



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:07 PM UTC

PDB ID : 2QCU / pdb_00002qcu
Title : Crystal structure of Glycerol-3-phosphate Dehydrogenase from Escherichia coli
Authors : Yeh, J.I.; Chinte, U.; Du, S.
Deposited on : 2007-06-19
Resolution : 1.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

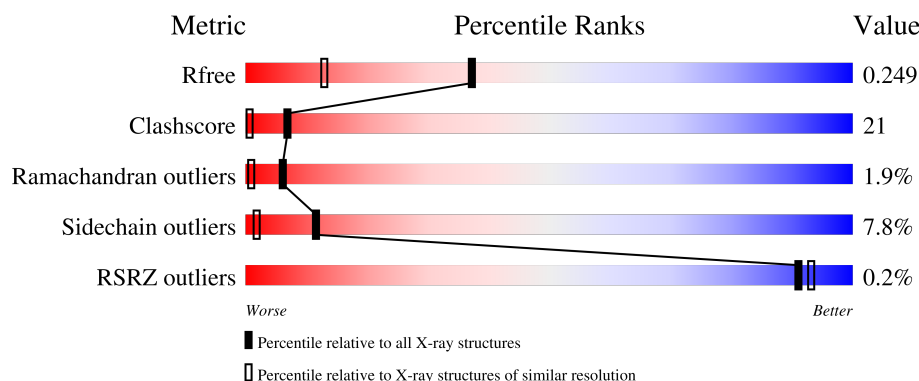
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	501	 75% 19% . .
1	B	501	 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
2	BOG	B	700	-	-	X	-
2	BOG	B	800	X	-	X	-
3	SO4	A	803	-	-	X	-
4	PO4	A	804	-	X	-	-
4	PO4	B	803	-	X	-	-
6	TAM	A	805	-	-	X	-
6	TAM	A	823	-	-	X	-
6	TAM	B	810	-	-	X	-
7	EDO	A	808	-	-	X	-
7	EDO	A	818	-	-	X	-
7	EDO	B	812	-	-	X	-

2 Entry composition [i](#)

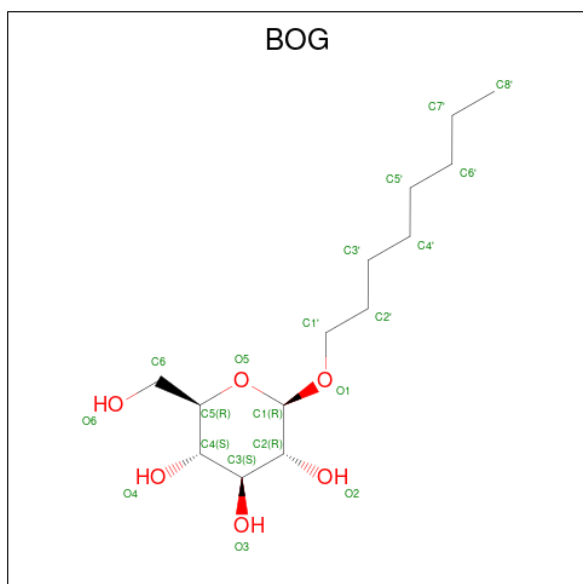
There are 9 unique types of molecules in this entry. The entry contains 8892 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aerobic glycerol-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	1	0	0
			3990	2532	712	734	12			
1	B	501	Total	C	N	O	S	0	0	0
			4007	2542	714	738	13			

- Molecule 2 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



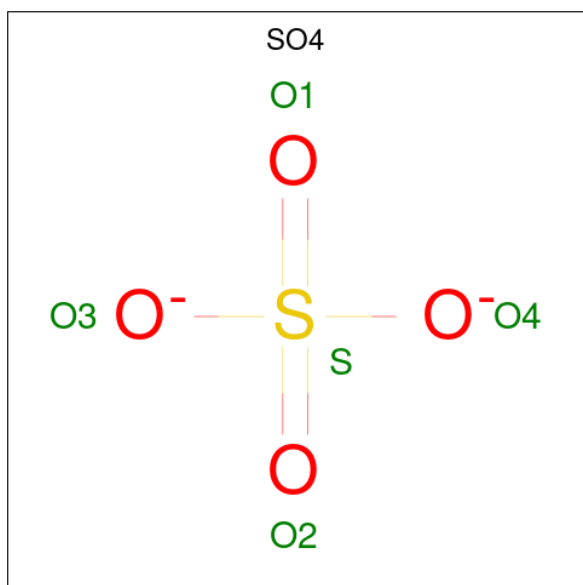
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		

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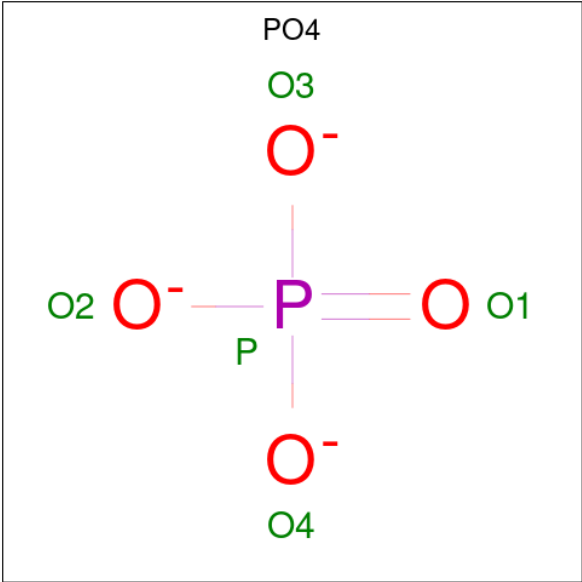
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



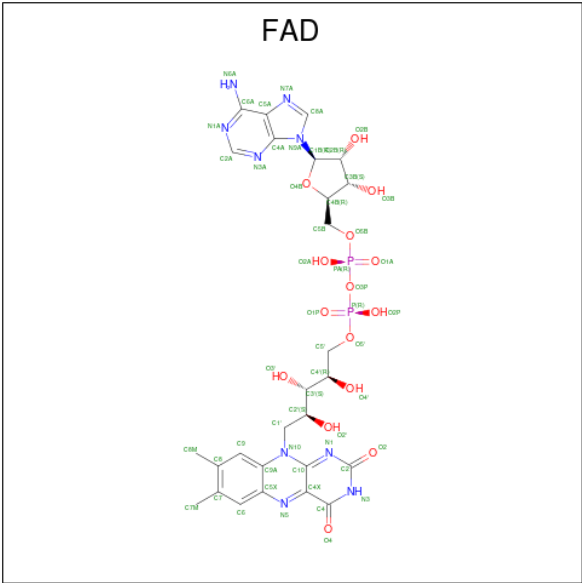
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



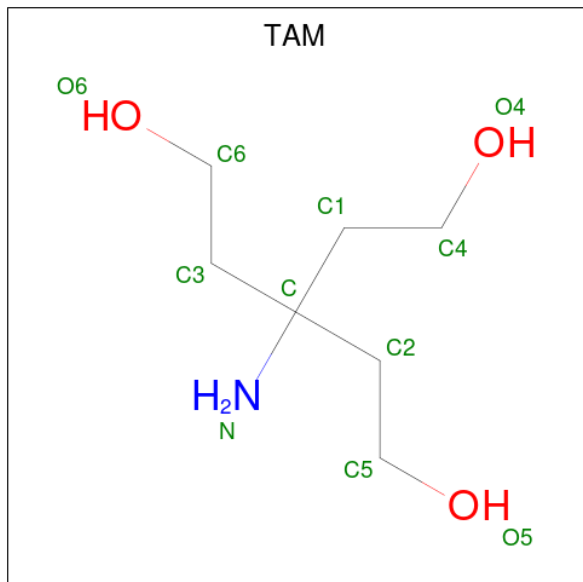
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	O	P		0	0
			5	4	1			
4	B	1	Total	O	P		0	0
			5	4	1			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



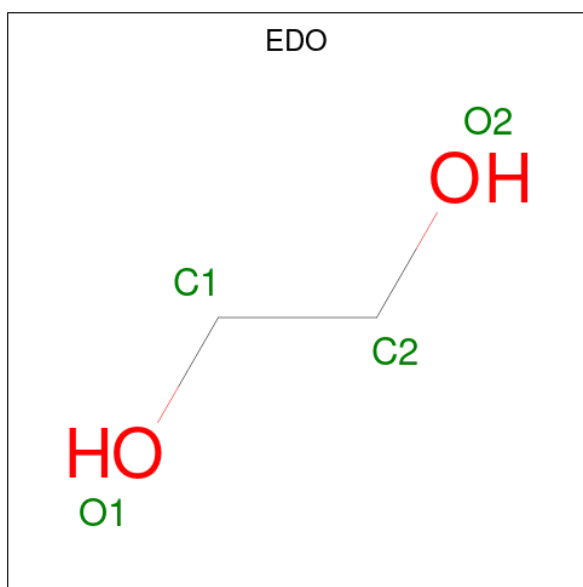
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is TRIS(HYDROXYETHYL)AMINOMETHANE (CCD ID: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			11	7	1	3		
6	A	1	Total	C	N	O	0	0
			11	7	1	3		
6	B	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



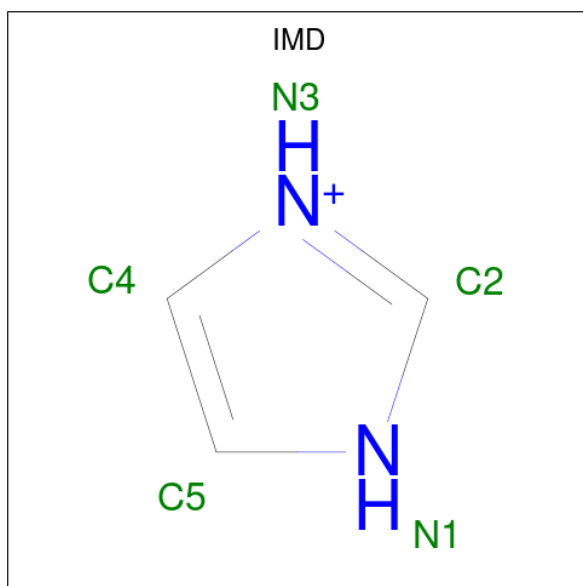
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0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

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

- Molecule 8 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	N	0	0
			5	3	2		
8	A	1	Total	C	N	0	0
			5	3	2		

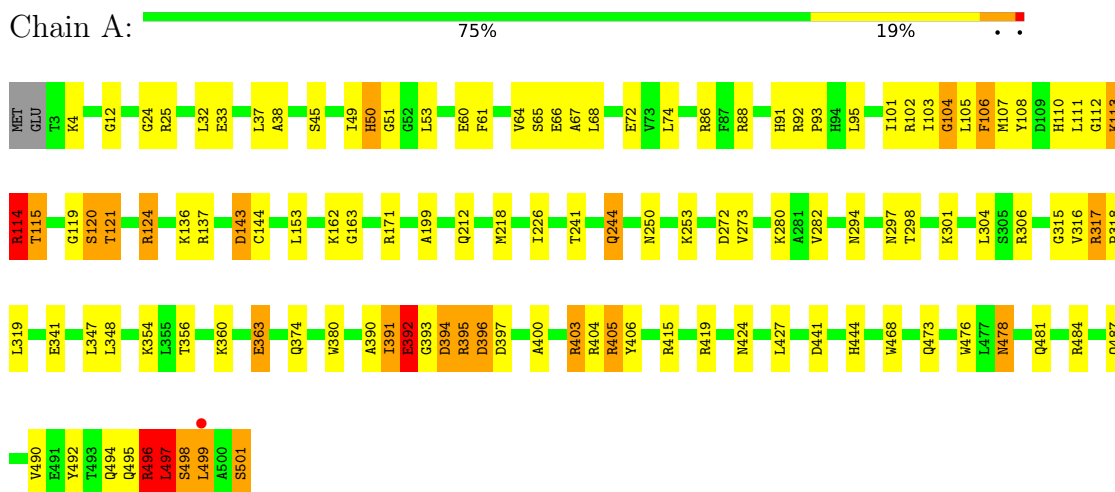
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	243	Total 243	O 243	0	0
9	B	233	Total 233	O 233	0	0

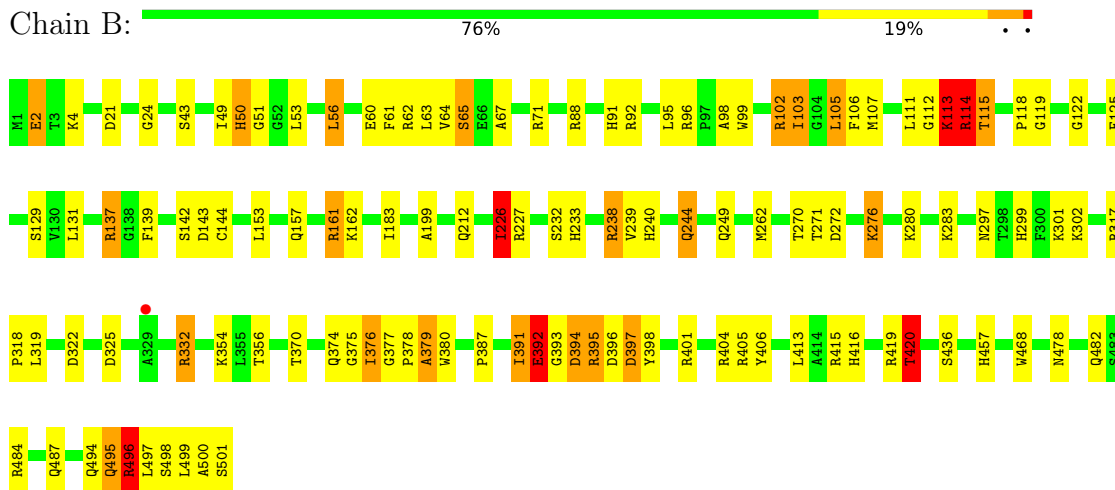
3 Residue-property plots

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: Aerobic glycerol-3-phosphate dehydrogenase



- Molecule 1: Aerobic glycerol-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	113.79Å 114.10Å 192.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.75 10.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (10.00-1.75) 98.9 (10.00-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.204 , 0.240 0.215 , 0.249	Depositor DCC
R_{free} test set	6861 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.478 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8892	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, SO4, TAM, BOG, EDO, PO4, FAD

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	0.71	1/4085 (0.0%)	0.98	7/5531 (0.1%)
1	B	0.67	0/4102	0.97	9/5553 (0.2%)
All	All	0.69	1/8187 (0.0%)	0.98	16/11084 (0.1%)

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	4
1	B	0	3
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	390	ALA	CA-CB	-6.10	1.45	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	HIS	N-CA-C	9.54	125.20	112.13
1	A	50	HIS	N-CA-C	9.02	124.49	112.13
1	B	2	GLU	N-CA-C	-7.12	95.63	110.80
1	B	395	ARG	N-CA-C	-6.24	105.32	113.12
1	B	226	ILE	N-CA-C	6.14	122.11	109.34

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	496	ARG	Peptide
1	A	497	LEU	Peptide
1	A	498	SER	Peptide
1	A	499	LEU	Peptide
1	B	496	ARG	Peptide

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	3990	0	3943	176	0
1	B	4007	0	3961	159	0
2	A	80	0	112	16	0
2	B	40	0	54	20	0
3	A	10	0	0	3	0
3	B	10	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
5	A	53	0	30	7	0
5	B	53	0	31	0	0
6	A	22	0	34	27	0
6	B	11	0	17	12	0
7	A	60	0	90	29	0
7	B	60	0	90	13	0
8	A	10	0	10	3	0
9	A	243	0	0	15	0
9	B	233	0	0	13	0
All	All	8892	0	8372	355	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 21.

The worst 5 of 355 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:395:ARG:CB	1:A:396:ASP:HB2	1.40	1.47
1:A:51:GLY:HA3	1:A:68:LEU:CD1	1.62	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ASP:H	1:A:397:ASP:CA	1.46	1.24
1:A:405:ARG:HD2	1:A:405:ARG:O	1.33	1.24
1:A:273:VAL:HG22	6:A:823:TAM:C3	1.68	1.24

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	497/501 (99%)	465 (94%)	23 (5%)	9 (2%)	6	1
1	B	499/501 (100%)	464 (93%)	25 (5%)	10 (2%)	6	1
All	All	996/1002 (99%)	929 (93%)	48 (5%)	19 (2%)	6	1

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	ARG
1	A	120	SER
1	A	319	LEU
1	A	396	ASP
1	B	113	LYS

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	417/419 (100%)	388 (93%)	29 (7%)	14	2
1	B	419/419 (100%)	383 (91%)	36 (9%)	10	1
All	All	836/838 (100%)	771 (92%)	65 (8%)	11	2

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	392	GLU
1	B	413	LEU
1	A	427	LEU
1	A	405	ARG
1	B	420	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	50	HIS
1	B	494	GLN
1	B	155	ASN
1	B	457	HIS
1	B	110	HIS

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 ⓘ

49 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	$\# Z > 2$
7	EDO	B	816	-	3,3,3	0.43	0	2,2,2	0.46	0
7	EDO	B	813	-	3,3,3	0.39	0	2,2,2	0.51	0
7	EDO	A	806	-	3,3,3	0.45	0	2,2,2	0.69	0
7	EDO	A	820	-	3,3,3	0.47	0	2,2,2	0.24	0
7	EDO	B	811	-	3,3,3	0.61	0	2,2,2	0.48	0
7	EDO	B	815	-	3,3,3	0.49	0	2,2,2	0.37	0
7	EDO	A	817	-	3,3,3	0.46	0	2,2,2	0.39	0
7	EDO	A	811	-	3,3,3	0.48	0	2,2,2	0.50	0
7	EDO	A	809	-	3,3,3	0.48	0	2,2,2	0.35	0
6	TAM	A	805	-	10,10,10	0.50	0	12,12,12	1.07	2 (16%)
5	FAD	B	600	-	58,58,58	1.32	5 (8%)	85,89,89	1.60	14 (16%)
7	EDO	A	813	-	3,3,3	0.46	0	2,2,2	0.41	0
7	EDO	B	814	-	3,3,3	0.48	0	2,2,2	0.21	0
7	EDO	B	819	-	3,3,3	0.54	0	2,2,2	0.40	0
7	EDO	A	815	-	3,3,3	0.47	0	2,2,2	0.28	0
7	EDO	A	818	-	3,3,3	0.29	0	2,2,2	1.08	0
7	EDO	B	806	-	3,3,3	0.48	0	2,2,2	0.51	0
7	EDO	B	805	-	3,3,3	0.43	0	2,2,2	0.23	0
3	SO4	B	801	-	4,4,4	0.24	0	6,6,6	0.36	0
5	FAD	A	600	-	58,58,58	1.16	6 (10%)	85,89,89	1.66	17 (20%)
6	TAM	A	823	-	10,10,10	0.60	0	12,12,12	2.32	3 (25%)
7	EDO	A	819	-	3,3,3	0.44	0	2,2,2	0.34	0
7	EDO	B	820	-	3,3,3	0.40	0	2,2,2	0.43	0
4	PO4	B	803	-	4,4,4	3.06	4 (100%)	6,6,6	0.46	0
4	PO4	A	804	-	4,4,4	2.33	3 (75%)	6,6,6	1.35	2 (33%)
6	TAM	B	810	-	10,10,10	0.52	0	12,12,12	2.10	3 (25%)
2	BOG	A	800	-	20,20,20	0.51	0	25,25,25	1.55	3 (12%)
2	BOG	A	701	-	20,20,20	0.59	1 (5%)	25,25,25	0.98	1 (4%)
3	SO4	A	802	-	4,4,4	0.23	0	6,6,6	0.30	0
2	BOG	B	800	-	20,20,20	0.96	1 (5%)	25,25,25	1.50	5 (20%)
3	SO4	A	803	-	4,4,4	0.21	0	6,6,6	0.30	0
7	EDO	A	822	-	3,3,3	0.48	0	2,2,2	0.25	0
7	EDO	A	808	-	3,3,3	0.38	0	2,2,2	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	B	812	-	3,3,3	0.58	0	2,2,2	0.11	0
7	EDO	A	816	-	3,3,3	0.44	0	2,2,2	0.07	0
7	EDO	A	812	-	3,3,3	0.43	0	2,2,2	0.58	0
2	BOG	A	801	-	20,20,20	0.50	0	25,25,25	0.90	1 (4%)
8	IMD	A	821	-	5,5,5	0.71	0	5,5,5	0.28	0
7	EDO	A	810	-	3,3,3	0.41	0	2,2,2	0.64	0
7	EDO	B	804	-	3,3,3	0.44	0	2,2,2	0.39	0
7	EDO	B	809	-	3,3,3	0.40	0	2,2,2	0.57	0
2	BOG	A	700	-	20,20,20	0.54	0	25,25,25	0.57	0
7	EDO	B	807	-	3,3,3	0.49	0	2,2,2	0.32	0
7	EDO	B	808	-	3,3,3	0.50	0	2,2,2	0.07	0
2	BOG	B	700	-	20,20,20	0.55	1 (5%)	25,25,25	1.45	5 (20%)
7	EDO	A	814	-	3,3,3	0.44	0	2,2,2	0.32	0
8	IMD	A	807	-	5,5,5	0.67	0	5,5,5	0.45	0
7	EDO	B	817	-	3,3,3	0.62	0	2,2,2	0.82	0
3	SO4	B	802	-	4,4,4	0.25	0	6,6,6	0.19	0

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
7	EDO	B	816	-	-	1/1/1/1	-
7	EDO	B	813	-	-	0/1/1/1	-
7	EDO	A	806	-	-	1/1/1/1	-
7	EDO	A	820	-	-	1/1/1/1	-
7	EDO	B	811	-	-	1/1/1/1	-
7	EDO	B	815	-	-	1/1/1/1	-
7	EDO	A	817	-	-	1/1/1/1	-
7	EDO	A	811	-	-	0/1/1/1	-
7	EDO	A	809	-	-	0/1/1/1	-
6	TAM	A	805	-	-	7/12/12/12	-
5	FAD	B	600	-	-	0/34/50/50	0/6/6/6
7	EDO	A	813	-	-	1/1/1/1	-
7	EDO	B	814	-	-	1/1/1/1	-
7	EDO	B	819	-	-	0/1/1/1	-
7	EDO	A	815	-	-	0/1/1/1	-
7	EDO	A	818	-	-	1/1/1/1	-
7	EDO	B	806	-	-	1/1/1/1	-
7	EDO	B	805	-	-	1/1/1/1	-
5	FAD	A	600	-	-	7/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TAM	A	823	-	-	8/12/12/12	-
7	EDO	A	819	-	-	1/1/1/1	-
7	EDO	B	820	-	-	1/1/1/1	-
6	TAM	B	810	-	-	6/12/12/12	-
2	BOG	A	800	-	-	7/11/31/31	0/1/1/1
2	BOG	A	701	-	-	5/11/31/31	0/1/1/1
2	BOG	B	800	-	3/3/5/5	5/11/31/31	1/1/1/1
7	EDO	A	822	-	-	1/1/1/1	-
7	EDO	A	808	-	-	1/1/1/1	-
7	EDO	B	812	-	-	1/1/1/1	-
7	EDO	A	816	-	-	1/1/1/1	-
7	EDO	A	812	-	-	1/1/1/1	-
2	BOG	A	801	-	-	4/11/31/31	0/1/1/1
8	IMD	A	821	-	-	-	0/1/1/1
7	EDO	A	810	-	-	0/1/1/1	-
7	EDO	B	804	-	-	1/1/1/1	-
7	EDO	B	809	-	-	0/1/1/1	-
2	BOG	A	700	-	-	3/11/31/31	0/1/1/1
7	EDO	B	807	-	-	0/1/1/1	-
7	EDO	B	808	-	-	0/1/1/1	-
2	BOG	B	700	-	-	6/11/31/31	0/1/1/1
7	EDO	A	814	-	-	1/1/1/1	-
8	IMD	A	807	-	-	-	0/1/1/1
7	EDO	B	817	-	-	1/1/1/1	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	600	FAD	C4X-N5	5.08	1.41	1.30
4	B	803	PO4	P-O1	4.67	1.61	1.50
5	B	600	FAD	PA-O3P	3.65	1.63	1.59
5	A	600	FAD	C4X-N5	3.53	1.38	1.30
5	B	600	FAD	C10-N1	3.48	1.40	1.33

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	600	FAD	N3A-C2A-N1A	-7.11	117.82	128.58
6	A	823	TAM	C5-C2-C	-6.81	107.94	115.97
5	A	600	FAD	N3A-C2A-N1A	-5.49	120.28	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	BOG	O1-C1-C2	5.42	116.50	108.27
5	A	600	FAD	C5A-C4A-N3A	-4.67	120.28	126.72

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	800	BOG	C4
2	B	800	BOG	C2
2	B	800	BOG	C3

5 of 79 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	BOG	O5-C1-O1-C1'
2	A	800	BOG	C2-C1-O1-C1'
5	A	600	FAD	C5B-O5B-PA-O2A
5	A	600	FAD	O4'-C4'-C5'-O5'
6	A	805	TAM	C1-C-C2-C5

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	800	BOG	C1-C2-C3-C4-C5-O5

31 monomers are involved in 131 short contacts:

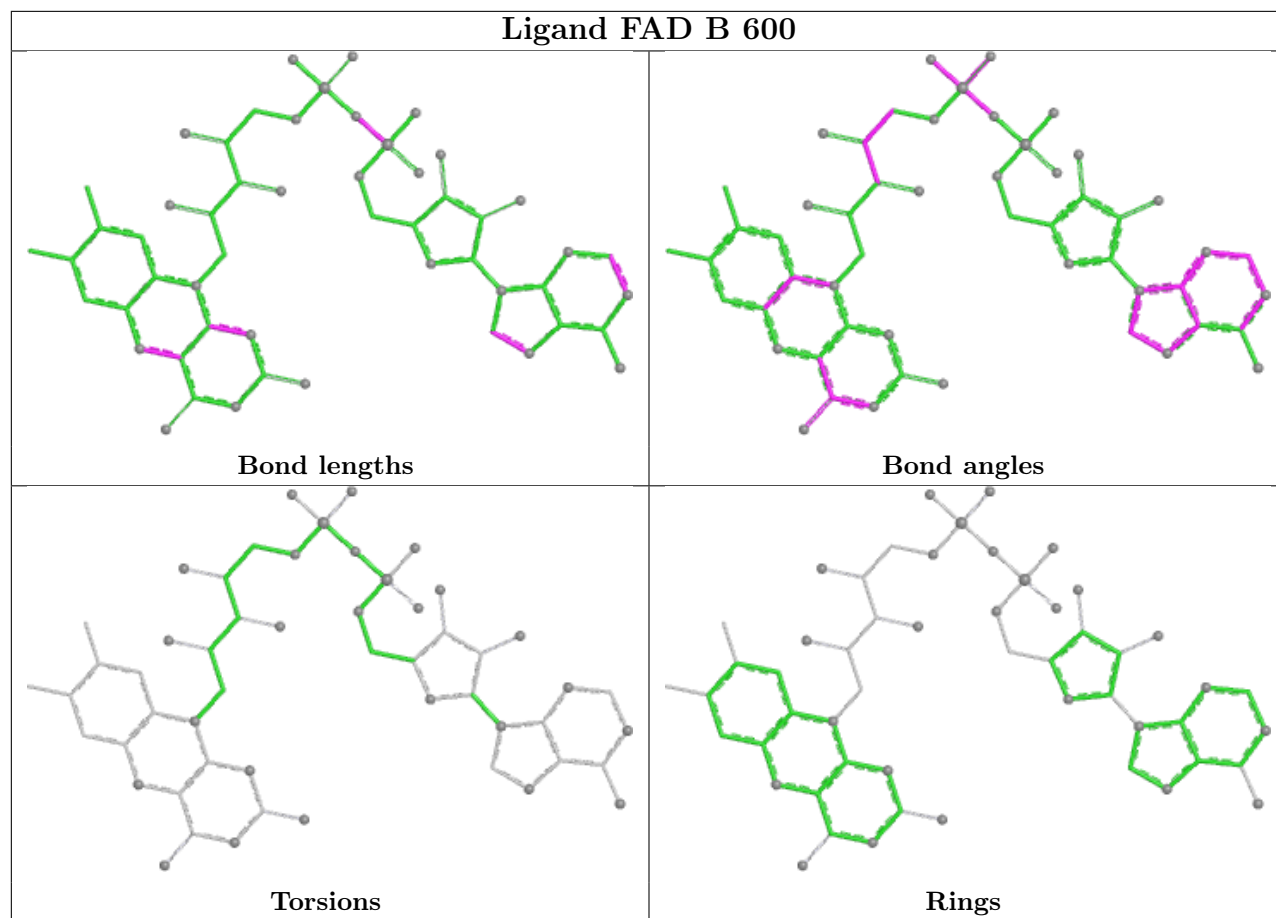
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	806	EDO	3	0
7	A	820	EDO	3	0
7	B	811	EDO	2	0
7	A	811	EDO	1	0
7	A	809	EDO	2	0
6	A	805	TAM	13	0
7	A	815	EDO	1	0
7	A	818	EDO	8	0
7	B	805	EDO	2	0
5	A	600	FAD	7	0
6	A	823	TAM	14	0
7	A	819	EDO	1	0
4	B	803	PO4	1	0
6	B	810	TAM	12	0
2	A	800	BOG	6	0

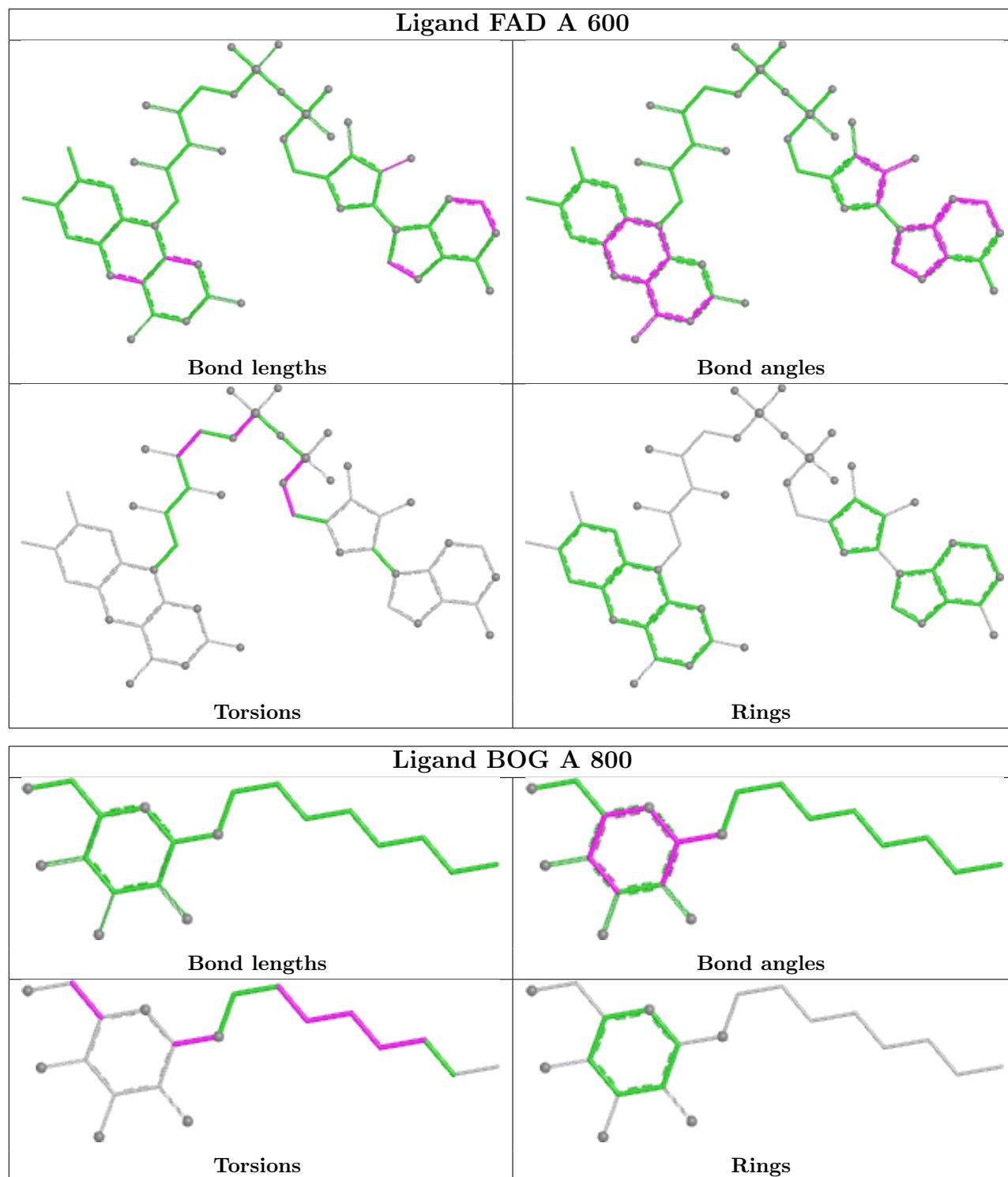
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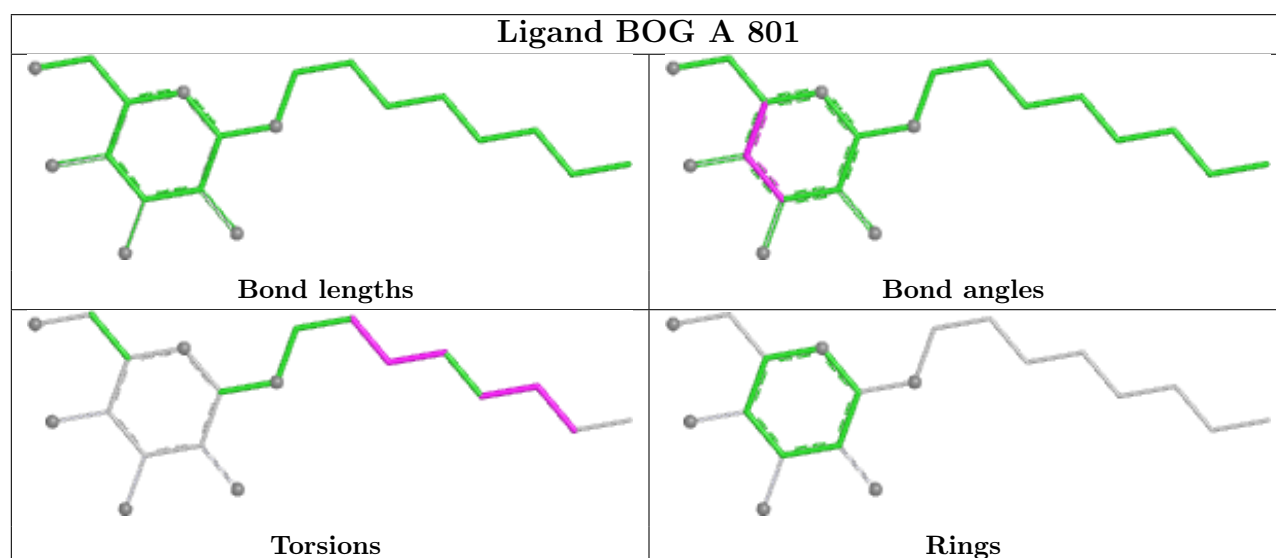
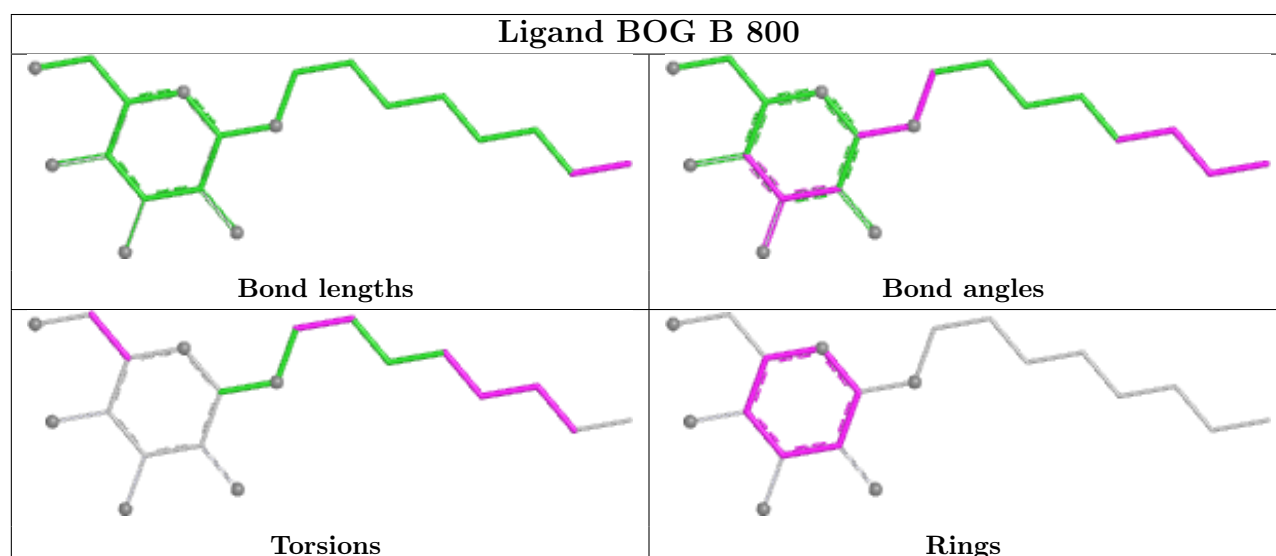
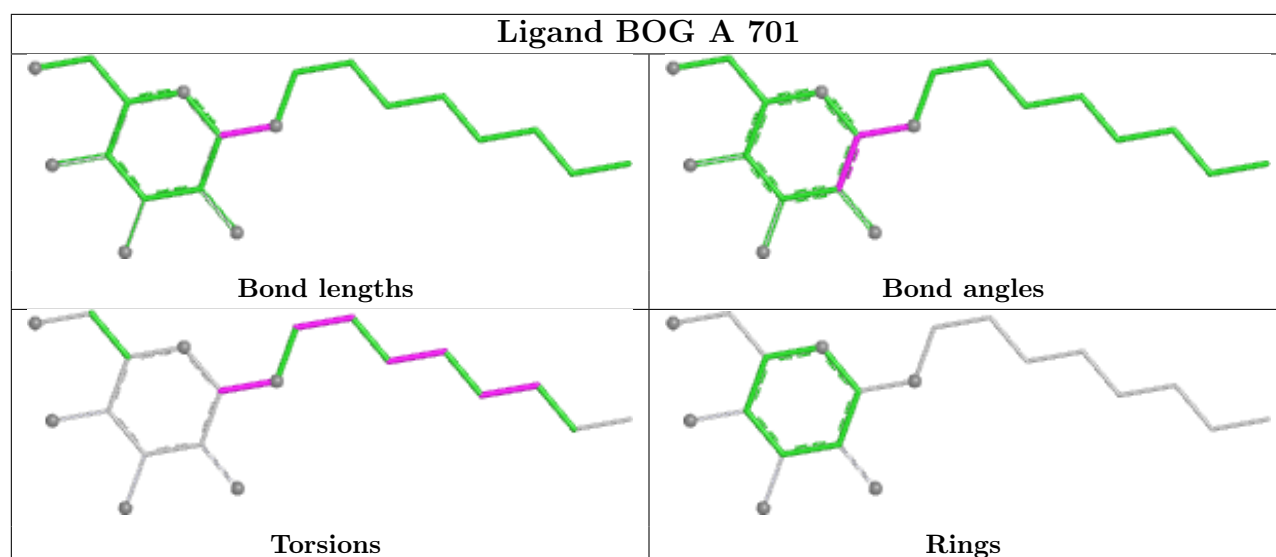
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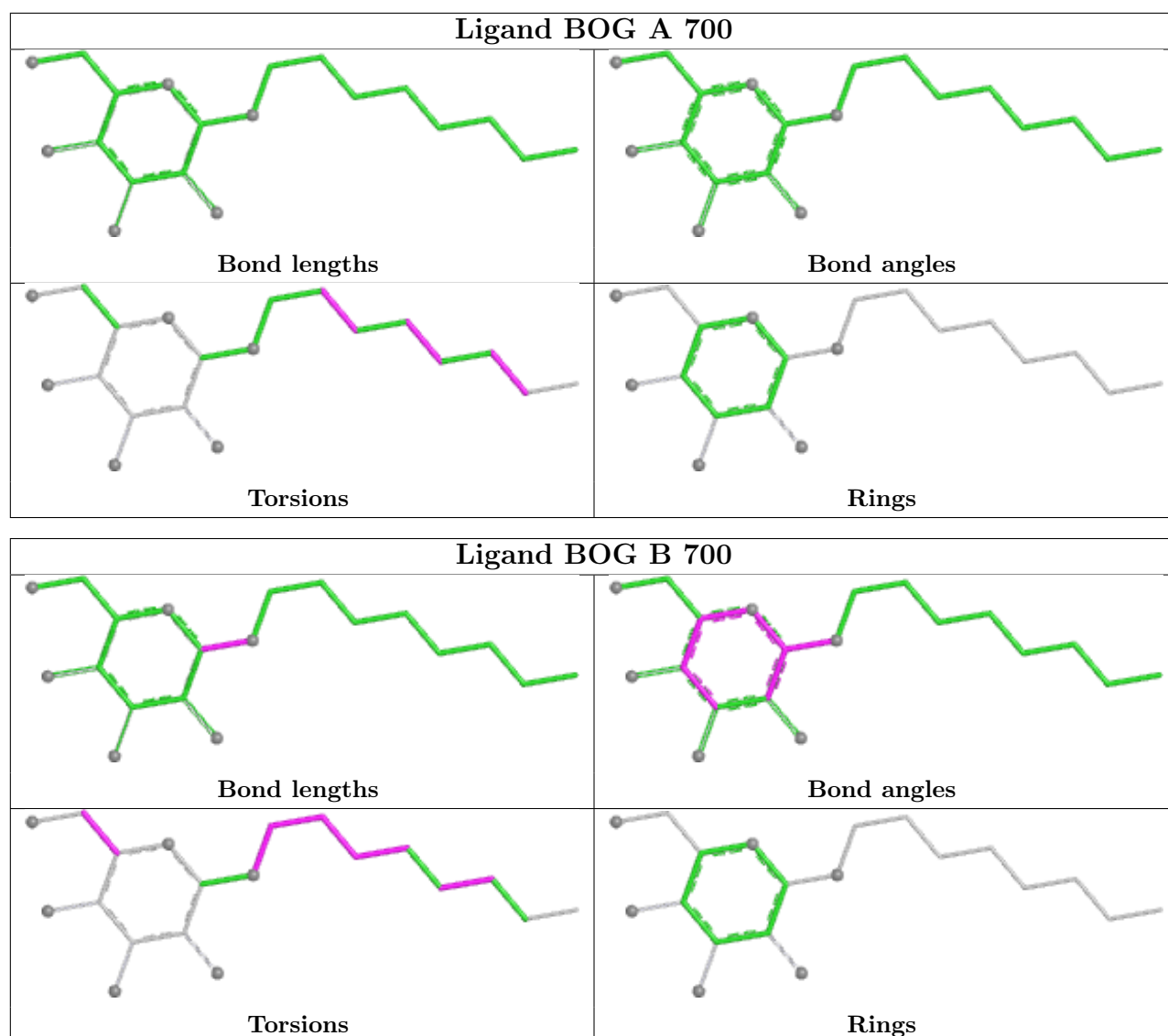
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	BOG	6	0
2	B	800	BOG	10	0
3	A	803	SO4	3	0
7	A	822	EDO	1	0
7	A	808	EDO	4	0
7	B	812	EDO	5	0
7	A	816	EDO	1	0
7	A	812	EDO	1	0
2	A	801	BOG	4	0
8	A	821	IMD	3	0
7	B	804	EDO	1	0
7	B	807	EDO	1	0
7	B	808	EDO	1	0
2	B	700	BOG	10	0
7	A	814	EDO	3	0
7	B	817	EDO	1	0

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 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.









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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	499/501 (99%)	-0.86	1 (0%) 91 93	13, 26, 54, 98	1 (0%)
1	B	501/501 (100%)	-0.84	1 (0%) 91 93	13, 26, 54, 101	0
All	All	1000/1002 (99%)	-0.85	2 (0%) 91 93	13, 26, 54, 101	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	499	LEU	2.2
1	B	329	ALA	2.1

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 oligosaccharides 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, 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
2	BOG	A	700	20/20	0.93	0.09	99,113,115,116	0
7	EDO	B	819	4/4	0.94	0.10	39,44,44,50	0
2	BOG	A	800	20/20	0.95	0.12	33,52,55,56	20

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BOG	B	800	20/20	0.96	0.10	83,89,90,92	0
6	TAM	A	805	11/11	0.96	0.10	44,58,59,61	0
7	EDO	B	815	4/4	0.96	0.07	53,54,55,57	0
2	BOG	A	701	20/20	0.96	0.08	67,75,81,81	0
2	BOG	A	801	20/20	0.97	0.10	54,59,62,63	20
6	TAM	B	810	11/11	0.97	0.08	45,54,55,55	0
7	EDO	A	812	4/4	0.97	0.07	44,45,46,50	0
7	EDO	A	813	4/4	0.97	0.06	57,59,61,61	0
7	EDO	A	814	4/4	0.97	0.10	33,38,44,55	0
3	SO4	A	803	5/5	0.97	0.09	76,77,82,84	0
7	EDO	B	816	4/4	0.97	0.07	55,55,58,61	0
7	EDO	B	817	4/4	0.97	0.08	43,44,46,50	0
4	PO4	B	803	5/5	0.97	0.10	30,30,30,30	0
8	IMD	A	821	5/5	0.97	0.09	59,63,64,64	0
2	BOG	B	700	20/20	0.98	0.06	54,66,74,78	0
3	SO4	B	801	5/5	0.98	0.07	69,70,72,74	0
7	EDO	A	816	4/4	0.98	0.10	34,36,37,42	0
7	EDO	A	817	4/4	0.98	0.06	30,37,40,42	0
7	EDO	A	819	4/4	0.98	0.05	52,57,59,60	0
7	EDO	A	820	4/4	0.98	0.07	46,52,55,55	0
7	EDO	B	806	4/4	0.98	0.08	34,39,48,48	0
7	EDO	B	807	4/4	0.98	0.07	38,43,45,48	0
7	EDO	B	808	4/4	0.98	0.09	26,40,41,43	0
7	EDO	B	809	4/4	0.98	0.04	53,57,59,60	0
7	EDO	B	811	4/4	0.98	0.10	19,32,38,45	0
7	EDO	B	812	4/4	0.98	0.05	44,46,49,50	0
7	EDO	B	813	4/4	0.98	0.06	43,43,50,52	0
6	TAM	A	823	11/11	0.98	0.08	47,51,55,55	0
3	SO4	B	802	5/5	0.98	0.10	93,93,95,96	0
7	EDO	A	809	4/4	0.98	0.07	31,35,41,42	0
7	EDO	A	810	4/4	0.98	0.06	47,49,50,54	0
7	EDO	B	820	4/4	0.98	0.05	43,43,49,51	0
8	IMD	A	807	5/5	0.98	0.07	49,52,55,57	0
4	PO4	A	804	5/5	0.98	0.08	30,30,30,30	0
3	SO4	A	802	5/5	0.99	0.08	66,68,69,70	0
5	FAD	A	600	53/53	0.99	0.03	12,16,20,44	0
7	EDO	A	818	4/4	0.99	0.07	24,31,37,44	0
7	EDO	A	811	4/4	0.99	0.05	20,28,31,37	0
7	EDO	B	814	4/4	0.99	0.06	23,35,41,47	0
5	FAD	B	600	53/53	0.99	0.03	13,16,19,22	0
7	EDO	A	822	4/4	0.99	0.09	40,42,43,48	0
7	EDO	B	804	4/4	0.99	0.05	32,34,35,39	0

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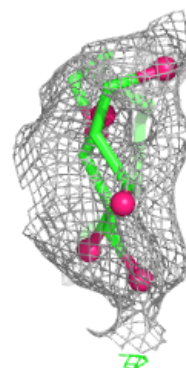
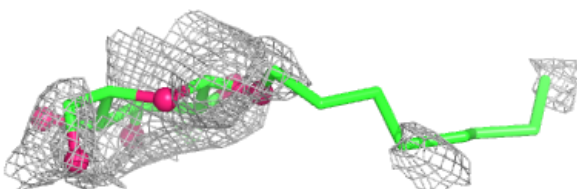
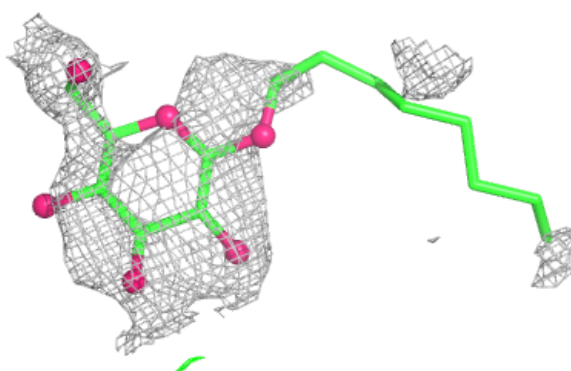
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	B	805	4/4	0.99	0.05	24,30,38,41	0
7	EDO	A	806	4/4	0.99	0.06	34,38,46,48	0
7	EDO	A	808	4/4	0.99	0.09	25,33,36,49	0
7	EDO	A	815	4/4	0.99	0.05	33,47,47,48	0

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.

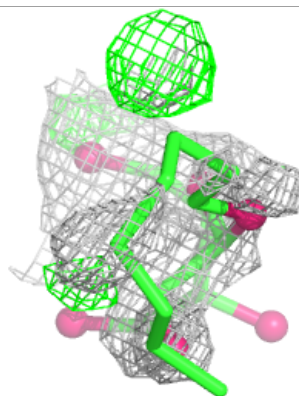
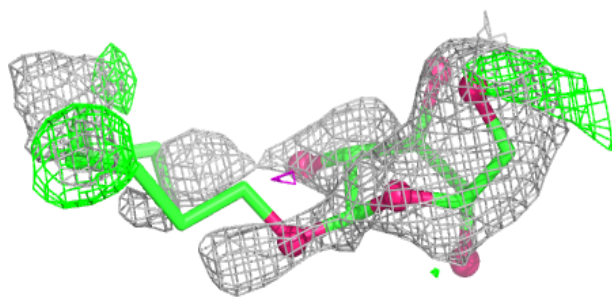
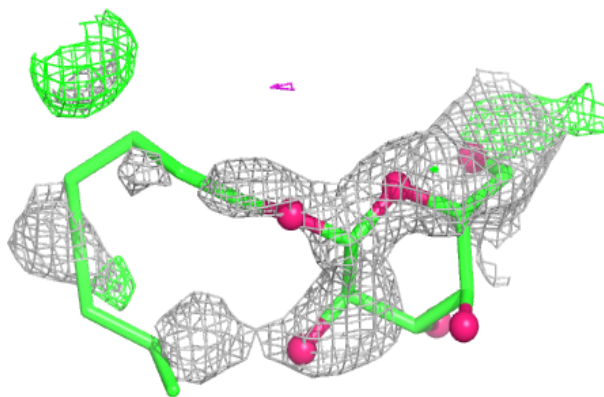
Electron density around BOG A 700:

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

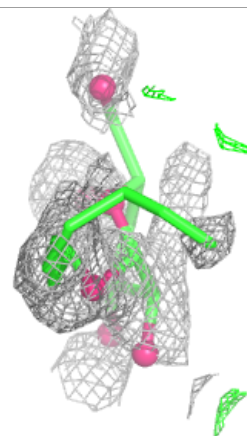
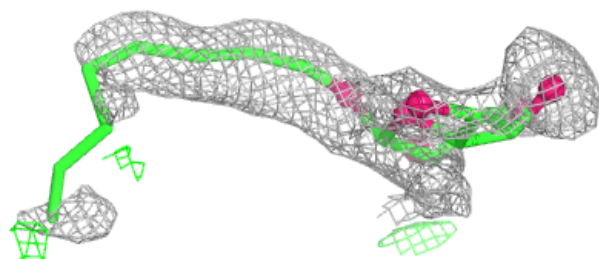
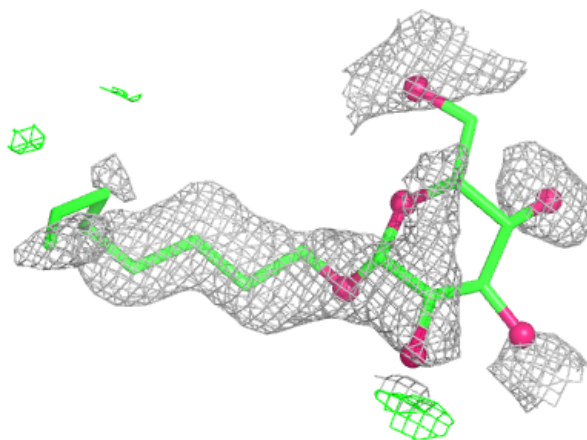


Electron density around BOG A 800:

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

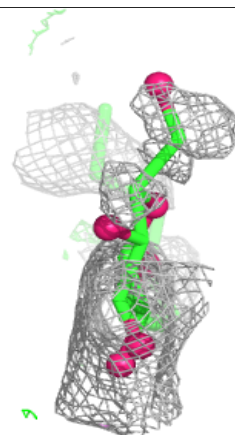
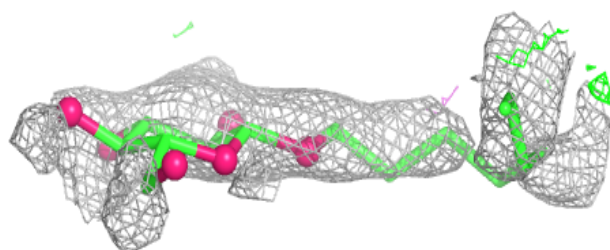
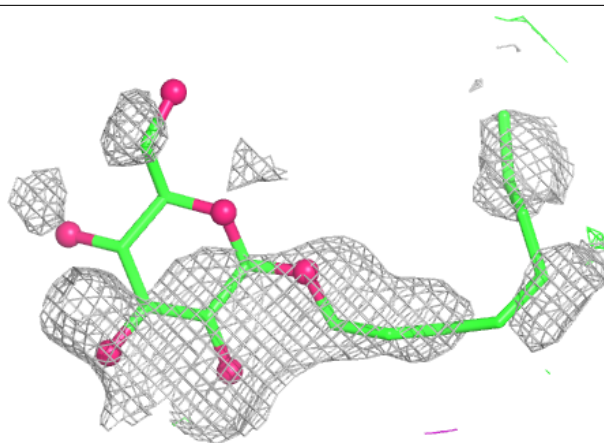
**Electron density around BOG B 800:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



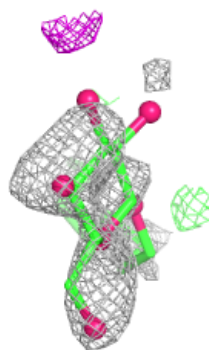
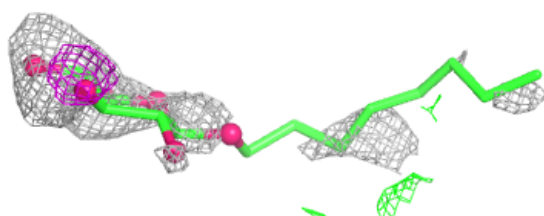
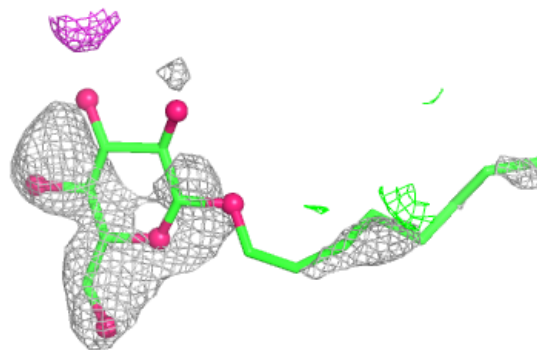
Electron density around BOG A 701:

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and green (positive)

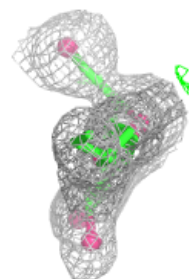
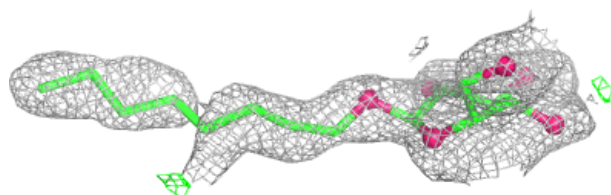
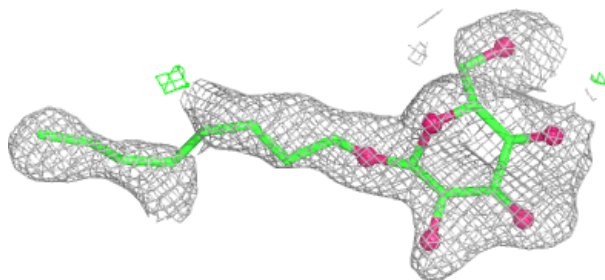


Electron density around BOG A 801:

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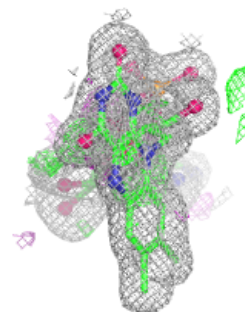
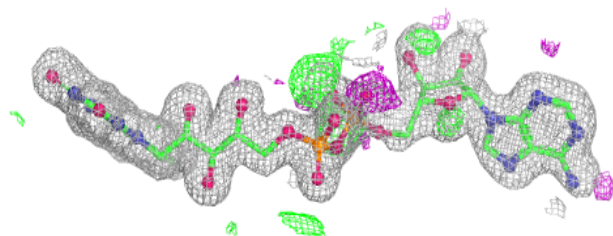
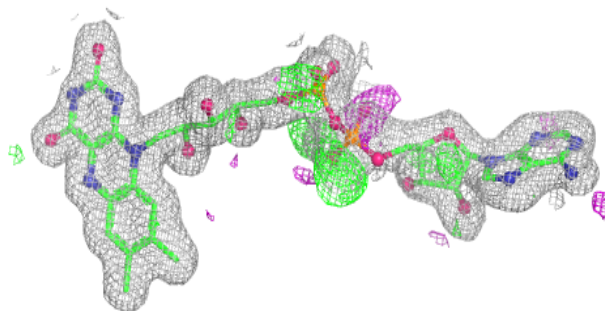
**Electron density around BOG B 700:**

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

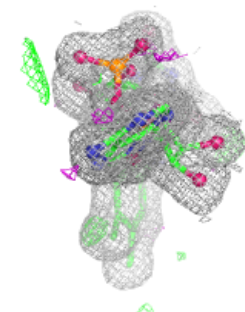
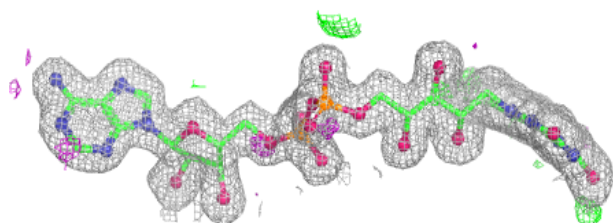
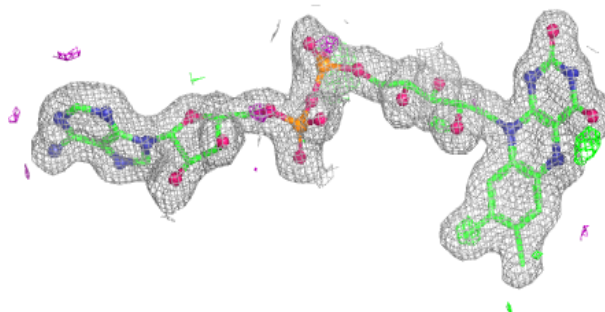


Electron density around FAD A 600:

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

**Electron density around FAD B 600:**

$2mF_o-DF_c$ (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.