



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:24 PM UTC

PDB ID : 4CDN / pdb_00004cdn
Title : Crystal structure of M. mazei photolyase with its in vivo reconstituted 8-HDF antenna chromophore
Authors : Kiontke, S.; Batschauer, A.; Essen, L.-O.
Deposited on : 2013-11-01
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

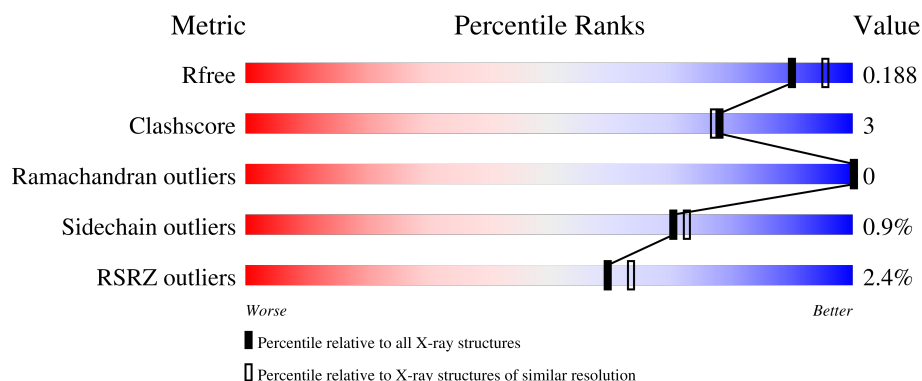
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

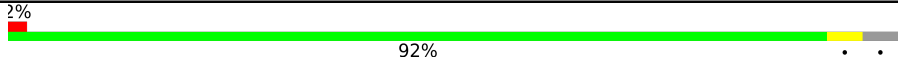
The reported resolution of this entry is 1.90 Å.

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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	482	 2% 92% 6% 2%
1	B	482	 3% 85% 6% 9%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8267 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 DEOXYRIBODIPYRIMIDINE PHOTOLYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	9	0
			3762	2420	630	697	15			
1	B	438	Total	C	N	O	S	0	7	0
			3564	2291	596	662	15			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP Q8PYK9
A	-16	GLY	-	expression tag	UNP Q8PYK9
A	-15	SER	-	expression tag	UNP Q8PYK9
A	-14	SER	-	expression tag	UNP Q8PYK9
A	-13	HIS	-	expression tag	UNP Q8PYK9
A	-12	HIS	-	expression tag	UNP Q8PYK9
A	-11	HIS	-	expression tag	UNP Q8PYK9
A	-10	HIS	-	expression tag	UNP Q8PYK9
A	-9	HIS	-	expression tag	UNP Q8PYK9
A	-8	HIS	-	expression tag	UNP Q8PYK9
A	-7	SER	-	expression tag	UNP Q8PYK9
A	-6	SER	-	expression tag	UNP Q8PYK9
A	-5	GLY	-	expression tag	UNP Q8PYK9
A	-4	LEU	-	expression tag	UNP Q8PYK9
A	-3	VAL	-	expression tag	UNP Q8PYK9
A	-2	PRO	-	expression tag	UNP Q8PYK9
A	-1	ARG	-	expression tag	UNP Q8PYK9
A	0	GLY	-	expression tag	UNP Q8PYK9
A	1	SER	-	expression tag	UNP Q8PYK9
A	2	HIS	-	expression tag	UNP Q8PYK9
A	377	THR	MET	cloning artifact	UNP Q8PYK9
B	-17	MET	-	expression tag	UNP Q8PYK9
B	-16	GLY	-	expression tag	UNP Q8PYK9
B	-15	SER	-	expression tag	UNP Q8PYK9
B	-14	SER	-	expression tag	UNP Q8PYK9

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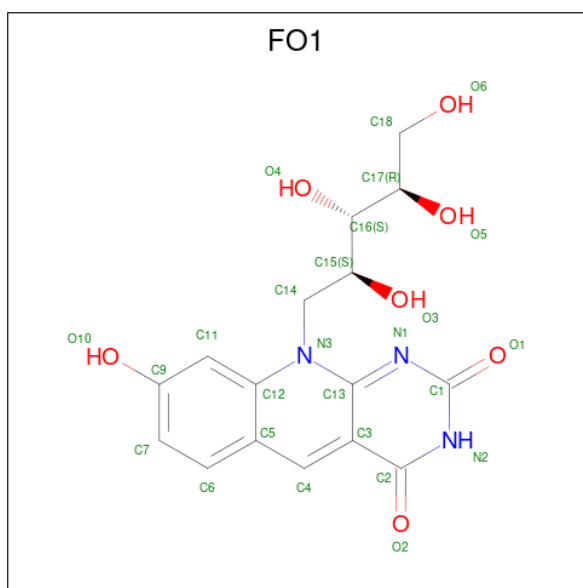
Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP Q8PYK9
B	-12	HIS	-	expression tag	UNP Q8PYK9
B	-11	HIS	-	expression tag	UNP Q8PYK9
B	-10	HIS	-	expression tag	UNP Q8PYK9
B	-9	HIS	-	expression tag	UNP Q8PYK9
B	-8	HIS	-	expression tag	UNP Q8PYK9
B	-7	SER	-	expression tag	UNP Q8PYK9
B	-6	SER	-	expression tag	UNP Q8PYK9
B	-5	GLY	-	expression tag	UNP Q8PYK9
B	-4	LEU	-	expression tag	UNP Q8PYK9
B	-3	VAL	-	expression tag	UNP Q8PYK9
B	-2	PRO	-	expression tag	UNP Q8PYK9
B	-1	ARG	-	expression tag	UNP Q8PYK9
B	0	GLY	-	expression tag	UNP Q8PYK9
B	1	SER	-	expression tag	UNP Q8PYK9
B	2	HIS	-	expression tag	UNP Q8PYK9
B	377	THR	MET	cloning artifact	UNP Q8PYK9

- # FAD
-
- The image displays the chemical structure of Flavin Adenine Dinucleotide (FAD). The molecule is composed of three main parts: a riboflavin (isoalloxazine) ring system, a ribitol linker, and an adenine ring system. The riboflavin ring is shown in blue, with nitrogen atoms labeled N1A, N3A, N7A, and N9A, and carbon atoms labeled C2A, C4A, C6A, and C8A. It is connected to a ribitol chain (a five-carbon chain with hydroxyl groups) via a glycosidic bond. The ribitol chain is shown in red, with carbon atoms labeled C1', C2', C3', C4', and C5'. The adenine ring is shown in blue, with nitrogen atoms labeled N1, N3, N7, and N9, and carbon atoms labeled C2, C4, C6, and C8. It is connected to the ribitol chain via a glycosidic bond. The structure is labeled with various atoms and bonds, including C1', C2', C3', C4', C5', C6', C7', C8', C9', C10', C11', C12', C13', C14', C15', C16', C17', C18', C19', C20', C21', C22', C23', C24', C25', C26', C27', C28', C29', C30', C31', C32', C33', C34', C35', C36', C37', C38', C39', C40', C41', C42', C43', C44', C45', C46', C47', C48', C49', C50', C51', C52', C53', C54', C55', C56', C57', C58', C59', C60', C61', C62', C63', C64', C65', C66', C67', C68', C69', C70', C71', C72', C73', C74', C75', C76', C77', C78', C79', C80', C81', C82', C83', C84', C85', C86', C87', C88', C89', C90', C91', C92', C93', C94', C95', C96', C97', C98', C99', C100', C101', C102', C103', C104', C105', C106', C107', C108', C109', C110', C111', C112', C113', C114', C115', C116', C117', C118', C119', C120', C121', C122', C123', C124', C125', C126', C127', C128', C129', C130', C131', C132', C133', C134', C135', C136', C137', C138', C139', C140', C141', C142', C143', C144', C145', C146', C147', C148', C149', C150', C151', C152', C153', C154', C155', C156', C157', C158', C159', C160', C161', C162', C163', C164', C165', C166', C167', C168', C169', C170', C171', C172', C173', C174', C175', C176', C177', C178', C179', C180', C181', C182', C183', C184', C185', C186', C187', C188', C189', C190', C191', C192', C193', C194', C195', C196', C197', C198', C199', C200', C201', C202', C203', C204', C205', C206', C207', C208', C209', C210', C211', C212', C213', C214', C215', C216', C217', C218', C219', C220', C221', C222', C223', C224', C225', C226', C227', C228', C229', C230', C231', C232', C233', C234', C235', C236', C237', C238', C239', C240', C241', C242', C243', C244', C245', C246', C247', C248', C249', C250', C251', C252', C253', C254', C255', C256', C257', C258', C259', C260', C261', C262', C263', C264', C265', C266', C267', C268', C269', C270', C271', C272', C273', C274', C275', C276', C277', C278', C279', C280', C281', C282', C283', C284', C285', C286', C287', C288', C289', C290', C291', C292', 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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

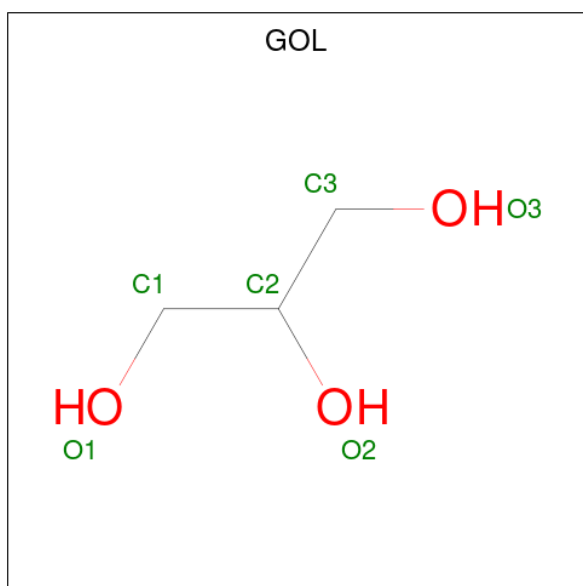
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- WORLD WIDE
PDB
PROTEIN DATA BANK

-D-ribitol (CCD ID: FO1) (formula: $C_{16}H_{17}N_3O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	16	3	7		
3	B	1	Total	C	N	O	0	0
			26	16	3	7		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



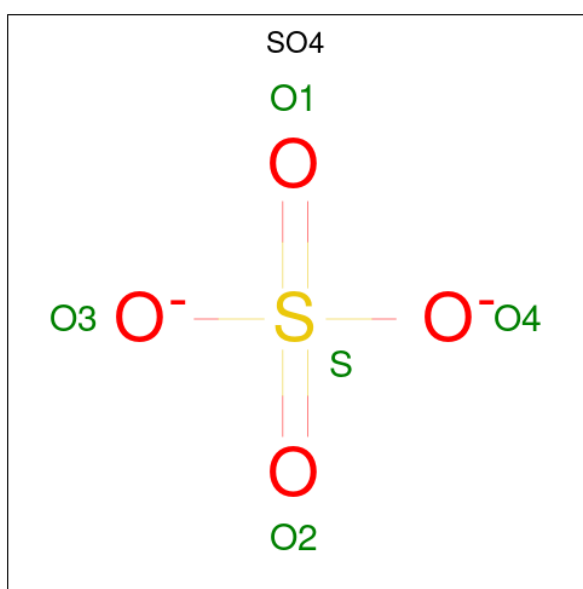
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

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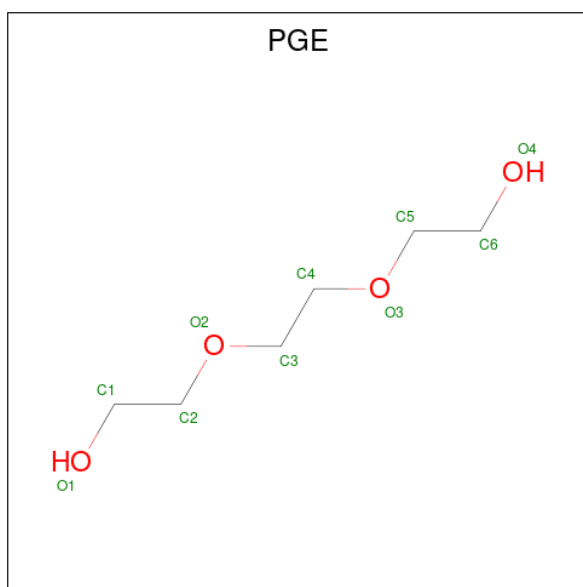
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



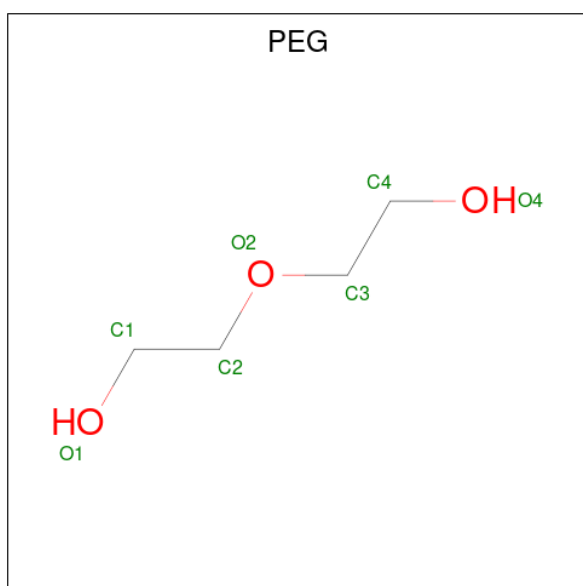
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

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

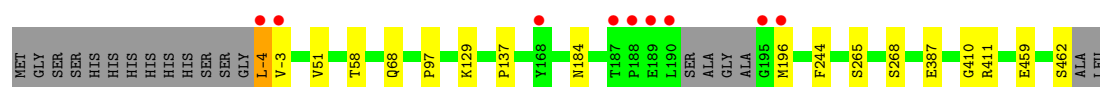
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	377	Total O 377 377	0	0
8	B	313	Total O 313 313	0	0

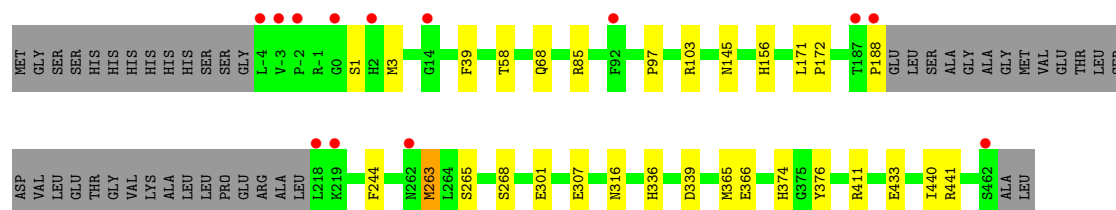
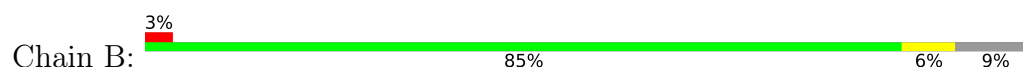
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DEOXYRIBODIPYRIMIDINE PHOTOLYASE



• Molecule 1: DEOXYRIBODIPYRIMIDINE PHOTOLYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.97Å 114.74Å 141.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.47 – 1.90 34.47 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (34.47-1.90) 98.1 (34.47-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.149 , 0.178 0.158 , 0.188	Depositor DCC
R_{free} test set	2025 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8267	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 3.49% 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: FO1, GOL, PGE, SO4, 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	0.64	0/3890	0.79	0/5266
1	B	0.64	0/3685	0.79	0/4990
All	All	0.64	0/7575	0.79	0/10256

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	3762	0	3681	13	0
1	B	3564	0	3444	27	0
2	A	53	0	31	2	0
2	B	53	0	31	3	0
3	A	26	0	16	0	0
3	B	26	0	16	0	0
4	A	18	0	24	0	0
4	B	12	0	16	2	0
5	A	5	0	0	0	0
5	B	10	0	0	0	0
6	A	20	0	28	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	28	0	40	3	0
8	A	377	0	0	2	0
8	B	313	0	0	7	0
All	All	8267	0	7327	41	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (41) 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:137:PRO:HB3	6:A:1469:PGE:H4	1.63	0.79
1:A:387:GLU:HG2	7:A:1470:PEG:H11	1.73	0.70
1:B:365[A]:MET:HA	1:B:365[A]:MET:HE3	1.73	0.69
1:A:387:GLU:HG2	7:A:1470:PEG:C1	2.26	0.65
1:B:336:HIS:HD2	1:B:339:ASP:OD2	1.84	0.61
1:A:51:VAL:H	1:A:184:ASN:HD21	1.48	0.60
1:B:365[A]:MET:HE3	1:B:365[A]:MET:CA	2.30	0.60
1:B:374:HIS:CD2	1:B:376:TYR:H	2.21	0.58
1:B:336:HIS:HE1	1:B:433:GLU:OE2	1.87	0.58
1:B:103:ARG:CB	8:B:2092:HOH:O	2.53	0.57
1:A:462:SER:C	8:A:2371:HOH:O	2.48	0.56
1:B:374:HIS:HD2	1:B:376:TYR:H	1.53	0.55
1:B:3:MET:HB3	1:B:39:PHE:CZ	2.44	0.53
1:B:336:HIS:CD2	1:B:339:ASP:OD2	2.62	0.51
1:A:459:GLU:HG3	8:A:2368:HOH:O	2.14	0.47
1:B:244:PHE:CD1	1:B:265:SER:HA	2.49	0.47
1:B:366:GLU:OE2	4:B:1463:GOL:H32	2.15	0.47
1:B:58:THR:HG22	1:B:97:PRO:HD3	1.97	0.46
1:B:156:HIS:CD2	1:B:316:ASN:HD21	2.34	0.46
1:B:263:MET:HB3	8:B:2179:HOH:O	2.16	0.45
1:A:68:GLN:HG2	1:A:411:ARG:NH2	2.31	0.45
1:B:365[A]:MET:HA	1:B:365[A]:MET:CE	2.43	0.45
1:A:244:PHE:CD1	1:A:265:SER:HA	2.51	0.45
1:A:268:SER:HB3	2:A:998:FAD:H5'2	1.98	0.44
1:B:268:SER:HB3	2:B:998:FAD:H5'2	2.00	0.44
1:B:188:PRO:CD	8:B:2083:HOH:O	2.64	0.43
1:B:336:HIS:CE1	1:B:433:GLU:OE2	2.69	0.43
1:A:410:GLY:HA2	2:A:998:FAD:O4	2.19	0.42
1:B:263:MET:CG	8:B:2179:HOH:O	2.66	0.42
1:B:145:ASN:HD22	1:B:307:GLU:HG2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:HIS:HE1	8:B:2185:HOH:O	2.01	0.42
1:A:58[A]:THR:HG22	1:A:97:PRO:HD3	2.01	0.42
1:A:387:GLU:HG2	7:A:1470:PEG:H12	2.00	0.42
1:A:-4:LEU:HG	6:A:1469:PGE:H32	2.00	0.42
1:B:188:PRO:HD3	8:B:2083:HOH:O	2.19	0.42
1:B:301:GLU:HB3	2:B:998:FAD:C8A	2.51	0.41
1:B:68:GLN:HG2	1:B:411:ARG:NH2	2.36	0.41
2:B:998:FAD:H62A	4:B:1464:GOL:H2	1.85	0.41
1:B:263:MET:CB	8:B:2179:HOH:O	2.69	0.41
1:B:171:LEU:N	1:B:172:PRO:CD	2.84	0.40
1:B:440:ILE:O	1:B:441:ARG:C	2.65	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	468/482 (97%)	462 (99%)	6 (1%)	0	100	100
1	B	441/482 (92%)	433 (98%)	8 (2%)	0	100	100
All	All	909/964 (94%)	895 (98%)	14 (2%)	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	404/416 (97%)	400 (99%)	4 (1%)	68	70
1	B	381/416 (92%)	378 (99%)	3 (1%)	73	75
All	All	785/832 (94%)	778 (99%)	7 (1%)	70	73

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-4	LEU
1	A	-3	VAL
1	A	129	LYS
1	A	196	MET
1	B	1	SER
1	B	85	ARG
1	B	263	MET

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

Mol	Chain	Res	Type
1	A	16	GLN
1	A	145	ASN
1	A	184	ASN
1	A	257	ASN
1	A	316	ASN
1	A	343	HIS
1	B	48	ASN
1	B	145	ASN
1	B	156	HIS
1	B	161	HIS
1	B	257	ASN
1	B	336	HIS
1	B	374	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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	GOL	B	1464	-	5,5,5	0.19	0	5,5,5	1.24	1 (20%)
7	PEG	A	1472	-	6,6,6	0.57	0	5,5,5	0.40	0
7	PEG	A	1471	-	6,6,6	0.53	0	5,5,5	0.50	0
7	PEG	A	1468	-	6,6,6	0.50	0	5,5,5	0.34	0
4	GOL	A	1464	-	5,5,5	0.32	0	5,5,5	0.55	0
4	GOL	B	1463	-	5,5,5	0.25	0	5,5,5	0.45	0
3	FO1	B	999	-	28,28,28	1.50	5 (17%)	38,41,41	1.81	10 (26%)
7	PEG	A	1470	-	6,6,6	0.52	0	5,5,5	0.60	0
5	SO4	B	1465	-	4,4,4	0.51	0	6,6,6	0.25	0
4	GOL	A	1463	-	5,5,5	0.40	0	5,5,5	0.23	0
4	GOL	A	1465	-	5,5,5	0.30	0	5,5,5	0.24	0
5	SO4	A	1466	-	4,4,4	0.46	0	6,6,6	0.24	0
6	PGE	A	1469	-	9,9,9	0.55	0	8,8,8	0.41	0
5	SO4	B	1466	-	4,4,4	0.43	0	6,6,6	0.19	0
2	FAD	B	998	-	58,58,58	1.39	9 (15%)	85,89,89	1.53	14 (16%)
3	FO1	A	999	-	28,28,28	1.43	3 (10%)	38,41,41	1.51	6 (15%)
6	PGE	A	1467	-	9,9,9	0.65	0	8,8,8	0.47	0
2	FAD	A	998	-	58,58,58	1.37	7 (12%)	85,89,89	1.57	18 (21%)

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
4	GOL	B	1464	-	-	2/4/4/4	-
7	PEG	A	1472	-	-	3/4/4/4	-
7	PEG	A	1471	-	-	1/4/4/4	-
7	PEG	A	1468	-	-	2/4/4/4	-
4	GOL	A	1464	-	-	0/4/4/4	-
4	GOL	B	1463	-	-	2/4/4/4	-
3	FO1	B	999	-	-	2/14/14/14	0/3/3/3
7	PEG	A	1470	-	-	3/4/4/4	-
4	GOL	A	1463	-	-	4/4/4/4	-
4	GOL	A	1465	-	-	0/4/4/4	-
6	PGE	A	1469	-	-	4/7/7/7	-
2	FAD	B	998	-	-	1/34/50/50	0/6/6/6
3	FO1	A	999	-	-	3/14/14/14	0/3/3/3
6	PGE	A	1467	-	-	5/7/7/7	-
2	FAD	A	998	-	-	1/34/50/50	0/6/6/6

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	998	FAD	C9A-C5X	4.74	1.48	1.41
2	A	998	FAD	C9A-C5X	4.71	1.48	1.41
3	B	999	FO1	C5-C12	4.52	1.48	1.41
3	A	999	FO1	C5-C12	4.41	1.48	1.41
2	B	998	FAD	C5A-C4A	4.21	1.46	1.39
2	A	998	FAD	C5A-C4A	3.78	1.45	1.39
3	A	999	FO1	C14-C15	-3.27	1.48	1.52
2	A	998	FAD	C8-C7	3.09	1.48	1.40
2	B	998	FAD	C8-C7	3.01	1.48	1.40
2	A	998	FAD	C4A-N9A	-2.95	1.31	1.37
2	A	998	FAD	C4X-N5	2.88	1.37	1.30
2	A	998	FAD	C5A-N7A	-2.80	1.34	1.39
2	B	998	FAD	C8A-N7A	2.80	1.37	1.31
3	B	999	FO1	C4-C3	2.72	1.41	1.35
2	B	998	FAD	C5A-N7A	-2.62	1.34	1.39
2	B	998	FAD	C4X-N5	2.53	1.36	1.30
2	A	998	FAD	C2-N3	-2.47	1.33	1.39
3	B	999	FO1	C3-C13	2.36	1.49	1.44
3	B	999	FO1	C3-C2	2.36	1.49	1.45
2	B	998	FAD	C4A-N9A	-2.09	1.33	1.37
2	B	998	FAD	C4-N3	-2.06	1.35	1.38
3	A	999	FO1	C4-C3	2.06	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	998	FAD	P-O3P	2.02	1.61	1.59
3	B	999	FO1	C1-N2	-2.02	1.34	1.39

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	999	FO1	C2-C3-C13	-5.79	114.45	117.48
2	B	998	FAD	C5A-C4A-N3A	-5.49	119.15	126.72
2	B	998	FAD	N3A-C4A-N9A	4.62	135.03	127.17
2	A	998	FAD	C5A-C4A-N3A	-4.51	120.51	126.72
2	A	998	FAD	N3A-C4A-N9A	4.36	134.58	127.17
2	A	998	FAD	N3A-C2A-N1A	-4.22	122.20	128.58
3	B	999	FO1	C5-C4-C3	-3.72	118.43	122.06
2	A	998	FAD	C4A-N9A-C8A	3.60	109.52	105.74
3	A	999	FO1	O2-C2-C3	-3.59	118.08	125.98
2	B	998	FAD	C2A-N3A-C4A	3.51	120.40	111.83
2	A	998	FAD	C2A-N3A-C4A	3.37	120.06	111.83
3	B	999	FO1	C3-C2-N2	3.34	120.29	114.45
3	A	999	FO1	C5-C4-C3	-3.33	118.81	122.06
2	B	998	FAD	N3A-C2A-N1A	-3.23	123.69	128.58
3	A	999	FO1	C2-C3-C13	-3.19	115.81	117.48
2	A	998	FAD	O4-C4-C4X	-2.95	118.73	126.53
2	B	998	FAD	C9A-C5X-N5	-2.82	119.47	122.45
2	A	998	FAD	C4-C4X-N5	2.80	122.08	118.21
2	B	998	FAD	C4A-N9A-C8A	2.62	108.49	105.74
2	B	998	FAD	O4-C4-C4X	-2.53	119.85	126.53
2	A	998	FAD	C10-N1-C2	2.51	122.29	116.85
3	B	999	FO1	O2-C2-C3	-2.50	120.47	125.98
3	A	999	FO1	C17-C16-C15	-2.49	109.43	113.57
3	B	999	FO1	C13-N1-C1	2.43	122.11	116.85
2	A	998	FAD	C9A-C5X-N5	-2.43	119.88	122.45
2	B	998	FAD	C2B-C1B-N9A	-2.37	107.41	113.30
2	A	998	FAD	O2P-P-O1P	2.33	123.31	112.44
2	A	998	FAD	C4X-C4-N3	2.31	119.13	113.25
3	B	999	FO1	C4-C3-C2	2.27	124.21	119.30
2	A	998	FAD	C5X-C9A-N10	2.26	120.01	117.97
3	B	999	FO1	C17-C16-C15	-2.25	109.83	113.57
3	A	999	FO1	C3-C2-N2	2.22	118.34	114.45
2	A	998	FAD	N6A-C6A-N1A	2.21	123.31	118.38
2	A	998	FAD	N9A-C8A-N7A	-2.20	110.81	113.94
2	A	998	FAD	C2A-N1A-C6A	2.19	122.32	118.73
4	B	1464	GOL	O1-C1-C2	-2.18	100.57	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	999	FO1	C15-C14-N3	2.16	120.43	110.20
2	B	998	FAD	C5A-C6A-N6A	-2.13	118.01	123.29
2	B	998	FAD	O4B-C1B-N9A	2.13	112.18	108.09
2	B	998	FAD	O2-C2-N1	-2.11	118.30	121.80
2	A	998	FAD	C4X-C10-N10	2.11	119.50	116.48
2	B	998	FAD	N3-C2-N1	2.11	123.98	119.50
2	A	998	FAD	C2B-C1B-N9A	-2.11	108.07	113.30
3	B	999	FO1	C5-C12-N3	2.10	121.19	118.72
2	B	998	FAD	C4X-C10-N1	-2.09	119.46	124.59
3	B	999	FO1	C2-N2-C1	-2.07	121.97	125.64
2	B	998	FAD	C4-N3-C2	-2.05	122.01	125.64
2	A	998	FAD	C5'-C4'-C3'	-2.03	108.39	112.22
3	A	999	FO1	C15-C14-N3	2.00	119.66	110.20

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	FO1	N3-C14-C15-O3
3	A	999	FO1	N3-C14-C15-C16
3	B	999	FO1	N3-C14-C15-O3
3	B	999	FO1	N3-C14-C15-C16
4	A	1463	GOL	O1-C1-C2-C3
4	A	1463	GOL	C1-C2-C3-O3
4	A	1463	GOL	O2-C2-C3-O3
4	B	1464	GOL	O1-C1-C2-C3
7	A	1470	PEG	O1-C1-C2-O2
6	A	1469	PGE	C6-C5-O3-C4
6	A	1467	PGE	C3-C4-O3-C5
6	A	1467	PGE	O3-C5-C6-O4
7	A	1472	PEG	O2-C3-C4-O4
4	A	1463	GOL	O1-C1-C2-O2
4	B	1464	GOL	O1-C1-C2-O2
7	A	1470	PEG	O2-C3-C4-O4
6	A	1467	PGE	C6-C5-O3-C4
6	A	1469	PGE	O2-C3-C4-O3
4	B	1463	GOL	O1-C1-C2-O2
6	A	1467	PGE	O1-C1-C2-O2
7	A	1472	PEG	O1-C1-C2-O2
6	A	1467	PGE	C1-C2-O2-C3
2	A	998	FAD	C4'-C5'-O5'-P
6	A	1469	PGE	C3-C4-O3-C5

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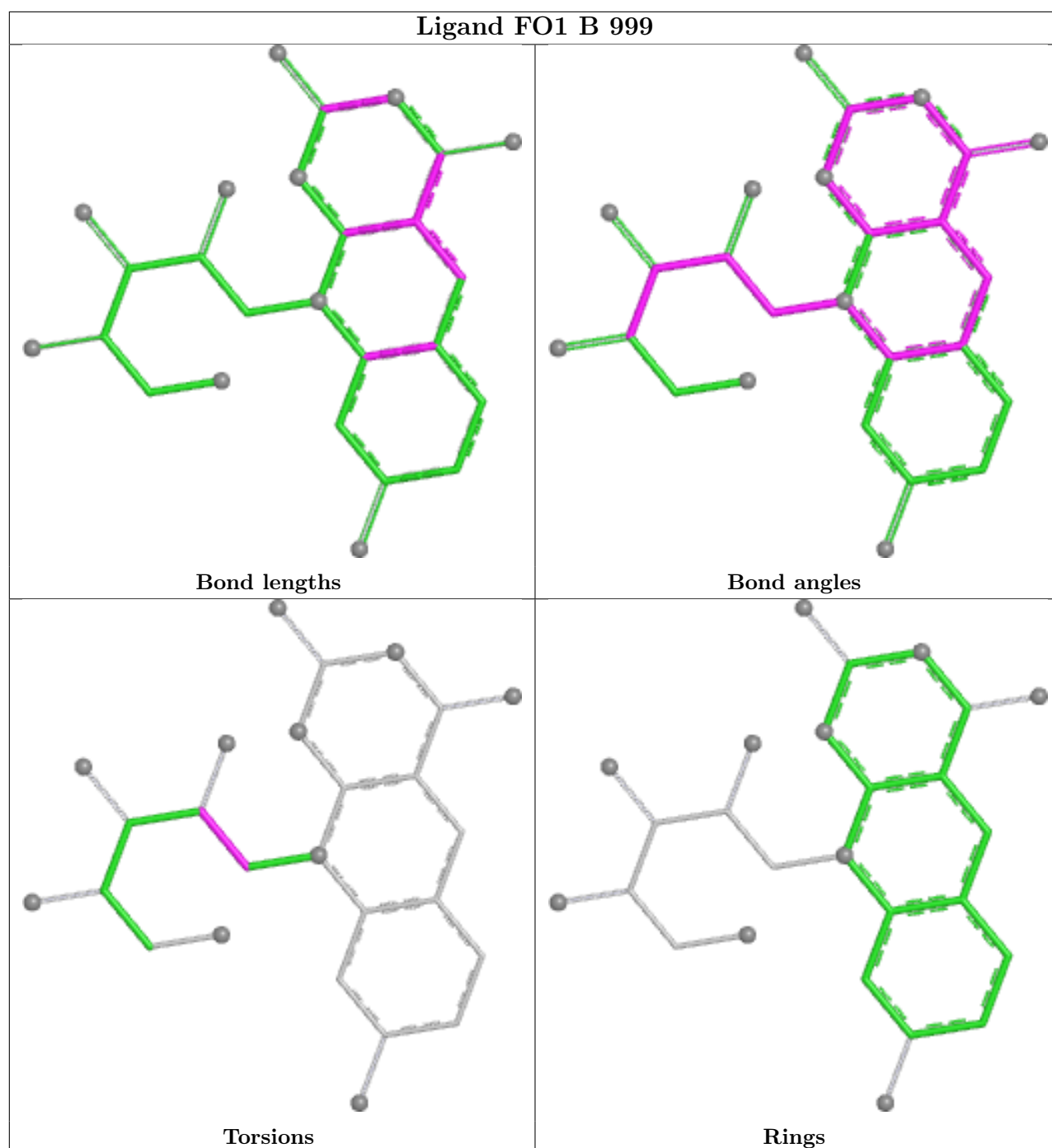
Mol	Chain	Res	Type	Atoms
6	A	1469	PGE	C4-C3-O2-C2
7	A	1470	PEG	C4-C3-O2-C2
4	B	1463	GOL	O1-C1-C2-C3
7	A	1468	PEG	C4-C3-O2-C2
7	A	1468	PEG	O1-C1-C2-O2
2	B	998	FAD	C4'-C5'-O5'-P
7	A	1472	PEG	C4-C3-O2-C2
3	A	999	FO1	O4-C16-C17-C18
7	A	1471	PEG	O1-C1-C2-O2

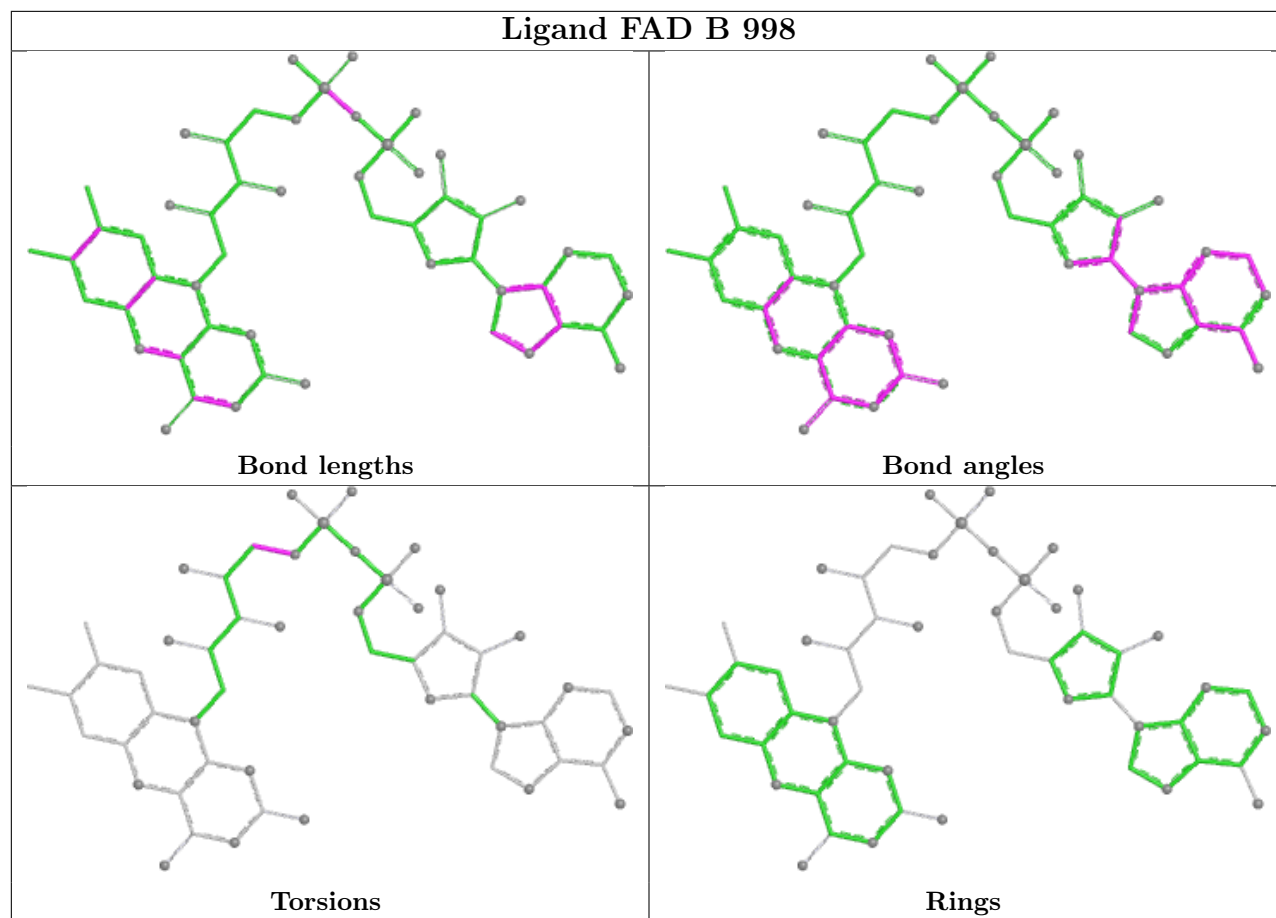
There are no ring outliers.

6 monomers are involved in 11 short contacts:

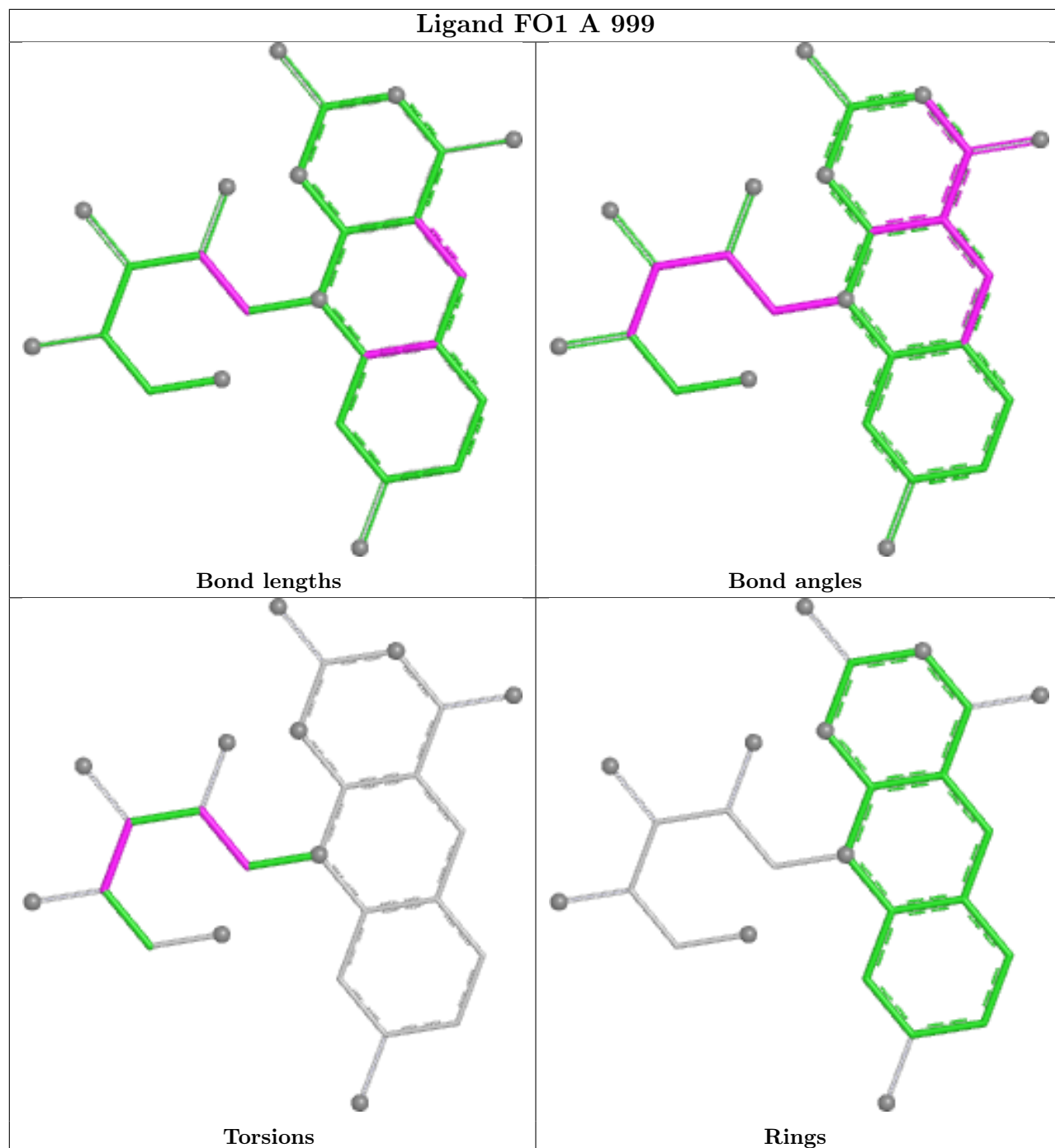
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1464	GOL	1	0
4	B	1463	GOL	1	0
7	A	1470	PEG	3	0
6	A	1469	PGE	2	0
2	B	998	FAD	3	0
2	A	998	FAD	2	0

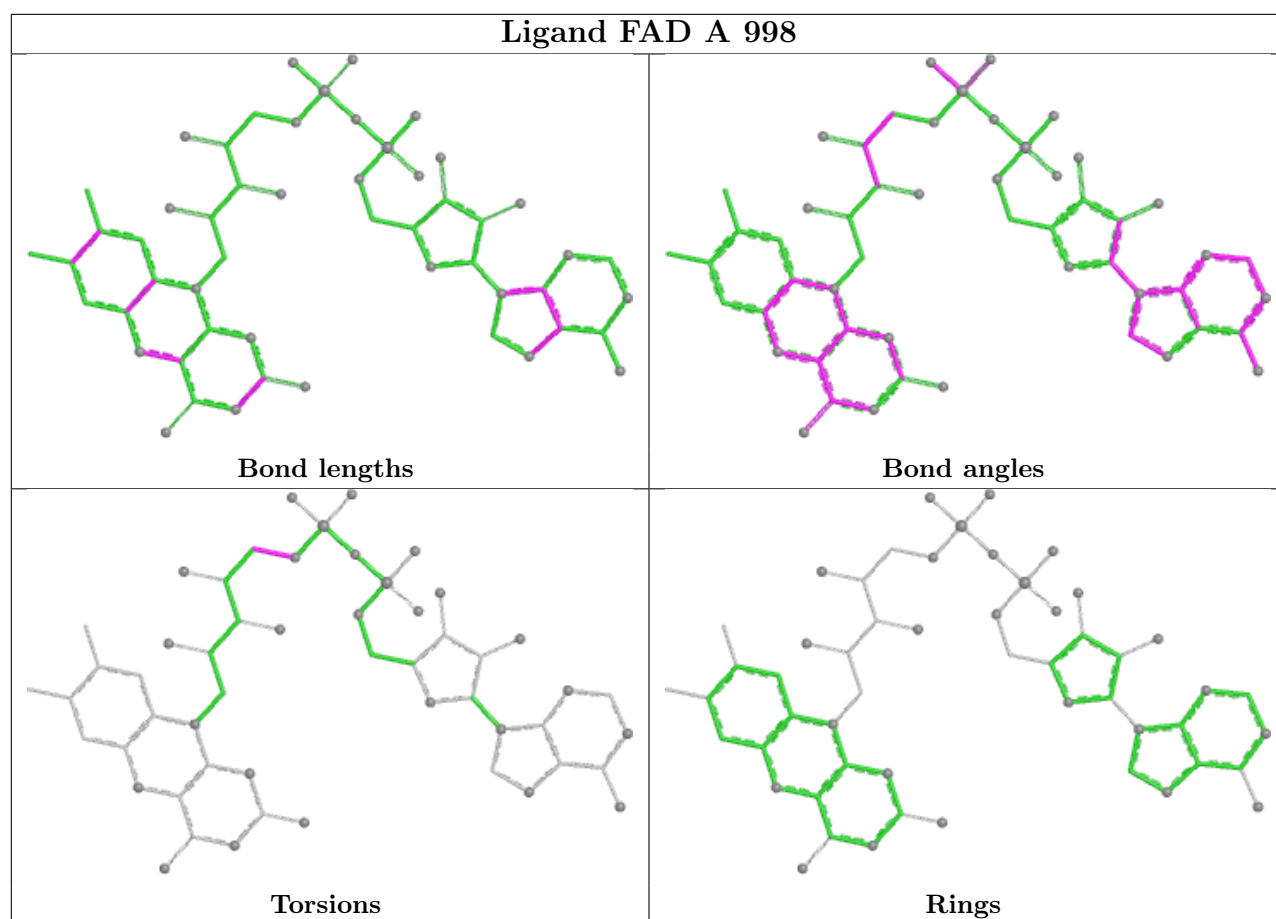
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 FO1 A 999





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	463/482 (96%)	-0.29	9 (1%) 66 70	15, 26, 45, 90	15 (3%)
1	B	438/482 (90%)	-0.14	13 (2%) 52 56	14, 29, 53, 83	10 (2%)
All	All	901/964 (93%)	-0.22	22 (2%) 59 63	14, 27, 50, 90	25 (2%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	LEU	7.8
1	A	195	GLY	5.8
1	A	-4	LEU	5.0
1	A	189	GLU	4.9
1	A	-3	VAL	4.8
1	B	219	LYS	4.8
1	B	218	LEU	4.8
1	B	187	THR	4.5
1	B	-4	LEU	4.1
1	A	196	MET	3.6
1	B	-3	VAL	3.2
1	A	188	PRO	3.0
1	B	188	PRO	2.8
1	B	462	SER	2.7
1	A	187	THR	2.7
1	A	168	TYR	2.6
1	B	92	PHE	2.5
1	B	0	GLY	2.4
1	B	262	ASN	2.4
1	B	-2	PRO	2.2
1	B	2	HIS	2.1
1	B	14	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

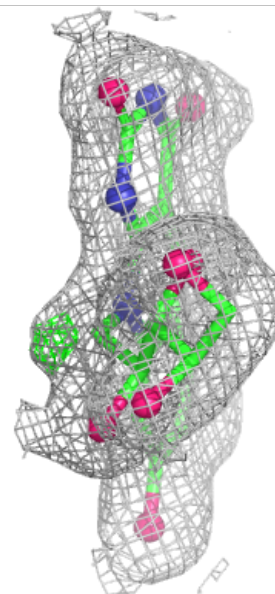
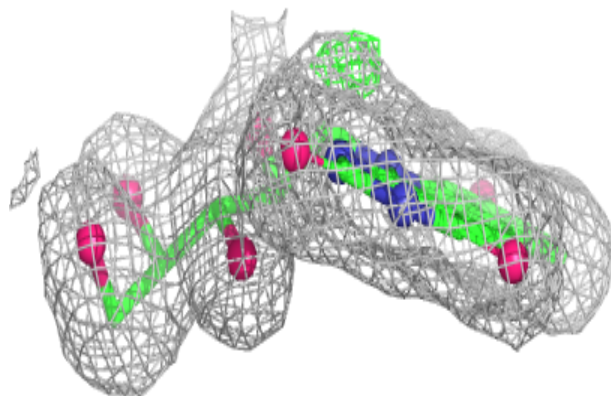
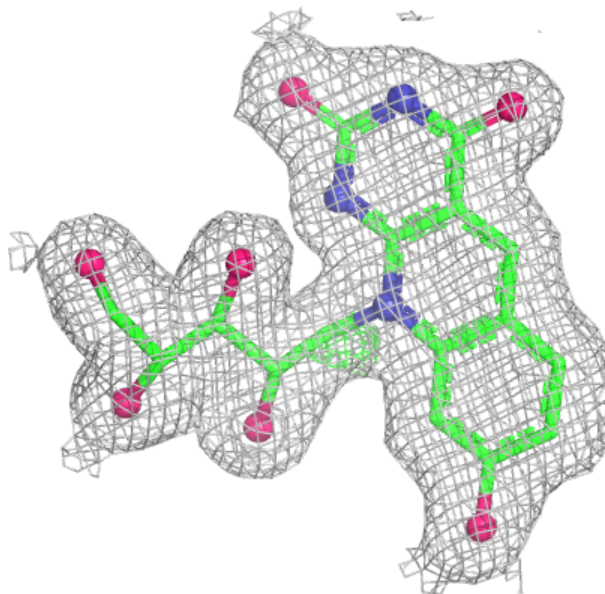
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PGE	A	1469	10/10	0.79	0.17	47,52,55,57	0
7	PEG	A	1472	7/7	0.80	0.24	60,63,68,68	0
7	PEG	A	1471	7/7	0.81	0.18	56,67,75,75	0
6	PGE	A	1467	10/10	0.86	0.15	43,51,54,55	0
7	PEG	A	1470	7/7	0.86	0.14	32,44,56,57	0
7	PEG	A	1468	7/7	0.88	0.14	36,47,57,59	0
4	GOL	B	1464	6/6	0.89	0.12	28,33,38,38	0
5	SO4	B	1466	5/5	0.89	0.14	82,85,91,94	0
4	GOL	B	1463	6/6	0.90	0.10	32,40,42,43	0
5	SO4	B	1465	5/5	0.91	0.09	50,60,62,62	0
4	GOL	A	1465	6/6	0.91	0.12	53,54,55,58	0
4	GOL	A	1463	6/6	0.92	0.11	39,43,43,48	0
4	GOL	A	1464	6/6	0.94	0.10	30,35,36,38	0
5	SO4	A	1466	5/5	0.95	0.07	44,56,59,61	0
3	FO1	A	999	26/26	0.97	0.04	18,19,21,23	0
3	FO1	B	999	26/26	0.97	0.05	19,22,25,26	0
2	FAD	A	998	53/53	0.99	0.04	17,19,22,23	0
2	FAD	B	998	53/53	0.99	0.04	18,20,22,23	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.

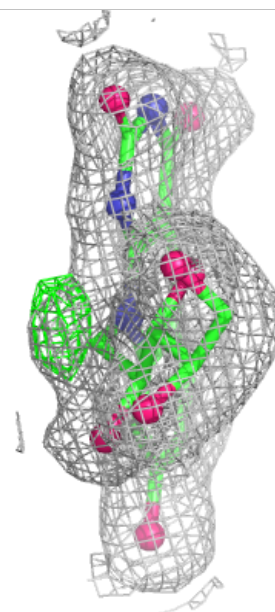
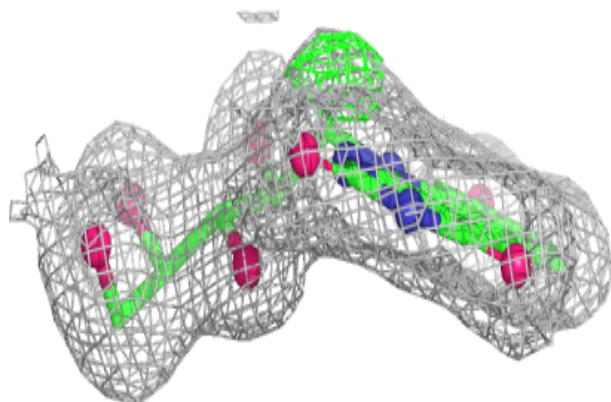
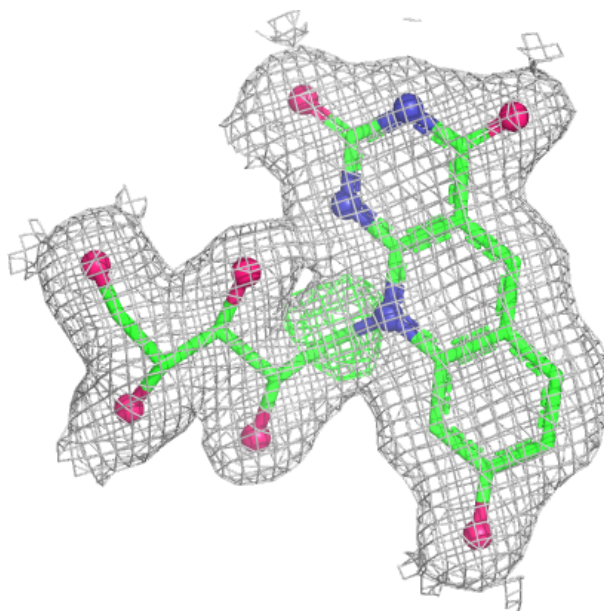
Electron density around FO1 A 999:

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



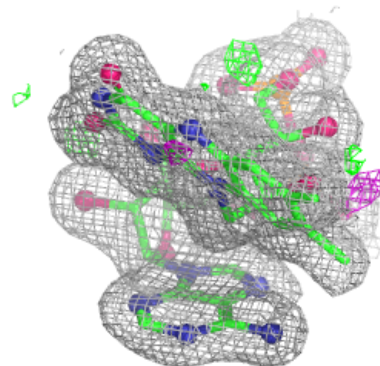
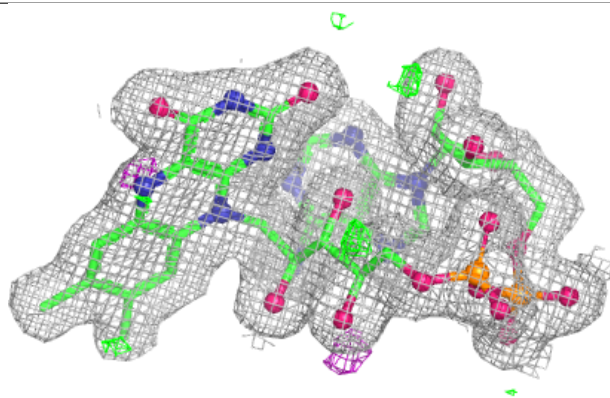
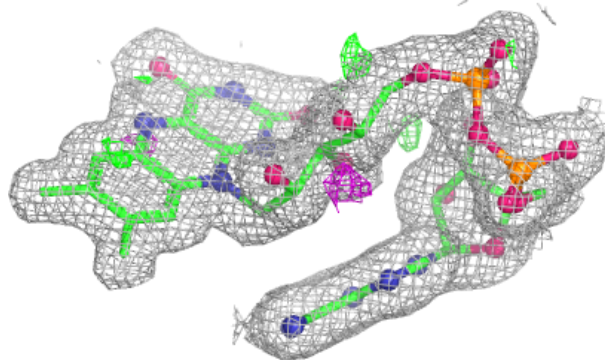
Electron density around FO1 B 999:

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

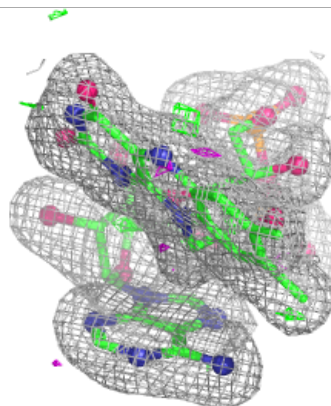
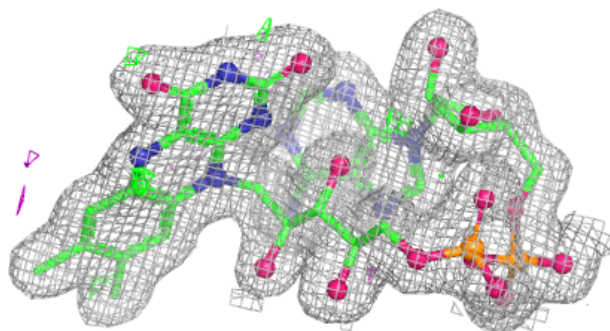
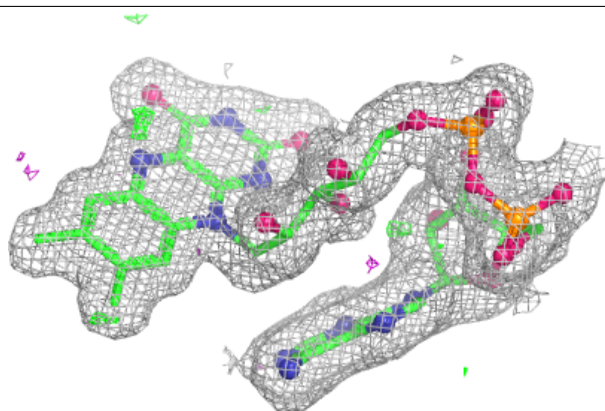


Electron density around FAD A 998:

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

**Electron density around FAD B 998:**

$2mF_o-DF_c$ (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.