



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:58 pm BST

PDB ID : 5YJW
Title : Structure of the Ndi1 protein from *Saccharomyces cerevisiae* in complex with the competitive inhibitor, stigmatellin.
Authors : Yamasita, T.; Inaoka, D.K.; Shiba, T.; Oohashi, T.; Iwata, S.; Yagi, T.; Kosaka, H.; Harada, S.; Kita, K.; Hirano, K.
Deposited on : 2017-10-11
Resolution : 1.85 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

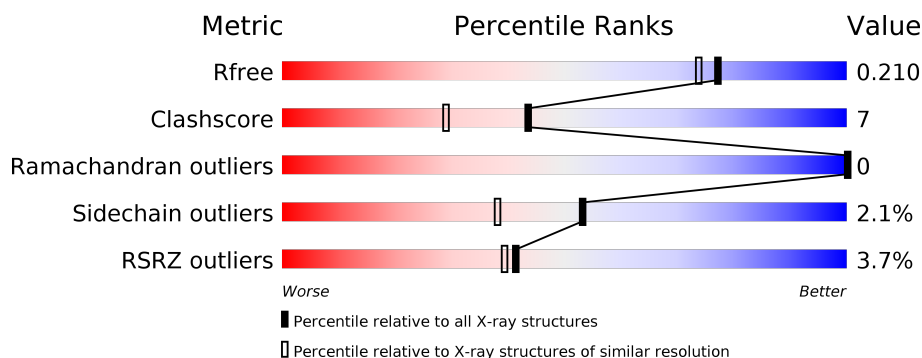
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 on 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	484	<div> <div>4%</div> <div>87%</div> <div>6% • 6%</div> </div>

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
11	SMA	A	626[A]	-	-	-	X
11	SMA	A	626[B]	-	-	-	X

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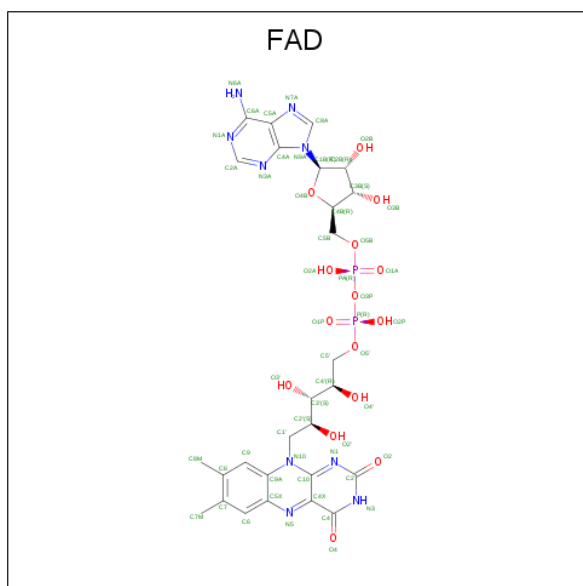
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	609	-	-	-	X
8	PEG	A	615	-	-	-	X

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 Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	14	0
			3698	2388	627	677	6			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).

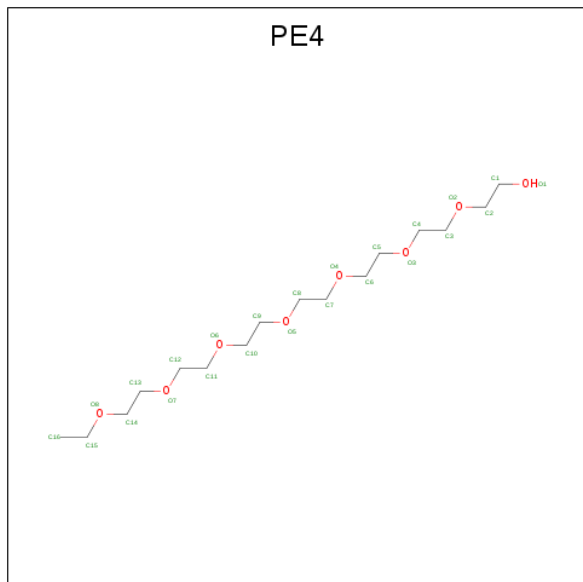


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

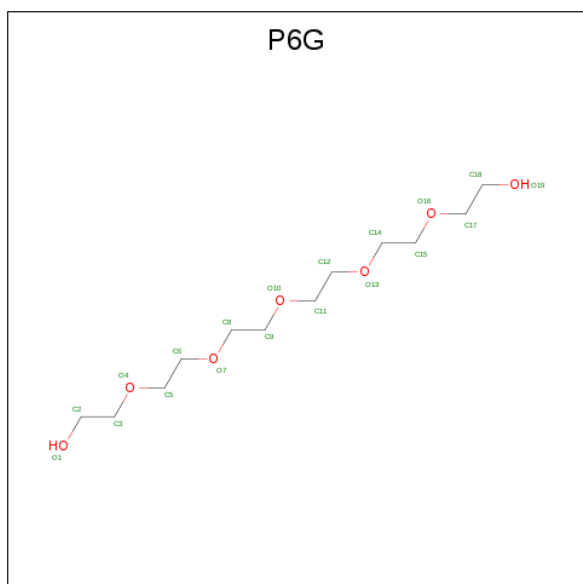
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Mg 4 4	0	0

- Molecule 4 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C₁₆H₃₄O₈).



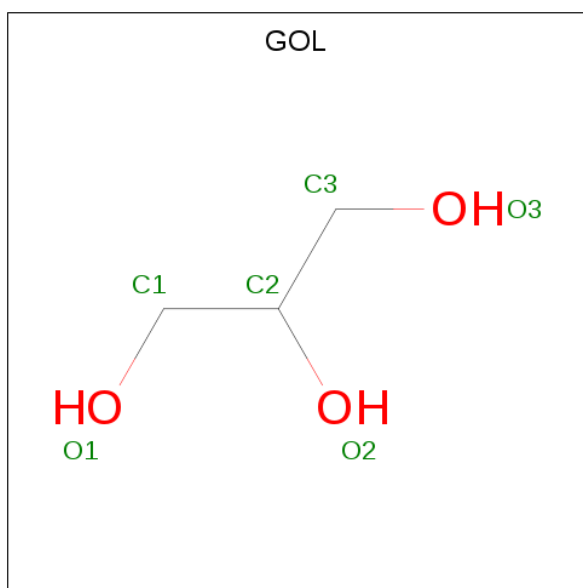
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			24	16	8		

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



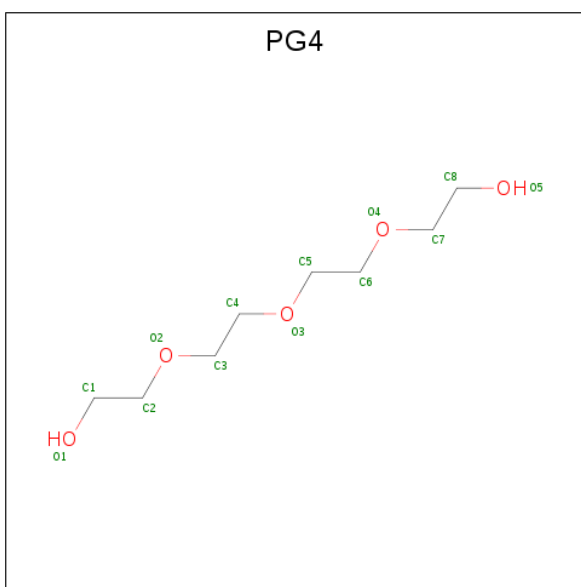
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



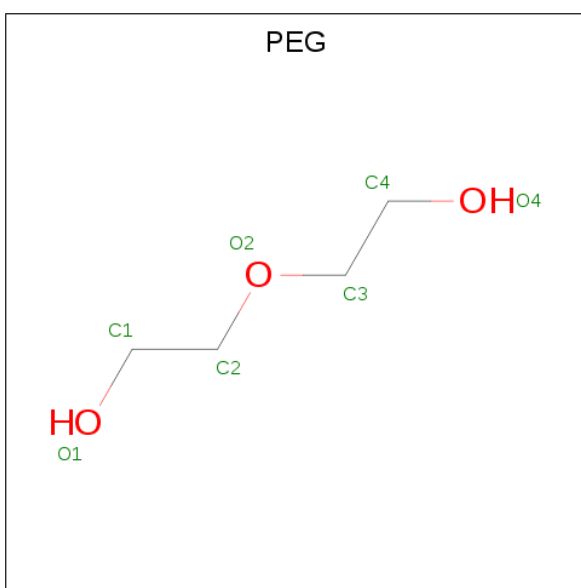
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		
7	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



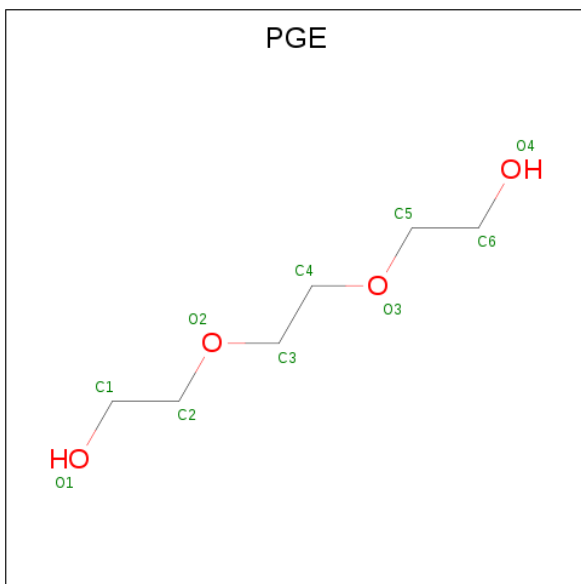
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		

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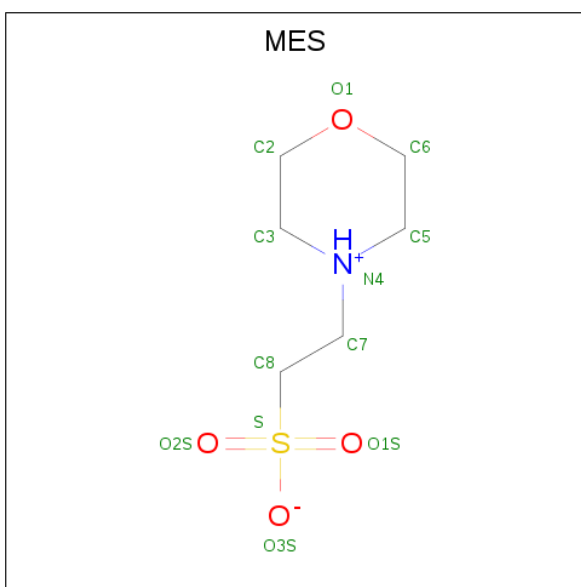
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



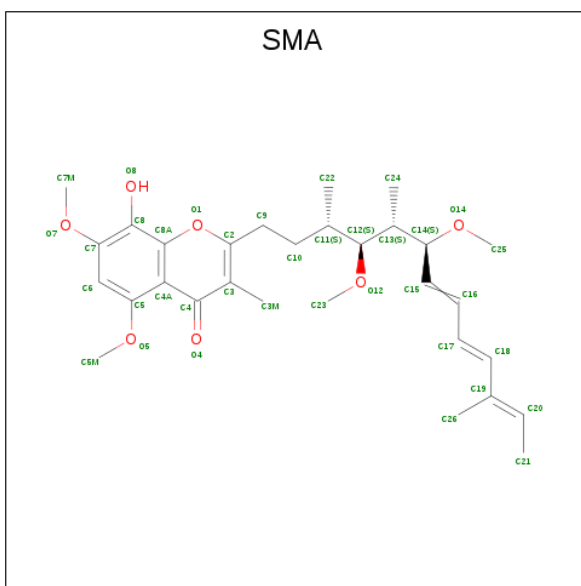
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			10	6	4		
9	A	1	Total	C	O	0	0
			10	6	4		
9	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
10	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			37	30	7		
11	A	1	Total	C	O	0	1
			74	60	14		

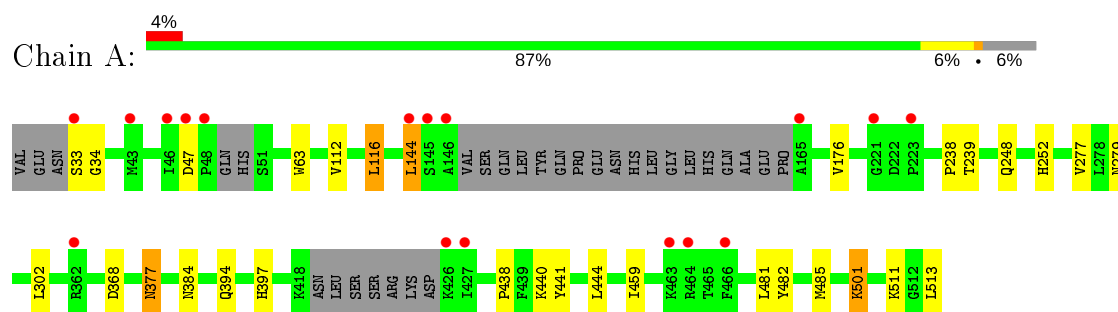
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	345	Total	O	0	0
			345	345		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	116.67Å 128.46Å 86.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 1.85 29.48 – 1.85	Depositor EDS
% Data completeness (in resolution range)	92.5 (29.48-1.85) 92.6 (29.48-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.182 , 0.204 0.190 , 0.210	Depositor DCC
R_{free} test set	2632 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4397	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: GOL, MG, PGE, P6G, PE4, PG4, SMA, MES, PEG, 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	0.35	0/3778	0.60	0/5102

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	3698	0	3757	24	0
2	A	53	0	31	2	0
3	A	4	0	0	0	0
4	A	24	0	34	0	0
5	A	19	0	26	0	0
6	A	42	0	56	3	0
7	A	26	0	36	0	0
8	A	21	0	30	0	0
9	A	30	0	42	0	0
10	A	24	0	26	0	0
11	A	111	0	123	38	0
12	A	345	0	0	1	0
All	All	4397	0	4161	55	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 7.

All (55) 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)
11:A:626[B]:SMA:H39	11:A:626[B]:SMA:C12	1.59	1.25
11:A:626[B]:SMA:H36	11:A:626[B]:SMA:H29	1.33	1.11
11:A:626[B]:SMA:C25	11:A:626[B]:SMA:C12	2.30	1.08
11:A:626[B]:SMA:O8	11:A:626[B]:SMA:H10	1.51	1.07
11:A:626[A]:SMA:H6	11:A:626[A]:SMA:O4	1.54	1.07
11:A:626[B]:SMA:C25	11:A:626[B]:SMA:H16	1.84	1.06
11:A:626[A]:SMA:H25	11:A:626[A]:SMA:H21	1.11	1.06
11:A:626[A]:SMA:H25	11:A:626[A]:SMA:C16	2.00	0.89
11:A:626[B]:SMA:H39	11:A:626[B]:SMA:H16	0.91	0.89
11:A:626[A]:SMA:C20	11:A:626[A]:SMA:H21	2.01	0.88
11:A:626[B]:SMA:H36	11:A:626[B]:SMA:C22	2.04	0.88
1:A:238:PRO:HG2	6:A:608:GOL:H32	1.56	0.87
11:A:626[A]:SMA:H18	11:A:626[A]:SMA:H34	1.59	0.82
11:A:626[A]:SMA:C5M	11:A:626[A]:SMA:O4	2.27	0.81
11:A:626[B]:SMA:O8	11:A:626[B]:SMA:C7M	2.29	0.80
11:A:626[A]:SMA:C14	11:A:626[A]:SMA:H34	2.16	0.73
11:A:625:SMA:H36	11:A:625:SMA:H29	1.71	0.72
11:A:626[B]:SMA:C25	11:A:626[B]:SMA:O12	2.39	0.71
11:A:626[B]:SMA:C24	11:A:626[B]:SMA:H29	2.12	0.70
11:A:626[A]:SMA:H14	11:A:626[A]:SMA:H33	1.72	0.70
11:A:626[A]:SMA:H6	11:A:626[A]:SMA:C4	2.21	0.69
11:A:626[B]:SMA:H40	11:A:626[B]:SMA:O12	1.93	0.68
1:A:239:THR:HG23	2:A:601:FAD:HM73	1.77	0.67
11:A:626[A]:SMA:H33	11:A:626[A]:SMA:C10	2.26	0.66
1:A:394:GLN:NE2	1:A:441:TYR:OH	2.32	0.62
11:A:626[B]:SMA:C22	11:A:626[B]:SMA:C24	2.74	0.61
1:A:47[B]:ASP:N	1:A:47[B]:ASP:OD1	2.28	0.60
1:A:248[B]:GLN:HE21	1:A:252:HIS:HD2	1.49	0.59
1:A:482[B]:TYR:OH	11:A:626[B]:SMA:H4	2.08	0.54
11:A:626[A]:SMA:C23	11:A:626[A]:SMA:C10	2.85	0.53
1:A:459:ILE:HD12	11:A:626[A]:SMA:H29	1.91	0.52
11:A:625:SMA:C24	11:A:625:SMA:H29	2.38	0.51
6:A:608:GOL:O1	11:A:626[B]:SMA:H6	2.11	0.50
1:A:444:LEU:HD13	11:A:626[A]:SMA:H33	1.93	0.49
11:A:626[A]:SMA:C5M	11:A:626[A]:SMA:C4	2.88	0.49
1:A:144:LEU:HD23	12:A:745:HOH:O	2.12	0.48
1:A:33[A]:SER:OG	1:A:34:GLY:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:626[B]:SMA:C16	11:A:626[B]:SMA:H35	2.44	0.47
1:A:112:VAL:HG22	1:A:116:LEU:HD22	1.97	0.47
1:A:176:VAL:HG22	1:A:384:ASN:HD22	1.80	0.46
1:A:501[A]:LYS:C	1:A:501[A]:LYS:CD	2.83	0.46
1:A:397:HIS:CD2	11:A:626[B]:SMA:H13	2.53	0.44
1:A:511[B]:LYS:HE3	1:A:511[B]:LYS:HB2	1.77	0.44
11:A:626[B]:SMA:H33	11:A:626[B]:SMA:H15	1.76	0.44
2:A:601:FAD:N3	6:A:608:GOL:H11	2.33	0.43
1:A:144:LEU:H	1:A:144:LEU:HD22	1.83	0.43
1:A:368:ASP:HB3	1:A:438:PRO:HB3	2.01	0.42
11:A:626[A]:SMA:H12	11:A:626[A]:SMA:H30	1.55	0.42
1:A:482[B]:TYR:OH	11:A:626[B]:SMA:C5M	2.68	0.41
1:A:444:LEU:HD13	11:A:626[A]:SMA:C23	2.50	0.41
1:A:485:MET:HG2	11:A:626[B]:SMA:H15	2.03	0.41
1:A:377:ASN:H	1:A:377:ASN:HD22	1.69	0.41
1:A:501[A]:LYS:HD3	1:A:501[A]:LYS:C	2.41	0.40
1:A:277:VAL:HG13	1:A:302:LEU:HD21	2.02	0.40
1:A:63:TRP:CH2	11:A:626[B]:SMA:H3	2.57	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	459/484 (95%)	445 (97%)	14 (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	398/412 (97%)	389 (98%)	9 (2%)	50 34

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	LEU
1	A	144	LEU
1	A	279	ASN
1	A	377	ASN
1	A	440	LYS
1	A	481	LEU
1	A	501[A]	LYS
1	A	501[B]	LYS
1	A	513	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	200	ASN
1	A	252	HIS
1	A	253	GLN
1	A	279	ASN
1	A	290	GLN
1	A	292	HIS
1	A	377	ASN
1	A	384	ASN
1	A	394	GLN
1	A	397	HIS
1	A	415	ASN
1	A	442	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 4 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	MES	A	623	-	12,12,12	2.03	1 (8%)	14,16,16	1.97	4 (28%)
6	GOL	A	608	-	5,5,5	0.40	0	5,5,5	1.07	0
4	PE4	A	606	-	23,23,23	0.36	0	22,22,22	0.53	0
2	FAD	A	601	3	51,58,58	1.91	6 (11%)	60,89,89	2.04	12 (20%)
8	PEG	A	615	-	6,6,6	0.46	0	5,5,5	0.28	0
8	PEG	A	618	-	6,6,6	0.43	0	5,5,5	0.39	0
6	GOL	A	620	-	5,5,5	0.31	0	5,5,5	0.25	0
11	SMA	A	626[A]	-	35,38,38	4.80	6 (17%)	46,52,52	2.31	12 (26%)
11	SMA	A	626[B]	-	35,38,38	4.86	6 (17%)	46,52,52	2.57	15 (32%)
9	PGE	A	617	-	9,9,9	0.48	0	8,8,8	0.21	0
6	GOL	A	609	-	5,5,5	0.33	0	5,5,5	0.19	0
6	GOL	A	622	-	5,5,5	0.32	0	5,5,5	0.21	0
8	PEG	A	614	-	6,6,6	0.48	0	5,5,5	0.31	0
10	MES	A	624	-	12,12,12	2.48	1 (8%)	14,16,16	1.82	5 (35%)
7	PG4	A	612	-	12,12,12	0.55	0	11,11,11	0.37	0
9	PGE	A	616	-	9,9,9	0.46	0	8,8,8	0.29	0
11	SMA	A	625	-	35,38,38	5.05	8 (22%)	46,52,52	1.59	7 (15%)
6	GOL	A	611	-	5,5,5	0.24	0	5,5,5	0.33	0
9	PGE	A	619	-	9,9,9	0.48	0	8,8,8	0.32	0
7	PG4	A	613	-	12,12,12	0.53	0	11,11,11	0.33	0
6	GOL	A	621	-	5,5,5	0.28	0	5,5,5	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	P6G	A	607	-	18,18,18	0.50	0	17,17,17	0.30	0
6	GOL	A	610	-	5,5,5	0.34	0	5,5,5	0.18	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
10	MES	A	623	-	-	2/6/14/14	0/1/1/1
6	GOL	A	608	-	-	2/4/4/4	-
4	PE4	A	606	-	-	8/21/21/21	-
2	FAD	A	601	3	-	1/30/50/50	0/6/6/6
8	PEG	A	615	-	-	3/4/4/4	-
8	PEG	A	618	-	-	1/4/4/4	-
6	GOL	A	620	-	-	2/4/4/4	-
11	SMA	A	626[A]	-	-	16/33/34/34	0/2/2/2
11	SMA	A	626[B]	-	-	8/33/34/34	0/2/2/2
9	PGE	A	617	-	-	4/7/7/7	-
6	GOL	A	609	-	-	2/4/4/4	-
6	GOL	A	622	-	-	4/4/4/4	-
8	PEG	A	614	-	-	2/4/4/4	-
10	MES	A	624	-	-	1/6/14/14	0/1/1/1
7	PG4	A	612	-	-	4/10/10/10	-
9	PGE	A	616	-	-	4/7/7/7	-
11	SMA	A	625	-	-	7/33/34/34	0/2/2/2
6	GOL	A	611	-	-	2/4/4/4	-
9	PGE	A	619	-	-	2/7/7/7	-
7	PG4	A	613	-	-	4/10/10/10	-
6	GOL	A	621	-	-	2/4/4/4	-
5	P6G	A	607	-	-	6/16/16/16	-
6	GOL	A	610	-	-	4/4/4/4	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	625	SMA	C20-C19	26.75	1.54	1.33
11	A	626[B]	SMA	C20-C19	25.92	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	626[A]	SMA	C20-C19	25.82	1.53	1.33
2	A	601	FAD	C4X-C10	9.81	1.48	1.38
10	A	624	MES	C8-S	-8.17	1.65	1.77
11	A	625	SMA	C17-C18	7.53	1.54	1.34
11	A	626[B]	SMA	C17-C18	7.47	1.53	1.34
11	A	626[A]	SMA	C17-C18	7.33	1.53	1.34
10	A	623	MES	C8-S	-6.32	1.68	1.77
11	A	626[B]	SMA	C3M-C3	-6.24	1.36	1.51
11	A	625	SMA	C16-C15	5.41	1.55	1.33
11	A	626[A]	SMA	C3M-C3	-5.06	1.39	1.51
11	A	626[B]	SMA	C16-C15	5.01	1.53	1.33
11	A	626[A]	SMA	C16-C15	4.98	1.53	1.33
11	A	625	SMA	C3M-C3	-4.16	1.41	1.51
11	A	625	SMA	C18-C19	4.14	1.54	1.45
2	A	601	FAD	C4-C4X	4.11	1.48	1.41
2	A	601	FAD	C9A-C5X	3.97	1.50	1.42
11	A	625	SMA	C11-C12	3.84	1.60	1.53
11	A	626[B]	SMA	C18-C19	3.57	1.53	1.45
11	A	626[A]	SMA	C18-C19	3.49	1.53	1.45
11	A	625	SMA	C17-C16	3.47	1.54	1.44
2	A	601	FAD	C8-C7	3.31	1.49	1.40
11	A	626[B]	SMA	C17-C16	3.23	1.53	1.44
11	A	626[A]	SMA	C17-C16	3.09	1.53	1.44
2	A	601	FAD	C9A-N10	2.59	1.42	1.38
2	A	601	FAD	C5A-C4A	2.48	1.47	1.40
11	A	625	SMA	C13-C12	2.04	1.59	1.54

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C4-N3-C2	8.35	122.19	115.14
11	A	626[B]	SMA	C5M-O5-C5	-7.49	107.26	117.75
11	A	626[A]	SMA	C7M-O7-C7	-7.39	106.37	117.53
11	A	626[B]	SMA	O1-C2-C9	7.22	120.47	111.91
11	A	626[A]	SMA	C9-C10-C11	-6.91	105.41	114.72
2	A	601	FAD	C1'-N10-C9A	6.21	123.18	118.29
11	A	626[B]	SMA	C7M-O7-C7	-6.09	108.34	117.53
11	A	626[A]	SMA	C10-C9-C2	-5.70	101.35	113.59
11	A	626[B]	SMA	C4-C3-C2	5.52	122.68	116.63
2	A	601	FAD	C4-C4X-C10	-5.43	116.36	119.95
11	A	626[B]	SMA	C3M-C3-C2	-4.55	115.78	122.30
11	A	625	SMA	C7M-O7-C7	4.35	124.09	117.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C4X-N5-C5X	4.20	120.97	116.77
11	A	626[A]	SMA	C9-C2-C3	4.14	126.26	120.39
10	A	623	MES	C2-C3-N4	3.70	115.72	110.10
10	A	624	MES	C6-C5-N4	3.63	115.61	110.10
11	A	626[A]	SMA	C4-C3-C2	3.62	120.60	116.63
2	A	601	FAD	C4X-C4-N3	-3.62	118.48	123.43
11	A	625	SMA	C9-C2-C3	3.60	125.49	120.39
2	A	601	FAD	C4-C4X-N5	3.54	122.64	118.60
11	A	626[B]	SMA	C3-C4-C4A	-3.52	117.04	120.58
11	A	626[B]	SMA	C22-C11-C12	-3.42	105.55	111.15
2	A	601	FAD	N3A-C2A-N1A	-3.41	123.34	128.68
10	A	623	MES	O1S-S-C8	3.27	110.86	106.92
11	A	626[B]	SMA	C14-C15-C16	-3.26	119.22	125.61
11	A	625	SMA	O1-C2-C9	3.10	115.59	111.91
11	A	626[A]	SMA	C14-C15-C16	-3.08	119.58	125.61
11	A	626[B]	SMA	C17-C18-C19	-3.03	117.90	126.42
10	A	623	MES	C6-C5-N4	3.03	114.70	110.10
2	A	601	FAD	C1B-N9A-C4A	-3.02	121.34	126.64
11	A	625	SMA	C4-C3-C2	3.01	119.93	116.63
2	A	601	FAD	C4'-C3'-C2'	-2.91	107.32	113.36
11	A	626[B]	SMA	C4-C4A-C5	-2.82	120.76	124.96
10	A	624	MES	C2-C3-N4	2.76	114.28	110.10
11	A	625	SMA	C6-C7-C8	-2.76	117.89	120.60
10	A	623	MES	O2S-S-C8	2.68	110.15	106.92
11	A	626[A]	SMA	C23-O12-C12	-2.67	107.51	114.52
10	A	624	MES	O2S-S-C8	2.65	110.10	106.92
11	A	626[B]	SMA	C23-O12-C12	-2.64	107.60	114.52
10	A	624	MES	C5-N4-C3	2.59	114.66	108.83
2	A	601	FAD	C4A-C5A-N7A	-2.54	106.76	109.40
11	A	626[A]	SMA	C3-C4-C4A	-2.46	118.11	120.58
11	A	625	SMA	C24-C13-C14	-2.38	106.08	110.93
11	A	626[B]	SMA	O7-C7-C8	2.31	116.87	114.54
11	A	626[A]	SMA	C24-C13-C14	-2.31	106.22	110.93
2	A	601	FAD	C9A-N10-C10	-2.29	118.91	121.91
11	A	626[B]	SMA	C22-C11-C10	2.24	113.88	110.36
11	A	626[A]	SMA	C13-C14-C15	-2.24	107.24	112.13
11	A	626[A]	SMA	C11-C12-C13	-2.23	108.33	114.29
11	A	626[B]	SMA	C24-C13-C14	-2.22	106.40	110.93
2	A	601	FAD	C2A-N1A-C6A	2.08	122.32	118.75
11	A	626[A]	SMA	C5M-O5-C5	-2.06	114.86	117.75
11	A	625	SMA	C17-C18-C19	-2.02	120.74	126.42
11	A	626[B]	SMA	C9-C10-C11	-2.01	112.01	114.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	624	MES	O1S-S-C8	2.01	109.33	106.92

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	623	MES	C8-C7-N4-C3
10	A	623	MES	N4-C7-C8-S
11	A	626[A]	SMA	C4A-C5-O5-C5M
11	A	626[A]	SMA	C10-C11-C12-C13
11	A	626[A]	SMA	C10-C11-C12-O12
11	A	626[A]	SMA	C22-C11-C12-C13
11	A	626[A]	SMA	C22-C11-C12-O12
11	A	626[A]	SMA	C13-C12-O12-C23
11	A	626[A]	SMA	C17-C18-C19-C20
11	A	626[A]	SMA	C17-C18-C19-C26
6	A	609	GOL	O1-C1-C2-C3
6	A	622	GOL	O1-C1-C2-C3
11	A	625	SMA	C22-C11-C12-O12
11	A	625	SMA	C24-C13-C14-C15
6	A	610	GOL	O1-C1-C2-C3
6	A	610	GOL	C1-C2-C3-O3
11	A	626[A]	SMA	C6-C5-O5-C5M
11	A	626[B]	SMA	C6-C7-O7-C7M
11	A	626[B]	SMA	C8-C7-O7-C7M
11	A	625	SMA	C4A-C5-O5-C5M
7	A	612	PG4	O3-C5-C6-O4
7	A	612	PG4	O2-C3-C4-O3
4	A	606	PE4	O6-C11-C12-O7
11	A	625	SMA	C6-C5-O5-C5M
5	A	607	P6G	O4-C5-C6-O7
6	A	609	GOL	O1-C1-C2-O2
8	A	615	PEG	O1-C1-C2-O2
8	A	618	PEG	O1-C1-C2-O2
9	A	617	PGE	O3-C5-C6-O4
11	A	626[B]	SMA	C15-C16-C17-C18
8	A	614	PEG	O2-C3-C4-O4
7	A	613	PG4	O4-C7-C8-O5
4	A	606	PE4	C16-C15-O8-C14
6	A	620	GOL	C1-C2-C3-O3
6	A	622	GOL	C1-C2-C3-O3
6	A	611	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	A	621	GOL	O1-C1-C2-C3
4	A	606	PE4	O6-C10-C9-O5
9	A	619	PGE	O2-C3-C4-O3
6	A	620	GOL	O2-C2-C3-O3
6	A	622	GOL	O1-C1-C2-O2
6	A	611	GOL	O2-C2-C3-O3
6	A	621	GOL	O1-C1-C2-O2
9	A	616	PGE	O2-C3-C4-O3
9	A	616	PGE	O1-C1-C2-O2
7	A	613	PG4	O3-C5-C6-O4
11	A	626[A]	SMA	C24-C13-C14-C15
11	A	626[A]	SMA	C24-C13-C14-O14
11	A	626[A]	SMA	C12-C13-C14-O14
9	A	616	PGE	O3-C5-C6-O4
5	A	607	P6G	O16-C17-C18-O19
11	A	626[A]	SMA	C9-C10-C11-C22
6	A	610	GOL	O1-C1-C2-O2
6	A	622	GOL	O2-C2-C3-O3
4	A	606	PE4	O2-C3-C4-O3
11	A	626[B]	SMA	C11-C12-O12-C23
11	A	626[B]	SMA	C13-C12-O12-C23
11	A	625	SMA	C11-C12-O12-C23
7	A	612	PG4	C4-C3-O2-C2
6	A	608	GOL	O2-C2-C3-O3
8	A	615	PEG	O2-C3-C4-O4
9	A	616	PGE	C4-C3-O2-C2
11	A	626[B]	SMA	C13-C14-O14-C25
7	A	612	PG4	O1-C1-C2-O2
8	A	615	PEG	C1-C2-O2-C3
11	A	626[A]	SMA	C15-C14-O14-C25
11	A	626[B]	SMA	C15-C14-O14-C25
8	A	614	PEG	C4-C3-O2-C2
11	A	626[A]	SMA	C16-C17-C18-C19
4	A	606	PE4	C7-C8-O5-C9
9	A	617	PGE	O2-C3-C4-O3
5	A	607	P6G	O7-C8-C9-O10
5	A	607	P6G	C9-C8-O7-C6
11	A	626[A]	SMA	C8-C7-O7-C7M
10	A	624	MES	C8-C7-N4-C5
11	A	625	SMA	C12-C13-C14-O14
9	A	619	PGE	C6-C5-O3-C4
4	A	606	PE4	C6-C5-O3-C4

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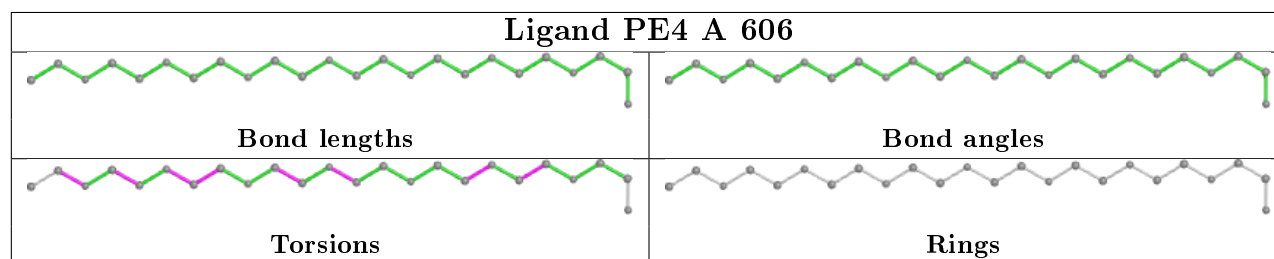
Mol	Chain	Res	Type	Atoms
6	A	608	GOL	C1-C2-C3-O3
9	A	617	PGE	C4-C3-O2-C2
6	A	610	GOL	O2-C2-C3-O3
7	A	613	PG4	C1-C2-O2-C3
4	A	606	PE4	C11-C12-O7-C13
4	A	606	PE4	O7-C13-C14-O8
11	A	625	SMA	C3-C2-C9-C10
2	A	601	FAD	O4B-C4B-C5B-O5B
7	A	613	PG4	O2-C3-C4-O3
9	A	617	PGE	O1-C1-C2-O2
5	A	607	P6G	O10-C11-C12-O13
5	A	607	P6G	C2-C3-O4-C5
11	A	626[B]	SMA	C11-C10-C9-C2

There are no ring outliers.

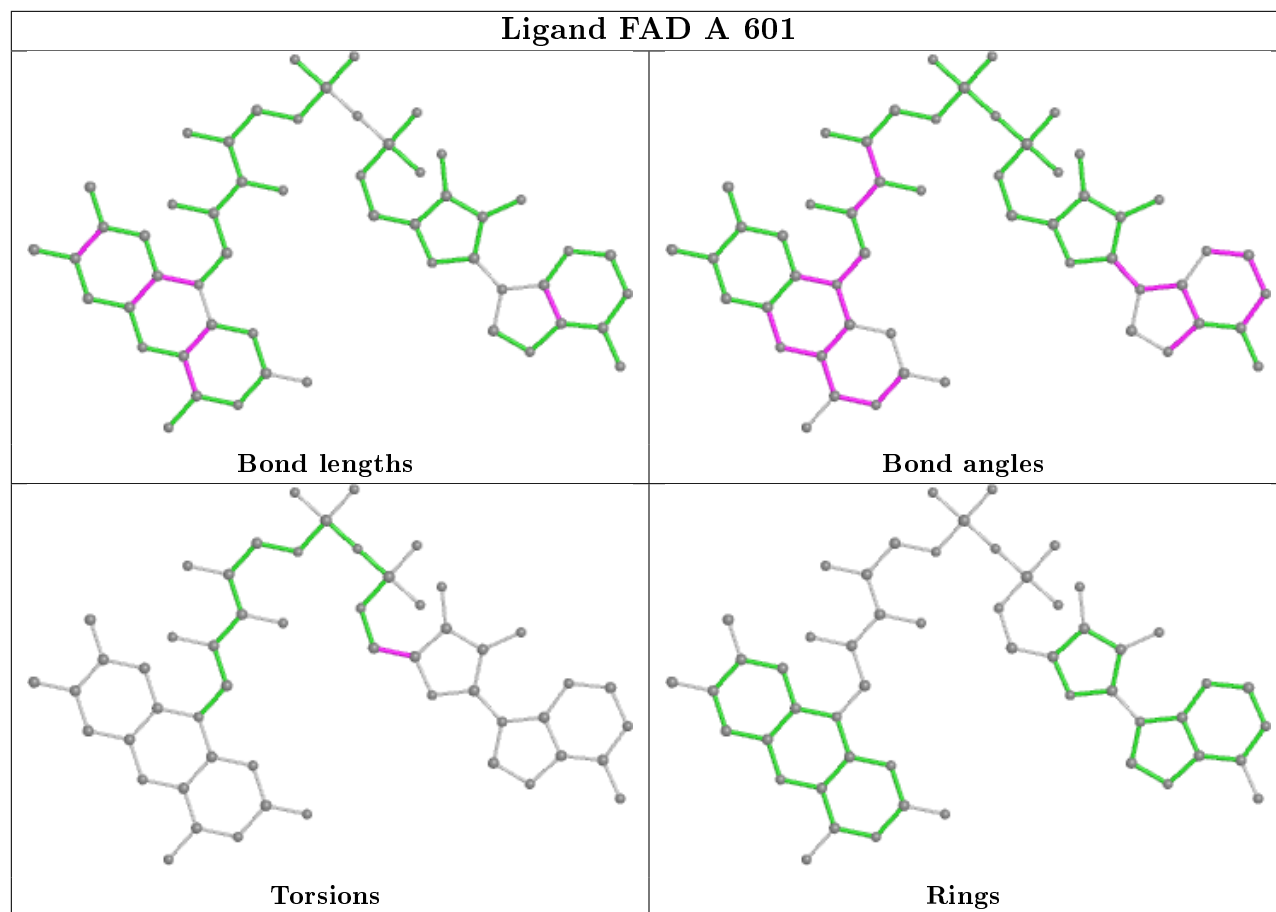
5 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	608	GOL	3	0
2	A	601	FAD	2	0
11	A	626[A]	SMA	16	0
11	A	626[B]	SMA	20	0
11	A	625	SMA	2	0

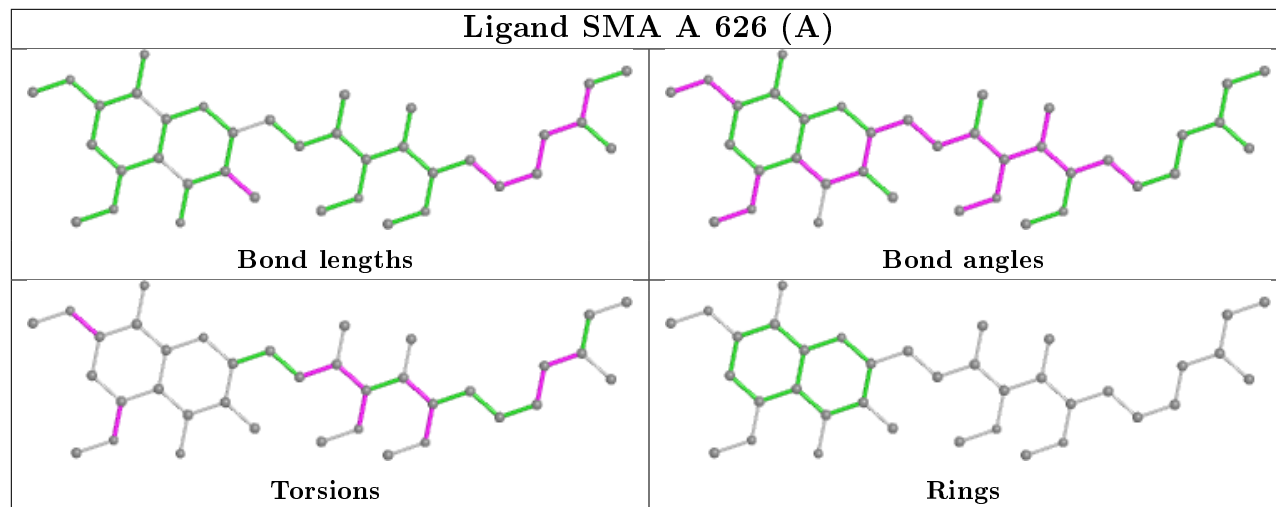
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

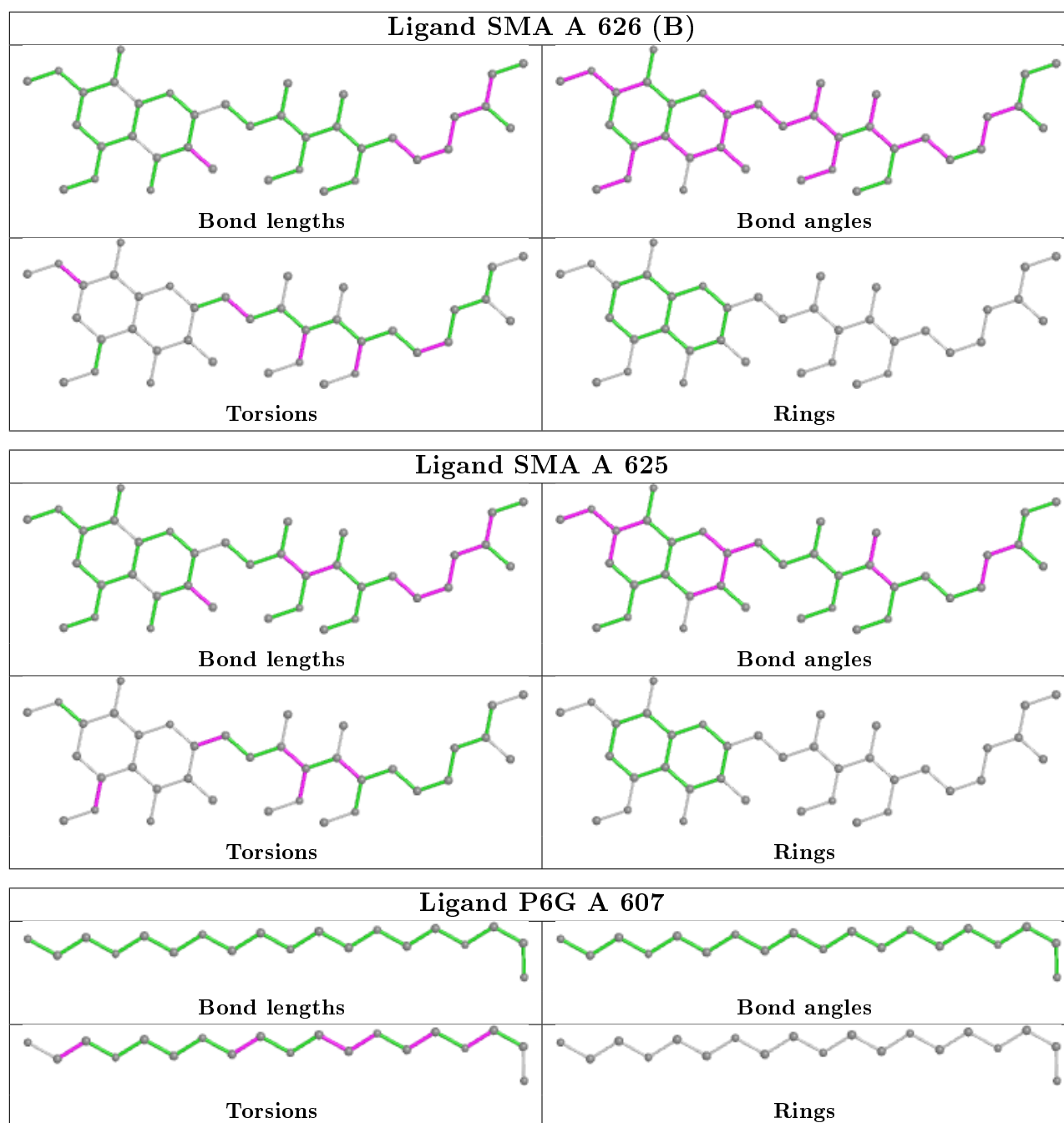


Ligand FAD A 601



Ligand SMA A 626 (A)





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	454/484 (93%)	0.03	17 (3%) 41 39	11, 19, 39, 63	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	144	LEU	7.5
1	A	146	ALA	6.2
1	A	46	ILE	5.8
1	A	464	ARG	4.3
1	A	463	LYS	4.3
1	A	221	GLY	3.9
1	A	466	PHE	3.6
1	A	426	LYS	3.4
1	A	145	SER	3.4
1	A	47[A]	ASP	3.4
1	A	48	PRO	3.3
1	A	33[A]	SER	2.9
1	A	362	ARG	2.8
1	A	165	ALA	2.4
1	A	223	PRO	2.2
1	A	43	MET	2.1
1	A	427	ILE	2.1

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 carbohydrates in this entry.

6.4 Ligands ⓘ

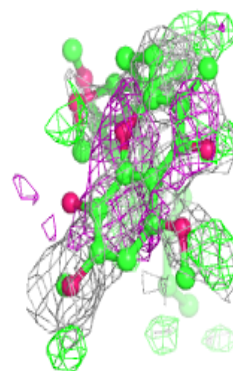
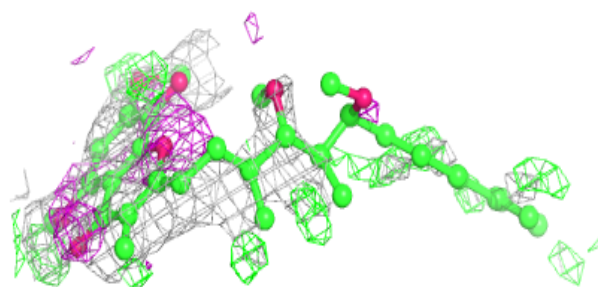
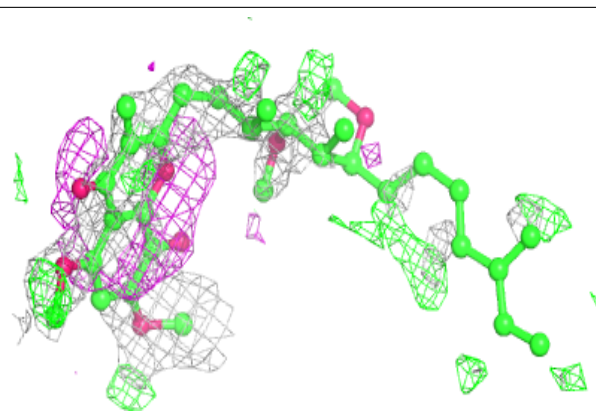
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	PEG	A	615	7/7	0.54	0.42	38,42,47,47	0
6	GOL	A	609	6/6	0.54	0.59	61,64,65,66	0
11	SMA	A	626[B]	37/37	0.58	0.50	45,48,52,52	37
11	SMA	A	626[A]	37/37	0.58	0.50	50,52,56,57	37
10	MES	A	624	12/12	0.62	0.34	73,75,84,85	0
6	GOL	A	622	6/6	0.63	0.33	50,51,51,51	0
7	PG4	A	613	13/13	0.66	0.22	62,63,65,66	0
9	PGE	A	617	10/10	0.69	0.19	57,58,60,60	0
9	PGE	A	616	10/10	0.70	0.22	69,71,72,73	0
6	GOL	A	610	6/6	0.70	0.32	58,58,59,60	0
3	MG	A	604	1/1	0.71	0.23	44,44,44,44	0
8	PEG	A	614	7/7	0.72	0.30	64,66,69,70	0
8	PEG	A	618	7/7	0.73	0.26	28,32,38,41	0
5	P6G	A	607	19/19	0.75	0.17	45,57,69,70	0
11	SMA	A	625	37/37	0.77	0.26	38,51,87,87	0
7	PG4	A	612	13/13	0.77	0.21	32,38,39,41	0
6	GOL	A	611	6/6	0.78	0.16	37,38,39,40	0
6	GOL	A	608	6/6	0.81	0.19	45,48,50,51	0
10	MES	A	623	12/12	0.83	0.18	35,37,43,44	0
9	PGE	A	619	10/10	0.85	0.25	53,55,56,56	0
4	PE4	A	606	24/24	0.85	0.18	22,25,28,29	0
6	GOL	A	621	6/6	0.86	0.17	33,35,36,37	0
6	GOL	A	620	6/6	0.92	0.14	30,33,35,35	0
3	MG	A	602	1/1	0.96	0.11	22,22,22,22	0
3	MG	A	605	1/1	0.96	0.15	27,27,27,27	0
2	FAD	A	601	53/53	0.97	0.11	11,12,17,17	0
3	MG	A	603	1/1	0.98	0.06	18,18,18,18	0

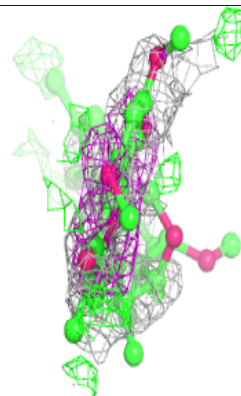
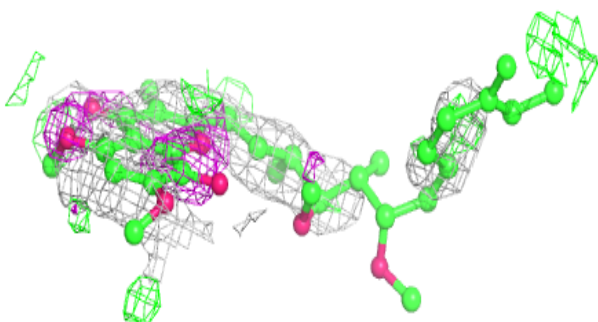
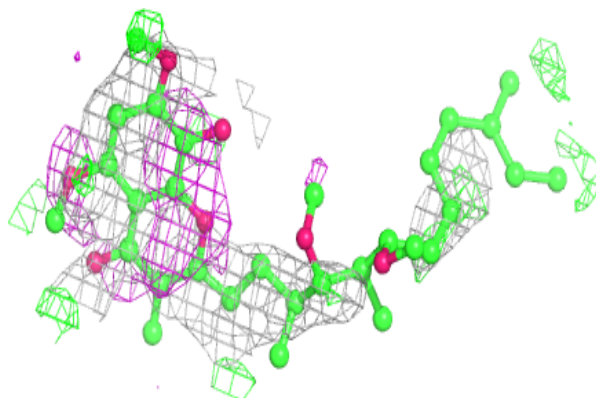
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SMA A 626 (B):

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

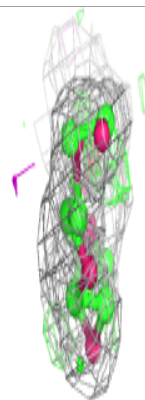
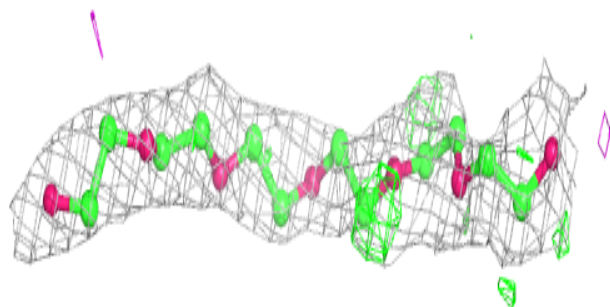
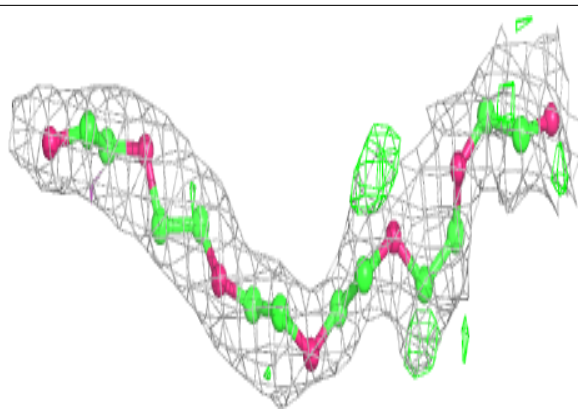
**Electron density around SMA A 626 (A):**

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

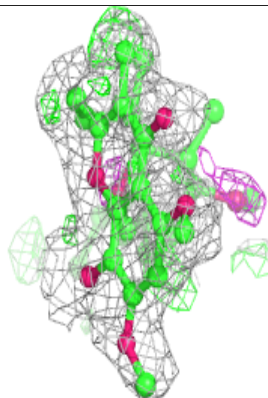
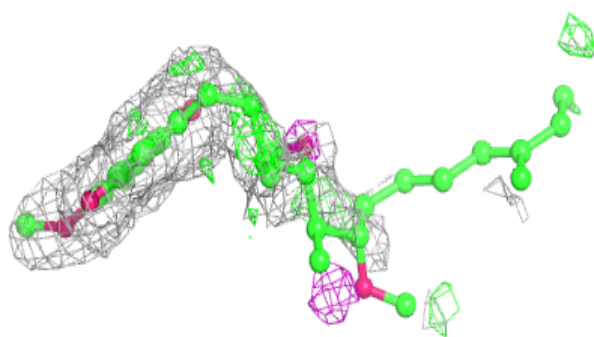
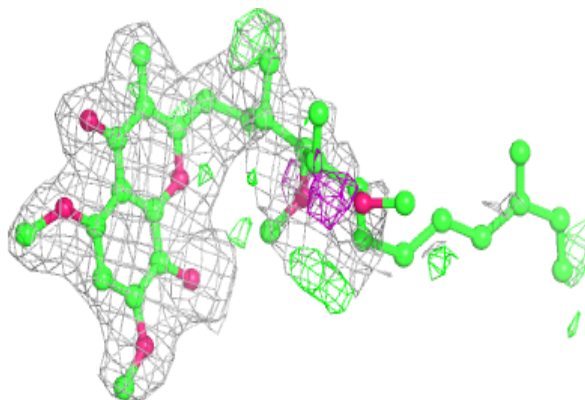


Electron density around P6G A 607:

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

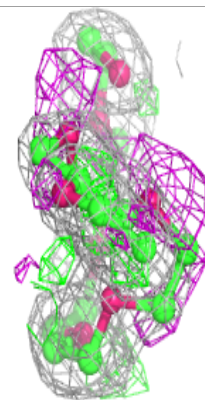
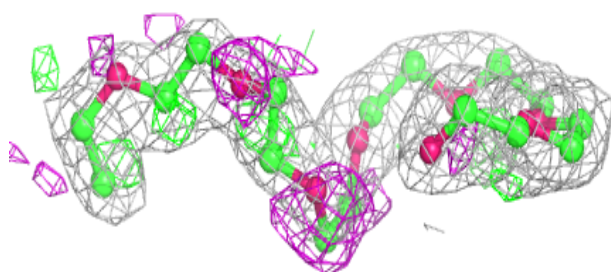
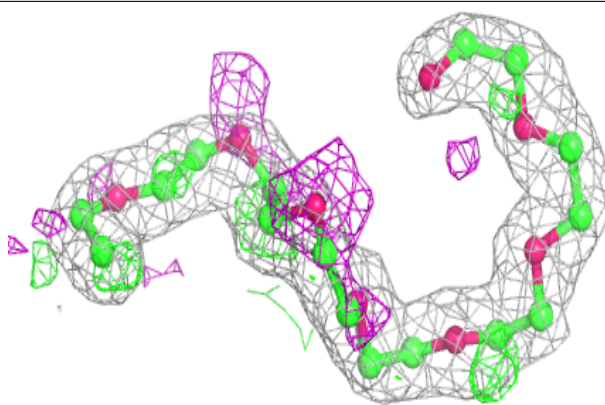
**Electron density around SMA A 625:**

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

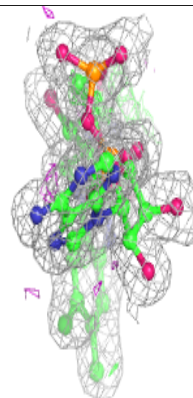
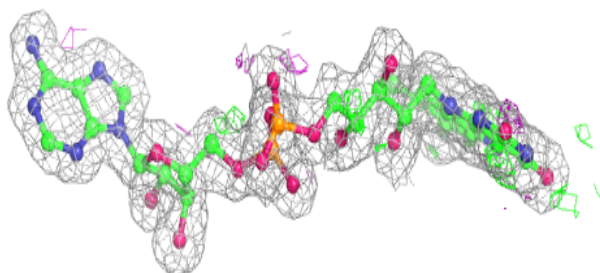
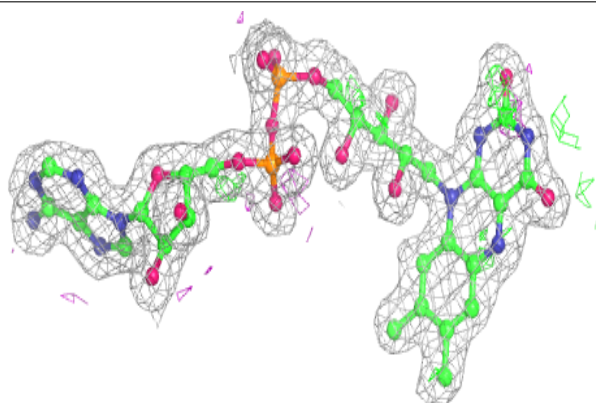


Electron density around PE4 A 606:

$2mF_o-DF_c$ (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)



6.5 Other polymers

There are no such residues in this entry.