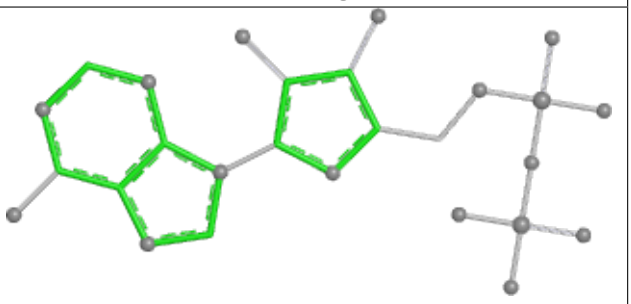
Bond angles



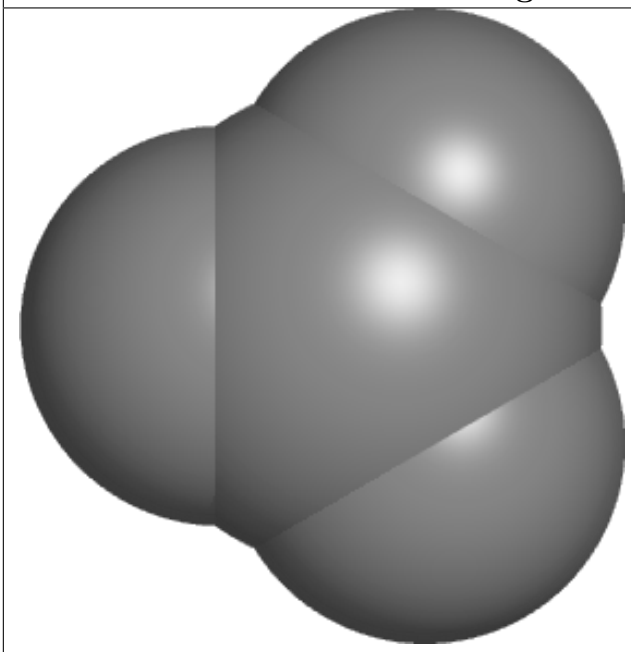
Torsions



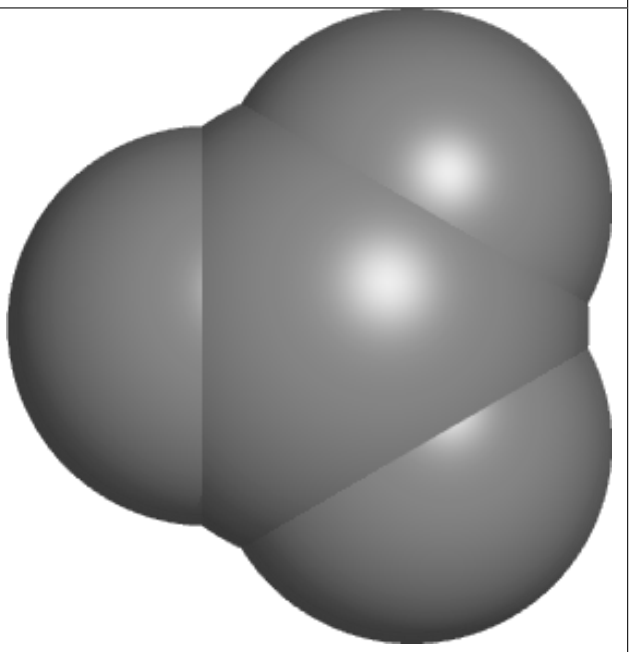
Rings

Ligand ADP C 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

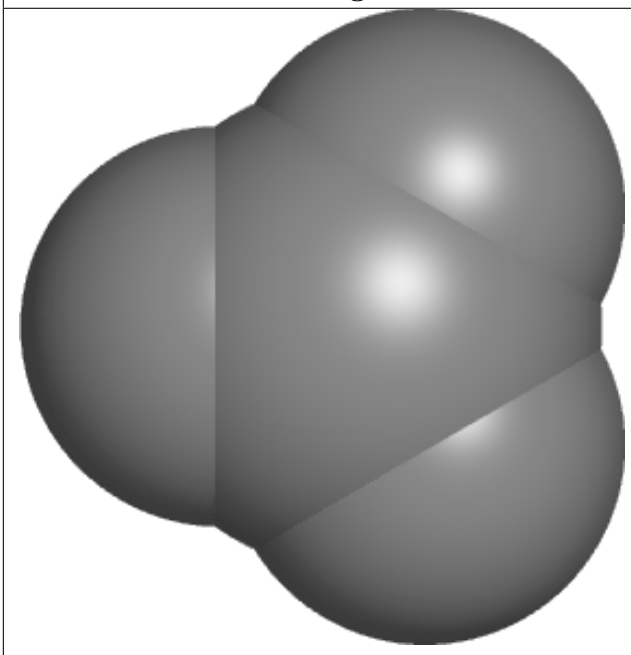
Ligand BEF D 1103



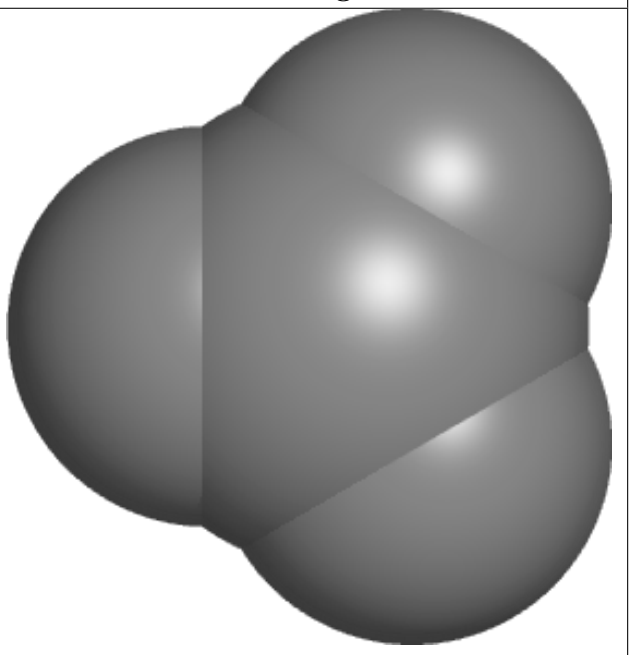
Bond lengths



Bond angles

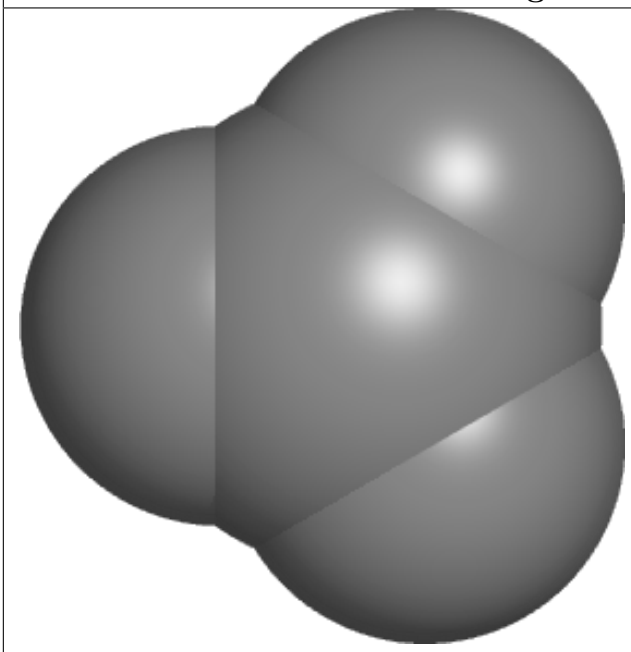


Torsions

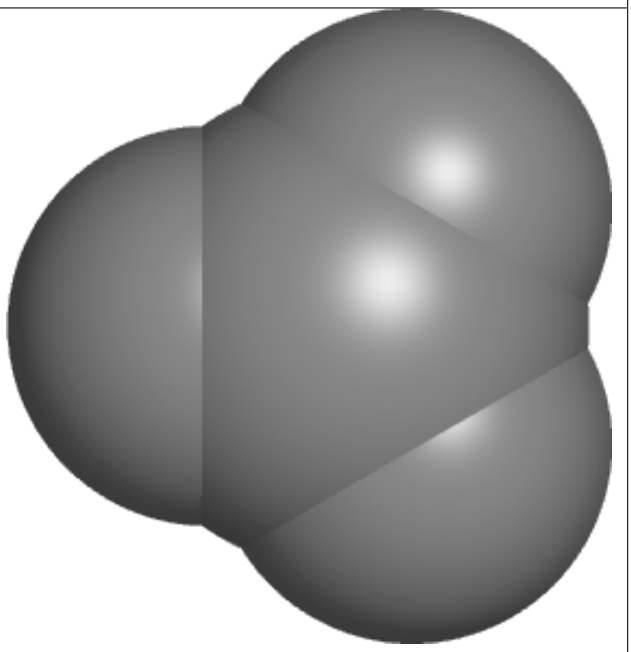


Rings

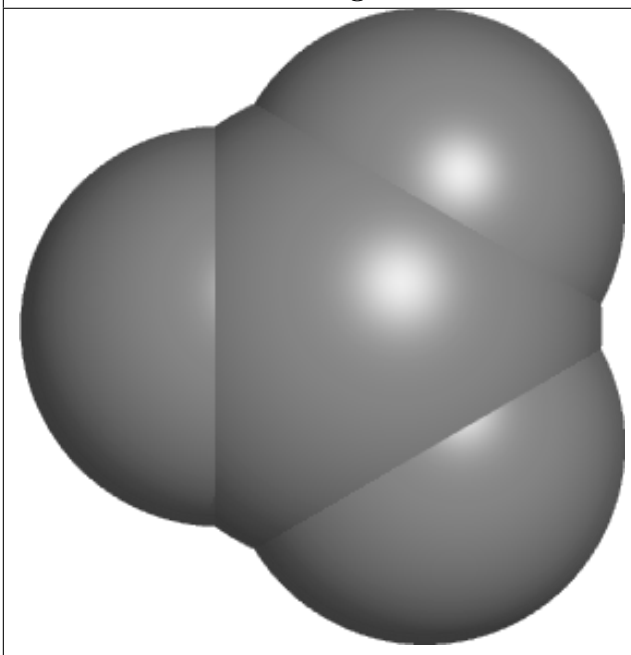
Ligand BEF E 801



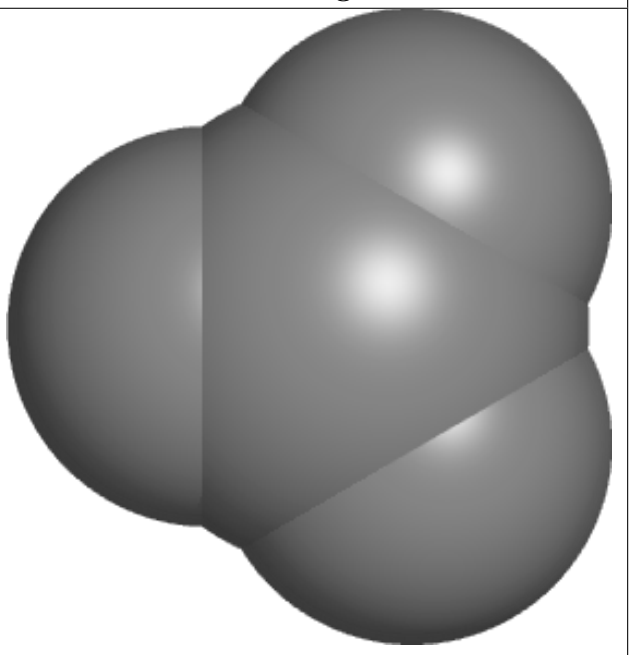
Bond lengths



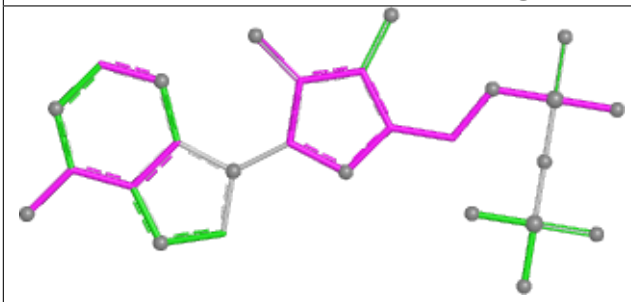
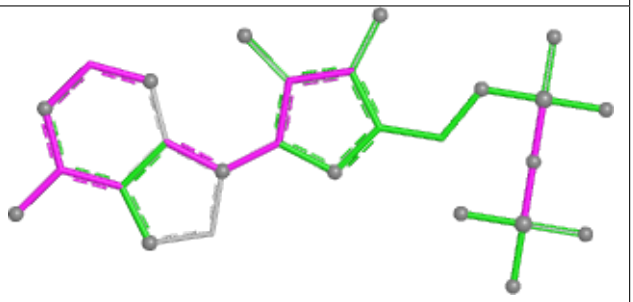
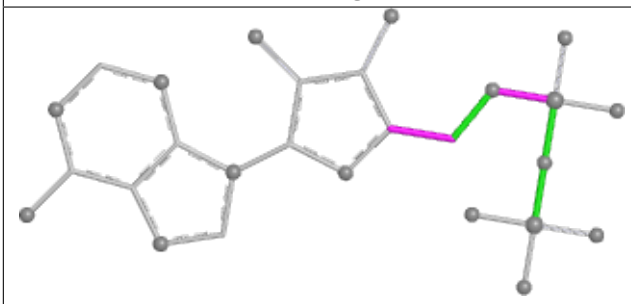
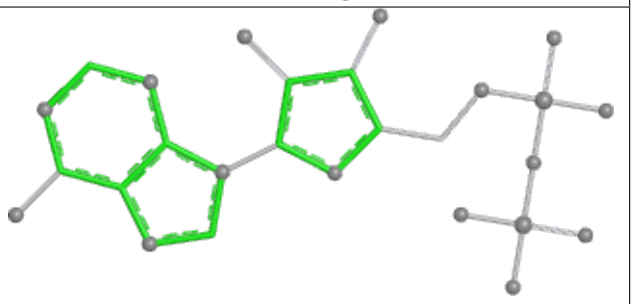
Bond angles



Torsions



Rings

Ligand ADP F 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

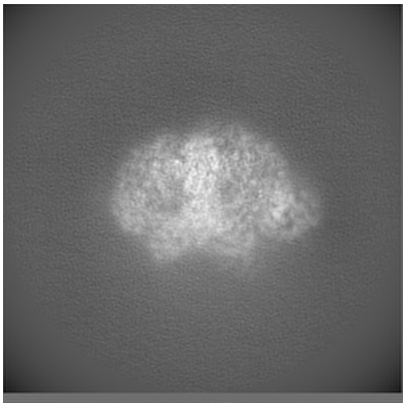
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13620. These allow visual inspection of the internal detail of the map and identification of artifacts.

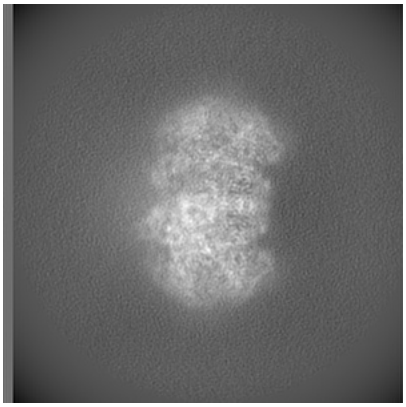
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

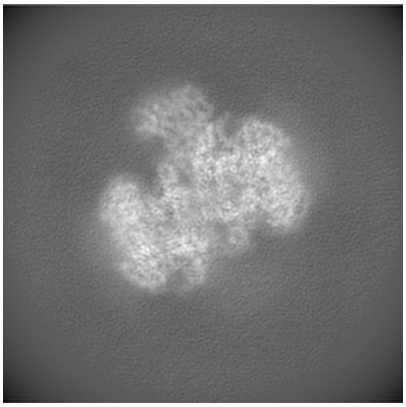
6.1.1 Primary map



X



Y

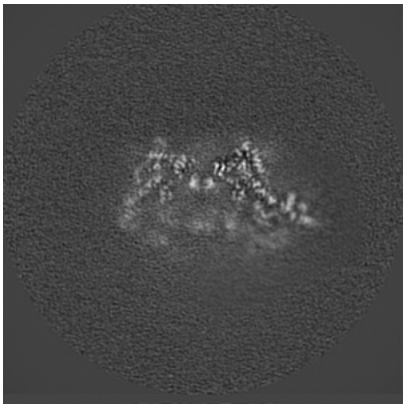


Z

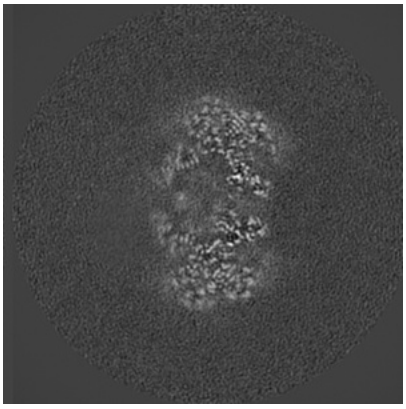
The images above show the map projected in three orthogonal directions.

6.2 Central slices

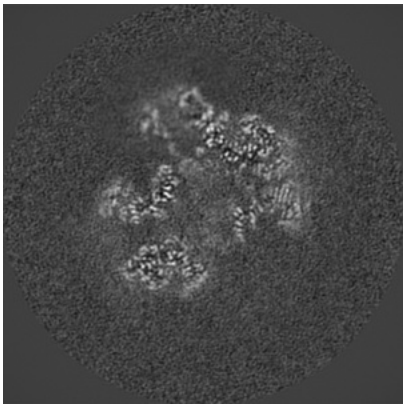
6.2.1 Primary map



X Index: 180



Y Index: 180

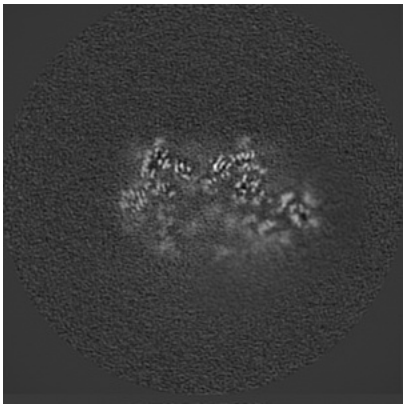


Z Index: 180

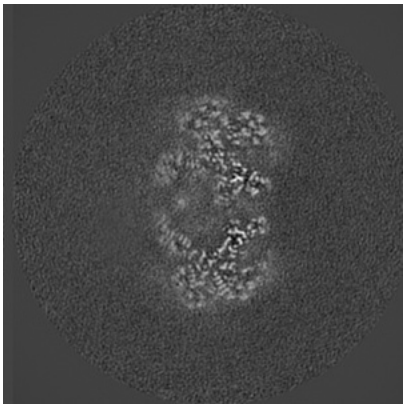
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

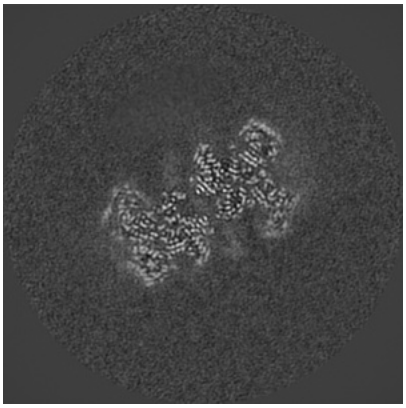
6.3.1 Primary map



X Index: 175



Y Index: 176



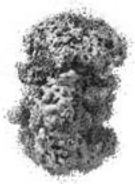
Z Index: 214

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

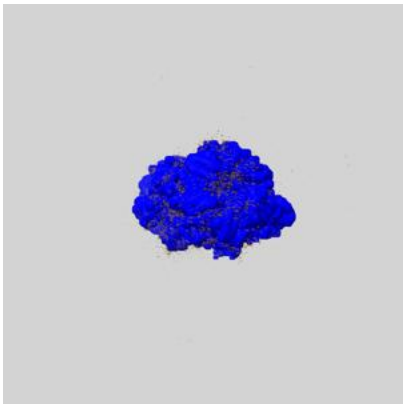
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

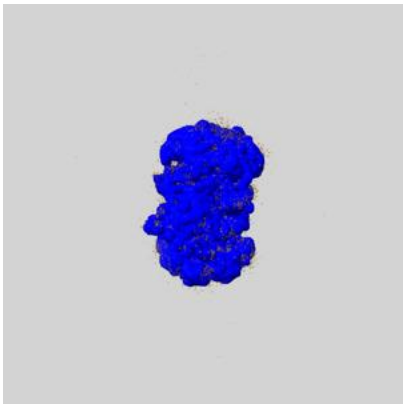
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

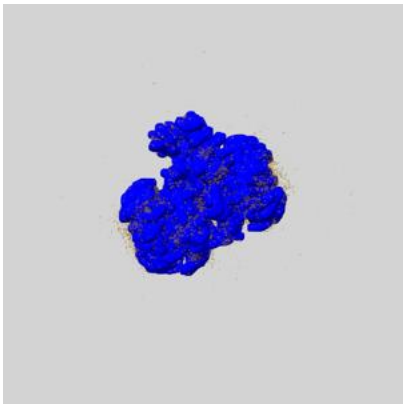
6.5.1 emd_13620_msk_1.map (i)



X



Y

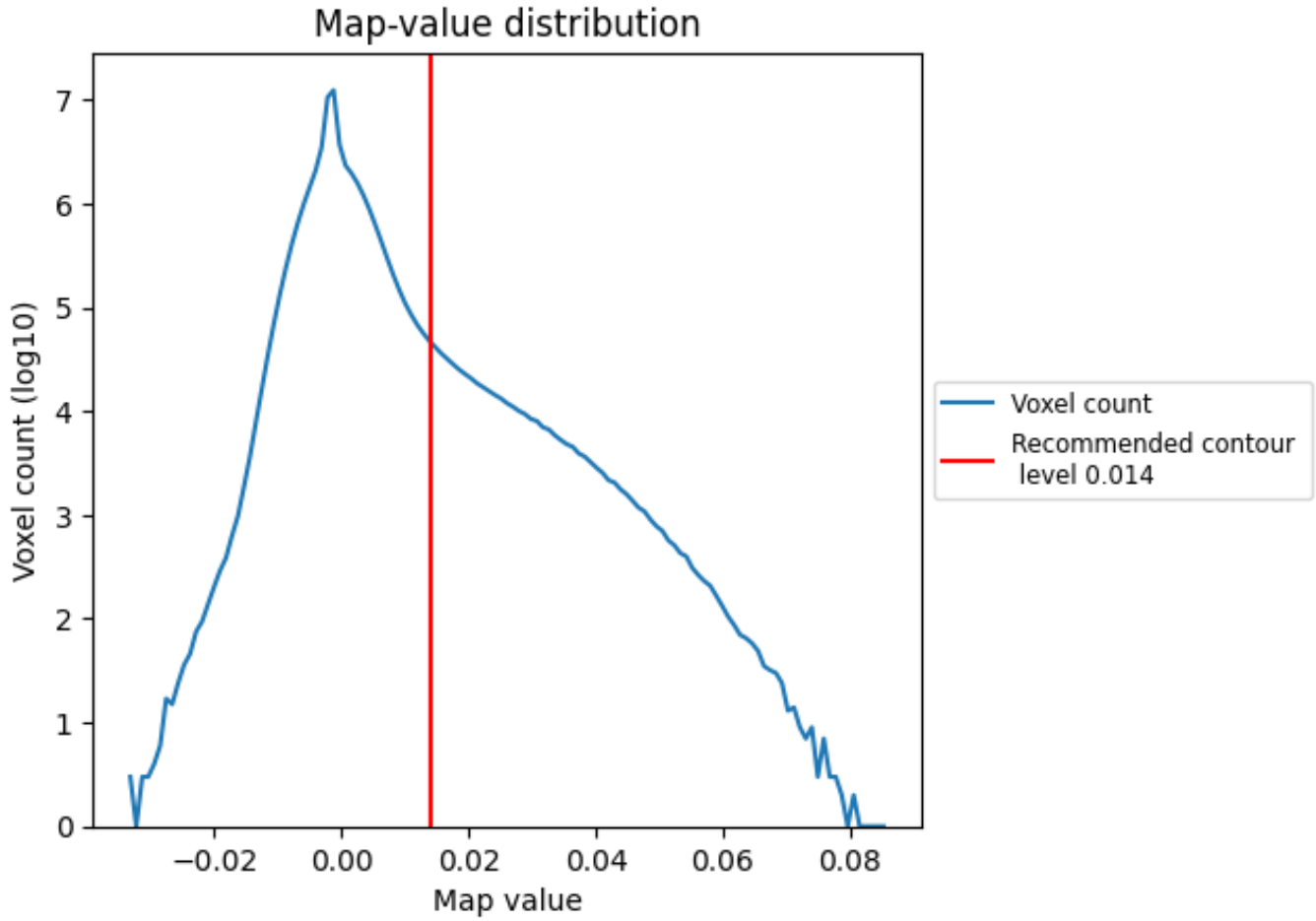


Z

7 Map analysis

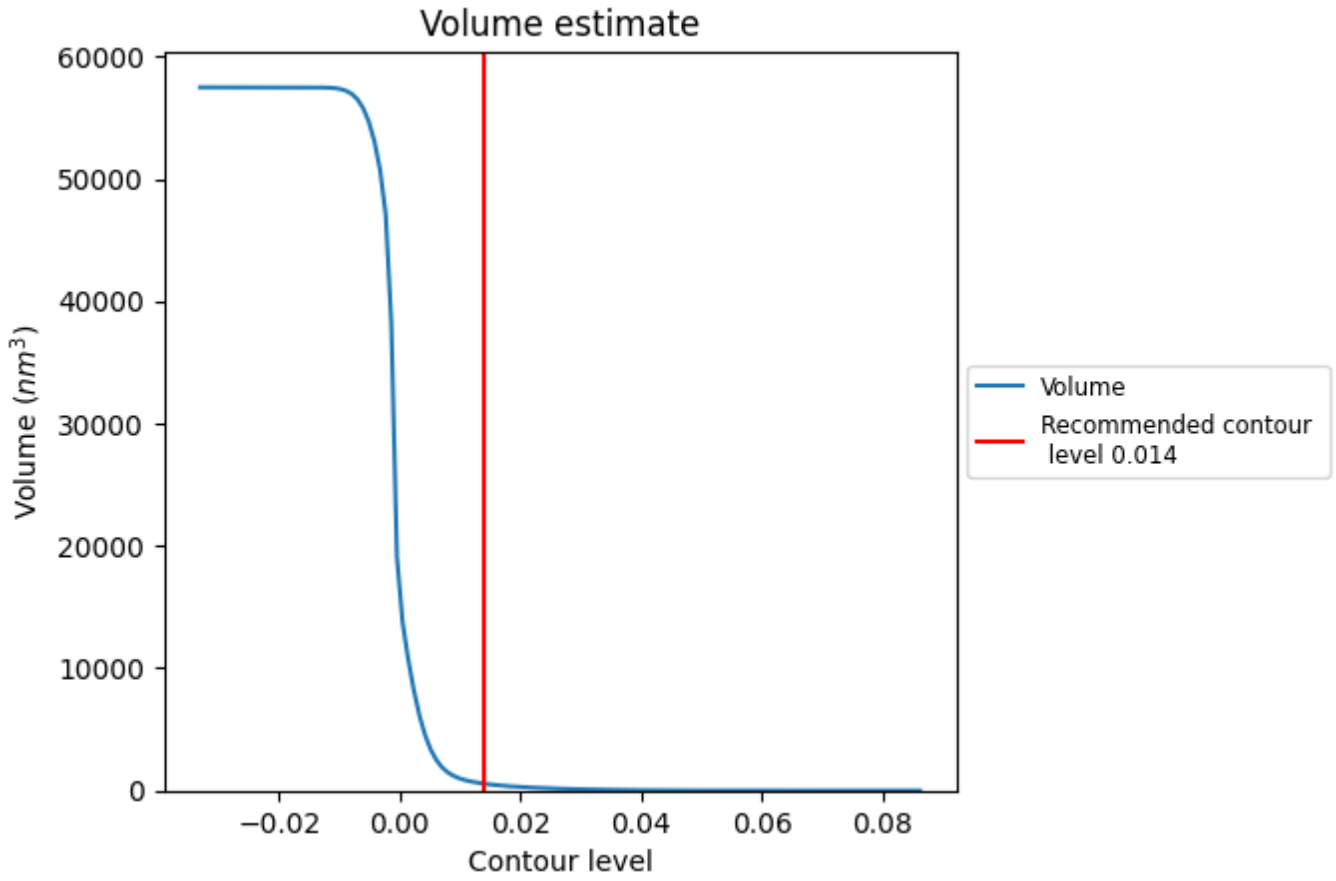
This section contains the results of statistical analysis of the map.

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.

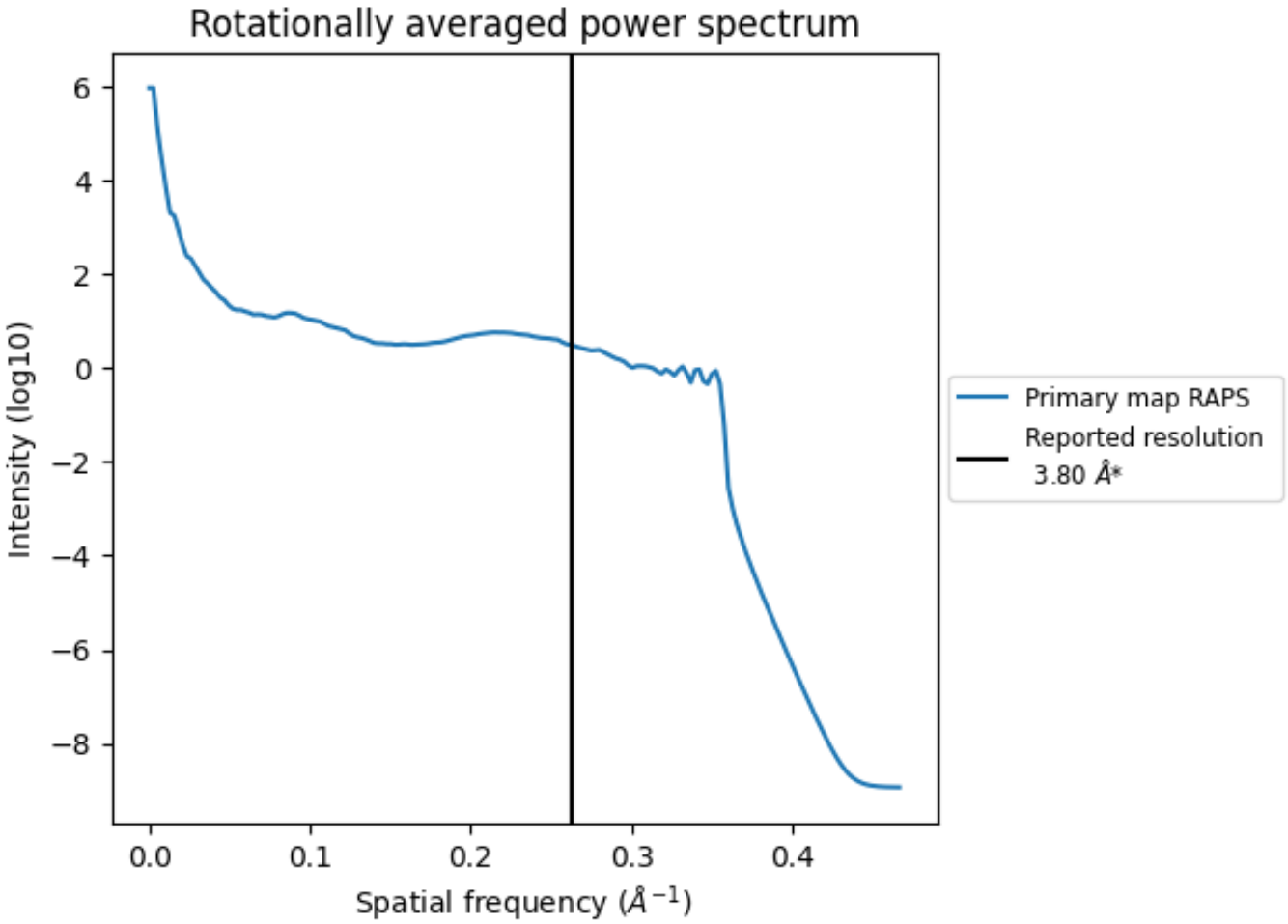
7.2 Volume estimate



The volume at the recommended contour level is 557 nm^3; this corresponds to an approximate mass of 504 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 0.263 Å^{-1}

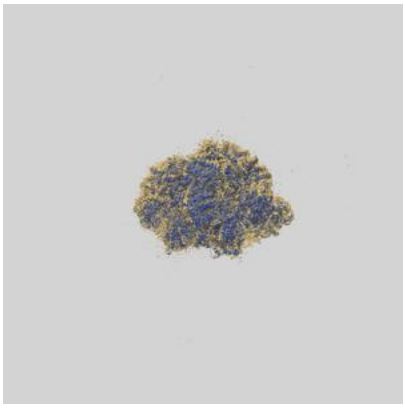
8 Fourier-Shell correlation

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

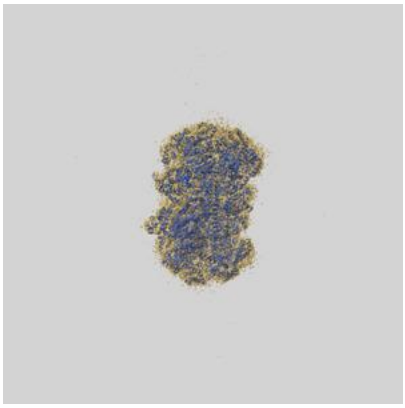
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13620 and PDB model 7PT7. Per-residue inclusion information can be found in section 3 on page 10.

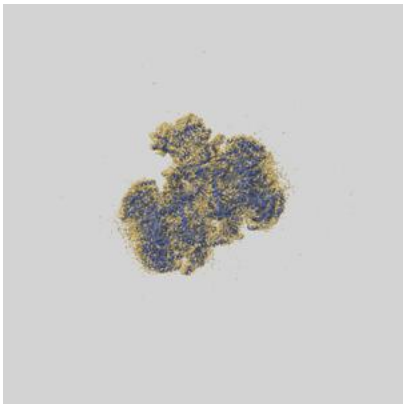
9.1 Map-model overlay



X



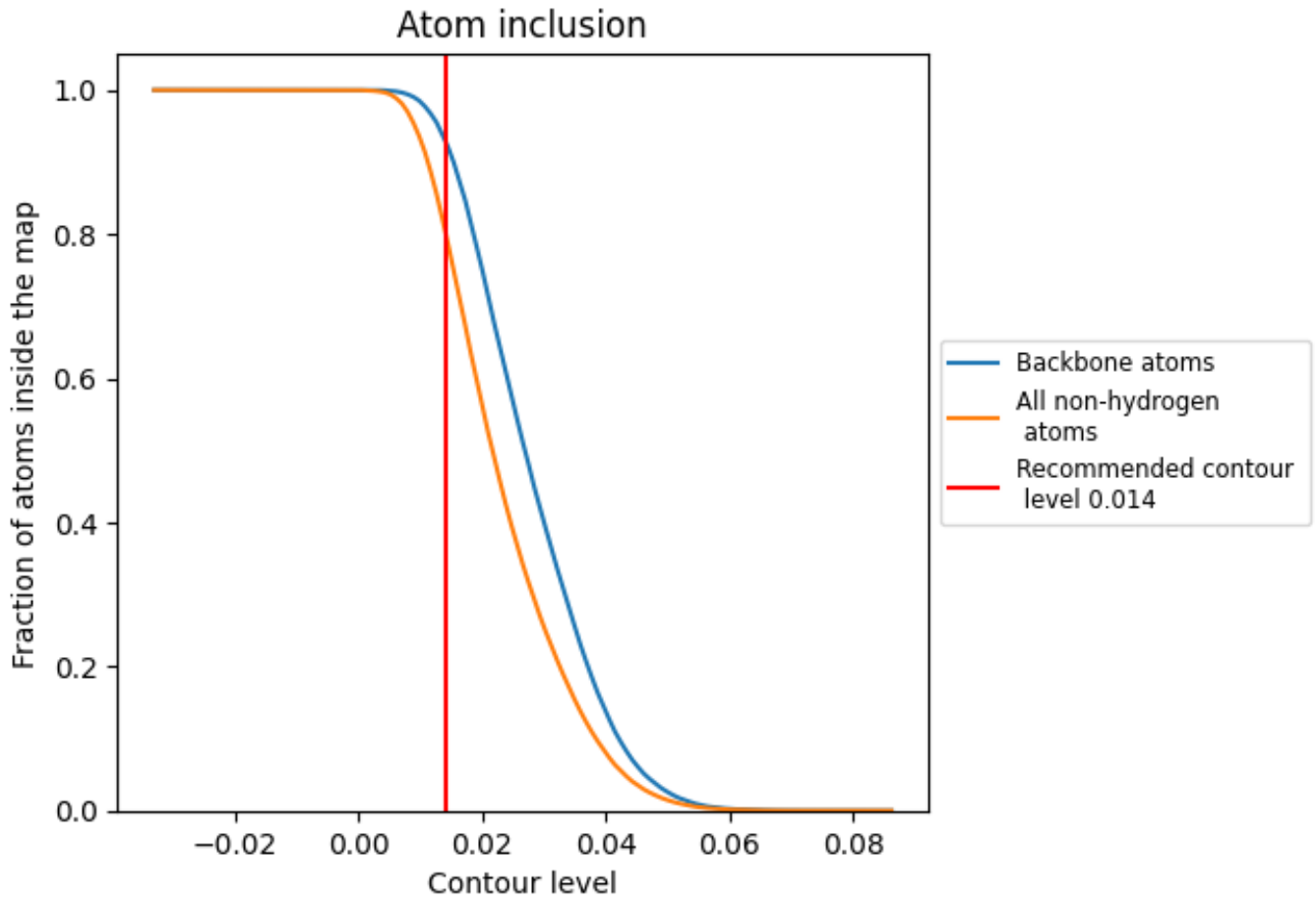
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.