



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:42 AM UTC

PDB ID : 8A8O / pdb_00008a8o
Title : PAPS reductase from Methanothermococcus thermolithotrophicus refined to 1.45 Å
Authors : Jespersen, M.; Wagner, T.
Deposited on : 2022-06-23
Resolution : 1.45 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

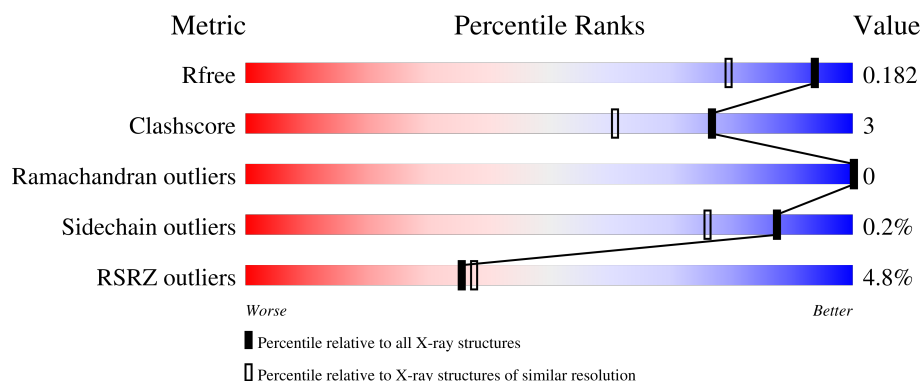
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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 $\leq 5\%$. 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	571	3% 90% 7% .
1	B	571	7% 90% 5% 5%
2	C	104	% 94% . .
2	D	104	5% 89% 9% .

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 11470 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.

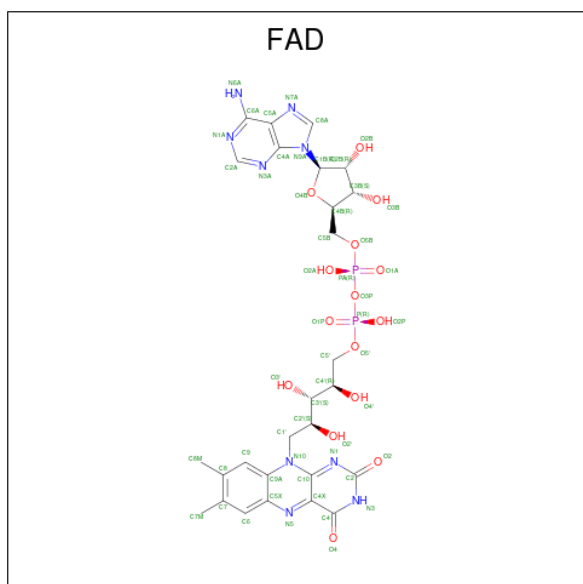
- Molecule 1 is a protein called Alpha-subunit of the PAPS reductase from Methanothermococcus thermolithotrophicus.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	6	0
			4446	2817	756	849	24			
1	B	544	Total	C	N	O	S	0	5	0
			4344	2759	732	830	23			

- Molecule 2 is a protein called Beta-subunit of the PAPS reductase from Methanothermococcus thermolithotrophicus.

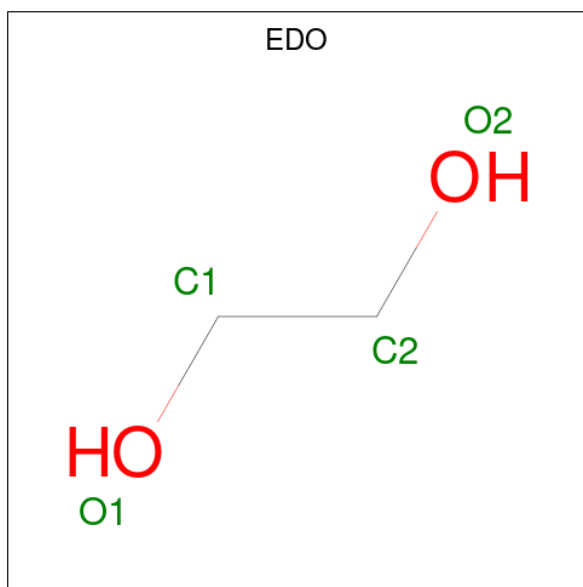
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	101	Total	C	N	O	S	0	0	0
			785	488	132	155	10			
2	D	102	Total	C	N	O	S	0	0	0
			793	492	133	158	10			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



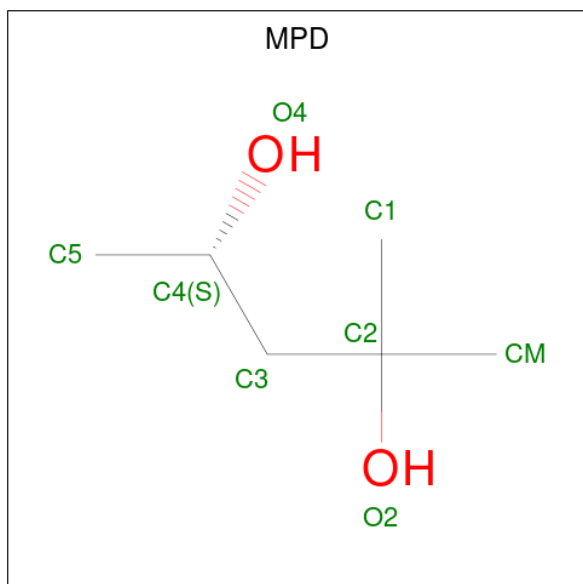
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



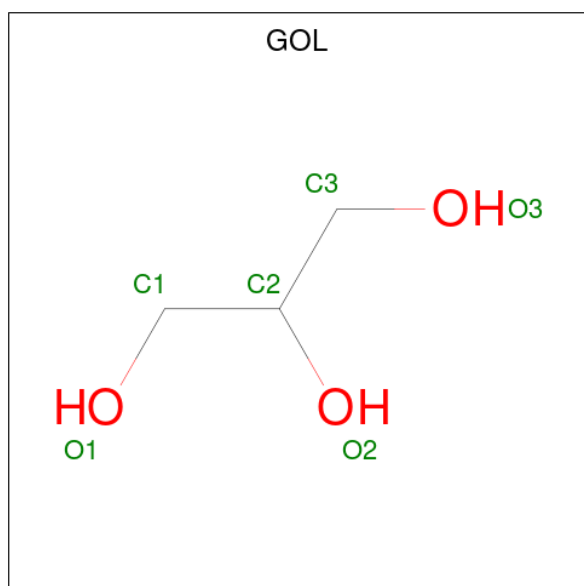
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0
5	C	1	Total C O 8 6 2	0	0
5	D	1	Total C O 8 6 2	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	1
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	1
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

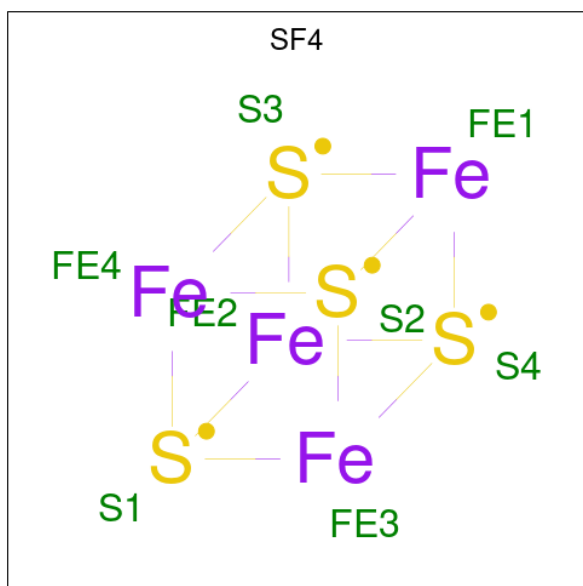
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Na 1 1	0	0
8	B	1	Total Na 1 1	0	0
8	C	1	Total Na 1 1	0	0

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total Fe S 8 4 4	0	0
9	C	1	Total Fe S 8 4 4	0	0
9	D	1	Total Fe S 8 4 4	0	0
9	D	1	Total Fe S 8 4 4	0	0

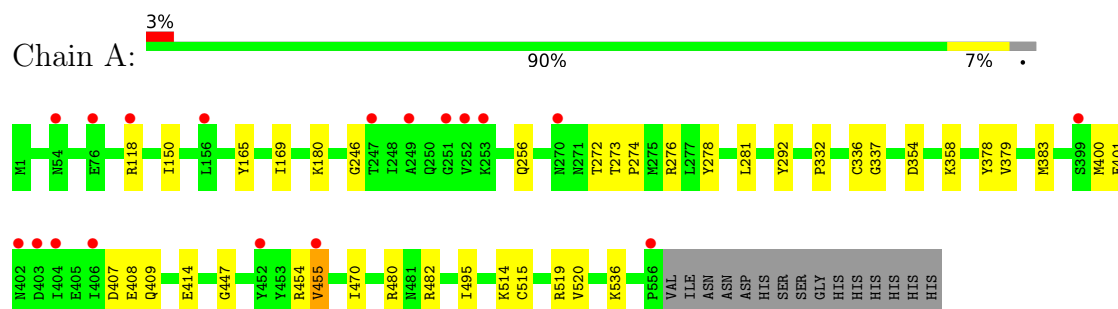
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	382	Total 382	O 382	0	16
10	B	298	Total 298	O 298	0	11
10	C	94	Total 94	O 94	0	1
10	D	105	Total 105	O 105	0	4

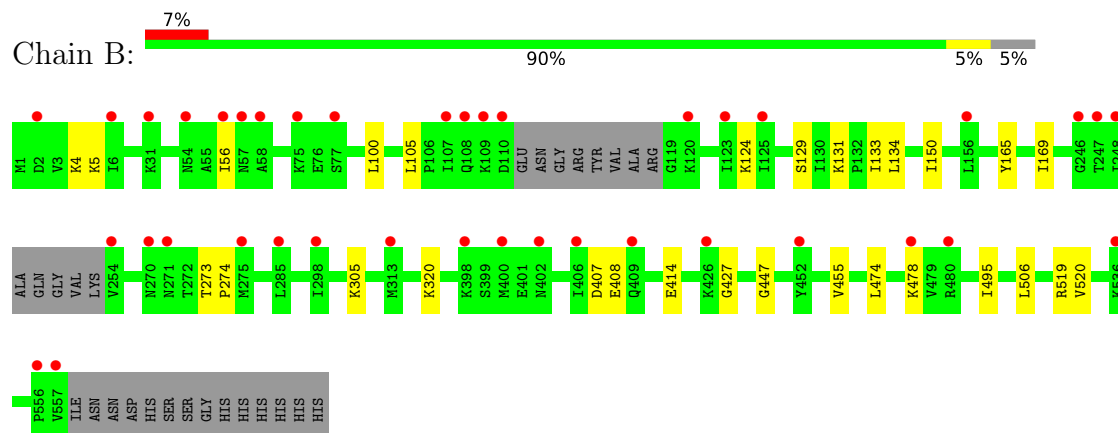
3 Residue-property plots

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.

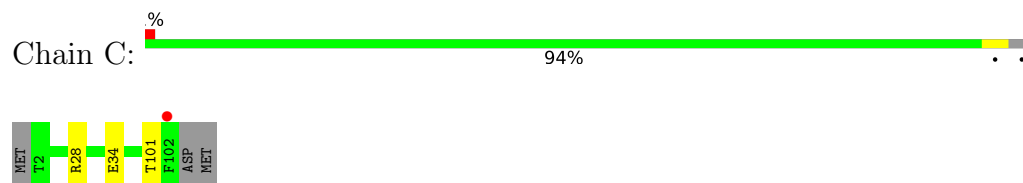
- Molecule 1: Alpha-subunit of the PAPS reductase from *Methanothermococcus thermolithotrophicus*



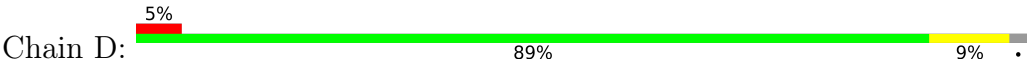
- Molecule 1: Alpha-subunit of the PAPS reductase from *Methanothermococcus thermolithotrophicus*



- Molecule 2: Beta-subunit of the PAPS reductase from *Methanothermococcus thermolithotrophicus*



- Molecule 2: Beta-subunit of the PAPS reductase from *Methanothermococcus thermolithotrophicus*



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.71Å 123.65Å 88.84Å 90.00° 104.44° 90.00°	Depositor
Resolution (Å)	52.04 – 1.45 52.04 – 1.45	Depositor EDS
% Data completeness (in resolution range)	62.3 (52.04-1.45) 62.3 (52.04-1.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.45Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.151 , 0.178 0.160 , 0.182	Depositor DCC
R_{free} test set	7256 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11470	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: CA, SF4, NA, EDO, MPD, FAD, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	1/4521 (0.0%)	0.49	0/6090
1	B	0.24	0/4416	0.45	0/5947
2	C	0.27	0/794	0.48	0/1068
2	D	0.32	0/802	0.50	0/1079
All	All	0.27	1/10533 (0.0%)	0.48	0/14184

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	455	VAL	C-N	-6.17	1.25	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4446	0	4482	31	0
1	B	4344	0	4388	23	0
2	C	785	0	781	2	0
2	D	793	0	785	6	0
3	A	53	0	31	2	0
3	B	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	6	0	0
5	A	8	0	14	0	0
5	B	16	0	28	0	0
5	C	8	0	14	0	0
5	D	8	0	14	0	0
6	A	24	0	32	4	0
6	B	12	0	16	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	C	16	0	0	0	0
9	D	16	0	0	0	0
10	A	382	0	0	0	0
10	B	298	0	0	1	0
10	C	94	0	0	0	0
10	D	105	0	0	1	0
All	All	11470	0	10622	61	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 3.

All (61) 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:118:ARG:HH12	1:A:246:GLY:C	2.04	0.65
1:A:378:TYR:HB3	3:A:601:FAD:O2	2.05	0.57
1:A:256:GLN:OE1	1:A:276:ARG:HD2	2.06	0.56
1:A:454:ARG:HD2	1:A:520:VAL:HG11	1.87	0.56
1:B:150:ILE:HD13	1:B:169:ILE:HG23	1.90	0.54
1:A:407:ASP:OD2	1:A:409:GLN:OE1	2.25	0.54
1:A:455:VAL:HG23	1:A:519:ARG:HD2	1.91	0.52
1:B:447:GLY:HA3	1:B:455:VAL:HG12	1.93	0.51
2:D:97:LYS:NZ	10:D:1003:HOH:O	2.43	0.50
1:B:56[B]:ILE:HD13	1:B:100:LEU:HD13	1.94	0.50
1:B:56[B]:ILE:HD12	1:B:105:LEU:CD2	2.43	0.48
1:A:354:ASP:HB3	6:A:606:GOL:H2	1.95	0.48
1:B:506:LEU:O	1:B:519:ARG:NH2	2.46	0.48
1:A:447:GLY:HA3	1:A:455:VAL:HG13	1.96	0.48
1:B:305:LYS:HD3	1:B:305:LYS:C	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:THR:HB	1:B:274:PRO:HD3	1.97	0.47
1:B:4:LYS:HD2	1:B:5:LYS:N	2.30	0.46
1:B:124:LYS:HB3	2:C:101:THR:HB	1.98	0.46
1:A:150:ILE:HD12	1:A:150:ILE:N	2.30	0.46
1:A:407:ASP:OD1	1:A:408:GLU:N	2.50	0.45
1:A:118:ARG:NH1	1:A:246:GLY:O	2.44	0.45
1:A:379[A]:VAL:HG23	3:A:601:FAD:N1	2.31	0.45
1:B:455:VAL:HG23	1:B:519:ARG:HD3	1.97	0.45
1:A:454:ARG:HB3	1:A:520:VAL:HG11	1.99	0.45
1:B:56[B]:ILE:HG22	1:B:56[B]:ILE:O	2.17	0.45
2:D:28:ARG:HD3	2:D:34:GLU:OE1	2.17	0.44
1:A:273:THR:HB	1:A:274:PRO:HD3	1.99	0.44
1:A:180:LYS:HE2	1:A:401:GLU:HA	1.98	0.44
1:A:514:LYS:HA	1:A:514:LYS:HD2	1.79	0.44
1:A:337:GLY:H	6:A:605:GOL:H11	1.83	0.44
1:B:407:ASP:OD1	1:B:408:GLU:N	2.51	0.44
1:A:150:ILE:HD13	1:A:169:ILE:HG23	2.00	0.44
1:A:165:TYR:CG	1:A:414:GLU:HG2	2.54	0.43
1:A:470:ILE:HG21	1:A:495:ILE:HD11	1.99	0.43
1:B:320:LYS:HE2	10:B:871:HOH:O	2.17	0.43
1:A:482[B]:ARG:HG3	1:A:482[B]:ARG:HH11	1.83	0.43
2:D:28:ARG:HD3	2:D:34:GLU:HB2	2.01	0.43
1:A:272:THR:O	1:A:276:ARG:HG3	2.18	0.43
1:A:454:ARG:HB3	1:A:520:VAL:CG1	2.48	0.43
1:B:133:ILE:HG13	1:B:134:LEU:N	2.34	0.43
1:B:427:GLY:HA3	1:B:478:LYS:HB3	2.01	0.42
2:D:17:THR:C	2:D:18:LYS:HD3	2.44	0.42
1:B:474:LEU:HD21	1:B:495:ILE:CD1	2.48	0.42
1:A:358:LYS:HE3	6:A:606:GOL:O1	2.18	0.42
1:A:536:LYS:HB2	1:A:536:LYS:HE2	1.82	0.42
1:A:379[B]:VAL:O	1:A:383:MET:HG3	2.20	0.41
1:B:150:ILE:HD12	1:B:150:ILE:N	2.36	0.41
1:B:129:SER:O	1:B:133:ILE:HG23	2.20	0.41
1:A:281:LEU:HD12	1:A:515[B]:CYS:SG	2.61	0.41
1:B:131:LYS:HA	1:B:131:LYS:HD2	1.93	0.41
1:B:165:TYR:CG	1:B:414:GLU:HG2	2.55	0.41
1:B:165:TYR:CD2	1:B:414:GLU:HG2	2.56	0.41
1:B:407:ASP:OD1	1:B:407:ASP:C	2.64	0.41
2:D:99:LYS:HA	2:D:99:LYS:HD2	1.98	0.41
1:A:336:CYS:HB2	6:A:605:GOL:H12	2.02	0.41
1:A:292:TYR:HB3	1:A:332:PRO:HB2	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:MET:HE2	1:A:400:MET:HB3	1.88	0.40
2:C:28:ARG:HD3	2:C:34:GLU:OE1	2.21	0.40
1:A:278:TYR:HB2	1:A:515[A]:CYS:SG	2.60	0.40
1:B:455:VAL:O	1:B:520:VAL:HG22	2.21	0.40
2:D:4:ARG:HD2	2:D:57:GLU:OE2	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	560/571 (98%)	546 (98%)	14 (2%)	0	100	100
1	B	543/571 (95%)	526 (97%)	17 (3%)	0	100	100
2	C	99/104 (95%)	98 (99%)	1 (1%)	0	100	100
2	D	100/104 (96%)	98 (98%)	2 (2%)	0	100	100
All	All	1302/1350 (96%)	1268 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	473/481 (98%)	472 (100%)	1 (0%)	87	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	463/481 (96%)	463 (100%)	0	100	100
2	C	89/92 (97%)	89 (100%)	0	100	100
2	D	90/92 (98%)	89 (99%)	1 (1%)	65	38
All	All	1115/1146 (97%)	1113 (100%)	2 (0%)	87	76

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	480	ARG
2	D	100	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	147	ASN
1	B	346	HIS
1	B	348	GLN
1	B	542	ASN
1	B	555	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 5 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	MPD	B	604	-	7,7,7	0.30	0	9,10,10	0.41	0
5	MPD	C	203	-	7,7,7	0.41	0	9,10,10	0.35	0
5	MPD	D	901	-	7,7,7	0.33	0	9,10,10	0.37	0
6	GOL	A	604[A]	-	5,5,5	0.76	0	5,5,5	0.94	0
3	FAD	A	601	-	58,58,58	1.54	10 (17%)	85,89,89	1.62	21 (24%)
6	GOL	A	606	-	5,5,5	0.09	0	5,5,5	0.32	0
4	EDO	A	602	-	3,3,3	0.44	0	2,2,2	0.61	0
6	GOL	B	605	-	5,5,5	0.99	0	5,5,5	1.09	0
5	MPD	A	603	-	7,7,7	0.28	0	9,10,10	0.27	0
6	GOL	A	607[B]	-	5,5,5	0.77	0	5,5,5	1.02	0
6	GOL	A	605	-	5,5,5	0.61	0	5,5,5	0.85	0
9	SF4	C	201	2	0,12,12	-	-	-		
9	SF4	D	902	2	0,12,12	-	-	-		
9	SF4	D	903	2	0,12,12	-	-	-		
6	GOL	B	603	-	5,5,5	0.98	0	5,5,5	1.07	0
3	FAD	B	601	-	58,58,58	1.45	10 (17%)	85,89,89	1.59	15 (17%)
5	MPD	B	602	-	7,7,7	0.29	0	9,10,10	0.30	0
9	SF4	C	202	2	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	MPD	B	604	-	-	0/5/5/5	-
5	MPD	C	203	-	-	0/5/5/5	-
5	MPD	D	901	-	-	0/5/5/5	-
6	GOL	A	604[A]	-	-	2/4/4/4	-
3	FAD	A	601	-	-	2/34/50/50	0/6/6/6
6	GOL	A	606	-	-	4/4/4/4	-
4	EDO	A	602	-	-	1/1/1/1	-
6	GOL	B	605	-	-	4/4/4/4	-
5	MPD	A	603	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	607[B]	-	-	1/4/4/4	-
6	GOL	A	605	-	-	4/4/4/4	-
9	SF4	C	201	2	-	-	0/6/5/5
9	SF4	D	902	2	-	-	0/6/5/5
9	SF4	D	903	2	-	-	0/6/5/5
6	GOL	B	603	-	-	2/4/4/4	-
3	FAD	B	601	-	-	2/34/50/50	0/6/6/6
5	MPD	B	602	-	-	3/5/5/5	-
9	SF4	C	202	2	-	-	0/6/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	FAD	C9A-C5X	5.39	1.49	1.41
3	B	601	FAD	C9A-C5X	5.33	1.49	1.41
3	A	601	FAD	C5A-C4A	4.86	1.47	1.39
3	B	601	FAD	C5A-C4A	4.34	1.46	1.39
3	B	601	FAD	C8-C7	3.73	1.49	1.40
3	A	601	FAD	C8-C7	3.17	1.48	1.40
3	A	601	FAD	C5A-C6A	3.00	1.49	1.41
3	A	601	FAD	C4-N3	-2.69	1.33	1.38
3	B	601	FAD	C5A-C6A	2.61	1.48	1.41
3	A	601	FAD	C4X-N5	2.51	1.36	1.30
3	B	601	FAD	C4X-N5	2.45	1.36	1.30
3	A	601	FAD	C2-N3	-2.45	1.33	1.39
3	B	601	FAD	C4-N3	-2.42	1.34	1.38
3	A	601	FAD	C4A-N9A	-2.27	1.33	1.37
3	B	601	FAD	C8A-N7A	2.23	1.36	1.31
3	A	601	FAD	C8A-N7A	2.18	1.35	1.31
3	A	601	FAD	C5X-N5	-2.15	1.35	1.39
3	B	601	FAD	C4A-N9A	-2.08	1.33	1.37
3	B	601	FAD	C5A-N7A	-2.05	1.35	1.39
3	B	601	FAD	C5X-N5	-2.02	1.35	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	FAD	C5A-C4A-N3A	-5.23	119.52	126.72
3	A	601	FAD	C5A-C4A-N3A	-4.84	120.05	126.72
3	B	601	FAD	N3A-C4A-N9A	4.11	134.15	127.17
3	A	601	FAD	C4'-C3'-C2'	-3.95	107.00	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	FAD	C4A-C5A-N7A	-3.86	106.16	110.58
3	A	601	FAD	N3A-C4A-N9A	3.60	133.30	127.17
3	B	601	FAD	C4A-C5A-N7A	-3.49	106.59	110.58
3	B	601	FAD	C4-C4X-N5	3.29	122.75	118.21
3	B	601	FAD	C2A-N3A-C4A	3.28	119.84	111.83
3	A	601	FAD	C2A-N3A-C4A	3.24	119.73	111.83
3	A	601	FAD	C4-C4X-N5	3.16	122.57	118.21
3	B	601	FAD	C4'-C3'-C2'	-3.10	108.41	113.57
3	B	601	FAD	N3A-C2A-N1A	-3.09	123.91	128.58
3	B	601	FAD	C4A-N9A-C8A	3.08	108.97	105.74
3	A	601	FAD	N3A-C2A-N1A	-3.05	123.96	128.58
3	A	601	FAD	C4A-N9A-C8A	3.05	108.94	105.74
3	B	601	FAD	O2A-PA-O3P	3.01	115.42	107.27
3	B	601	FAD	C5A-N7A-C8A	2.71	107.71	103.45
3	A	601	FAD	C6A-C5A-N7A	2.70	137.30	132.09
3	A	601	FAD	C5X-C9A-N10	2.50	120.23	117.97
3	B	601	FAD	N9A-C8A-N7A	-2.49	110.40	113.94
3	A	601	FAD	C2A-N1A-C6A	2.47	122.78	118.73
3	A	601	FAD	O5'-C5'-C4'	-2.46	102.78	109.36
3	B	601	FAD	C9A-C5X-N5	-2.43	119.87	122.45
3	A	601	FAD	C5A-N7A-C8A	2.41	107.24	103.45
3	A	601	FAD	C9A-C5X-N5	-2.36	119.95	122.45
3	A	601	FAD	O2A-PA-O3P	2.30	113.50	107.27
3	A	601	FAD	C4X-C10-N1	-2.21	119.18	124.59
3	B	601	FAD	C5X-C9A-N10	2.18	119.94	117.97
3	A	601	FAD	C5'-C4'-C3'	-2.11	108.23	112.22
3	A	601	FAD	C4X-C4-N3	2.09	118.56	113.25
3	B	601	FAD	C4X-C10-N10	2.06	119.43	116.48
3	A	601	FAD	C9-C9A-N10	-2.06	119.09	121.85
3	A	601	FAD	N9A-C8A-N7A	-2.05	111.03	113.94
3	A	601	FAD	C4X-C10-N10	2.02	119.37	116.48
3	B	601	FAD	C4X-C4-N3	2.01	118.36	113.25

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	FAD	N10-C1'-C2'-O2'
6	A	606	GOL	O1-C1-C2-C3
6	A	606	GOL	C1-C2-C3-O3
6	A	606	GOL	O2-C2-C3-O3
6	B	605	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	A	604[A]	GOL	O1-C1-C2-C3
6	A	605	GOL	O1-C1-C2-C3
6	A	605	GOL	C1-C2-C3-O3
6	B	605	GOL	C1-C2-C3-O3
6	B	605	GOL	O1-C1-C2-O2
6	A	605	GOL	O2-C2-C3-O3
6	A	606	GOL	O1-C1-C2-O2
6	A	605	GOL	O1-C1-C2-O2
6	B	605	GOL	O2-C2-C3-O3
3	A	601	FAD	N10-C1'-C2'-O2'
5	B	602	MPD	C1-C2-C3-C4
6	A	607[B]	GOL	O2-C2-C3-O3
6	B	603	GOL	O1-C1-C2-C3
6	A	604[A]	GOL	O1-C1-C2-O2
3	B	601	FAD	P-O3P-PA-O1A
4	A	602	EDO	O1-C1-C2-O2
6	B	603	GOL	O1-C1-C2-O2
5	B	602	MPD	O2-C2-C3-C4
3	A	601	FAD	N10-C1'-C2'-C3'
5	B	602	MPD	CM-C2-C3-C4

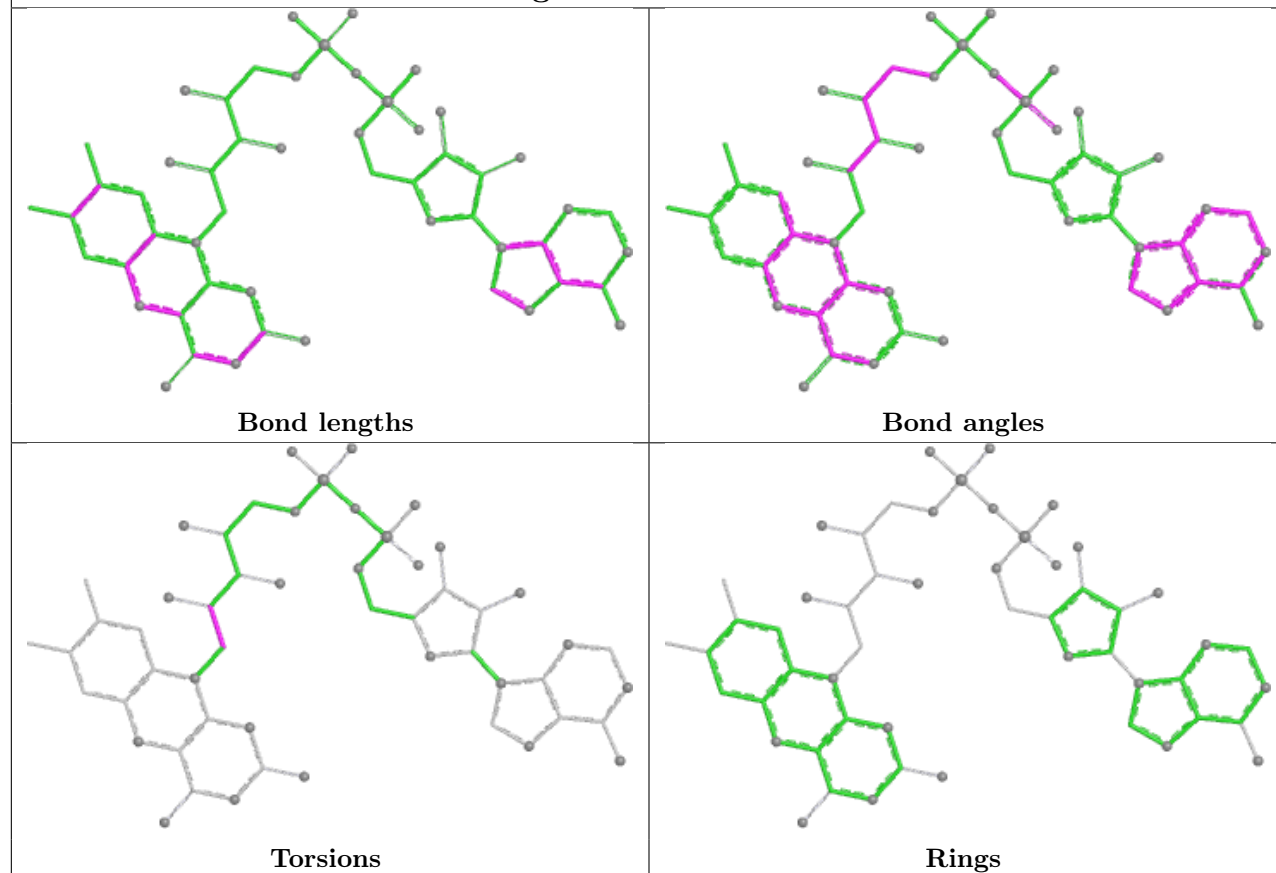
There are no ring outliers.

3 monomers are involved in 6 short contacts:

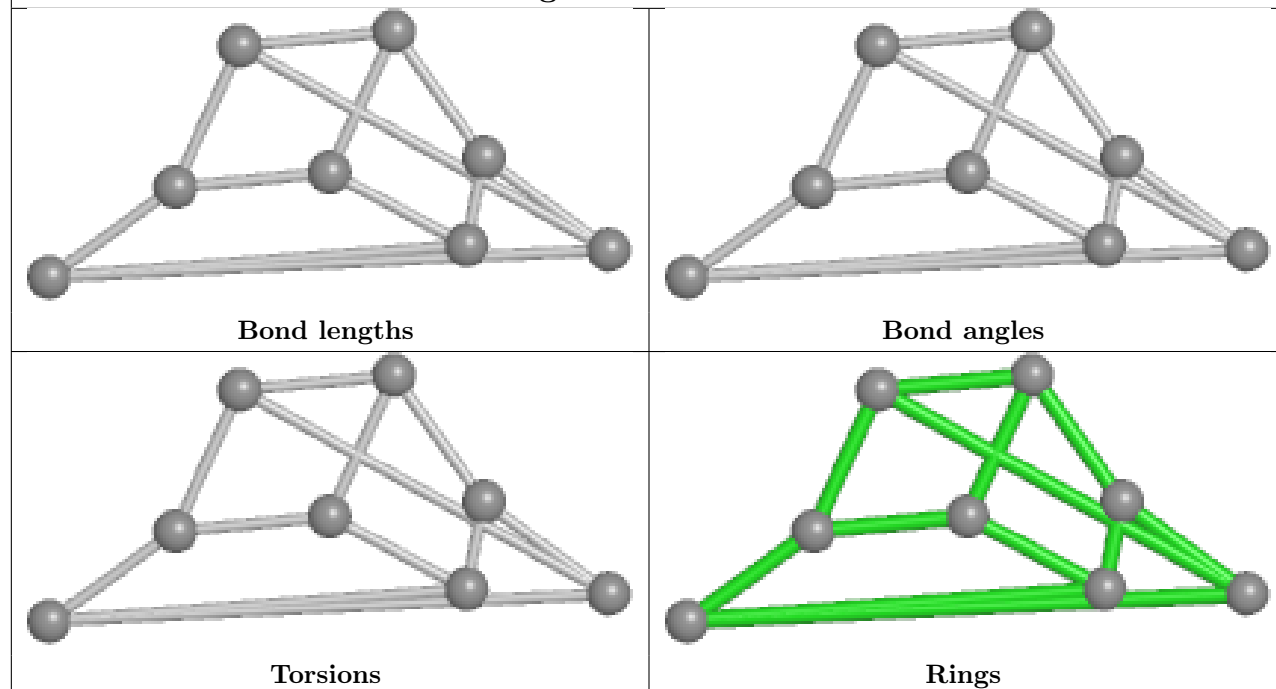
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	FAD	2	0
6	A	606	GOL	2	0
6	A	605	GOL	2	0

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

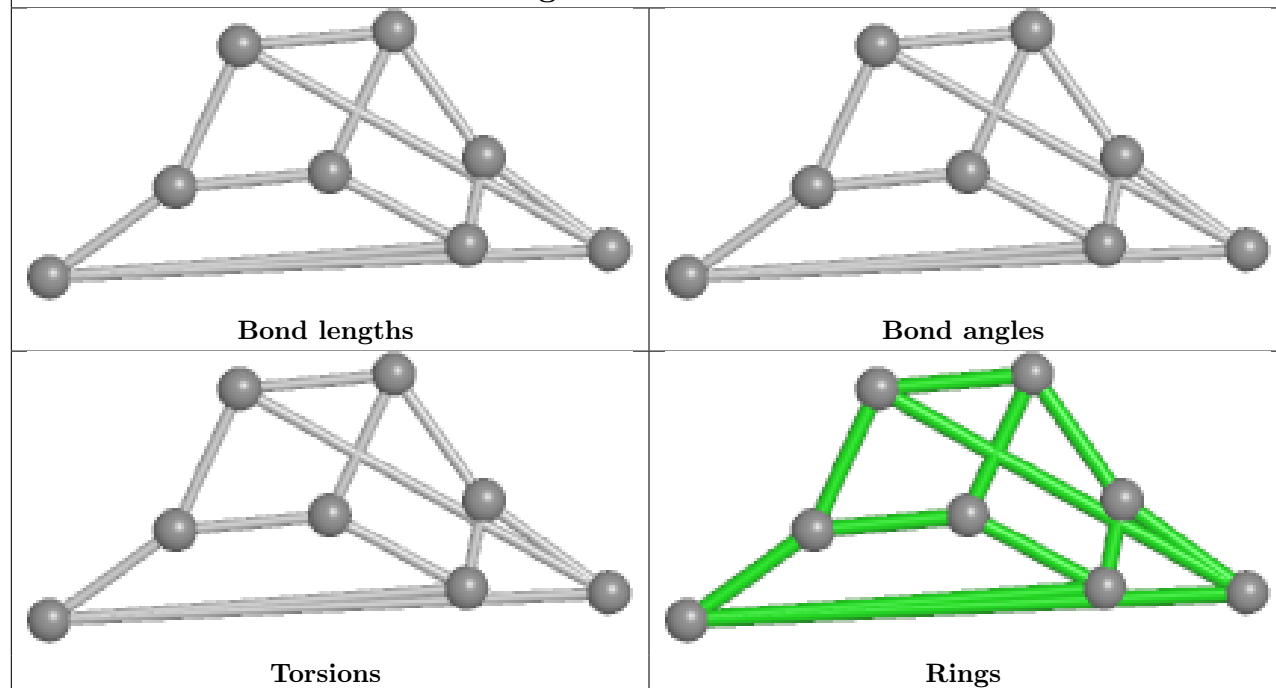
Ligand FAD A 601



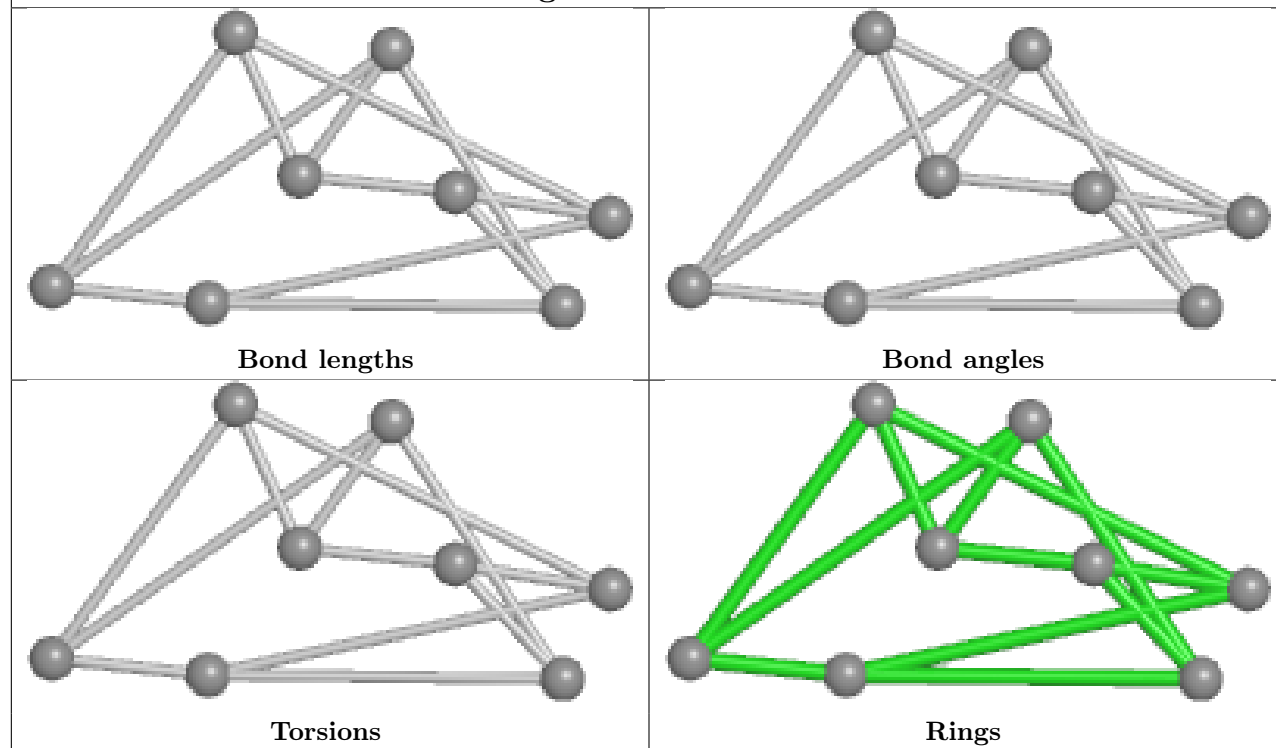
Ligand SF4 C 201

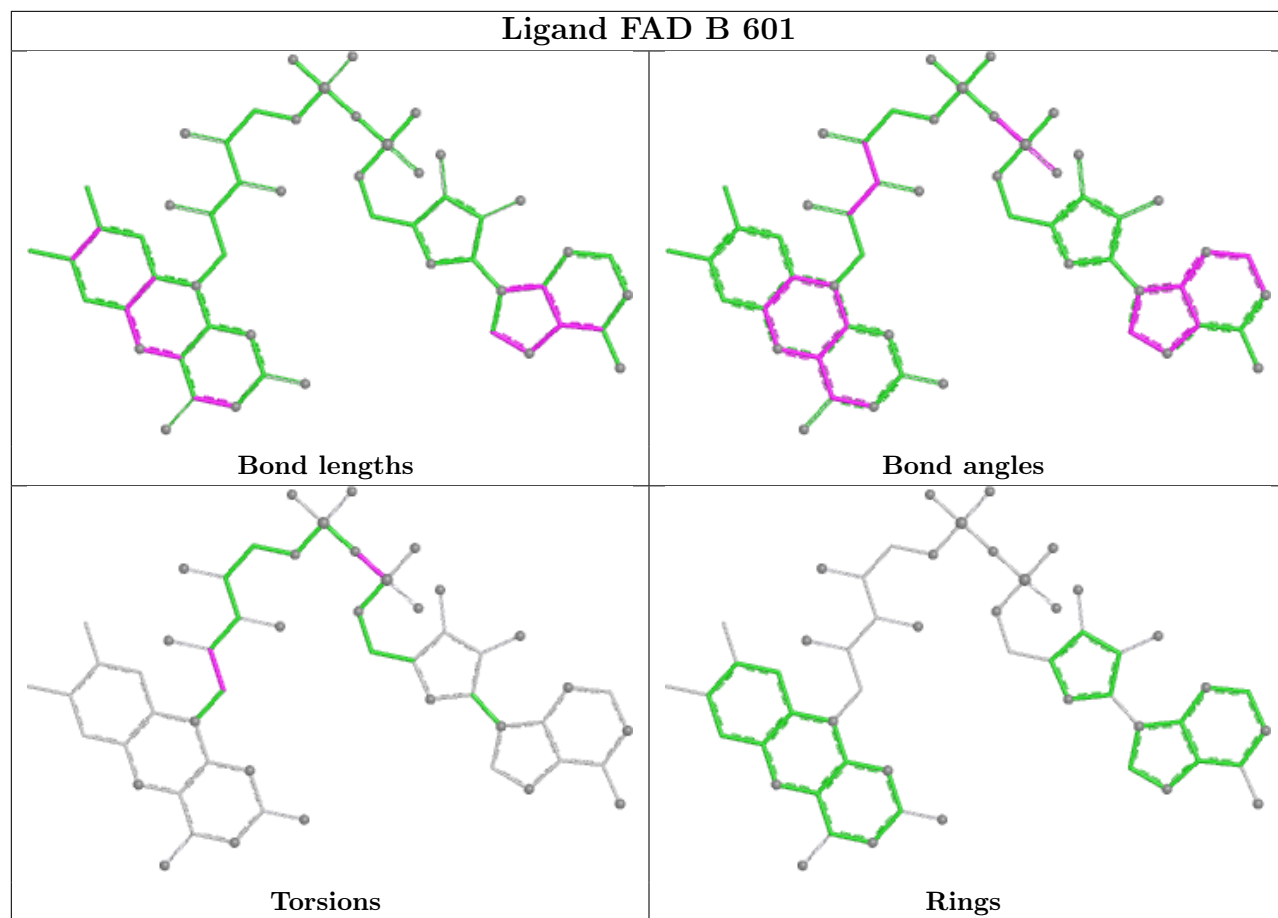


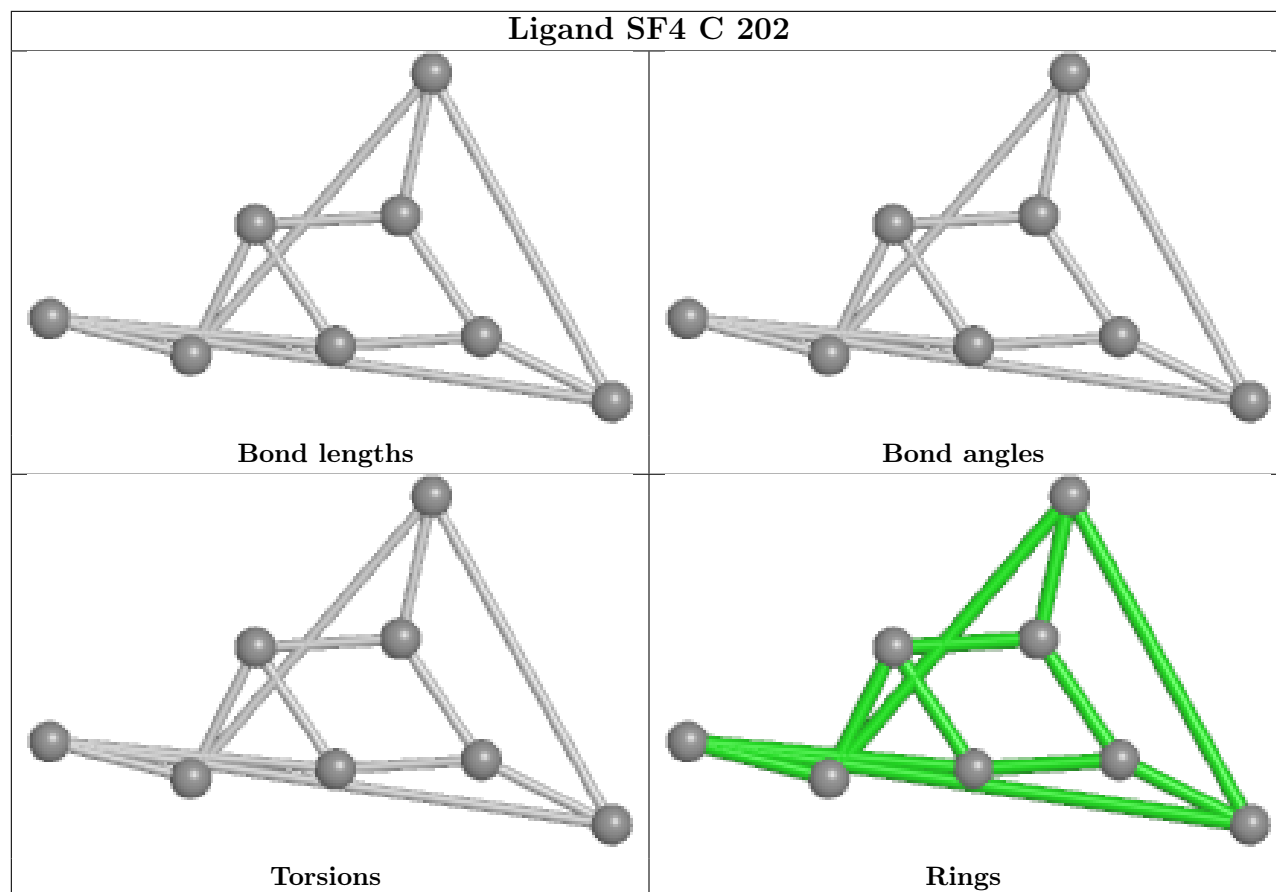
Ligand SF4 D 902



Ligand SF4 D 903







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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, 95th 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	556/571 (97%)	0.01	18 (3%)	50 53	8, 22, 59, 120	6 (1%)
1	B	544/571 (95%)	0.47	39 (7%)	21 21	13, 30, 71, 95	5 (0%)
2	C	101/104 (97%)	0.21	1 (0%)	79 83	16, 29, 58, 76	0
2	D	102/104 (98%)	0.06	5 (4%)	35 36	11, 23, 56, 90	0
All	All	1303/1350 (96%)	0.22	63 (4%)	35 37	8, 27, 65, 120	11 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	248	ILE	8.2
1	A	252	VAL	6.3
1	B	247	THR	5.9
1	B	557	VAL	5.0
1	A	251	GLY	4.9
1	B	254	VAL	4.8
2	D	102	PHE	4.7
1	B	246	GLY	4.4
1	B	536[A]	LYS	4.4
1	B	57[A]	ASN	4.4
1	A	556	PRO	4.3
1	B	107	ILE	4.2
1	B	402	ASN	4.2
1	B	56[A]	ILE	4.1
1	B	452	TYR	3.8
1	A	406	ILE	3.7
1	B	110	ASP	3.7
1	B	156	LEU	3.5
1	B	123	ILE	3.3
2	C	102	PHE	3.3
1	A	404	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	399	SER	3.2
2	D	100	LYS	3.1
1	B	125	ILE	3.0
1	B	313	MET	3.0
1	B	275	MET	2.9
1	B	406	ILE	2.9
2	D	103	ASP	2.8
1	B	271	ASN	2.8
1	B	478	LYS	2.8
1	B	120	LYS	2.7
1	A	156	LEU	2.5
1	A	452	TYR	2.5
1	A	270	ASN	2.5
1	B	58[A]	ALA	2.4
1	A	403	ASP	2.4
1	A	76	GLU	2.4
1	B	77	SER	2.4
1	B	75	LYS	2.3
1	B	398	LYS	2.3
2	D	101	THR	2.3
1	A	249	ALA	2.3
1	B	285	LEU	2.3
1	B	426	LYS	2.3
1	A	118	ARG	2.2
1	B	109	LYS	2.2
1	B	556	PRO	2.2
1	A	402	ASN	2.2
1	B	6	ILE	2.1
1	B	409	GLN	2.1
1	A	247	THR	2.1
1	A	253	LYS	2.1
1	B	480	ARG	2.1
2	D	29	GLU	2.1
1	B	54	ASN	2.1
1	B	270	ASN	2.1
1	B	298	ILE	2.0
1	B	400	MET	2.0
1	B	2	ASP	2.0
1	B	31	LYS	2.0
1	B	108	GLN	2.0
1	A	455	VAL	2.0
1	A	54	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

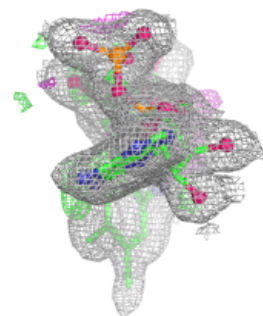
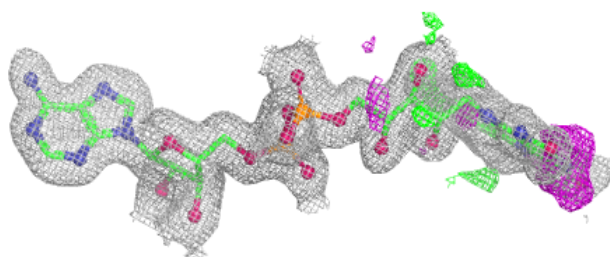
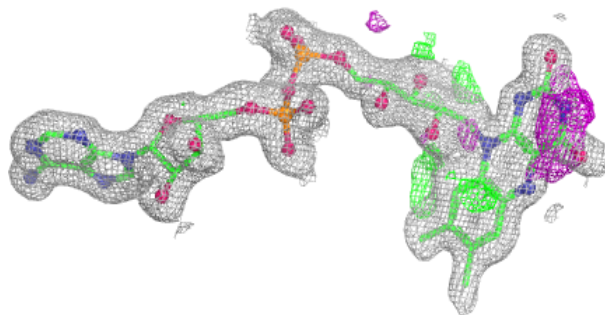
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	A	607[B]	6/6	0.61	0.17	19,19,19,19	6
6	GOL	A	605	6/6	0.66	0.16	20,20,20,21	0
6	GOL	A	606	6/6	0.68	0.15	20,20,21,21	0
6	GOL	B	603	6/6	0.77	0.21	67,74,85,111	0
6	GOL	A	604[A]	6/6	0.79	0.27	49,65,77,85	6
4	EDO	A	602	4/4	0.81	0.15	45,45,46,46	0
8	NA	B	607	1/1	0.81	0.10	29,29,29,29	1
5	MPD	B	602	8/8	0.82	0.15	50,51,51,51	0
6	GOL	B	605	6/6	0.85	0.23	62,65,84,90	0
5	MPD	B	604	8/8	0.86	0.16	50,60,68,70	0
8	NA	C	204	1/1	0.89	0.09	29,29,29,29	1
5	MPD	A	603	8/8	0.91	0.10	35,37,38,39	0
5	MPD	C	203	8/8	0.93	0.10	32,33,33,34	0
8	NA	A	609	1/1	0.94	0.06	29,29,29,29	1
5	MPD	D	901	8/8	0.95	0.07	26,26,27,28	0
3	FAD	B	601	53/53	0.97	0.07	19,21,34,35	0
7	CA	B	606	1/1	0.98	0.06	29,29,29,29	0
3	FAD	A	601	53/53	0.98	0.06	10,14,25,26	0
7	CA	A	608	1/1	0.99	0.08	29,29,29,29	0
9	SF4	C	202	8/8	0.99	0.02	23,23,24,26	0
9	SF4	C	201	8/8	1.00	0.02	16,17,17,18	0
9	SF4	D	902	8/8	1.00	0.02	11,12,12,12	0
9	SF4	D	903	8/8	1.00	0.02	18,20,21,21	0

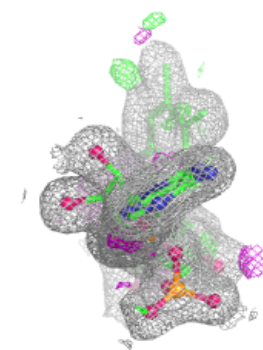
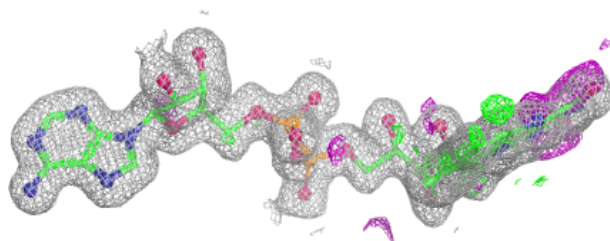
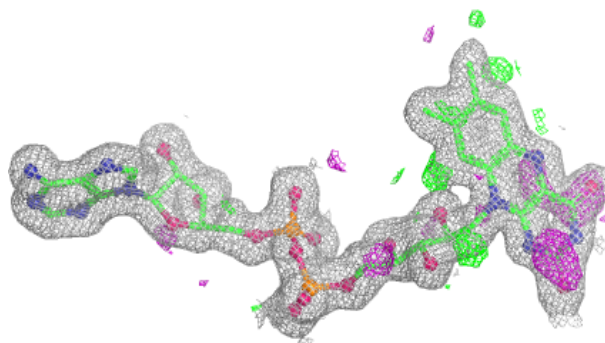
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 601:

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

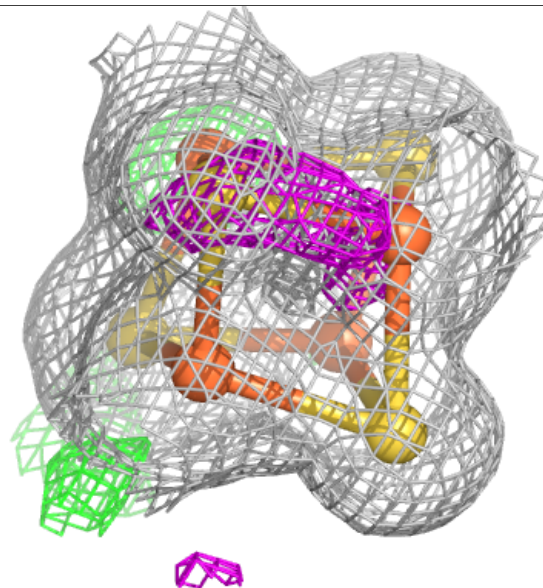
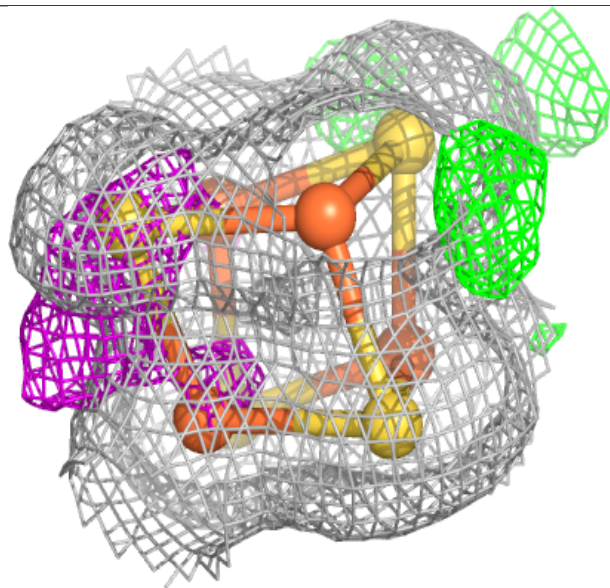
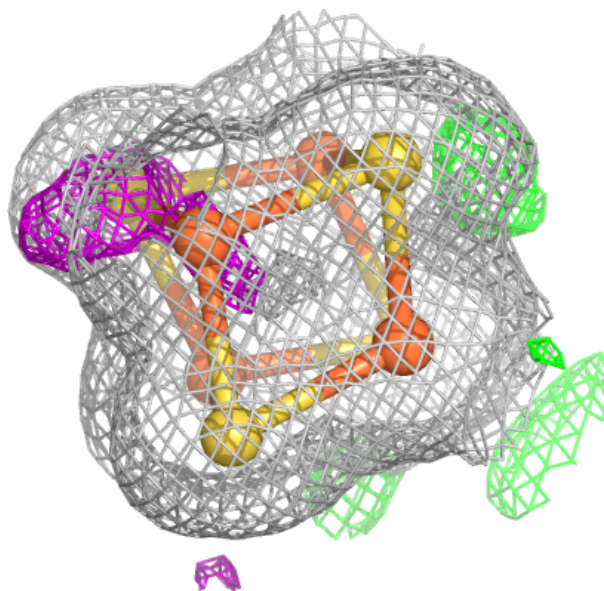
**Electron density around FAD A 601:**

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



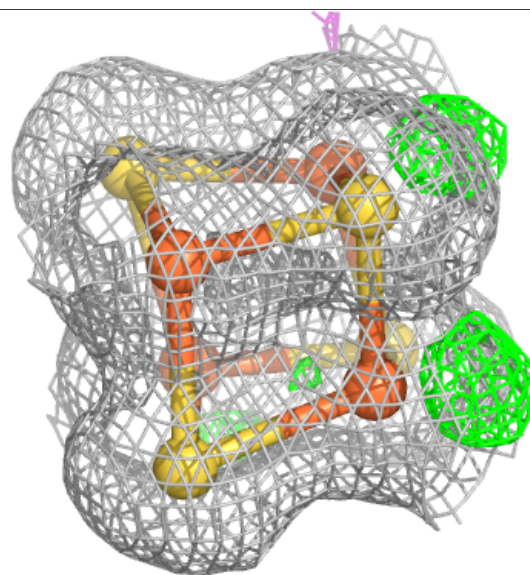
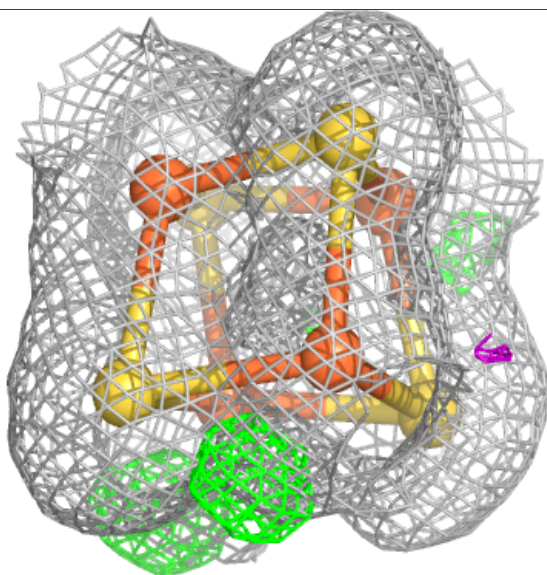
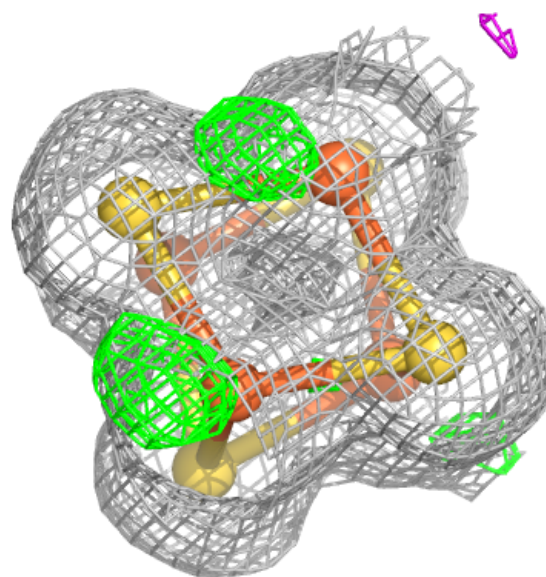
Electron density around SF4 C 202:

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



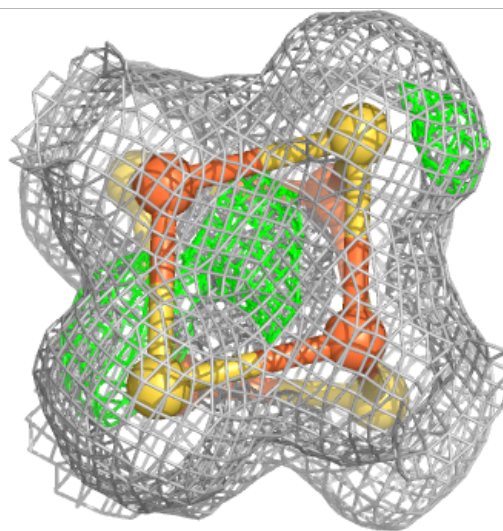
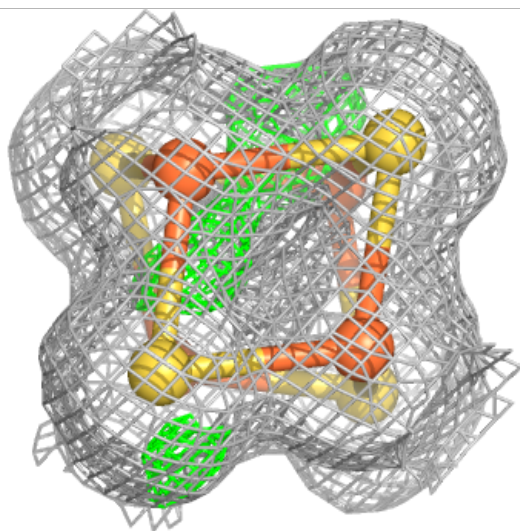
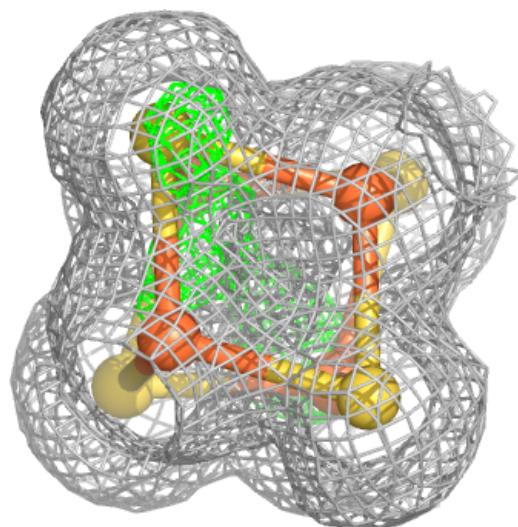
Electron density around SF4 C 201:

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



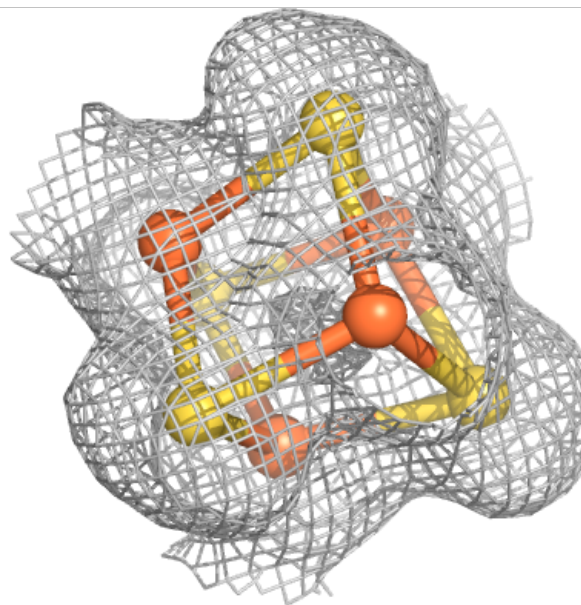
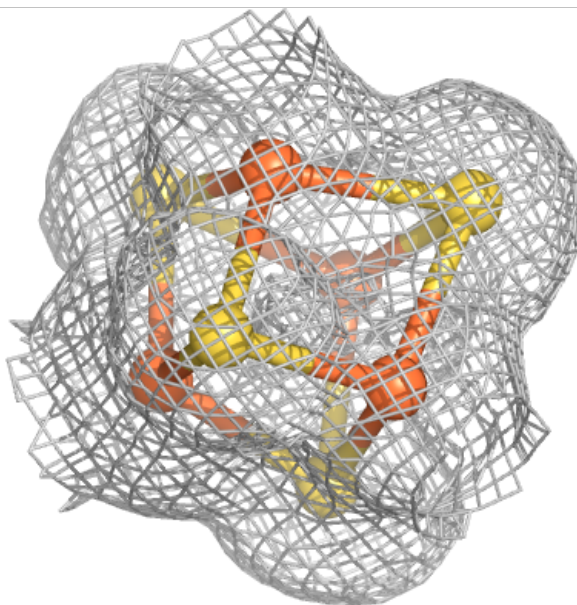
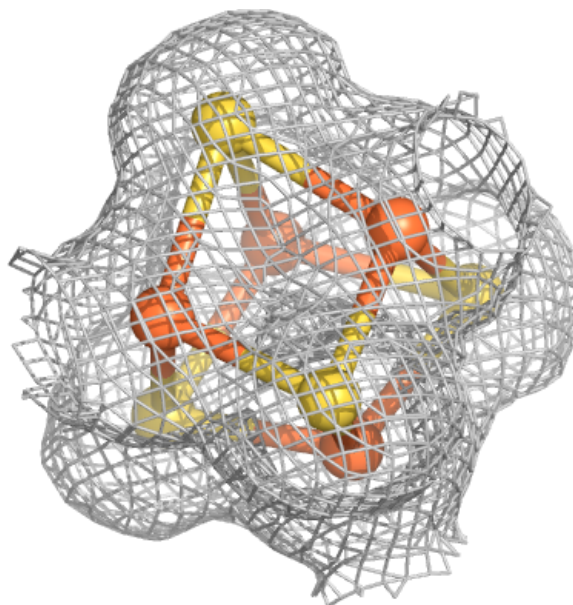
Electron density around SF4 D 902:

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



Electron density around SF4 D 903:

$2mF_o-DF_c$ (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.