



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 01:06 PM EDT

PDB ID : 1T3Q / pdb_00001t3q
Title : Crystal structure of quinoline 2-Oxidoreductase from Pseudomonas Putida 86
Authors : Bonin, I.; Martins, B.M.; Purvanov, V.; Fetzner, S.; Huber, R.; Dobbek, H.
Deposited on : 2004-04-27
Resolution : 1.80 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

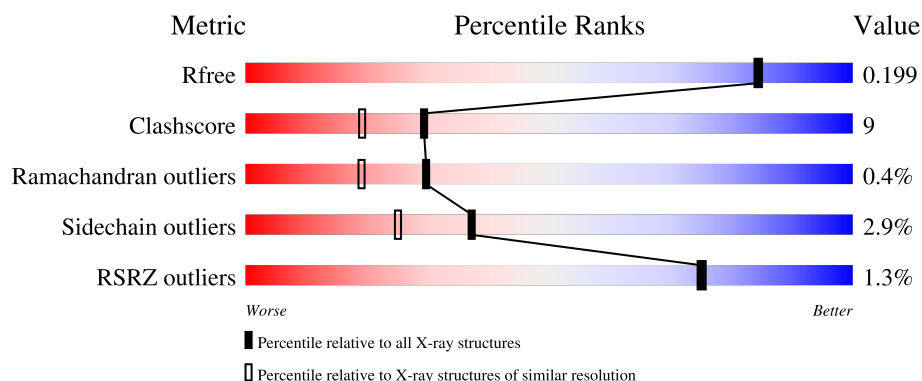
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	168	3% 79% 14% • •
1	D	168	3% 82% 14% • •
2	B	788	81% 17% •
2	E	788	• 81% 17% •
3	C	288	2% 77% 21% ••

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Mol	Chain	Length	Quality of chain
3	F	288	

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
5	GOL	A	3909	-	X	-	-
5	GOL	B	3902	-	X	-	-
5	GOL	B	3906	-	X	-	-
5	GOL	C	3907	-	X	-	-
5	GOL	C	3908	-	X	-	-
5	GOL	E	3901	-	X	-	-
5	GOL	E	3904	-	X	-	-
5	GOL	E	3905	-	X	-	-
5	GOL	F	3903	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21323 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 quinoline 2-oxidoreductase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	23	0	0
			1201	733	220	234	14			
1	D	162	Total	C	N	O	S	34	0	0
			1201	733	220	234	14			

- Molecule 2 is a protein called quinoline 2-oxidoreductase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	786	Total	C	N	O	S	99	0	0
			5899	3704	1043	1128	24			
2	E	786	Total	C	N	O	S	84	0	0
			5899	3704	1043	1128	24			

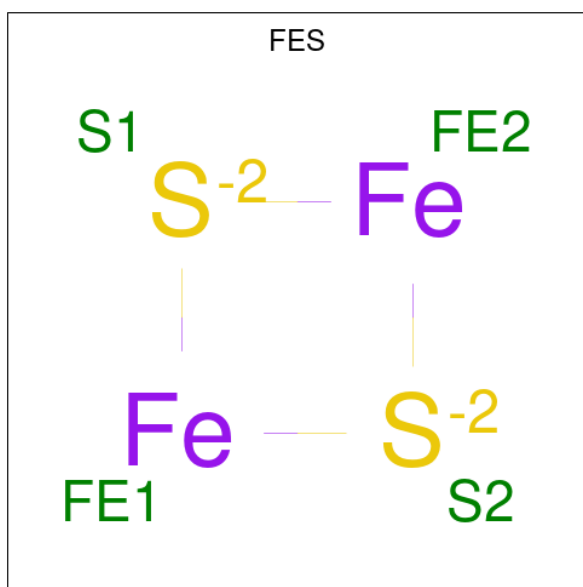
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	465	GLU	ASP	SEE REMARK 999	UNP P72224
B	466	VAL	CYS	SEE REMARK 999	UNP P72224
E	465	GLU	ASP	SEE REMARK 999	UNP P72224
E	466	VAL	CYS	SEE REMARK 999	UNP P72224

- Molecule 3 is a protein called quinoline 2-oxidoreductase medium subunit.

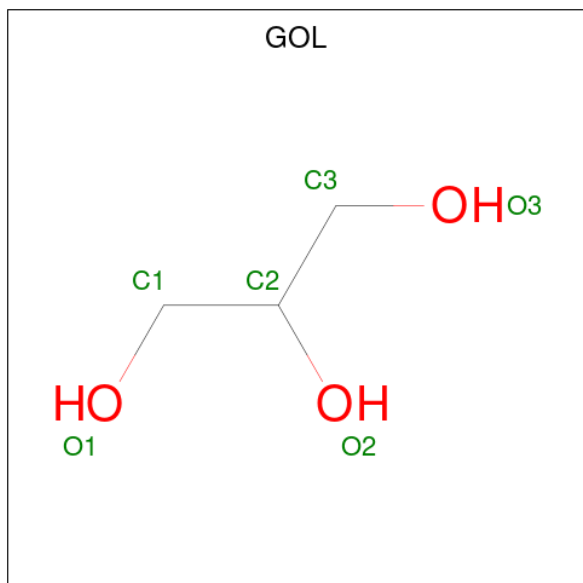
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	285	Total	C	N	O	S	64	0	0
			2139	1353	381	393	12			
3	F	285	Total	C	N	O	S	51	0	0
			2139	1353	381	393	12			

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



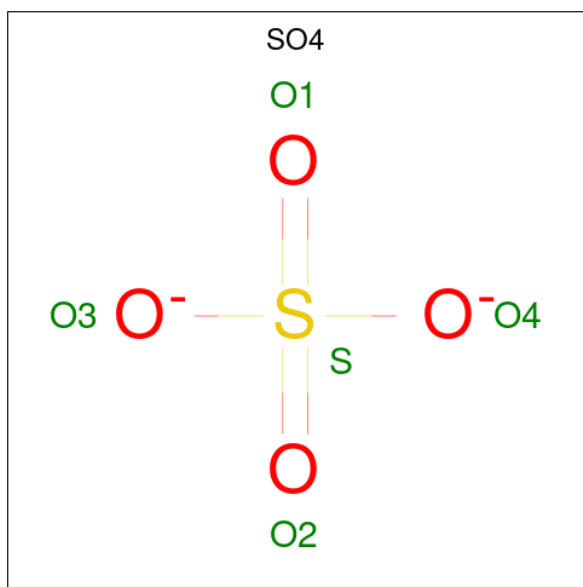
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	D	1	Total	Fe	S	0	0
			4	2	2		
4	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



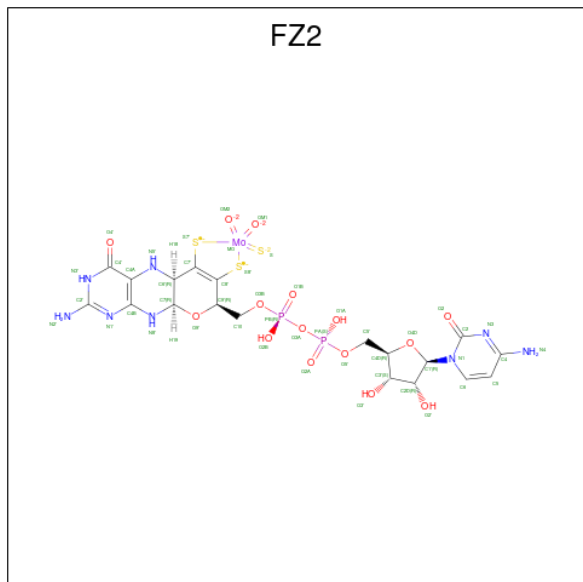
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0

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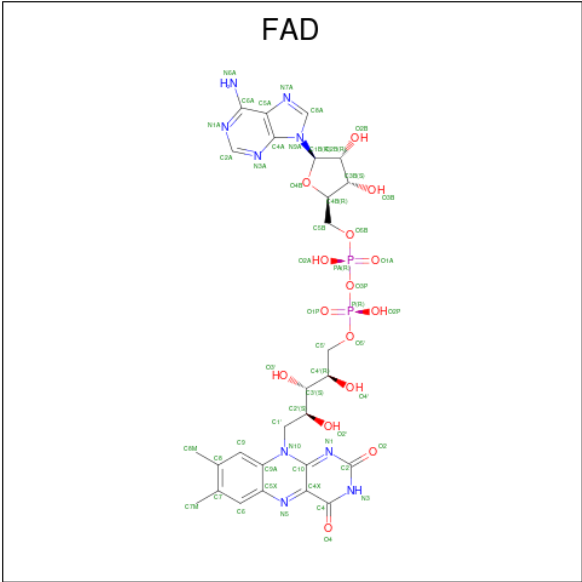
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is Mo-dioxo-thioxo-molybdopterin cytosine dinucleotide (CCD ID: FZ2) (formula: $C_{19}H_{24}MoN_8O_{15}P_2S_3$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
7	B	1	Total	C	Mo	N	O	P	S	0	0
			48	19	1	8	15	2	3		
7	E	1	Total	C	Mo	N	O	P	S	0	0
			48	19	1	8	15	2	3		

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

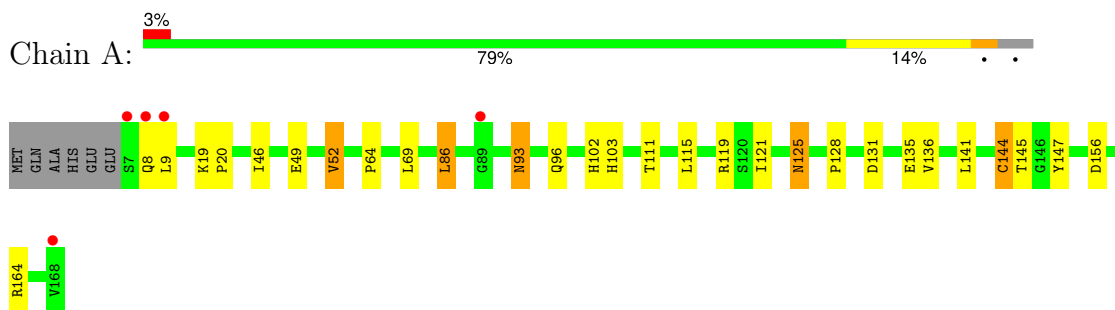
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	192	Total	O	0	0
			192	192		
9	B	806	Total	O	0	0
			806	806		
9	C	272	Total	O	0	0
			272	272		
9	D	178	Total	O	0	0
			178	178		
9	E	776	Total	O	0	0
			776	776		
9	F	309	Total	O	0	0
			309	309		

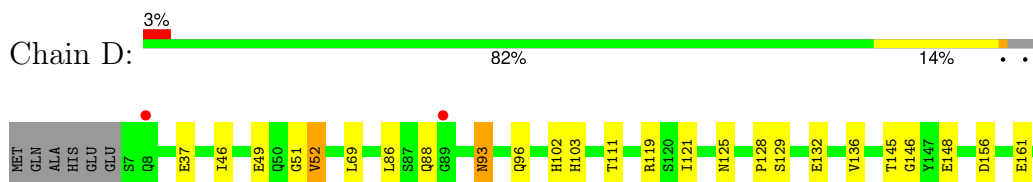
3 Residue-property plots [i](#)

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.

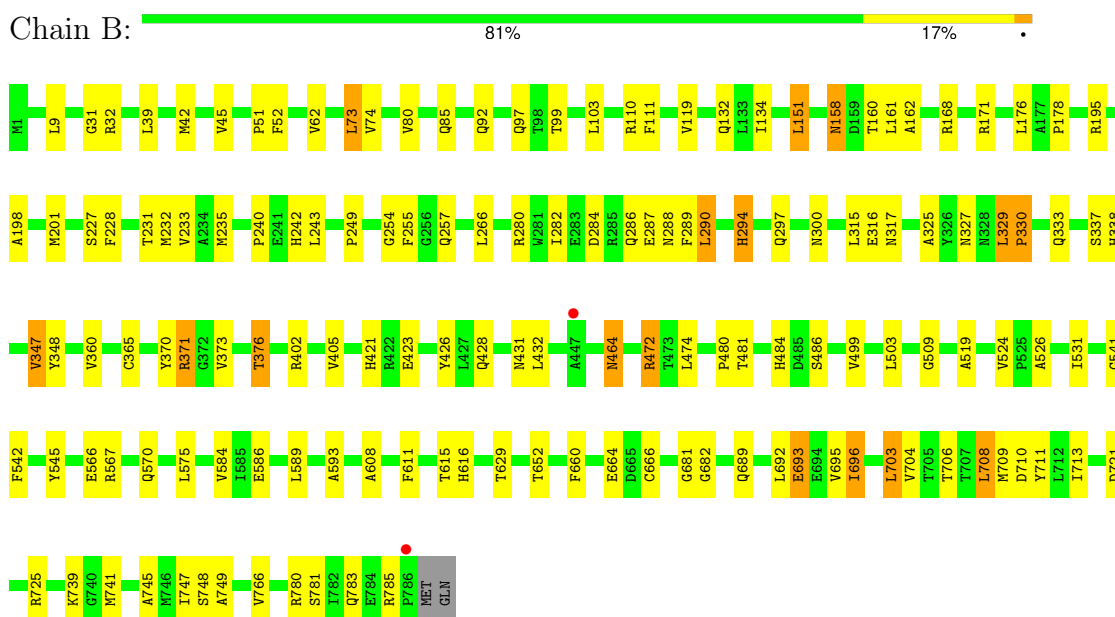
- Molecule 1: quinoline 2-oxidoreductase small subunit



- Molecule 1: quinoline 2-oxidoreductase small subunit



- Molecule 2: quinoline 2-oxidoreductase large subunit



Chain E: 81% 17%

Label	Color
I696	Green
L703	Green
L708	Orange
M709	Green
D710	Green
Y711	Green
D721	Green
L727	Green
K739	Green
G740	Green
M741	Green
G742	Green
E743	Green
S744	Green
A745	Green
M746	Green
I747	Green
S748	Green
A749	Green
P750	Green
G759	Green
R780	Orange
Q783	Green
E784	Green
R785	Green
P786	Green
NET	Grey
GLN	Grey
G509	Green
H510	Green
E511	Green
V529	Green
M538	Green
T539	Green
Y540	Orange
G541	Green
F542	Green
Y545	Green
A546	Green
E566	Green
Q570	Green
L575	Green
L589	Orange
V590	Green
H591	Green
G594	Green
V595	Green
P596	Green
A597	Green
K598	Green
G599	Green
A608	Green
F611	Green
T615	Green
H616	Green
T629	Green
Y630	Green
D631	Green
P632	Green
T652	Green
F660	Green
C666	Green
G682	Green
I683	Green
A684	Green
Q689	Green
L692	Green
E693	Orange
F694	Green
V695	Green
V350	Green
V360	Green
C365	Green
Y370	Green
R371	Orange
G372	Green
V373	Green
T376	Green
R391	Green
R402	Green
V405	Green
L417	Green
H421	Green
Y426	Green
L427	Green
Q428	Green
M431	Green
L432	Green
P439	Green
E440	Green
A441	Green
F442	Green
R443	Green
Q444	Green
R445	Green
Q446	Green
A447	Green
E448	Green
A451	Green
M464	Orange
L474	Green
T479	Green
P480	Green
T481	Green
H484	Green
D485	Green
S486	Green
V497	Green
S502	Green
L503	Orange
M201	Green
S227	Green
T231	Green
M232	Green
P240	Green
E241	Green
H242	Green
L243	Green
P249	Green
G254	Green
Q257	Green
P263	Green
D284	Green
R285	Green
Q286	Orange
E287	Green
N288	Green
F289	Green
A292	Orange
T293	Green
H294	Green
Q297	Green
N300	Green
D307	Green
L315	Green
E316	Green
N317	Green
G323	Green
G324	Green
A325	Green
Y326	Green
N328	Green
L329	Orange
P330	Orange
W331	Green
T332	Green
Q333	Green
H338	Green
I344	Green
L345	Green
G346	Green
V347	Orange
A181	Green
R195	Orange

Chain C:

Amino Acid	Percentage
M1	2%
P4	
S7	
P11	
Q15	
E16	
V17	
V20	
D24	
L37	
A41	
F42	
R43	
C49	
S57	
Q64	
S65	
T68	
L69	
N80	
D83	
P84	
L93	
H102	
Q103	
L115	
A129	
M135	
A148	
L160	
L166	
E170	
A175	
E179	
F182	

Chain F:

3% 82% 15% ..

M1 P11 Q15 E16 V17 V20 R28 L37 R43 S57 S65 I68 L69 R79 M80 D83 L93 H102 N107 A129 A148 T158 D159 L160 L166 E170 A175 L176 H177 W178 E179 Y183 A184 R185 R186 K187 G188 D189 V190 A191 L192 S200 R205 A208 I211 A212 L213 V216 N227 V231 V234 I235 L251 E252 P253 H258 G259 S260 R264 A283 M284 Y285 ALA GLY ALA

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	278.32Å 72.10Å 202.65Å 90.00° 127.98° 90.00°	Depositor
Resolution (Å)	19.29 – 1.80 19.29 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.2 (19.29-1.80) 96.1 (19.29-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.23 (at 1.75Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.186 , 0.207 0.178 , 0.199	Depositor DCC
R_{free} test set	13956 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.6	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	0.96	EDS
Total number of atoms	21323	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, FES, FAD, FZ2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/1214	0.97	9/1638 (0.5%)
1	D	0.36	0/1214	0.93	5/1638 (0.3%)
2	B	0.37	0/6002	0.92	17/8169 (0.2%)
2	E	0.36	0/6002	0.92	17/8169 (0.2%)
3	C	0.35	0/2177	0.92	9/2951 (0.3%)
3	F	0.35	0/2177	0.92	9/2951 (0.3%)
All	All	0.36	0/18786	0.92	66/25516 (0.3%)

There are no bond length outliers.

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	THR	N-CA-C	9.16	124.59	113.23
1	D	145	THR	N-CA-C	8.87	124.52	112.90
2	B	31	GLY	N-CA-C	-8.12	102.14	112.54
1	D	52	VAL	N-CA-C	7.74	118.65	111.45
1	A	52	VAL	N-CA-C	7.58	118.50	111.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1201	0	1196	20	0
1	D	1201	0	1196	19	0
2	B	5899	0	5916	109	0
2	E	5899	0	5916	105	0
3	C	2139	0	2176	44	0
3	F	2139	0	2176	38	0
4	A	8	0	0	0	0
4	D	8	0	0	1	0
5	A	6	0	4	1	0
5	B	12	0	8	1	0
5	C	12	0	8	0	0
5	E	18	0	12	1	0
5	F	6	0	4	2	0
6	B	20	0	0	1	0
6	E	20	0	0	0	0
7	B	48	0	0	2	0
7	E	48	0	0	1	0
8	C	53	0	31	0	0
8	F	53	0	31	0	0
9	A	192	0	0	4	0
9	B	806	0	0	11	0
9	C	272	0	0	4	0
9	D	178	0	0	2	0
9	E	776	0	0	10	0
9	F	309	0	0	6	0
All	All	21323	0	18674	316	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 9.

The worst 5 of 316 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)
2:E:347:VAL:HG13	2:E:405:VAL:HG23	1.45	0.98
2:E:402:ARG:HE	2:E:431:ASN:HD21	1.15	0.94
2:E:97:GLN:HE22	2:E:162:ALA:H	1.18	0.91
2:B:402:ARG:HE	2:B:431:ASN:HD21	1.15	0.90
1:D:86:LEU:HD21	1:D:119:ARG:HD2	1.50	0.90

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	160/168 (95%)	157 (98%)	3 (2%)	0	100	100
1	D	160/168 (95%)	156 (98%)	4 (2%)	0	100	100
2	B	784/788 (100%)	764 (97%)	16 (2%)	4 (0%)	24	14
2	E	784/788 (100%)	762 (97%)	17 (2%)	5 (1%)	21	11
3	C	283/288 (98%)	276 (98%)	7 (2%)	0	100	100
3	F	283/288 (98%)	280 (99%)	3 (1%)	0	100	100
All	All	2454/2488 (99%)	2395 (98%)	50 (2%)	9 (0%)	30	19

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	371	ARG
2	E	371	ARG
2	E	373	VAL
2	B	373	VAL
2	B	741	MET

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	129/134 (96%)	127 (98%)	2 (2%)	55	47
1	D	129/134 (96%)	127 (98%)	2 (2%)	55	47
2	B	618/620 (100%)	602 (97%)	16 (3%)	40	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	618/620 (100%)	602 (97%)	16 (3%)	40	28
3	C	218/218 (100%)	206 (94%)	12 (6%)	19	8
3	F	218/218 (100%)	210 (96%)	8 (4%)	30	18
All	All	1930/1944 (99%)	1874 (97%)	56 (3%)	37	25

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	281	GLN
3	F	185	ARG
2	E	286	GLN
3	F	166	LEU
3	F	68	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	639	ASN
2	E	702	GLN
3	F	222	GLN
2	B	702	GLN
2	B	689	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

25 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$
6	SO4	B	3102	-	4,4,4	0.38	0	6,6,6	0.08	0
6	SO4	E	3107	-	4,4,4	0.40	0	6,6,6	0.05	0
4	FES	D	4909	1	0,4,4	-	-	-		
5	GOL	A	3909	-	5,5,5	4.75	5 (100%)	5,5,5	6.11	3 (60%)
5	GOL	B	3902	-	5,5,5	4.75	5 (100%)	5,5,5	6.13	3 (60%)
5	GOL	C	3907	-	5,5,5	4.76	5 (100%)	5,5,5	6.10	3 (60%)
5	GOL	E	3905	-	5,5,5	4.75	5 (100%)	5,5,5	6.06	3 (60%)
6	SO4	E	3104	-	4,4,4	0.37	0	6,6,6	0.10	0
5	GOL	F	3903	-	5,5,5	4.77	5 (100%)	5,5,5	6.12	3 (60%)
5	GOL	B	3906	-	5,5,5	4.82	5 (100%)	5,5,5	6.12	3 (60%)
6	SO4	E	3106	-	4,4,4	0.38	0	6,6,6	0.07	0
8	FAD	F	4932	-	58,58,58	2.47	21 (36%)	85,89,89	1.12	6 (7%)
8	FAD	C	4931	-	58,58,58	2.41	22 (37%)	85,89,89	1.12	6 (7%)
7	FZ2	B	3907	-	47,53,53	2.33	15 (31%)	54,86,86	2.41	12 (22%)
7	FZ2	E	3906	-	47,53,53	2.33	17 (36%)	54,86,86	2.38	11 (20%)
4	FES	A	4907	1	0,4,4	-	-	-		
5	GOL	E	3901	-	5,5,5	4.76	5 (100%)	5,5,5	6.12	3 (60%)
6	SO4	B	3105	-	4,4,4	0.37	0	6,6,6	0.09	0
5	GOL	E	3904	-	5,5,5	4.79	5 (100%)	5,5,5	6.16	3 (60%)
6	SO4	B	3101	-	4,4,4	0.39	0	6,6,6	0.08	0
6	SO4	B	3100	-	4,4,4	0.36	0	6,6,6	0.07	0
4	FES	D	4910	1	0,4,4	-	-	-		
6	SO4	E	3103	-	4,4,4	0.36	0	6,6,6	0.11	0
4	FES	A	4908	1	0,4,4	-	-	-		
5	GOL	C	3908	-	5,5,5	4.77	5 (100%)	5,5,5	6.12	3 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	F	3903	-	-	2/4/4/4	-
5	GOL	B	3906	-	-	3/4/4/4	-
4	FES	A	4908	1	-	-	0/1/1/1
8	FAD	F	4932	-	-	12/34/50/50	0/6/6/6
8	FAD	C	4931	-	-	11/34/50/50	0/6/6/6
7	FZ2	B	3907	-	-	5/22/78/78	0/6/6/6
7	FZ2	E	3906	-	-	6/22/78/78	0/6/6/6
4	FES	D	4910	1	-	-	0/1/1/1
5	GOL	E	3904	-	-	2/4/4/4	-
5	GOL	A	3909	-	-	3/4/4/4	-
5	GOL	E	3901	-	-	2/4/4/4	-
4	FES	A	4907	1	-	-	0/1/1/1
5	GOL	B	3902	-	-	2/4/4/4	-
5	GOL	C	3907	-	-	3/4/4/4	-
5	GOL	E	3905	-	-	3/4/4/4	-
4	FES	D	4909	1	-	-	0/1/1/1
5	GOL	C	3908	-	-	3/4/4/4	-

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	4932	FAD	P-O3P	-11.74	1.46	1.59
8	C	4931	FAD	P-O3P	-10.91	1.47	1.59
5	C	3907	GOL	C3-C2	-8.14	1.20	1.51
5	E	3905	GOL	C3-C2	-8.13	1.20	1.51
5	B	3906	GOL	C3-C2	-8.04	1.21	1.51

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	3904	GOL	O3-C3-C2	11.25	161.02	110.38
5	B	3906	GOL	O3-C3-C2	11.16	160.61	110.38
5	E	3901	GOL	O3-C3-C2	11.13	160.48	110.38
5	A	3909	GOL	O3-C3-C2	11.11	160.41	110.38
5	C	3908	GOL	O3-C3-C2	11.09	160.32	110.38

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

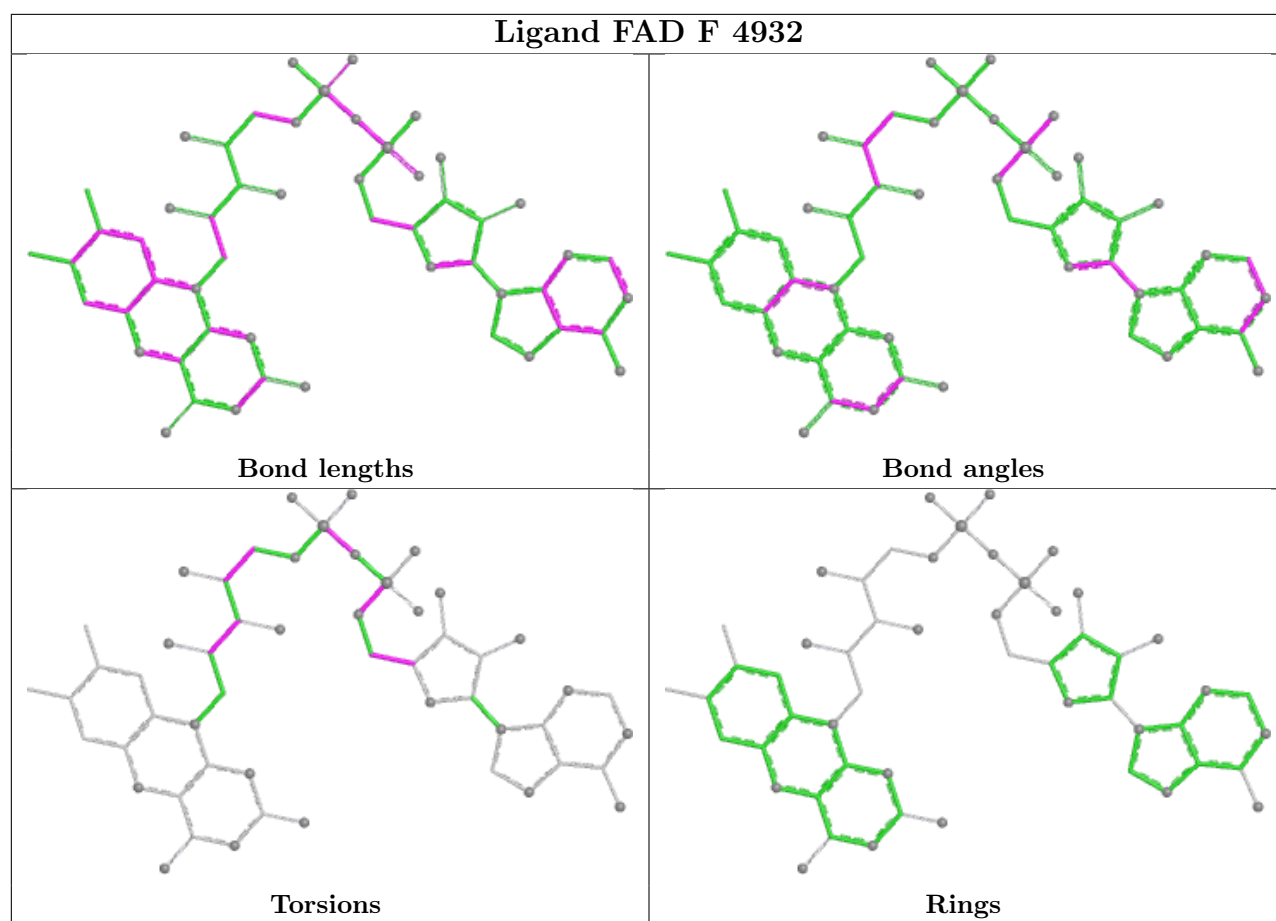
Mol	Chain	Res	Type	Atoms
5	A	3909	GOL	O1-C1-C2-C3
5	A	3909	GOL	C1-C2-C3-O3
5	B	3902	GOL	O1-C1-C2-C3
5	B	3902	GOL	C1-C2-C3-O3
5	B	3906	GOL	C1-C2-C3-O3

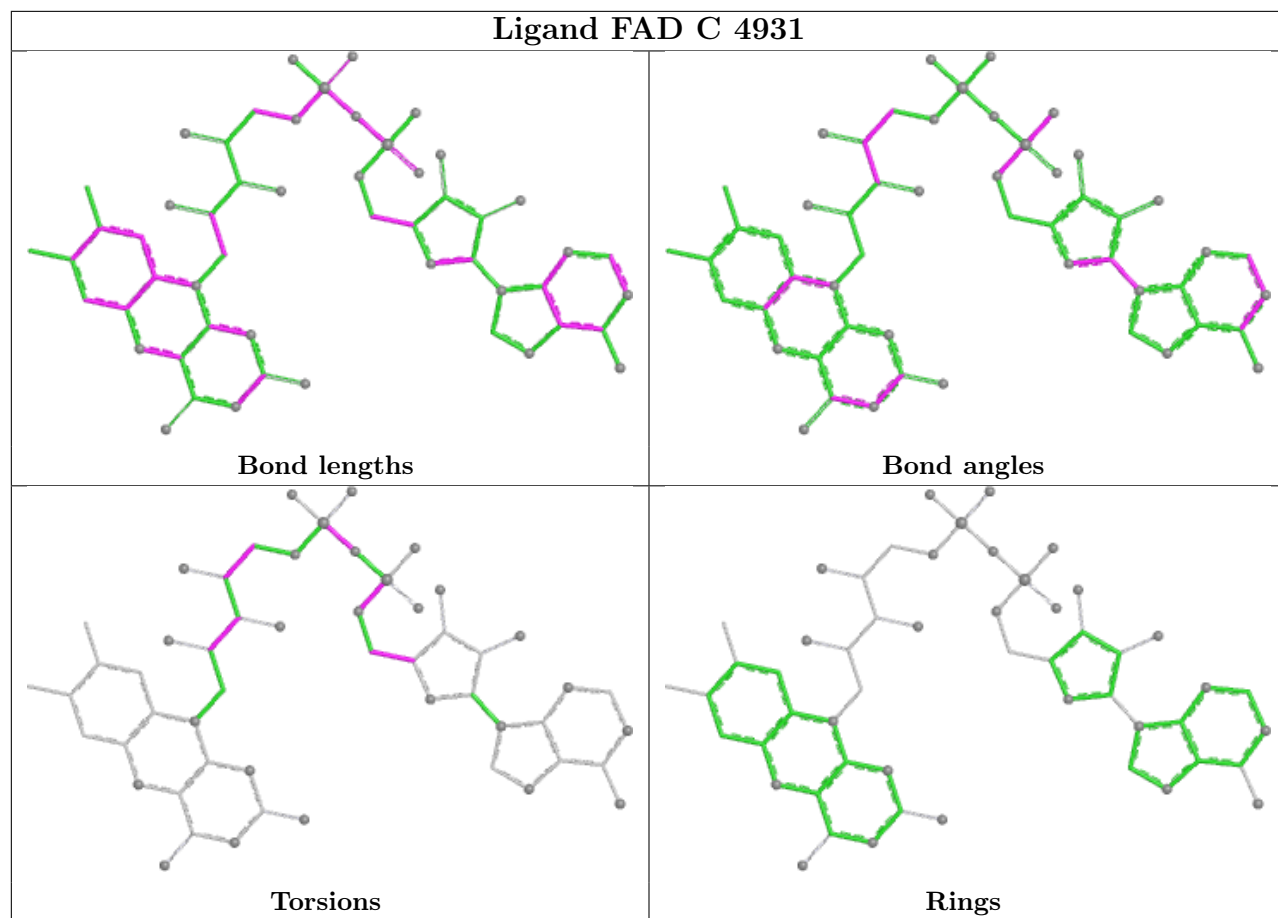
There are no ring outliers.

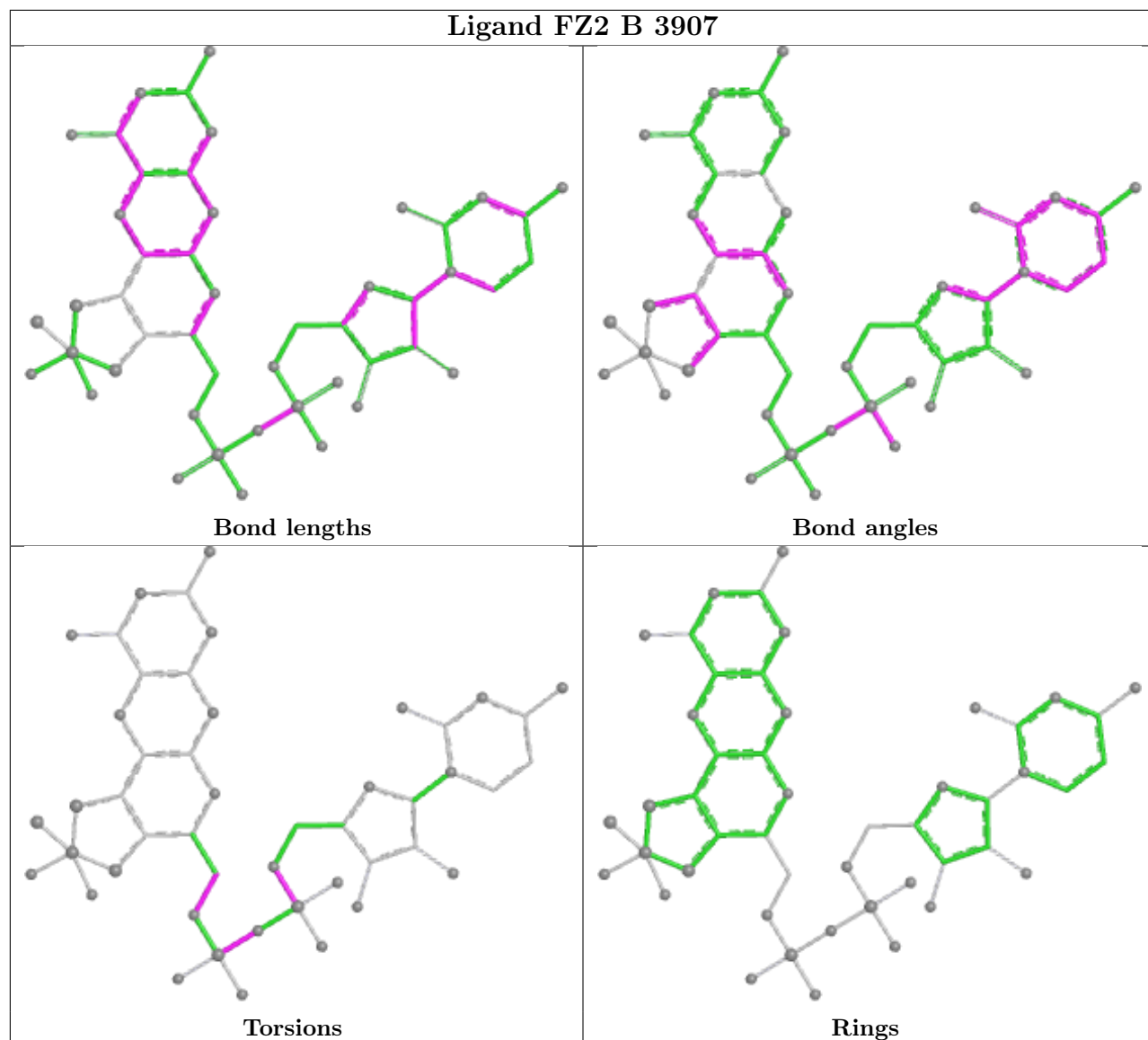
8 monomers are involved in 10 short contacts:

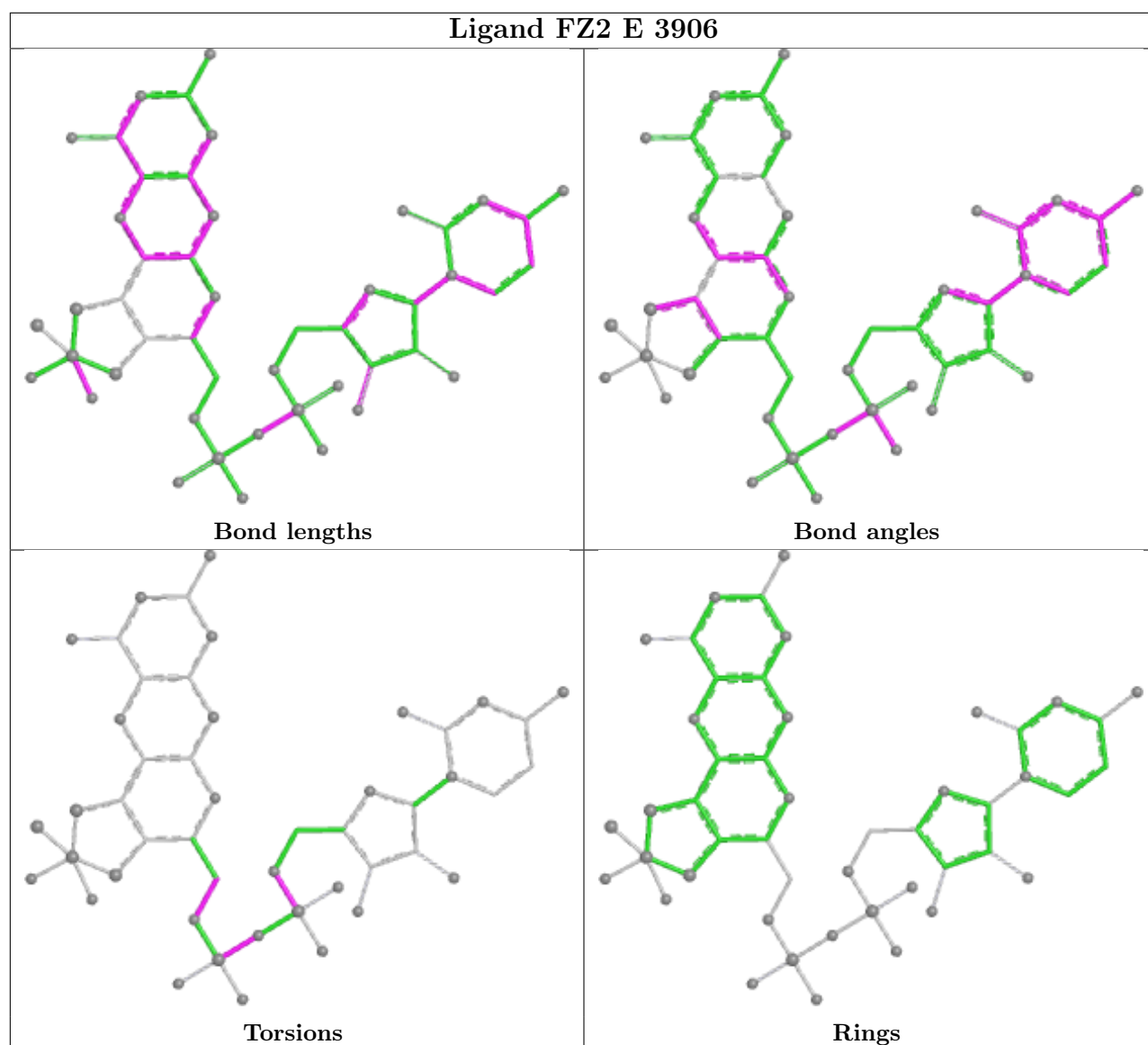
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3909	GOL	1	0
5	F	3903	GOL	2	0
5	B	3906	GOL	1	0
7	B	3907	FZ2	2	0
7	E	3906	FZ2	1	0
5	E	3904	GOL	1	0
6	B	3101	SO4	1	0
4	D	4910	FES	1	0

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	162/168 (96%)	-0.23	5 (3%)	51	51	13, 20, 32, 62	6 (3%)
1	D	162/168 (96%)	-0.22	5 (3%)	51	51	9, 21, 32, 59	8 (4%)
2	B	786/788 (99%)	-0.38	2 (0%)	90	90	9, 21, 32, 54	26 (3%)
2	E	786/788 (99%)	-0.19	6 (0%)	82	83	12, 23, 36, 58	26 (3%)
3	C	285/288 (98%)	-0.01	6 (2%)	63	64	12, 26, 39, 49	18 (6%)
3	F	285/288 (98%)	0.00	9 (3%)	50	50	13, 26, 36, 50	15 (5%)
All	All	2466/2488 (99%)	-0.21	33 (1%)	75	75	9, 22, 35, 62	99 (4%)

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	SER	17.4
2	E	598	LYS	5.4
2	E	451	ALA	5.2
1	D	168	VAL	5.0
1	A	8	GLN	4.5

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 ⓘ

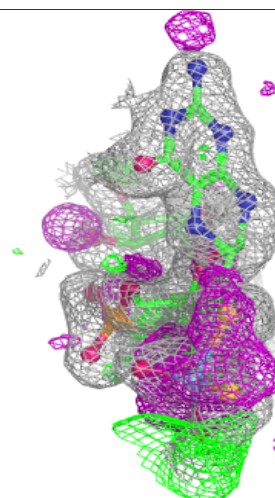
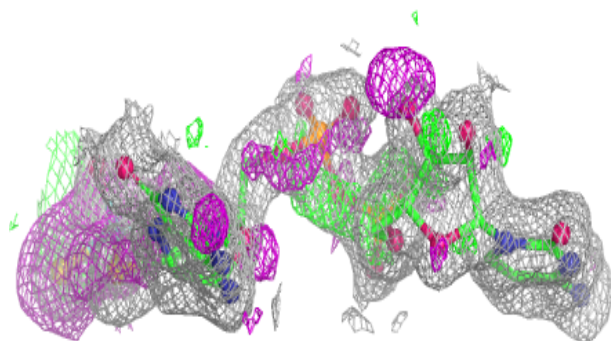
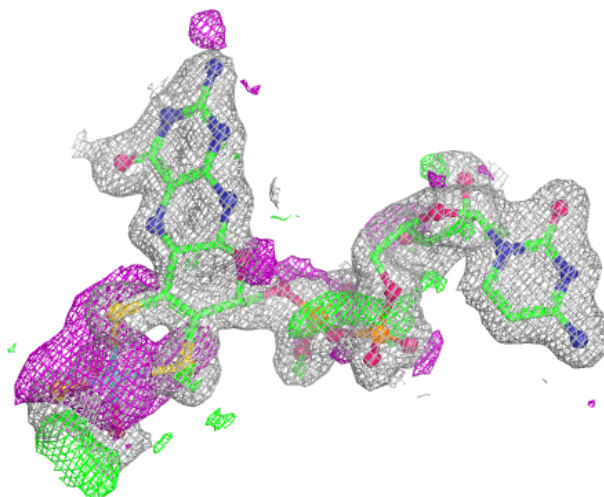
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	B	3902	6/6	0.49	0.24	49,52,52,53	0
5	GOL	C	3908	6/6	0.59	0.19	55,57,57,57	0
6	SO4	B	3102	5/5	0.62	0.17	100,100,101,101	0
5	GOL	E	3901	6/6	0.64	0.20	67,67,68,68	0
5	GOL	F	3903	6/6	0.75	0.16	64,65,65,66	0
6	SO4	E	3106	5/5	0.76	0.17	100,100,100,101	0
5	GOL	A	3909	6/6	0.78	0.17	44,50,51,52	0
6	SO4	B	3105	5/5	0.80	0.15	69,69,70,70	0
6	SO4	B	3100	5/5	0.80	0.16	92,93,93,93	0
6	SO4	E	3103	5/5	0.84	0.16	73,74,74,74	0
5	GOL	B	3906	6/6	0.84	0.13	41,44,46,47	0
6	SO4	E	3104	5/5	0.87	0.10	68,68,69,69	0
5	GOL	E	3904	6/6	0.87	0.18	27,33,39,46	0
6	SO4	B	3101	5/5	0.88	0.10	59,59,60,61	0
5	GOL	C	3907	6/6	0.89	0.12	26,31,33,35	0
5	GOL	E	3905	6/6	0.92	0.08	24,26,27,27	0
6	SO4	E	3107	5/5	0.94	0.14	37,38,38,40	0
7	FZ2	B	3907	48/48	0.95	0.10	13,21,26,28	0
7	FZ2	E	3906	48/48	0.96	0.09	19,24,28,29	0
8	FAD	F	4932	53/53	0.96	0.06	9,20,22,24	1
8	FAD	C	4931	53/53	0.97	0.06	10,19,22,24	0
4	FES	A	4908	4/4	0.99	0.02	16,17,17,18	0
4	FES	A	4907	4/4	0.99	0.03	14,15,16,18	0
4	FES	D	4910	4/4	1.00	0.02	14,15,16,17	0
4	FES	D	4909	4/4	1.00	0.02	16,16,17,17	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.

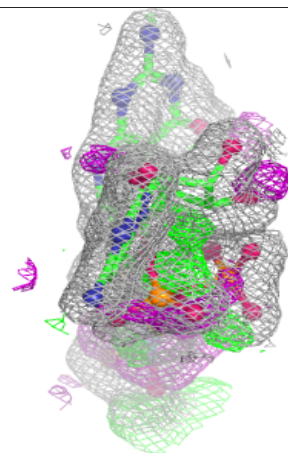
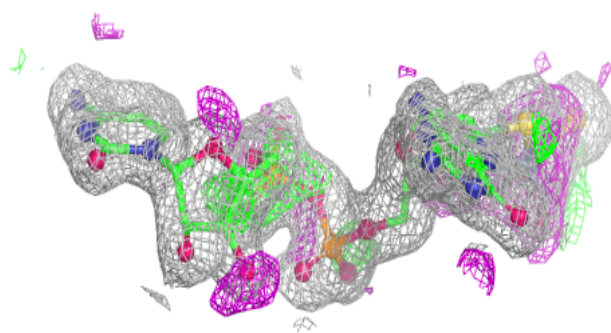
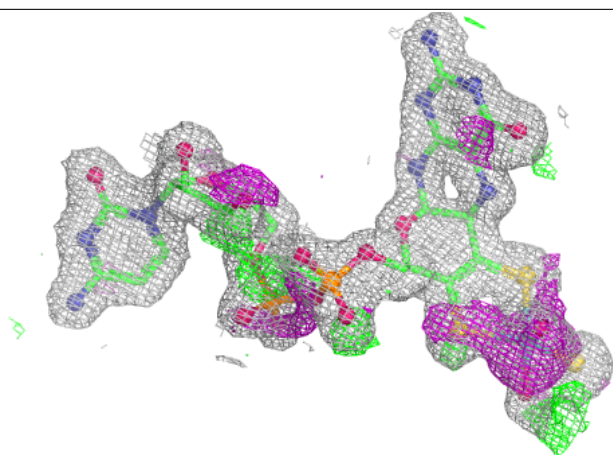
Electron density around FZ2 B 3907:

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

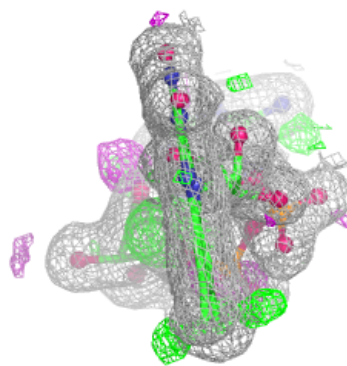
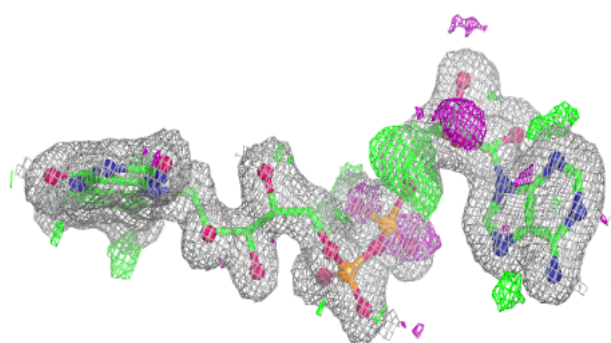
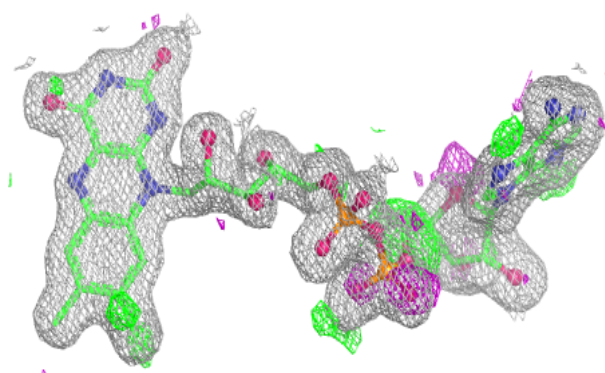


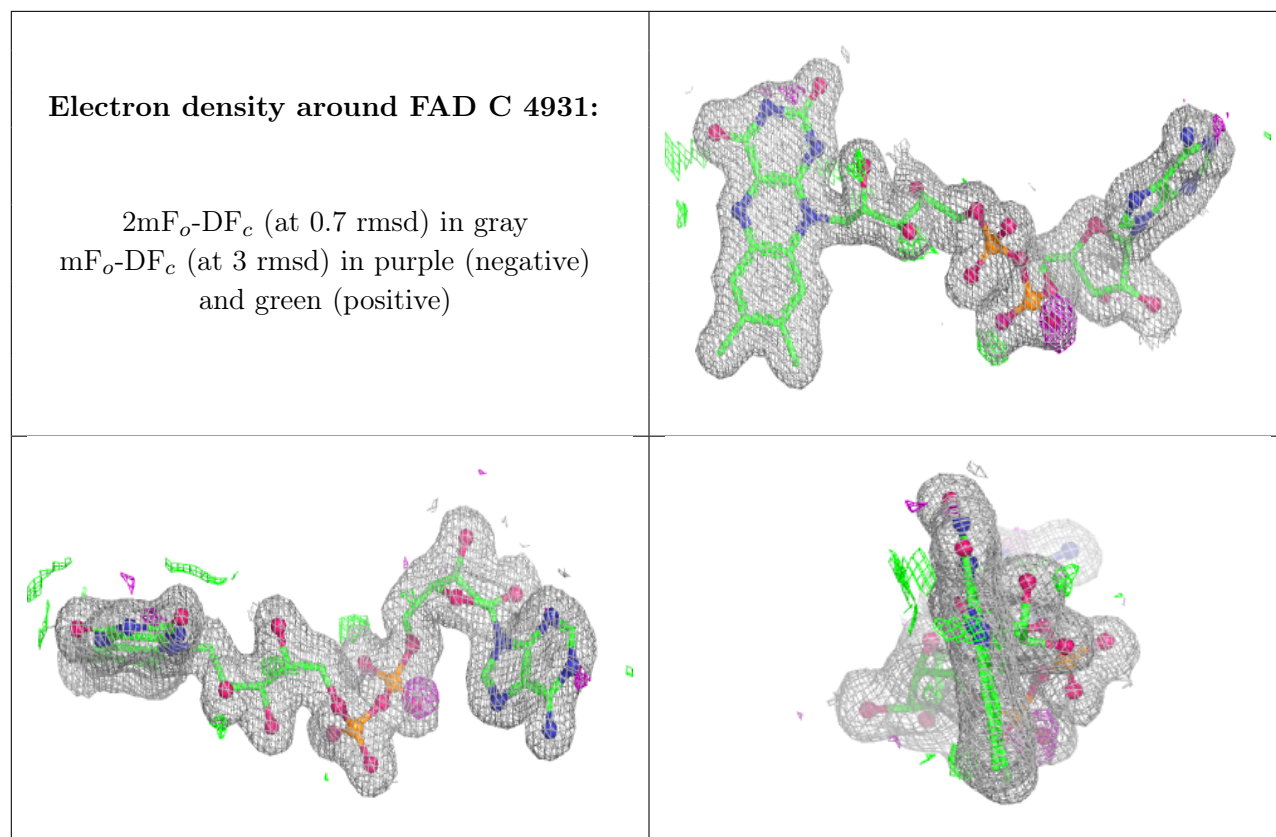
Electron density around FZ2 E 3906:

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

**Electron density around FAD F 4932:**

$2mF_o-DF_c$ (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.