WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2022 – 06:15 pm GMT

PDB ID	:	6XTF
Title	:	Crystal structure a Thioredoxin Reductase from Gloeobacter violaceus bound to its electron donor
Authors	:	Buey, R.M.; Gonzalez-Holgado, G.; Fernandez-Justel, D.; Balsera, M.
Deposited on	:	2020-01-16
Resolution	:	2.23 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 2.23 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.
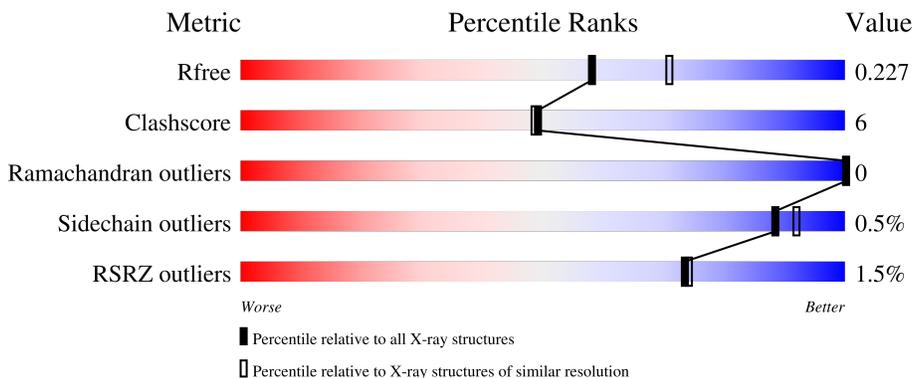
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	320	88% ... 10% ·
1	B	320	3% ... 89% ... 9% ·
2	C	100	79% ... 17% ·
2	D	100	76% ... 19% · ·

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
4	ACT	A	405	-	-	-	X

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 13044 atoms, of which 6311 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 Thioredoxin reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	315	Total	C	H	N	O	S	0	1	0
			4729	1512	2352	412	441	12			
1	B	315	Total	C	H	N	O	S	0	2	0
			4722	1508	2347	409	444	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q7NMP6
A	-1	SER	-	expression tag	UNP Q7NMP6
A	0	HIS	-	expression tag	UNP Q7NMP6
B	-2	GLY	-	expression tag	UNP Q7NMP6
B	-1	SER	-	expression tag	UNP Q7NMP6
B	0	HIS	-	expression tag	UNP Q7NMP6

- Molecule 2 is a protein called Ferredoxin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	96	Total	C	H	N	O	S	0	0	0
			1390	442	674	114	153	7			
2	D	96	Total	C	H	N	O	S	0	0	0
			1340	432	639	111	151	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q7NFA3
C	-1	SER	-	expression tag	UNP Q7NFA3
C	0	HIS	-	expression tag	UNP Q7NFA3
D	-2	GLY	-	expression tag	UNP Q7NFA3
D	-1	SER	-	expression tag	UNP Q7NFA3
D	0	HIS	-	expression tag	UNP Q7NFA3

- Molecule 3 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).
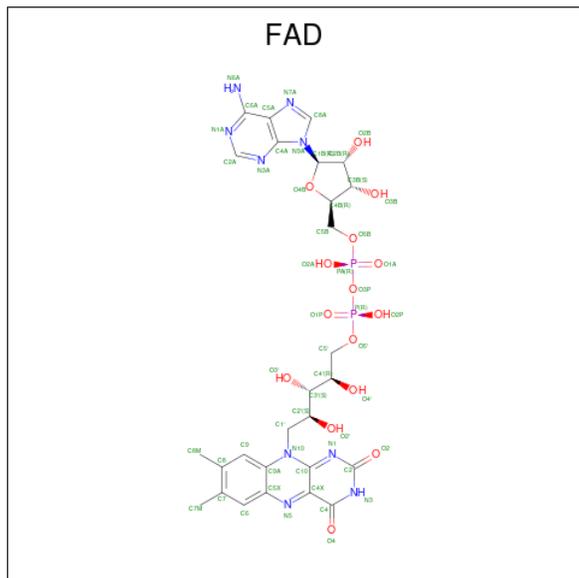
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		
3	B	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
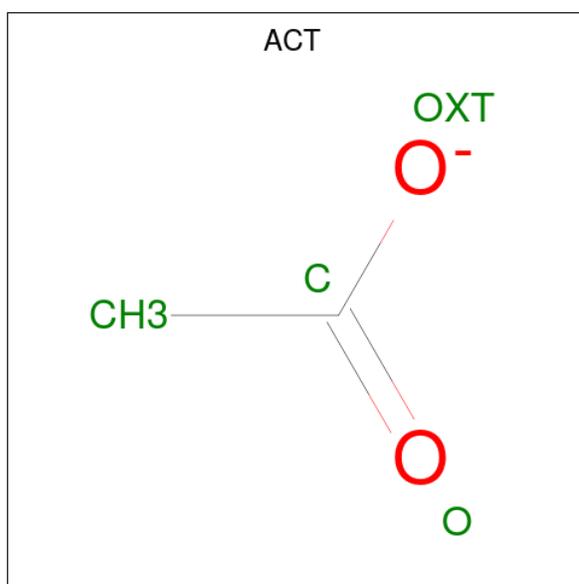
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 7	C 2	H 3	O 2	0	0
4	A	1	Total 7	C 2	H 3	O 2	0	0
4	A	1	Total 7	C 2	H 3	O 2	0	0
4	A	1	Total 7	C 2	H 3	O 2	0	0
4	A	1	Total 7	C 2	H 3	O 2	0	0
4	A	1	Total 7	C 2	H 3	O 2	0	0
4	A	1	Total 7	C 2	H 3	O 2	0	0
4	B	1	Total 7	C 2	H 3	O 2	0	0
4	B	1	Total 7	C 2	H 3	O 2	0	0
4	B	1	Total 7	C 2	H 3	O 2	0	0
4	B	1	Total 7	C 2	H 3	O 2	0	0
4	D	1	Total 7	C 2	H 3	O 2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
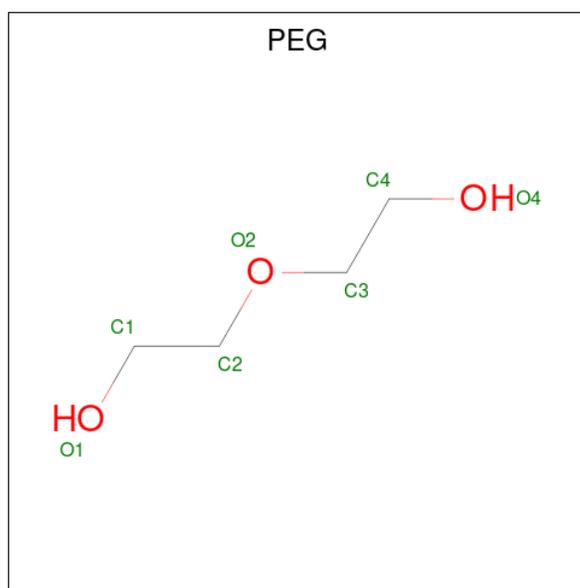
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 17	C 4	H 10	O 3	0	0
5	A	1	Total 17	C 4	H 10	O 3	0	0
5	A	1	Total 17	C 4	H 10	O 3	0	0
5	B	1	Total 17	C 4	H 10	O 3	0	0
5	B	1	Total 17	C 4	H 10	O 3	0	0
5	B	1	Total 17	C 4	H 10	O 3	0	0
5	C	1	Total 17	C 4	H 10	O 3	0	0
5	C	1	Total 17	C 4	H 10	O 3	0	0
5	C	1	Total 17	C 4	H 10	O 3	0	0
5	C	1	Total 17	C 4	H 10	O 3	0	0
5	D	1	Total 17	C 4	H 10	O 3	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$) (labeled as "Ligand of Interest" by depositor).


PG4
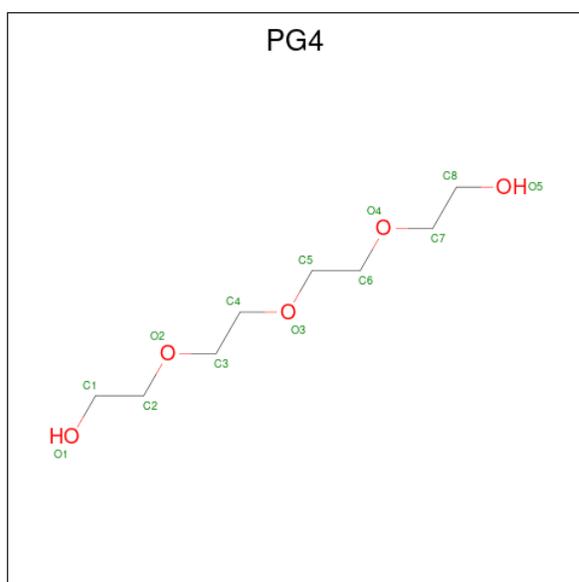
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 31	C 8	H 18	O 5	0	0
6	B	1	Total 31	C 8	H 18	O 5	0	0
6	B	1	Total 31	C 8	H 18	O 5	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).
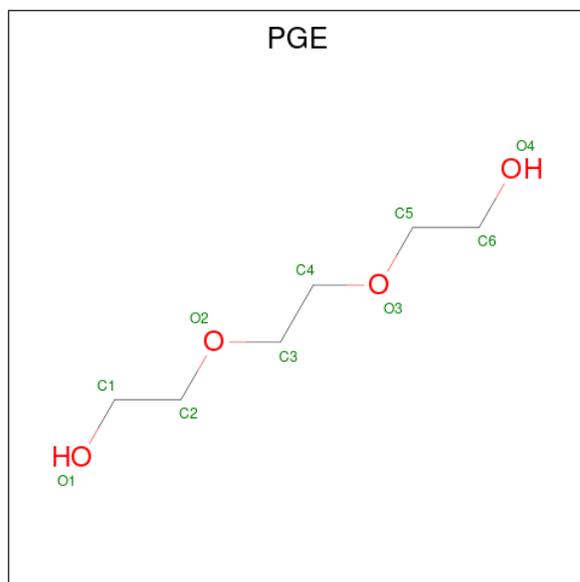
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 23	C 6	H 13	O 4	0	0
7	A	1	Total 23	C 6	H 13	O 4	0	0
7	B	1	Total 23	C 6	H 13	O 4	0	0

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

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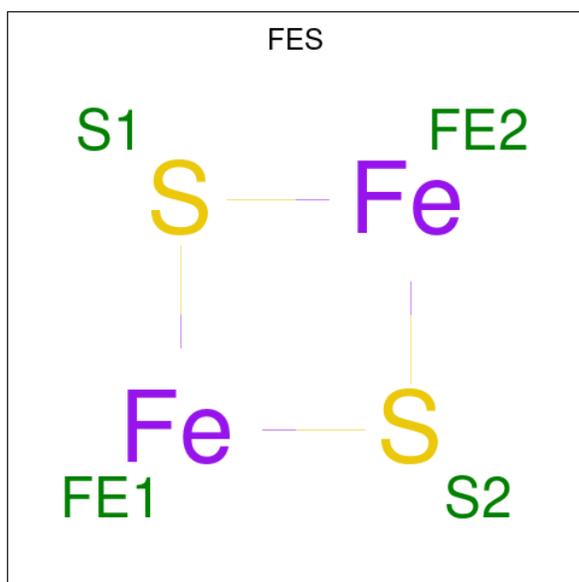
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total 4	Fe 2	S 2	0	0
8	D	1	Total 4	Fe 2	S 2	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	94	Total 94	O 94	0	0
9	B	98	Total 98	O 98	0	0
9	C	46	Total 46	O 46	0	0
9	D	18	Total 18	O 18	0	0

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: Thioredoxin reductase

Chain A:

- Molecule 1: Thioredoxin reductase

Chain B:

- Molecule 2: Ferredoxin

Chain C:

- Molecule 2: Ferredoxin

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	166.74Å 181.31Å 80.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.37 – 2.23 90.66 – 2.23	Depositor EDS
% Data completeness (in resolution range)	67.0 (83.37-2.23) 67.0 (90.66-2.23)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.22Å)	Xtriage
Refinement program	PHENIX dev_3689	Depositor
R, R_{free}	0.201 , 0.232 0.199 , 0.227	Depositor DCC
R_{free} test set	2035 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13044	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 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, FAD, PG4, PEG, FES, ACT

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	0.38	0/2434	0.62	0/3311
1	B	0.42	0/2433	0.67	0/3308
2	C	0.39	0/727	0.62	0/987
2	D	0.45	0/712	0.77	0/970
All	All	0.40	0/6306	0.65	0/8576

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2377	2352	2352	24	3
1	B	2375	2347	2347	24	1
2	C	716	674	673	13	0
2	D	701	639	638	14	2
3	A	53	30	31	0	0
3	B	53	30	31	3	0
4	A	28	21	21	0	0
4	B	16	12	12	1	0
4	D	4	3	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	21	30	30	5	0
5	B	21	30	30	2	0
5	C	28	40	40	3	0
5	D	7	10	10	0	0
6	A	13	18	18	0	0
6	B	26	36	36	4	0
7	A	20	26	28	1	0
7	B	10	13	14	0	0
8	C	4	0	0	1	0
8	D	4	0	0	1	0
9	A	94	0	0	1	0
9	B	98	0	0	6	0
9	C	46	0	0	0	0
9	D	18	0	0	0	0
All	All	6733	6311	6314	75	3

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 6.

The worst 5 of 75 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:70:ASP:OD2	5:A:414:PEG:H12	1.64	0.96
1:A:70:ASP:OD2	5:A:414:PEG:C1	2.26	0.83
3:B:401:FAD:HM73	2:D:39:SER:HB3	1.70	0.72
6:B:405:PG4:O2	6:B:405:PG4:O5	2.08	0.71
3:B:401:FAD:H3B	9:B:505:HOH:O	1.93	0.69

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ASP:H	1:B:286:GLN:HE22[6_445]	1.23	0.37
1:A:308:ARG:HH12	2:D:94:ASP:OD1[6_445]	1.26	0.34
1:A:308:ARG:NH1	2:D:94:ASP:OD1[6_445]	2.07	0.13

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	314/320 (98%)	306 (98%)	8 (2%)	0	100	100
1	B	315/320 (98%)	308 (98%)	7 (2%)	0	100	100
2	C	94/100 (94%)	88 (94%)	6 (6%)	0	100	100
2	D	94/100 (94%)	89 (95%)	5 (5%)	0	100	100
All	All	817/840 (97%)	791 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	244/252 (97%)	244 (100%)	0	100	100
1	B	245/252 (97%)	243 (99%)	2 (1%)	81	87
2	C	79/83 (95%)	79 (100%)	0	100	100
2	D	75/83 (90%)	74 (99%)	1 (1%)	69	76
All	All	643/670 (96%)	640 (100%)	3 (0%)	88	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	203	LEU
1	B	254	MET
2	D	54	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	227	GLN
2	D	32	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

33 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	$\#|Z| > 2$
4	ACT	A	402	-	1,3,3	4.49	1 (100%)	0,3,3	-	-
8	FES	C	101	2	0,4,4	-	-	-		
4	ACT	A	412	-	1,3,3	5.72	1 (100%)	0,3,3	-	-
8	FES	D	5202	2	0,4,4	-	-	-		
3	FAD	A	401	-	51,58,58	1.22	5 (9%)	60,89,89	2.20	7 (11%)
5	PEG	D	5203	-	6,6,6	0.49	0	5,5,5	0.19	0
5	PEG	A	407	-	6,6,6	0.48	0	5,5,5	0.17	0
5	PEG	A	414	-	6,6,6	0.55	0	5,5,5	0.39	0
6	PG4	B	405	-	12,12,12	0.76	0	11,11,11	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
7	PGE	A	409	-	9,9,9	0.46	0	8,8,8	0.22	0
5	PEG	C	103	-	6,6,6	0.50	0	5,5,5	0.19	0
4	ACT	A	404	-	1,3,3	5.45	1 (100%)	0,3,3	-	-
4	ACT	D	5201	-	1,3,3	5.89	1 (100%)	0,3,3	-	-
6	PG4	B	402	-	12,12,12	0.53	0	11,11,11	0.39	0
5	PEG	C	104	-	6,6,6	0.48	0	5,5,5	0.20	0
3	FAD	B	401	-	51,58,58	1.20	4 (7%)	60,89,89	2.19	7 (11%)
6	PG4	A	406	-	12,12,12	0.53	0	11,11,11	0.27	0
5	PEG	C	105	-	6,6,6	0.50	0	5,5,5	0.17	0
7	PGE	B	409	-	9,9,9	0.52	0	8,8,8	0.21	0
4	ACT	B	406	-	1,3,3	5.50	1 (100%)	0,3,3	-	-
4	ACT	B	404	-	1,3,3	4.97	1 (100%)	0,3,3	-	-
5	PEG	B	410	-	6,6,6	0.50	0	5,5,5	0.37	0
5	PEG	C	102	-	6,6,6	0.49	0	5,5,5	0.11	0
5	PEG	B	403	-	6,6,6	0.48	0	5,5,5	0.18	0
5	PEG	B	408	-	6,6,6	0.50	0	5,5,5	0.19	0
4	ACT	A	410	-	1,3,3	4.53	1 (100%)	0,3,3	-	-
4	ACT	A	411	-	1,3,3	4.46	1 (100%)	0,3,3	-	-
5	PEG	A	403	-	6,6,6	0.49	0	5,5,5	0.13	0
4	ACT	A	405	-	1,3,3	5.72	1 (100%)	0,3,3	-	-
4	ACT	B	407	-	1,3,3	5.58	1 (100%)	0,3,3	-	-
7	PGE	A	408	-	9,9,9	0.53	0	8,8,8	0.25	0
4	ACT	B	411	-	1,3,3	6.02	1 (100%)	0,3,3	-	-
4	ACT	A	413	-	1,3,3	2.90	1 (100%)	0,3,3	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FES	C	101	2	-	-	0/1/1/1
8	FES	D	5202	2	-	-	0/1/1/1
3	FAD	A	401	-	-	1/30/50/50	0/6/6/6
5	PEG	D	5203	-	-	2/4/4/4	-
5	PEG	A	407	-	-	2/4/4/4	-
5	PEG	A	414	-	-	2/4/4/4	-
6	PG4	B	405	-	-	2/10/10/10	-
7	PGE	A	409	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	C	103	-	-	2/4/4/4	-
6	PG4	B	402	-	-	7/10/10/10	-
5	PEG	C	104	-	-	3/4/4/4	-
3	FAD	B	401	-	-	2/30/50/50	0/6/6/6
6	PG4	A	406	-	-	8/10/10/10	-
5	PEG	C	105	-	-	3/4/4/4	-
7	PGE	B	409	-	-	1/7/7/7	-
5	PEG	B	410	-	-	3/4/4/4	-
5	PEG	C	102	-	-	3/4/4/4	-
5	PEG	B	403	-	-	2/4/4/4	-
5	PEG	B	408	-	-	3/4/4/4	-
5	PEG	A	403	-	-	1/4/4/4	-
7	PGE	A	408	-	-	5/7/7/7	-

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	411	ACT	CH3-C	6.02	1.56	1.48
4	D	5201	ACT	CH3-C	5.89	1.56	1.48
4	A	412	ACT	CH3-C	5.72	1.56	1.48
4	A	405	ACT	CH3-C	5.72	1.56	1.48
3	A	401	FAD	C4X-C10	5.64	1.44	1.38

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	FAD	C2-N3-C4	12.82	125.96	115.14
3	B	401	FAD	C2-N3-C4	12.61	125.79	115.14
3	B	401	FAD	C4X-C4-N3	-6.84	114.07	123.43
3	A	401	FAD	C4X-C4-N3	-6.79	114.15	123.43
3	A	401	FAD	C10-C4X-N5	4.93	124.67	121.26

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	409	PGE	O2-C3-C4-O3
6	A	406	PG4	O3-C5-C6-O4
5	A	407	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	414	PEG	O1-C1-C2-O2
5	C	104	PEG	O1-C1-C2-O2

There are no ring outliers.

14 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	101	FES	1	0
8	D	5202	FES	1	0
5	A	407	PEG	1	0
5	A	414	PEG	3	0
6	B	405	PG4	3	0
7	A	409	PGE	1	0
5	C	103	PEG	1	0
6	B	402	PG4	1	0
5	C	104	PEG	1	0
3	B	401	FAD	3	0
5	C	105	PEG	1	0
5	B	410	PEG	2	0
5	A	403	PEG	1	0
4	B	411	ACT	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 FAD A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand PG4 B 405

Bond lengths

Bond angles

Torsions

Rings

Ligand PG4 B 402

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand PG4 A 406

Bond lengths

Bond angles

Torsions

Rings
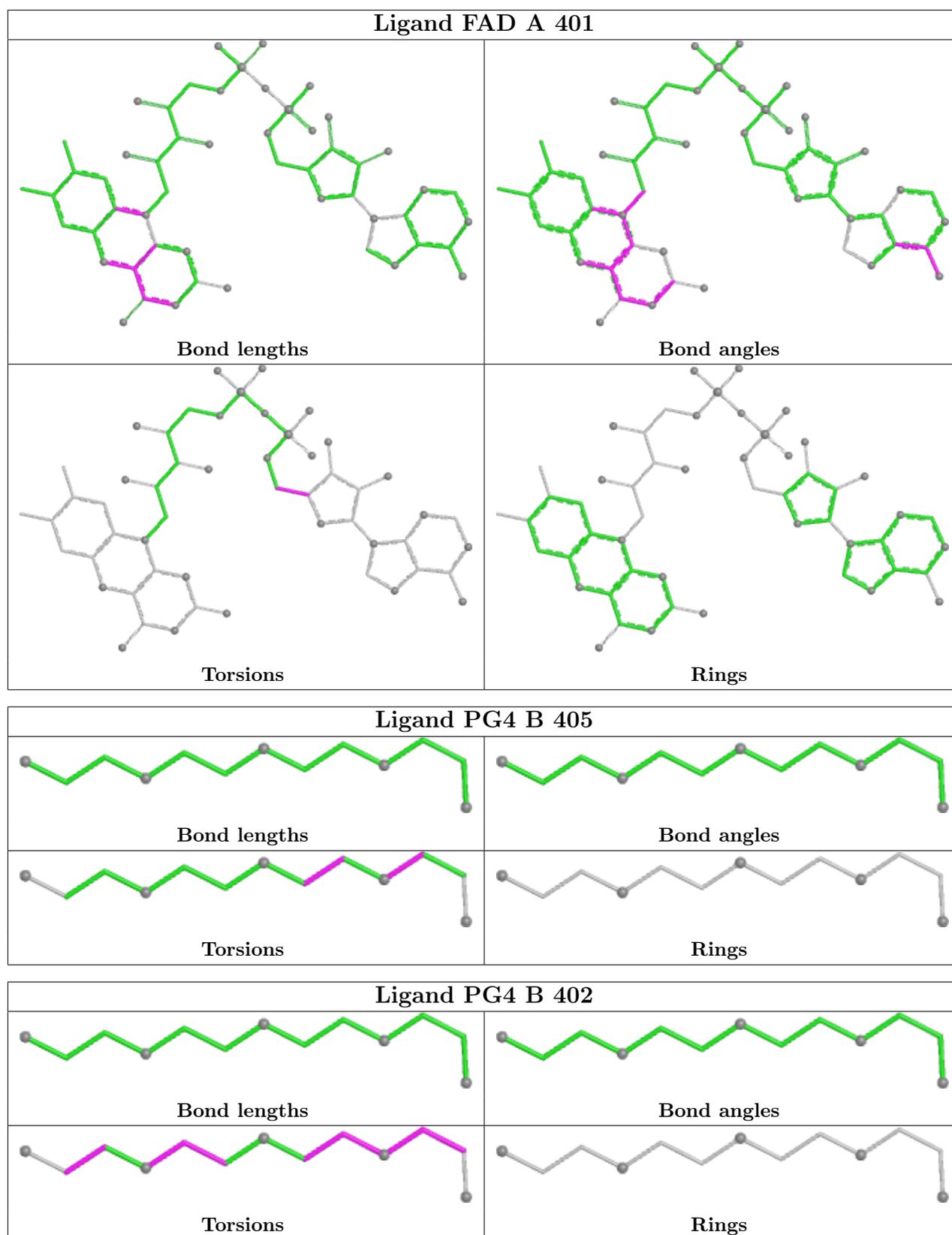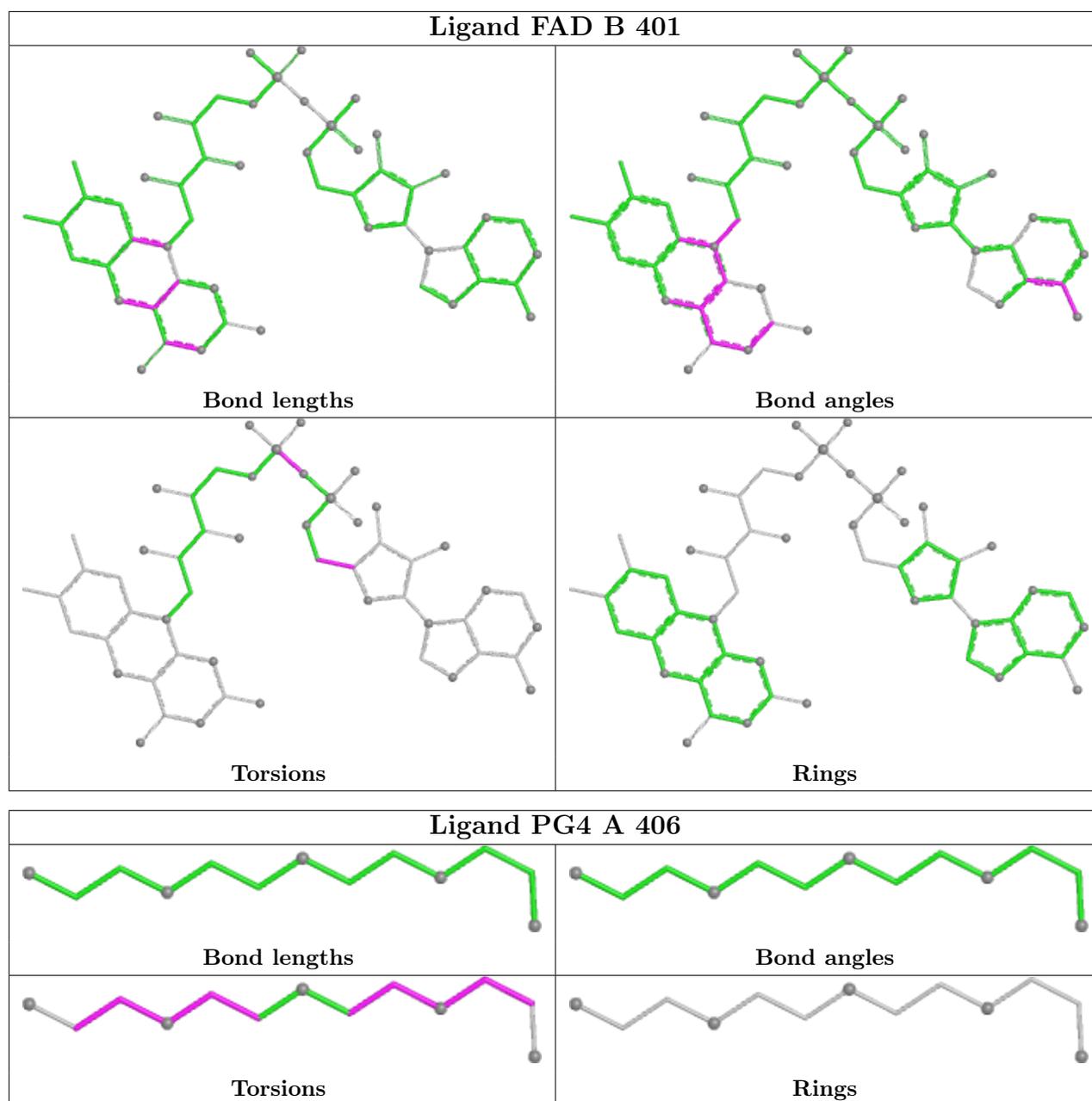
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 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(Å²)	Q<0.9
1	A	315/320 (98%)	0.13	2 (0%)	89	89	14, 30, 60, 98	0
1	B	315/320 (98%)	0.19	9 (2%)	51	52	17, 31, 66, 89	0
2	C	96/100 (96%)	0.23	1 (1%)	82	83	16, 28, 44, 72	0
2	D	96/100 (96%)	0.29	0	100	100	30, 50, 74, 87	0
All	All	822/840 (97%)	0.18	12 (1%)	73	74	14, 32, 66, 98	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	ILE	4.7
1	A	317	HIS	3.5
1	B	182	LEU	3.2
1	B	181	THR	3.0
1	B	118	ILE	2.7

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 monosaccharides 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(Å²)	Q<0.9
4	ACT	A	405	4/4	0.64	0.41	81,102,128,128	0
7	PGE	B	409	10/10	0.66	0.15	95,115,123,125	0
5	PEG	A	407	7/7	0.69	0.18	64,78,91,91	0
4	ACT	B	407	4/4	0.69	0.23	56,65,68,68	0
7	PGE	A	409	10/10	0.70	0.18	70,106,130,134	0
5	PEG	A	414	7/7	0.71	0.22	87,110,138,140	0
4	ACT	A	412	4/4	0.72	0.17	59,68,82,82	0
5	PEG	C	104	7/7	0.73	0.23	25,36,49,49	0
5	PEG	B	408	7/7	0.74	0.14	86,104,117,118	0
7	PGE	A	408	10/10	0.76	0.15	80,109,134,135	0
5	PEG	C	105	7/7	0.78	0.17	39,48,58,58	0
5	PEG	D	5203	7/7	0.79	0.18	53,69,91,91	0
5	PEG	A	403	7/7	0.79	0.16	52,71,91,91	0
4	ACT	D	5201	4/4	0.81	0.15	53,61,65,65	0
4	ACT	A	404	4/4	0.81	0.16	72,81,100,100	0
6	PG4	B	405	13/13	0.81	0.18	33,48,69,69	0
4	ACT	A	413	4/4	0.82	0.16	74,82,92,92	0
6	PG4	B	402	13/13	0.82	0.16	49,74,91,92	0
5	PEG	C	103	7/7	0.85	0.18	57,70,89,89	0
5	PEG	B	403	7/7	0.86	0.13	42,54,66,66	0
4	ACT	B	411	4/4	0.87	0.16	48,55,59,59	0
5	PEG	B	410	7/7	0.88	0.19	21,48,85,85	0
4	ACT	B	404	4/4	0.88	0.21	46,57,68,68	0
4	ACT	B	406	4/4	0.89	0.14	41,51,55,65	0
6	PG4	A	406	13/13	0.90	0.19	32,54,77,77	0
5	PEG	C	102	7/7	0.92	0.14	26,33,70,73	0
4	ACT	A	402	4/4	0.93	0.17	60,64,87,87	0
3	FAD	A	401	53/53	0.94	0.20	13,52,85,112	0
4	ACT	A	411	4/4	0.95	0.24	48,54,66,66	0
8	FES	D	5202	4/4	0.96	0.12	27,35,38,45	0
8	FES	C	101	4/4	0.97	0.20	24,26,32,38	0
4	ACT	A	410	4/4	0.97	0.22	11,20,34,39	0
3	FAD	B	401	53/53	0.98	0.14	8,23,34,42	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.
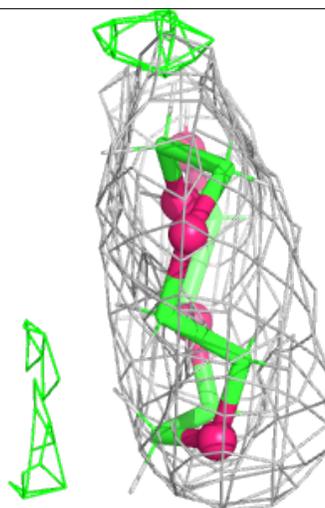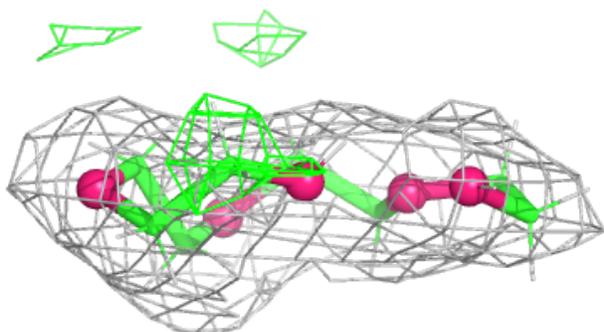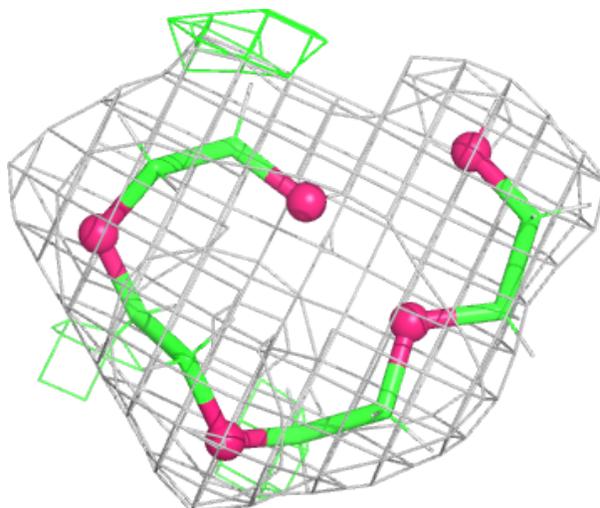
Electron density around PG4 B 405:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
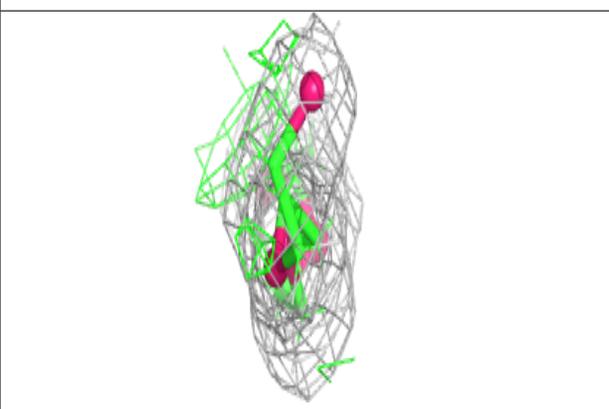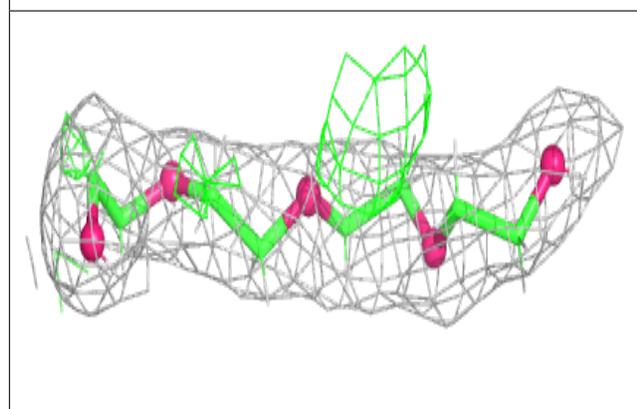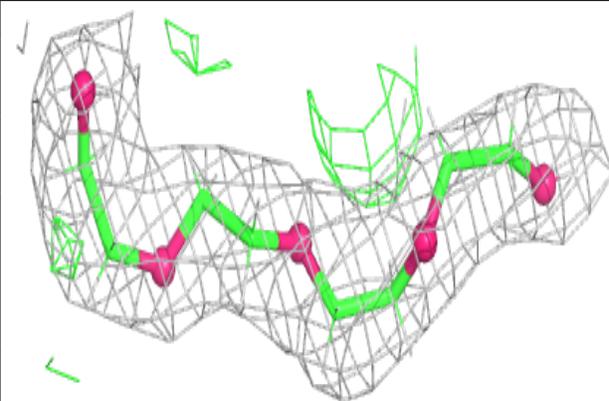and green (positive)
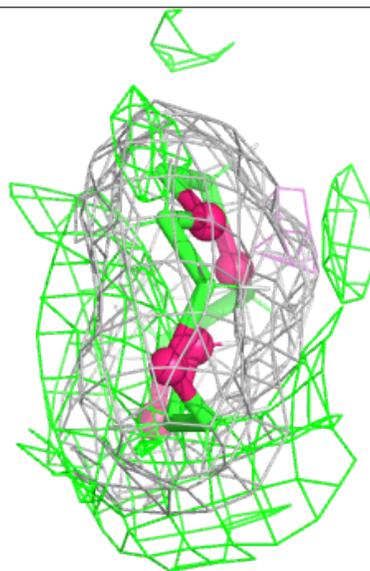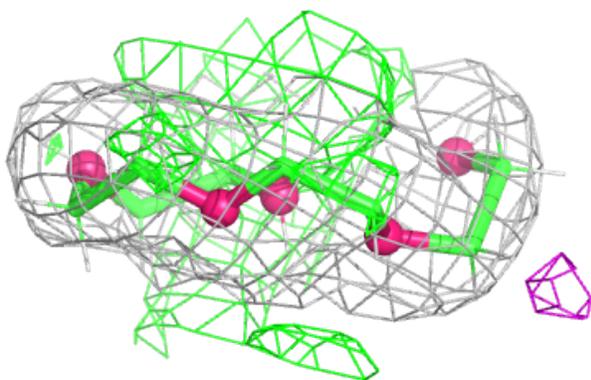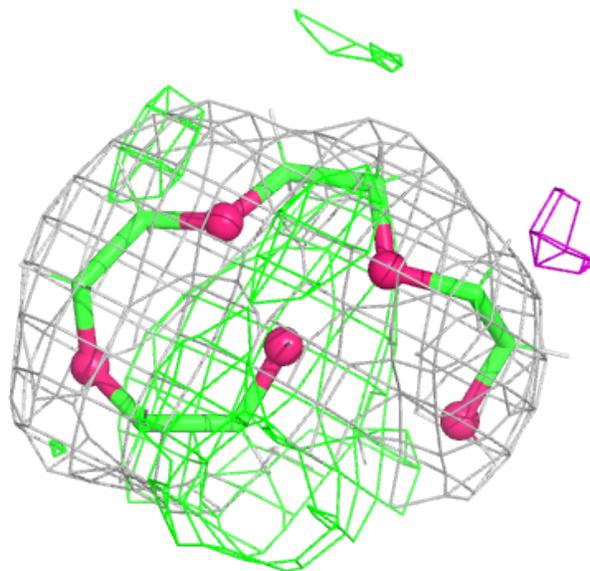
Electron density around PG4 B 402:

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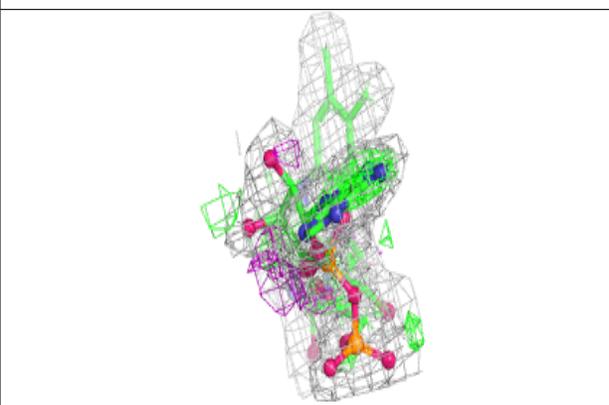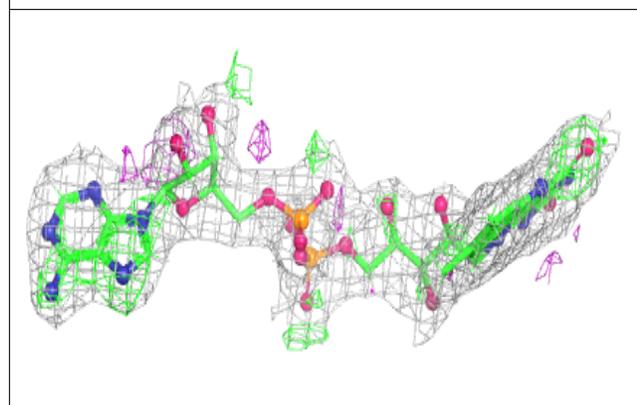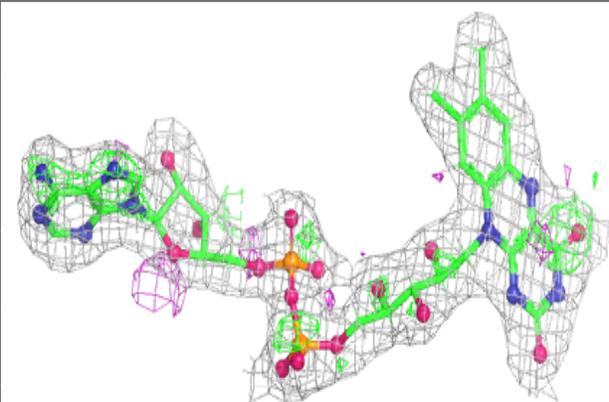mF_o-DF_c (at 3 rmsd) in purple (negative)
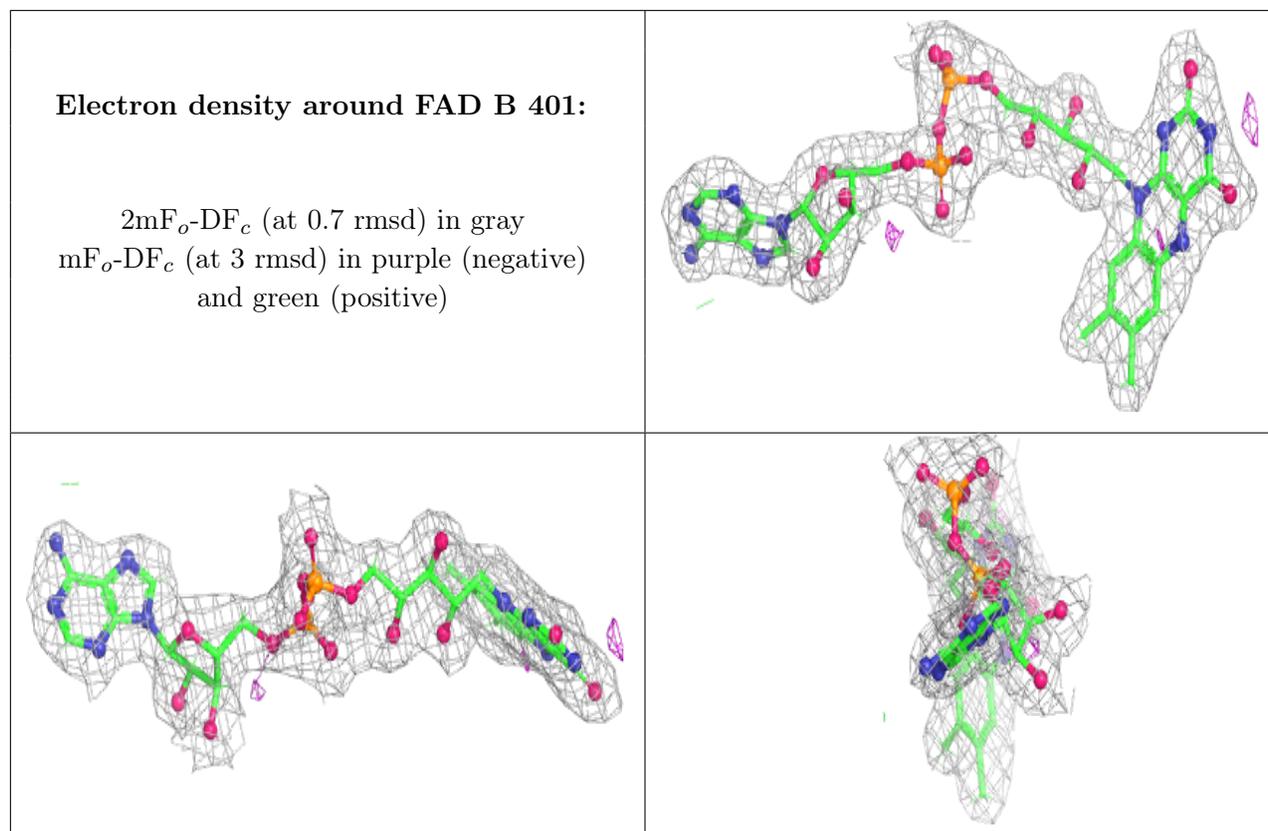and green (positive)

Electron density around PG4 A 406:

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

Electron density around FAD A 401:

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

Electron density around FAD B 401:

$2mF_o$-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 ⓘ

There are no such residues in this entry.