Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 03:46 AM EDT

PDB ID	:	8F6N
Title	:	Dihydropyrimidine Dehydrogenase (DPD) C671S Mutant Soaked with Thymine Quasi-Anaerobically
Authors	:	Kaley, N.; Smith, M.; Forouzesh, D.; Liu, D.; Moran, G.
Deposited on	:	2022-11-16
Resolution	:	2.12 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

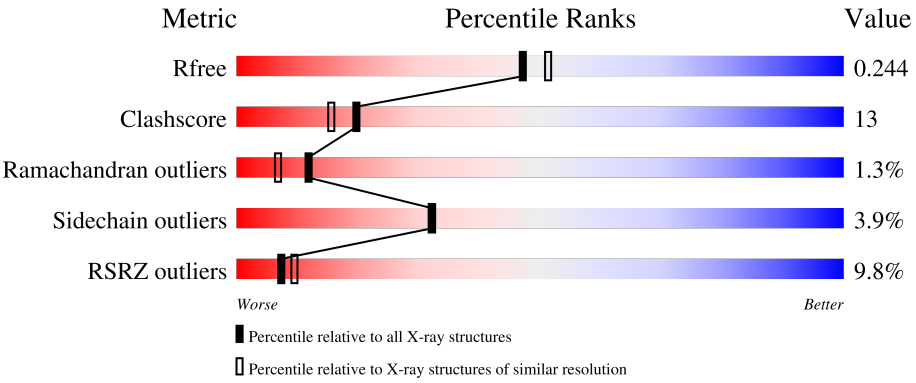
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1025	8% 61% 30% 6%
1	B	1025	10% 61% 30% 6%
1	C	1025	10% 63% 29% 6%
1	D	1025	10% 63% 29%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SF4	A	1103	-	-	X	-
2	SF4	C	1102	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 31607 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Dihydropyrimidine dehydrogenase [NADP(+)].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	996	Total	C	N	O	S	0	4	0
			7608	4829	1283	1443	53			
1	B	1001	Total	C	N	O	S	0	5	0
			7662	4860	1298	1450	54			
1	C	1002	Total	C	N	O	S	0	4	0
			7654	4856	1292	1453	53			
1	D	992	Total	C	N	O	S	0	5	0
			7590	4816	1282	1441	51			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLY	conflict	UNP Q28943
A	671	SER	CYS	engineered mutation	UNP Q28943
A	1019	LEU	-	expression tag	UNP Q28943
A	1020	ALA	-	expression tag	UNP Q28943
A	1021	VAL	-	expression tag	UNP Q28943
A	1022	ASN	-	expression tag	UNP Q28943
A	1023	PRO	-	expression tag	UNP Q28943
A	1024	VAL	-	expression tag	UNP Q28943
A	1025	CYS	-	expression tag	UNP Q28943
B	60	ASP	GLY	conflict	UNP Q28943
B	671	SER	CYS	engineered mutation	UNP Q28943
B	1019	LEU	-	expression tag	UNP Q28943
B	1020	ALA	-	expression tag	UNP Q28943
B	1021	VAL	-	expression tag	UNP Q28943
B	1022	ASN	-	expression tag	UNP Q28943
B	1023	PRO	-	expression tag	UNP Q28943
B	1024	VAL	-	expression tag	UNP Q28943
B	1025	CYS	-	expression tag	UNP Q28943
C	60	ASP	GLY	conflict	UNP Q28943
C	671	SER	CYS	engineered mutation	UNP Q28943
C	1019	LEU	-	expression tag	UNP Q28943

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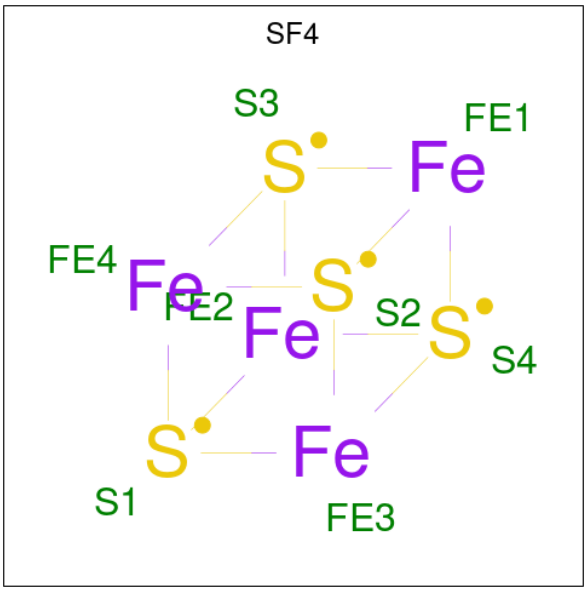
Chain	Residue	Modelled	Actual	Comment	Reference
C	1020	ALA	-	expression tag	UNP Q28943
C	1021	VAL	-	expression tag	UNP Q28943
C	1022	ASN	-	expression tag	UNP Q28943
C	1023	PRO	-	expression tag	UNP Q28943
C	1024	VAL	-	expression tag	UNP Q28943
C	1025	CYS	-	expression tag	UNP Q28943
D	60	ASP	GLY	conflict	UNP Q28943
D	671	SER	CYS	engineered mutation	UNP Q28943
D	1019	LEU	-	expression tag	UNP Q28943
D	1020	ALA	-	expression tag	UNP Q28943
D	1021	VAL	-	expression tag	UNP Q28943
D	1022	ASN	-	expression tag	UNP Q28943
D	1023	PRO	-	expression tag	UNP Q28943
D	1024	VAL	-	expression tag	UNP Q28943
D	1025	CYS	-	expression tag	UNP Q28943

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0

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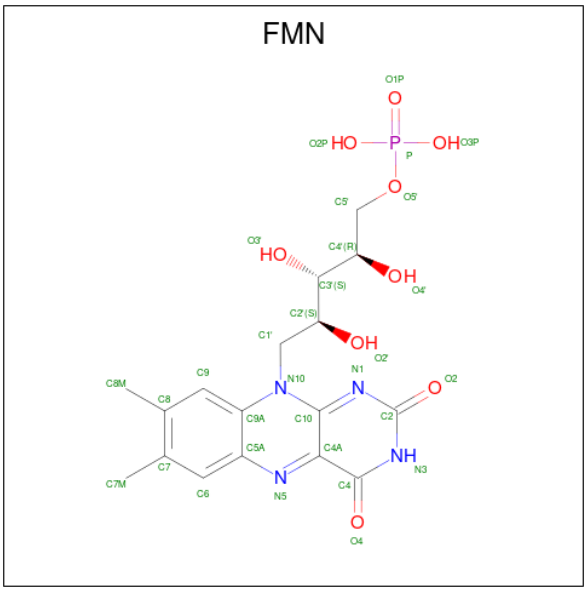
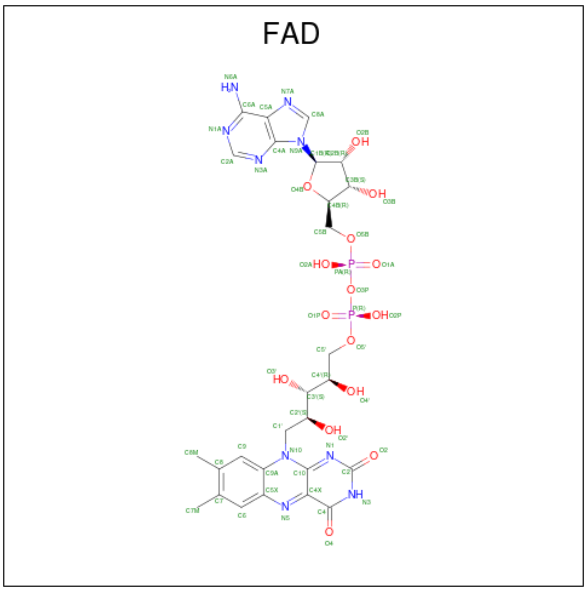
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



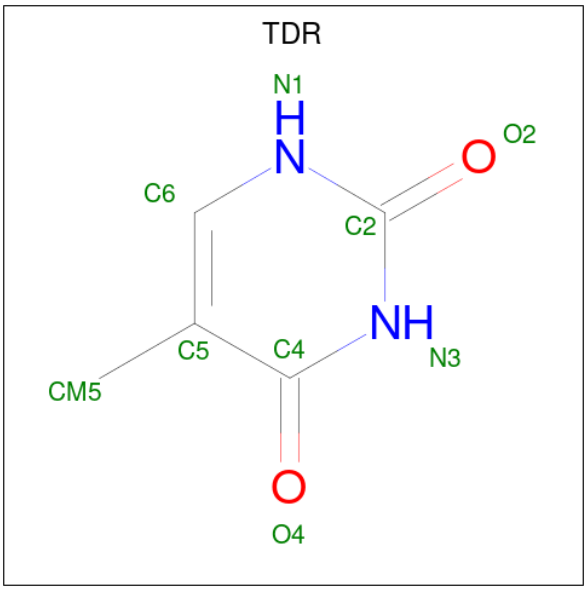
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is THYMINE (three-letter code: TDR) (formula: $C_5H_6N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			9	5	2	2		
5	B	1	Total	C	N	O	0	0
			9	5	2	2		
5	C	1	Total	C	N	O	0	0
			9	5	2	2		
5	D	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	149	Total	O	0	0
			149	149		

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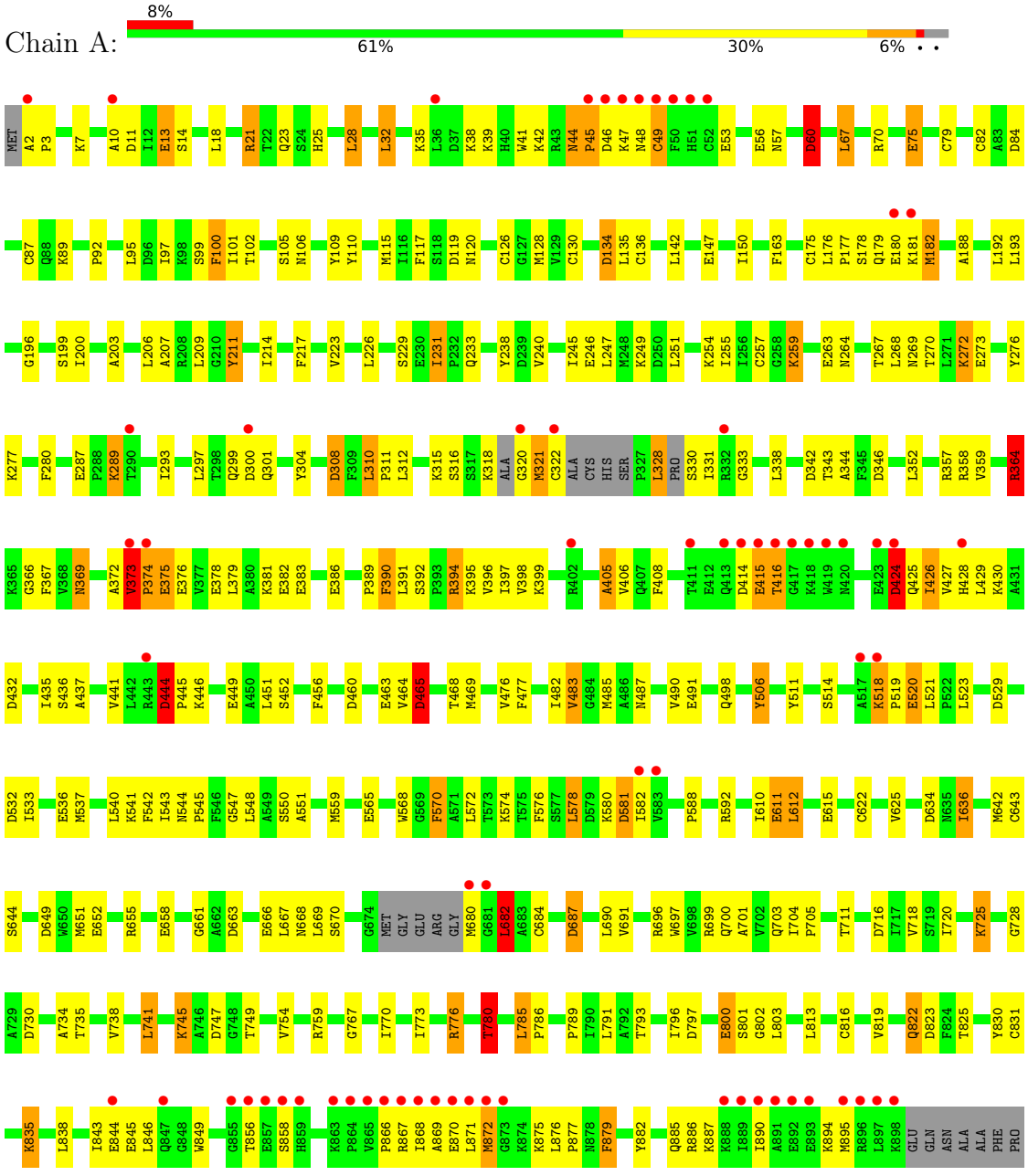
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	141	Total O 141 141	0	0
6	C	159	Total O 159 159	0	0
6	D	144	Total O 144 144	0	0

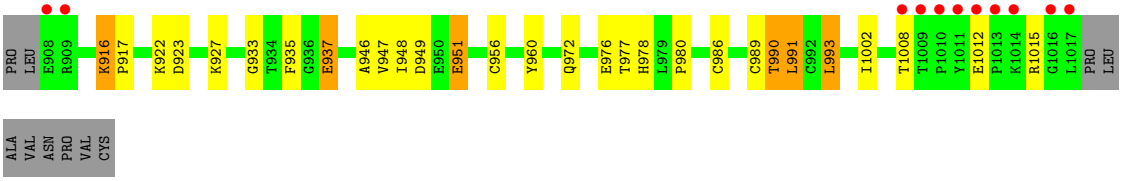
3 Residue-property plots (i)

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: Dihydropyrimidine dehydrogenase [NADP(+)]

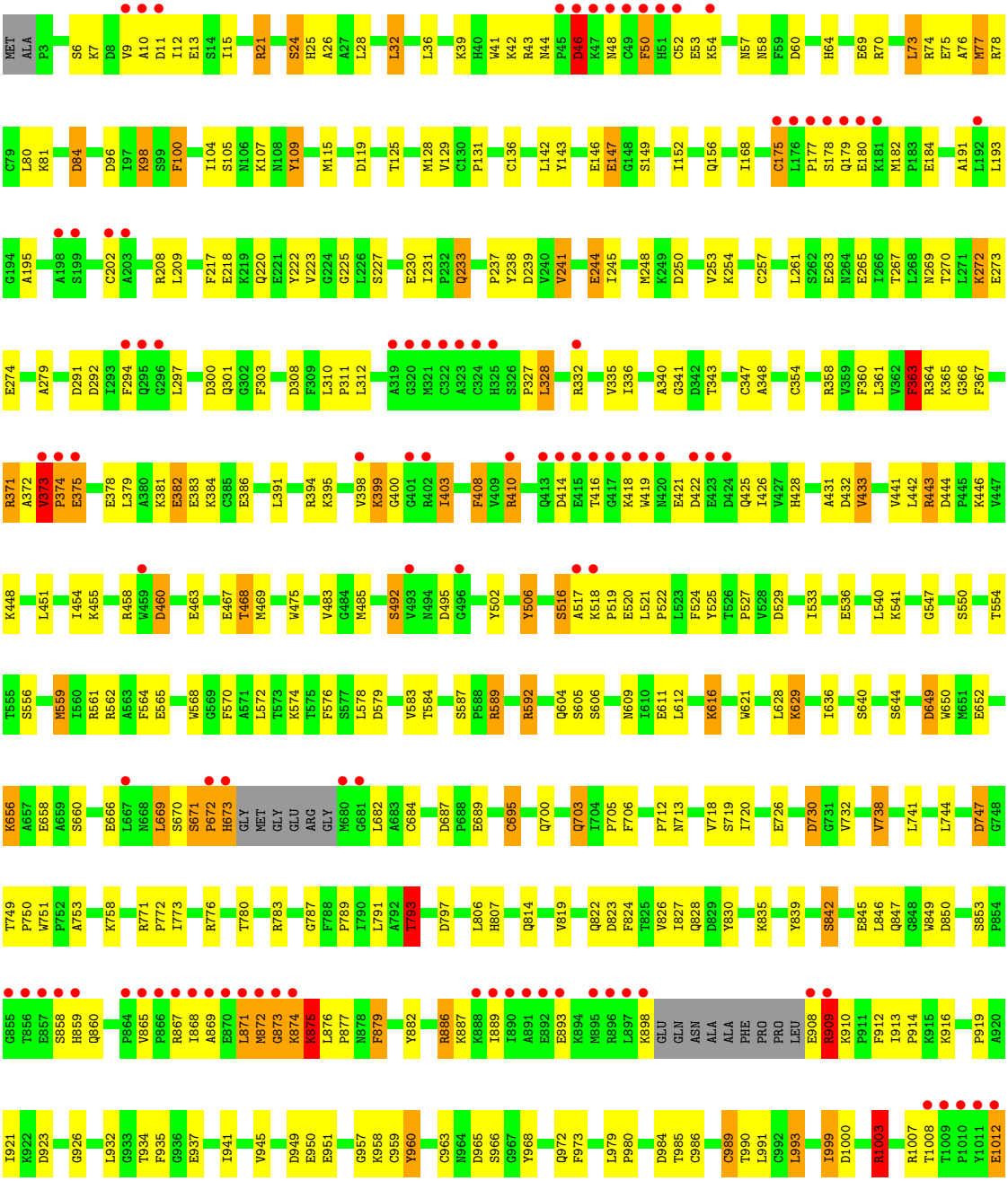
Chain A:

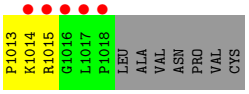




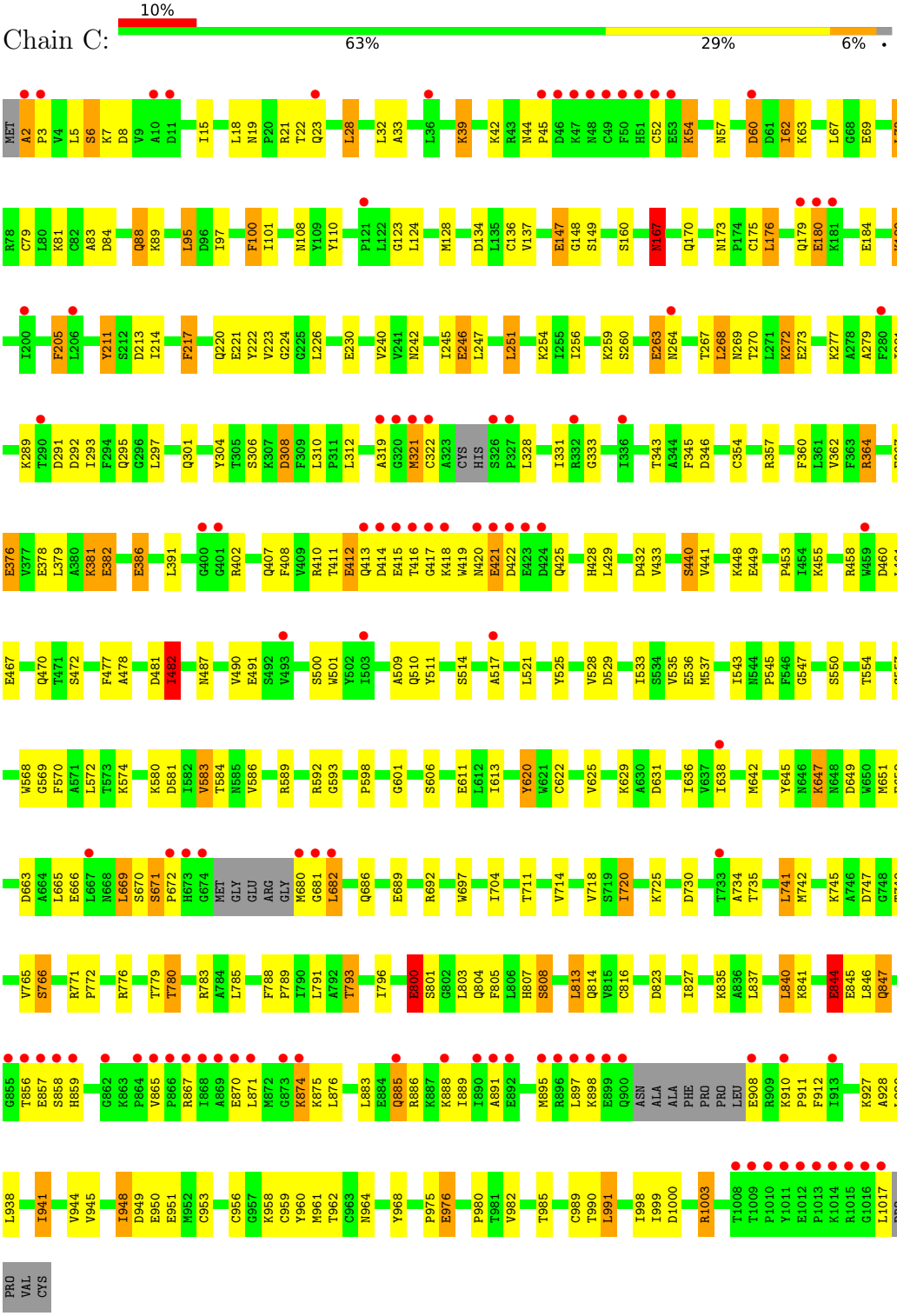
• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]

Chain B:





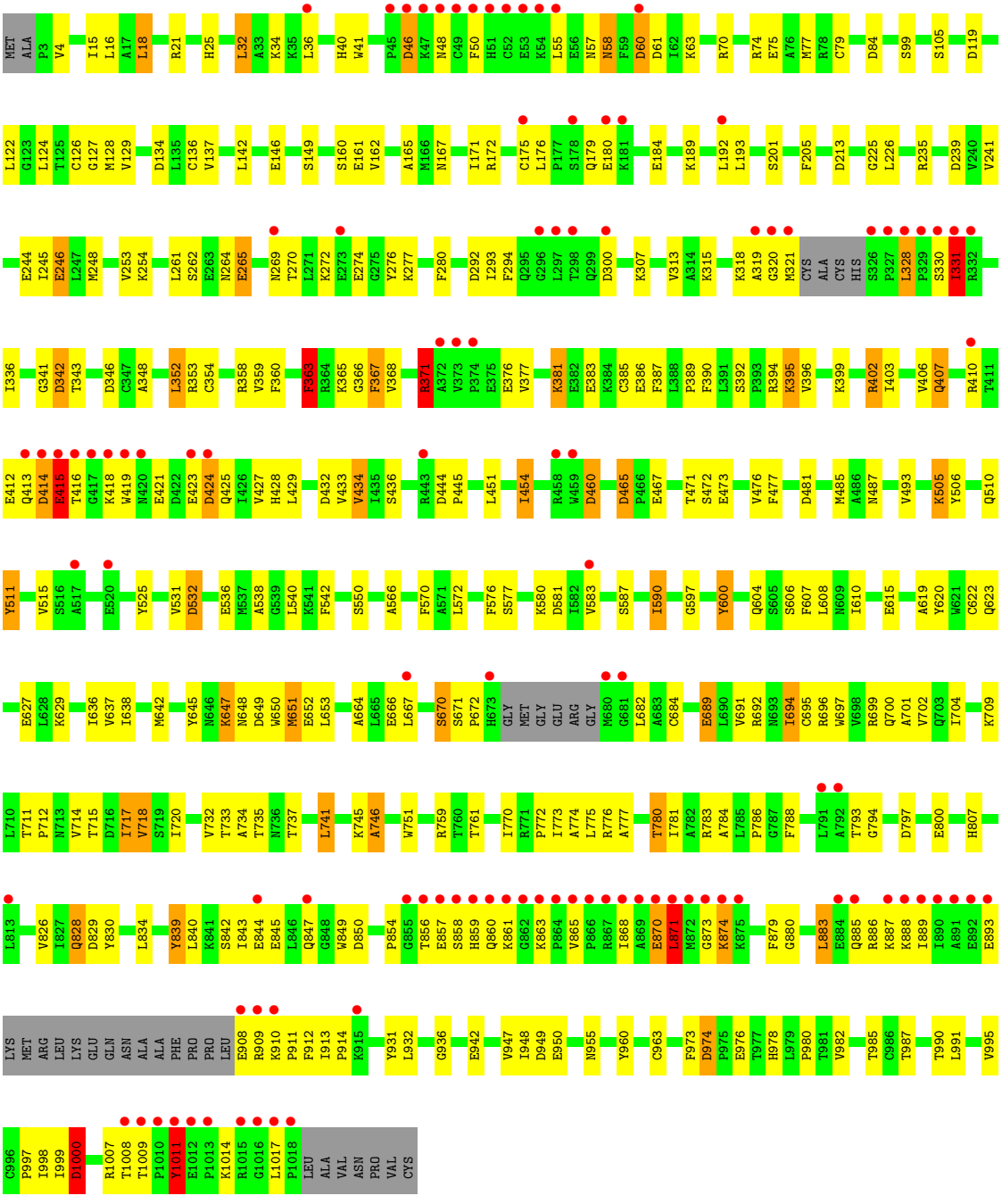
• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]



• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]

Chain D:


10%
63%
29%


MET ALA P3 V4 I15 L16 A17 L18 R21 H25 L32 A33 K34 K35 L36 H40 W41 P45 D46 K47 N48 C49 F50 H51 C52 E53 K54 L55 E56 N57 N58 F59 D60 D61 I62 K63 R70 R74 E75 A76 M77 R78 C79 D84 S99 S105 D119
L122 G123 L124 T125 C126 G127 M128 V129 D134 L135 C136 V137 L142 E146 S149 S160 E161 V162 A165 M166 N167 I171 R172 C175 L176 P177 S178 Q179 E180 K181 E184 K189 L192 L193 S201 F205 D213 G225 L226 R235 D239 V240 V241
E244 I245 E246 L247 M248 V253 K254 L261 S262 E263 N264 E265 N269 T270 L271 K272 E273 E274 G275 Y276 K277 F280 D292 I293 F294 Q295 G296 L297 T298 Q299 D300 K307 V313 A314 K315 K318 A319 G320 M321 CYS ALA CYS HIS S326 P327 L328 P329 S330 I331 R332
I336 G341 D342 T343 D346 C347 A348 L352 R353 C354 R358 V359 F360 F363 R364 K365 G366 F367 V368 R371 A372 V373 P374 E375 E376 V377 K381 E382 E383 K384 C385 E386 F387 L388 P389 F390 L391 S392 P393 R394 K395 V396 K399 R402 I403 V406 Q407 R410 T411
E412 Q413 D414 E415 T416 G417 K418 W419 N420 E421 D422 E423 D424 Q425 I426 V427 H428 L429 D432 V433 V434 I435 S436 R443 D444 P445 L451 I454 R458 W459 D460 D465 P466 E467 T471 S472 E473 V476 F477 D481 M485 A486 N487 V493 K505 Y506 Q510
Y511 V515 S516 A517 E520 Y525 V531 D532 E536 M537 A538 G539 L540 K541 F542 S550 A566 F570 A571 L572 F576 S577 K580 D581 I582 V583 S587 I590 G597 Y600 Q604 S605 S606 F607 L608 N609 I610 E615 A619 Y620 W621 C622 Q623
E627 L628 K629 I636 V637 I638 M642 Y645 N646 K647 N648 D649 W650 M651 E652 L653 A664 L665 E666 L667 S670 S671 P672 H673 GLY MET GLY GLU ARG GLY M680 G681 L682 A683 C684 E689 L690 V691 R692 N693 I694 C695 R696 W697 V698 R699 Q700 A701 V702 Q703 I704 K709
L710 T711 P712 N713 V714 T715 D716 I717 V718 S719 I720 V732 T733 A734 T735 N736 T737 L741 K745 A746 W751 R759 T760 T761 I770 R771 P772 I773 A774 L775 R776 A777 T780 I781 A782 R783 A784 L785 P786 G787 F788 L791 A792 T793 G794 D797 E800 H807
L813 V826 I827 Q828 D829 Y830 L834 Y839 L840 K841 S842 I843 E844 E845 L846 Q847 G848 W849 D850 P854 G855 T856 E857 S858 H859 Q860 K861 G862 K863 P864 V865 P866 R867 I868 A869 E870 L871 M872 G873 K874 K875 F879 G880 L883 E884 Q885 R886 K887 K888 I889 E890 A891 E892 E893
LYS MET ARG LEU LYS GLU GLN ASN ALA ALA PHE PRO PRO LEU E908 R909 K910 P911 F912 I913 P914 K915 Y931 L932 G936 E942 V947 I948 D949 E950 N955 Y960 C963 F973 D974 P975 E976 T977 H978 L979 P980 T981 V982 T985 C986 T987 T990 L991 V995
C996 P997 I998 I999 D1000 R1007 T1008 T1009 P1010 Y1011 E1012 P1013 K1014 R1015 G1016 L1017 P1018 LEU ALA VAL ASN PRO VAL CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.44Å 158.14Å 165.71Å 90.00° 96.78° 90.00°	Depositor
Resolution (Å)	26.98 – 2.12 26.98 – 2.12	Depositor EDS
% Data completeness (in resolution range)	61.4 (26.98-2.12) 61.4 (26.98-2.12)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.182 , 0.244 0.182 , 0.244	Depositor DCC
R_{free} test set	7333 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 61.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	31607	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, FAD, TDR, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.53	105/7773 (1.4%)	1.40	91/10525 (0.9%)
1	B	1.54	109/7839 (1.4%)	1.36	72/10620 (0.7%)
1	C	1.50	93/7823 (1.2%)	1.39	80/10598 (0.8%)
1	D	1.44	82/7765 (1.1%)	1.36	63/10522 (0.6%)
All	All	1.50	389/31200 (1.2%)	1.38	306/42265 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	12
1	C	0	4
1	D	0	7
All	All	0	31

All (389) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	671	SER	C-N	-19.68	0.96	1.34
1	B	175	CYS	CB-SG	14.29	2.06	1.82
1	A	652	GLU	CG-CD	14.04	1.73	1.51
1	B	670	SER	C-N	-13.25	1.03	1.34
1	B	695	CYS	CB-SG	12.80	2.04	1.82
1	A	666	GLU	CD-OE1	12.18	1.39	1.25
1	B	671	SER	C-N	-11.98	1.11	1.34
1	D	670	SER	C-N	-11.45	1.07	1.34
1	C	263	GLU	CG-CD	11.37	1.69	1.51
1	C	666	GLU	CD-OE2	11.10	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	536	GLU	CG-CD	10.95	1.68	1.51
1	C	908	GLU	CB-CG	10.72	1.72	1.52
1	A	246	GLU	CG-CD	10.08	1.67	1.51
1	C	845	GLU	CG-CD	9.96	1.66	1.51
1	B	147	GLU	CD-OE2	9.78	1.36	1.25
1	A	643	CYS	CB-SG	-9.74	1.65	1.82
1	B	75	GLU	CD-OE1	9.59	1.36	1.25
1	B	147	GLU	CG-CD	9.37	1.66	1.51
1	D	695	CYS	CB-SG	9.24	1.98	1.82
1	A	819	VAL	CB-CG1	9.11	1.72	1.52
1	D	828	GLN	CG-CD	9.09	1.72	1.51
1	C	625	VAL	CB-CG2	-8.99	1.33	1.52
1	C	670	SER	C-N	-8.96	1.13	1.34
1	C	525	TYR	CE1-CZ	8.85	1.50	1.38
1	C	622	CYS	CB-SG	8.69	1.97	1.82
1	C	583	VAL	CB-CG2	8.65	1.71	1.52
1	C	950	GLU	CD-OE2	8.49	1.34	1.25
1	A	259	LYS	CE-NZ	8.48	1.70	1.49
1	C	217	PHE	CE1-CZ	8.41	1.53	1.37
1	C	908	GLU	CG-CD	8.41	1.64	1.51
1	A	520	GLU	CG-CD	8.37	1.64	1.51
1	B	60	ASP	CB-CG	8.33	1.69	1.51
1	B	726	GLU	CD-OE2	8.32	1.34	1.25
1	C	69	GLU	CG-CD	8.29	1.64	1.51
1	C	375	GLU	CG-CD	8.21	1.64	1.51
1	A	386	GLU	CG-CD	8.20	1.64	1.51
1	D	666	GLU	CD-OE1	8.09	1.34	1.25
1	B	467	GLU	CD-OE2	8.08	1.34	1.25
1	B	536	GLU	CG-CD	8.02	1.64	1.51
1	A	449	GLU	CD-OE2	8.01	1.34	1.25
1	B	363	PHE	CE2-CZ	8.00	1.52	1.37
1	A	520	GLU	CB-CG	7.98	1.67	1.52
1	D	460	ASP	CB-CG	7.92	1.68	1.51
1	B	354	CYS	CB-SG	-7.88	1.68	1.82
1	A	725	LYS	CD-CE	7.87	1.71	1.51
1	D	371	ARG	CG-CD	7.83	1.71	1.51
1	D	79	CYS	CB-SG	7.79	1.95	1.82
1	D	995	VAL	CB-CG1	7.75	1.69	1.52
1	B	658	GLU	CD-OE1	7.74	1.34	1.25
1	A	257	CYS	CB-SG	-7.73	1.69	1.82
1	C	800	GLU	CD-OE1	7.69	1.34	1.25
1	B	568	TRP	CG-CD1	-7.69	1.25	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	622	CYS	CB-SG	7.68	1.95	1.82
1	C	816	CYS	CB-SG	7.58	1.95	1.82
1	A	845	GLU	CG-CD	7.53	1.63	1.51
1	D	666	GLU	CD-OE2	7.53	1.33	1.25
1	D	751	TRP	CZ3-CH2	7.52	1.52	1.40
1	A	60	ASP	CB-CG	7.52	1.67	1.51
1	D	976	GLU	CG-CD	7.52	1.63	1.51
1	D	637	VAL	CB-CG1	-7.51	1.37	1.52
1	C	620	TYR	CD1-CE1	7.50	1.50	1.39
1	A	382	GLU	CD-OE2	7.50	1.33	1.25
1	C	758	LYS	CD-CE	7.49	1.70	1.51
1	D	175	CYS	CB-SG	7.46	1.95	1.82
1	B	828	GLN	CG-CD	7.46	1.68	1.51
1	B	147	GLU	CD-OE1	7.44	1.33	1.25
1	B	984	ASP	CB-CG	7.43	1.67	1.51
1	C	620	TYR	CE2-CZ	7.42	1.48	1.38
1	A	13	GLU	CG-CD	7.42	1.63	1.51
1	A	373	VAL	C-N	7.41	1.48	1.34
1	A	276	TYR	CD2-CE2	-7.38	1.28	1.39
1	C	525	TYR	CZ-OH	7.37	1.50	1.37
1	B	524	PHE	CE1-CZ	7.33	1.51	1.37
1	B	824	PHE	CD1-CE1	7.31	1.53	1.39
1	C	801	SER	CB-OG	7.31	1.51	1.42
1	A	273	GLU	CB-CG	-7.30	1.38	1.52
1	B	824	PHE	CD2-CE2	7.29	1.53	1.39
1	B	819	VAL	CB-CG1	7.29	1.68	1.52
1	D	280	PHE	CD2-CE2	7.29	1.53	1.39
1	B	609	ASN	CB-CG	7.24	1.67	1.51
1	A	490	VAL	CB-CG1	7.23	1.68	1.52
1	C	376	GLU	CB-CG	-7.22	1.38	1.52
1	C	354	CYS	CB-SG	-7.21	1.70	1.82
1	B	502	TYR	CD2-CE2	7.20	1.50	1.39
1	C	382	GLU	CD-OE1	7.16	1.33	1.25
1	D	264	ASN	CB-CG	7.15	1.67	1.51
1	C	272	LYS	CD-CE	7.14	1.69	1.51
1	A	652	GLU	CB-CG	7.13	1.65	1.52
1	B	381	LYS	CB-CG	7.09	1.71	1.52
1	A	976	GLU	CG-CD	7.09	1.62	1.51
1	B	960	TYR	CZ-OH	7.07	1.49	1.37
1	B	265	GLU	CG-CD	7.06	1.62	1.51
1	A	147	GLU	CG-CD	7.05	1.62	1.51
1	C	951	GLU	CD-OE2	7.04	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	109	TYR	CD2-CE2	-7.04	1.28	1.39
1	B	184	GLU	CG-CD	7.03	1.62	1.51
1	C	611	GLU	CD-OE1	6.99	1.33	1.25
1	D	606	SER	CB-OG	6.99	1.51	1.42
1	A	565	GLU	CD-OE2	6.95	1.33	1.25
1	B	217	PHE	CE1-CZ	6.94	1.50	1.37
1	A	922	LYS	CE-NZ	6.94	1.66	1.49
1	C	487	ASN	CB-CG	6.93	1.67	1.51
1	A	830	TYR	CD2-CE2	-6.93	1.28	1.39
1	A	800	GLU	CG-CD	6.88	1.62	1.51
1	A	322	CYS	CB-SG	6.87	1.94	1.82
1	C	944	VAL	CB-CG1	-6.87	1.38	1.52
1	B	583	VAL	CB-CG2	6.86	1.67	1.52
1	C	976	GLU	CG-CD	6.86	1.62	1.51
1	A	844	GLU	CG-CD	6.82	1.62	1.51
1	A	830	TYR	CD1-CE1	-6.80	1.29	1.39
1	C	147	GLU	CB-CG	-6.79	1.39	1.52
1	B	973	PHE	CD2-CE2	6.78	1.52	1.39
1	D	689	GLU	CG-CD	6.78	1.62	1.51
1	C	960	TYR	CZ-OH	6.76	1.49	1.37
1	B	104	ILE	CB-CG2	-6.73	1.31	1.52
1	B	263	GLU	CG-CD	6.72	1.62	1.51
1	A	570	PHE	CE1-CZ	6.71	1.50	1.37
1	C	945	VAL	CB-CG2	-6.70	1.38	1.52
1	D	424	ASP	CB-CG	6.70	1.65	1.51
1	D	587	SER	CB-OG	6.69	1.50	1.42
1	D	75	GLU	CG-CD	6.68	1.61	1.51
1	B	492	SER	CB-OG	6.67	1.50	1.42
1	D	879	PHE	CD2-CE2	-6.63	1.25	1.39
1	B	495	ASP	CB-CG	6.63	1.65	1.51
1	A	441	VAL	CB-CG1	-6.63	1.39	1.52
1	C	931	TYR	CE2-CZ	-6.62	1.29	1.38
1	A	937	GLU	CG-CD	6.60	1.61	1.51
1	A	725	LYS	CE-NZ	6.58	1.65	1.49
1	D	597	GLY	C-N	6.57	1.46	1.34
1	C	382	GLU	CD-OE2	6.56	1.32	1.25
1	D	828	GLN	CB-CG	6.55	1.70	1.52
1	D	576	PHE	CD1-CE1	6.55	1.52	1.39
1	A	382	GLU	CD-OE1	6.54	1.32	1.25
1	C	666	GLU	CG-CD	6.52	1.61	1.51
1	B	606	SER	CB-OG	6.51	1.50	1.42
1	D	745	LYS	CE-NZ	6.50	1.65	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	656	LYS	CD-CE	6.50	1.67	1.51
1	A	532	ASP	CB-CG	6.49	1.65	1.51
1	A	49	CYS	CB-SG	6.47	1.93	1.82
1	A	280	PHE	CE2-CZ	6.47	1.49	1.37
1	A	800	GLU	CD-OE2	6.44	1.32	1.25
1	A	611	GLU	CD-OE2	6.43	1.32	1.25
1	B	879	PHE	CD2-CE2	-6.43	1.26	1.39
1	C	968	TYR	CD2-CE2	6.42	1.49	1.39
1	C	375	GLU	CD-OE2	6.41	1.32	1.25
1	A	464	VAL	CB-CG2	-6.39	1.39	1.52
1	D	718	VAL	CB-CG2	-6.39	1.39	1.52
1	A	511	TYR	CD2-CE2	-6.38	1.29	1.39
1	A	109	TYR	CB-CG	-6.37	1.42	1.51
1	B	830	TYR	CD2-CE2	6.37	1.49	1.39
1	B	621	TRP	CZ3-CH2	6.37	1.50	1.40
1	B	958	LYS	CD-CE	6.36	1.67	1.51
1	C	989	CYS	CB-SG	6.35	1.93	1.82
1	A	456	PHE	CD2-CE2	6.34	1.51	1.39
1	C	467	GLU	CB-CG	6.32	1.64	1.52
1	C	211	TYR	CE2-CZ	6.32	1.46	1.38
1	A	263	GLU	CD-OE1	6.32	1.32	1.25
1	D	467	GLU	CB-CG	6.32	1.64	1.52
1	D	826	VAL	CB-CG2	-6.32	1.39	1.52
1	A	105	SER	CB-OG	6.31	1.50	1.42
1	A	117	PHE	CD2-CE2	-6.30	1.26	1.39
1	B	7	LYS	CD-CE	6.30	1.67	1.51
1	D	800	GLU	CD-OE1	6.29	1.32	1.25
1	C	730	ASP	CB-CG	6.29	1.65	1.51
1	A	2	ALA	CA-CB	6.27	1.65	1.52
1	A	800	GLU	CD-OE1	6.26	1.32	1.25
1	C	75	GLU	CD-OE1	6.25	1.32	1.25
1	C	525	TYR	CD2-CE2	6.25	1.48	1.39
1	C	273	GLU	CG-CD	6.24	1.61	1.51
1	D	60	ASP	CB-CG	6.24	1.64	1.51
1	B	230	GLU	CG-CD	6.24	1.61	1.51
1	B	241	VAL	CB-CG1	6.22	1.66	1.52
1	C	205	PHE	CB-CG	-6.20	1.40	1.51
1	D	511	TYR	CE1-CZ	-6.19	1.30	1.38
1	C	788	PHE	CB-CG	-6.19	1.40	1.51
1	D	830	TYR	CE1-CZ	6.17	1.46	1.38
1	C	528	VAL	CB-CG1	6.16	1.65	1.52
1	D	712	PRO	CG-CD	6.15	1.71	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	371	ARG	CG-CD	6.15	1.67	1.51
1	B	525	TYR	CE2-CZ	6.14	1.46	1.38
1	C	758	LYS	CE-NZ	6.10	1.64	1.49
1	B	222	TYR	CE1-CZ	6.09	1.46	1.38
1	C	666	GLU	CD-OE1	6.09	1.32	1.25
1	D	949	ASP	CB-CG	6.09	1.64	1.51
1	C	375	GLU	CB-CG	6.08	1.63	1.52
1	C	583	VAL	CB-CG1	6.07	1.65	1.52
1	B	959	CYS	CB-SG	6.06	1.92	1.82
1	D	800	GLU	CG-CD	6.05	1.61	1.51
1	B	751	TRP	CZ3-CH2	6.04	1.49	1.40
1	B	467	GLU	CD-OE1	6.04	1.32	1.25
1	A	477	PHE	CE1-CZ	6.04	1.48	1.37
1	C	725	LYS	CE-NZ	6.04	1.64	1.49
1	A	776	ARG	CG-CD	-6.04	1.36	1.51
1	D	376	GLU	CD-OE1	6.03	1.32	1.25
1	C	931	TYR	CE1-CZ	6.03	1.46	1.38
1	C	421	GLU	CG-CD	6.02	1.60	1.51
1	C	511	TYR	CD2-CE2	-6.02	1.30	1.39
1	D	1000	ASP	CB-CG	-6.02	1.39	1.51
1	A	364	ARG	CG-CD	6.01	1.67	1.51
1	B	24	SER	CB-OG	-6.00	1.34	1.42
1	D	467	GLU	CG-CD	5.99	1.60	1.51
1	D	652	GLU	CB-CG	-5.99	1.40	1.52
1	C	2	ALA	C-N	5.98	1.45	1.34
1	D	950	GLU	CG-CD	5.98	1.60	1.51
1	C	491	GLU	CG-CD	5.97	1.60	1.51
1	B	223	VAL	CB-CG2	-5.96	1.40	1.52
1	B	835	LYS	CD-CE	-5.96	1.36	1.51
1	B	468	THR	CB-CG2	-5.95	1.32	1.52
1	B	689	GLU	CG-CD	5.93	1.60	1.51
1	B	244	GLU	CD-OE1	5.93	1.32	1.25
1	C	751	TRP	CB-CG	5.93	1.60	1.50
1	B	640	SER	CB-OG	5.92	1.50	1.42
1	A	134	ASP	CB-CG	5.91	1.64	1.51
1	C	167	ASN	CB-CG	-5.91	1.37	1.51
1	D	751	TRP	CD2-CE2	5.90	1.48	1.41
1	B	506	TYR	CD2-CE2	5.90	1.48	1.39
1	C	574	LYS	CD-CE	5.89	1.66	1.51
1	A	382	GLU	CB-CG	-5.89	1.41	1.52
1	C	845	GLU	CB-CG	5.88	1.63	1.52
1	D	371	ARG	CZ-NH2	5.88	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	839	TYR	CD1-CE1	5.88	1.48	1.39
1	A	922	LYS	CD-CE	5.87	1.66	1.51
1	B	973	PHE	CE1-CZ	5.84	1.48	1.37
1	B	218	GLU	CD-OE1	5.83	1.32	1.25
1	D	647	LYS	CD-CE	5.80	1.65	1.51
1	B	554	THR	CB-CG2	-5.79	1.33	1.52
1	A	147	GLU	CD-OE2	5.79	1.32	1.25
1	A	960	TYR	CE1-CZ	5.78	1.46	1.38
1	A	147	GLU	CD-OE1	5.77	1.31	1.25
1	C	800	GLU	CB-CG	-5.76	1.41	1.52
1	B	383	GLU	CD-OE1	5.75	1.31	1.25
1	B	706	PHE	CD2-CE2	5.75	1.50	1.39
1	D	363	PHE	CE2-CZ	5.75	1.48	1.37
1	B	650	TRP	CZ3-CH2	5.74	1.49	1.40
1	D	365	LYS	CE-NZ	5.73	1.63	1.49
1	B	272	LYS	CD-CE	5.73	1.65	1.51
1	A	272	LYS	CD-CE	5.72	1.65	1.51
1	B	797	ASP	CB-CG	5.72	1.63	1.51
1	A	581	ASP	CB-CG	5.72	1.63	1.51
1	C	246	GLU	CG-CD	5.71	1.60	1.51
1	B	1008	THR	C-N	5.70	1.47	1.34
1	B	751	TRP	CD2-CE2	5.69	1.48	1.41
1	C	481	ASP	CB-CG	5.69	1.63	1.51
1	A	240	VAL	CB-CG1	5.68	1.64	1.52
1	A	381	LYS	CB-CG	-5.68	1.37	1.52
1	C	647	LYS	CE-NZ	5.67	1.63	1.49
1	B	265	GLU	CD-OE2	5.67	1.31	1.25
1	B	968	TYR	CZ-OH	5.66	1.47	1.37
1	A	163	PHE	CE1-CZ	5.63	1.48	1.37
1	B	826	VAL	CB-CG1	-5.63	1.41	1.52
1	A	1012	GLU	CG-CD	5.62	1.60	1.51
1	B	587	SER	CB-OG	5.62	1.49	1.42
1	C	557	SER	CB-OG	5.61	1.49	1.42
1	B	574	LYS	CE-NZ	5.59	1.63	1.49
1	A	446	LYS	CE-NZ	5.58	1.62	1.49
1	D	342	ASP	CG-OD2	5.58	1.38	1.25
1	A	544	ASN	CB-CG	5.58	1.63	1.51
1	A	136	CYS	CB-SG	5.57	1.91	1.82
1	A	276	TYR	CD1-CE1	-5.57	1.30	1.39
1	A	956	CYS	CB-SG	-5.57	1.72	1.81
1	B	202	CYS	CB-SG	5.57	1.91	1.82
1	B	986	CYS	CB-SG	-5.57	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	246	GLU	CB-CG	5.56	1.62	1.52
1	A	838	LEU	CG-CD1	5.55	1.72	1.51
1	D	467	GLU	CD-OE1	5.54	1.31	1.25
1	C	844	GLU	CD-OE2	5.53	1.31	1.25
1	A	110	TYR	CE1-CZ	-5.52	1.31	1.38
1	B	373	VAL	CB-CG2	5.52	1.64	1.52
1	B	6	SER	CB-OG	5.51	1.49	1.42
1	B	592	ARG	CG-CD	5.51	1.65	1.51
1	D	161	GLU	CD-OE1	5.51	1.31	1.25
1	A	666	GLU	CD-OE2	5.50	1.31	1.25
1	B	408	PHE	CE1-CZ	5.50	1.47	1.37
1	B	421	GLU	CD-OE1	5.50	1.31	1.25
1	D	421	GLU	CG-CD	5.50	1.60	1.51
1	D	931	TYR	CD2-CE2	5.49	1.47	1.39
1	B	732	VAL	CB-CG1	-5.49	1.41	1.52
1	A	75	GLU	CD-OE2	5.49	1.31	1.25
1	A	106	ASN	CG-OD1	5.48	1.36	1.24
1	A	697	TRP	CG-CD1	-5.47	1.29	1.36
1	A	951	GLU	CB-CG	5.46	1.62	1.52
1	D	542	PHE	CE2-CZ	5.46	1.47	1.37
1	B	605	SER	CB-OG	5.46	1.49	1.42
1	A	951	GLU	CG-CD	5.45	1.60	1.51
1	C	88	GLN	CD-NE2	5.45	1.46	1.32
1	A	211	TYR	CG-CD2	5.45	1.46	1.39
1	D	870	GLU	CG-CD	5.45	1.60	1.51
1	C	60	ASP	CB-CG	5.45	1.63	1.51
1	D	702	VAL	CB-CG1	5.45	1.64	1.52
1	B	525	TYR	CD1-CE1	5.44	1.47	1.39
1	B	968	TYR	CE2-CZ	5.44	1.45	1.38
1	C	260	SER	CA-CB	-5.44	1.44	1.52
1	D	171	ILE	CB-CG2	-5.44	1.35	1.52
1	C	263	GLU	CB-CG	5.44	1.62	1.52
1	B	107	LYS	CD-CE	5.42	1.64	1.51
1	A	879	PHE	CE1-CZ	5.41	1.47	1.37
1	D	265	GLU	CG-CD	5.41	1.60	1.51
1	B	847	GLN	CG-CD	5.41	1.63	1.51
1	D	34	LYS	CE-NZ	5.41	1.62	1.49
1	B	950	GLU	CD-OE2	5.41	1.31	1.25
1	A	476	VAL	CB-CG1	5.40	1.64	1.52
1	D	487	ASN	CB-CG	5.40	1.63	1.51
1	D	600	TYR	CG-CD1	-5.40	1.32	1.39
1	C	184	GLU	CD-OE1	5.39	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	951	GLU	CB-CG	5.38	1.62	1.52
1	D	377	VAL	CB-CG1	-5.38	1.41	1.52
1	B	839	TYR	CD2-CE2	-5.38	1.31	1.39
1	C	6	SER	CB-OG	5.38	1.49	1.42
1	A	53	GLU	CG-CD	5.37	1.60	1.51
1	A	506	TYR	CB-CG	-5.36	1.43	1.51
1	D	434	VAL	CB-CG2	-5.35	1.41	1.52
1	C	221	GLU	CD-OE2	5.35	1.31	1.25
1	D	395	LYS	CD-CE	5.34	1.64	1.51
1	B	428	HIS	CA-CB	5.33	1.65	1.53
1	B	576	PHE	CD1-CE1	5.32	1.49	1.39
1	C	386	GLU	CG-CD	5.32	1.59	1.51
1	D	715	THR	CB-CG2	-5.32	1.34	1.52
1	A	41	TRP	CE3-CZ3	5.32	1.47	1.38
1	A	885	GLN	CG-CD	5.32	1.63	1.51
1	B	658	GLU	CD-OE2	5.32	1.31	1.25
1	A	491	GLU	CG-CD	5.31	1.59	1.51
1	C	803	LEU	CG-CD2	5.31	1.71	1.51
1	C	758	LYS	CG-CD	5.30	1.70	1.52
1	D	246	GLU	CB-CG	5.29	1.62	1.52
1	D	645	TYR	CD1-CE1	5.29	1.47	1.39
1	D	1011	TYR	CE1-CZ	5.29	1.45	1.38
1	A	126	CYS	CB-SG	5.28	1.91	1.82
1	D	525	TYR	CE1-CZ	5.28	1.45	1.38
1	D	908	GLU	CG-CD	5.28	1.59	1.51
1	A	684	CYS	CB-SG	-5.27	1.73	1.81
1	A	483	VAL	CB-CG1	-5.27	1.41	1.52
1	B	433	VAL	CB-CG2	-5.26	1.41	1.52
1	C	517	ALA	C-N	5.26	1.46	1.34
1	A	99	SER	CB-OG	-5.25	1.35	1.42
1	A	568	TRP	CD2-CE2	-5.24	1.35	1.41
1	B	527	PRO	CG-CD	5.23	1.68	1.50
1	B	443	ARG	CB-CG	5.23	1.66	1.52
1	C	561	ARG	CG-CD	5.23	1.65	1.51
1	D	505	LYS	CD-CE	5.23	1.64	1.51
1	A	82	CYS	CB-SG	5.22	1.91	1.82
1	B	13	GLU	CD-OE2	5.22	1.31	1.25
1	A	703	GLN	CG-CD	5.21	1.63	1.51
1	B	502	TYR	CD1-CE1	5.21	1.47	1.39
1	B	382	GLU	CD-OE1	5.20	1.31	1.25
1	C	134	ASP	CB-CG	5.19	1.62	1.51
1	B	536	GLU	CD-OE2	5.18	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	162	VAL	CB-CG2	-5.18	1.42	1.52
1	D	205	PHE	CE2-CZ	5.18	1.47	1.37
1	B	842	SER	CB-OG	5.17	1.49	1.42
1	A	463	GLU	CB-CG	-5.16	1.42	1.52
1	B	152	ILE	C-N	5.16	1.42	1.33
1	A	48	ASN	CB-CG	5.16	1.62	1.51
1	A	661	GLY	CA-C	5.16	1.60	1.51
1	D	161	GLU	CD-OE2	5.15	1.31	1.25
1	A	386	GLU	CD-OE1	5.15	1.31	1.25
1	C	953	CYS	CB-SG	-5.15	1.73	1.81
1	B	136	CYS	CB-SG	-5.15	1.73	1.81
1	C	765	VAL	CB-CG2	5.15	1.63	1.52
1	A	576	PHE	CB-CG	-5.15	1.42	1.51
1	B	21	ARG	CG-CD	5.15	1.64	1.51
1	D	61	ASP	CB-CG	5.14	1.62	1.51
1	D	800	GLU	CD-OE2	5.12	1.31	1.25
1	D	963	CYS	CB-SG	5.11	1.91	1.82
1	C	956	CYS	CB-SG	5.10	1.91	1.82
1	C	100	PHE	CE2-CZ	5.08	1.47	1.37
1	B	347	CYS	CB-SG	5.08	1.90	1.82
1	D	714	VAL	CB-CG2	5.08	1.63	1.52
1	D	600	TYR	CG-CD2	5.08	1.45	1.39
1	D	313	VAL	CB-CG1	-5.08	1.42	1.52
1	B	738	VAL	CB-CG1	5.07	1.63	1.52
1	C	254	LYS	CE-NZ	5.07	1.61	1.49
1	A	217	PHE	CE1-CZ	5.07	1.47	1.37
1	A	120	ASN	CB-CG	-5.06	1.39	1.51
1	C	449	GLU	CB-CG	-5.06	1.42	1.52
1	D	363	PHE	CB-CG	-5.05	1.42	1.51
1	D	947	VAL	CB-CG2	-5.05	1.42	1.52
1	B	39	LYS	CD-CE	5.05	1.63	1.51
1	A	21	ARG	CA-CB	5.05	1.65	1.53
1	A	382	GLU	CG-CD	5.04	1.59	1.51
1	C	745	LYS	CD-CE	5.04	1.63	1.51
1	A	536	GLU	CB-CG	5.04	1.61	1.52
1	B	272	LYS	CB-CG	5.04	1.66	1.52
1	A	53	GLU	CB-CG	5.04	1.61	1.52
1	A	364	ARG	CB-CG	5.03	1.66	1.52
1	B	968	TYR	CG-CD1	5.02	1.45	1.39
1	B	564	PHE	CB-CG	-5.02	1.42	1.51
1	C	805	PHE	CE2-CZ	5.01	1.46	1.37
1	C	620	TYR	CG-CD1	5.01	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	105	SER	CB-OG	5.01	1.48	1.42

All (306) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	670	SER	O-C-N	-18.09	93.76	122.70
1	D	32	LEU	CB-CG-CD1	-14.83	85.79	111.00
1	C	670	SER	CA-C-N	12.78	145.31	117.20
1	A	444	ASP	CB-CG-OD2	-11.51	107.94	118.30
1	D	15	ILE	CG1-CB-CG2	-11.37	86.39	111.40
1	B	670	SER	O-C-N	-11.19	104.80	122.70
1	D	432	ASP	CB-CG-OD1	-10.60	108.76	118.30
1	C	720	ILE	CG1-CB-CG2	-9.82	89.81	111.40
1	C	932	LEU	CB-CG-CD2	-9.72	94.47	111.00
1	A	663	ASP	CB-CG-OD2	9.70	127.03	118.30
1	A	119	ASP	CB-CG-OD1	9.66	126.99	118.30
1	B	670	SER	CA-C-N	9.61	138.33	117.20
1	D	653	LEU	CB-CG-CD2	-9.60	94.69	111.00
1	A	523	LEU	CB-CG-CD1	-9.52	94.82	111.00
1	C	1000	ASP	CB-CG-OD2	-9.45	109.80	118.30
1	A	130	CYS	CA-CB-SG	9.06	130.31	114.00
1	C	631	ASP	CB-CG-OD2	-9.03	110.17	118.30
1	A	634	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	D	684	CYS	CA-CB-SG	-8.86	98.04	114.00
1	C	649	ASP	CB-CG-OD1	-8.77	110.41	118.30
1	A	993	LEU	CB-CG-CD2	-8.68	96.25	111.00
1	D	342	ASP	CB-CG-OD1	-8.52	110.64	118.30
1	D	134	ASP	CB-CG-OD1	-8.46	110.69	118.30
1	C	670	SER	C-N-CA	8.41	142.73	121.70
1	C	21	ARG	CG-CD-NE	-8.32	94.32	111.80
1	C	189	LYS	CD-CE-NZ	8.30	130.78	111.70
1	A	663	ASP	CB-CG-OD1	-8.14	110.98	118.30
1	B	15	ILE	CG1-CB-CG2	-8.01	93.79	111.40
1	C	226	LEU	CB-CG-CD1	-7.97	97.45	111.00
1	A	612	LEU	CB-CG-CD2	-7.97	97.46	111.00
1	D	590	ILE	CG1-CB-CG2	-7.89	94.03	111.40
1	B	628	LEU	CB-CG-CD1	-7.88	97.60	111.00
1	A	682	LEU	CB-CG-CD1	-7.87	97.61	111.00
1	D	371	ARG	NE-CZ-NH1	-7.72	116.44	120.30
1	C	95	LEU	CB-CG-CD2	7.64	123.99	111.00
1	D	1008	THR	C-N-CA	7.62	140.75	121.70
1	C	247	LEU	CB-CG-CD1	-7.61	98.07	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	669	LEU	CB-CG-CD2	7.60	123.93	111.00
1	B	872	MET	CG-SD-CE	-7.60	88.05	100.20
1	C	741	LEU	CB-CG-CD1	-7.58	98.11	111.00
1	B	175	CYS	CA-CB-SG	7.54	127.58	114.00
1	A	785	LEU	CB-CG-CD2	-7.51	98.24	111.00
1	D	991	LEU	CA-CB-CG	-7.51	98.03	115.30
1	B	36	LEU	CB-CG-CD1	7.48	123.72	111.00
1	C	28	LEU	CB-CG-CD1	-7.41	98.41	111.00
1	C	482	ILE	CG1-CB-CG2	-7.39	95.13	111.40
1	D	775	LEU	CA-CB-CG	7.38	132.29	115.30
1	A	876	LEU	CB-CG-CD1	-7.38	98.46	111.00
1	A	176	LEU	CB-CG-CD1	-7.38	98.46	111.00
1	A	642	MET	CG-SD-CE	-7.33	88.48	100.20
1	A	119	ASP	CB-CG-OD2	-7.22	111.81	118.30
1	B	533	ILE	CG1-CB-CG2	-7.20	95.56	111.40
1	A	128	MET	CG-SD-CE	7.14	111.63	100.20
1	A	312	LEU	CB-CG-CD2	-7.13	98.87	111.00
1	D	741	LEU	CB-CG-CD1	-7.11	98.91	111.00
1	A	32	LEU	CB-CG-CD2	-7.10	98.92	111.00
1	D	226	LEU	CB-CG-CD1	-7.10	98.94	111.00
1	A	831	CYS	CA-CB-SG	-7.08	101.26	114.00
1	C	649	ASP	CB-CG-OD2	7.06	124.66	118.30
1	A	803	LEU	CB-CG-CD2	-7.05	99.01	111.00
1	A	652	GLU	OE1-CD-OE2	-7.03	114.86	123.30
1	B	354	CYS	CA-CB-SG	-7.01	101.38	114.00
1	C	745	LYS	CD-CE-NZ	7.00	127.80	111.70
1	A	321	MET	CG-SD-CE	7.00	111.39	100.20
1	C	991	LEU	CB-CG-CD2	6.92	122.76	111.00
1	D	119	ASP	CB-CG-OD1	6.92	124.53	118.30
1	A	308	ASP	CB-CG-OD2	-6.92	112.08	118.30
1	D	444	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	C	583	VAL	CG1-CB-CG2	6.85	121.86	110.90
1	A	625	VAL	CA-CB-CG2	-6.83	100.65	110.90
1	C	850	ASP	CB-CG-OD2	6.83	124.45	118.30
1	A	142	LEU	O-C-N	-6.82	111.78	122.70
1	D	651	MET	CG-SD-CE	-6.79	89.34	100.20
1	B	261	LEU	CB-CG-CD2	-6.77	99.49	111.00
1	A	636	ILE	CG1-CB-CG2	-6.75	96.56	111.40
1	B	578	LEU	CB-CG-CD2	-6.75	99.53	111.00
1	A	115	MET	CG-SD-CE	-6.73	89.44	100.20
1	B	999	ILE	CG1-CB-CG2	-6.71	96.64	111.40
1	D	485	MET	CG-SD-CE	6.70	110.92	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	MET	CA-CB-CG	-6.70	101.91	113.30
1	D	974	ASP	CB-CG-OD2	-6.70	112.28	118.30
1	B	649	ASP	CB-CG-OD1	-6.68	112.29	118.30
1	B	107	LYS	CD-CE-NZ	6.68	127.06	111.70
1	D	192	LEU	CB-CG-CD2	6.67	122.33	111.00
1	C	932	LEU	CA-CB-CG	6.65	130.60	115.30
1	A	922	LYS	CD-CE-NZ	6.62	126.92	111.70
1	B	529	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	791	LEU	CB-CG-CD2	-6.60	99.78	111.00
1	B	300	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	C	803	LEU	CB-CG-CD2	6.57	122.17	111.00
1	B	128	MET	CA-CB-CG	-6.55	102.16	113.30
1	D	381	LYS	CD-CE-NZ	6.54	126.74	111.70
1	A	520	GLU	C-N-CA	-6.54	105.35	121.70
1	C	938	LEU	CB-CG-CD2	-6.52	99.92	111.00
1	C	950	GLU	CA-CB-CG	6.51	127.73	113.40
1	D	1000	ASP	CB-CA-C	-6.51	97.38	110.40
1	A	254	LYS	CD-CE-NZ	-6.50	96.75	111.70
1	A	429	LEU	CB-CG-CD1	-6.49	99.96	111.00
1	C	835	LYS	CD-CE-NZ	-6.49	96.77	111.70
1	A	780	THR	OG1-CB-CG2	-6.48	95.09	110.00
1	A	49	CYS	CA-CB-SG	6.47	125.64	114.00
1	D	850	ASP	C-N-CA	-6.47	108.72	122.30
1	A	465	ASP	CB-CG-OD1	6.41	124.07	118.30
1	C	813	LEU	CB-CG-CD1	6.40	121.87	111.00
1	A	754	VAL	CG1-CB-CG2	6.37	121.10	110.90
1	C	961	MET	CA-CB-CG	-6.37	102.48	113.30
1	D	454	ILE	CG1-CB-CG2	-6.33	97.48	111.40
1	A	923	ASP	CB-CG-OD2	6.33	123.99	118.30
1	B	371	ARG	CA-CB-CG	6.32	127.30	113.40
1	C	682	LEU	CA-CB-CG	6.32	129.83	115.30
1	C	62	ILE	CG1-CB-CG2	-6.31	97.52	111.40
1	D	481	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	785	LEU	CB-CG-CD1	6.30	121.71	111.00
1	B	77	MET	CG-SD-CE	6.28	110.24	100.20
1	D	883	LEU	CB-CG-CD2	-6.26	100.36	111.00
1	A	272	LYS	CD-CE-NZ	6.25	126.07	111.70
1	A	574	LYS	CD-CE-NZ	6.23	126.03	111.70
1	A	182	MET	CG-SD-CE	-6.22	90.24	100.20
1	B	616	LYS	CD-CE-NZ	6.18	125.92	111.70
1	C	982	VAL	CG1-CB-CG2	-6.18	101.01	110.90
1	C	747	ASP	CB-CG-OD2	6.17	123.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	541	LYS	CD-CE-NZ	6.16	125.87	111.70
1	B	403	ILE	CG1-CB-CG2	-6.15	97.86	111.40
1	C	7	LYS	CD-CE-NZ	6.14	125.82	111.70
1	C	758	LYS	CG-CD-CE	6.13	130.29	111.90
1	D	365	LYS	CD-CE-NZ	6.13	125.80	111.70
1	D	829	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	A	540	LEU	CB-CG-CD1	6.11	121.39	111.00
1	A	887	LYS	CD-CE-NZ	-6.10	97.66	111.70
1	C	785	LEU	CB-CG-CD1	-6.10	100.64	111.00
1	B	850	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	D	974	ASP	CB-CG-OD1	6.08	123.78	118.30
1	B	846	LEU	CB-CG-CD1	-6.08	100.67	111.00
1	A	845	GLU	OE1-CD-OE2	-6.07	116.02	123.30
1	C	211	TYR	CD1-CE1-CZ	-6.05	114.36	119.80
1	B	73	LEU	CB-CG-CD2	-6.04	100.72	111.00
1	A	426	ILE	CG1-CB-CG2	-6.04	98.11	111.40
1	A	578	LEU	CA-CB-CG	-6.04	101.40	115.30
1	B	744	LEU	CB-CG-CD2	-6.04	100.74	111.00
1	D	780	THR	CA-CB-CG2	-6.04	103.95	112.40
1	A	209	LEU	CB-CG-CD1	-6.03	100.75	111.00
1	B	96	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	687	ASP	CB-CG-OD1	6.02	123.72	118.30
1	D	666	GLU	OE1-CD-OE2	6.02	130.52	123.30
1	A	18	LEU	CB-CG-CD1	-5.99	100.81	111.00
1	B	559	MET	CG-SD-CE	-5.99	90.62	100.20
1	C	8	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	B	700	GLN	CA-CB-CG	5.97	126.54	113.40
1	A	226	LEU	CB-CG-CD1	-5.97	100.86	111.00
1	B	495	ASP	CB-CG-OD2	5.96	123.66	118.30
1	C	95	LEU	CB-CG-CD1	-5.96	100.87	111.00
1	D	761	THR	CA-CB-CG2	-5.96	104.06	112.40
1	C	251	LEU	CB-CG-CD2	-5.95	100.89	111.00
1	D	746	ALA	CB-CA-C	-5.95	101.18	110.10
1	A	622	CYS	CA-CB-SG	-5.94	103.30	114.00
1	A	310	LEU	CA-CB-CG	-5.94	101.64	115.30
1	A	745	LYS	CD-CE-NZ	5.92	125.31	111.70
1	C	39	LYS	CD-CE-NZ	5.91	125.30	111.70
1	A	741	LEU	CB-CG-CD2	-5.89	100.98	111.00
1	A	643	CYS	CA-CB-SG	-5.89	103.41	114.00
1	C	554	THR	CA-CB-CG2	-5.89	104.16	112.40
1	D	161	GLU	OE1-CD-OE2	5.88	130.36	123.30
1	D	328	LEU	CA-CB-CG	5.88	128.84	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	293	ILE	CG1-CB-CG2	-5.88	98.46	111.40
1	B	46	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	C	669	LEU	CB-CG-CD1	-5.87	101.02	111.00
1	D	1000	ASP	CB-CG-OD2	-5.87	113.01	118.30
1	A	791	LEU	CB-CG-CD1	5.87	120.97	111.00
1	B	965	ASP	CB-CG-OD1	5.86	123.57	118.30
1	C	846	LEU	CB-CG-CD1	-5.86	101.04	111.00
1	D	352	LEU	CA-CB-CG	-5.86	101.83	115.30
1	C	636	ILE	CG1-CB-CG2	5.86	124.28	111.40
1	C	268	LEU	CA-CB-CG	-5.83	101.89	115.30
1	A	916	LYS	N-CA-C	-5.83	95.27	111.00
1	C	559	MET	CG-SD-CE	5.83	109.52	100.20
1	C	28	LEU	CB-CG-CD2	5.80	120.86	111.00
1	C	529	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	C	897	LEU	CA-CB-CG	5.80	128.63	115.30
1	A	991	LEU	CA-CB-CG	-5.79	101.99	115.30
1	D	776	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	246	GLU	OE1-CD-OE2	-5.76	116.38	123.30
1	C	211	TYR	CA-CB-CG	-5.76	102.45	113.40
1	C	663	ASP	CB-CG-OD1	-5.76	113.12	118.30
1	B	629	LYS	CD-CE-NZ	-5.73	98.51	111.70
1	A	28	LEU	CA-CB-CG	-5.71	102.16	115.30
1	A	520	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	B	687	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	B	84	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	395	LYS	CD-CE-NZ	-5.68	98.63	111.70
1	A	60	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	25	HIS	CB-CA-C	5.67	121.73	110.40
1	A	67	LEU	CB-CG-CD2	-5.65	101.39	111.00
1	C	669	LEU	CD1-CG-CD2	-5.65	93.54	110.50
1	B	328	LEU	CA-CB-CG	5.65	128.29	115.30
1	C	663	ASP	CB-CG-OD2	5.65	123.38	118.30
1	D	99	SER	CA-CB-OG	-5.63	95.98	111.20
1	A	268	LEU	CB-CG-CD1	5.62	120.55	111.00
1	A	991	LEU	CB-CG-CD1	-5.62	101.45	111.00
1	D	253	VAL	CA-CB-CG2	-5.62	102.47	110.90
1	B	747	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	517	ALA	C-N-CA	5.61	135.72	121.70
1	C	948	ILE	CG1-CB-CG2	5.59	123.70	111.40
1	D	122	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	B	989	CYS	CA-CB-SG	-5.58	103.95	114.00
1	C	402	ARG	CG-CD-NE	5.57	123.50	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	985	THR	CA-CB-CG2	-5.57	104.60	112.40
1	A	581	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	835	LYS	CD-CE-NZ	-5.56	98.92	111.70
1	C	823	ASP	CB-CG-OD1	5.55	123.30	118.30
1	B	248	MET	CG-SD-CE	5.54	109.07	100.20
1	D	949	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	559	MET	CG-SD-CE	5.53	109.05	100.20
1	C	402	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	C	766	SER	CA-CB-OG	-5.53	96.28	111.20
1	D	1011	TYR	C-N-CA	5.52	135.50	121.70
1	A	328	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	797	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	D	682	LEU	CB-CG-CD1	5.50	120.36	111.00
1	D	36	LEU	CB-CG-CD2	5.50	120.35	111.00
1	B	741	LEU	CA-CB-CG	5.50	127.94	115.30
1	C	381	LYS	CD-CE-NZ	5.49	124.32	111.70
1	C	680	MET	CA-CB-CG	5.48	122.62	113.30
1	B	669	LEU	CA-CB-CG	-5.48	102.70	115.30
1	B	147	GLU	CA-CB-CG	5.47	125.44	113.40
1	D	293	ILE	CG1-CB-CG2	-5.47	99.37	111.40
1	D	61	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	574	LYS	CG-CD-CE	-5.46	95.51	111.90
1	D	307	LYS	CD-CE-NZ	5.46	124.26	111.70
1	C	647	LYS	CD-CE-NZ	5.46	124.25	111.70
1	A	687	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	B	442	LEU	CB-CG-CD2	-5.44	101.75	111.00
1	C	704	ILE	CG1-CB-CG2	-5.43	99.45	111.40
1	B	250	ASP	CB-CA-C	-5.41	99.57	110.40
1	D	445	PRO	CA-N-CD	-5.41	103.92	111.50
1	D	780	THR	OG1-CB-CG2	-5.41	97.56	110.00
1	A	548	LEU	CB-CG-CD1	-5.41	101.81	111.00
1	A	747	ASP	CB-CG-OD1	5.41	123.16	118.30
1	D	670	SER	C-N-CA	-5.39	108.23	121.70
1	C	741	LEU	CB-CG-CD2	-5.36	101.89	111.00
1	D	402	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	D	608	LEU	CB-CG-CD2	-5.36	101.89	111.00
1	B	684	CYS	CA-CB-SG	-5.35	104.37	114.00
1	B	250	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	176	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	562	ARG	CD-NE-CZ	-5.32	116.15	123.60
1	B	257	CYS	CA-CB-SG	-5.32	104.43	114.00
1	C	308	ASP	CB-CA-C	-5.31	99.78	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	574	LYS	CD-CE-NZ	5.30	123.89	111.70
1	C	771	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	224	GLY	C-N-CA	-5.29	111.20	122.30
1	B	379	LEU	CA-CB-CG	-5.29	103.14	115.30
1	D	717	ILE	CG1-CB-CG2	-5.28	99.78	111.40
1	B	993	LEU	CB-CG-CD1	-5.28	102.03	111.00
1	A	394	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	405	ALA	N-CA-CB	5.27	117.48	110.10
1	B	24	SER	CA-CB-OG	-5.27	96.97	111.20
1	C	343	THR	CA-CB-CG2	-5.26	105.03	112.40
1	B	572	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	D	694	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	A	32	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	B	379	LEU	CB-CG-CD2	5.26	119.94	111.00
1	A	359	VAL	CG1-CB-CG2	-5.26	102.49	110.90
1	B	823	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	14	SER	N-CA-CB	-5.24	102.64	110.50
1	B	195	ALA	CB-CA-C	5.24	117.95	110.10
1	D	99	SER	C-N-CA	-5.24	108.61	121.70
1	B	254	LYS	CD-CE-NZ	-5.23	99.68	111.70
1	B	669	LEU	CB-CG-CD1	-5.23	102.12	111.00
1	A	529	ASP	CB-CG-OD2	5.22	122.99	118.30
1	D	84	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	453	PRO	CA-C-N	5.20	128.64	117.20
1	B	253	VAL	CG1-CB-CG2	5.20	119.22	110.90
1	A	21	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	B	730	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	C	991	LEU	CA-CB-CG	-5.19	103.37	115.30
1	C	941	ILE	CG1-CB-CG2	-5.18	100.00	111.40
1	C	666	GLU	CG-CD-OE1	-5.17	107.95	118.30
1	C	714	VAL	CA-CB-CG2	-5.16	103.16	110.90
1	A	444	ASP	N-CA-C	5.14	124.88	111.00
1	A	667	LEU	CA-CB-CG	-5.14	103.48	115.30
1	B	826	VAL	CA-CB-CG2	5.13	118.60	110.90
1	D	432	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	532	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	986	CYS	CA-CB-SG	-5.13	104.77	114.00
1	C	23	GLN	C-N-CA	-5.12	108.90	121.70
1	B	540	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	D	775	LEU	CB-CG-CD1	-5.11	102.31	111.00
1	A	797	ASP	CB-CG-OD2	5.10	122.89	118.30
1	D	600	TYR	CB-CG-CD1	-5.10	117.94	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	231	ILE	CG1-CB-CG2	-5.07	100.24	111.40
1	C	840	LEU	CA-CB-CG	-5.07	103.63	115.30
1	B	441	VAL	CA-CB-CG1	-5.06	103.31	110.90
1	C	73	LEU	CB-CG-CD2	-5.06	102.40	111.00
1	A	424	ASP	N-CA-CB	-5.06	101.50	110.60
1	B	923	ASP	CB-CG-OD1	5.06	122.85	118.30
1	B	584	THR	C-N-CA	-5.05	109.07	121.70
1	B	209	LEU	CB-CG-CD1	-5.04	102.42	111.00
1	A	206	LEU	CB-CG-CD2	5.04	119.56	111.00
1	B	32	LEU	CA-CB-CG	-5.04	103.72	115.30
1	B	98	LYS	CD-CE-NZ	-5.03	100.12	111.70
1	C	847	GLN	CA-CB-CG	-5.03	102.34	113.40
1	B	793	THR	OG1-CB-CG2	-5.02	98.44	110.00
1	C	277	LYS	CD-CE-NZ	5.02	123.25	111.70
1	D	342	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	81	LYS	CD-CE-NZ	5.01	123.22	111.70
1	D	781	ILE	CG1-CB-CG2	-5.00	100.39	111.40

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ARG	Sidechain
1	A	364	ARG	Sidechain
1	A	415	GLU	Peptide
1	A	44	ASN	Peptide
1	A	696	ARG	Sidechain
1	A	70	ARG	Sidechain
1	A	759	ARG	Sidechain
1	A	886	ARG	Sidechain
1	B	1003	ARG	Sidechain
1	B	21	ARG	Sidechain
1	B	372	ALA	Peptide
1	B	373	VAL	Peptide
1	B	410[A]	ARG	Sidechain
1	B	410[B]	ARG	Sidechain
1	B	443	ARG	Sidechain
1	B	589	ARG	Sidechain
1	B	776	ARG	Sidechain
1	B	871	LEU	Peptide
1	B	886	ARG	Sidechain
1	B	919	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	C	1003	ARG	Sidechain
1	C	319	ALA	Peptide
1	C	333	GLY	Peptide
1	C	422	ASP	Peptide
1	D	318	LYS	Peptide
1	D	371	ARG	Sidechain
1	D	696	ARG	Sidechain
1	D	70	ARG	Sidechain
1	D	74	ARG	Sidechain
1	D	783	ARG	Sidechain
1	D	871	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7608	0	7645	212	0
1	B	7662	0	7694	218	0
1	C	7654	0	7686	219	0
1	D	7590	0	7612	190	0
2	A	32	0	0	3	0
2	B	32	0	0	2	0
2	C	32	0	0	3	0
2	D	32	0	0	1	0
3	A	31	0	19	1	0
3	B	31	0	19	1	0
3	C	31	0	19	1	0
3	D	31	0	19	1	0
4	A	53	0	31	2	0
4	B	53	0	31	3	0
4	C	53	0	31	1	0
4	D	53	0	31	2	0
5	A	9	0	6	1	0
5	B	9	0	6	0	0
5	C	9	0	6	0	0
5	D	9	0	6	0	0
6	A	149	0	0	23	0
6	B	141	0	0	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	159	0	0	18	0
6	D	144	0	0	8	0
All	All	31607	0	30861	788	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 13.

All (788) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LYS:NZ	1:A:259:LYS:CE	1.70	1.53
1:B:695:CYS:CB	1:B:695:CYS:SG	2.04	1.46
1:B:175:CYS:SG	1:B:175:CYS:CB	2.06	1.42
1:B:414:ASP:HB3	1:B:416:THR:HG22	1.32	1.09
1:B:115:MET:SD	6:B:1334:HOH:O	2.08	1.08
1:B:394:ARG:NH1	6:B:1201:HOH:O	1.90	1.02
1:B:399:LYS:NZ	6:B:1202:HOH:O	1.94	0.99
1:C:410:ARG:NH2	6:C:1202:HOH:O	1.85	0.97
1:B:341:GLY:HA2	1:B:371:ARG:HB3	1.49	0.93
1:C:381:LYS:HE2	1:D:381:LYS:HE2	1.50	0.93
1:C:246:GLU:OE2	6:C:1201:HOH:O	1.84	0.93
1:D:1011:TYR:OH	6:D:1201:HOH:O	1.85	0.92
1:A:373:VAL:O	1:A:376:GLU:N	2.06	0.88
1:C:886:ARG:HA	1:C:889:ILE:HD12	1.56	0.87
1:A:916:LYS:HD2	1:A:917:PRO:HD2	1.55	0.87
1:B:783:ARG:NH2	6:B:1207:HOH:O	2.07	0.86
1:C:220:GLN:NE2	6:C:1203:HOH:O	1.88	0.85
1:D:604:GLN:OE1	6:D:1202:HOH:O	1.93	0.84
1:A:728:GLY:O	6:A:1202:HOH:O	1.94	0.83
1:B:373:VAL:O	1:B:375:GLU:N	2.11	0.82
1:B:233:GLN:HE22	1:B:238:TYR:H	1.27	0.82
1:A:46:ASP:HB3	1:A:49:CYS:HB3	1.60	0.82
1:C:850:ASP:OD1	6:C:1204:HOH:O	2.00	0.80
1:A:776:ARG:HD3	6:A:1214:HOH:O	1.80	0.80
1:B:518:LYS:NZ	6:B:1209:HOH:O	2.12	0.80
1:B:416:THR:HG23	1:B:418:LYS:H	1.45	0.80
1:B:332:ARG:NH2	6:B:1211:HOH:O	2.14	0.79
1:A:651:MET:O	1:A:655:ARG:HG3	1.83	0.79
1:C:448:LYS:HE2	1:C:460:ASP:OD1	1.83	0.78
1:B:592:ARG:O	6:B:1204:HOH:O	2.00	0.78
1:B:46:ASP:OD2	1:B:48:ASN:HB2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:875:LYS:O	1:B:876:LEU:HD23	1.83	0.77
1:D:570:PHE:HB2	1:D:636:ILE:HB	1.65	0.77
1:B:73:LEU:O	1:B:77:MET:HG3	1.86	0.76
1:D:193:LEU:HD12	1:D:261:LEU:HB2	1.67	0.76
1:A:872:MET:O	6:A:1204:HOH:O	2.03	0.76
1:A:651:MET:HG2	1:A:701:ALA:HB2	1.66	0.75
1:D:246:GLU:HG3	1:D:909:ARG:HG2	1.67	0.75
1:B:358:ARG:NH1	6:B:1203:HOH:O	1.96	0.75
1:C:124:LEU:HD13	1:C:160:SER:HB2	1.68	0.75
1:B:703:GLN:NE2	6:B:1213:HOH:O	2.18	0.75
1:B:42:LYS:HE3	1:B:44:ASN:OD1	1.86	0.74
1:B:604:GLN:OE1	6:B:1205:HOH:O	2.06	0.74
1:C:718:VAL:HG23	1:C:780:THR:HG23	1.69	0.73
1:C:592:ARG:O	6:C:1207:HOH:O	2.07	0.73
1:A:658:GLU:O	6:A:1205:HOH:O	2.07	0.73
1:B:966:SER:O	6:B:1206:HOH:O	2.06	0.73
1:D:844:GLU:O	1:D:847:GLN:HG2	1.88	0.73
1:B:867:ARG:HA	1:B:872:MET:HE3	1.68	0.73
1:B:893:GLU:N	6:B:1215:HOH:O	2.22	0.73
1:B:1000:ASP:HB3	1:B:1003:ARG:HH21	1.54	0.72
1:D:396:VAL:HG13	1:D:406:VAL:HG22	1.69	0.72
1:A:615:GLU:OE2	1:B:1013:PRO:HB2	1.88	0.72
1:B:990:THR:HG22	1:B:990:THR:O	1.90	0.72
1:C:413:GLN:HB2	1:C:419:TRP:CZ3	2.23	0.72
1:C:583:VAL:HA	6:C:1210:HOH:O	1.90	0.72
1:C:870:GLU:OE1	1:C:874:LYS:HD3	1.89	0.72
1:C:976:GLU:OE2	6:C:1205:HOH:O	2.06	0.72
1:B:125:THR:O	1:B:129:VAL:HG22	1.90	0.72
1:C:220:GLN:HG3	1:C:222:TYR:CE2	2.25	0.71
1:B:267:THR:OG1	1:B:270:THR:HG23	1.91	0.71
1:C:584:THR:N	6:C:1210:HOH:O	2.23	0.71
1:B:233:GLN:HA	1:B:233:GLN:HE21	1.55	0.71
1:C:583:VAL:CA	6:C:1210:HOH:O	2.38	0.70
1:B:291:ASP:OD1	1:B:292:ASP:N	2.24	0.69
1:D:581:ASP:OD2	6:D:1203:HOH:O	2.09	0.69
2:C:1102:SF4:FE3	2:C:1102:SF4:S2	1.84	0.69
1:A:60:ASP:OD2	1:A:894:LYS:NZ	2.26	0.69
1:C:416:THR:OG1	1:C:418:LYS:HE2	1.93	0.68
1:B:589:ARG:HD2	1:B:611:GLU:HG3	1.75	0.68
1:C:413:GLN:HG2	1:C:417:GLY:HA2	1.76	0.68
1:A:299:GLN:NE2	1:A:308:ASP:HB3	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:GLU:OE1	6:B:1208:HOH:O	2.12	0.68
2:A:1103:SF4:FE2	2:A:1103:SF4:S3	1.87	0.67
1:B:394:ARG:HB3	1:B:395:LYS:HD2	1.76	0.67
1:D:860:GLN:OE1	6:D:1204:HOH:O	2.12	0.67
1:C:173:ASN:HB3	1:C:176:LEU:HD12	1.75	0.67
1:C:306:SER:OG	6:C:1208:HOH:O	2.13	0.66
1:B:868:ILE:N	1:B:872:MET:HE1	2.10	0.66
1:C:364:ARG:H	1:C:364:ARG:HD3	1.60	0.66
1:A:47:LYS:HE2	1:B:374:PRO:HD3	1.78	0.66
1:D:580:LYS:NZ	1:D:649:ASP:OD2	2.28	0.66
1:B:1014:LYS:O	6:B:1210:HOH:O	2.12	0.65
2:B:1101:SF4:FE1	2:B:1101:SF4:S2	1.87	0.65
1:D:550:SER:HB2	1:D:572:LEU:HB3	1.77	0.65
1:A:35:LYS:O	1:A:39:LYS:NZ	2.27	0.65
1:C:291:ASP:OD1	1:C:293:ILE:HG23	1.96	0.65
1:D:415:GLU:CD	1:D:416:THR:H	2.00	0.65
1:A:682:LEU:H	1:A:682:LEU:HD23	1.62	0.64
2:D:1101:SF4:FE2	2:D:1101:SF4:S1	1.89	0.64
1:B:9:VAL:CG2	1:B:12:ILE:HG12	2.28	0.64
1:C:535:VAL:HG22	1:C:536:GLU:N	2.13	0.64
1:D:999:ILE:O	1:D:1000:ASP:HB2	1.97	0.64
1:C:220:GLN:HG3	1:C:222:TYR:CZ	2.32	0.64
1:C:593:GLY:HA2	1:C:742:MET:SD	2.37	0.64
2:B:1103:SF4:FE4	2:B:1103:SF4:S1	1.89	0.64
1:A:398:VAL:O	1:A:399:LYS:HG3	1.97	0.63
2:A:1102:SF4:FE2	2:A:1102:SF4:S4	1.90	0.63
2:A:1103:SF4:FE3	2:A:1103:SF4:S4	1.90	0.63
1:B:652:GLU:OE2	6:B:1212:HOH:O	2.15	0.63
1:B:793:THR:HB	1:B:814:GLN:HB2	1.80	0.63
1:A:424:ASP:OD2	1:A:425:GLN:NE2	2.31	0.63
1:B:868:ILE:HG22	1:B:869:ALA:H	1.64	0.63
1:B:451:LEU:HD13	1:B:454:ILE:HD11	1.80	0.63
1:A:669:LEU:HD13	1:A:691:VAL:HG22	1.80	0.63
1:B:343:THR:HA	4:B:1106:FAD:HM73	1.81	0.63
1:A:846:LEU:HD22	1:A:849:TRP:CE2	2.34	0.63
1:B:867:ARG:HA	1:B:872:MET:CE	2.28	0.63
1:A:427:VAL:HG13	1:B:410[A]:ARG:HD2	1.80	0.62
1:D:845:GLU:OE1	1:D:845:GLU:N	2.33	0.62
1:A:367:PHE:HB2	1:B:386:GLU:OE1	1.99	0.62
1:A:776:ARG:NH1	6:A:1214:HOH:O	2.32	0.62
1:D:870:GLU:C	1:D:874:LYS:HG3	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LYS:NZ	6:A:1213:HOH:O	2.30	0.62
1:A:867:ARG:HH12	1:A:951:GLU:HG3	1.63	0.62
1:A:318:LYS:O	1:A:320:GLY:N	2.33	0.62
1:A:389:PRO:HB2	1:A:390:PHE:CD2	2.35	0.62
1:A:376:GLU:OE1	1:A:376:GLU:HA	2.00	0.61
1:A:543:ILE:N	6:A:1201:HOH:O	1.86	0.61
1:A:871:LEU:HB2	1:A:872:MET:HE1	1.83	0.61
1:B:378:GLU:O	1:B:382:GLU:HG2	2.00	0.61
1:D:842:SER:OG	1:D:914:PRO:HB3	2.00	0.61
1:C:373:VAL:O	1:C:375:GLU:N	2.33	0.61
1:C:67:LEU:HD23	1:D:146:GLU:HG2	1.83	0.61
1:C:272:LYS:NZ	6:C:1209:HOH:O	2.14	0.61
2:C:1102:SF4:FE1	2:C:1102:SF4:S4	1.91	0.61
1:B:272:LYS:NZ	6:B:1220:HOH:O	2.32	0.61
1:C:647:LYS:O	1:C:651:MET:HG3	2.01	0.61
1:C:88:GLN:HG3	1:C:95:LEU:O	2.02	0.60
1:C:189:LYS:HE2	1:C:213:ASP:OD2	2.01	0.60
1:D:570:PHE:CB	1:D:636:ILE:HB	2.31	0.60
1:D:860:GLN:HG2	6:D:1204:HOH:O	2.01	0.60
1:B:629:LYS:HE2	1:B:629:LYS:HA	1.82	0.60
1:C:267:THR:OG1	1:C:270:THR:HG23	2.02	0.60
1:B:74:ARG:HD2	6:B:1249:HOH:O	2.00	0.60
1:B:989:CYS:O	1:B:990:THR:HB	2.02	0.60
1:B:845:GLU:HG3	1:B:912:PHE:CD1	2.37	0.60
1:A:378:GLU:OE2	1:A:378:GLU:HA	2.02	0.60
1:B:787:GLY:O	1:B:789:PRO:HD3	2.02	0.59
1:A:786:PRO:HB2	1:D:942:GLU:HG2	1.83	0.59
1:C:613:ILE:HG21	1:C:642:MET:HE2	1.83	0.59
1:C:962[A]:THR:HG21	1:C:991:LEU:HB3	1.83	0.59
1:A:373:VAL:O	1:A:375:GLU:N	2.35	0.59
1:A:927:LYS:NZ	1:D:936:GLY:O	2.31	0.59
1:C:57:ASN:HD22	1:C:898:LYS:HD2	1.67	0.59
1:A:611:GLU:O	5:A:1107:TDR:H6	2.02	0.59
1:B:747:ASP:OD1	1:B:749:THR:HG23	2.02	0.59
1:C:791:LEU:HD12	1:C:791:LEU:N	2.18	0.59
1:C:533:ILE:O	1:C:545:PRO:HD3	2.03	0.59
1:C:948:ILE:HD13	1:C:980:PRO:HG2	1.86	0.58
1:A:223:VAL:HG23	1:A:245[A]:ILE:HD13	1.85	0.58
1:A:267:THR:OG1	1:A:270:THR:HG23	2.03	0.58
1:A:948:ILE:HD13	1:A:980:PRO:HG2	1.84	0.58
1:C:285:LEU:HB3	1:C:440:SER:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:949:ASP:HB2	1:C:1003:ARG:HH21	1.67	0.58
1:B:873:GLY:C	1:B:874:LYS:HD3	2.24	0.58
1:D:262:SER:HB3	1:D:265:GLU:H	1.67	0.58
1:C:191:ALA:O	1:C:279:ALA:HA	2.04	0.58
1:A:28:LEU:HD22	1:B:519:PRO:HB3	1.85	0.58
1:A:483:VAL:HG12	1:A:485:MET:HG3	1.86	0.58
1:A:741:LEU:O	1:B:772:PRO:HA	2.04	0.57
1:A:786:PRO:HB2	1:D:942:GLU:CG	2.34	0.57
1:C:205:PHE:CD1	1:C:521:LEU:HD13	2.39	0.57
1:B:341:GLY:CA	1:B:371:ARG:HB3	2.31	0.57
1:B:934:THR:HG23	1:B:937:GLU:OE1	2.05	0.57
1:C:413:GLN:CG	1:C:417:GLY:HA2	2.34	0.57
1:A:428:HIS:HB2	1:B:425:GLN:NE2	2.18	0.57
1:A:316:SER:OG	1:A:328:LEU:HD23	2.04	0.57
1:C:783:ARG:HG3	1:C:929:LEU:HD22	1.86	0.57
1:D:394:ARG:HB3	1:D:407:GLN:O	2.05	0.57
1:A:180:GLU:HG2	1:A:181:LYS:HD3	1.86	0.57
1:A:993:LEU:C	1:A:993:LEU:HD23	2.25	0.57
1:B:705:PRO:HA	1:B:730:ASP:OD2	2.05	0.57
1:A:822:GLN:O	1:A:823:ASP:HB3	2.05	0.57
1:B:233:GLN:HE22	1:B:238:TYR:N	1.98	0.57
1:C:796:ILE:HD13	1:C:813:LEU:HB3	1.86	0.57
1:A:379:LEU:O	1:A:383:GLU:HG3	2.04	0.57
1:D:360:PHE:CD1	1:D:386:GLU:HB3	2.41	0.56
1:D:506:TYR:O	1:D:510:GLN:HG2	2.06	0.56
1:D:985:THR:O	1:D:1014:LYS:NZ	2.37	0.56
1:B:673:HIS:NE2	1:B:682:LEU:O	2.37	0.56
1:C:411:THR:HA	1:C:420:ASN:O	2.05	0.56
1:A:188:ALA:HB1	1:A:277:LYS:HG3	1.86	0.56
1:C:386:GLU:OE1	1:D:368:VAL:HG23	2.04	0.56
1:C:482:ILE:HG12	1:C:482:ILE:O	2.04	0.56
1:D:390:PHE:HB2	1:D:410[B]:ARG:NH1	2.21	0.56
1:A:289:LYS:NZ	6:A:1209:HOH:O	2.21	0.56
1:B:70:ARG:HB2	1:B:999:ILE:HG13	1.87	0.56
1:A:498:GLN:HA	1:B:28:LEU:HD11	1.87	0.56
1:A:796:ILE:HD13	1:A:813:LEU:HB3	1.87	0.56
1:C:776:ARG:NH1	6:C:1218:HOH:O	2.37	0.56
1:C:54:LYS:HB3	1:C:891:ALA:HB1	1.87	0.56
1:B:336:ILE:HD12	1:B:431:ALA:CB	2.34	0.56
1:B:233:GLN:HE21	1:B:233:GLN:CA	2.14	0.56
1:C:844:GLU:O	1:C:847:GLN:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:VAL:HG23	1:A:376:GLU:HB2	1.88	0.55
1:C:170:GLN:OE1	1:C:251:LEU:HD11	2.06	0.55
1:A:424:ASP:OD1	1:A:424:ASP:N	2.27	0.55
1:A:990:THR:HG22	1:A:990:THR:O	2.07	0.55
1:C:749:THR:HG21	1:C:758:LYS:HD2	1.89	0.55
1:D:870:GLU:O	1:D:871:LEU:HB2	2.06	0.55
1:B:177:PRO:HD2	1:B:182:MET:SD	2.46	0.55
1:D:193:LEU:CD1	1:D:261:LEU:HB2	2.36	0.55
1:A:333:GLY:HA3	1:A:432:ASP:OD2	2.07	0.55
1:C:223:VAL:HG23	1:C:245[A]:ILE:HD13	1.87	0.55
1:D:353:ARG:NH1	1:D:383:GLU:OE2	2.40	0.55
1:A:776:ARG:HG2	1:A:776:ARG:O	2.07	0.55
1:D:241:VAL:O	1:D:245:ILE:HG12	2.07	0.55
1:D:413:GLN:HG3	1:D:419:TRP:CE2	2.41	0.55
1:A:580:LYS:HB3	6:A:1203:HOH:O	2.06	0.55
1:D:331:ILE:HD12	1:D:433:VAL:HG21	1.89	0.55
1:A:705:PRO:HA	1:A:730:ASP:OD2	2.07	0.54
1:B:561:ARG:O	1:B:565:GLU:HG3	2.06	0.54
1:C:856:THR:HG22	1:C:857:GLU:O	2.08	0.54
1:A:428:HIS:H	1:B:425:GLN:NE2	2.05	0.54
1:A:338:LEU:O	1:A:437:ALA:HB3	2.06	0.54
1:C:193:LEU:HD13	1:C:217:PHE:HB2	1.90	0.54
1:D:638:ILE:HG12	1:D:664:ALA:HB3	1.88	0.54
1:A:612:LEU:HD11	1:B:935:PHE:CE1	2.43	0.54
1:B:867:ARG:C	1:B:872:MET:HE1	2.27	0.54
1:A:427:VAL:HG11	1:B:410[B]:ARG:HD2	1.90	0.54
1:A:427:VAL:CG1	1:B:410[A]:ARG:HD2	2.37	0.54
1:A:134:ASP:HA	1:B:42:LYS:HZ1	1.73	0.54
1:C:689:GLU:HA	1:C:692:ARG:HH12	1.73	0.54
1:D:718:VAL:CG2	1:D:780:THR:HG22	2.38	0.54
1:A:56:GLU:OE2	1:A:895:MET:SD	2.66	0.54
1:A:877:PRO:HD2	1:A:882:TYR:CG	2.43	0.54
1:B:239:ASP:HB2	1:B:909:ARG:HH22	1.73	0.54
1:D:642:MET:HE1	1:D:670:SER:HB2	1.90	0.54
1:A:44:ASN:HB2	1:A:45:PRO:HD2	1.90	0.53
1:B:340:ALA:HB2	1:B:363:PHE:CD1	2.44	0.53
1:C:654:SER:HB2	1:C:665:LEU:HD11	1.89	0.53
1:D:999:ILE:O	1:D:999:ILE:HG22	2.09	0.53
1:A:843:ILE:HG21	1:A:846:LEU:HD12	1.89	0.53
1:C:949:ASP:HB2	1:C:1003:ARG:NH2	2.23	0.53
1:D:165:ALA:O	1:D:167[A]:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:LYS:NZ	1:A:649:ASP:OD1	2.36	0.53
6:C:1229:HOH:O	1:D:807:HIS:HD2	1.91	0.53
1:D:55:LEU:O	1:D:58:ASN:HB2	2.08	0.53
1:A:75:GLU:OE2	1:A:150:ILE:HA	2.09	0.53
1:A:396:VAL:HG22	1:A:406:VAL:HG22	1.91	0.53
1:B:9:VAL:HG23	1:B:12:ILE:HG12	1.91	0.53
1:A:28:LEU:HD22	1:B:519:PRO:CB	2.38	0.53
1:A:297:LEU:HA	1:A:301:GLN:OE1	2.08	0.53
1:C:97:ILE:HA	1:C:100:PHE:CD2	2.44	0.53
1:C:331:ILE:HD12	1:C:433:VAL:HG21	1.89	0.53
1:D:849:TRP:N	1:D:849:TRP:CD1	2.75	0.53
1:B:98:LYS:HE2	1:B:822:GLN:NE2	2.23	0.53
1:C:18:LEU:HD11	1:C:975:PRO:HA	1.91	0.53
1:D:642:MET:CE	1:D:670:SER:HB2	2.39	0.53
1:A:193:LEU:HD22	1:A:193:LEU:N	2.24	0.53
1:D:269:ASN:O	1:D:270:THR:C	2.47	0.53
1:C:613:ILE:HG21	1:C:642:MET:CE	2.38	0.52
1:A:935:PHE:CE1	1:B:612:LEU:HD11	2.44	0.52
1:B:233:GLN:HA	1:B:233:GLN:NE2	2.22	0.52
1:A:408:PHE:O	1:A:426:ILE:HA	2.09	0.52
1:B:10:ALA:N	6:B:1225:HOH:O	2.41	0.52
1:C:414:ASP:O	1:C:416:THR:N	2.40	0.52
1:B:871:LEU:HD11	1:B:886:ARG:HG2	1.91	0.52
1:C:410:ARG:NH1	1:C:425:GLN:OE1	2.41	0.52
1:D:213:ASP:OD1	1:D:254:LYS:NZ	2.24	0.52
1:A:373:VAL:CG2	1:A:376:GLU:HB2	2.40	0.52
1:B:241:VAL:O	1:B:245:ILE:HG12	2.09	0.52
1:D:583:VAL:O	1:D:615:GLU:HG2	2.10	0.52
1:D:691:VAL:HG21	1:D:720:ILE:HG23	1.91	0.52
1:A:259:LYS:NZ	6:A:1220:HOH:O	2.40	0.52
1:A:518:LYS:HD2	1:A:518:LYS:C	2.30	0.52
1:B:695:CYS:SG	1:B:695:CYS:CA	2.93	0.52
1:A:357:ARG:HH22	1:A:430:LYS:HD3	1.75	0.52
1:A:468:THR:O	1:A:469:MET:HB2	2.09	0.52
1:A:343:THR:HA	4:A:1106:FAD:HM73	1.92	0.51
1:D:415:GLU:OE2	1:D:415:GLU:N	2.43	0.51
1:C:375:GLU:O	1:C:378:GLU:HB3	2.09	0.51
1:D:341:GLY:HA2	1:D:371:ARG:HB3	1.92	0.51
1:D:651:MET:HG2	1:D:701:ALA:HB2	1.92	0.51
1:A:100:PHE:CD1	1:A:100:PHE:C	2.84	0.51
1:A:414:ASP:O	1:A:416:THR:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:VAL:HG23	1:B:780:THR:CG2	2.40	0.51
1:C:89:LYS:HD3	1:D:41:TRP:CZ2	2.45	0.51
1:D:124:LEU:HD13	1:D:160:SER:HB2	1.92	0.51
1:A:238:TYR:O	1:A:238:TYR:CD1	2.63	0.51
1:A:427:VAL:CG1	1:B:410[B]:ARG:HD2	2.40	0.51
1:B:791:LEU:N	1:B:791:LEU:HD12	2.26	0.51
1:C:180:GLU:OE2	1:C:180:GLU:N	2.27	0.51
1:A:92:PRO:HD3	1:A:135:LEU:HD22	1.91	0.51
1:B:69:GLU:OE2	1:B:853:SER:HB3	2.11	0.51
1:D:137:VAL:HG13	1:D:149:SER:HB3	1.93	0.51
1:A:518:LYS:HD2	1:A:518:LYS:O	2.10	0.51
1:A:592:ARG:NH1	6:A:1217:HOH:O	2.35	0.51
1:B:76:ALA:HB1	1:B:105:SER:HB3	1.92	0.51
1:B:233:GLN:NE2	1:B:237:PRO:HA	2.26	0.51
1:B:859:HIS:O	1:B:860:GLN:HG2	2.10	0.51
1:D:328:LEU:HD21	1:D:354:CYS:HA	1.92	0.51
1:C:367:PHE:HB3	1:D:386:GLU:OE1	2.10	0.50
1:C:373:VAL:HG23	1:C:376:GLU:HB2	1.93	0.50
1:A:7:LYS:HG2	1:B:561:ARG:NE	2.26	0.50
1:A:687:ASP:HB3	1:A:690:LEU:HD12	1.92	0.50
1:B:12:ILE:HD13	1:B:12:ILE:N	2.27	0.50
1:B:57:ASN:HB2	1:B:898:LYS:NZ	2.25	0.50
1:C:110:TYR:CD1	1:C:110:TYR:C	2.85	0.50
1:D:506:TYR:CD1	1:D:506:TYR:C	2.84	0.50
1:A:978:HIS:NE2	1:B:84:ASP:OD2	2.33	0.50
1:C:22:THR:HB	1:D:828:GLN:HG3	1.92	0.50
1:B:842:SER:HA	1:B:916:LYS:HG2	1.93	0.50
1:C:856:THR:HG21	1:C:859:HIS:HD2	1.76	0.50
1:D:40:HIS:O	1:D:880:GLY:HA3	2.10	0.50
1:D:759:ARG:HG2	1:D:759:ARG:HH11	1.76	0.50
1:C:793:THR:HG22	1:C:814:GLN:HB2	1.93	0.50
1:C:959:CYS:O	1:C:962[B]:THR:HG22	2.12	0.50
1:D:960:TYR:CD1	1:D:973:PHE:HB2	2.47	0.50
1:B:57:ASN:OD1	1:B:328:LEU:HD22	2.11	0.50
1:B:468:THR:O	1:B:469:MET:HB2	2.12	0.50
1:A:211:TYR:HB2	1:A:214:ILE:HD11	1.93	0.50
1:B:308:ASP:O	1:B:312:LEU:HD12	2.10	0.50
1:B:913:ILE:HG22	1:B:914:PRO:O	2.11	0.50
1:B:1013:PRO:HG2	1:B:1015:ARG:HH21	1.76	0.50
1:C:856:THR:HG22	1:C:857:GLU:N	2.26	0.50
1:D:885:GLN:O	1:D:889:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ASP:HB3	1:A:49:CYS:CB	2.38	0.50
1:A:223:VAL:HG11	1:A:255:ILE:HG21	1.94	0.50
1:C:652:GLU:O	1:C:656:LYS:HG2	2.11	0.50
1:D:225:GLY:HA2	4:D:1106:FAD:H3B	1.94	0.50
1:C:42:LYS:NZ	1:C:44:ASN:OD1	2.43	0.49
1:C:535:VAL:CG2	1:C:536:GLU:N	2.75	0.49
1:A:23:GLN:O	6:A:1208:HOH:O	2.18	0.49
1:B:42:LYS:HE2	1:B:46:ASP:HB2	1.94	0.49
1:B:269:ASN:HB3	1:B:273:GLU:OE2	2.11	0.49
1:D:955:ASN:HB3	1:D:978:HIS:HB3	1.94	0.49
1:C:79:CYS:CB	1:C:101:ILE:HG21	2.42	0.49
1:B:989:CYS:SG	1:B:990:THR:N	2.86	0.49
1:D:269:ASN:O	1:D:272:LYS:N	2.45	0.49
1:B:178:SER:OG	1:B:179:GLN:N	2.46	0.49
1:B:649:ASP:OD1	1:B:649:ASP:N	2.45	0.49
1:B:845:GLU:HG3	1:B:912:PHE:CG	2.48	0.49
1:C:263:GLU:O	1:C:264:ASN:HB2	2.13	0.49
1:D:577[A]:SER:OG	1:D:642:MET:O	2.16	0.49
1:A:580:LYS:N	6:A:1203:HOH:O	2.02	0.49
1:B:455:LYS:HE2	1:B:463:GLU:OE1	2.12	0.49
1:C:63:LYS:HE3	1:C:128:MET:HG2	1.94	0.49
1:D:277:LYS:HD2	1:D:511:TYR:CE1	2.47	0.49
1:C:490:VAL:HG12	6:C:1206:HOH:O	2.13	0.49
1:C:692:ARG:HB3	1:C:692:ARG:NH1	2.27	0.49
1:D:532:ASP:OD1	1:D:532:ASP:C	2.51	0.49
1:D:911:PRO:O	1:D:913:ILE:HG13	2.12	0.49
1:A:357:ARG:O	1:A:358:ARG:HG3	2.13	0.49
1:C:362:VAL:HG13	1:C:391:LEU:HB2	1.94	0.49
1:B:753:ALA:HB1	1:B:758:LYS:HB3	1.95	0.48
1:B:877:PRO:HD2	1:B:882:TYR:CG	2.47	0.48
1:C:804:GLN:O	1:C:808:SER:OG	2.30	0.48
2:C:1102:SF4:S2	2:C:1102:SF4:S4	3.11	0.48
1:D:277:LYS:HD2	1:D:511:TYR:HE1	1.77	0.48
1:B:358:ARG:HD3	6:B:1203:HOH:O	2.14	0.48
1:D:664:ALA:HA	1:D:704:ILE:HD12	1.95	0.48
1:A:328:LEU:C	1:A:330:SER:N	2.67	0.48
1:A:867:ARG:HA	1:A:872:MET:SD	2.54	0.48
1:C:5:LEU:HD13	1:D:620:TYR:CD2	2.48	0.48
1:C:428:HIS:O	1:D:410[A]:ARG:NH1	2.46	0.48
1:C:870:GLU:HA	1:C:874:LYS:HZ3	1.78	0.48
1:A:67:LEU:HD23	1:B:146:GLU:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ILE:HG12	1:A:482:ILE:O	2.13	0.48
1:A:543:ILE:HG23	6:A:1201:HOH:O	2.12	0.48
1:C:772:PRO:HA	1:D:741:LEU:O	2.13	0.48
1:D:292:ASP:O	1:D:294:PHE:N	2.46	0.48
1:C:346:ASP:OD2	4:C:1106:FAD:H6	2.12	0.48
1:C:669:LEU:HD13	1:C:669:LEU:HA	1.49	0.48
1:A:550:SER:HB2	1:A:572:LEU:HB3	1.96	0.48
1:B:335:VAL:HG22	1:B:433:VAL:HB	1.95	0.48
1:B:270:THR:O	1:B:274:GLU:HB2	2.13	0.48
1:B:719:SER:OG	1:B:720:ILE:N	2.46	0.48
1:C:32:LEU:O	1:C:33:ALA:C	2.52	0.48
1:A:84:ASP:OD1	1:A:89:LYS:NZ	2.41	0.48
1:A:394:ARG:HG3	1:A:394:ARG:HH11	1.79	0.48
1:C:281:ILE:HD13	1:C:281:ILE:N	2.28	0.48
1:B:373:VAL:C	1:B:375:GLU:H	2.11	0.48
1:B:448:LYS:NZ	1:B:460:ASP:OD1	2.45	0.48
1:B:749:THR:OG1	6:B:1214:HOH:O	2.20	0.48
1:C:379:LEU:HA	1:C:382:GLU:HG2	1.94	0.48
1:C:807:HIS:HB3	1:C:928:ALA:HB2	1.96	0.48
1:D:454:ILE:HG22	1:D:473:GLU:HG2	1.96	0.48
1:A:372:ALA:O	1:A:374:PRO:HD3	2.14	0.48
1:A:375:GLU:O	1:A:379:LEU:HD22	2.13	0.48
1:A:1015:ARG:O	1:B:616:LYS:HA	2.12	0.48
1:A:868:ILE:O	1:A:870:GLU:N	2.46	0.47
1:C:230:GLU:HG2	1:C:310:LEU:HB2	1.96	0.47
1:A:725:LYS:NZ	6:A:1229:HOH:O	2.48	0.47
1:B:227:SER:HA	1:B:231:ILE:HD12	1.95	0.47
1:B:673:HIS:CD2	1:B:673:HIS:N	2.83	0.47
1:C:413:GLN:HB2	1:C:419:TRP:CH2	2.49	0.47
1:C:464:VAL:CG1	1:C:478:ALA:HB3	2.44	0.47
1:C:568:TRP:CE2	1:C:827:ILE:HB	2.48	0.47
1:C:999:ILE:HD11	1:D:600:TYR:CE2	2.49	0.47
1:D:477:PHE:N	1:D:477:PHE:CD1	2.83	0.47
1:A:38:LYS:NZ	6:A:1207:HOH:O	2.17	0.47
1:A:249:LYS:NZ	6:A:1224:HOH:O	2.43	0.47
1:D:180:GLU:N	1:D:180:GLU:CD	2.68	0.47
1:A:610:ILE:O	1:A:610:ILE:HG13	2.15	0.47
1:A:796:ILE:HD13	1:A:796:ILE:HG21	1.65	0.47
1:B:43:ARG:HD3	1:B:879:PHE:HB3	1.97	0.47
1:C:173:ASN:HB3	1:C:176:LEU:CD1	2.43	0.47
1:D:536:GLU:HG3	1:D:540:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:HIS:CB	1:B:425:GLN:HE22	2.27	0.47
1:C:651:MET:O	1:C:655:ARG:HB2	2.14	0.47
1:A:711:THR:HG23	1:A:711:THR:O	2.15	0.47
1:B:336:ILE:HD12	1:B:431:ALA:HB2	1.97	0.47
1:C:776:ARG:O	1:C:780:THR:HB	2.14	0.47
1:D:352:LEU:HA	1:D:352:LEU:HD23	1.37	0.47
1:A:668:ASN:OD1	1:A:670:SER:HB2	2.15	0.47
1:B:868:ILE:HD12	1:B:871:LEU:HD22	1.96	0.47
1:B:972:GLN:O	1:B:980:PRO:HA	2.15	0.47
1:C:373:VAL:O	1:C:376:GLU:N	2.45	0.47
1:A:304:TYR:O	1:A:435:ILE:HA	2.14	0.46
1:A:346:ASP:OD2	4:A:1106:FAD:H6	2.15	0.46
1:A:582:ILE:HA	1:A:582:ILE:HD12	1.62	0.46
1:B:301:GLN:O	1:B:403:ILE:HG12	2.14	0.46
1:D:471:THR:HG23	1:D:476:VAL:O	2.15	0.46
1:A:588:PRO:HB3	1:B:990:THR:OG1	2.15	0.46
1:B:806:LEU:HD13	1:B:921:ILE:HG23	1.97	0.46
1:C:647:LYS:HE3	1:C:697:TRP:CD1	2.50	0.46
1:C:859:HIS:CE1	1:C:998:ILE:HG23	2.51	0.46
1:D:201:SER:HB2	1:D:493:VAL:HG13	1.97	0.46
1:D:415:GLU:CD	1:D:416:THR:N	2.67	0.46
1:B:858:SER:O	1:B:865:VAL:HG23	2.15	0.46
1:C:572:LEU:HD13	1:C:638:ILE:HB	1.98	0.46
1:C:837:LEU:HD23	1:C:837:LEU:HA	1.71	0.46
1:B:990:THR:O	1:B:990:THR:CG2	2.63	0.46
1:D:883:LEU:HG	1:D:887:LYS:HE3	1.96	0.46
1:D:849:TRP:N	1:D:849:TRP:HD1	2.14	0.46
1:A:315:LYS:HZ2	1:A:321:MET:HE2	1.81	0.46
1:B:475:TRP:HB3	1:B:506:TYR:CZ	2.51	0.46
1:A:367:PHE:CZ	1:B:367:PHE:CZ	3.03	0.46
1:A:390:PHE:O	1:A:391:LEU:HD23	2.15	0.46
1:B:78:ARG:NH1	1:B:147:GLU:HG2	2.30	0.46
1:B:225:GLY:HA2	4:B:1106:FAD:H3B	1.98	0.46
1:B:444:ASP:OD1	1:B:446:LYS:HB2	2.16	0.46
1:C:57:ASN:HD22	1:C:898:LYS:CD	2.27	0.46
1:C:741:LEU:O	1:D:772:PRO:HA	2.15	0.46
1:D:860:GLN:CG	6:D:1204:HOH:O	2.62	0.46
1:D:868:ILE:HG12	1:D:893:GLU:HG2	1.98	0.46
1:A:680:MET:N	6:A:1228:HOH:O	2.47	0.46
1:A:767:GLY:O	1:A:770:ILE:HG12	2.15	0.46
1:B:50:PHE:O	1:B:384:LYS:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:GLU:OE1	1:B:109:TYR:OH	2.24	0.46
1:C:941:ILE:HD12	1:C:941:ILE:HG23	1.76	0.46
1:A:10:ALA:HA	1:A:13:GLU:HB2	1.98	0.46
1:B:989:CYS:O	1:B:990:THR:CB	2.64	0.46
1:C:167:ASN:HB3	1:C:912:PHE:CD2	2.51	0.46
1:C:285:LEU:CB	1:C:440:SER:HB3	2.45	0.46
1:C:410:ARG:NH1	1:D:428:HIS:O	2.49	0.46
1:D:451:LEU:O	1:D:454:ILE:HG13	2.16	0.46
1:A:682:LEU:HD23	1:A:682:LEU:N	2.30	0.46
1:C:2:ALA:HB1	1:D:623:GLN:OE1	2.16	0.46
1:C:269:ASN:HD22	1:C:269:ASN:H	1.64	0.46
1:C:791:LEU:HD12	1:C:791:LEU:H	1.80	0.46
1:D:717:ILE:HD13	1:D:717:ILE:HG21	1.61	0.46
1:B:656:LYS:HD2	6:B:1219:HOH:O	2.16	0.45
1:B:993:LEU:O	1:B:993:LEU:HD23	2.16	0.45
1:C:416:THR:OG1	1:C:418:LYS:CE	2.64	0.45
1:A:816:CYS:HB3	3:A:1105:FMN:O1P	2.16	0.45
1:B:191:ALA:O	1:B:279:ALA:HA	2.16	0.45
1:B:589:ARG:CD	1:B:611:GLU:HG3	2.44	0.45
1:C:386:GLU:OE2	1:D:367:PHE:HB2	2.16	0.45
1:C:428:HIS:H	1:D:425:GLN:HE21	1.64	0.45
1:A:177:PRO:HG2	1:A:182:MET:SD	2.56	0.45
1:B:233:GLN:CA	1:B:233:GLN:NE2	2.79	0.45
1:C:461:LEU:HD23	1:C:461:LEU:HA	1.61	0.45
1:C:601:GLY:HA3	1:D:997:PRO:HB3	1.98	0.45
1:C:941:ILE:HD13	1:C:941:ILE:HA	1.35	0.45
1:D:16:LEU:HD23	1:D:16:LEU:HA	1.71	0.45
1:D:860:GLN:HB2	1:D:865:VAL:CG2	2.46	0.45
1:A:45:PRO:HD2	1:B:143:TYR:OH	2.16	0.45
1:A:776:ARG:O	1:A:780:THR:HG22	2.16	0.45
1:B:10:ALA:HB3	6:B:1225:HOH:O	2.15	0.45
1:B:492:SER:OG	4:B:1106:FAD:H5'2	2.17	0.45
1:B:957:GLY:O	1:B:960:TYR:HB3	2.16	0.45
1:C:948:ILE:HD13	1:C:980:PRO:CG	2.46	0.45
1:A:342:ASP:OD1	1:A:373:VAL:HG13	2.16	0.45
1:C:547:GLY:HA3	1:C:570:PHE:CE1	2.52	0.45
1:D:845:GLU:HG3	1:D:912:PHE:CE1	2.51	0.45
1:A:785:LEU:HA	1:A:785:LEU:HD23	1.67	0.45
1:B:294:PHE:CD1	1:B:303:PHE:CE1	3.05	0.45
1:D:416:THR:HG23	1:D:418:LYS:HB2	1.98	0.45
1:A:287:GLU:OE2	1:A:444:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:HIS:CB	1:B:425:GLN:NE2	2.79	0.45
1:C:256:ILE:HG22	1:C:259:LYS:HG3	1.98	0.45
1:D:396:VAL:HG11	1:D:403:ILE:HD13	1.98	0.45
1:D:948:ILE:HG21	1:D:980:PRO:HG2	1.99	0.45
1:A:32:LEU:HD13	1:B:485:MET:HE3	1.98	0.45
1:B:398:VAL:HG22	1:B:403:ILE:HD13	1.99	0.45
1:B:738:VAL:HG21	1:B:773:ILE:CD1	2.47	0.45
1:C:289:LYS:HG3	1:C:441:VAL:HG13	1.98	0.45
1:A:518:LYS:NZ	1:A:520:GLU:HB3	2.32	0.45
1:B:180:GLU:CD	1:B:180:GLU:H	2.20	0.45
1:D:300:ASP:N	1:D:300:ASP:OD1	2.49	0.45
1:B:475:TRP:HB3	1:B:506:TYR:OH	2.17	0.45
1:C:62:ILE:C	1:C:62:ILE:HD12	2.37	0.45
1:C:470:GLN:HG3	1:C:477:PHE:CE2	2.52	0.45
1:D:18:LEU:HD12	1:D:18:LEU:HA	1.64	0.45
1:A:264:ASN:HB2	6:A:1212:HOH:O	2.17	0.44
1:A:866:PRO:CG	1:A:890:ILE:HD11	2.47	0.44
1:A:877:PRO:HB2	1:A:879:PHE:CE2	2.52	0.44
1:B:945:VAL:HG13	1:B:1007:ARG:HG2	1.98	0.44
1:C:741:LEU:HD12	1:C:741:LEU:HA	1.63	0.44
1:D:572:LEU:N	1:D:572:LEU:CD2	2.80	0.44
1:A:716:ASP:OD1	1:A:718:VAL:HB	2.17	0.44
1:D:402:ARG:HB3	1:D:402:ARG:NH1	2.33	0.44
1:A:344:ALA:HA	1:A:437:ALA:HB1	1.97	0.44
1:A:547:GLY:HA3	1:A:570:PHE:CE1	2.52	0.44
1:B:636:ILE:HD13	1:B:636:ILE:HA	1.55	0.44
1:C:720:ILE:HD12	1:C:720:ILE:HG23	1.42	0.44
1:A:56:GLU:HG2	1:A:57:ASN:N	2.32	0.44
1:A:192:LEU:HD12	1:A:192:LEU:N	2.32	0.44
1:A:397:ILE:HD12	1:A:405:ALA:HB3	1.99	0.44
1:C:413:GLN:NE2	6:C:1226:HOH:O	2.45	0.44
1:D:124:LEU:HB3	1:D:244:GLU:OE2	2.17	0.44
1:A:578:LEU:HD23	1:A:578:LEU:HA	1.65	0.44
1:B:872:MET:SD	1:B:872:MET:N	2.91	0.44
1:B:889:ILE:O	1:B:889:ILE:HG22	2.17	0.44
1:D:363:PHE:HZ	1:D:387:PHE:HB3	1.82	0.44
1:B:52:CYS:HB2	1:B:384:LYS:HG3	1.99	0.44
1:B:365:LYS:HB3	1:B:366:GLY:H	1.61	0.44
1:B:669:LEU:HD23	1:B:669:LEU:HA	1.81	0.44
1:C:19:ASN:OD1	1:C:964:ASN:ND2	2.48	0.44
1:C:292:ASP:O	1:C:295:GLN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:LEU:HD23	1:C:312:LEU:HA	1.72	0.44
1:C:410:ARG:HG3	1:C:411:THR:N	2.32	0.44
1:C:654:SER:HB2	1:C:665:LEU:CD1	2.47	0.44
1:D:366:GLY:HA2	1:D:390:PHE:CZ	2.53	0.44
1:A:801:SER:O	1:A:802:GLY:C	2.54	0.44
1:A:615:GLU:O	1:B:1015:ARG:HD3	2.17	0.44
1:B:849:TRP:N	1:B:849:TRP:CD1	2.85	0.44
1:C:44:ASN:HB2	1:C:45:PRO:CD	2.47	0.44
1:C:147:GLU:HG2	1:C:148:GLY:N	2.33	0.44
1:C:958:LYS:HB3	1:C:958:LYS:HE3	1.73	0.44
1:D:406:VAL:HG21	1:D:434:VAL:HG11	1.99	0.44
1:B:750:PRO:O	1:B:753:ALA:HB2	2.17	0.44
1:C:568:TRP:NE1	1:C:827:ILE:HB	2.32	0.44
1:C:583:VAL:CB	6:C:1210:HOH:O	2.64	0.44
1:A:32:LEU:HD13	1:B:485:MET:CE	2.48	0.43
1:A:366:GLY:HA3	1:A:390:PHE:CZ	2.52	0.43
1:C:73:LEU:O	1:C:77:MET:HG3	2.18	0.43
1:B:53:GLU:HG2	1:B:54:LYS:H	1.83	0.43
1:C:75:GLU:OE1	1:C:75:GLU:HA	2.18	0.43
1:C:509:ALA:O	1:C:510:GLN:C	2.56	0.43
1:D:63:LYS:HE3	1:D:128:MET:HG2	2.00	0.43
1:D:246:GLU:OE2	6:D:1207:HOH:O	2.21	0.43
1:D:607:PHE:N	1:D:607:PHE:CD1	2.86	0.43
1:D:651:MET:CE	1:D:701:ALA:HB2	2.48	0.43
1:B:579:ASP:N	1:B:579:ASP:OD1	2.50	0.43
1:B:771:ARG:O	1:B:772:PRO:C	2.56	0.43
1:C:470:GLN:HG3	1:C:477:PHE:CZ	2.53	0.43
1:D:248:MET:O	1:D:248:MET:HG2	2.15	0.43
1:A:506:TYR:CD2	1:A:506:TYR:C	2.91	0.43
1:B:239:ASP:O	1:B:909:ARG:NH2	2.52	0.43
1:B:547:GLY:HA3	1:B:570:PHE:CE1	2.54	0.43
1:C:83:ALA:O	1:C:84:ASP:C	2.57	0.43
1:C:800:GLU:HB2	6:C:1291:HOH:O	2.19	0.43
1:D:315:LYS:HD3	1:D:321:MET:HG2	2.00	0.43
1:D:737:THR:HG23	3:D:1105:FMN:H1'2	2.00	0.43
1:D:982:VAL:O	6:D:1208:HOH:O	2.21	0.43
1:A:203:ALA:HB1	1:A:214:ILE:HG21	1.99	0.43
1:B:208:ARG:HB3	1:B:522:PRO:HG2	1.99	0.43
1:B:979:LEU:HD23	1:B:979:LEU:HA	1.80	0.43
1:D:167[B]:ASN:ND2	1:D:911:PRO:HA	2.34	0.43
1:D:352:LEU:HD21	1:D:359:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:454:ILE:HG22	1:D:473:GLU:CG	2.48	0.43
1:D:699:ARG:NE	1:D:699:ARG:HA	2.34	0.43
1:A:537:MET:HG3	1:A:789:PRO:HB3	2.00	0.43
1:B:100:PHE:CZ	1:B:156:GLN:HB2	2.54	0.43
1:B:297:LEU:HD21	1:B:398:VAL:HG21	2.01	0.43
1:B:365:LYS:HG2	1:B:419:TRP:CZ2	2.53	0.43
1:C:62:ILE:HD13	1:C:379:LEU:HD22	2.01	0.43
1:C:89:LYS:HD3	1:D:41:TRP:CE2	2.53	0.43
1:C:124:LEU:HD23	1:C:240:VAL:HG13	2.01	0.43
1:C:586:VAL:O	1:C:589:ARG:HD3	2.18	0.43
1:C:734:ALA:HA	1:C:735:THR:HA	1.67	0.43
1:D:25:HIS:N	1:D:25:HIS:ND1	2.67	0.43
1:A:25:HIS:ND1	1:A:25:HIS:N	2.67	0.43
1:B:336:ILE:CD1	1:B:431:ALA:HB2	2.48	0.43
1:B:521:LEU:HA	1:B:522:PRO:HD3	1.73	0.43
1:B:999:ILE:HG21	1:B:999:ILE:HD13	1.45	0.43
1:C:6:SER:N	1:D:627:GLU:OE1	2.51	0.43
1:C:193:LEU:N	1:C:193:LEU:HD22	2.33	0.43
1:C:297:LEU:HA	1:C:301:GLN:OE1	2.18	0.43
1:C:547:GLY:O	1:C:814:GLN:HA	2.19	0.43
1:C:620:TYR:CA	1:D:1017:LEU:HD12	2.48	0.43
1:D:840:LEU:HD23	1:D:840:LEU:HA	1.81	0.43
1:B:949:ASP:OD1	1:B:951:GLU:HB2	2.19	0.43
1:C:692:ARG:CB	1:C:692:ARG:CZ	2.97	0.43
1:D:294:PHE:CD1	1:D:396:VAL:HG21	2.54	0.43
1:A:196:GLY:N	6:A:1227:HOH:O	2.47	0.43
1:A:207:ALA:HB1	1:A:251:LEU:HB3	2.00	0.43
1:A:933:GLY:HA3	1:A:937:GLU:OE1	2.19	0.43
1:B:80:LEU:HD11	1:B:142:LEU:HD21	2.00	0.43
1:B:671:SER:HA	1:B:672:PRO:HD3	1.56	0.43
1:C:242:ASN:O	1:C:246:GLU:HG2	2.18	0.43
1:C:537:MET:CG	1:C:789:PRO:HB3	2.49	0.43
1:C:858:SER:OG	1:C:867:ARG:NH2	2.49	0.43
1:D:629:LYS:HE3	1:D:629:LYS:HB3	1.77	0.43
1:A:269:ASN:OD1	1:A:269:ASN:N	2.52	0.43
1:A:533:ILE:HD13	1:A:835:LYS:HG3	2.01	0.43
1:B:131:PRO:HB3	1:B:373:VAL:HG21	2.01	0.43
1:C:137:VAL:HG13	1:C:149:SER:HB3	2.00	0.43
1:C:581:ASP:O	1:C:583:VAL:HG13	2.19	0.43
1:C:885:GLN:OE1	1:C:889:ILE:HD11	2.18	0.43
1:C:1017:LEU:HA	1:C:1017:LEU:HD23	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:888:LYS:O	1:D:888:LYS:HG2	2.19	0.43
1:A:542:PHE:HA	6:A:1201:HOH:O	2.18	0.42
1:A:991:LEU:HD23	1:A:991:LEU:HA	1.88	0.42
1:C:360:PHE:CD1	1:C:386:GLU:HB3	2.54	0.42
1:D:849:TRP:CG	1:D:854:PRO:HA	2.54	0.42
1:A:300:ASP:OD1	1:A:300:ASP:N	2.52	0.42
1:A:369:ASN:OD1	1:A:369:ASN:N	2.51	0.42
1:B:58:ASN:C	1:B:58:ASN:OD1	2.57	0.42
1:C:108:ASN:HA	1:C:852:GLN:NE2	2.34	0.42
1:C:653:LEU:HD12	1:C:653:LEU:HA	1.60	0.42
1:C:671:SER:HA	1:C:672:PRO:HD3	1.46	0.42
1:C:776:ARG:HD3	6:C:1218:HOH:O	2.18	0.42
1:D:270:THR:O	1:D:274:GLU:HG3	2.18	0.42
1:D:774:ALA:O	1:D:777:ALA:HB3	2.19	0.42
1:A:972:GLN:O	1:A:980:PRO:HA	2.19	0.42
1:B:845:GLU:CD	1:B:845:GLU:H	2.20	0.42
1:B:908:GLU:O	1:B:910:LYS:N	2.52	0.42
1:C:500:SER:O	1:C:501:TRP:C	2.57	0.42
1:A:871:LEU:HB2	1:A:872:MET:CE	2.49	0.42
1:C:364:ARG:H	1:C:364:ARG:CD	2.28	0.42
1:C:455:LYS:HG3	1:C:472:SER:CB	2.49	0.42
1:C:779:THR:HG21	1:C:932:LEU:HG	2.00	0.42
1:D:172:ARG:NH1	1:D:176:LEU:HB2	2.34	0.42
1:D:394:ARG:HA	1:D:394:ARG:HD3	1.75	0.42
1:A:231:ILE:HD13	1:A:231:ILE:HG21	1.76	0.42
1:A:612:LEU:HA	1:A:612:LEU:HD23	1.65	0.42
1:B:516:SER:OG	1:B:517:ALA:N	2.53	0.42
1:C:379:LEU:H	1:C:379:LEU:HG	1.53	0.42
1:D:348:ALA:HB1	1:D:385:CYS:SG	2.60	0.42
1:D:671:SER:HA	1:D:672:PRO:HD3	1.81	0.42
1:A:87:CYS:HB2	1:A:97:ILE:HD13	2.02	0.42
1:A:451:LEU:O	1:A:452:SER:C	2.58	0.42
1:A:691:VAL:HG21	1:A:720:ILE:HG23	2.02	0.42
1:A:949:ASP:C	1:A:949:ASP:OD1	2.57	0.42
1:B:941:ILE:HA	1:B:941:ILE:HD13	1.75	0.42
1:C:193:LEU:CD1	1:C:217:PHE:HB2	2.50	0.42
1:C:267:THR:O	1:C:268:LEU:C	2.57	0.42
1:C:268:LEU:HD23	1:C:268:LEU:HA	1.58	0.42
1:C:856:THR:HG22	1:C:857:GLU:H	1.85	0.42
1:D:336:ILE:HD13	1:D:429:LEU:HD23	2.00	0.42
1:D:402:ARG:HB3	1:D:402:ARG:HH11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:LEU:O	1:A:581:ASP:HB2	2.20	0.42
1:B:193:LEU:HD13	1:B:193:LEU:HA	1.87	0.42
1:B:941:ILE:HD12	1:B:941:ILE:HG23	1.73	0.42
1:C:22:THR:HG21	1:D:566:ALA:O	2.19	0.42
1:C:304:TYR:HB3	1:C:308:ASP:HB2	2.01	0.42
1:C:629:LYS:HD2	1:C:629:LYS:HA	1.89	0.42
1:D:647:LYS:HA	1:D:697:TRP:CE3	2.54	0.42
1:D:694:ILE:HG21	1:D:694:ILE:HD13	1.79	0.42
1:D:732:VAL:HG13	1:D:788:PHE:CE2	2.55	0.42
1:A:38:LYS:HE2	1:A:39:LYS:HZ2	1.84	0.42
1:A:866:PRO:HG3	1:A:890:ILE:CD1	2.50	0.42
1:A:989:CYS:O	1:A:990:THR:HB	2.19	0.42
1:C:79:CYS:O	1:C:81:LYS:NZ	2.53	0.42
1:C:598:PRO:HD2	1:D:77:MET:SD	2.59	0.42
1:D:610:ILE:HG13	1:D:610:ILE:O	2.20	0.42
1:D:998:ILE:HD12	1:D:998:ILE:HG23	1.78	0.42
1:A:199:SER:O	1:A:200:ILE:C	2.56	0.42
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.54	0.42
1:A:570:PHE:HB2	1:A:636:ILE:HB	2.01	0.42
1:B:403:ILE:HD12	1:B:403:ILE:HG23	1.75	0.42
1:B:426:ILE:HD13	1:B:426:ILE:HG21	1.72	0.42
1:B:550:SER:O	3:B:1105:FMN:C10	2.68	0.42
1:C:167:ASN:OD1	1:C:911:PRO:HA	2.20	0.42
1:C:412:GLU:O	1:C:412:GLU:HG2	2.19	0.42
1:A:533:ILE:O	1:A:545:PRO:HD3	2.20	0.42
1:D:784:ALA:O	1:D:786:PRO:HD3	2.20	0.42
1:D:1007:ARG:NE	1:D:1011:TYR:HB3	2.35	0.42
1:A:704:ILE:HB	1:A:705:PRO:HD2	2.02	0.41
1:C:455:LYS:HG3	1:C:472:SER:OG	2.20	0.41
1:C:465:ASP:OD1	1:C:465:ASP:C	2.59	0.41
1:C:672:PRO:HA	1:C:682:LEU:O	2.20	0.41
1:C:841:LYS:NZ	1:D:746:ALA:O	2.53	0.41
1:D:142:LEU:HD23	1:D:142:LEU:HA	1.86	0.41
1:D:689:GLU:HA	1:D:692:ARG:NH1	2.35	0.41
1:A:101:ILE:O	1:A:102:THR:C	2.58	0.41
1:A:247:LEU:HD23	1:A:247:LEU:HA	1.82	0.41
1:A:745:LYS:HE2	1:A:749:THR:OG1	2.20	0.41
1:B:220:GLN:NE2	1:B:220:GLN:HA	2.34	0.41
1:C:230:GLU:HG2	1:C:310:LEU:CB	2.50	0.41
1:C:428:HIS:H	1:D:425:GLN:NE2	2.18	0.41
1:C:1017:LEU:HD12	1:D:619:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:VAL:HG21	1:A:773:ILE:HD13	2.02	0.41
1:B:408:PHE:O	1:B:426:ILE:HA	2.20	0.41
1:C:613:ILE:HD13	1:C:642:MET:HE2	2.01	0.41
1:C:883:LEU:HD12	1:C:883:LEU:HA	1.71	0.41
1:D:650:TRP:HZ3	1:D:667:LEU:HD22	1.85	0.41
1:D:770:ILE:HG21	1:D:770:ILE:HD13	1.75	0.41
1:D:797:ASP:N	1:D:797:ASP:OD1	2.51	0.41
1:D:834:LEU:HD12	1:D:834:LEU:HA	1.78	0.41
1:A:518:LYS:HD2	1:A:519:PRO:O	2.21	0.41
1:B:64:HIS:HE1	1:B:382:GLU:OE2	2.03	0.41
1:D:331:ILE:HD13	1:D:331:ILE:HA	1.64	0.41
1:D:861:LYS:HE2	1:D:863:LYS:HE3	2.01	0.41
1:A:977:THR:O	1:A:978:HIS:HB2	2.20	0.41
1:B:310:LEU:N	1:B:311:PRO:CD	2.84	0.41
1:B:348:ALA:HB2	1:B:361:LEU:HD21	2.03	0.41
1:B:518:LYS:O	1:B:520:GLU:HG2	2.21	0.41
1:B:877:PRO:HD2	1:B:882:TYR:CB	2.50	0.41
1:C:550:SER:O	3:C:1105:FMN:C10	2.69	0.41
1:D:189:LYS:HB3	1:D:276:TYR:CD1	2.55	0.41
1:D:465:ASP:OD1	1:D:465:ASP:C	2.58	0.41
1:D:843:ILE:HD13	1:D:843:ILE:HA	1.84	0.41
1:D:974:ASP:OD1	1:D:974:ASP:C	2.58	0.41
1:A:233:GLN:O	1:A:233:GLN:HG3	2.20	0.41
1:B:993:LEU:HD23	1:B:993:LEU:C	2.40	0.41
1:D:410[A]:ARG:CZ	1:D:412:GLU:OE1	2.69	0.41
1:A:444:ASP:HA	1:A:445:PRO:HD3	1.94	0.41
1:A:521:LEU:HB2	1:B:26:ALA:HB3	2.01	0.41
1:C:211:TYR:HB2	1:C:214:ILE:HD11	2.02	0.41
1:C:620:TYR:HA	1:D:1017:LEU:HD12	2.02	0.41
1:D:389:PRO:HB2	1:D:390:PHE:CD2	2.56	0.41
1:D:1007:ARG:CZ	1:D:1011:TYR:HB3	2.50	0.41
1:A:193:LEU:HD13	1:A:193:LEU:HA	1.93	0.41
1:A:465:ASP:OD1	1:A:465:ASP:C	2.59	0.41
1:A:877:PRO:HG2	1:A:882:TYR:CD2	2.56	0.41
1:B:391:LEU:HD23	1:B:391:LEU:HA	1.94	0.41
1:B:867:ARG:CA	1:B:872:MET:CE	2.97	0.41
1:B:875:LYS:C	1:B:876:LEU:HD23	2.38	0.41
1:B:1012:GLU:OE2	1:B:1014:LYS:HE3	2.21	0.41
1:C:345:PHE:HB3	1:C:376:GLU:HG3	2.03	0.41
1:C:681:GLY:HA3	1:C:686:GLN:HB2	2.03	0.41
1:D:46:ASP:HB3	1:D:48:ASN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:ASP:HB3	1:D:415:GLU:OE2	2.20	0.41
1:D:987:THR:HG22	1:D:1014:LYS:HZ2	1.85	0.41
1:A:223:VAL:CG2	1:A:245[A]:ILE:HD13	2.49	0.41
1:A:229:SER:O	1:A:311:PRO:HA	2.21	0.41
1:A:255:ILE:HG21	1:A:255:ILE:HD13	1.69	0.41
1:A:734:ALA:HA	1:A:735:THR:HA	1.75	0.41
1:A:823:ASP:OD1	1:A:825:THR:OG1	2.31	0.41
1:A:866:PRO:HG3	1:A:890:ILE:HD11	2.02	0.41
1:B:32:LEU:HA	1:B:32:LEU:HD12	1.93	0.41
1:B:125:THR:OG1	1:B:244:GLU:OE2	2.33	0.41
1:B:827:ILE:HA	1:B:827:ILE:HD12	1.79	0.41
1:C:192:LEU:HD12	1:C:192:LEU:N	2.35	0.41
1:C:408:PHE:CE1	1:C:429:LEU:HD23	2.56	0.41
1:C:535:VAL:HG22	1:C:536:GLU:H	1.85	0.41
1:D:773:ILE:HG21	1:D:773:ILE:HD13	1.93	0.41
1:D:857:GLU:O	1:D:859:HIS:N	2.54	0.41
1:D:871:LEU:HD21	1:D:886:ARG:NH1	2.36	0.41
1:A:394:ARG:HG3	1:A:394:ARG:NH1	2.35	0.41
1:C:193:LEU:HD13	1:C:193:LEU:HA	1.85	0.41
1:C:281:ILE:HG23	1:C:281:ILE:HD12	1.80	0.41
1:C:606:SER:HB2	1:C:766:SER:O	2.19	0.41
1:C:840:LEU:HD23	1:C:840:LEU:HA	1.64	0.41
1:C:889:ILE:O	1:C:889:ILE:HG22	2.21	0.41
1:D:407:GLN:HA	1:D:427:VAL:O	2.21	0.41
1:A:946:ALA:HB1	1:A:1002:ILE:CG2	2.51	0.40
1:C:837:LEU:O	1:C:841:LYS:HG3	2.21	0.40
1:D:454:ILE:HA	1:D:472:SER:OG	2.21	0.40
1:D:734:ALA:HA	1:D:735:THR:HA	1.80	0.40
1:B:168:ILE:HD13	1:B:168:ILE:HG21	1.78	0.40
1:B:358:ARG:NE	1:B:360:PHE:CZ	2.89	0.40
1:C:543:ILE:HD11	1:C:569:GLY:HA2	2.03	0.40
1:D:235:ARG:NH1	4:D:1106:FAD:O4	2.38	0.40
1:D:454:ILE:HG22	1:D:473:GLU:HB2	2.02	0.40
1:D:531:VAL:HG21	1:D:839:TYR:HB2	2.02	0.40
1:D:590:ILE:HG21	1:D:590:ILE:HD13	1.78	0.40
1:D:709:LYS:HG3	1:D:733:THR:HB	2.03	0.40
1:A:331:ILE:HG22	1:A:331:ILE:O	2.21	0.40
1:B:483:VAL:O	1:B:483:VAL:CG1	2.69	0.40
1:B:556:SER:HB2	1:B:559:MET:CE	2.51	0.40
1:B:991:LEU:HA	1:B:991:LEU:HD23	1.90	0.40
1:C:328:LEU:HD23	1:C:328:LEU:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:PRO:HB2	1:D:32:LEU:HD13	2.03	0.40
1:C:876:LEU:O	1:C:886:ARG:NH1	2.48	0.40
1:D:4:VAL:H	1:D:4:VAL:HG23	1.63	0.40
1:A:178:SER:HB3	1:A:181:LYS:HG2	2.04	0.40
1:A:352:LEU:HD23	1:A:352:LEU:HA	1.73	0.40
1:D:126:CYS:O	1:D:127:GLY:C	2.60	0.40
1:A:89:LYS:HD2	1:B:41:TRP:CE2	2.56	0.40
1:A:196:GLY:CA	6:A:1227:HOH:O	2.69	0.40
1:A:699:ARG:NH1	6:A:1202:HOH:O	2.46	0.40
1:A:858:SER:OG	1:A:867:ARG:NH2	2.55	0.40
1:B:807:HIS:O	1:B:926:GLY:HA2	2.22	0.40
1:C:2:ALA:HB1	1:D:623:GLN:HE22	1.87	0.40
1:C:410:ARG:O	1:C:421:GLU:HA	2.21	0.40
1:C:718:VAL:CG2	1:C:780:THR:HG23	2.46	0.40
1:D:861:LYS:HB3	1:D:863:LYS:HE3	2.04	0.40
1:D:910:LYS:O	1:D:910:LYS:HG3	2.21	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	988/1025 (96%)	895 (91%)	80 (8%)	13 (1%)	12	7
1	B	1000/1025 (98%)	904 (90%)	83 (8%)	13 (1%)	12	7
1	C	998/1025 (97%)	913 (92%)	70 (7%)	15 (2%)	10	5
1	D	989/1025 (96%)	892 (90%)	85 (9%)	12 (1%)	13	8
All	All	3975/4100 (97%)	3604 (91%)	318 (8%)	53 (1%)	12	7

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	PRO
1	A	415	GLU
1	B	875	LYS
1	C	52	CYS
1	C	176	LEU
1	D	319	ALA
1	D	871	LEU
1	A	869	ALA
1	B	327	PRO
1	B	400	GLY
1	B	422	ASP
1	B	713	ASN
1	B	873	GLY
1	B	909	ARG
1	C	580	LYS
1	C	645	TYR
1	C	871	LEU
1	C	875	LYS
1	D	50	PHE
1	D	342	ASP
1	A	3	PRO
1	A	289	LYS
1	A	374	PRO
1	A	822	GLN
1	B	672	PRO
1	C	321	MET
1	C	415	GLU
1	D	320	GLY
1	D	538	ALA
1	D	858	SER
1	A	551	ALA
1	A	875	LYS
1	B	50	PHE
1	B	516	SER
1	C	54	LYS
1	C	990	THR
1	D	794	GLY
1	D	873	GLY
1	A	373	VAL
1	A	390	PHE
1	A	444	ASP
1	B	458	ARG
1	C	374	PRO

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Mol	Chain	Res	Type
1	D	415	GLU
1	D	990	THR
1	A	990	THR
1	B	149	SER
1	C	3	PRO
1	D	331	ILE
1	B	374	PRO
1	C	865	VAL
1	C	123	GLY
1	C	482	ILE

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	834/854 (98%)	801 (96%)	33 (4%)	31	31
1	B	842/854 (99%)	815 (97%)	27 (3%)	39	40
1	C	839/854 (98%)	807 (96%)	32 (4%)	33	33
1	D	834/854 (98%)	792 (95%)	42 (5%)	24	22
All	All	3349/3416 (98%)	3215 (96%)	134 (4%)	32	31

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	42	LYS
1	A	60	ASP
1	A	79	CYS
1	A	95	LEU
1	A	100	PHE
1	A	175	CYS
1	A	179	GLN
1	A	272	LYS
1	A	364	ARG
1	A	369	ASN

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Mol	Chain	Res	Type
1	A	375	GLU
1	A	392	SER
1	A	416	THR
1	A	424	ASP
1	A	436	SER
1	A	460	ASP
1	A	465	ASP
1	A	487	ASN
1	A	514	SER
1	A	518	LYS
1	A	541	LYS
1	A	644	SER
1	A	682	LEU
1	A	700	GLN
1	A	780	THR
1	A	793	THR
1	A	800	GLU
1	A	856	THR
1	A	872	MET
1	A	947[A]	VAL
1	A	947[B]	VAL
1	A	1008	THR
1	B	11	ASP
1	B	24	SER
1	B	46	ASP
1	B	100	PHE
1	B	119	ASP
1	B	233	GLN
1	B	363	PHE
1	B	364	ARG
1	B	375	GLU
1	B	399	LYS
1	B	432	ASP
1	B	460	ASP
1	B	644	SER
1	B	660	SER
1	B	673	HIS
1	B	703	GLN
1	B	712	PRO
1	B	793	THR
1	B	874	LYS
1	B	875	LYS

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Mol	Chain	Res	Type
1	B	887	LYS
1	B	909	ARG
1	B	932[A]	LEU
1	B	932[B]	LEU
1	B	963	CYS
1	B	1003	ARG
1	B	1012	GLU
1	C	15	ILE
1	C	28	LEU
1	C	39	LYS
1	C	60	ASP
1	C	136	CYS
1	C	167	ASN
1	C	175	CYS
1	C	179	GLN
1	C	180	GLU
1	C	321	MET
1	C	322	CYS
1	C	357	ARG
1	C	364	ARG
1	C	407	GLN
1	C	412	GLU
1	C	432	ASP
1	C	440	SER
1	C	458	ARG
1	C	514	SER
1	C	711	THR
1	C	780	THR
1	C	793	THR
1	C	800	GLU
1	C	808	SER
1	C	844	GLU
1	C	874	LYS
1	C	885	GLN
1	C	888	LYS
1	C	895	MET
1	C	910	LYS
1	C	927	LYS
1	C	985	THR
1	D	18	LEU
1	D	21	ARG
1	D	46	ASP

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Mol	Chain	Res	Type
1	D	57	ASN
1	D	58	ASN
1	D	60	ASP
1	D	129	VAL
1	D	136	CYS
1	D	179	GLN
1	D	184	GLU
1	D	239	ASP
1	D	330	SER
1	D	331	ILE
1	D	343	THR
1	D	346	ASP
1	D	358	ARG
1	D	363	PHE
1	D	367	PHE
1	D	392	SER
1	D	395	LYS
1	D	399	LYS
1	D	407	GLN
1	D	414	ASP
1	D	415	GLU
1	D	423	GLU
1	D	424	ASP
1	D	436	SER
1	D	460	ASP
1	D	465	ASP
1	D	505	LYS
1	D	515	VAL
1	D	648	ASN
1	D	700	GLN
1	D	711	THR
1	D	793	THR
1	D	856	THR
1	D	874	LYS
1	D	932[A]	LEU
1	D	932[B]	LEU
1	D	1000	ASP
1	D	1009	THR
1	D	1011	TYR

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

Mol	Chain	Res	Type
1	A	299	GLN
1	B	64	HIS
1	B	220	GLN
1	B	233	GLN
1	B	425	GLN
1	C	57	ASN
1	C	269	ASN
1	C	413	GLN
1	C	508	GLN
1	D	23	GLN
1	D	57	ASN
1	D	179	GLN
1	D	220	GLN
1	D	407	GLN
1	D	413	GLN
1	D	498	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	TDR	B	1107	-	9,9,9	1.49	2 (22%)	12,12,12	1.43	1 (8%)
2	SF4	A	1103	1	0,12,12	-	-	-		
2	SF4	C	1103	1	0,12,12	-	-	-		
2	SF4	A	1104	1	0,12,12	-	-	-		
4	FAD	A	1106	-	53,58,58	0.96	3 (5%)	68,89,89	1.22	9 (13%)
2	SF4	A	1102	1	0,12,12	-	-	-		
3	FMN	D	1105	-	33,33,33	1.97	11 (33%)	48,50,50	2.26	17 (35%)
5	TDR	D	1107	-	9,9,9	2.57	5 (55%)	12,12,12	1.70	2 (16%)
2	SF4	C	1102	1	0,12,12	-	-	-		
5	TDR	A	1107	-	9,9,9	1.01	1 (11%)	12,12,12	1.58	2 (16%)
2	SF4	B	1103	1	0,12,12	-	-	-		
5	TDR	C	1107	-	9,9,9	1.37	1 (11%)	12,12,12	2.61	4 (33%)
3	FMN	C	1105	-	33,33,33	1.75	6 (18%)	48,50,50	2.27	18 (37%)
2	SF4	B	1104	1	0,12,12	-	-	-		
2	SF4	D	1102	1	0,12,12	-	-	-		
2	SF4	D	1104	1	0,12,12	-	-	-		
4	FAD	D	1106	-	53,58,58	0.98	4 (7%)	68,89,89	0.95	5 (7%)
3	FMN	B	1105	-	33,33,33	1.46	6 (18%)	48,50,50	2.38	20 (41%)
2	SF4	C	1101	1	0,12,12	-	-	-		
2	SF4	B	1101	1	0,12,12	-	-	-		
2	SF4	C	1104	1	0,12,12	-	-	-		
4	FAD	C	1106	-	53,58,58	1.15	2 (3%)	68,89,89	0.80	1 (1%)
3	FMN	A	1105	-	33,33,33	1.87	7 (21%)	48,50,50	2.39	17 (35%)
2	SF4	A	1101	1	0,12,12	-	-	-		
2	SF4	B	1102	1	0,12,12	-	-	-		
4	FAD	B	1106	-	53,58,58	1.14	3 (5%)	68,89,89	1.35	7 (10%)
2	SF4	D	1101	1	0,12,12	-	-	-		
2	SF4	D	1103	1	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TDR	B	1107	-	-	-	0/1/1/1
2	SF4	A	1103	1	-	-	0/6/5/5
2	SF4	C	1103	1	-	-	0/6/5/5
2	SF4	A	1104	1	-	-	0/6/5/5
4	FAD	A	1106	-	-	3/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	A	1102	1	-	-	0/6/5/5
3	FMN	D	1105	-	-	4/18/18/18	0/3/3/3
5	TDR	D	1107	-	-	-	0/1/1/1
2	SF4	C	1102	1	-	-	0/6/5/5
5	TDR	A	1107	-	-	-	0/1/1/1
2	SF4	B	1103	1	-	-	0/6/5/5
5	TDR	C	1107	-	-	-	0/1/1/1
3	FMN	C	1105	-	-	2/18/18/18	0/3/3/3
2	SF4	B	1104	1	-	-	0/6/5/5
2	SF4	D	1102	1	-	-	0/6/5/5
2	SF4	D	1104	1	-	-	0/6/5/5
4	FAD	D	1106	-	-	1/30/50/50	0/6/6/6
3	FMN	B	1105	-	-	2/18/18/18	0/3/3/3
2	SF4	C	1101	1	-	-	0/6/5/5
2	SF4	B	1101	1	-	-	0/6/5/5
2	SF4	C	1104	1	-	-	0/6/5/5
4	FAD	C	1106	-	-	1/30/50/50	0/6/6/6
3	FMN	A	1105	-	-	1/18/18/18	0/3/3/3
2	SF4	A	1101	1	-	-	0/6/5/5
2	SF4	B	1102	1	-	-	0/6/5/5
4	FAD	B	1106	-	-	1/30/50/50	0/6/6/6
2	SF4	D	1101	1	-	-	0/6/5/5
2	SF4	D	1103	1	-	-	0/6/5/5

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1105	FMN	C4A-N5	5.99	1.42	1.30
4	C	1106	FAD	C10-N1	-5.77	1.21	1.33
3	C	1105	FMN	C4A-N5	5.25	1.41	1.30
5	D	1107	TDR	C2-N1	4.61	1.43	1.36
3	D	1105	FMN	C5'-C4'	4.21	1.57	1.51
4	B	1106	FAD	C10-N1	3.85	1.41	1.33
5	D	1107	TDR	C4-C5	3.75	1.51	1.44
3	C	1105	FMN	C6-C5A	3.72	1.45	1.40
3	D	1105	FMN	O4-C4	3.71	1.30	1.23
3	D	1105	FMN	C10-N10	3.66	1.45	1.37
3	A	1105	FMN	C10-N1	3.54	1.40	1.33
4	B	1106	FAD	C4-N3	3.48	1.45	1.38
3	B	1105	FMN	C4A-C10	-3.43	1.34	1.44
3	D	1105	FMN	C4A-N5	3.42	1.37	1.30
3	A	1105	FMN	C5A-N5	3.42	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1106	FAD	PA-O5B	-3.40	1.45	1.59
5	B	1107	TDR	C2-N1	3.24	1.41	1.36
3	A	1105	FMN	C6-C7	-3.19	1.34	1.39
3	C	1105	FMN	C10-N1	3.18	1.39	1.33
3	D	1105	FMN	C4'-C3'	-3.05	1.47	1.53
3	D	1105	FMN	C9-C9A	2.93	1.44	1.39
5	D	1107	TDR	C6-N1	2.90	1.41	1.36
4	A	1106	FAD	C4-N3	2.88	1.44	1.38
3	B	1105	FMN	O4'-C4'	-2.73	1.37	1.43
3	C	1105	FMN	P-O1P	2.72	1.59	1.50
3	A	1105	FMN	C4'-C3'	2.71	1.58	1.53
5	D	1107	TDR	C6-C5	2.61	1.38	1.34
5	C	1107	TDR	C6-N1	2.59	1.40	1.36
3	D	1105	FMN	C10-N1	2.58	1.38	1.33
4	D	1106	FAD	C8A-N7A	-2.54	1.30	1.34
3	B	1105	FMN	C9-C8	2.54	1.43	1.39
3	C	1105	FMN	C5'-C4'	2.53	1.55	1.51
3	C	1105	FMN	O4-C4	2.51	1.28	1.23
5	A	1107	TDR	C2-N1	2.47	1.40	1.36
4	B	1106	FAD	C4A-N3A	-2.43	1.32	1.35
4	A	1106	FAD	C8A-N7A	-2.43	1.30	1.34
3	D	1105	FMN	O2-C2	-2.42	1.19	1.24
5	B	1107	TDR	C6-N1	2.42	1.40	1.36
3	D	1105	FMN	P-O1P	2.31	1.58	1.50
3	B	1105	FMN	C10-N1	2.30	1.37	1.33
4	D	1106	FAD	O4B-C1B	2.25	1.44	1.41
5	D	1107	TDR	CM5-C5	2.24	1.56	1.50
3	A	1105	FMN	C9-C9A	2.24	1.43	1.39
3	A	1105	FMN	P-O1P	2.23	1.57	1.50
3	D	1105	FMN	C5A-N5	-2.23	1.35	1.39
3	B	1105	FMN	C8M-C8	2.18	1.55	1.51
3	D	1105	FMN	C1'-C2'	2.16	1.55	1.52
4	A	1106	FAD	C10-N1	2.16	1.37	1.33
3	B	1105	FMN	C4A-N5	2.14	1.34	1.30
4	D	1106	FAD	C4A-N3A	-2.11	1.32	1.35
4	C	1106	FAD	C8A-N7A	-2.03	1.31	1.34

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1107	TDR	CM5-C5-C4	-6.48	111.63	118.77
3	C	1105	FMN	C4A-C10-N10	5.72	124.85	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1105	FMN	C4A-C10-N10	5.57	124.62	116.48
3	A	1105	FMN	C10-N1-C2	5.33	127.56	116.90
3	D	1105	FMN	C4-C4A-C10	5.23	125.58	116.79
3	A	1105	FMN	C4-N3-C2	-5.19	116.05	125.64
3	D	1105	FMN	C10-C4A-N5	-5.10	114.04	124.86
4	B	1106	FAD	O3'-C3'-C2'	5.07	121.05	108.81
3	A	1105	FMN	C4A-C4-N3	4.90	125.63	113.19
3	C	1105	FMN	C1'-N10-C9A	4.88	128.65	120.51
3	D	1105	FMN	C4A-C10-N1	-4.83	113.53	124.73
3	B	1105	FMN	C9A-C5A-N5	-4.63	117.40	122.43
3	B	1105	FMN	C4-N3-C2	-4.63	117.09	125.64
3	C	1105	FMN	C4'-C3'-C2'	-4.57	103.86	113.36
3	C	1105	FMN	C5A-C9A-N10	4.56	122.66	117.95
3	B	1105	FMN	C4A-C10-N10	4.54	123.12	116.48
3	A	1105	FMN	C4A-C10-N1	-4.48	114.33	124.73
4	B	1106	FAD	O2B-C2B-C1B	-4.40	94.60	110.85
3	B	1105	FMN	C4A-C10-N1	-4.35	114.63	124.73
3	A	1105	FMN	C4A-C10-N10	4.23	122.66	116.48
5	D	1107	TDR	C5-C4-N3	4.19	118.89	115.31
4	B	1106	FAD	O4'-C4'-C5'	-4.16	100.57	109.92
5	C	1107	TDR	CM5-C5-C6	4.06	127.65	123.16
3	A	1105	FMN	C8M-C8-C9	4.03	126.95	119.49
4	A	1106	FAD	O2'-C2'-C3'	-3.98	99.42	109.10
3	B	1105	FMN	C5A-N5-C4A	3.91	124.58	118.07
3	A	1105	FMN	C4-C4A-N5	3.89	123.77	118.23
5	A	1107	TDR	C6-N1-C2	-3.85	118.74	122.68
3	B	1105	FMN	C10-N1-C2	3.83	124.55	116.90
3	B	1105	FMN	C6-C5A-C9A	3.78	124.29	118.94
3	B	1105	FMN	O4'-C4'-C5'	-3.72	101.56	109.92
4	B	1106	FAD	O2'-C2'-C1'	-3.68	100.90	109.80
3	A	1105	FMN	O3P-P-O2P	-3.67	93.62	107.64
3	A	1105	FMN	O4-C4-C4A	-3.65	116.92	126.60
3	B	1105	FMN	C4-C4A-C10	3.61	122.85	116.79
4	A	1106	FAD	O2P-P-O1P	3.55	129.80	112.24
3	C	1105	FMN	C9A-N10-C10	-3.55	115.24	120.77
3	B	1105	FMN	C10-C4A-N5	-3.54	117.35	124.86
3	C	1105	FMN	C9A-C9-C8	3.52	126.38	119.30
3	D	1105	FMN	C5A-N5-C4A	3.46	123.83	118.07
3	B	1105	FMN	C4A-C4-N3	3.40	121.82	113.19
3	D	1105	FMN	C4-N3-C2	-3.34	119.47	125.64
5	B	1107	TDR	O2-C2-N1	3.28	126.41	122.79
3	C	1105	FMN	C4-N3-C2	-3.27	119.59	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1105	FMN	C10-N1-C2	3.26	123.43	116.90
3	C	1105	FMN	C10-C4A-N5	-3.26	117.94	124.86
3	D	1105	FMN	C9-C9A-N10	3.25	126.23	121.84
5	C	1107	TDR	O4-C4-C5	-3.24	121.14	124.90
3	B	1105	FMN	C9-C8-C7	3.22	124.29	119.67
3	A	1105	FMN	C10-C4A-N5	-3.19	118.10	124.86
3	B	1105	FMN	O2'-C2'-C3'	3.12	116.69	109.10
3	C	1105	FMN	C4A-C10-N1	-3.11	117.51	124.73
3	C	1105	FMN	C9-C9A-C5A	-3.01	114.42	120.11
4	D	1106	FAD	O2'-C2'-C3'	-3.01	101.78	109.10
3	A	1105	FMN	C5A-C6-C7	3.00	126.21	120.71
4	A	1106	FAD	O2A-PA-O5B	-2.96	93.98	107.75
3	D	1105	FMN	C9A-N10-C10	-2.94	116.18	120.77
3	C	1105	FMN	C4-C4A-C10	2.93	121.72	116.79
4	B	1106	FAD	O2'-C2'-C3'	-2.91	102.02	109.10
3	D	1105	FMN	O4-C4-N3	-2.91	114.54	120.12
3	D	1105	FMN	C9-C9A-C5A	-2.88	114.67	120.11
3	C	1105	FMN	C9A-C5A-N5	-2.88	119.30	122.43
3	B	1105	FMN	O3P-P-O1P	2.87	121.90	110.68
3	B	1105	FMN	O4-C4-C4A	-2.83	119.08	126.60
4	B	1106	FAD	C5A-C6A-N6A	2.79	124.59	120.35
3	C	1105	FMN	O3'-C3'-C2'	2.76	115.49	108.81
3	A	1105	FMN	C9-C9A-N10	2.73	125.53	121.84
4	A	1106	FAD	O3'-C3'-C2'	-2.67	102.37	108.81
5	A	1107	TDR	C5-C6-N1	2.67	125.65	122.43
3	A	1105	FMN	O3'-C3'-C2'	-2.65	102.40	108.81
3	A	1105	FMN	C6-C5A-C9A	-2.56	115.31	118.94
3	B	1105	FMN	O3P-P-O5'	-2.56	99.92	106.73
3	A	1105	FMN	O5'-P-O1P	2.55	113.64	106.47
3	B	1105	FMN	O2P-P-O1P	-2.52	100.83	110.68
5	C	1107	TDR	C5-C6-N1	-2.51	119.40	122.43
3	A	1105	FMN	C8M-C8-C7	-2.50	115.61	120.74
3	D	1105	FMN	O5'-C5'-C4'	-2.49	102.71	109.36
3	D	1105	FMN	C8M-C8-C7	-2.48	115.64	120.74
4	D	1106	FAD	O3'-C3'-C2'	-2.47	102.85	108.81
4	A	1106	FAD	O5B-PA-O1A	2.44	118.59	109.07
3	D	1105	FMN	C8M-C8-C9	2.44	124.00	119.49
4	B	1106	FAD	O3B-C3B-C4B	-2.43	104.02	111.05
4	D	1106	FAD	C5A-C6A-N6A	2.34	123.91	120.35
3	A	1105	FMN	O2P-P-O1P	2.31	119.73	110.68
4	A	1106	FAD	C1B-N9A-C4A	2.29	130.67	126.64
3	C	1105	FMN	P-O5'-C5'	-2.29	111.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1105	FMN	O4'-C4'-C3'	-2.29	103.53	109.10
3	C	1105	FMN	C6-C5A-C9A	2.26	122.14	118.94
3	C	1105	FMN	C9-C8-C7	-2.25	116.44	119.67
4	A	1106	FAD	C5A-C6A-N6A	2.23	123.74	120.35
4	A	1106	FAD	C4'-C3'-C2'	2.19	117.91	113.36
3	C	1105	FMN	O5'-P-O1P	2.18	112.60	106.47
3	B	1105	FMN	O3P-P-O2P	2.18	115.95	107.64
5	D	1107	TDR	C5-C6-N1	-2.13	119.86	122.43
4	C	1106	FAD	P-O3P-PA	2.12	140.10	132.83
3	B	1105	FMN	O2-C2-N3	2.12	122.76	118.65
3	D	1105	FMN	O3'-C3'-C4'	-2.09	103.77	108.81
3	B	1105	FMN	O2-C2-N1	-2.09	118.37	121.83
4	D	1106	FAD	O2A-PA-O1A	2.08	122.55	112.24
3	D	1105	FMN	O3P-P-O2P	-2.08	99.69	107.64
4	A	1106	FAD	O5B-C5B-C4B	2.03	116.00	108.99
3	C	1105	FMN	C4A-C4-N3	2.02	118.31	113.19
4	D	1106	FAD	O5B-PA-O1A	-2.02	101.19	109.07

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1105	FMN	C5'-O5'-P-O3P
3	C	1105	FMN	C2'-C3'-C4'-O4'
4	A	1106	FAD	P-O3P-PA-O5B
4	A	1106	FAD	C5B-O5B-PA-O3P
4	C	1106	FAD	O4B-C4B-C5B-O5B
3	A	1105	FMN	C4'-C5'-O5'-P
3	B	1105	FMN	C4'-C5'-O5'-P
3	C	1105	FMN	C4'-C5'-O5'-P
3	D	1105	FMN	C5'-O5'-P-O1P
4	B	1106	FAD	O4B-C4B-C5B-O5B
3	D	1105	FMN	C4'-C5'-O5'-P
4	A	1106	FAD	O4B-C4B-C5B-O5B
4	D	1106	FAD	O4B-C4B-C5B-O5B
3	B	1105	FMN	O3'-C3'-C4'-C5'
3	D	1105	FMN	O3'-C3'-C4'-C5'

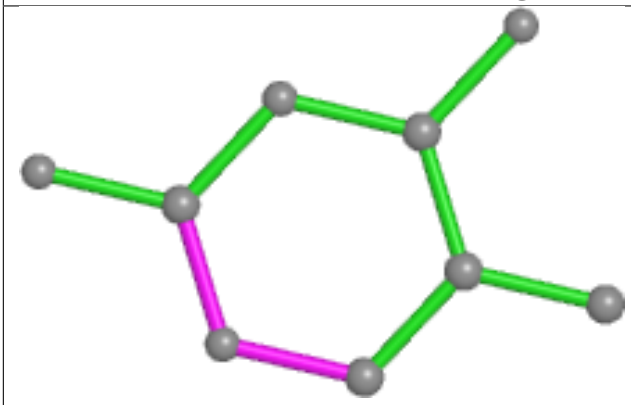
There are no ring outliers.

15 monomers are involved in 22 short contacts:

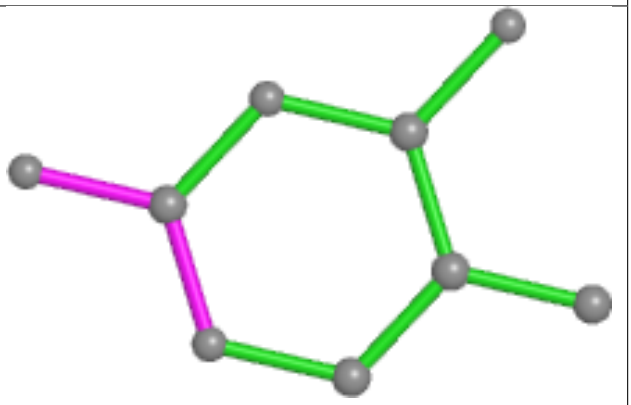
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1103	SF4	2	0
4	A	1106	FAD	2	0
2	A	1102	SF4	1	0
3	D	1105	FMN	1	0
2	C	1102	SF4	3	0
5	A	1107	TDR	1	0
2	B	1103	SF4	1	0
3	C	1105	FMN	1	0
4	D	1106	FAD	2	0
3	B	1105	FMN	1	0
2	B	1101	SF4	1	0
4	C	1106	FAD	1	0
3	A	1105	FMN	1	0
4	B	1106	FAD	3	0
2	D	1101	SF4	1	0

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.

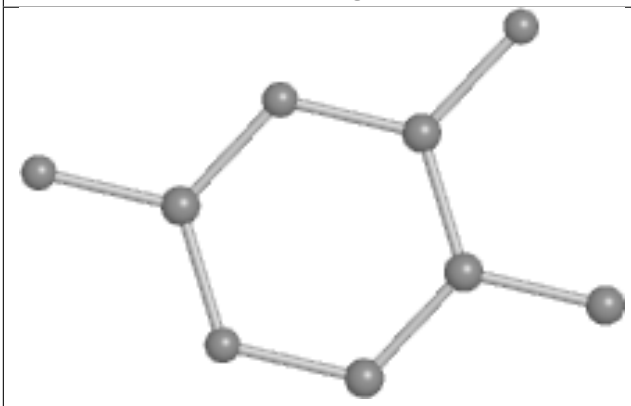
Ligand TDR B 1107



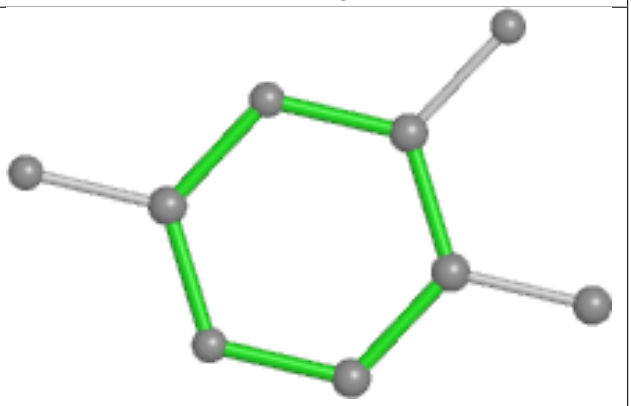
Bond lengths



Bond angles

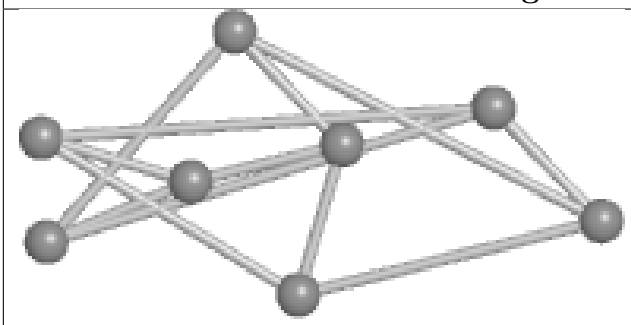


Torsions

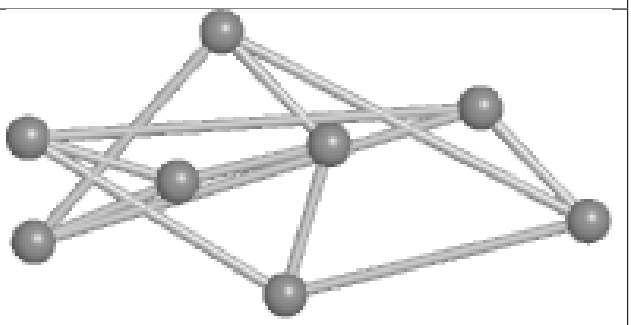


Rings

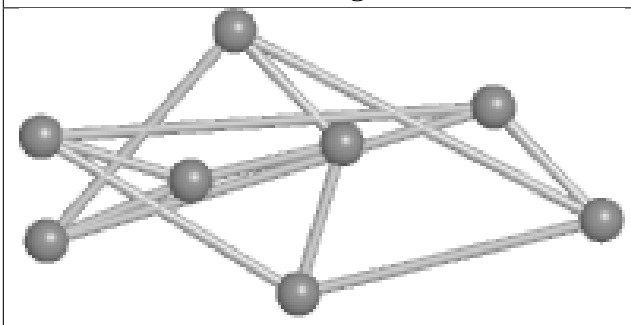
Ligand SF4 A 1103



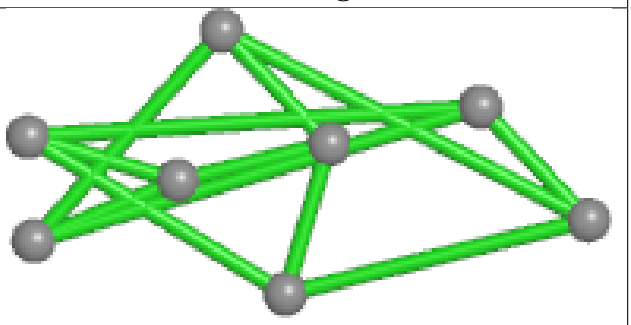
Bond lengths



Bond angles

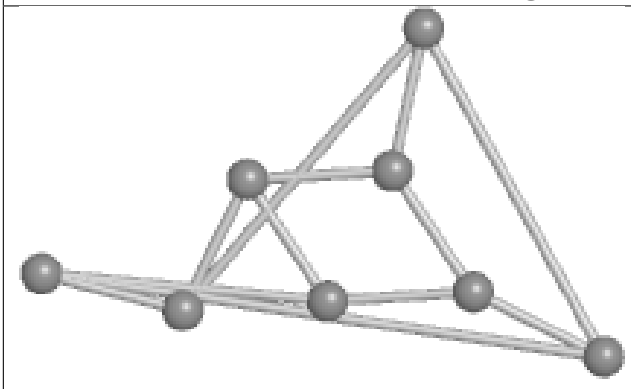


Torsions

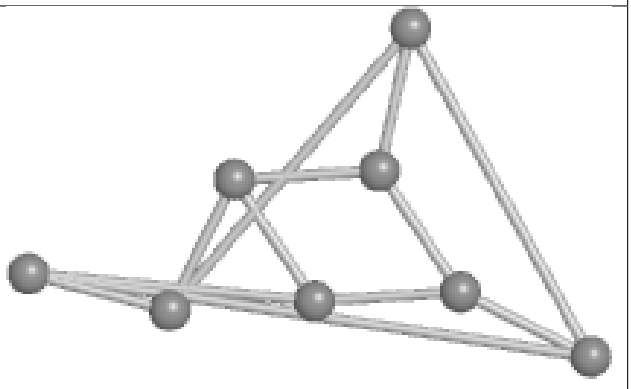


Rings

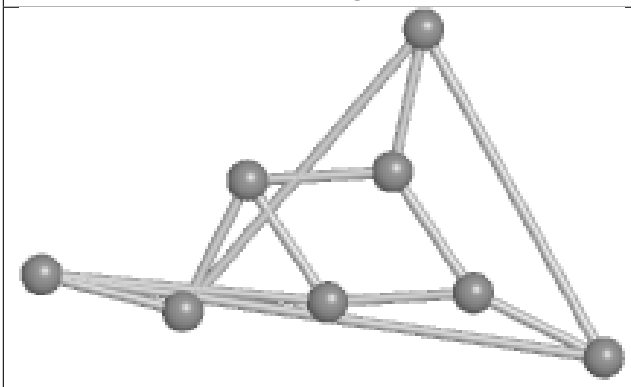
Ligand SF4 C 1103



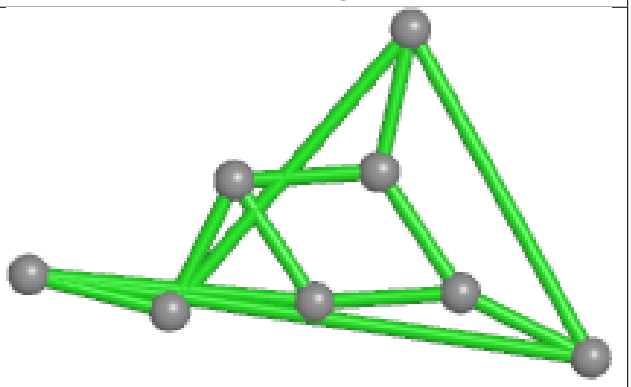
Bond lengths



Bond angles

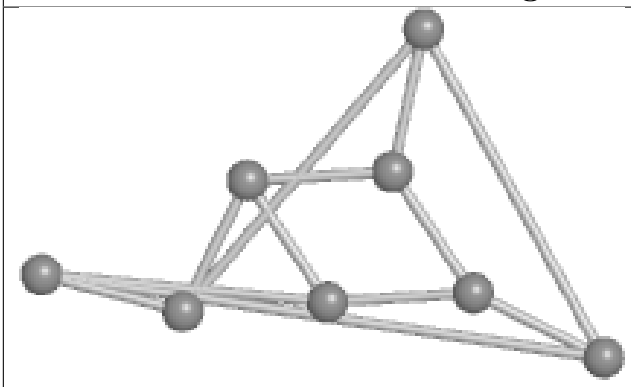


Torsions

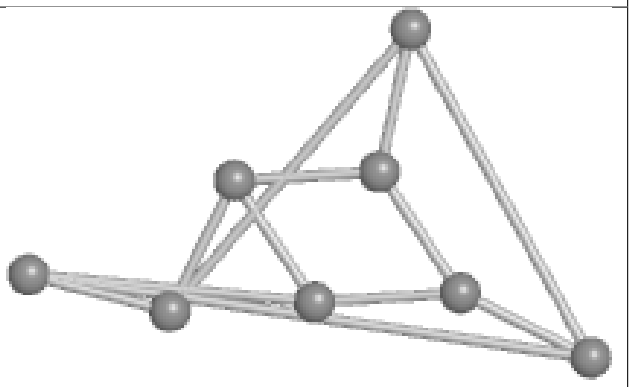


Rings

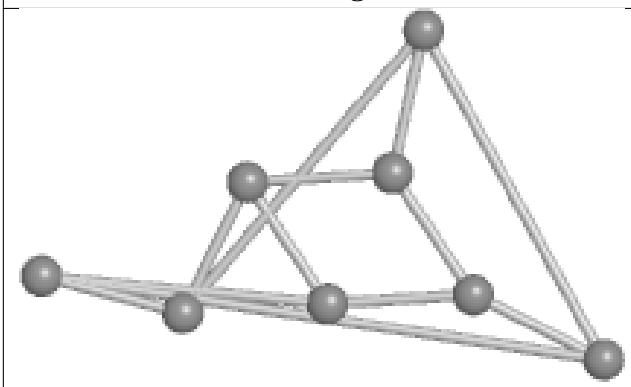
Ligand SF4 A 1104



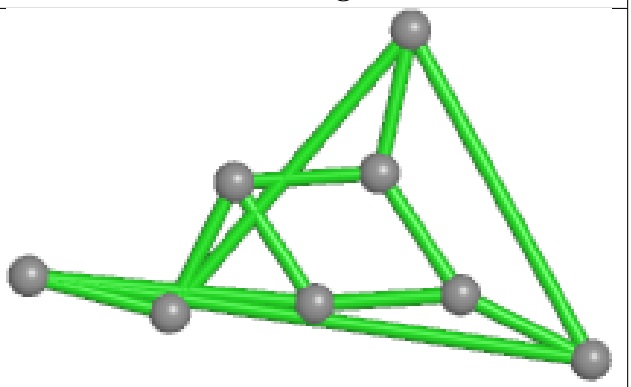
Bond lengths



Bond angles

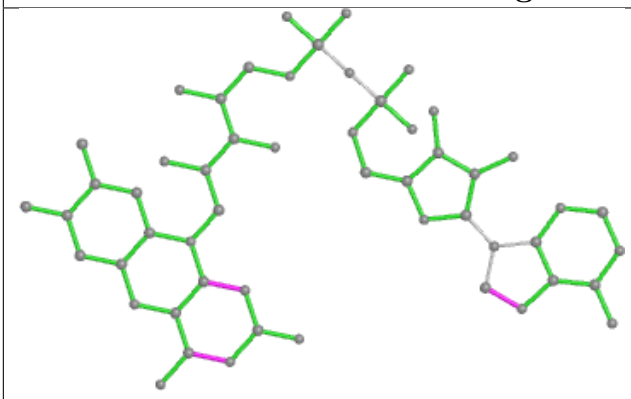


Torsions

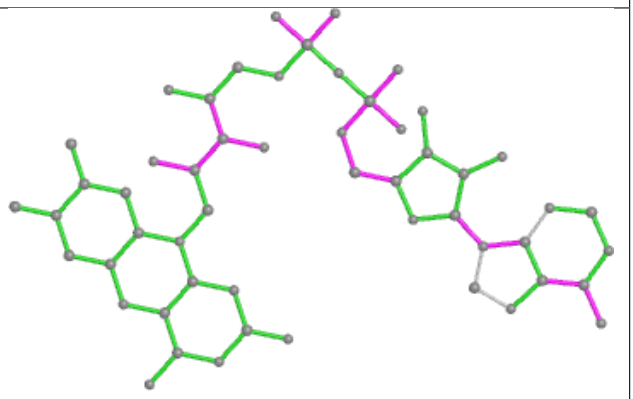


Rings

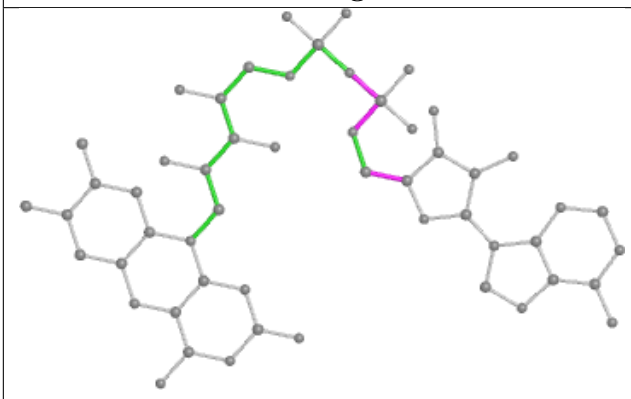
Ligand FAD A 1106



Bond lengths



Bond angles



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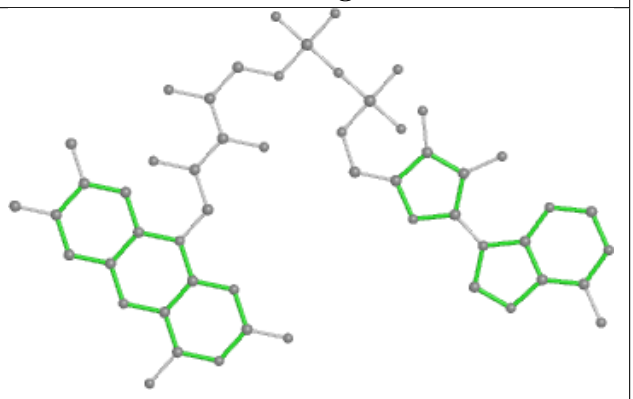
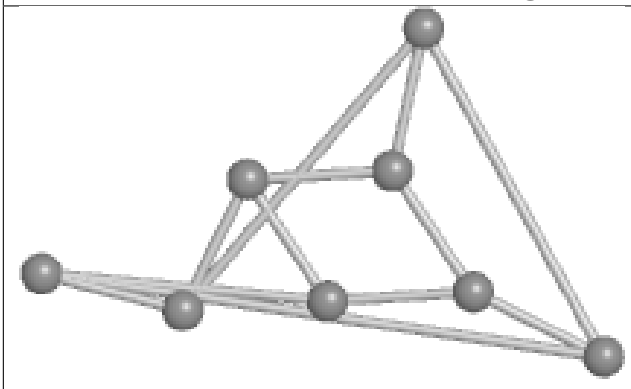


Rings

Ligand SF4 A 1102



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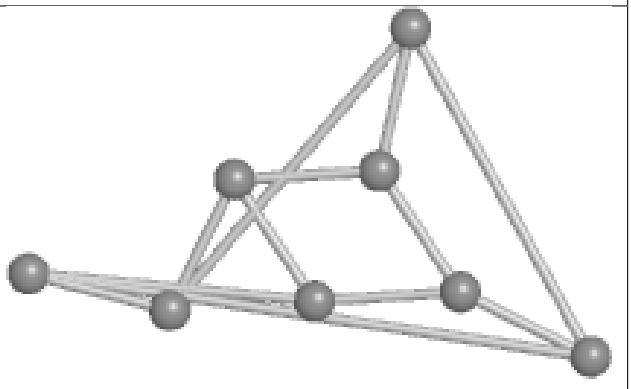
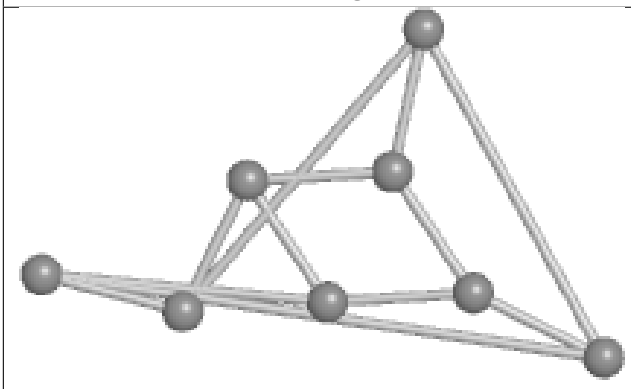


Bond angles



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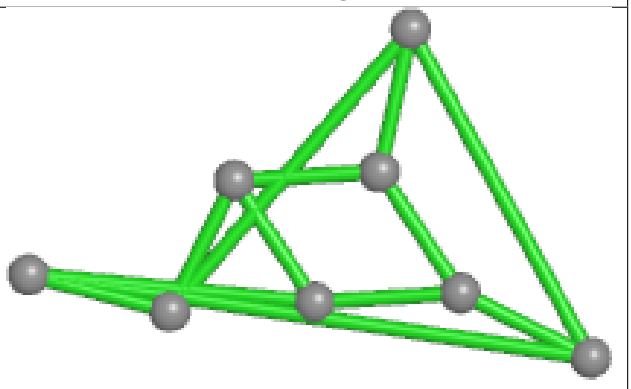
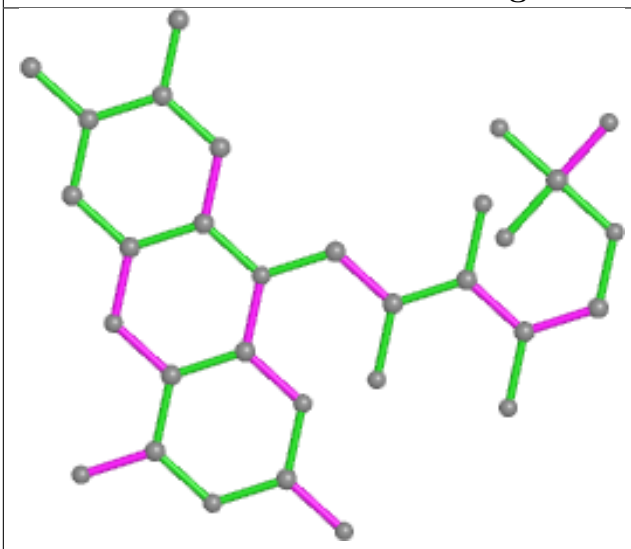


Rings

Ligand FMN D 1105



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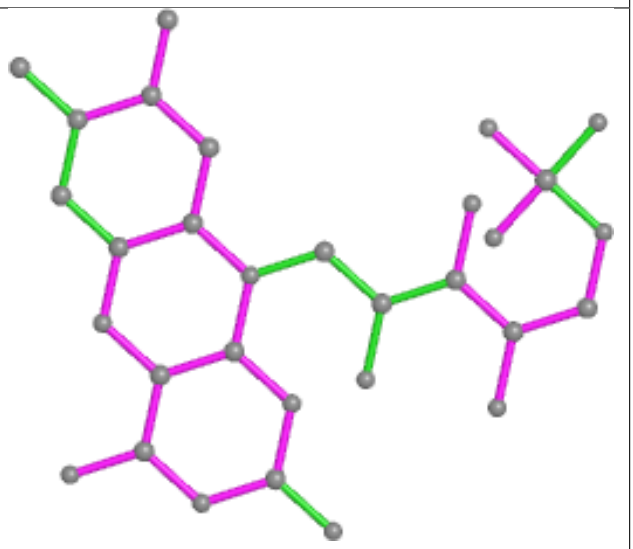
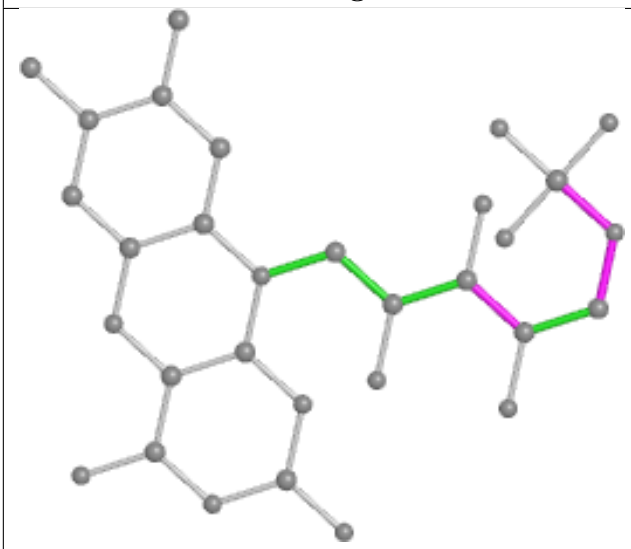


Bond angles



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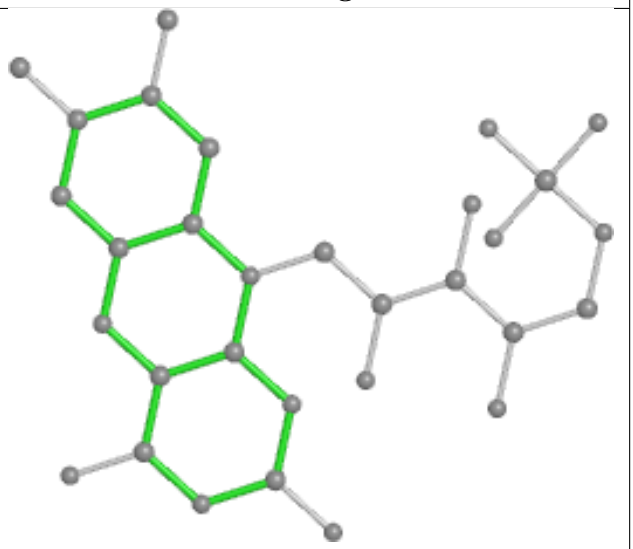
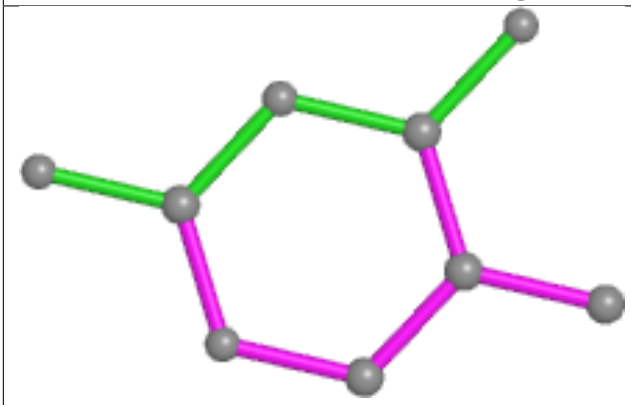


Rings

Ligand TDR D 1107



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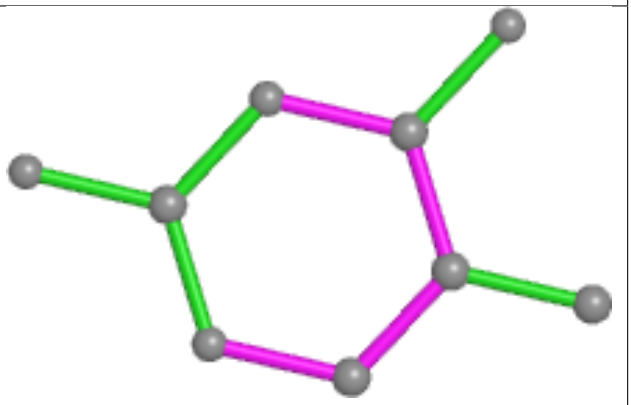
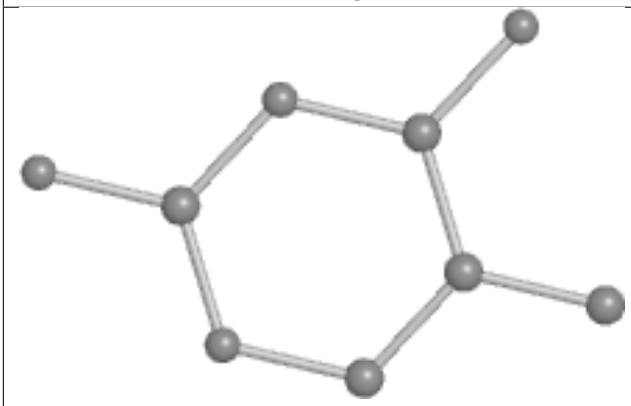
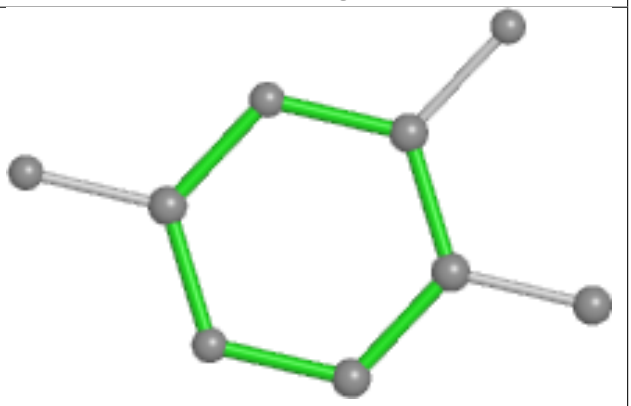


Bond angles

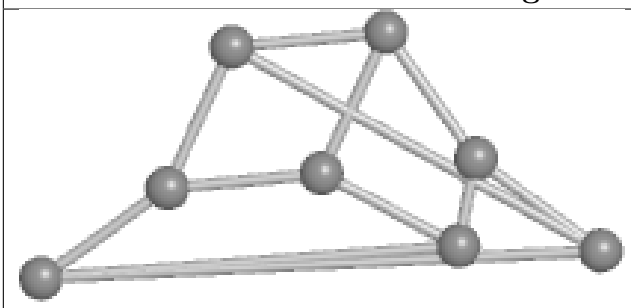


Torsions



Rings

Ligand SF4 C 1102



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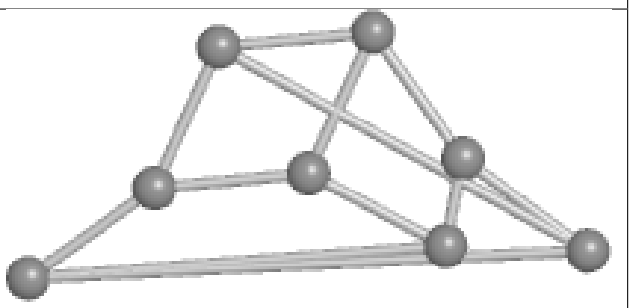
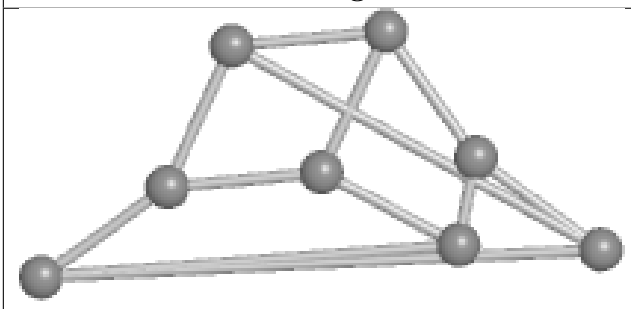
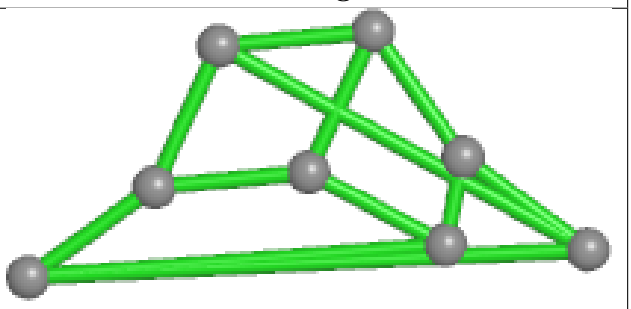


Bond angles

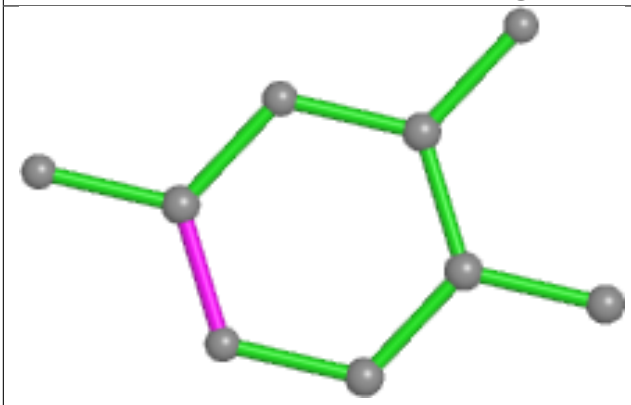


Torsions



Rings

Ligand TDR A 1107



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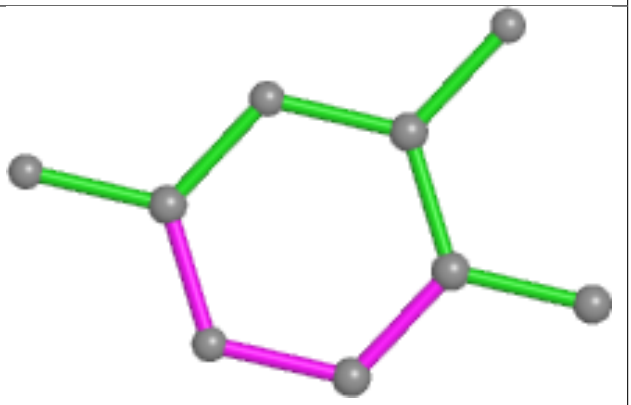
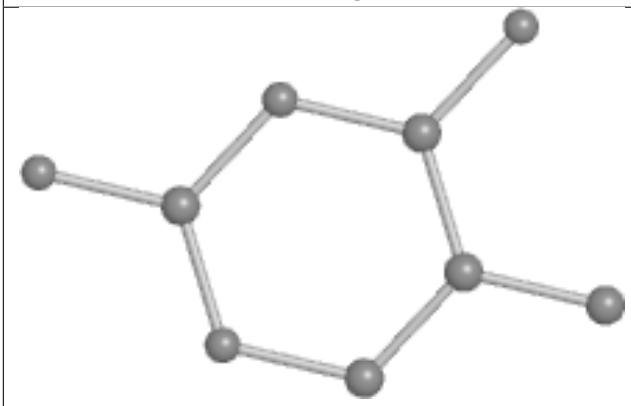
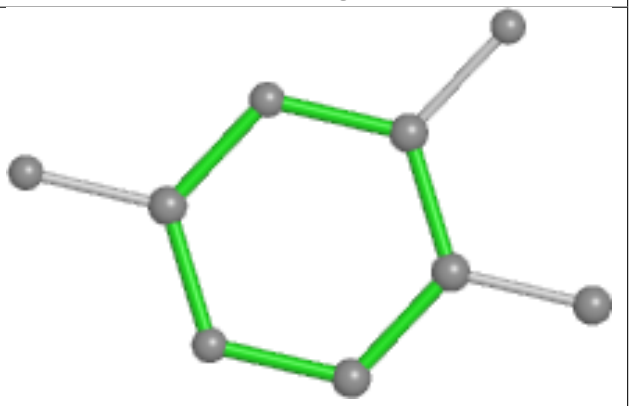


Bond angles

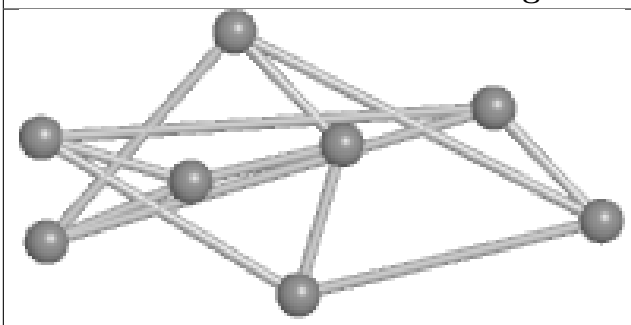


Torsions

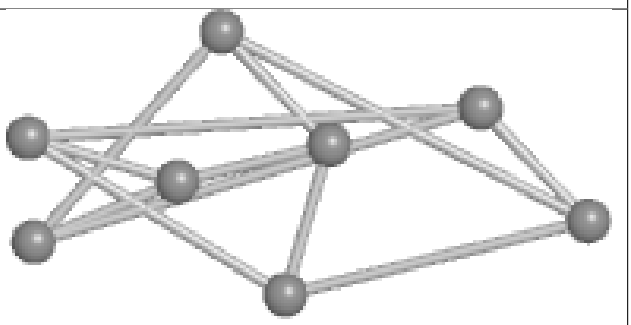


Rings

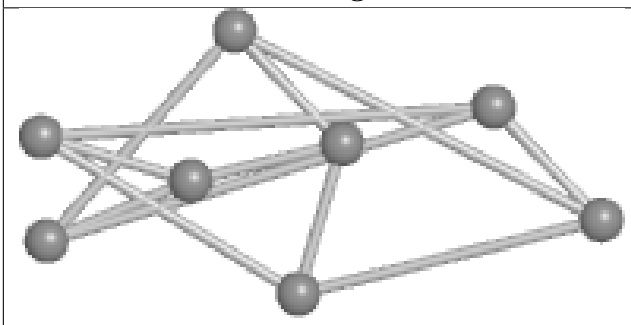
Ligand SF4 B 1103



Bond lengths



Bond angles



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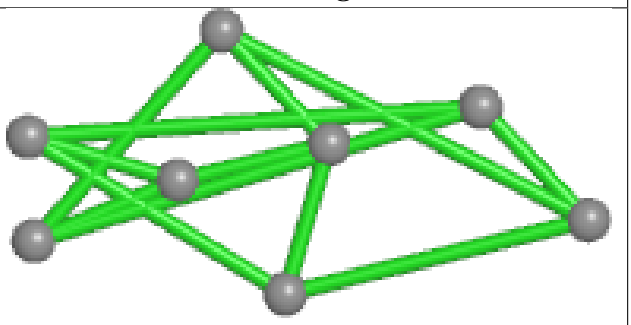
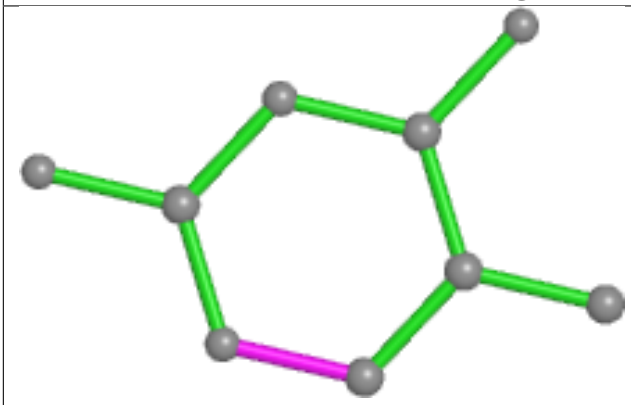


Rings

Ligand TDR C 1107



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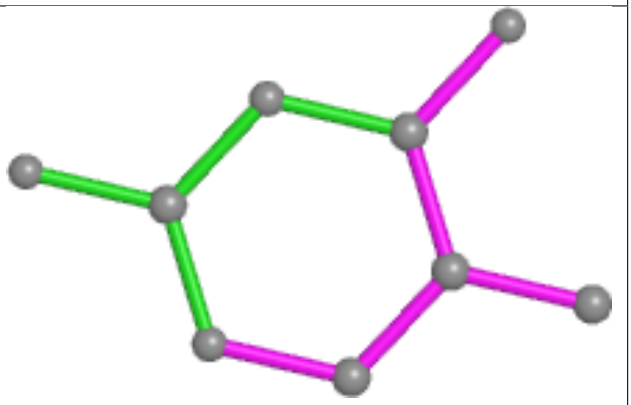
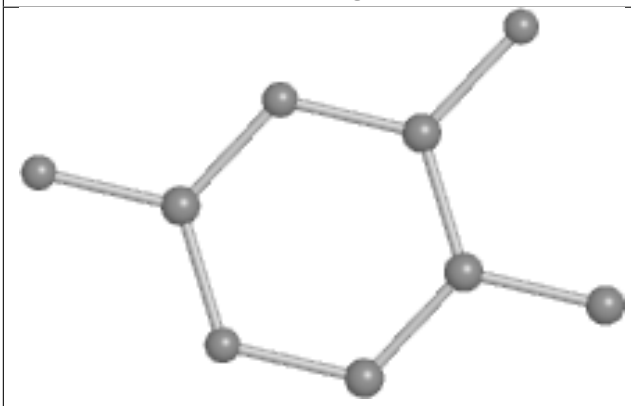
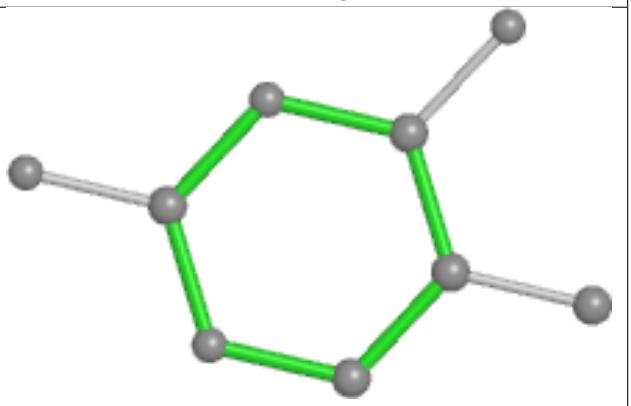


Bond angles

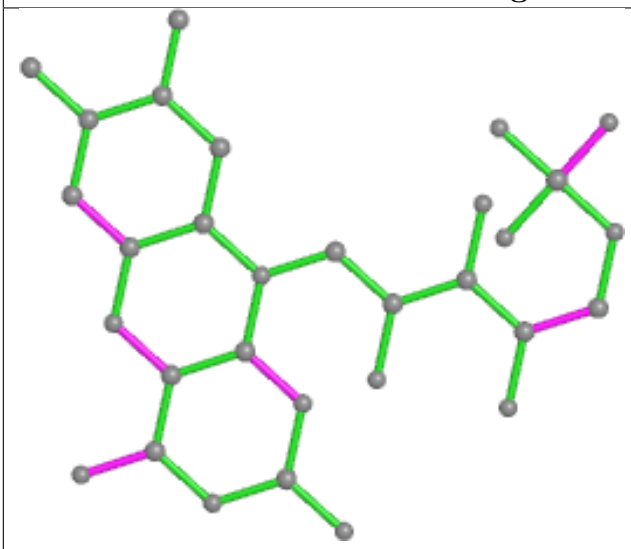


Torsions



Rings

Ligand FMN C 1105



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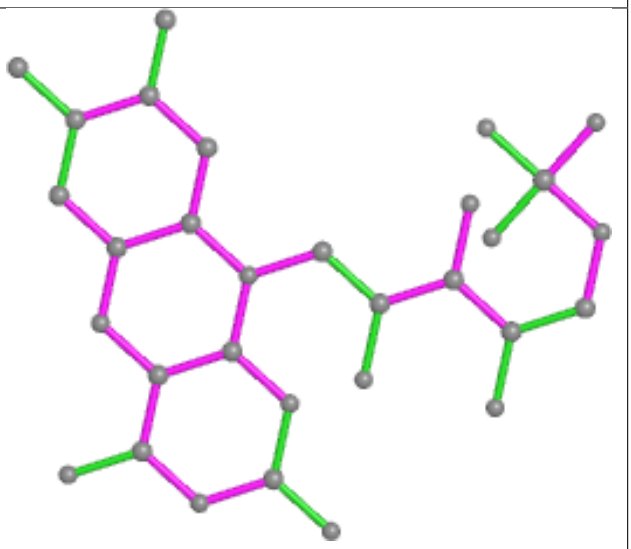
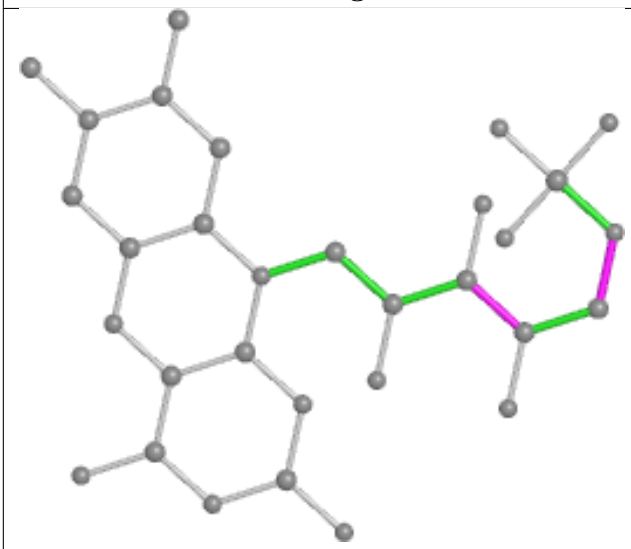
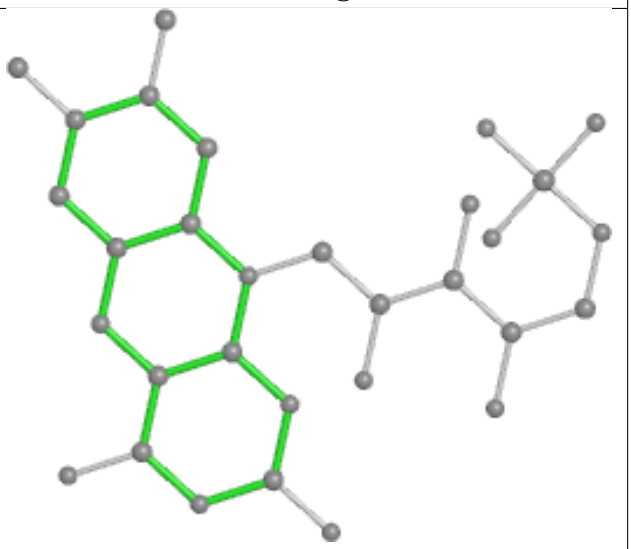


Bond angles

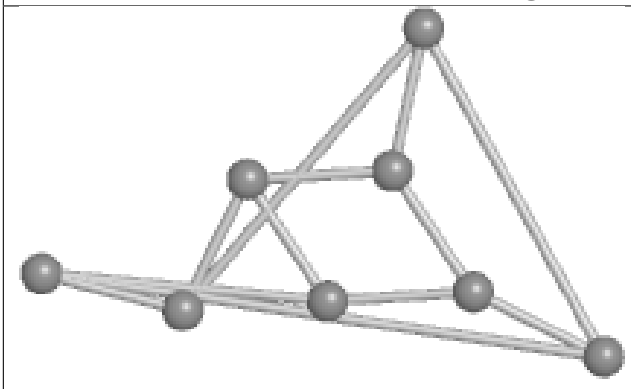


Torsions



Rings

Ligand SF4 B 1104



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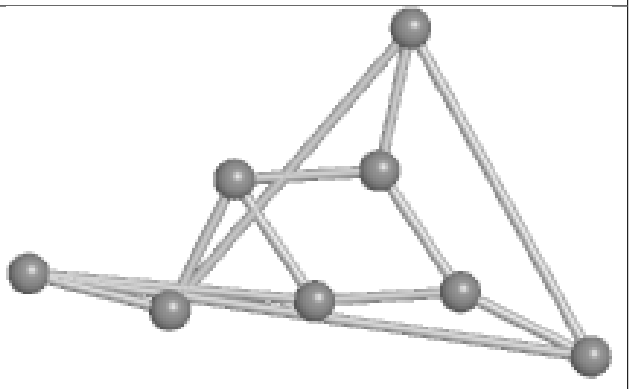
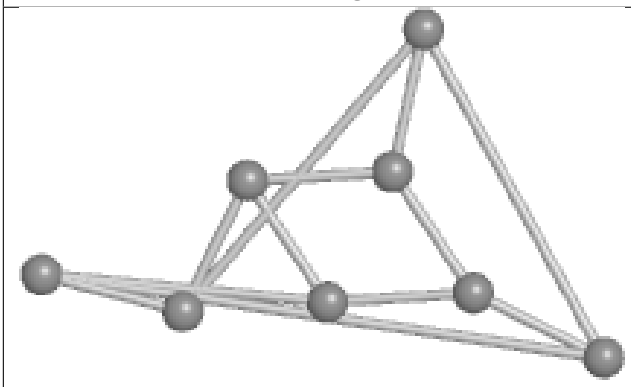
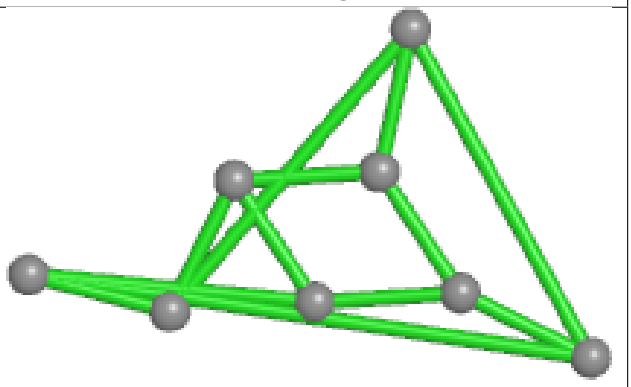


Bond angles

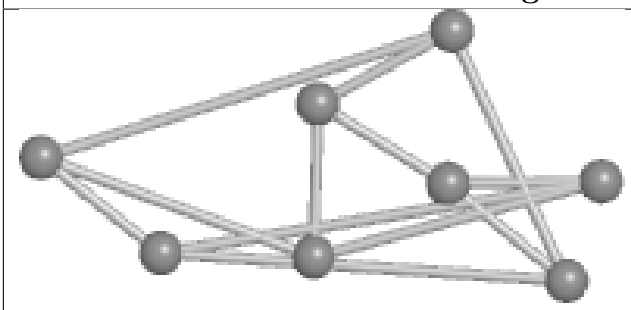


Torsions



Rings

Ligand SF4 D 1102



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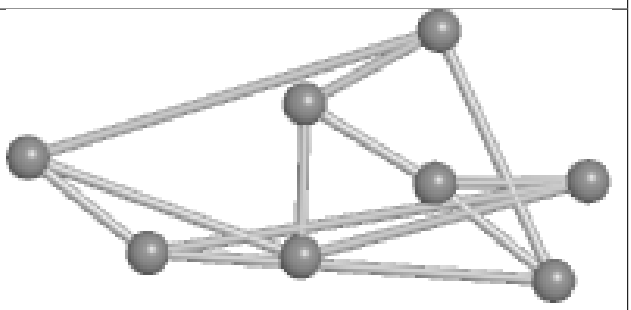

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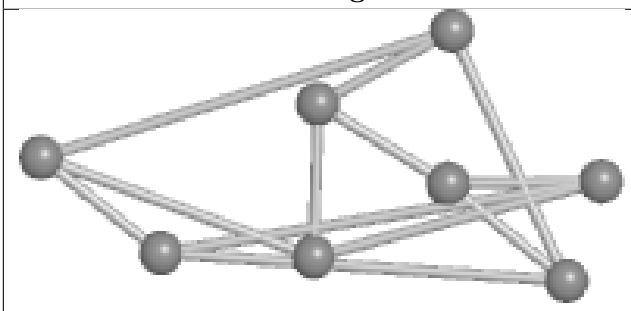
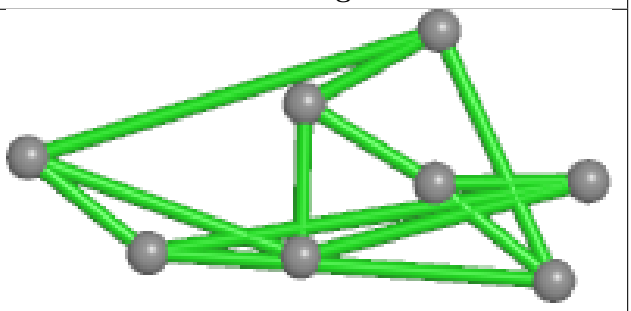


Torsions



Rings

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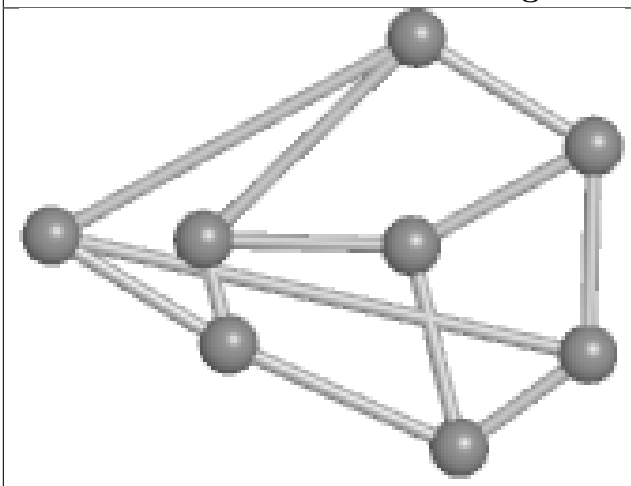

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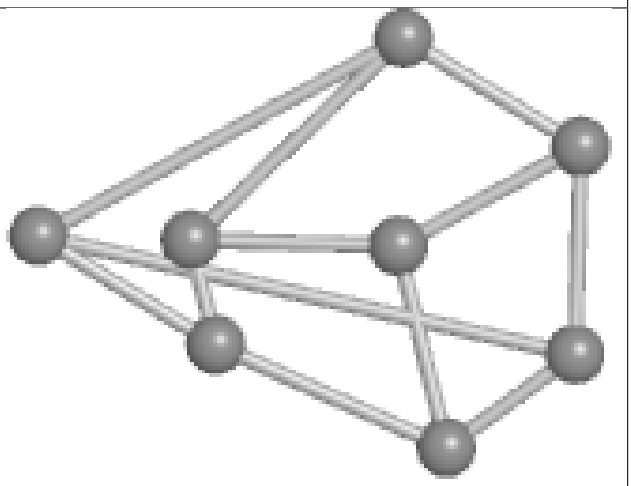
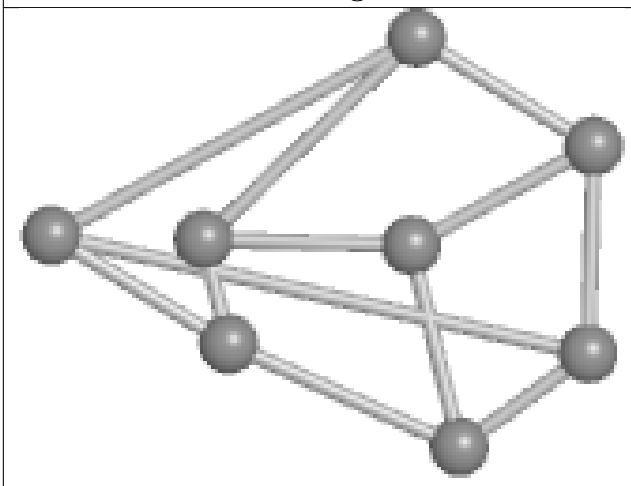


Bond angles



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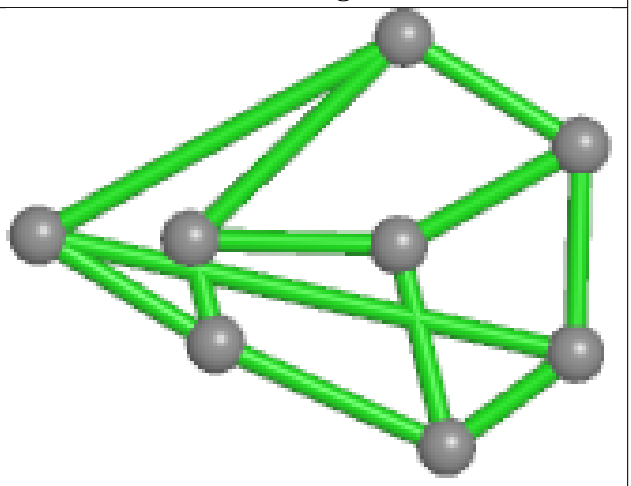
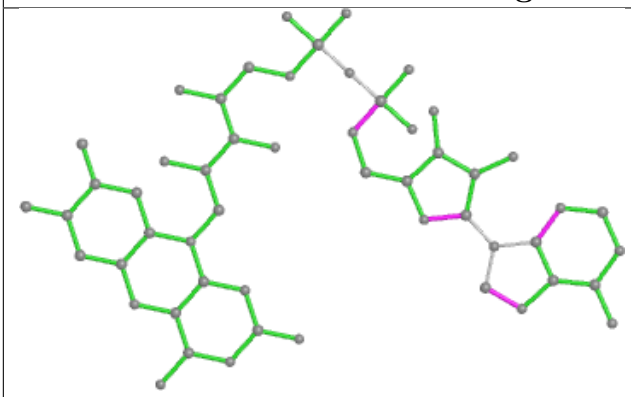


Rings

Ligand FAD D 1106



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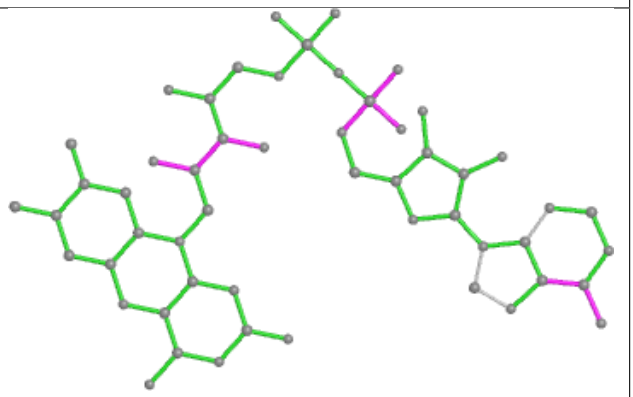

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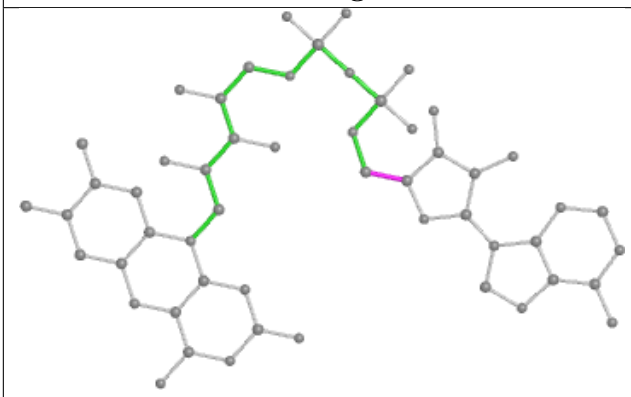

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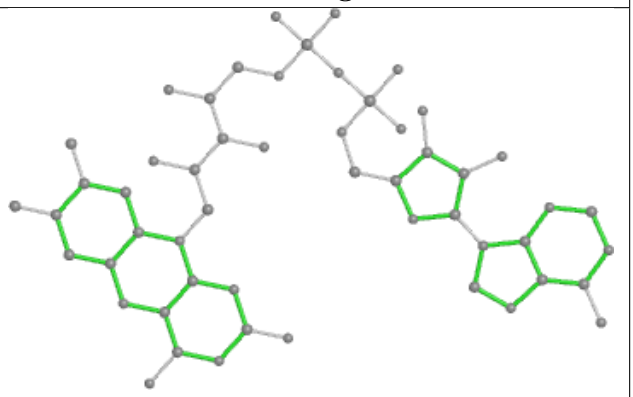
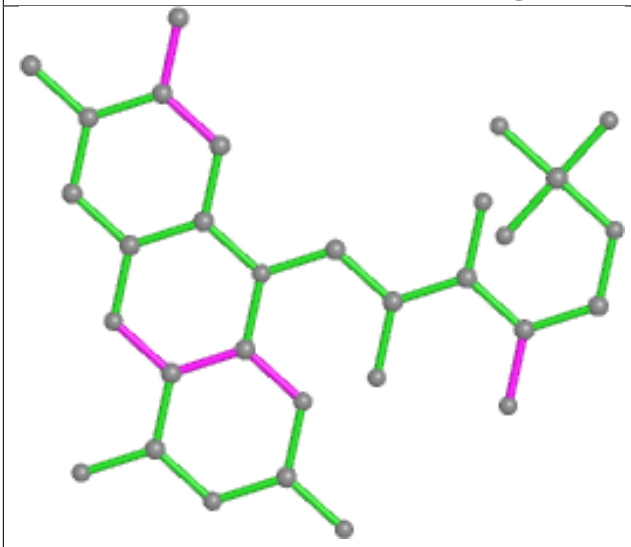


Rings

Ligand FMN B 1105



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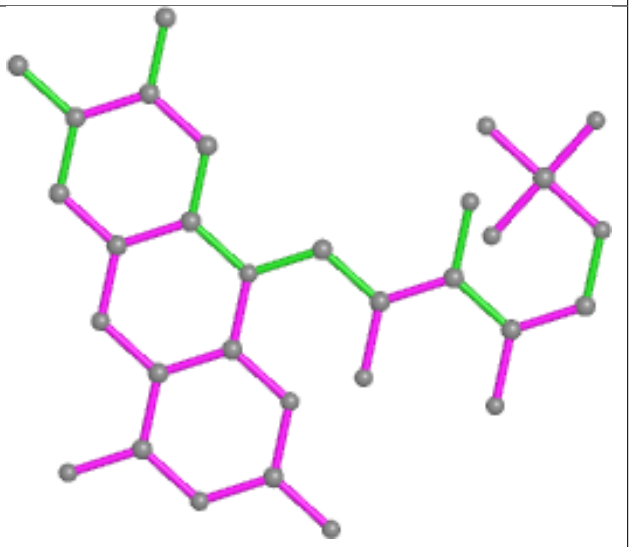
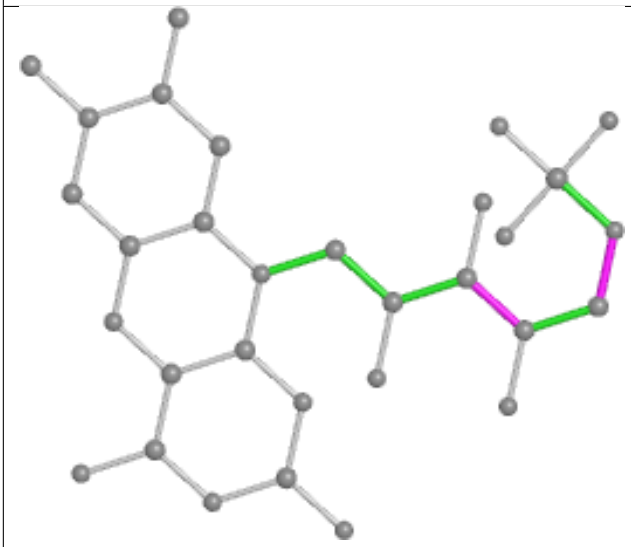


Bond angles



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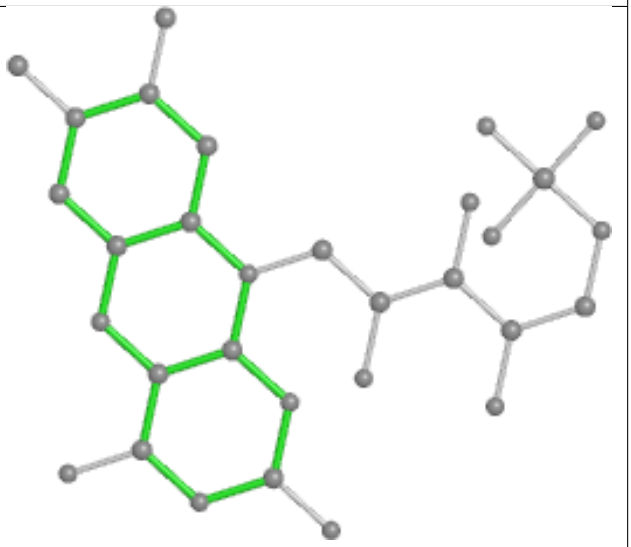
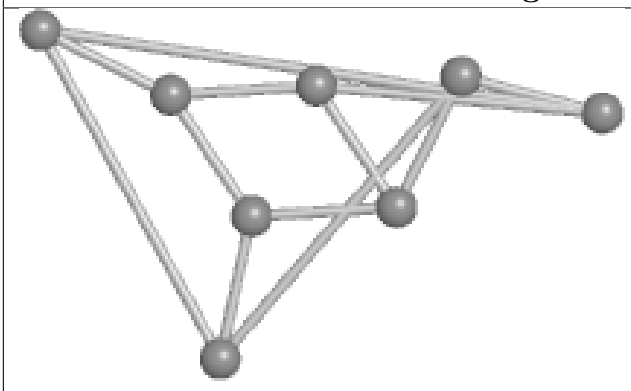


Rings

Ligand SF4 C 1101



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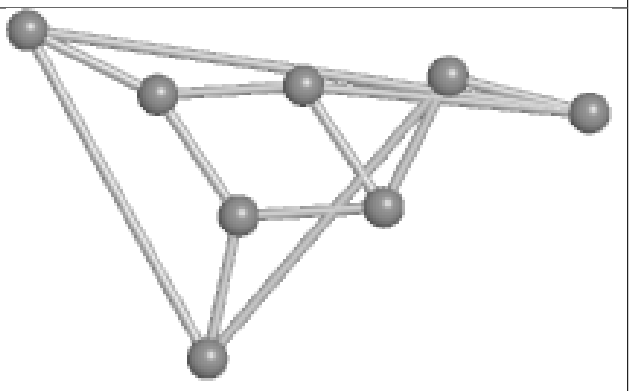

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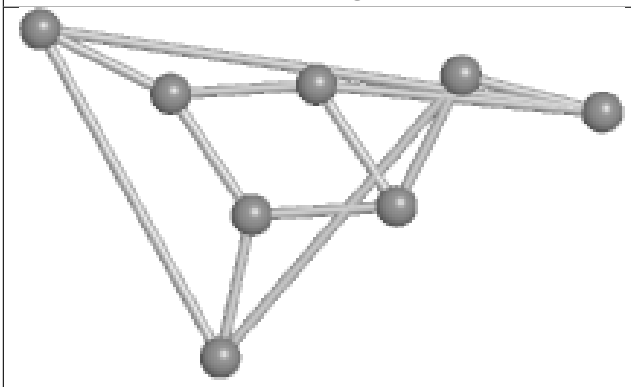

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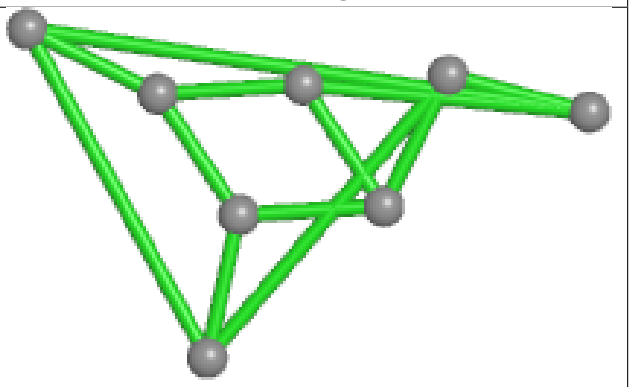
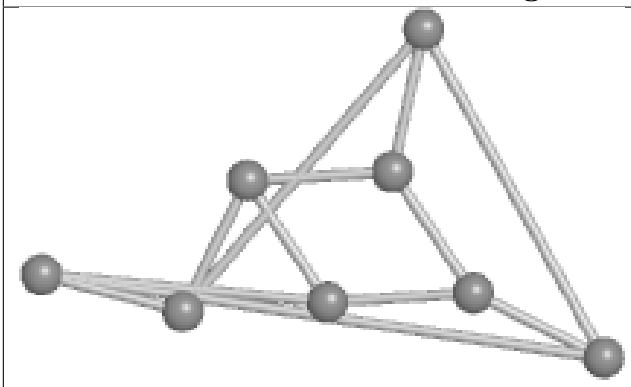


Rings

Ligand SF4 B 1101



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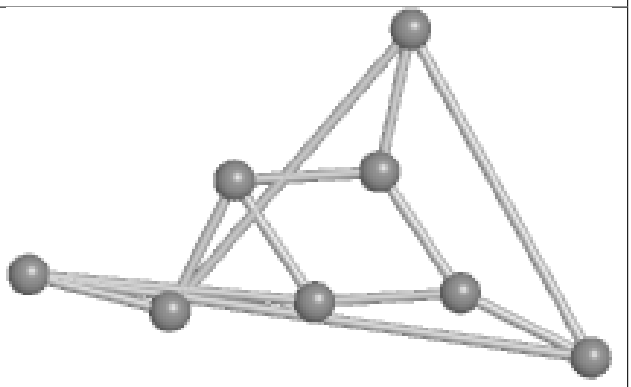
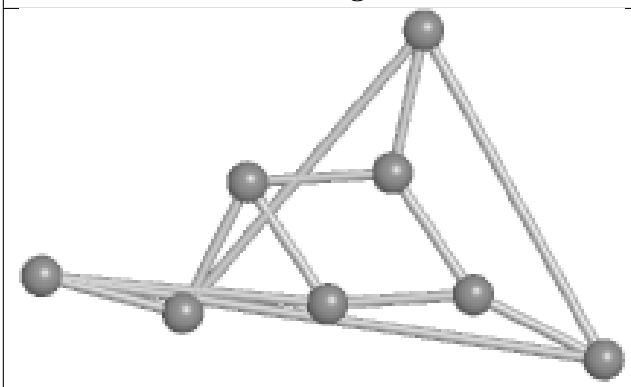
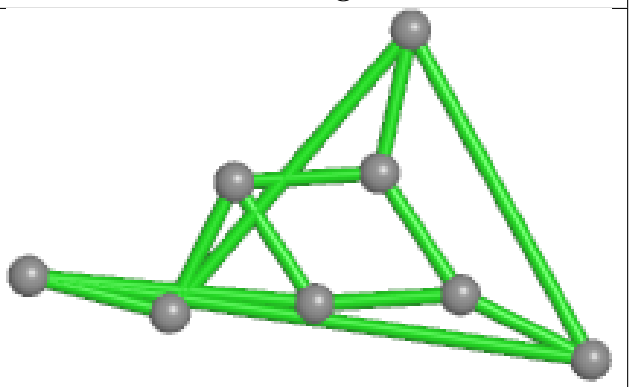


Bond angles

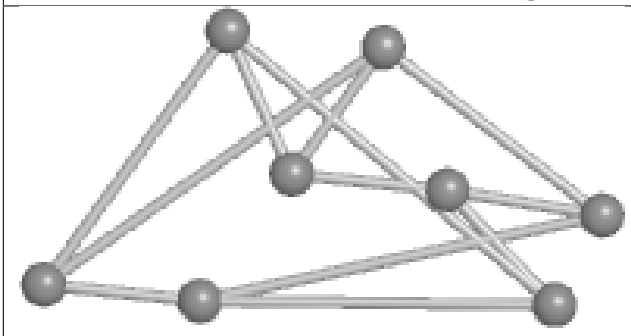


Torsions



Rings

Ligand SF4 C 1104



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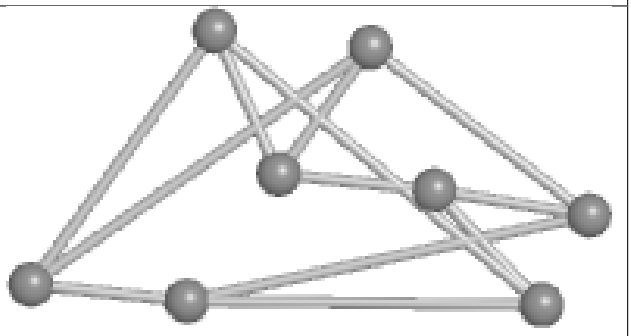

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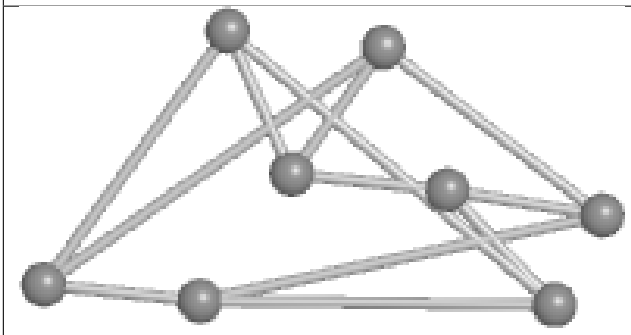

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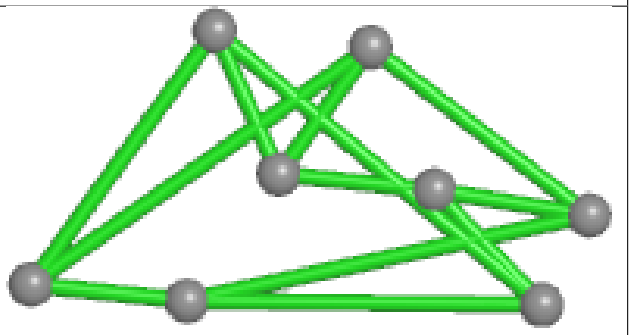
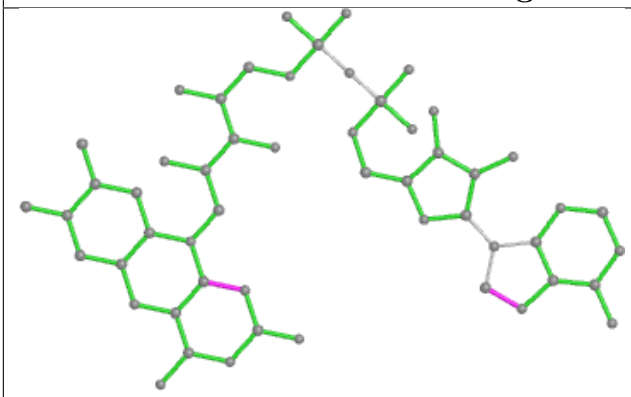


Rings

Ligand FAD C 1106



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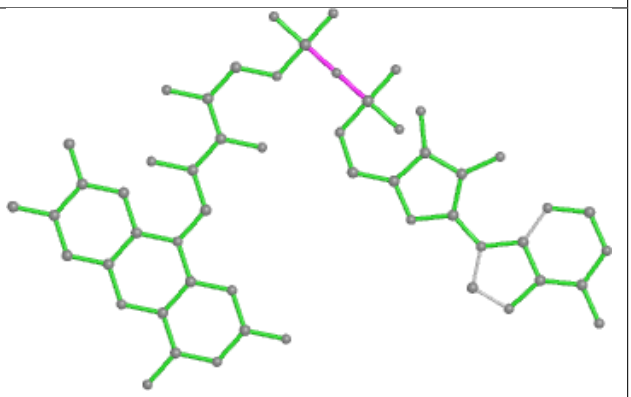
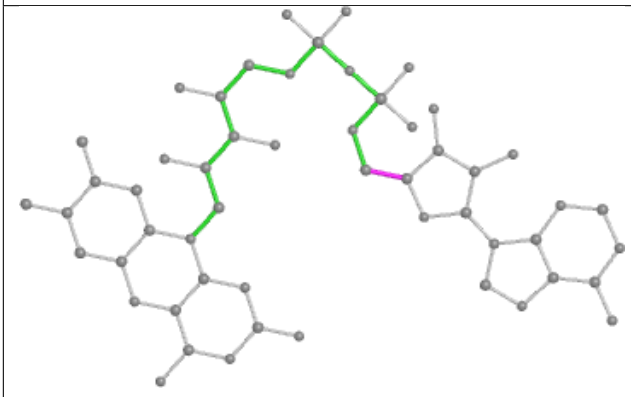


Bond angles



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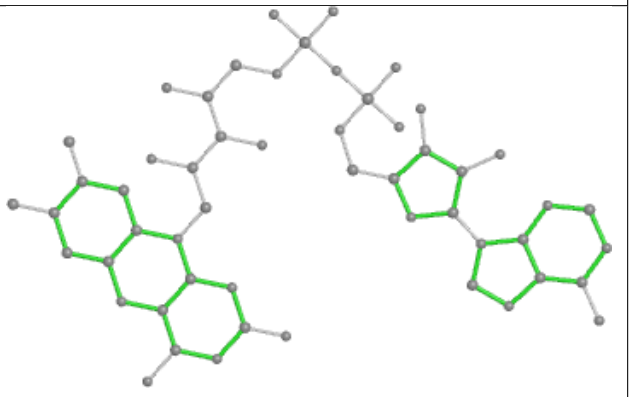
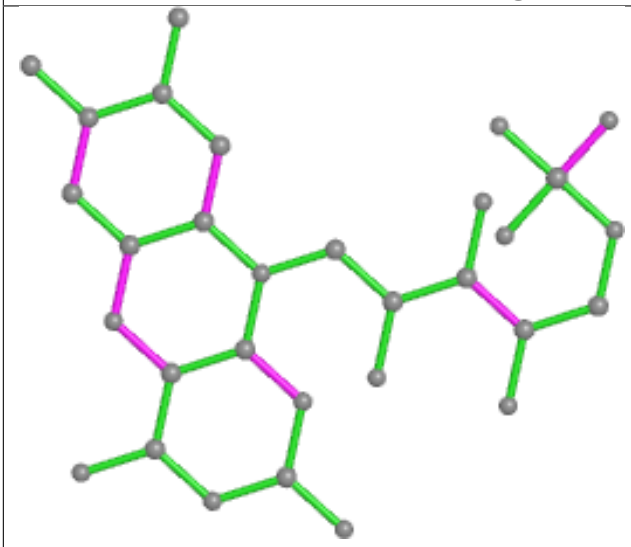


Rings

Ligand FMN A 1105



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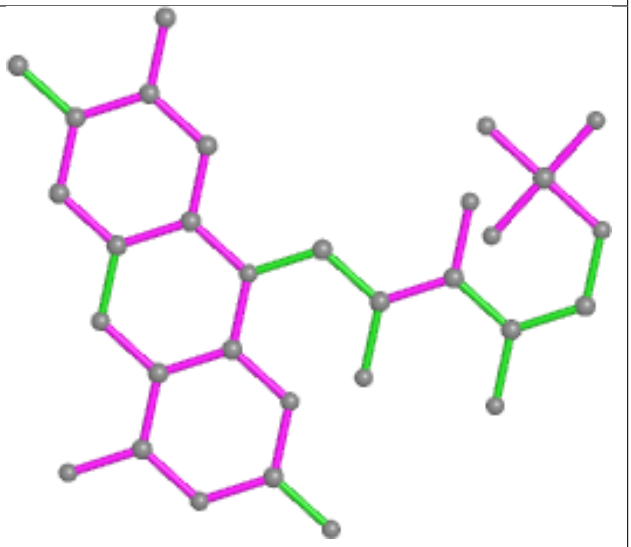
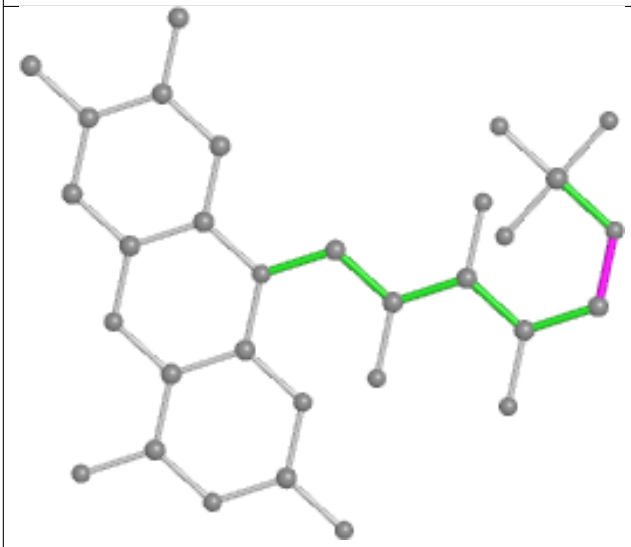
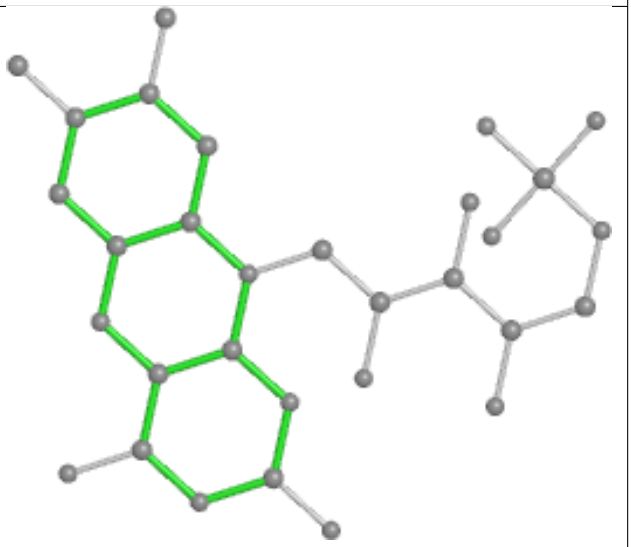


Bond angles

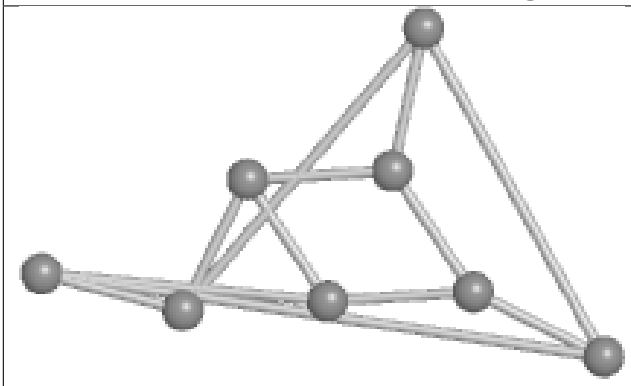


Torsions



Rings

Ligand SF4 A 1101



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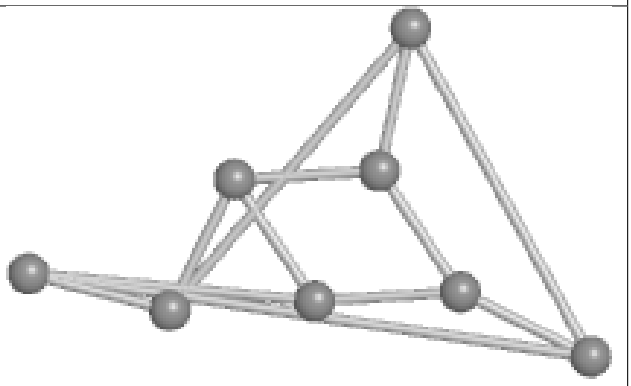
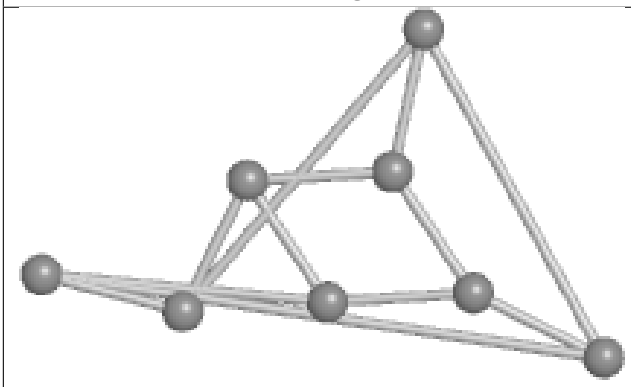


Bond angles



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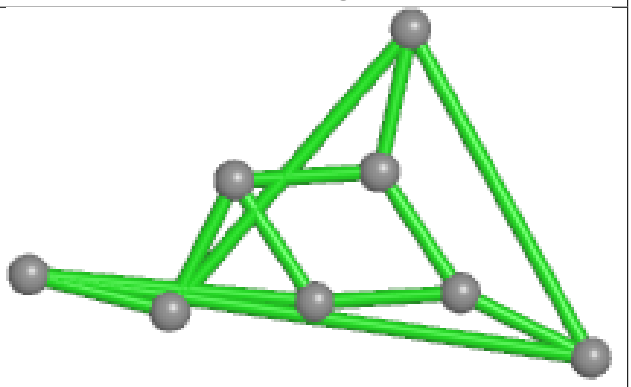
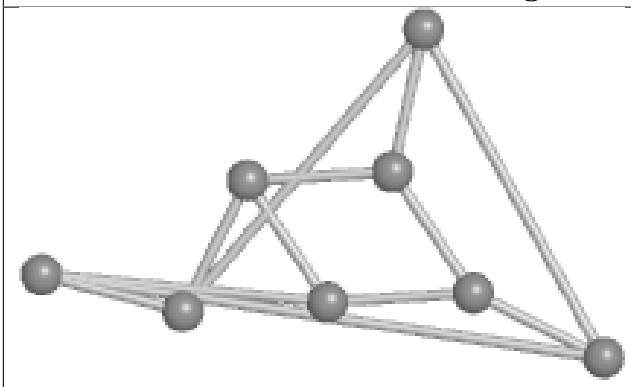


Rings

Ligand SF4 B 1102



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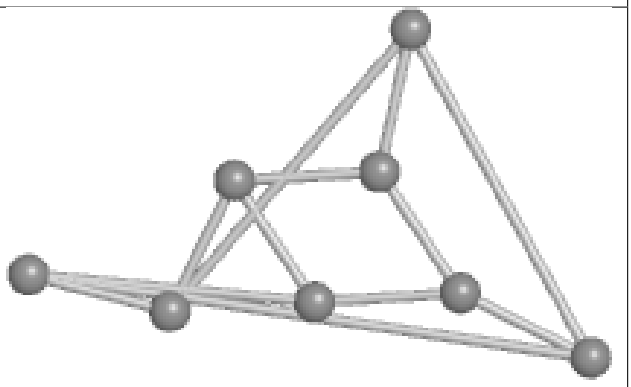
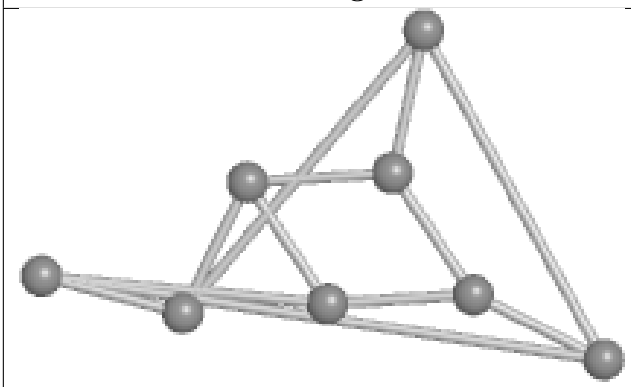


Bond angles



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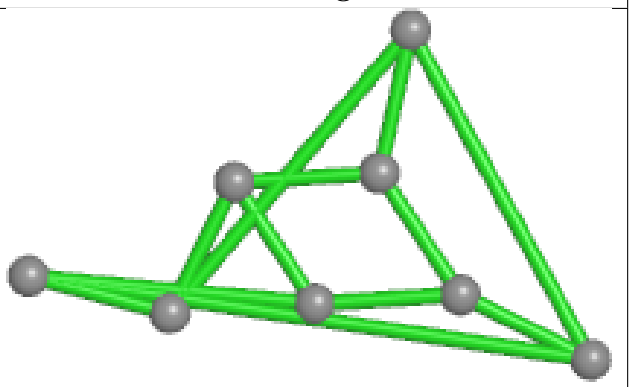
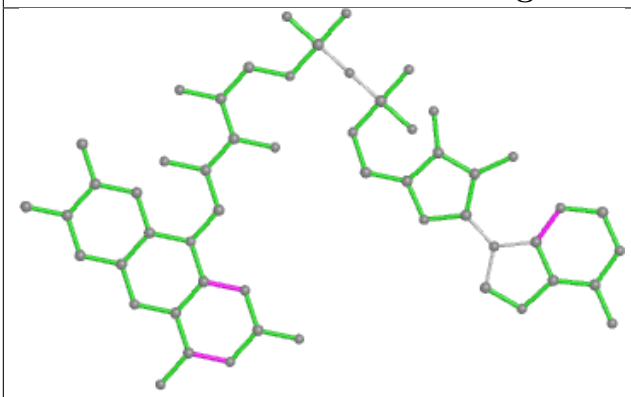


Rings

Ligand FAD B 1106



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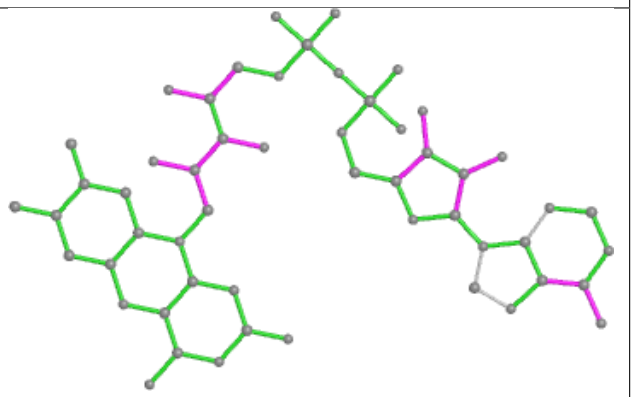
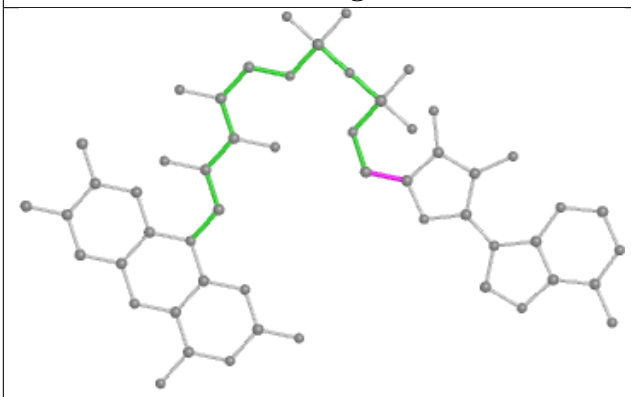
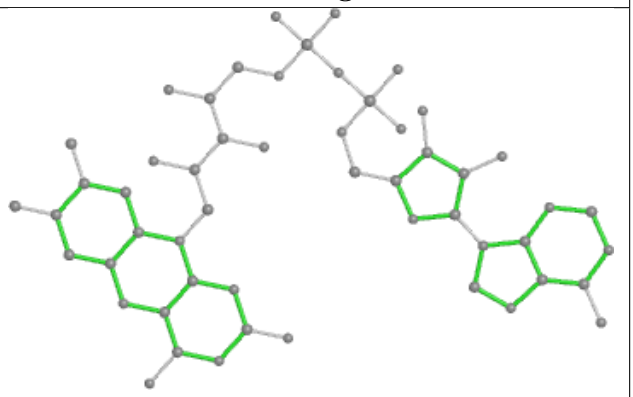


Bond angles

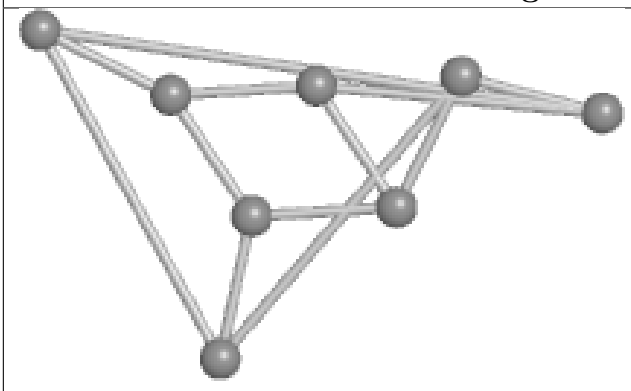


Torsions



Rings

Ligand SF4 D 1101



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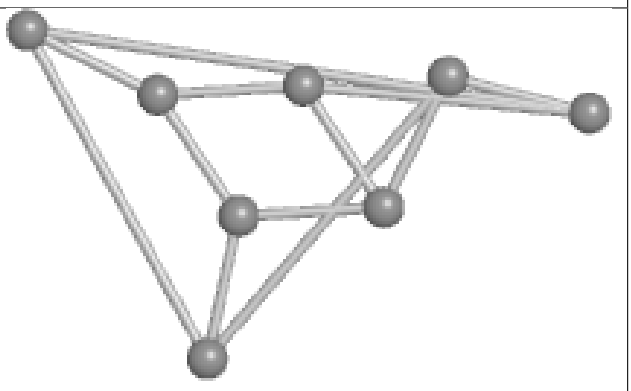
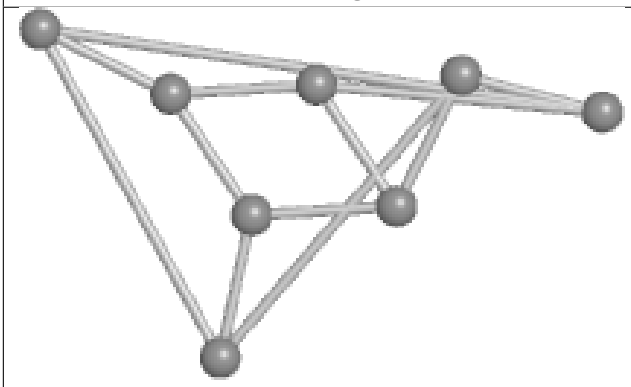


Bond angles



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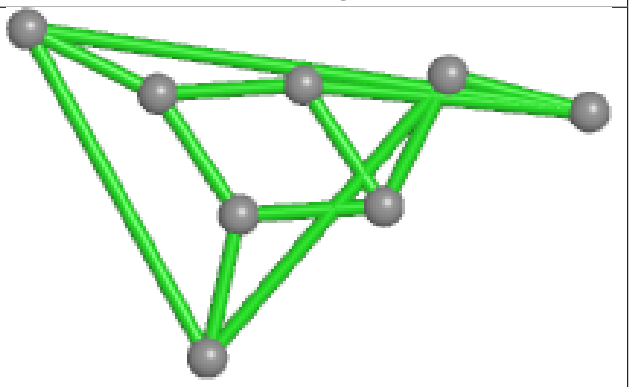
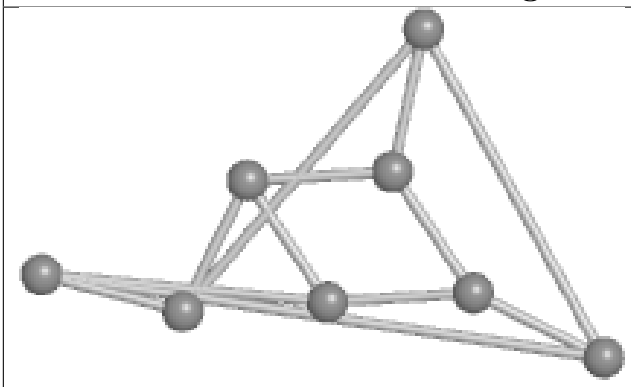
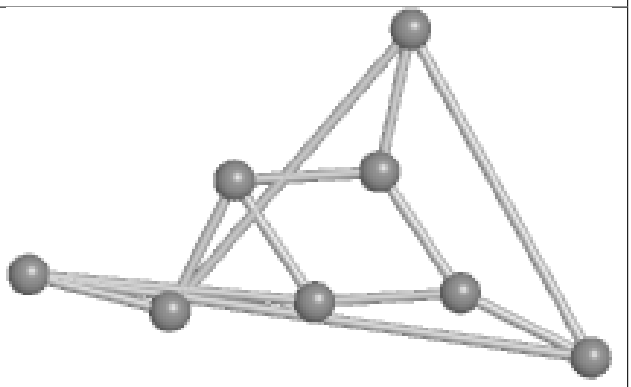


Rings

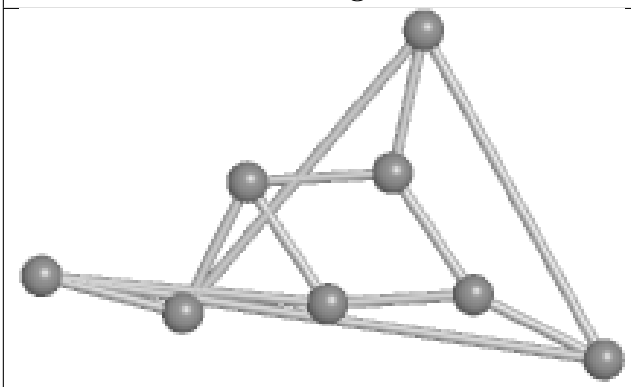
Ligand SF4 D 1103



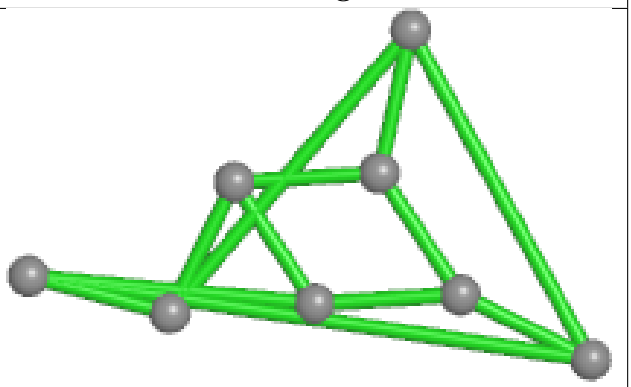
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2
1	B	2
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	670:SER	C	671:SER	N	1.13
1	B	671:SER	C	672:PRO	N	1.11
1	D	670:SER	C	671:SER	N	1.07
1	B	670:SER	C	671:SER	N	1.03
1	C	671:SER	C	672:PRO	N	0.96

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	996/1025 (97%)	0.32	79 (7%) 12 16	11, 30, 88, 160	0
1	B	1001/1025 (97%)	0.43	101 (10%) 7 8	13, 31, 89, 187	0
1	C	1002/1025 (97%)	0.39	103 (10%) 6 8	14, 32, 89, 164	0
1	D	992/1025 (96%)	0.56	107 (10%) 5 7	15, 34, 100, 192	0
All	All	3991/4100 (97%)	0.42	390 (9%) 7 9	11, 32, 91, 192	0

All (390) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	868	ILE	23.0
1	D	864	PRO	21.2
1	D	52	CYS	20.1
1	A	868	ILE	18.1
1	D	868	ILE	17.6
1	D	869	ALA	17.3
1	B	869	ALA	15.0
1	C	868	ILE	13.4
1	D	50	PHE	13.1
1	C	52	CYS	11.8
1	B	52	CYS	11.6
1	D	320	GLY	11.5
1	D	865	VAL	11.5
1	B	323	ALA	11.3
1	C	866	PRO	11.0
1	D	866	PRO	10.5
1	D	680	MET	10.1
1	B	324	CYS	9.7
1	C	869	ALA	9.6
1	A	2	ALA	9.5
1	C	1011	TYR	9.5

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Mol	Chain	Res	Type	RSRZ
1	B	865	VAL	9.4
1	A	864	PRO	9.0
1	C	865	VAL	8.8
1	D	867	ARG	8.6
1	B	867	ARG	8.6
1	D	48	ASN	8.5
1	A	869	ALA	8.5
1	B	897	LEU	8.5
1	C	867	ARG	8.4
1	B	50	PHE	8.4
1	C	49	CYS	8.4
1	A	867	ARG	8.3
1	A	51	HIS	8.1
1	D	1018	PRO	8.1
1	D	870	GLU	8.0
1	C	50	PHE	7.8
1	C	864	PRO	7.8
1	C	1012	GLU	7.8
1	A	417	GLY	7.8
1	A	873	GLY	7.8
1	C	680	MET	7.7
1	C	1013	PRO	7.6
1	D	1008	THR	7.6
1	D	418	LYS	7.5
1	D	416	THR	7.5
1	D	1013	PRO	7.4
1	A	859	HIS	7.4
1	A	897	LEU	7.3
1	C	897	LEU	7.3
1	A	47	LYS	7.2
1	B	866	PRO	7.2
1	A	416	THR	7.2
1	D	892	GLU	7.2
1	A	50	PHE	7.1
1	A	1017	LEU	7.1
1	D	673	HIS	7.1
1	C	900	GLN	7.0
1	D	328	LEU	7.0
1	A	322	CYS	6.9
1	A	414	ASP	6.8
1	D	856	THR	6.7
1	B	51	HIS	6.7

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Mol	Chain	Res	Type	RSRZ
1	B	673	HIS	6.7
1	D	49	CYS	6.6
1	C	2	ALA	6.5
1	B	871	LEU	6.4
1	D	319	ALA	6.4
1	A	870	GLU	6.3
1	A	52	CYS	6.3
1	D	858	SER	6.3
1	A	48	ASN	6.3
1	B	1018	PRO	6.2
1	D	891	ALA	6.2
1	B	870	GLU	6.1
1	C	673	HIS	6.1
1	C	870	GLU	6.1
1	C	674	GLY	6.0
1	B	320	GLY	6.0
1	B	48	ASN	6.0
1	C	320	GLY	5.9
1	A	898	LYS	5.9
1	D	51	HIS	5.8
1	A	1010	PRO	5.8
1	C	414	ASP	5.7
1	D	681	GLY	5.7
1	C	681	GLY	5.6
1	D	60	ASP	5.6
1	A	865	VAL	5.6
1	C	322	CYS	5.6
1	D	45	PRO	5.5
1	D	890	ILE	5.5
1	B	416	THR	5.5
1	C	873	GLY	5.5
1	A	890	ILE	5.4
1	B	322	CYS	5.4
1	A	895	MET	5.4
1	B	417	GLY	5.4
1	D	417	GLY	5.4
1	A	872	MET	5.4
1	D	862	GLY	5.3
1	D	414	ASP	5.2
1	B	49	CYS	5.2
1	D	175	CYS	5.2
1	A	1012	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	680	MET	5.2
1	C	899	GLU	5.2
1	B	46	ASP	5.1
1	B	892	GLU	5.1
1	C	416	THR	5.1
1	D	893	GLU	5.1
1	B	858	SER	5.1
1	C	1010	PRO	5.1
1	A	419	TRP	5.1
1	D	863	LYS	5.0
1	B	859	HIS	5.0
1	C	417	GLY	5.0
1	B	908	GLU	5.0
1	D	872	MET	4.9
1	A	855	GLY	4.9
1	B	47	LYS	4.9
1	A	49	CYS	4.9
1	D	1009	THR	4.8
1	B	319	ALA	4.8
1	C	1008	THR	4.8
1	B	896	ARG	4.8
1	C	908	GLU	4.8
1	C	1014	LYS	4.7
1	A	1013	PRO	4.7
1	D	54	LYS	4.7
1	D	327	PRO	4.7
1	B	414	ASP	4.7
1	C	891	ALA	4.6
1	B	890	ILE	4.6
1	A	517	ALA	4.6
1	C	859	HIS	4.6
1	C	871	LEU	4.6
1	A	866	PRO	4.6
1	B	459	TRP	4.6
1	A	46	ASP	4.5
1	D	1011	TYR	4.5
1	D	326	SER	4.5
1	B	410[A]	ARG	4.5
1	A	415	GLU	4.5
1	A	908	GLU	4.5
1	B	415	GLU	4.5
1	D	459	TRP	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	1012	GLU	4.4
1	B	680	MET	4.4
1	D	860	GLN	4.3
1	D	329	PRO	4.3
1	C	415	GLU	4.3
1	A	1011	TYR	4.3
1	C	424	ASP	4.3
1	B	895	MET	4.3
1	C	327	PRO	4.3
1	B	856	THR	4.3
1	D	1016	GLY	4.2
1	D	46	ASP	4.2
1	C	857	GLU	4.2
1	B	418	LYS	4.2
1	C	418	LYS	4.2
1	D	857	GLU	4.2
1	D	888	LYS	4.1
1	C	898	LYS	4.1
1	B	1015	ARG	4.1
1	B	373	VAL	4.0
1	C	46	ASP	4.0
1	A	1008	THR	4.0
1	D	873	GLY	4.0
1	D	859	HIS	4.0
1	D	415	GLU	4.0
1	D	1012	GLU	4.0
1	A	418	LYS	4.0
1	B	1016	GLY	4.0
1	C	517	ALA	4.0
1	C	326	SER	3.9
1	B	517	ALA	3.9
1	A	424	ASP	3.9
1	A	896	ARG	3.9
1	C	895	MET	3.9
1	B	873	GLY	3.9
1	A	871	LEU	3.9
1	B	1017	LEU	3.9
1	D	908	GLU	3.8
1	C	48	ASN	3.8
1	B	872	MET	3.8
1	D	1017	LEU	3.8
1	D	517	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	871	LEU	3.8
1	C	45	PRO	3.8
1	C	374	PRO	3.8
1	C	892	GLU	3.8
1	C	1017	LEU	3.8
1	C	51	HIS	3.8
1	D	844	GLU	3.7
1	A	1009	THR	3.7
1	B	888	LYS	3.7
1	D	1015	ARG	3.7
1	C	413	GLN	3.7
1	C	1009	THR	3.7
1	D	321	MET	3.6
1	A	374	PRO	3.6
1	B	374	PRO	3.6
1	B	1014	LYS	3.6
1	B	420	ASN	3.6
1	B	857	GLU	3.6
1	C	890	ILE	3.6
1	D	885	GLN	3.6
1	B	413	GLN	3.6
1	B	180	GLU	3.6
1	C	53	GLU	3.6
1	B	9	VAL	3.5
1	C	332	ARG	3.5
1	B	864	PRO	3.5
1	C	896	ARG	3.5
1	A	856	THR	3.4
1	C	401	GLY	3.4
1	B	893	GLU	3.4
1	D	889	ILE	3.4
1	C	672	PRO	3.4
1	C	319	ALA	3.3
1	A	892	GLU	3.3
1	B	891	ALA	3.3
1	B	175	CYS	3.3
1	D	420	ASN	3.3
1	A	681	GLY	3.3
1	D	296	GLY	3.3
1	B	1009	THR	3.3
1	B	1010	PRO	3.3
1	B	419	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	181	LYS	3.3
1	D	410[A]	ARG	3.3
1	D	583	VAL	3.2
1	B	202	CYS	3.2
1	D	374	PRO	3.2
1	D	874	LYS	3.2
1	A	373	VAL	3.2
1	A	909	ARG	3.2
1	B	178	SER	3.2
1	A	891	ALA	3.1
1	C	47	LYS	3.1
1	D	47	LYS	3.1
1	D	909	ARG	3.1
1	C	856	THR	3.1
1	B	909	ARG	3.1
1	D	330	SER	3.1
1	B	10	ALA	3.1
1	A	893	GLU	3.1
1	C	373	VAL	3.1
1	D	55	LEU	3.0
1	B	1011	TYR	3.0
1	D	36	LEU	3.0
1	D	884	GLU	3.0
1	C	10	ALA	3.0
1	A	1016	GLY	3.0
1	A	857	GLU	3.0
1	C	423	GLU	3.0
1	A	583	VAL	3.0
1	B	295	GLN	3.0
1	C	910	LYS	2.9
1	A	858	SER	2.9
1	A	413	GLN	2.9
1	B	667	LEU	2.9
1	B	889	ILE	2.9
1	B	198	ALA	2.9
1	C	206	LEU	2.9
1	A	420	ASN	2.8
1	D	372	ALA	2.8
1	B	874	LYS	2.8
1	A	443	ARG	2.8
1	D	855	GLY	2.8
1	D	331	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	178	SER	2.8
1	B	321	MET	2.7
1	B	332	ARG	2.7
1	D	792	ALA	2.7
1	B	402	ARG	2.7
1	C	1015	ARG	2.7
1	B	325	HIS	2.7
1	D	373	VAL	2.7
1	D	53	GLU	2.7
1	B	681	GLY	2.7
1	D	1010	PRO	2.7
1	C	667	LEU	2.7
1	D	192	LEU	2.7
1	B	424	ASP	2.7
1	A	888	LYS	2.7
1	B	422	ASP	2.7
1	A	423	GLU	2.6
1	D	791	LEU	2.6
1	D	419	TRP	2.6
1	A	320	GLY	2.6
1	C	1016	GLY	2.6
1	D	180	GLU	2.6
1	C	874	LYS	2.6
1	B	54	LYS	2.6
1	A	889	ILE	2.6
1	C	200	ILE	2.6
1	B	177	PRO	2.6
1	B	423	GLU	2.6
1	C	733	THR	2.5
1	A	847	GLN	2.5
1	C	888	LYS	2.5
1	D	887	LYS	2.5
1	B	11	ASP	2.5
1	C	11	ASP	2.5
1	A	863	LYS	2.5
1	C	459	TRP	2.5
1	D	332	ARG	2.5
1	D	300	ASP	2.5
1	D	423	GLU	2.5
1	D	269	ASN	2.5
1	A	582	ILE	2.5
1	B	203	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	518	LYS	2.4
1	D	273	GLU	2.4
1	C	179	GLN	2.4
1	A	300	ASP	2.4
1	D	861	LYS	2.4
1	C	290	THR	2.4
1	A	45	PRO	2.3
1	C	321	MET	2.3
1	B	176	LEU	2.3
1	D	424	ASP	2.3
1	A	332	ARG	2.3
1	C	36	LEU	2.3
1	C	400	GLY	2.3
1	D	443	ARG	2.3
1	D	910	LYS	2.3
1	C	913	ILE	2.3
1	B	496	GLY	2.3
1	C	862	GLY	2.2
1	A	428	HIS	2.2
1	C	181	LYS	2.2
1	C	682	LEU	2.2
1	D	667	LEU	2.2
1	D	875	LYS	2.2
1	B	199	SER	2.2
1	B	398	VAL	2.2
1	B	181	LYS	2.2
1	B	1008	THR	2.2
1	B	855	GLY	2.2
1	C	422	ASP	2.2
1	A	1014	LYS	2.2
1	A	290	THR	2.2
1	A	36	LEU	2.2
1	A	402	ARG	2.2
1	D	847	GLN	2.2
1	C	858	SER	2.2
1	C	283	ILE	2.1
1	C	503	ILE	2.1
1	D	458	ARG	2.1
1	C	3	PRO	2.1
1	B	192	LEU	2.1
1	D	915	LYS	2.1
1	B	493	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	179	GLN	2.1
1	B	375	GLU	2.1
1	A	181	LYS	2.1
1	C	420	ASN	2.1
1	C	280	PHE	2.1
1	D	298	THR	2.1
1	C	885	GLN	2.1
1	C	336	ILE	2.1
1	C	23	GLN	2.1
1	D	413	GLN	2.1
1	B	672	PRO	2.1
1	C	60	ASP	2.1
1	A	411	THR	2.1
1	A	844	GLU	2.0
1	C	264	ASN	2.0
1	C	121	PRO	2.0
1	C	493	VAL	2.0
1	A	180	GLU	2.0
1	C	180	GLU	2.0
1	C	282	GLY	2.0
1	C	855	GLY	2.0
1	C	638	ILE	2.0
1	D	297	LEU	2.0
1	D	813	LEU	2.0
1	A	10	ALA	2.0
1	C	421	GLU	2.0
1	B	294	PHE	2.0
1	B	401	GLY	2.0
1	B	898	LYS	2.0
1	B	45	PRO	2.0
1	D	520	GLU	2.0
1	B	296	GLY	2.0
1	B	518	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

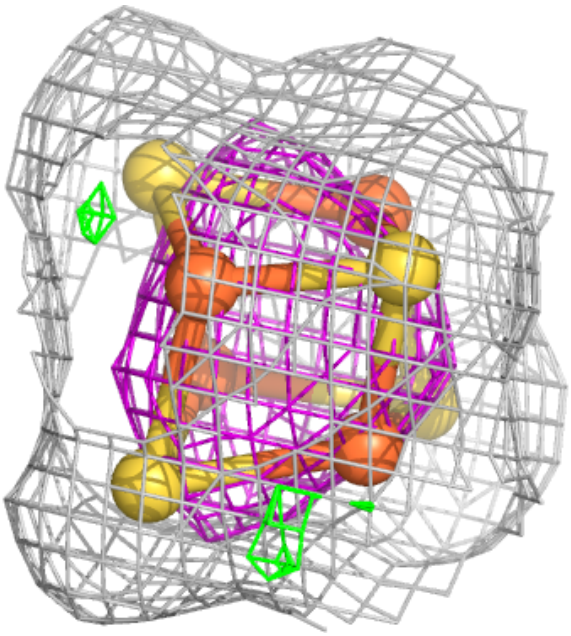
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

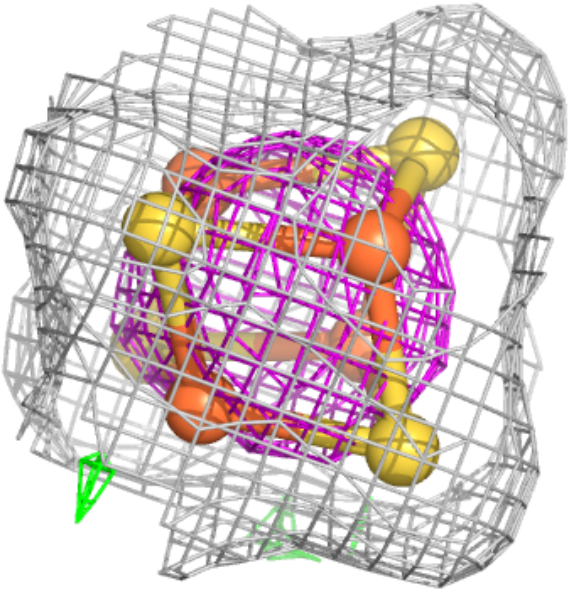
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SF4	A	1104	8/8	0.92	0.07	20,23,24,24	0
2	SF4	B	1101	8/8	0.92	0.07	19,21,21,22	0
2	SF4	B	1103	8/8	0.92	0.07	18,19,21,21	0
2	SF4	B	1104	8/8	0.92	0.07	19,21,23,23	0
2	SF4	A	1103	8/8	0.93	0.07	19,22,24,24	0
2	SF4	B	1102	8/8	0.93	0.07	20,21,23,23	0
2	SF4	C	1104	8/8	0.93	0.07	21,22,23,23	0
2	SF4	D	1103	8/8	0.93	0.08	17,22,24,25	0
2	SF4	D	1104	8/8	0.93	0.06	21,23,25,25	0
2	SF4	C	1103	8/8	0.94	0.07	17,20,21,21	0
2	SF4	A	1101	8/8	0.94	0.07	18,21,22,23	0
2	SF4	D	1101	8/8	0.94	0.07	22,24,27,27	0
2	SF4	C	1101	8/8	0.94	0.07	19,21,22,23	0
2	SF4	C	1102	8/8	0.94	0.07	21,22,23,24	0
2	SF4	A	1102	8/8	0.95	0.06	15,16,19,20	0
2	SF4	D	1102	8/8	0.95	0.06	19,20,21,21	0
3	FMN	C	1105	31/31	0.97	0.16	17,23,26,33	0
4	FAD	A	1106	53/53	0.97	0.12	20,27,31,38	0
4	FAD	B	1106	53/53	0.97	0.12	23,31,37,43	0
4	FAD	C	1106	53/53	0.97	0.12	20,32,37,39	0
4	FAD	D	1106	53/53	0.97	0.12	25,34,41,41	0
5	TDR	B	1107	9/9	0.97	0.13	22,25,27,28	0
5	TDR	D	1107	9/9	0.97	0.12	22,25,27,27	0
3	FMN	B	1105	31/31	0.98	0.14	16,24,29,33	0
5	TDR	A	1107	9/9	0.98	0.13	21,21,25,27	0
3	FMN	A	1105	31/31	0.98	0.17	19,28,36,37	0
3	FMN	D	1105	31/31	0.98	0.15	19,23,28,31	0
5	TDR	C	1107	9/9	0.99	0.14	18,20,23,25	0

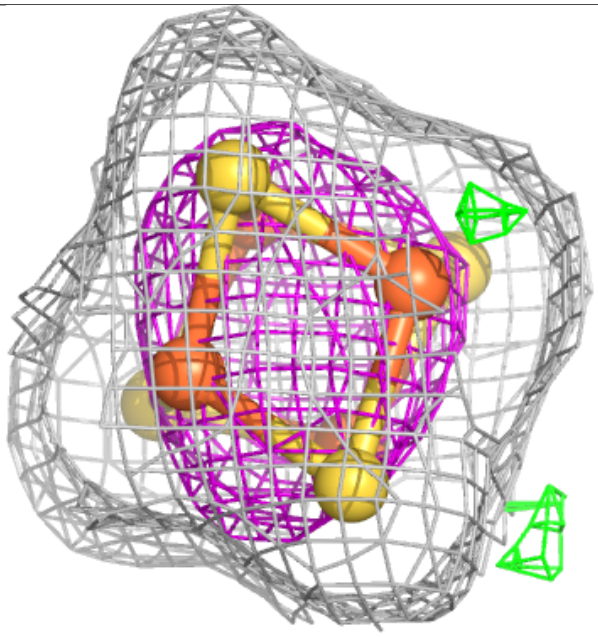
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SF4 A 1104:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

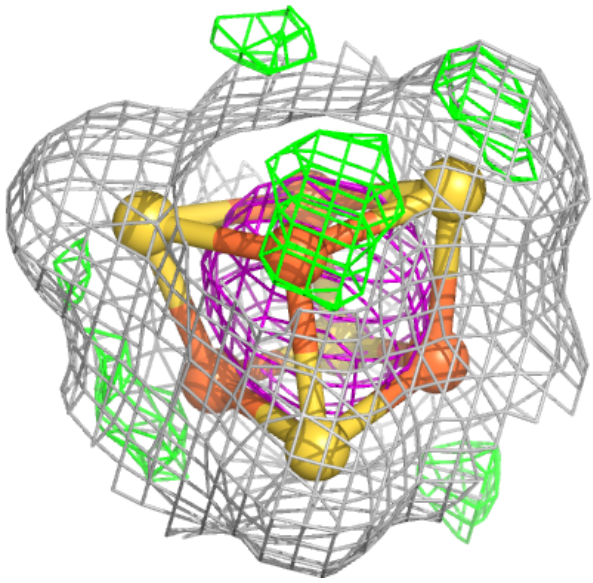


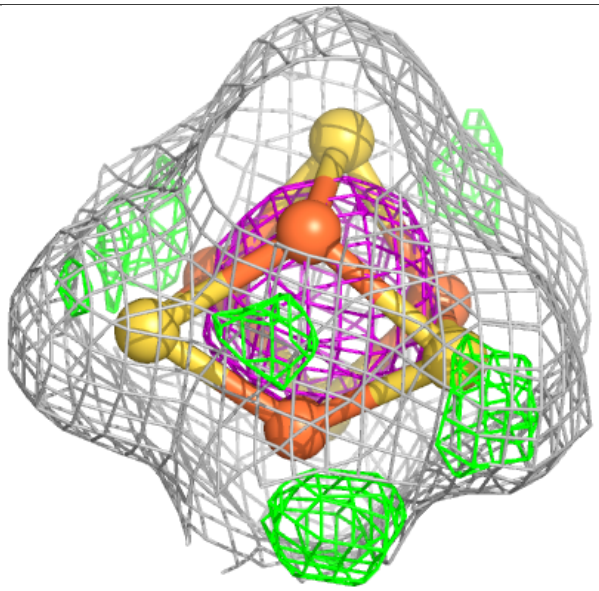


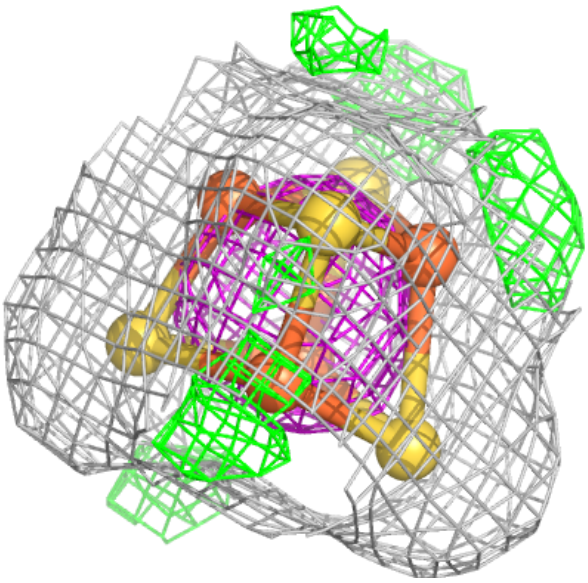


Electron density around SF4 B 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

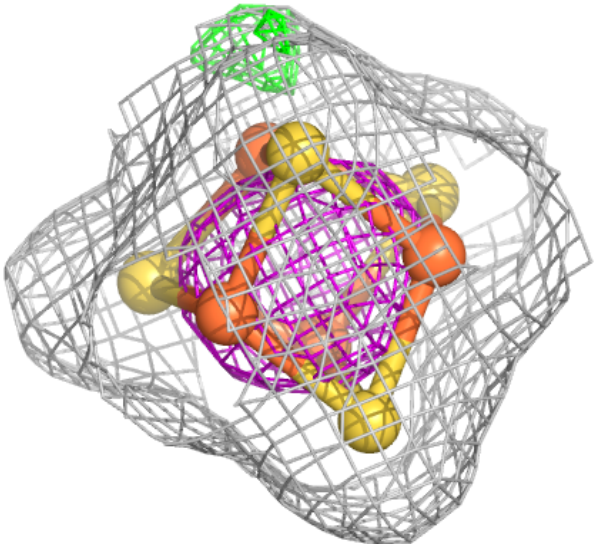


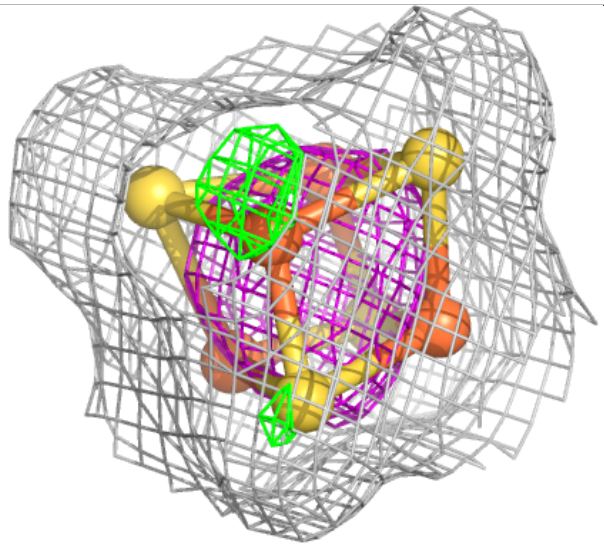


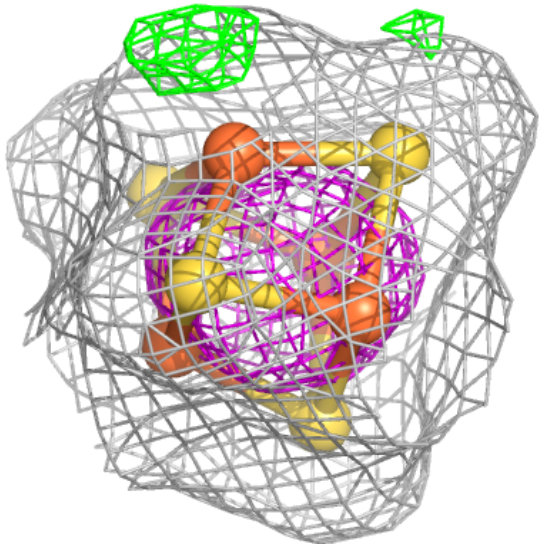


Electron density around SF4 B 1103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

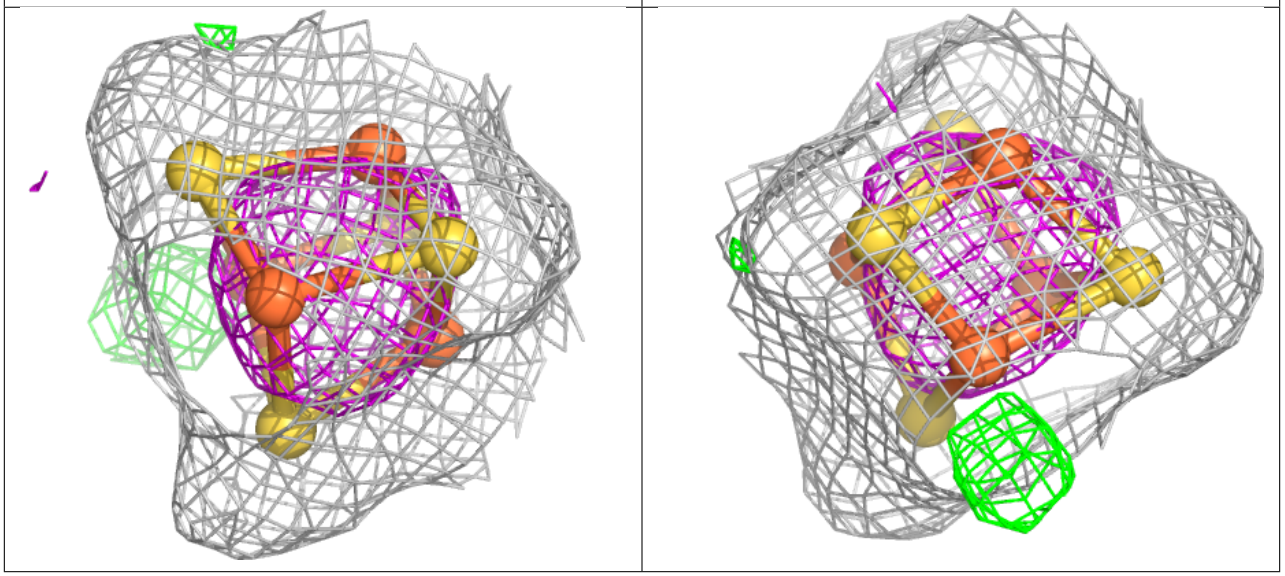






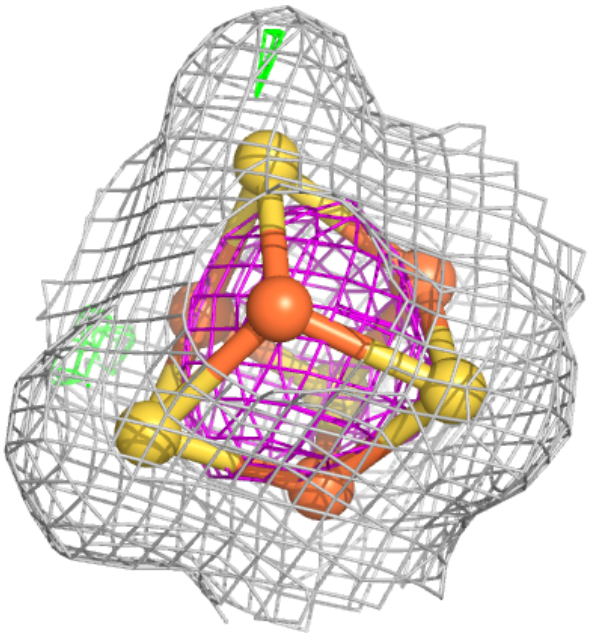
Electron density around SF4 B 1104:

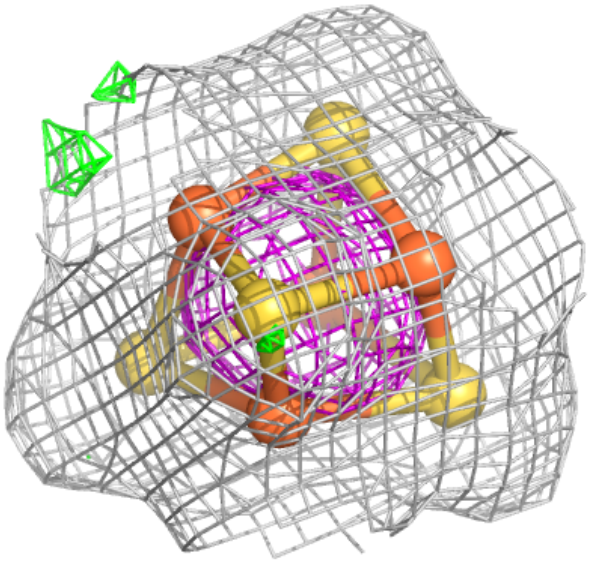
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

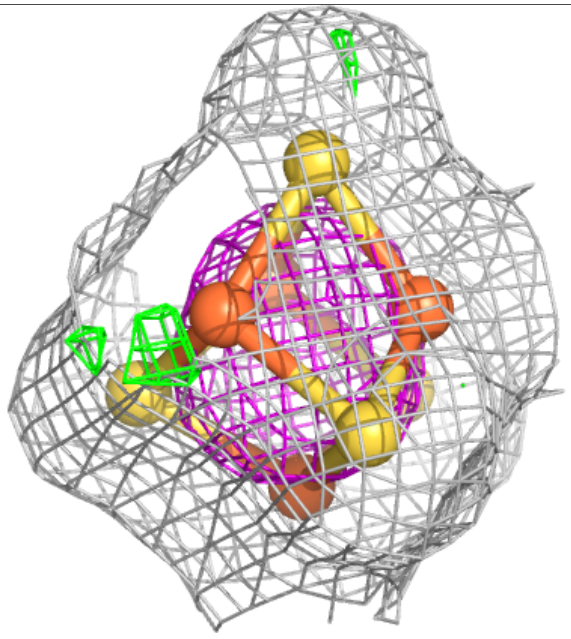


Electron density around SF4 A 1103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

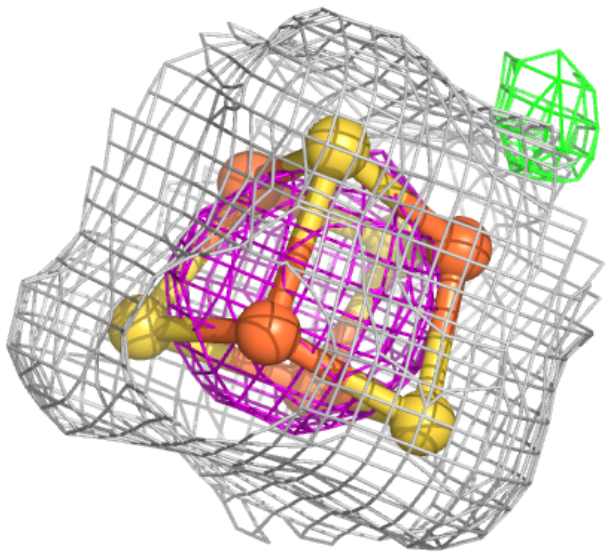


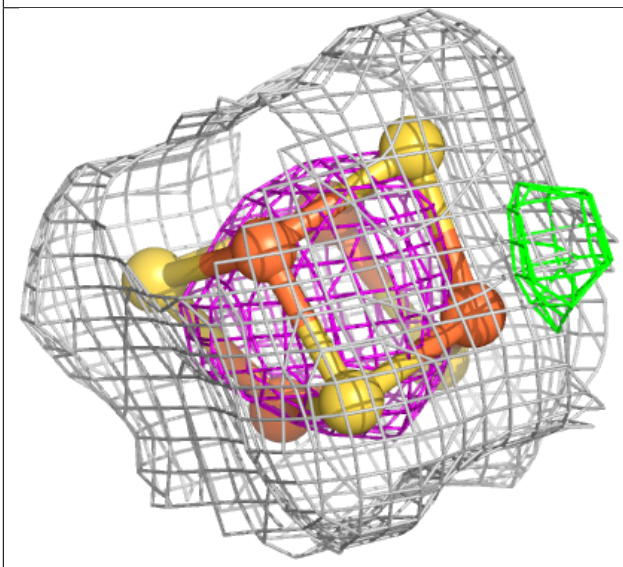


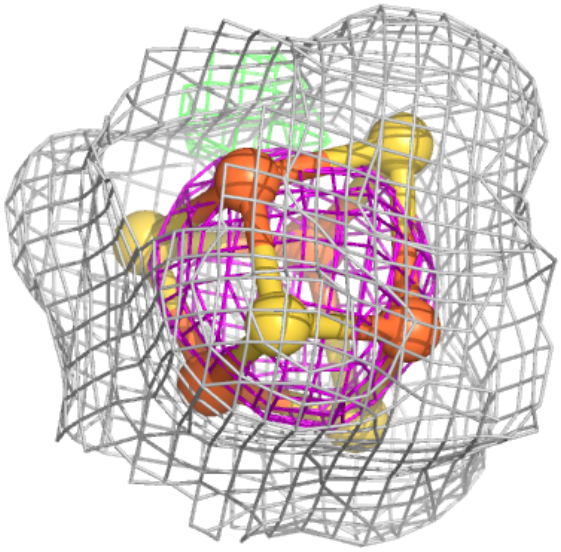


Electron density around SF4 B 1102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

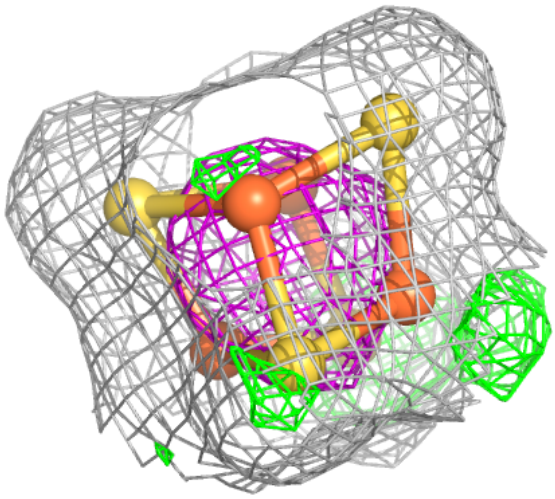


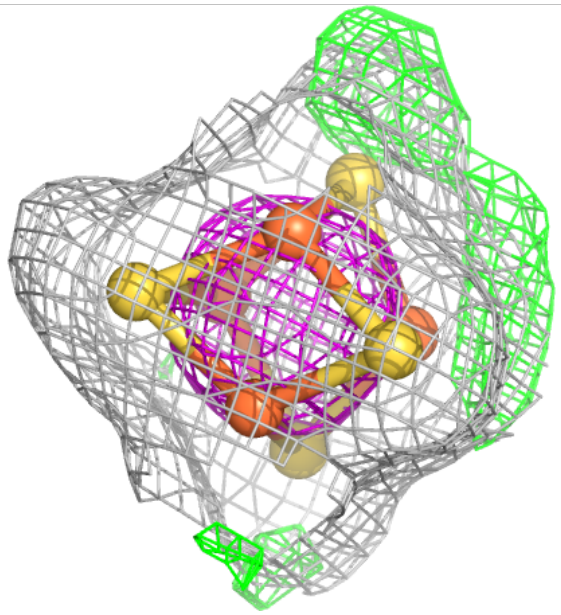


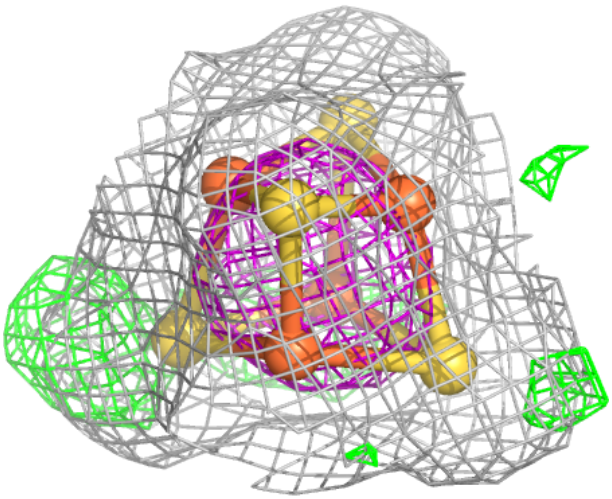


Electron density around SF4 C 1104:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

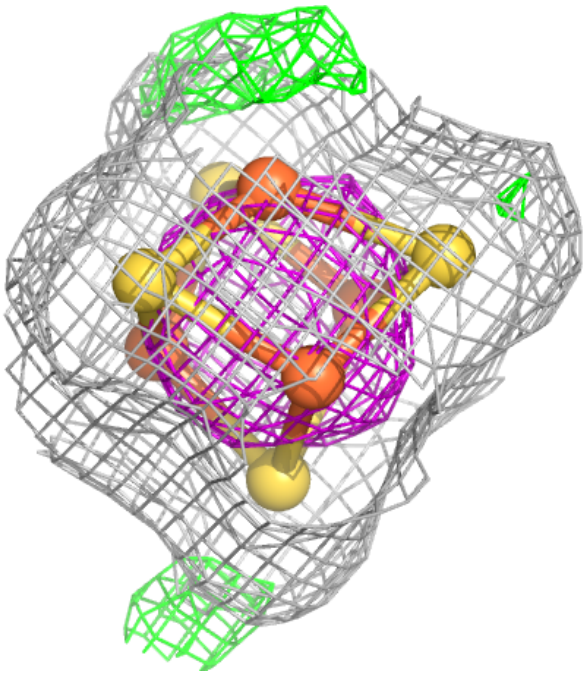


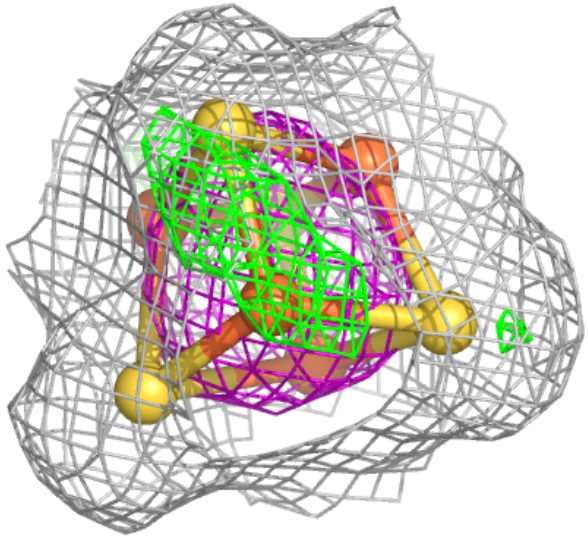


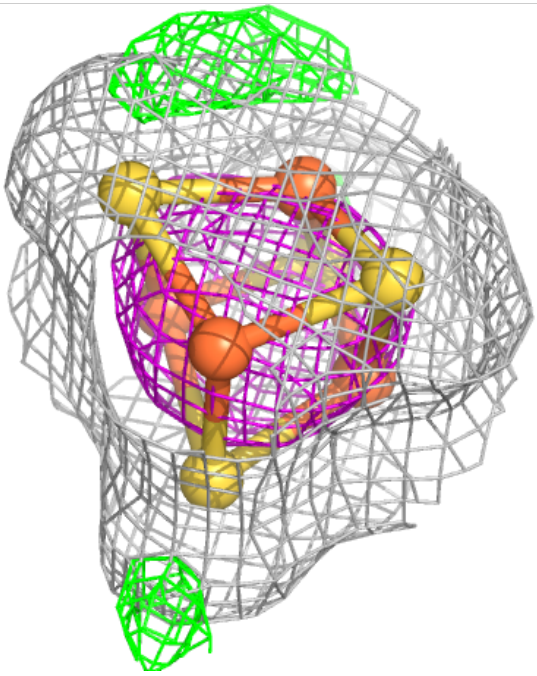


Electron density around SF4 D 1103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

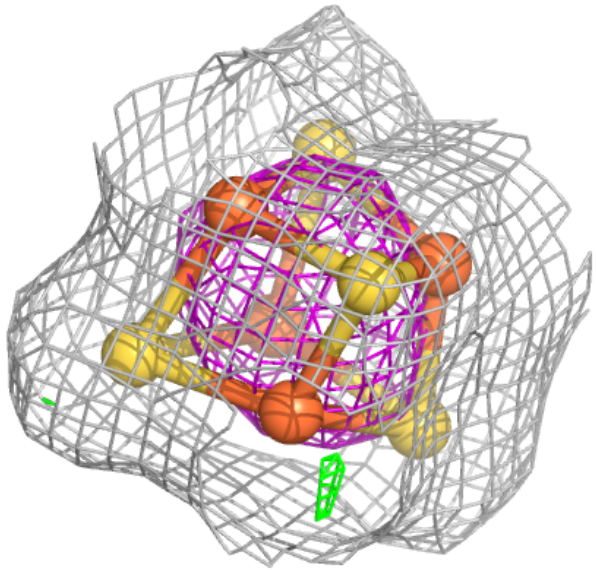


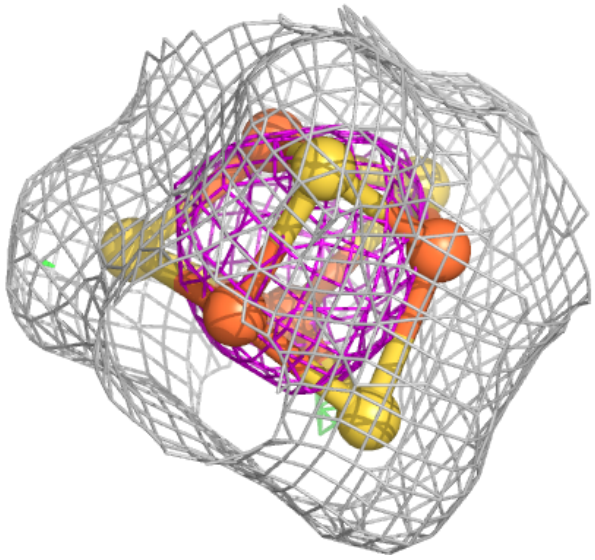


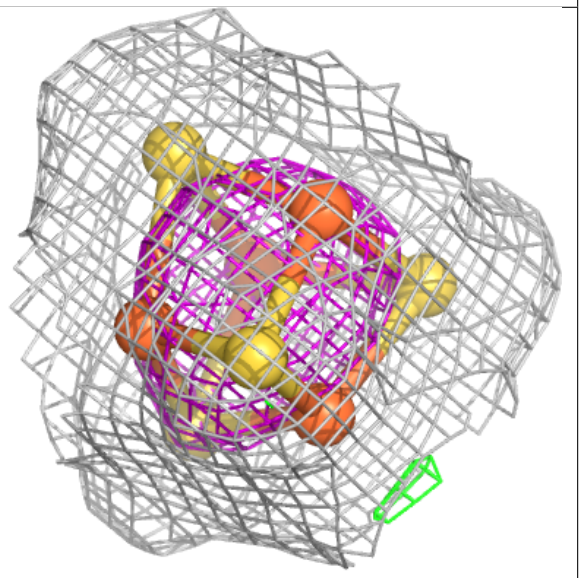


Electron density around SF4 D 1104:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

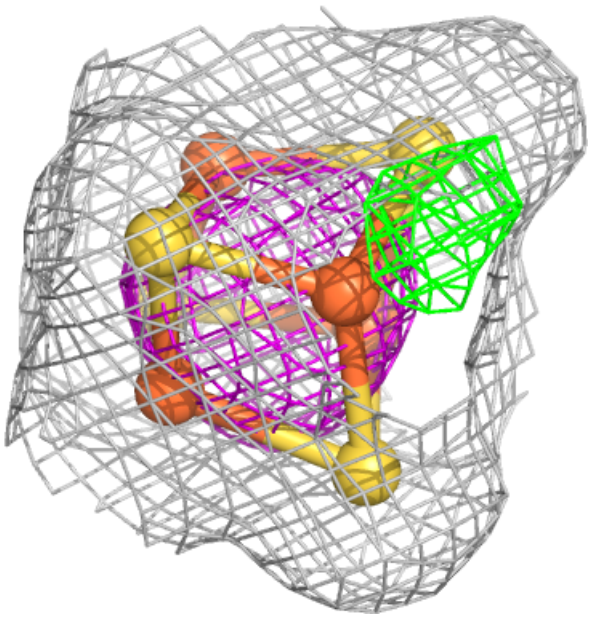


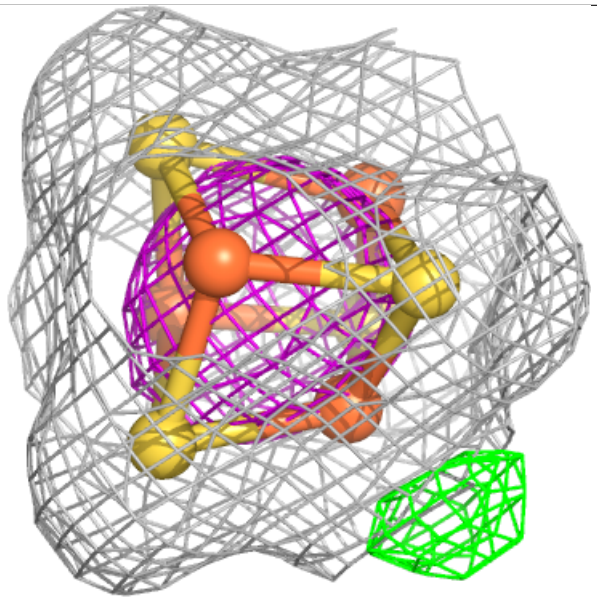


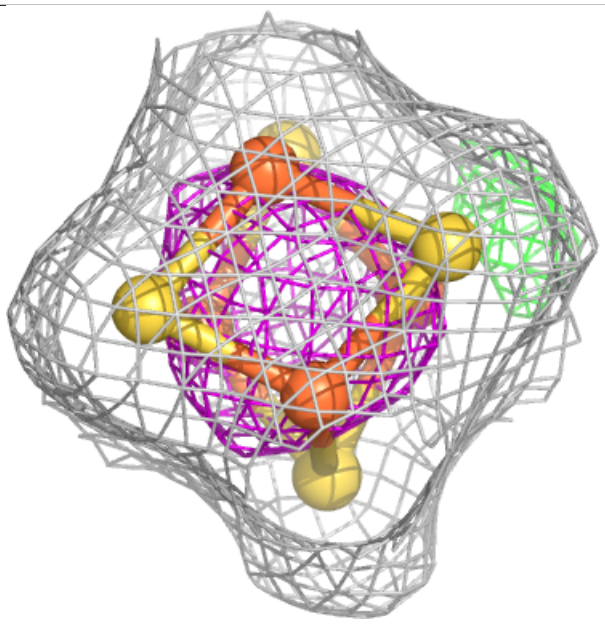


Electron density around SF4 C 1103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

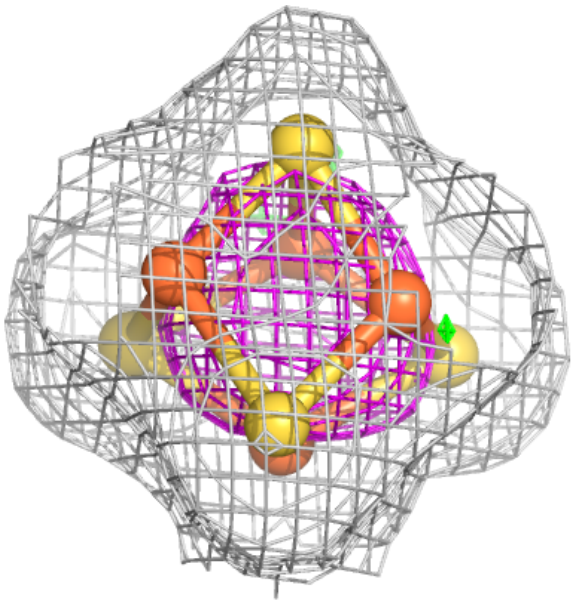


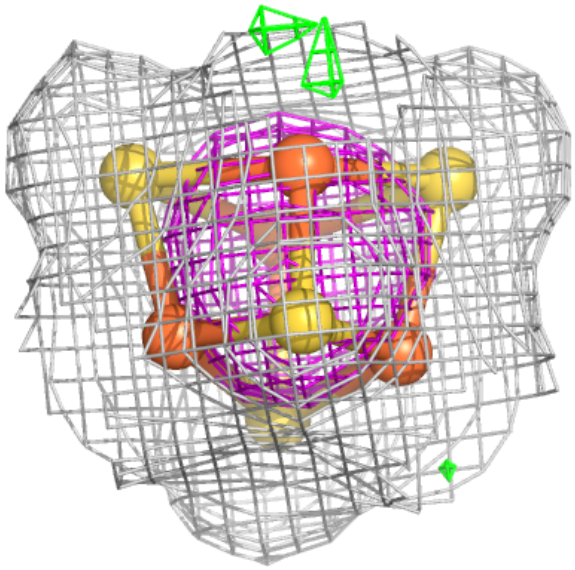


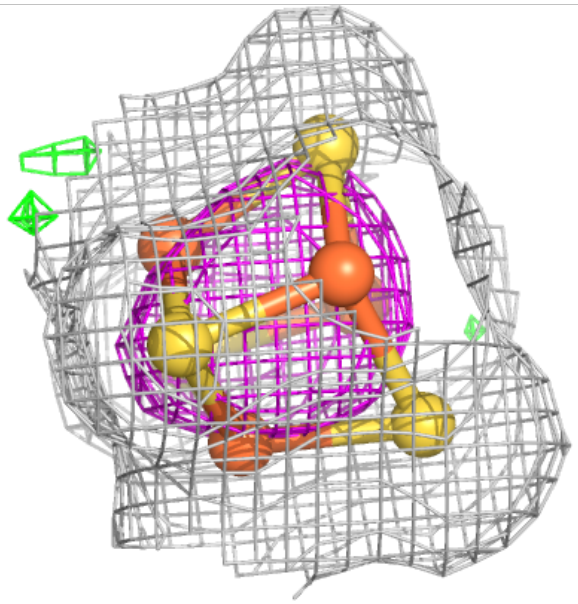


Electron density around SF4 A 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

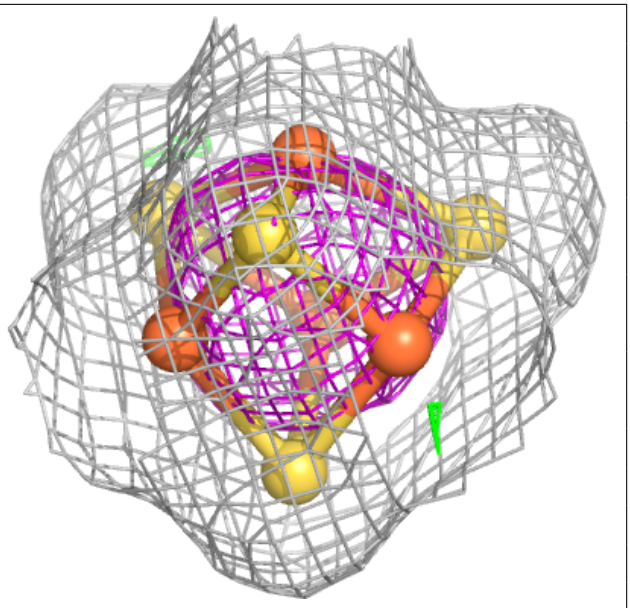


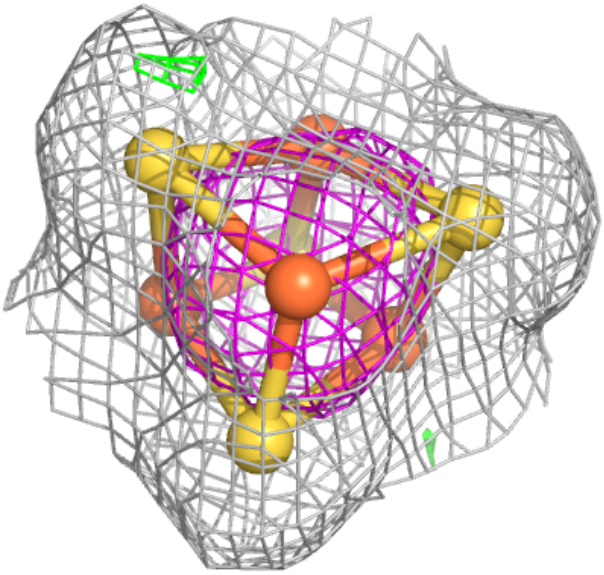


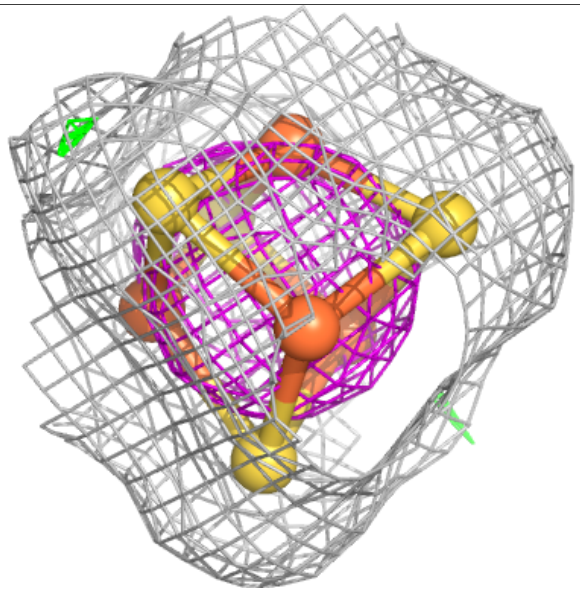


Electron density around SF4 D 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

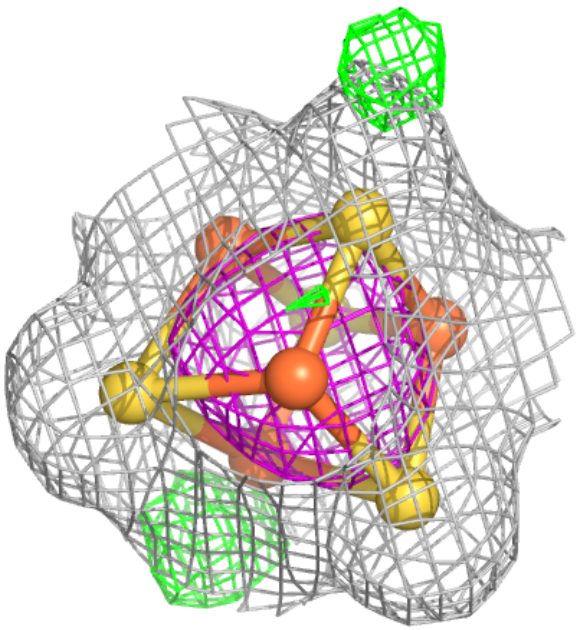


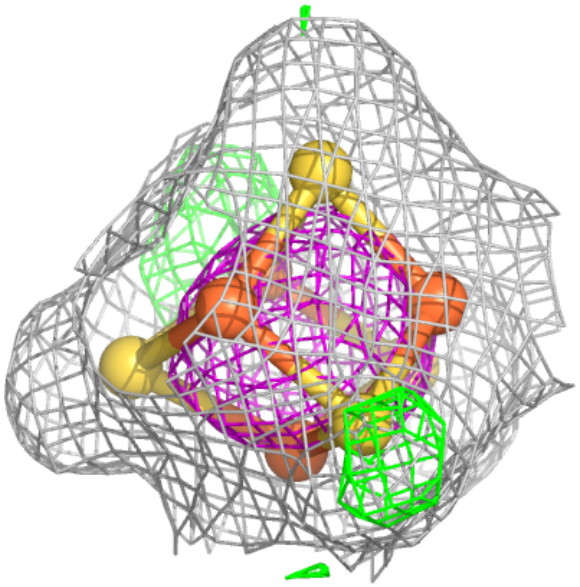


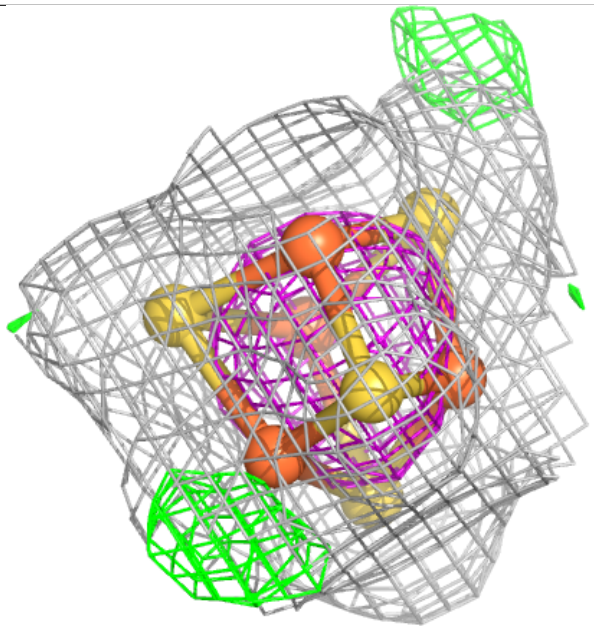


Electron density around SF4 C 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

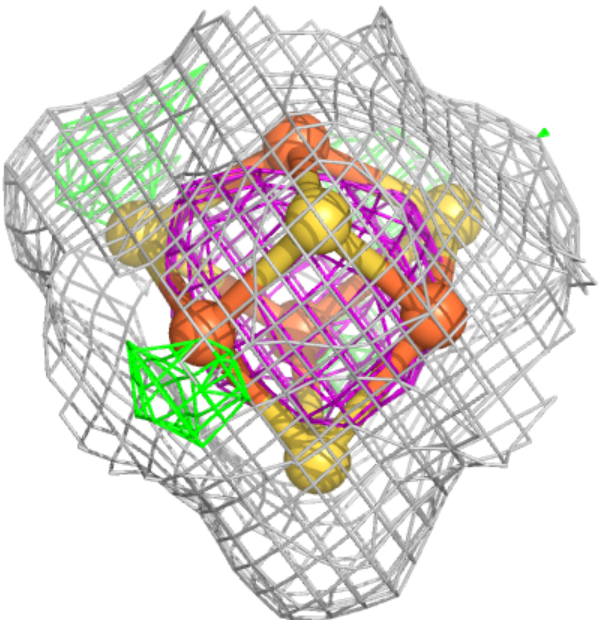


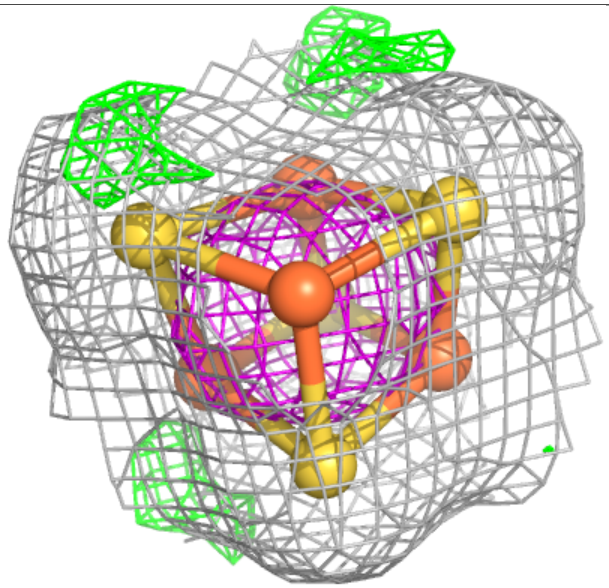


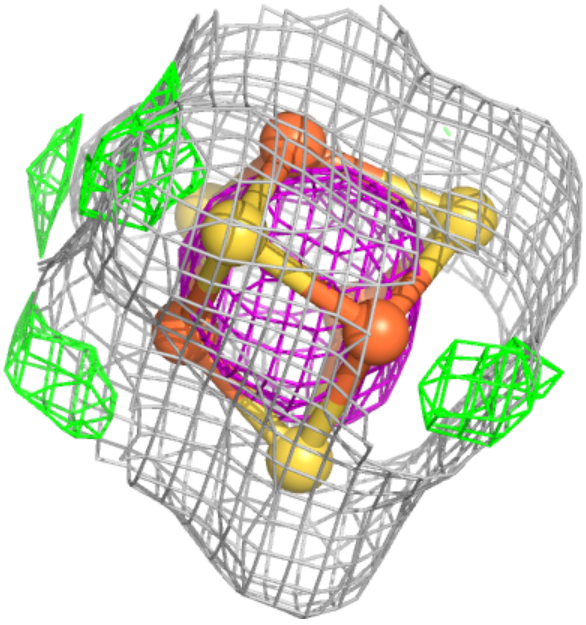


Electron density around SF4 C 1102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

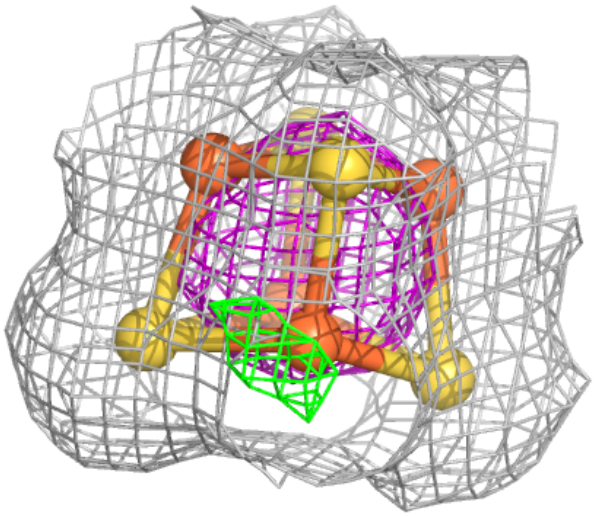


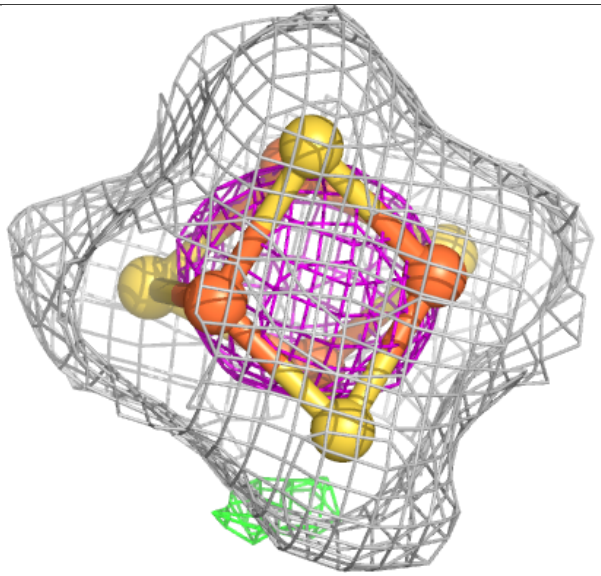


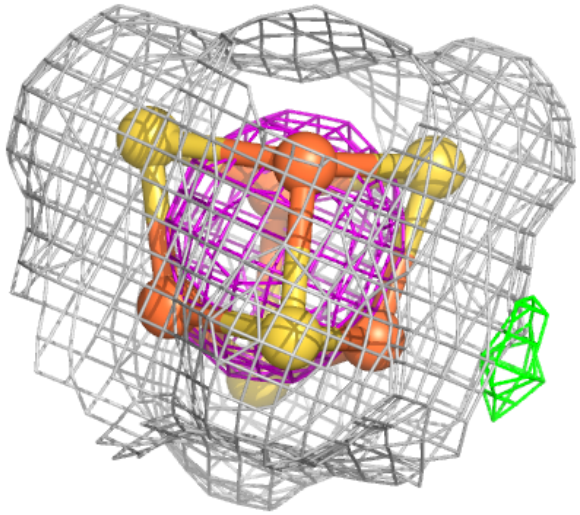


Electron density around SF4 A 1102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

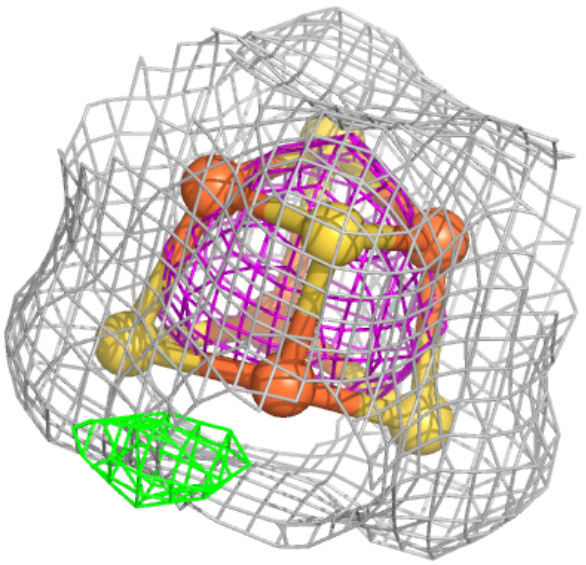


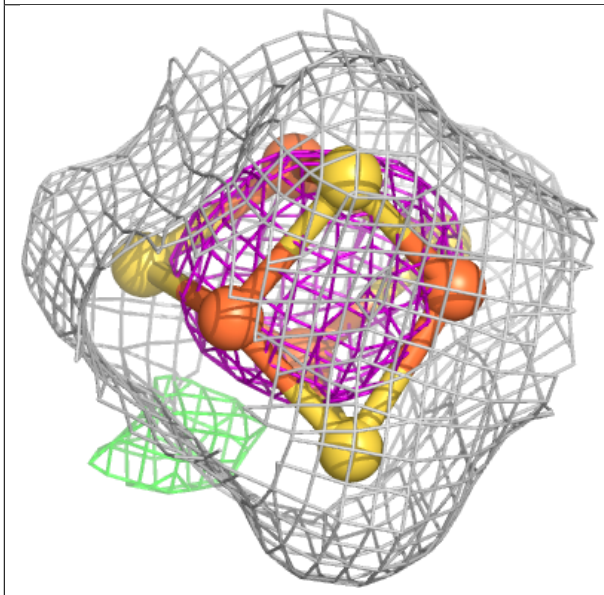


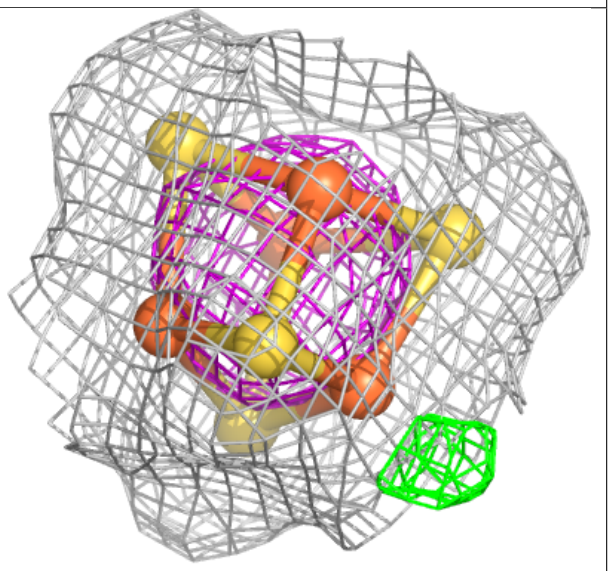


Electron density around SF4 D 1102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

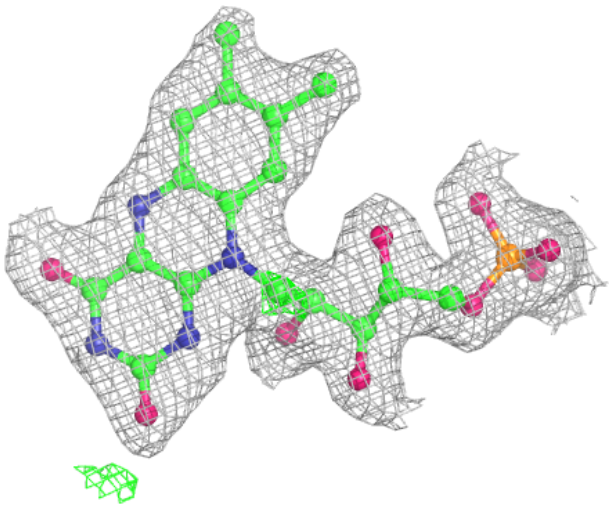


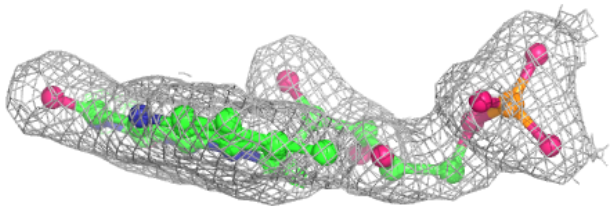


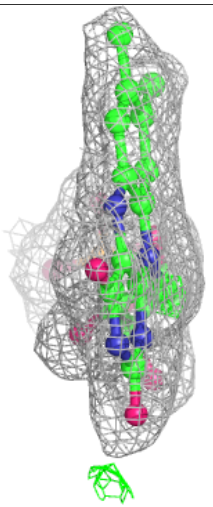


Electron density around FMN C 1105:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

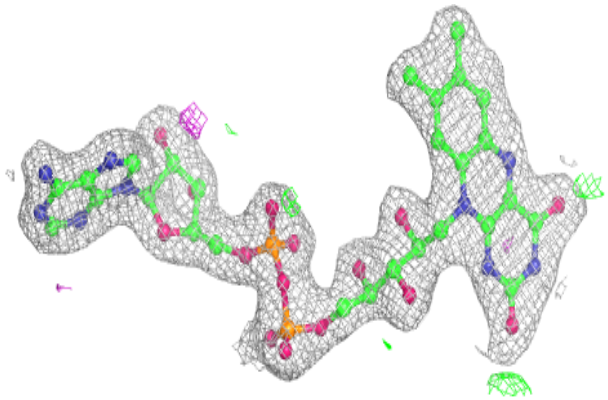


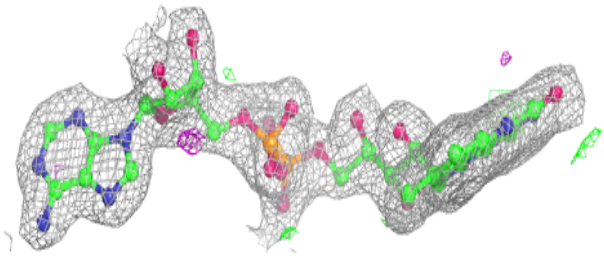


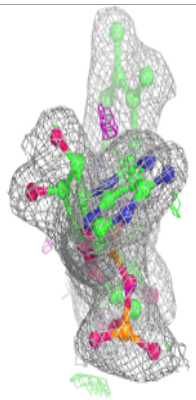


Electron density around FAD A 1106:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

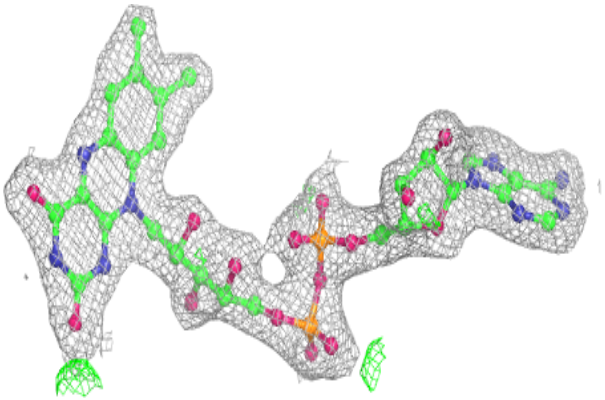


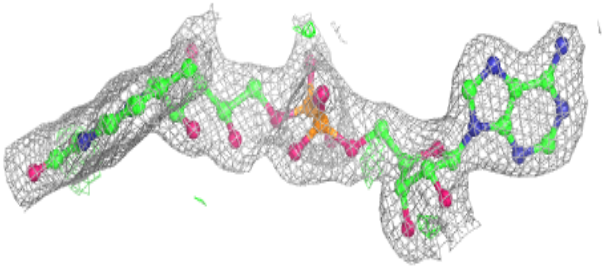


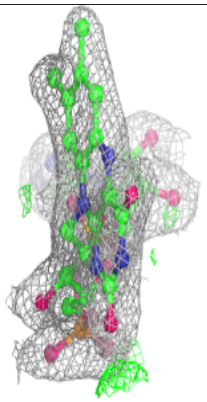


Electron density around FAD B 1106:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

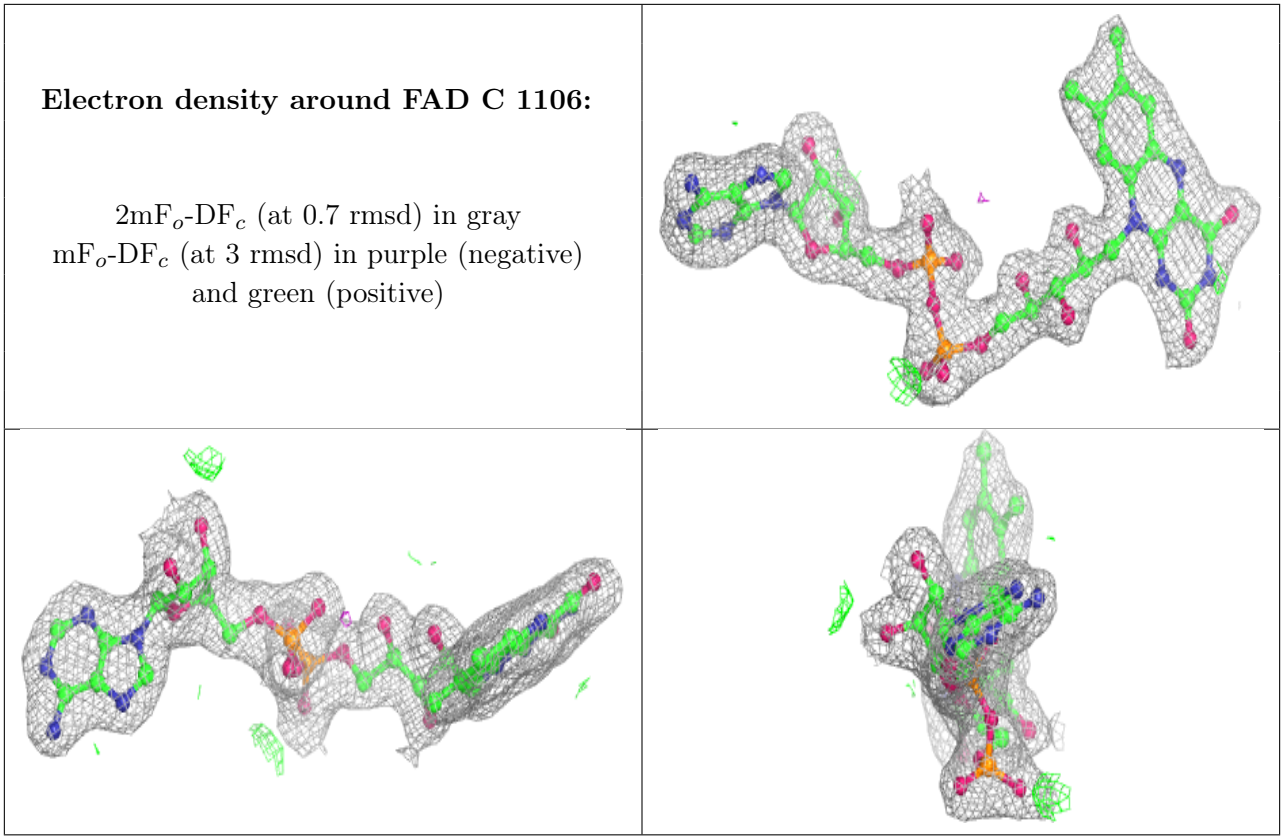






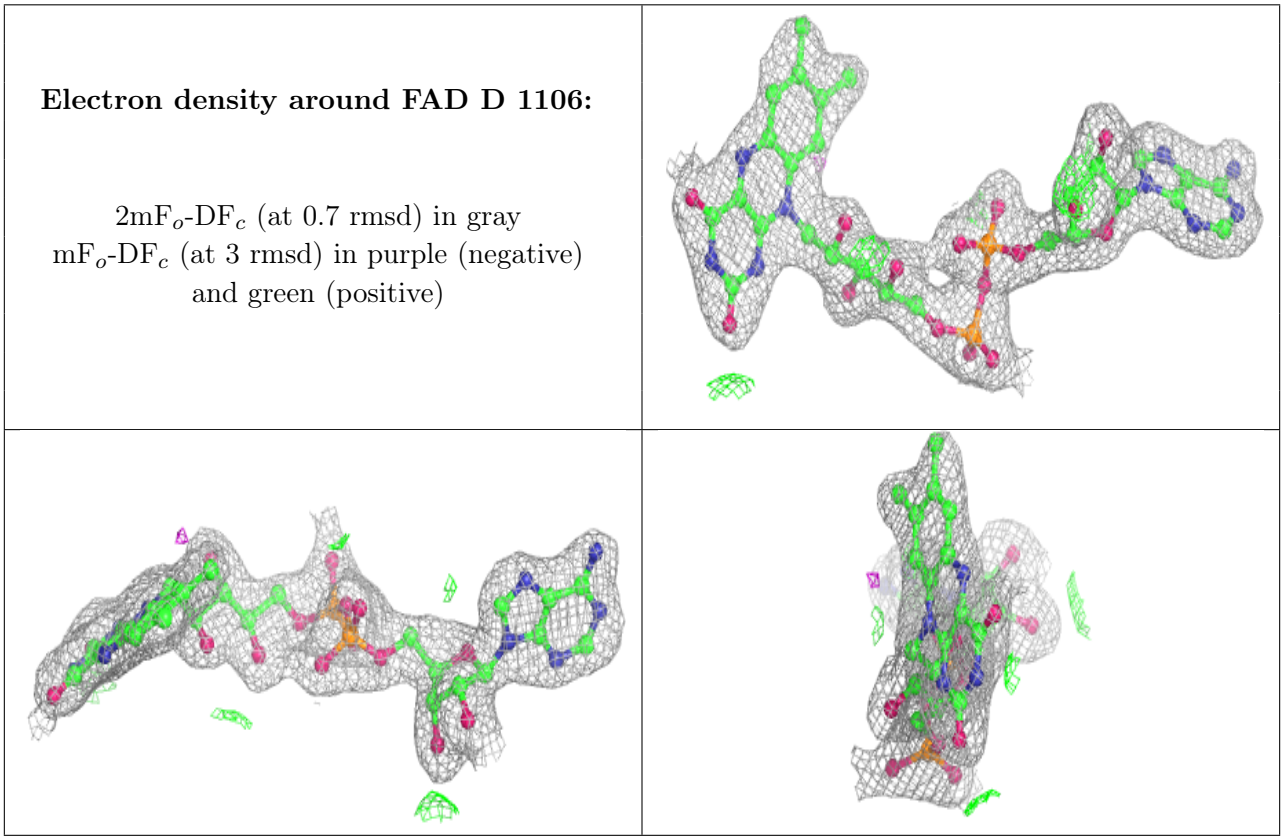
Electron density around FAD C 1106:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



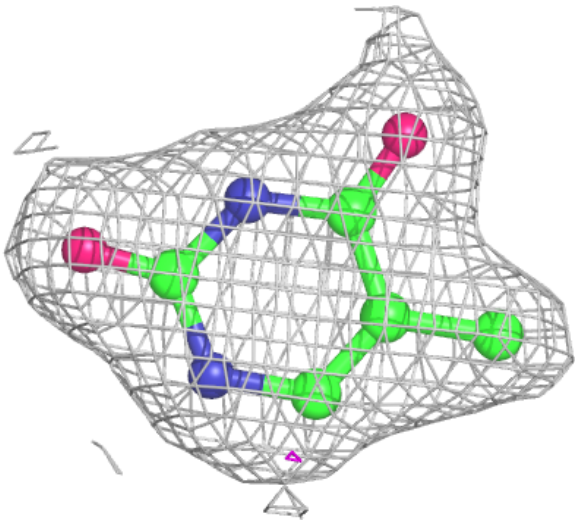
Electron density around FAD D 1106:

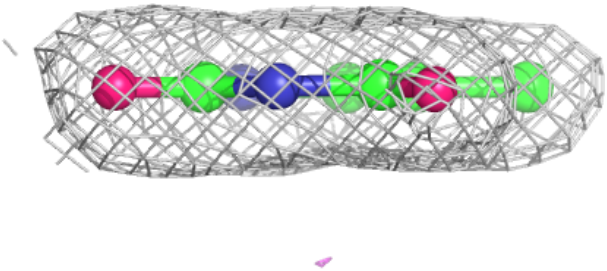
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

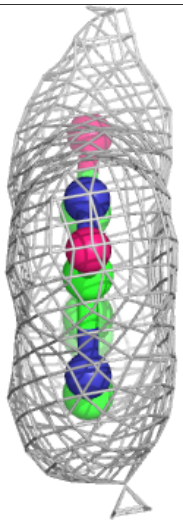


Electron density around TDR B 1107:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

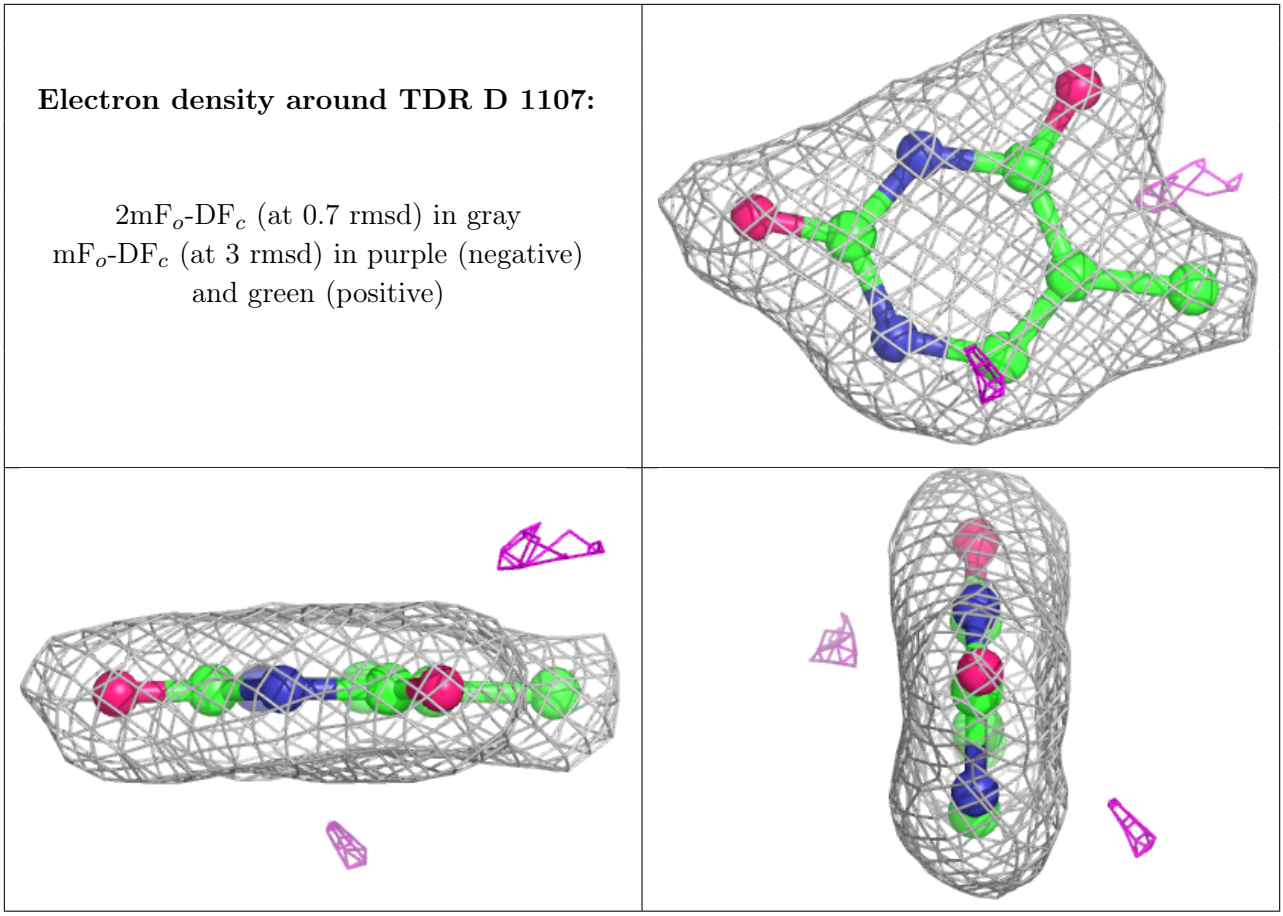






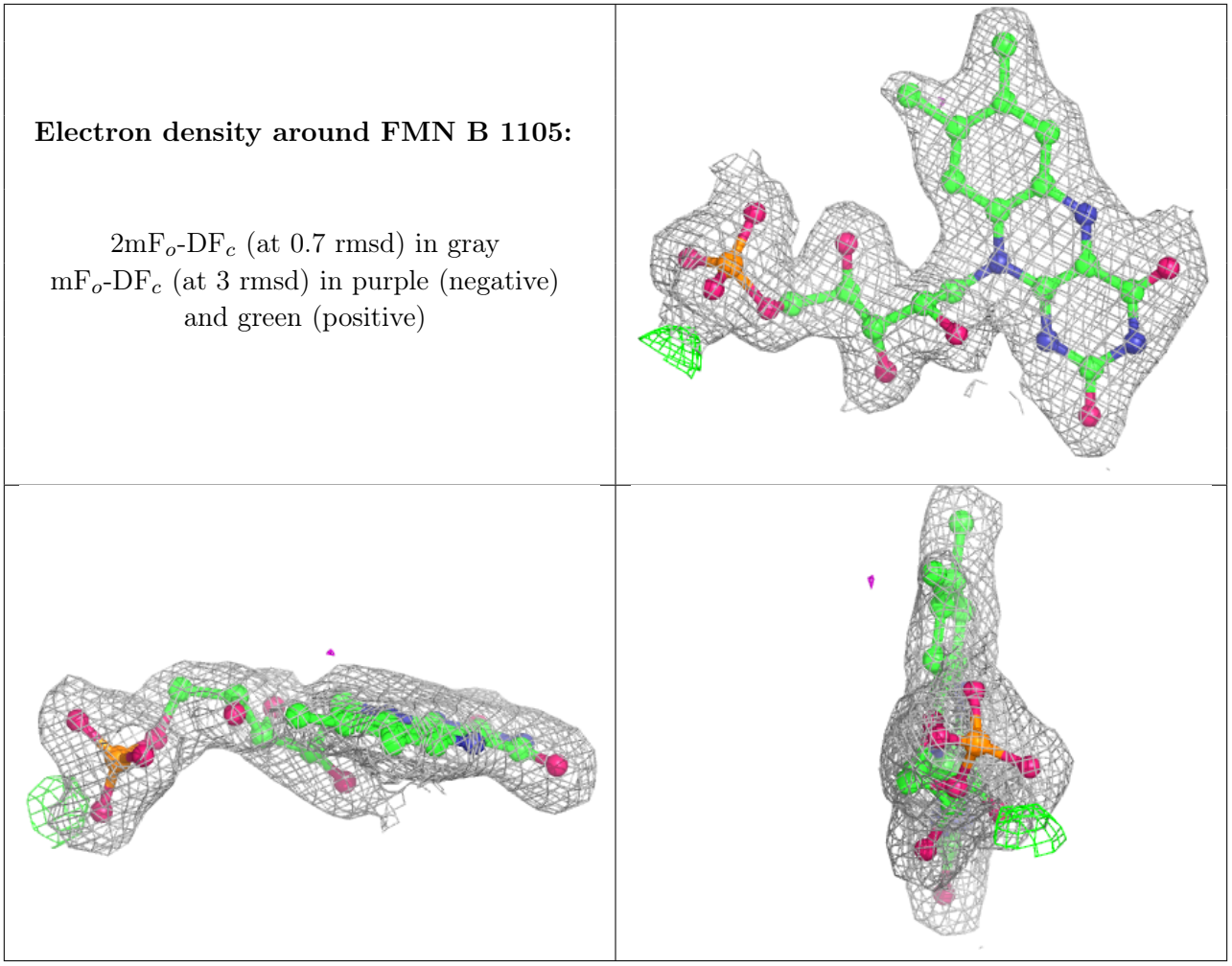
Electron density around TDR D 1107:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



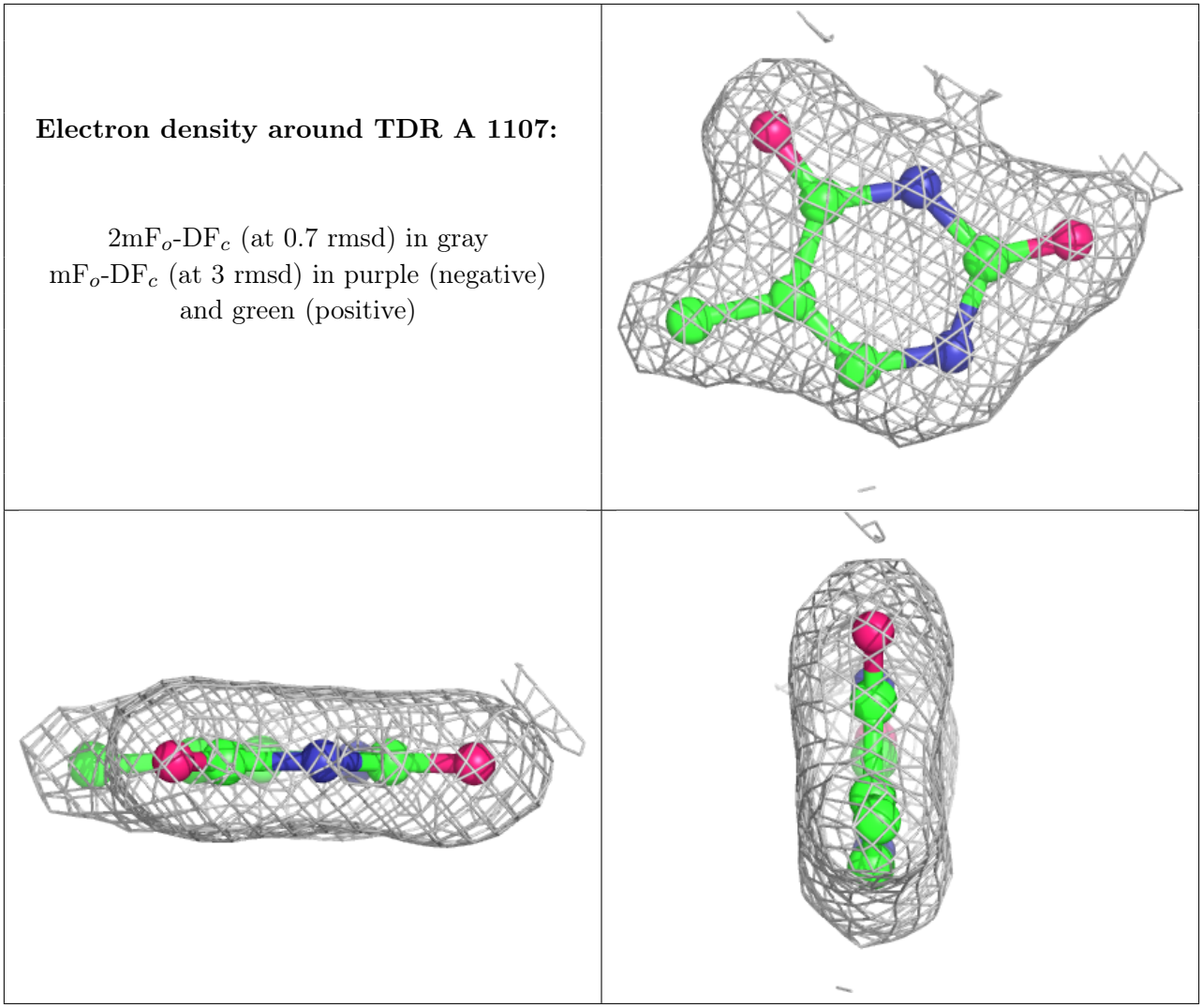
Electron density around FMN B 1105:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



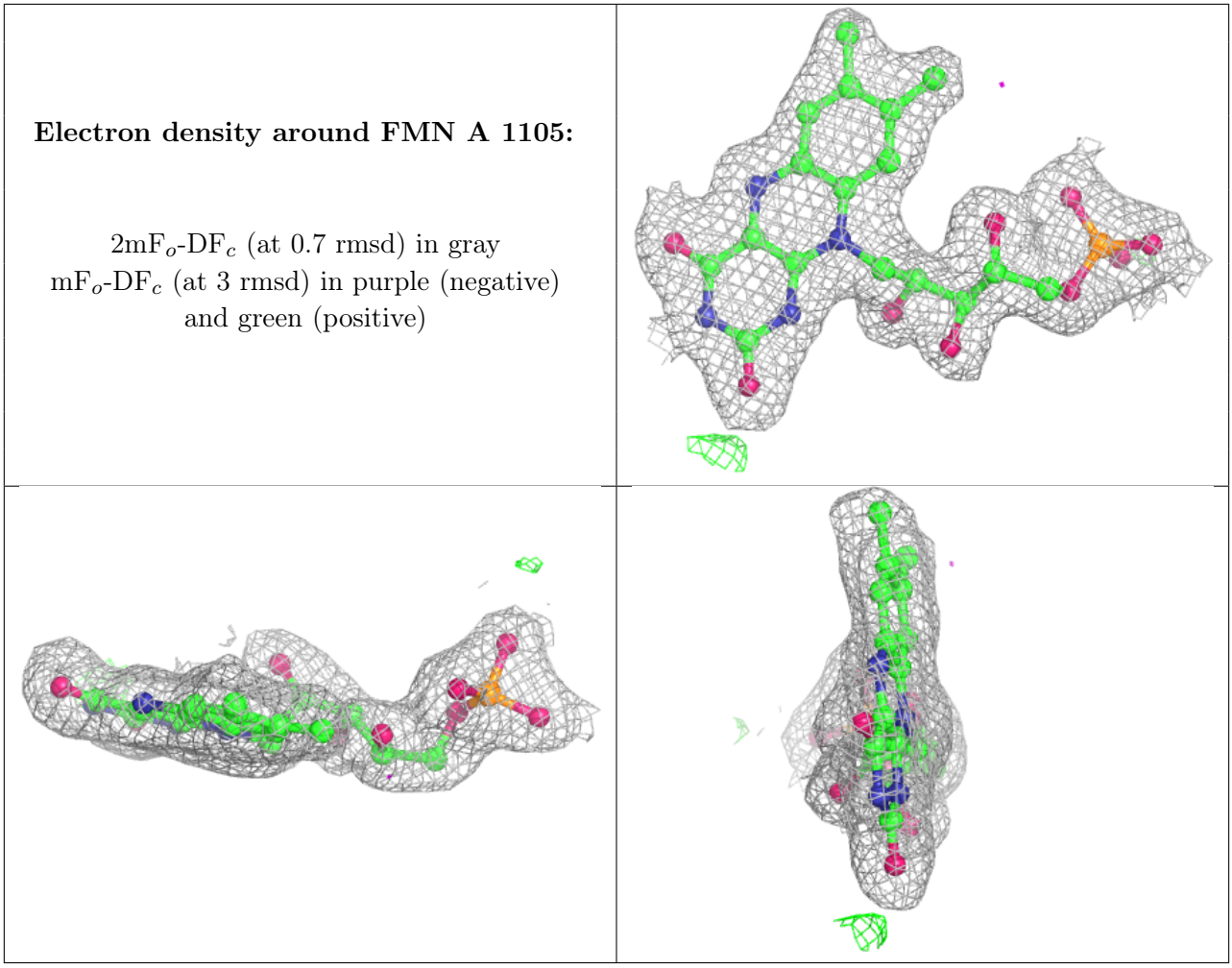
Electron density around TDR A 1107:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



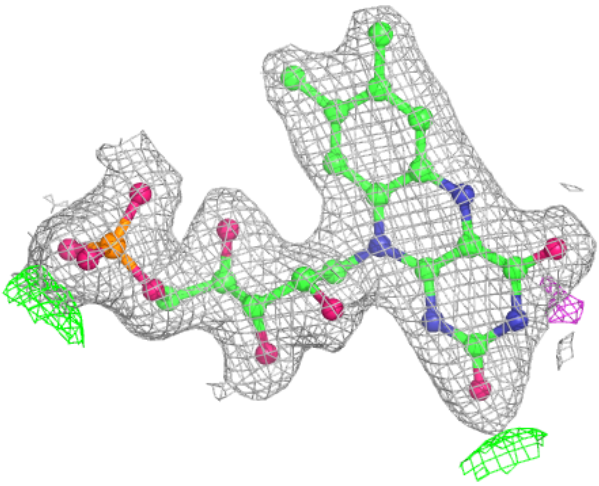
Electron density around FMN A 1105:

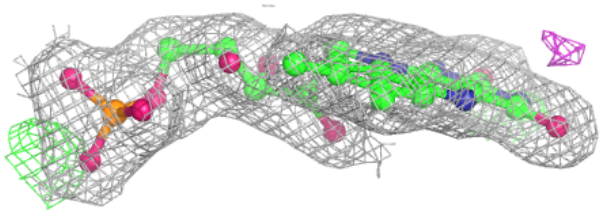
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

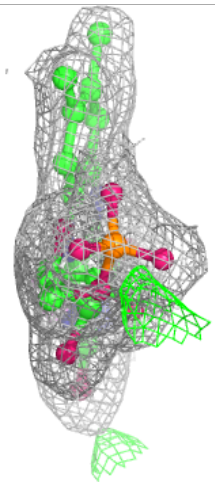


Electron density around FMN D 1105:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

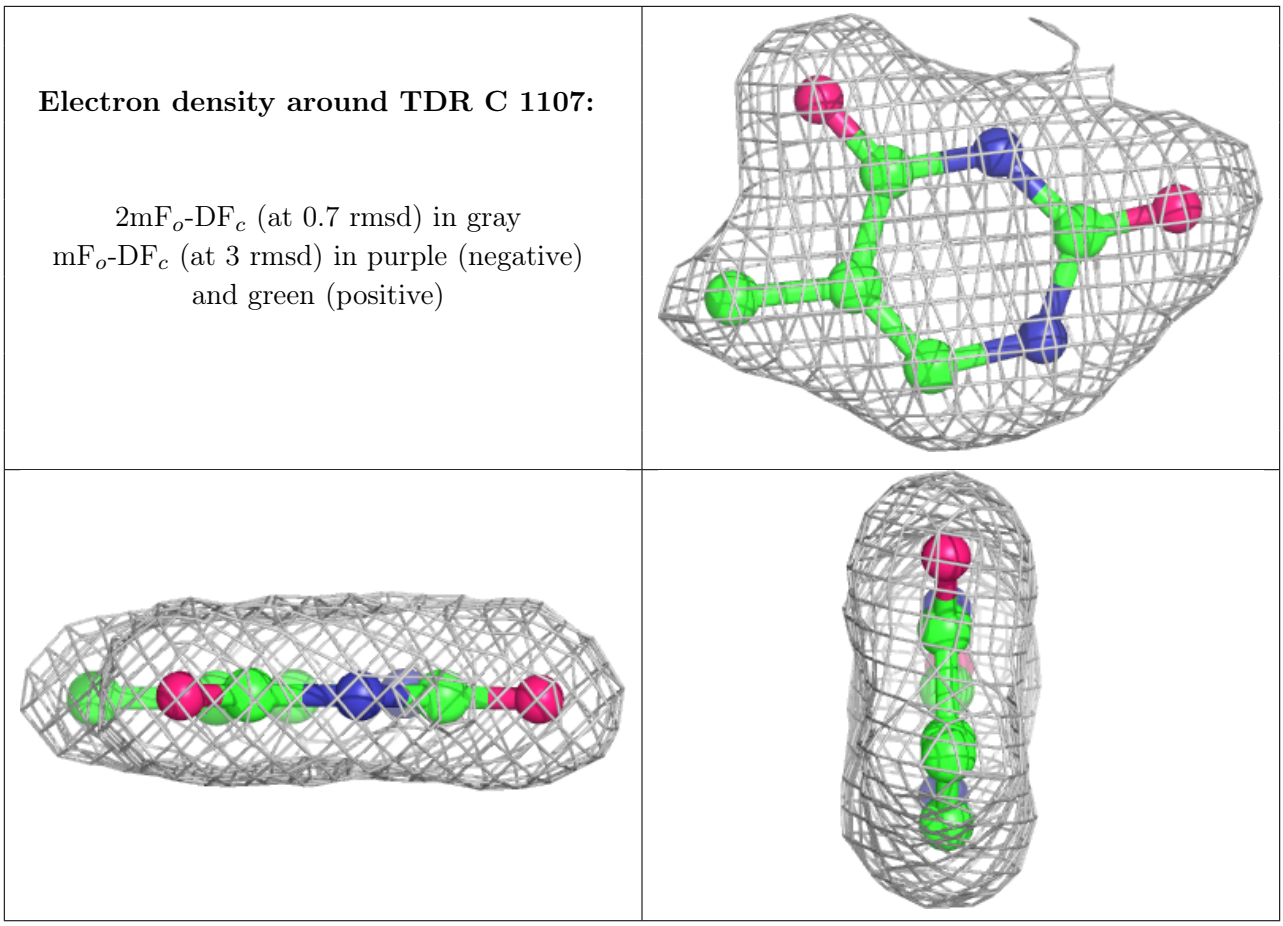






Electron density around TDR C 1107:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.