



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 01:10 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 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 : 9.0.015 (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

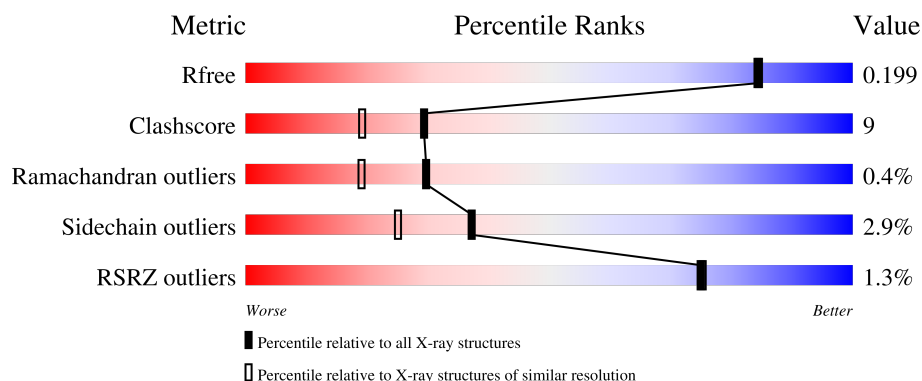
1 Overall quality at a glance

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	0% 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			

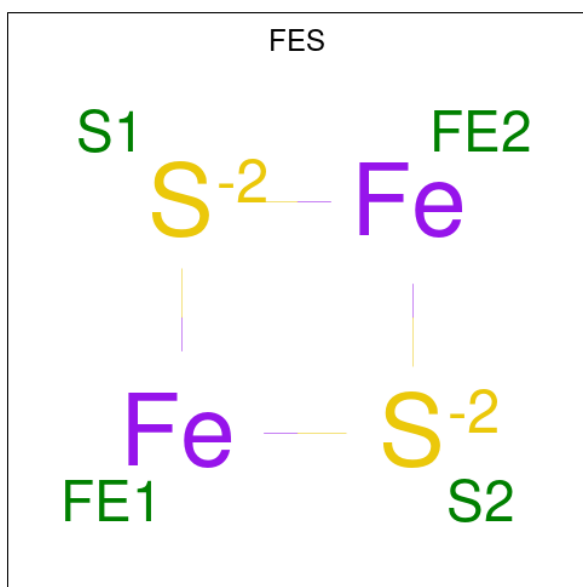
There are 4 discrepancies between the modelled and reference sequences:

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.

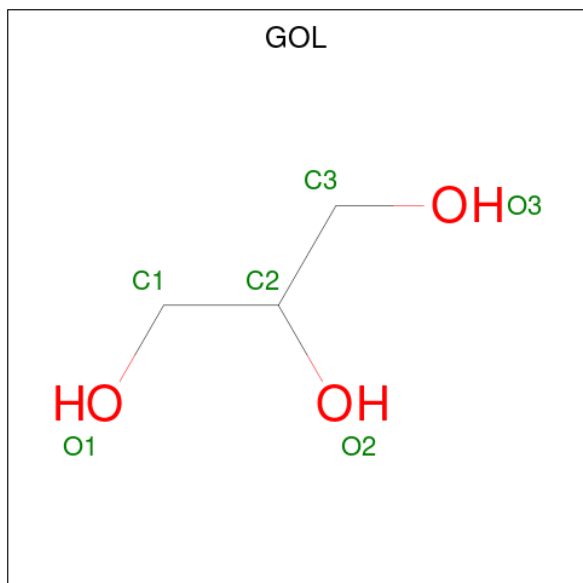
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	285	Total	C	N	O	S	64	0	0
			2139	1353	381	393	12			
3	F	285	Total	C	N	O	S	51	0	0
			2139	1353	381	393	12			

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



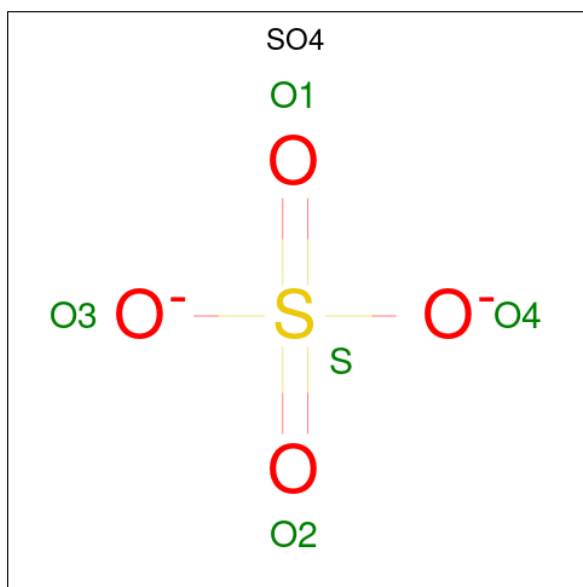
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	D	1	Total	Fe	S	0	0
			4	2	2		
4	D	1	Total	Fe	S	0	0
			4	2	2		

- 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).



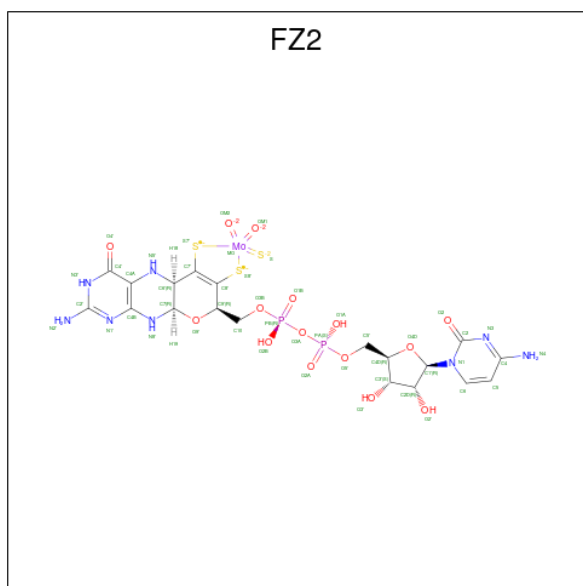
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0

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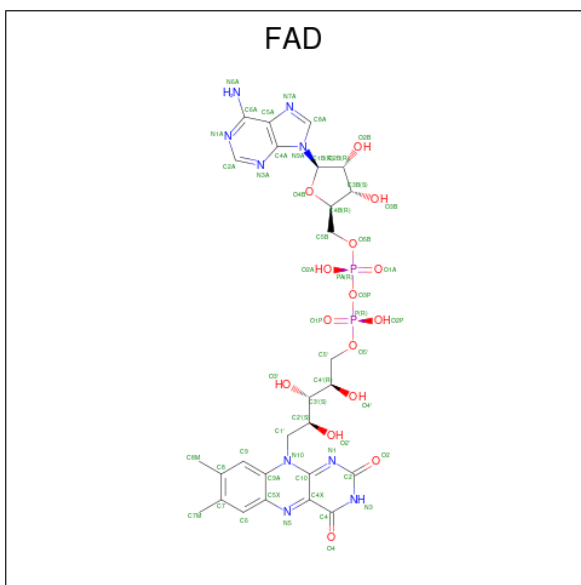
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		

- 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 53	C 27	N 9	O 15	P 2	0	0
8	F	1	Total 53	C 27	N 9	O 15	P 2	1	0

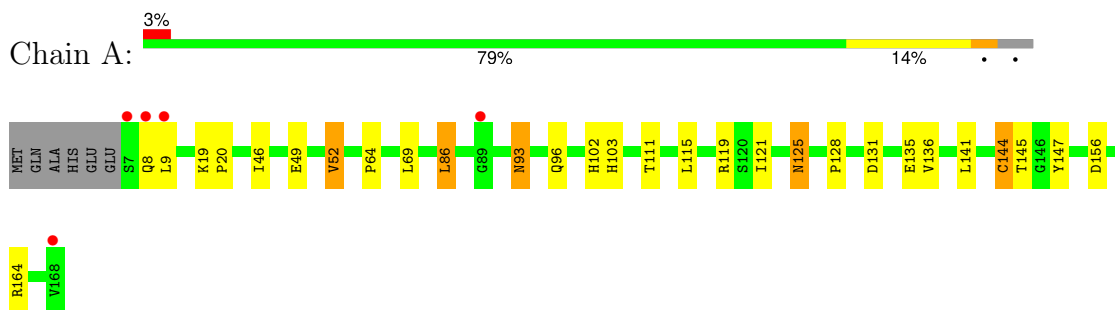
- Molecule 9 is water.

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

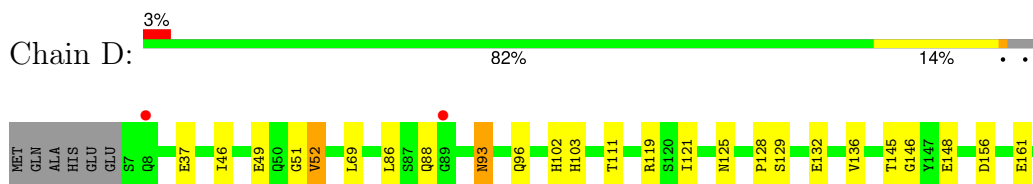
3 Residue-property plots [i](#)

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.

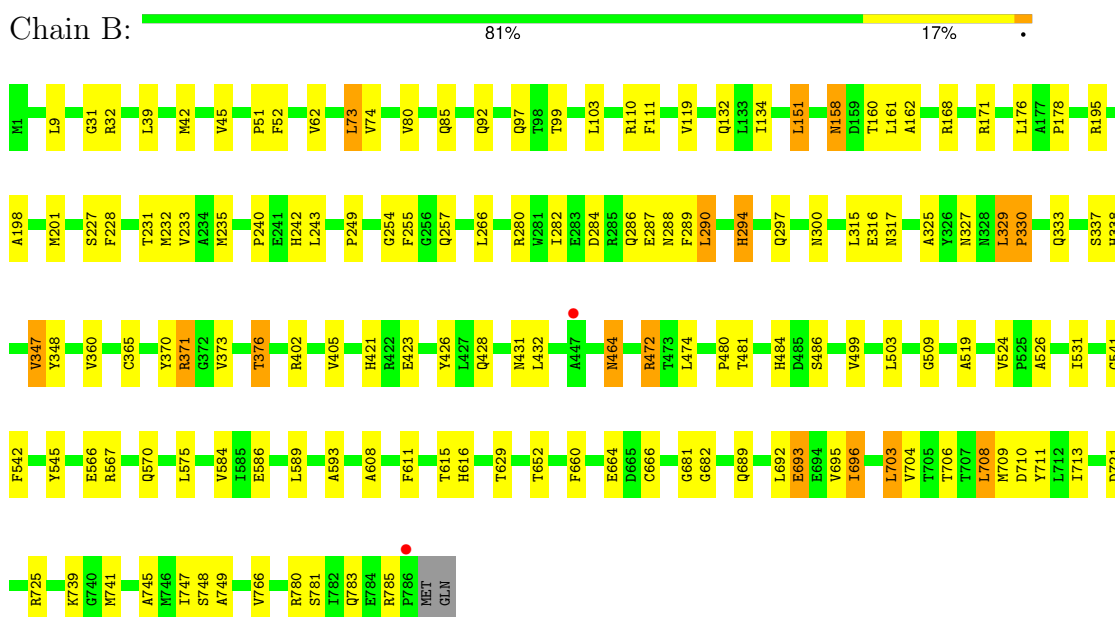
- Molecule 1: quinoline 2-oxidoreductase small subunit



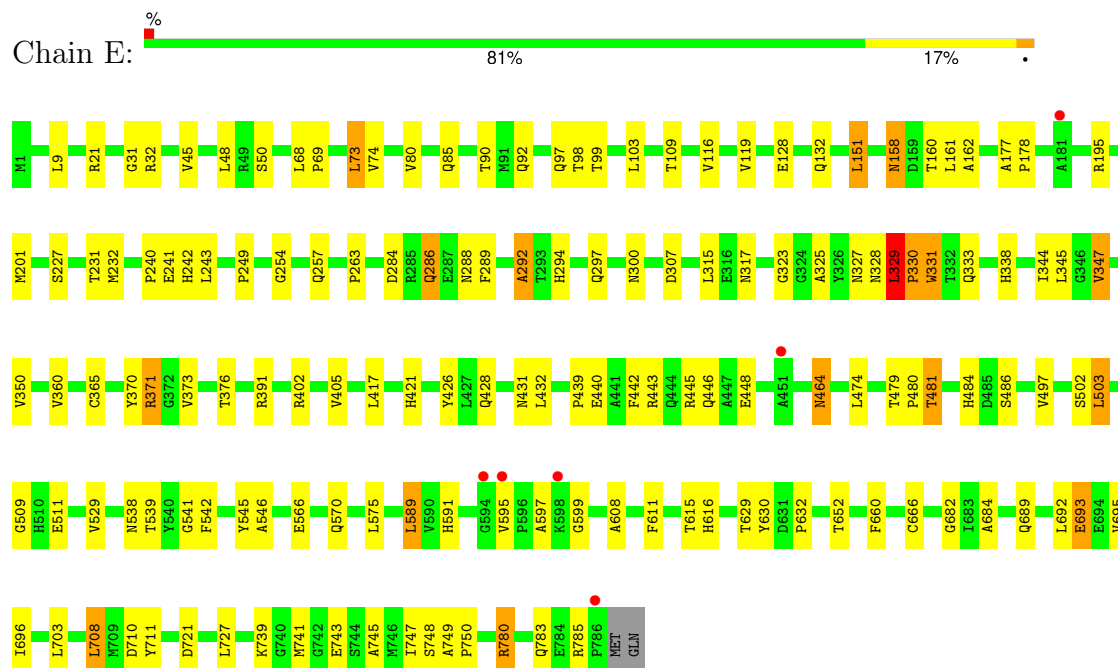
- Molecule 1: quinoline 2-oxidoreductase small subunit



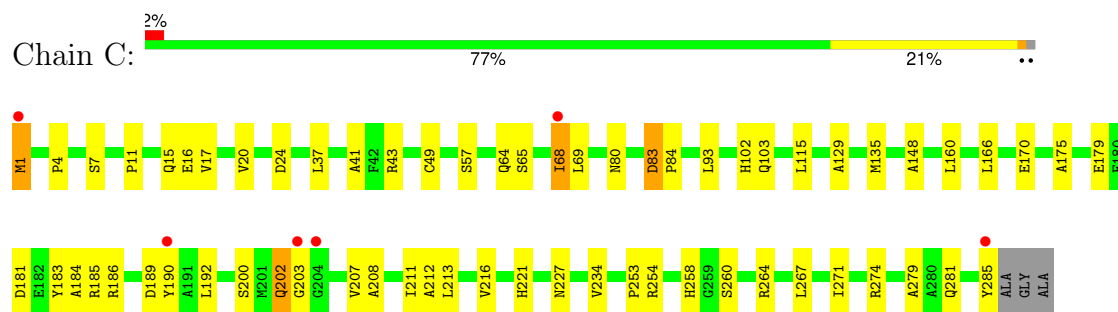
- Molecule 2: quinoline 2-oxidoreductase large subunit



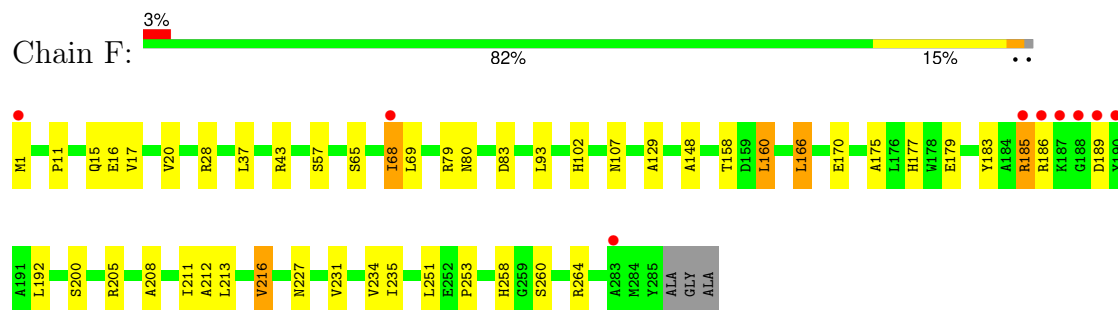
- Molecule 2: quinoline 2-oxidoreductase large subunit



- Molecule 3: quinoline 2-oxidoreductase medium subunit



- Molecule 3: quinoline 2-oxidoreductase medium subunit



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.

All (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
2	E	693	GLU	N-CA-C	7.23	121.25	109.76
2	B	464	ASN	N-CA-C	-7.16	98.43	109.24
2	B	693	GLU	N-CA-C	6.92	121.13	110.20
2	E	31	GLY	N-CA-C	-6.86	102.77	112.37
3	F	175	ALA	N-CA-C	-6.81	105.10	113.41
2	E	464	ASN	N-CA-C	-6.75	99.05	109.24
2	B	696	ILE	N-CA-C	6.50	117.21	108.11
2	B	376	THR	N-CA-C	6.45	117.97	111.07
1	A	111	THR	N-CA-C	6.37	117.89	111.07
2	B	721	ASP	N-CA-C	-6.32	101.59	110.50
2	B	290	LEU	N-CA-C	6.30	117.95	111.14
2	E	323	GLY	N-CA-C	6.29	123.56	115.32
2	E	696	ILE	N-CA-C	6.24	116.85	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	611	PHE	N-CA-C	6.20	121.69	112.94
1	D	111	THR	N-CA-C	6.16	118.79	111.33
2	E	241	GLU	N-CA-C	6.12	117.95	111.28
3	C	192	LEU	N-CA-C	-6.02	104.65	112.23
1	A	8	GLN	N-CA-C	-5.99	105.62	113.17
1	A	144	CYS	N-CA-C	5.99	120.65	112.68
2	B	509	GLY	N-CA-C	5.91	124.18	115.08
2	E	748	SER	N-CA-C	5.90	120.49	113.12
2	E	509	GLY	N-CA-C	5.89	124.15	115.08
2	B	692	LEU	N-CA-C	5.85	120.96	113.18
3	F	83	ASP	CA-C-N	5.84	125.04	118.97
3	F	83	ASP	C-N-CA	5.84	125.04	118.97
2	E	611	PHE	N-CA-C	5.83	121.16	112.94
2	E	692	LEU	N-CA-C	5.80	120.90	113.18
2	E	331	TRP	N-CA-C	5.78	118.52	111.82
1	A	125	ASN	CA-C-N	5.75	125.60	119.28
1	A	125	ASN	C-N-CA	5.75	125.60	119.28
2	B	325	ALA	N-CA-C	5.72	118.46	111.82
2	E	721	ASP	N-CA-C	-5.69	102.47	110.50
3	C	83	ASP	CA-C-N	5.67	124.87	118.97
3	C	83	ASP	C-N-CA	5.67	124.87	118.97
2	B	748	SER	N-CA-C	5.65	120.19	113.12
2	B	348	TYR	N-CA-C	5.61	119.11	110.42
3	C	4	PRO	N-CA-C	-5.59	102.81	111.13
3	C	175	ALA	N-CA-C	-5.59	105.58	112.90
3	C	24	ASP	CA-C-N	5.53	125.20	119.56
3	C	24	ASP	C-N-CA	5.53	125.20	119.56
2	B	294	HIS	N-CA-C	-5.52	101.37	109.81
3	F	57	SER	N-CA-C	5.43	117.89	111.33
2	E	695	VAL	N-CA-C	-5.42	99.94	108.23
2	E	747	ILE	N-CA-C	-5.42	106.41	111.45
3	F	235	ILE	N-CA-C	5.41	115.42	107.15
3	C	234	VAL	N-CA-C	-5.40	100.55	108.54
1	A	86	LEU	N-CA-C	5.31	116.76	110.97
2	B	747	ILE	N-CA-C	-5.31	106.51	111.45
3	F	234	VAL	N-CA-C	-5.29	101.91	108.89
2	B	695	VAL	N-CA-C	-5.29	100.14	108.23
1	D	37	GLU	N-CA-C	5.28	119.82	112.90
3	C	57	SER	N-CA-C	5.25	117.69	111.33
2	E	325	ALA	N-CA-C	5.22	117.88	111.82
1	A	147	TYR	N-CA-C	5.20	121.87	110.80
3	F	216	VAL	N-CA-C	-5.17	106.10	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
2	B	337	SER	N-CA-C	5.10	117.23	111.11
3	F	192	LEU	N-CA-C	-5.06	105.85	112.23
1	D	148	GLU	N-CA-C	5.06	117.18	111.11
2	E	297	GLN	N-CA-C	5.05	117.51	108.17
2	E	329	LEU	N-CA-C	-5.04	102.54	110.14
3	F	166	LEU	N-CA-C	-5.00	102.23	109.59

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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
2:B:97:GLN:HE22	2:B:162:ALA:H	1.17	0.89
2:B:347:VAL:HG13	2:B:405:VAL:HG23	1.54	0.89
3:C:211:ILE:H	3:C:227:ASN:HD21	1.18	0.89
3:F:231:VAL:HA	9:F:5039:HOH:O	1.73	0.89
3:F:211:ILE:H	3:F:227:ASN:HD21	1.22	0.84
2:E:240:PRO:HG2	2:E:243:LEU:HD12	1.60	0.82
2:E:405:VAL:HG21	2:E:426:TYR:HB3	1.64	0.80
2:B:240:PRO:HG2	2:B:243:LEU:HD12	1.66	0.78
3:C:264:ARG:HD2	9:C:4949:HOH:O	1.83	0.77
2:B:402:ARG:HE	2:B:431:ASN:ND2	1.84	0.76
2:E:402:ARG:HE	2:E:431:ASN:ND2	1.84	0.75
2:B:92:GLN:HB3	2:B:480:PRO:HG2	1.69	0.74
2:E:329:LEU:HD22	2:E:330:PRO:HA	1.70	0.73
2:B:171:ARG:HD2	9:B:5640:HOH:O	1.88	0.73
2:E:443:ARG:HH21	2:E:446:GLN:HE22	1.35	0.73
2:E:327:ASN:HD22	2:E:333:GLN:H	1.35	0.72
2:E:195:ARG:HH11	2:E:294:HIS:HD2	1.35	0.72
3:C:115:LEU:HD13	3:C:135:MET:HE3	1.71	0.71
1:A:64:PRO:HG3	3:C:103:GLN:NE2	2.06	0.70
2:E:502:SER:HB2	9:E:5679:HOH:O	1.91	0.70
2:B:329:LEU:HD22	2:B:330:PRO:HA	1.73	0.70
2:E:575:LEU:HD21	2:E:615:THR:HB	1.73	0.70
2:B:240:PRO:CG	2:B:243:LEU:HD12	2.22	0.69
3:F:264:ARG:HD2	9:F:5019:HOH:O	1.93	0.69
1:A:135:GLU:HG2	9:A:5034:HOH:O	1.93	0.69
1:D:93:ASN:ND2	1:D:96:GLN:H	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:257:GLN:HE22	2:E:288:ASN:HD21	1.41	0.68
2:B:151:LEU:HD13	2:B:360:VAL:HG11	1.75	0.68
1:A:93:ASN:C	1:A:93:ASN:HD22	2.00	0.68
2:B:327:ASN:HD22	2:B:333:GLN:H	1.41	0.67
3:F:260:SER:O	3:F:264:ARG:HG2	1.95	0.67
2:E:158:ASN:C	2:E:158:ASN:HD22	2.03	0.66
2:B:132:GLN:NE2	3:C:43:ARG:HH11	1.94	0.66
3:C:260:SER:O	3:C:264:ARG:HG2	1.97	0.65
2:E:151:LEU:HD13	2:E:360:VAL:HG11	1.78	0.65
2:B:286:GLN:OE1	3:C:1:MET:SD	2.54	0.65
1:D:93:ASN:C	1:D:93:ASN:HD22	2.04	0.65
2:B:421:HIS:HD2	2:B:426:TYR:OH	1.80	0.65
2:B:158:ASN:C	2:B:158:ASN:HD22	2.05	0.65
3:C:216:VAL:HG13	3:C:253:PRO:HG3	1.78	0.64
2:E:347:VAL:HG22	2:E:426:TYR:CD2	2.32	0.64
2:B:158:ASN:HD22	2:B:160:THR:H	1.45	0.64
2:B:428:GLN:HG3	9:B:5494:HOH:O	1.98	0.64
3:F:216:VAL:HG13	3:F:253:PRO:HG3	1.79	0.64
2:B:347:VAL:HG22	2:B:426:TYR:CD2	2.33	0.63
7:E:3906:FZ2:MO	7:E:3906:FZ2:OM1	1.70	0.63
3:F:11:PRO:HG2	3:F:17:VAL:HG22	1.81	0.63
2:E:132:GLN:NE2	3:F:43:ARG:HH11	1.96	0.63
2:E:329:LEU:CD2	2:E:330:PRO:HA	2.29	0.63
3:F:205:ARG:HD3	9:F:5234:HOH:O	1.99	0.63
3:F:200:SER:HB2	3:F:208:ALA:HB3	1.82	0.62
2:E:300:ASN:HB3	2:E:317:ASN:HD21	1.63	0.62
7:B:3907:FZ2:OM1	7:B:3907:FZ2:MO	1.69	0.62
3:F:68:ILE:HD13	3:F:170:GLU:HB3	1.80	0.62
2:B:232:MET:HE1	2:B:235:MET:CE	2.30	0.62
2:E:158:ASN:HD22	2:E:160:THR:H	1.46	0.61
1:D:129:SER:OG	1:D:132:GLU:HG3	2.01	0.61
2:E:73:LEU:C	2:E:73:LEU:HD23	2.26	0.61
3:C:216:VAL:CG1	3:C:253:PRO:HG3	2.31	0.61
2:E:479:THR:O	2:E:481:THR:HG22	2.00	0.61
2:E:195:ARG:HH11	2:E:294:HIS:CD2	2.17	0.61
9:B:5717:HOH:O	3:C:1:MET:HB3	2.00	0.61
2:E:421:HIS:HD2	2:E:426:TYR:OH	1.84	0.60
3:C:68:ILE:CD1	3:C:170:GLU:HB3	2.32	0.60
2:E:474:LEU:HD13	2:E:481:THR:HG23	1.84	0.60
2:B:567:ARG:HH11	5:B:3906:GOL:C3	2.15	0.60
1:A:86:LEU:HD21	1:A:119:ARG:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ASN:ND2	1:A:96:GLN:H	2.00	0.59
2:B:575:LEU:HD21	2:B:615:THR:HB	1.85	0.59
3:C:211:ILE:H	3:C:227:ASN:ND2	1.93	0.58
2:B:195:ARG:HH11	2:B:294:HIS:HD2	1.51	0.58
2:B:290:LEU:HD23	2:B:703:LEU:HD12	1.84	0.58
2:B:257:GLN:HE22	2:B:288:ASN:HD21	1.52	0.58
3:F:216:VAL:CG1	3:F:253:PRO:HG3	2.34	0.58
2:E:158:ASN:ND2	2:E:160:THR:H	2.01	0.58
2:B:315:LEU:C	2:B:315:LEU:HD23	2.28	0.57
2:B:472:ARG:NE	2:B:472:ARG:HA	2.19	0.57
2:B:586:GLU:HG2	9:B:5153:HOH:O	2.04	0.57
2:E:785:ARG:HG2	2:E:785:ARG:HH21	1.69	0.57
2:E:90:THR:HB	9:E:5250:HOH:O	2.03	0.57
2:B:725:ARG:HD2	9:B:5668:HOH:O	2.03	0.57
2:E:240:PRO:CG	2:E:243:LEU:HD12	2.34	0.57
2:B:73:LEU:C	2:B:73:LEU:HD23	2.29	0.56
2:B:709:MET:HE1	3:C:190:TYR:HE2	1.70	0.56
1:D:93:ASN:HD21	1:D:96:GLN:H	1.53	0.56
3:F:68:ILE:CD1	3:F:170:GLU:HB3	2.35	0.56
1:A:102:HIS:HD2	9:A:4952:HOH:O	1.88	0.56
2:E:132:GLN:HE21	3:F:43:ARG:HH11	1.53	0.56
2:B:652:THR:HB	3:C:183:TYR:CE1	2.40	0.56
2:B:158:ASN:ND2	2:B:160:THR:H	2.02	0.56
2:B:338:HIS:HD2	9:B:4952:HOH:O	1.89	0.56
3:C:11:PRO:HG2	3:C:17:VAL:HG22	1.87	0.56
2:E:440:GLU:HB2	9:E:5261:HOH:O	2.05	0.55
2:E:347:VAL:HG23	2:E:464:ASN:HB3	1.88	0.55
2:B:300:ASN:HB3	2:B:317:ASN:HD21	1.72	0.55
1:A:93:ASN:C	1:A:93:ASN:ND2	2.64	0.55
3:C:202:GLN:HB2	3:C:207:VAL:HG11	1.88	0.55
2:E:338:HIS:HD2	9:E:5021:HOH:O	1.89	0.55
2:B:294:HIS:CD2	2:B:365:CYS:SG	3.00	0.54
2:B:405:VAL:HG21	2:B:426:TYR:HB3	1.89	0.54
2:B:474:LEU:HD13	2:B:481:THR:HB	1.89	0.54
1:A:69:LEU:C	3:C:37:LEU:HD12	2.32	0.54
2:B:329:LEU:CD2	2:B:330:PRO:HA	2.37	0.54
2:B:73:LEU:HD23	2:B:74:VAL:N	2.23	0.54
1:D:102:HIS:HE1	1:D:156:ASP:OD1	1.91	0.54
3:F:211:ILE:H	3:F:227:ASN:ND2	1.98	0.54
3:F:16:GLU:O	3:F:20:VAL:HG23	2.08	0.54
2:B:32:ARG:O	2:B:249:PRO:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:ASN:ND2	1:D:93:ASN:C	2.64	0.54
2:B:227:SER:HB2	2:B:541:GLY:O	2.08	0.53
2:E:666:CYS:C	2:E:739:LYS:HB2	2.32	0.53
2:B:566:GLU:O	2:B:570:GLN:HG3	2.08	0.53
1:D:69:LEU:C	3:F:37:LEU:HD12	2.33	0.53
3:C:203:GLY:HA3	9:C:5043:HOH:O	2.08	0.52
1:A:102:HIS:HE1	1:A:156:ASP:OD1	1.93	0.52
2:B:195:ARG:HH11	2:B:294:HIS:CD2	2.27	0.52
2:B:97:GLN:NE2	2:B:162:ALA:H	1.97	0.52
2:E:284:ASP:CG	3:F:1:MET:HE3	2.35	0.52
1:A:46:ILE:CG2	1:A:49:GLU:HG3	2.40	0.52
3:F:65:SER:O	3:F:68:ILE:HG23	2.10	0.52
1:A:131:ASP:O	1:A:135:GLU:HG3	2.10	0.52
2:B:347:VAL:CG1	2:B:405:VAL:HG23	2.35	0.52
2:E:391:ARG:HD3	9:E:5247:HOH:O	2.08	0.51
3:F:212:ALA:C	3:F:213:LEU:HD12	2.35	0.51
2:E:201:MET:HE2	2:E:201:MET:HA	1.92	0.51
1:A:52:VAL:HG11	2:B:708:LEU:HB3	1.93	0.51
2:E:442:PHE:HA	2:E:445:ARG:HE	1.76	0.51
2:E:630:TYR:CE1	2:E:632:PRO:HD3	2.46	0.51
3:C:68:ILE:HD11	3:C:170:GLU:OE2	2.11	0.51
2:E:405:VAL:CG2	2:E:426:TYR:HB3	2.37	0.51
2:B:103:LEU:HD21	2:B:266:LEU:HD12	1.94	0.50
3:C:65:SER:O	3:C:68:ILE:HG23	2.10	0.50
9:D:5088:HOH:O	3:F:102:HIS:HB2	2.11	0.50
2:E:405:VAL:HG21	2:E:426:TYR:CB	2.39	0.50
2:E:666:CYS:O	2:E:739:LYS:HB2	2.12	0.50
2:E:376:THR:HG21	2:E:689:GLN:HE22	1.77	0.50
3:F:158:THR:OG1	3:F:160:LEU:HB2	2.12	0.50
3:F:129:ALA:HA	3:F:148:ALA:HB3	1.93	0.50
2:B:85:GLN:HG2	9:B:5339:HOH:O	2.12	0.50
3:C:129:ALA:HA	3:C:148:ALA:HB3	1.92	0.50
3:F:79:ARG:HD3	9:F:4954:HOH:O	2.12	0.50
3:C:68:ILE:HD11	3:C:170:GLU:HB3	1.94	0.50
3:F:107:ASN:HD21	5:F:3903:GOL:H12	1.75	0.50
2:E:608:ALA:O	2:E:616:HIS:HE1	1.95	0.50
2:E:21:ARG:HG3	2:E:511:GLU:HG2	1.95	0.49
2:B:347:VAL:HG22	2:B:426:TYR:CG	2.48	0.49
2:B:347:VAL:HG13	2:B:347:VAL:O	2.11	0.49
2:B:176:LEU:HD12	2:B:316:GLU:HB2	1.94	0.49
2:E:92:GLN:HB2	2:E:480:PRO:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:MET:HE2	2:B:201:MET:HA	1.94	0.48
2:B:484:HIS:O	2:B:541:GLY:HA2	2.12	0.48
2:E:484:HIS:O	2:E:541:GLY:HA2	2.13	0.48
2:E:566:GLU:O	2:E:570:GLN:HG3	2.14	0.48
2:E:780:ARG:HH11	2:E:783:GLN:HE22	1.60	0.48
2:B:39:LEU:O	2:B:42:MET:HB2	2.13	0.48
2:B:423:GLU:O	2:B:423:GLU:HG2	2.11	0.48
2:E:9:LEU:C	2:E:9:LEU:HD12	2.38	0.48
1:A:121:ILE:HG12	1:A:136:VAL:HG11	1.95	0.48
2:E:68:LEU:HD12	2:E:69:PRO:HD2	1.95	0.48
1:D:52:VAL:HG11	2:E:708:LEU:HB3	1.96	0.48
2:E:32:ARG:O	2:E:249:PRO:HB2	2.14	0.48
5:F:3903:GOL:H11	9:F:5120:HOH:O	2.13	0.48
2:E:48:LEU:O	2:E:116:VAL:HG22	2.13	0.48
2:B:703:LEU:HD13	2:B:706:THR:HG22	1.95	0.48
3:C:200:SER:HB3	3:C:208:ALA:HB3	1.96	0.48
2:E:97:GLN:NE2	2:E:162:ALA:H	1.99	0.47
2:E:99:THR:HG22	2:E:161:LEU:HD21	1.96	0.47
2:B:709:MET:HE1	3:C:190:TYR:CE2	2.50	0.47
3:C:181:ASP:OD1	3:C:274:ARG:HD2	2.14	0.47
3:F:11:PRO:HG2	3:F:17:VAL:CG2	2.44	0.47
2:E:693:GLU:HB3	2:E:711:TYR:CZ	2.49	0.47
2:B:329:LEU:HD22	2:B:330:PRO:CA	2.43	0.47
3:C:68:ILE:HD11	3:C:170:GLU:CD	2.39	0.47
2:E:45:VAL:HA	2:E:119:VAL:O	2.15	0.47
3:C:11:PRO:HG2	3:C:17:VAL:CG2	2.44	0.47
2:E:73:LEU:HD23	2:E:74:VAL:N	2.29	0.47
2:E:80:VAL:HG11	2:E:103:LEU:HB2	1.97	0.47
2:B:405:VAL:CG2	2:B:426:TYR:HB3	2.44	0.47
2:E:503:LEU:HD13	9:E:5002:HOH:O	2.14	0.47
2:B:370:TYR:O	2:B:371:ARG:C	2.58	0.46
2:B:97:GLN:HE22	2:B:162:ALA:N	1.99	0.46
2:B:616:HIS:HD2	9:B:5073:HOH:O	1.99	0.46
2:E:785:ARG:HG2	2:E:785:ARG:NH2	2.29	0.46
1:D:86:LEU:HD21	1:D:119:ARG:CD	2.35	0.46
2:B:9:LEU:HD12	2:B:9:LEU:C	2.40	0.46
2:B:347:VAL:HG23	2:B:464:ASN:HB3	1.96	0.46
2:E:486:SER:HA	2:E:629:THR:HA	1.98	0.46
1:D:102:HIS:HD2	9:D:4945:HOH:O	1.98	0.46
2:E:329:LEU:HD22	2:E:330:PRO:CA	2.43	0.46
1:A:115:LEU:O	1:A:119:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:3909:GOL:H11	9:A:4923:HOH:O	2.16	0.46
2:B:542:PHE:HB3	2:B:545:TYR:HE2	1.79	0.46
2:B:696:ILE:O	2:B:704:VAL:HG22	2.15	0.46
3:C:83:ASP:HA	3:C:84:PRO:HD3	1.85	0.46
1:D:125:ASN:O	1:D:128:PRO:HD3	2.16	0.46
1:D:161:GLU:OE2	1:D:161:GLU:HA	2.15	0.46
2:E:292:ALA:O	2:E:365:CYS:SG	2.73	0.46
2:B:608:ALA:O	2:B:616:HIS:HE1	1.98	0.46
2:E:370:TYR:O	2:E:371:ARG:C	2.59	0.46
2:B:231:THR:HG22	2:B:235:MET:HE2	1.98	0.45
3:C:1:MET:HA	3:C:41:ALA:O	2.16	0.45
2:E:542:PHE:HB3	2:E:545:TYR:HE2	1.81	0.45
2:E:710:ASP:OD1	3:F:258:HIS:HE1	1.99	0.45
3:C:16:GLU:O	3:C:20:VAL:HG23	2.17	0.45
3:C:267:LEU:O	3:C:271:ILE:HG12	2.16	0.45
2:E:546:ALA:HA	2:E:743:GLU:OE1	2.16	0.45
2:E:589:LEU:HD13	2:E:591:HIS:CD2	2.51	0.45
1:D:46:ILE:CG2	1:D:49:GLU:HG3	2.46	0.45
1:D:121:ILE:HG12	1:D:136:VAL:HG11	1.97	0.45
2:E:286:GLN:CD	3:F:1:MET:HE1	2.41	0.45
2:E:347:VAL:HG22	2:E:426:TYR:CG	2.51	0.45
3:F:1:MET:HE3	3:F:1:MET:HB2	1.82	0.45
2:B:228:PHE:HZ	2:B:329:LEU:HD13	1.81	0.45
2:E:345:LEU:HD22	2:E:350:VAL:HB	1.99	0.45
2:E:616:HIS:HD2	9:E:5017:HOH:O	1.99	0.45
2:E:652:THR:HB	3:F:183:TYR:CE1	2.52	0.45
2:B:519:ALA:HB2	2:B:526:ALA:HA	1.99	0.45
2:E:90:THR:HG22	2:E:98:THR:OG1	2.17	0.45
2:E:227:SER:HB2	2:E:541:GLY:O	2.16	0.45
2:E:242:HIS:H	2:E:242:HIS:CD2	2.35	0.45
2:B:178:PRO:HG2	9:B:5443:HOH:O	2.16	0.44
2:B:240:PRO:HG3	2:B:243:LEU:HD12	1.99	0.44
2:B:327:ASN:ND2	2:B:333:GLN:HG3	2.32	0.44
2:B:682:GLY:HA3	2:B:745:ALA:HB3	1.98	0.44
3:C:102:HIS:HB2	9:C:5025:HOH:O	2.17	0.44
3:F:177:HIS:HE1	3:F:179:GLU:OE1	2.00	0.44
2:E:347:VAL:HG13	2:E:347:VAL:O	2.17	0.44
3:F:185:ARG:O	3:F:186:ARG:HD3	2.18	0.44
1:A:164:ARG:NH2	9:A:5070:HOH:O	2.50	0.44
3:C:185:ARG:C	3:C:186:ARG:HD3	2.43	0.44
2:E:439:PRO:O	2:E:443:ARG:HG2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:589:LEU:HD21	2:E:599:GLY:HA3	1.99	0.44
3:F:227:ASN:O	3:F:231:VAL:HG23	2.18	0.44
2:B:486:SER:HA	2:B:629:THR:HA	1.98	0.44
3:C:179:GLU:HG3	3:C:279:ALA:HA	1.98	0.44
2:E:50:SER:HB2	2:E:109:THR:HG21	1.99	0.44
2:E:347:VAL:HG22	2:E:426:TYR:CE2	2.52	0.44
2:B:584:VAL:HG13	2:B:593:ALA:HB2	2.00	0.44
2:B:652:THR:HB	3:C:183:TYR:HE1	1.81	0.44
3:C:7:SER:OG	3:C:49:CYS:HB2	2.18	0.44
2:B:168:ARG:NH2	6:B:3101:SO4:O3	2.50	0.44
1:D:103:HIS:HA	9:E:5008:HOH:O	2.18	0.44
2:E:21:ARG:HD2	2:E:511:GLU:O	2.18	0.44
2:B:62:VAL:HG12	2:B:134:ILE:HG23	1.99	0.43
2:B:402:ARG:HH21	2:B:431:ASN:HD22	1.65	0.43
3:C:68:ILE:HD12	3:C:170:GLU:HB3	1.99	0.43
2:B:228:PHE:CZ	2:B:329:LEU:HD13	2.53	0.43
2:E:177:ALA:N	2:E:178:PRO:HD2	2.33	0.43
2:B:198:ALA:HA	2:B:370:TYR:CE1	2.53	0.43
2:B:376:THR:HG21	2:B:689:GLN:HE22	1.83	0.43
2:B:666:CYS:C	2:B:739:LYS:HB2	2.43	0.43
1:A:141:LEU:HD13	2:B:713:ILE:HD11	2.01	0.43
1:D:46:ILE:HG23	1:D:49:GLU:HG3	2.00	0.43
2:E:231:THR:HG22	2:E:232:MET:HE2	2.00	0.43
2:B:327:ASN:ND2	2:B:333:GLN:H	2.13	0.43
2:B:347:VAL:HG22	2:B:426:TYR:CE2	2.53	0.43
2:B:110:ARG:O	2:B:111:PHE:HB3	2.19	0.43
2:B:284:ASP:OD2	2:B:287:GLU:HG3	2.19	0.43
2:E:289:PHE:O	2:E:294:HIS:HE1	2.01	0.43
2:E:428:GLN:HG2	2:E:727:LEU:HD11	2.00	0.43
2:E:749:ALA:N	2:E:750:PRO:CD	2.82	0.42
3:F:68:ILE:O	3:F:68:ILE:HG13	2.13	0.42
2:B:233:VAL:HG22	2:B:266:LEU:HD23	2.00	0.42
2:B:242:HIS:CD2	2:B:242:HIS:H	2.37	0.42
2:B:255:PHE:HA	7:B:3907:FZ2:S7'	2.60	0.42
1:A:144:CYS:O	2:B:681:GLY:HA3	2.18	0.42
1:A:103:HIS:HA	9:B:4925:HOH:O	2.19	0.42
2:B:45:VAL:HA	2:B:119:VAL:O	2.19	0.42
2:E:128:GLU:OE1	3:F:1:MET:N	2.53	0.42
2:E:327:ASN:ND2	2:E:333:GLN:HG3	2.34	0.42
1:A:125:ASN:O	1:A:128:PRO:HD3	2.19	0.42
2:B:132:GLN:HE21	3:C:43:ARG:HH11	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:307:ASP:OD2	2:E:307:ASP:C	2.63	0.42
2:B:710:ASP:OD1	3:C:258:HIS:HE1	2.02	0.42
3:C:184:ALA:HB1	3:C:189:ASP:HB2	2.01	0.42
3:C:221:HIS:HD2	9:C:5167:HOH:O	2.02	0.42
2:E:327:ASN:ND2	2:E:333:GLN:H	2.12	0.42
2:B:80:VAL:HG11	2:B:103:LEU:HB2	2.01	0.41
3:C:186:ARG:O	3:C:189:ASP:HB2	2.20	0.41
1:D:146:GLY:HA2	2:E:684:ALA:HB2	2.02	0.41
2:E:85:GLN:HG2	9:E:5258:HOH:O	2.20	0.41
3:F:28:ARG:HD2	9:F:5214:HOH:O	2.20	0.41
2:B:664:GLU:HB2	9:B:5257:HOH:O	2.19	0.41
2:E:263:PRO:HD2	9:E:5149:HOH:O	2.20	0.41
2:E:344:ILE:HG22	2:E:417:LEU:HD11	2.02	0.41
2:E:497:VAL:HB	2:E:529:VAL:HG22	2.01	0.41
2:E:595:VAL:C	2:E:597:ALA:H	2.27	0.41
2:B:519:ALA:HB1	2:B:524:VAL:O	2.20	0.41
2:B:766:VAL:CG1	2:B:781:SER:HB2	2.50	0.41
3:C:80:ASN:HD22	3:C:80:ASN:HA	1.66	0.41
2:E:591:HIS:HB3	2:E:599:GLY:HA3	2.02	0.41
3:C:212:ALA:C	3:C:213:LEU:HD12	2.45	0.41
2:B:725:ARG:HA	2:B:725:ARG:HD3	1.85	0.41
5:E:3904:GOL:C2	3:F:186:ARG:HH12	2.34	0.41
2:E:328:ASN:HD21	2:E:331:TRP:HB2	1.86	0.41
2:E:682:GLY:HA3	2:E:745:ALA:HB3	2.02	0.41
3:F:216:VAL:HG11	3:F:251:LEU:HD13	2.02	0.41
2:B:99:THR:HG22	2:B:161:LEU:HD21	2.03	0.41
2:B:195:ARG:HG3	2:B:297:GLN:OE1	2.21	0.41
2:B:289:PHE:O	2:B:294:HIS:HE1	2.03	0.41
2:B:745:ALA:O	2:B:749:ALA:HB3	2.21	0.41
3:F:186:ARG:HB2	3:F:189:ASP:OD1	2.21	0.41
2:B:499:VAL:HB	2:B:531:ILE:HD13	2.03	0.40
2:B:693:GLU:HB3	2:B:711:TYR:CZ	2.56	0.40
2:E:257:GLN:HE22	2:E:288:ASN:ND2	2.14	0.40
2:B:280:ARG:CZ	2:B:282:ILE:HG13	2.52	0.40
1:D:51:GLY:HA2	4:D:4910:FES:S1	2.61	0.40
2:E:538:ASN:O	2:E:539:THR:OG1	2.34	0.40
2:B:51:PRO:HG2	2:B:52:PHE:CD1	2.56	0.40
1:A:19:LYS:HA	1:A:20:PRO:HD3	1.95	0.40
2:E:315:LEU:HD23	2:E:315:LEU:C	2.47	0.40

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

All (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
2	E	741	MET
2	E	292	ALA
2	E	254	GLY
2	B	254	GLY

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
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

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	93	ASN
2	B	73	LEU
2	B	151	LEU
2	B	158	ASN
2	B	329	LEU
2	B	330	PRO
2	B	347	VAL
2	B	432	LEU
2	B	472	ARG
2	B	503	LEU
2	B	589	LEU
2	B	660	PHE
2	B	703	LEU
2	B	708	LEU
2	B	780	ARG
2	B	783	GLN
2	B	785	ARG
3	C	1	MET
3	C	15	GLN
3	C	64	GLN
3	C	68	ILE
3	C	69	LEU
3	C	93	LEU
3	C	160	LEU
3	C	166	LEU
3	C	202	GLN
3	C	254	ARG
3	C	281	GLN
3	C	285	TYR

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Mol	Chain	Res	Type
1	D	88	GLN
1	D	93	ASN
2	E	73	LEU
2	E	151	LEU
2	E	158	ASN
2	E	286	GLN
2	E	329	LEU
2	E	330	PRO
2	E	347	VAL
2	E	432	LEU
2	E	448	GLU
2	E	481	THR
2	E	503	LEU
2	E	589	LEU
2	E	660	PHE
2	E	703	LEU
2	E	708	LEU
2	E	780	ARG
3	F	15	GLN
3	F	68	ILE
3	F	69	LEU
3	F	80	ASN
3	F	93	LEU
3	F	160	LEU
3	F	166	LEU
3	F	185	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	102	HIS
2	B	97	GLN
2	B	106	ASN
2	B	132	GLN
2	B	158	ASN
2	B	216	GLN
2	B	242	HIS
2	B	257	GLN
2	B	294	HIS
2	B	300	ASN
2	B	317	ASN

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Mol	Chain	Res	Type
2	B	327	ASN
2	B	328	ASN
2	B	333	GLN
2	B	338	HIS
2	B	341	ASN
2	B	392	GLN
2	B	421	HIS
2	B	431	ASN
2	B	484	HIS
2	B	616	HIS
2	B	639	ASN
2	B	689	GLN
2	B	702	GLN
3	C	80	ASN
3	C	103	GLN
3	C	107	ASN
3	C	177	HIS
3	C	222	GLN
3	C	227	ASN
3	C	258	HIS
3	C	273	GLN
1	D	93	ASN
1	D	102	HIS
2	E	97	GLN
2	E	106	ASN
2	E	132	GLN
2	E	135	GLN
2	E	158	ASN
2	E	216	GLN
2	E	242	HIS
2	E	257	GLN
2	E	294	HIS
2	E	300	ASN
2	E	317	ASN
2	E	327	ASN
2	E	328	ASN
2	E	333	GLN
2	E	338	HIS
2	E	341	ASN
2	E	421	HIS
2	E	431	ASN
2	E	446	GLN

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Mol	Chain	Res	Type
2	E	484	HIS
2	E	538	ASN
2	E	616	HIS
2	E	639	ASN
2	E	689	GLN
2	E	702	GLN
2	E	783	GLN
3	F	15	GLN
3	F	80	ASN
3	F	107	ASN
3	F	177	HIS
3	F	222	GLN
3	F	227	ASN
3	F	258	HIS
3	F	273	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-

All (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
5	C	3908	GOL	C3-C2	-8.03	1.21	1.51
5	E	3904	GOL	C3-C2	-8.02	1.21	1.51
5	F	3903	GOL	C3-C2	-8.01	1.21	1.51
5	E	3901	GOL	C3-C2	-7.98	1.21	1.51
5	B	3902	GOL	C3-C2	-7.98	1.21	1.51
5	A	3909	GOL	C3-C2	-7.92	1.21	1.51
7	B	3907	FZ2	C4B-N8'	7.21	1.43	1.35
7	E	3906	FZ2	C4B-N8'	7.02	1.42	1.35
7	E	3906	FZ2	C6'-N5'	5.52	1.52	1.46
7	B	3907	FZ2	C6'-N5'	5.43	1.52	1.46
5	C	3908	GOL	O1-C1	4.59	1.61	1.42
5	E	3904	GOL	O1-C1	4.58	1.61	1.42
5	E	3901	GOL	O1-C1	4.54	1.61	1.42
8	C	4931	FAD	PA-O2A	-4.53	1.34	1.55
5	B	3902	GOL	O1-C1	4.50	1.61	1.42
5	A	3909	GOL	O1-C1	4.44	1.61	1.42
5	F	3903	GOL	O1-C1	4.42	1.61	1.42
5	B	3906	GOL	O1-C1	4.42	1.61	1.42
5	E	3905	GOL	O1-C1	4.40	1.60	1.42
5	C	3907	GOL	O1-C1	4.38	1.60	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	4932	FAD	PA-O2A	-4.25	1.35	1.55
8	C	4931	FAD	PA-O3P	4.20	1.64	1.59
7	E	3906	FZ2	C4B-N1'	4.08	1.42	1.36
7	B	3907	FZ2	C4B-N1'	3.91	1.42	1.36
8	F	4932	FAD	PA-O3P	3.83	1.63	1.59
7	E	3906	FZ2	O9'-C9'	3.80	1.50	1.43
7	B	3907	FZ2	O9'-C9'	3.77	1.50	1.43
7	E	3906	FZ2	C7-N8'	3.72	1.51	1.45
7	E	3906	FZ2	C1'-N1	3.66	1.57	1.47
7	B	3907	FZ2	C1'-N1	3.64	1.57	1.47
8	F	4932	FAD	C9A-N10	3.53	1.47	1.41
5	B	3902	GOL	O3-C3	3.46	1.56	1.42
8	C	4931	FAD	P-O2P	-3.46	1.39	1.55
5	F	3903	GOL	O3-C3	3.46	1.56	1.42
7	B	3907	FZ2	PA-O3A	3.42	1.63	1.59
5	B	3906	GOL	O3-C3	3.41	1.56	1.42
8	F	4932	FAD	C4X-N5	3.41	1.38	1.30
5	A	3909	GOL	O3-C3	3.39	1.56	1.42
5	E	3901	GOL	O3-C3	3.37	1.56	1.42
8	C	4931	FAD	C9A-N10	3.35	1.47	1.41
7	B	3907	FZ2	C7-C6'	-3.35	1.51	1.53
5	C	3908	GOL	O3-C3	3.35	1.56	1.42
7	B	3907	FZ2	C7-N8'	3.33	1.50	1.45
5	E	3904	GOL	O3-C3	3.32	1.56	1.42
8	C	4931	FAD	C5A-C6A	3.32	1.50	1.41
5	E	3905	GOL	O3-C3	3.29	1.56	1.42
7	B	3907	FZ2	C4A-N5'	3.29	1.45	1.37
5	B	3906	GOL	C1-C2	-3.26	1.39	1.51
8	C	4931	FAD	C4X-N5	3.26	1.37	1.30
7	B	3907	FZ2	C4'-N3'	3.24	1.44	1.38
5	C	3907	GOL	O3-C3	3.24	1.56	1.42
8	C	4931	FAD	C8-C7	3.23	1.48	1.40
7	E	3906	FZ2	C4A-N5'	3.21	1.45	1.37
8	C	4931	FAD	C9A-C5X	3.18	1.46	1.41
7	E	3906	FZ2	O4D-C4D	3.17	1.52	1.45
8	F	4932	FAD	P-O2P	-3.14	1.40	1.55
5	F	3903	GOL	C1-C2	-3.14	1.39	1.51
5	A	3909	GOL	C1-C2	-3.12	1.39	1.51
7	B	3907	FZ2	O4D-C4D	3.12	1.51	1.45
5	E	3901	GOL	C1-C2	-3.11	1.39	1.51
8	F	4932	FAD	C9A-C5X	3.11	1.46	1.41
8	F	4932	FAD	C5A-C6A	3.10	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	4932	FAD	C8-C7	3.09	1.48	1.40
5	B	3906	GOL	O2-C2	-3.08	1.34	1.43
8	F	4932	FAD	C4A-N3A	3.07	1.40	1.34
5	E	3904	GOL	O2-C2	-3.07	1.34	1.43
5	B	3902	GOL	C1-C2	-3.07	1.40	1.51
7	E	3906	FZ2	OM2-MO	3.04	1.78	1.68
8	F	4932	FAD	O5'-C5'	3.04	1.56	1.44
5	C	3907	GOL	C1-C2	-3.02	1.40	1.51
5	A	3909	GOL	O2-C2	-3.02	1.34	1.43
8	C	4931	FAD	C5A-C4A	2.99	1.44	1.39
5	C	3908	GOL	C1-C2	-2.99	1.40	1.51
7	E	3906	FZ2	C7-C6'	-2.97	1.51	1.53
5	E	3904	GOL	C1-C2	-2.97	1.40	1.51
5	E	3905	GOL	C1-C2	-2.94	1.40	1.51
8	C	4931	FAD	O5'-C5'	2.94	1.55	1.44
5	C	3907	GOL	O2-C2	-2.91	1.34	1.43
8	F	4932	FAD	C1'-C2'	2.91	1.56	1.52
7	E	3906	FZ2	C6-N1	2.90	1.45	1.38
8	F	4932	FAD	C5A-C4A	2.89	1.44	1.39
5	C	3908	GOL	O2-C2	-2.87	1.35	1.43
5	F	3903	GOL	O2-C2	-2.87	1.35	1.43
5	E	3901	GOL	O2-C2	-2.86	1.35	1.43
8	F	4932	FAD	C6-C5X	2.85	1.44	1.40
7	B	3907	FZ2	C6-N1	2.85	1.44	1.38
5	E	3905	GOL	O2-C2	-2.83	1.35	1.43
5	B	3902	GOL	O2-C2	-2.76	1.35	1.43
8	C	4931	FAD	C4A-N3A	2.75	1.39	1.34
7	E	3906	FZ2	C4-N3	2.55	1.39	1.34
8	C	4931	FAD	C5B-C4B	2.54	1.59	1.51
7	E	3906	FZ2	PA-O3A	2.53	1.62	1.59
8	F	4932	FAD	C2A-N1A	2.50	1.38	1.33
7	E	3906	FZ2	C4'-N3'	2.50	1.43	1.38
7	B	3907	FZ2	C4-N3	2.50	1.39	1.34
7	B	3907	FZ2	C4A-C4'	2.50	1.49	1.41
8	F	4932	FAD	C10-N1	2.49	1.38	1.33
8	C	4931	FAD	C6-C5X	2.49	1.43	1.40
8	C	4931	FAD	C1'-C2'	2.47	1.56	1.52
8	C	4931	FAD	C2A-N1A	2.46	1.38	1.33
8	C	4931	FAD	C9-C9A	2.45	1.43	1.39
8	C	4931	FAD	C10-N1	2.40	1.38	1.33
8	F	4932	FAD	C2-N3	2.39	1.44	1.39
8	F	4932	FAD	C5B-C4B	2.35	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	4932	FAD	O4B-C1B	2.33	1.47	1.42
7	E	3906	FZ2	O3'-C3'	2.31	1.48	1.43
8	C	4931	FAD	C2-N3	2.31	1.44	1.39
8	C	4931	FAD	O4B-C1B	2.29	1.47	1.42
7	E	3906	FZ2	C4A-C4'	2.29	1.48	1.41
8	F	4932	FAD	C9-C8	2.23	1.42	1.39
8	F	4932	FAD	C9-C9A	2.22	1.43	1.39
8	C	4931	FAD	P-O5'	-2.15	1.51	1.59
8	C	4931	FAD	C9-C8	2.14	1.42	1.39
7	E	3906	FZ2	C5-C4	2.12	1.47	1.42
7	B	3907	FZ2	C2D-C1'	2.10	1.60	1.53

All (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
5	B	3902	GOL	O3-C3-C2	11.07	160.21	110.38
5	F	3903	GOL	O3-C3-C2	11.07	160.21	110.38
5	C	3907	GOL	O3-C3-C2	11.01	159.94	110.38
5	E	3905	GOL	O3-C3-C2	10.87	159.32	110.38
7	E	3906	FZ2	C7-C6'-N5'	10.81	118.48	107.87
7	B	3907	FZ2	C7-C6'-N5'	10.43	118.11	107.87
7	B	3907	FZ2	C8'-C7'-S7'	9.36	125.46	120.15
7	E	3906	FZ2	C8'-C7'-S7'	8.83	125.16	120.15
5	E	3905	GOL	O2-C2-C3	7.26	139.25	109.18
5	F	3903	GOL	O2-C2-C3	7.25	139.20	109.18
5	B	3902	GOL	O2-C2-C3	7.23	139.13	109.18
5	C	3907	GOL	O2-C2-C3	7.23	139.10	109.18
5	A	3909	GOL	O2-C2-C3	7.22	139.06	109.18
5	B	3906	GOL	O2-C2-C3	7.19	138.94	109.18
5	C	3908	GOL	O2-C2-C3	7.17	138.87	109.18
5	E	3901	GOL	O2-C2-C3	7.15	138.76	109.18
5	E	3904	GOL	O2-C2-C3	7.11	138.63	109.18
7	B	3907	FZ2	C4-N3-C2	4.11	126.73	120.26
7	E	3906	FZ2	C4-N3-C2	3.86	126.33	120.26
7	E	3906	FZ2	O9'-C7-C6'	3.63	111.38	108.96
5	B	3902	GOL	O1-C1-C2	3.52	126.25	110.38
5	E	3904	GOL	O1-C1-C2	3.46	125.95	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	3908	GOL	O1-C1-C2	3.44	125.85	110.38
5	E	3901	GOL	O1-C1-C2	3.40	125.68	110.38
7	B	3907	FZ2	O9'-C7-C6'	3.39	111.22	108.96
5	C	3907	GOL	O1-C1-C2	3.38	125.60	110.38
5	E	3905	GOL	O1-C1-C2	3.38	125.59	110.38
5	F	3903	GOL	O1-C1-C2	3.36	125.51	110.38
5	B	3906	GOL	O1-C1-C2	3.27	125.12	110.38
7	B	3907	FZ2	N1-C2-N3	-3.24	113.18	118.80
5	A	3909	GOL	O1-C1-C2	3.24	124.94	110.38
7	E	3906	FZ2	N1-C2-N3	-3.21	113.24	118.80
8	C	4931	FAD	C5'-C4'-C3'	-2.92	106.72	112.22
8	C	4931	FAD	O5B-PA-O1A	-2.87	97.57	108.94
8	F	4932	FAD	O5B-PA-O1A	-2.84	97.70	108.94
8	F	4932	FAD	C5'-C4'-C3'	-2.83	106.87	112.22
8	C	4931	FAD	O4B-C1B-N9A	-2.80	102.72	108.09
7	B	3907	FZ2	C7'-C8'-S8'	-2.79	118.57	120.15
8	F	4932	FAD	O4B-C1B-N9A	-2.76	102.79	108.09
7	B	3907	FZ2	O4D-C1'-N1	2.49	114.00	108.36
8	F	4932	FAD	C2A-N1A-C6A	2.46	122.77	118.73
7	E	3906	FZ2	O1A-PA-O3A	-2.45	100.66	107.27
8	C	4931	FAD	C2A-N1A-C6A	2.44	122.73	118.73
7	B	3907	FZ2	O1A-PA-O3A	-2.42	100.73	107.27
8	C	4931	FAD	C5X-C9A-N10	-2.37	115.82	117.97
8	F	4932	FAD	C5X-C9A-N10	-2.28	115.91	117.97
7	E	3906	FZ2	C6-N1-C2	2.28	124.31	120.46
7	B	3907	FZ2	C6-N1-C2	2.26	124.27	120.46
8	F	4932	FAD	C4-N3-C2	-2.21	121.71	125.64
7	E	3906	FZ2	O2-C2-N3	2.20	125.79	122.33
7	B	3907	FZ2	C5-C4-N3	-2.17	117.66	121.32
7	E	3906	FZ2	O4D-C1'-N1	2.15	113.23	108.36
7	B	3907	FZ2	O2-C2-N3	2.13	125.69	122.33
8	C	4931	FAD	C4-N3-C2	-2.12	121.87	125.64
7	E	3906	FZ2	N4-C4-N3	2.10	121.67	117.91
7	B	3907	FZ2	C5-C6-N1	-2.04	118.52	121.84
7	E	3906	FZ2	C5-C4-N3	-2.04	117.88	121.32

There are no chirality outliers.

All (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

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Mol	Chain	Res	Type	Atoms
5	B	3902	GOL	O1-C1-C2-C3
5	B	3902	GOL	C1-C2-C3-O3
5	B	3906	GOL	C1-C2-C3-O3
5	C	3907	GOL	O1-C1-C2-C3
5	C	3907	GOL	C1-C2-C3-O3
5	C	3908	GOL	O1-C1-C2-C3
5	C	3908	GOL	C1-C2-C3-O3
5	E	3901	GOL	C1-C2-C3-O3
5	E	3904	GOL	C1-C2-C3-O3
5	E	3905	GOL	C1-C2-C3-O3
5	F	3903	GOL	O1-C1-C2-C3
5	F	3903	GOL	C1-C2-C3-O3
7	B	3907	FZ2	C5'-O5'-PA-O1A
7	E	3906	FZ2	C5'-O5'-PA-O2A
7	E	3906	FZ2	C5'-O5'-PA-O1A
7	E	3906	FZ2	C5'-O5'-PA-O3A
8	C	4931	FAD	C5B-O5B-PA-O1A
8	C	4931	FAD	C5B-O5B-PA-O3P
8	C	4931	FAD	C1'-C2'-C3'-O3'
8	C	4931	FAD	C1'-C2'-C3'-C4'
8	F	4932	FAD	C1'-C2'-C3'-O3'
8	F	4932	FAD	C1'-C2'-C3'-C4'
8	F	4932	FAD	C3'-C4'-C5'-O5'
5	E	3901	GOL	O1-C1-C2-O2
8	F	4932	FAD	O4B-C4B-C5B-O5B
8	F	4932	FAD	C3B-C4B-C5B-O5B
8	F	4932	FAD	O2'-C2'-C3'-C4'
5	B	3906	GOL	O1-C1-C2-C3
5	E	3904	GOL	O1-C1-C2-O2
8	C	4931	FAD	C3B-C4B-C5B-O5B
8	F	4932	FAD	O2'-C2'-C3'-O3'
8	C	4931	FAD	O2'-C2'-C3'-C4'
8	C	4931	FAD	O4B-C4B-C5B-O5B
8	C	4931	FAD	O2'-C2'-C3'-O3'
8	C	4931	FAD	C3'-C4'-C5'-O5'
5	E	3905	GOL	O1-C1-C2-O2
5	A	3909	GOL	O1-C1-C2-O2
8	C	4931	FAD	PA-O3P-P-O2P
8	F	4932	FAD	PA-O3P-P-O2P
5	C	3908	GOL	O1-C1-C2-O2
7	B	3907	FZ2	C5'-O5'-PA-O2A
7	B	3907	FZ2	C5'-O5'-PA-O3A

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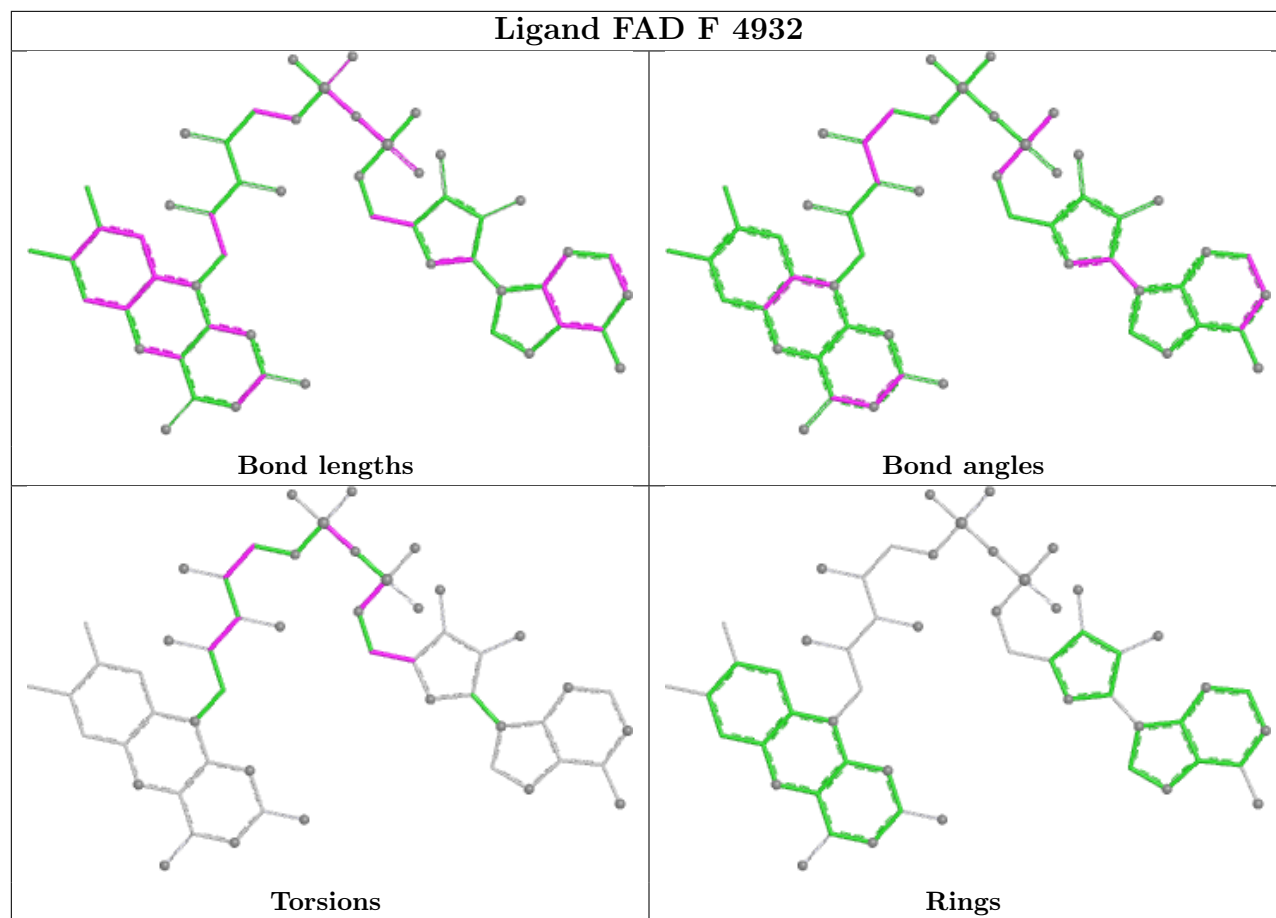
Mol	Chain	Res	Type	Atoms
8	F	4932	FAD	C5B-O5B-PA-O1A
8	F	4932	FAD	C5B-O5B-PA-O2A
8	F	4932	FAD	C5B-O5B-PA-O3P
7	B	3907	FZ2	C9'-C10-O3B-PB
7	B	3907	FZ2	PA-O3A-PB-O2B
5	C	3907	GOL	O1-C1-C2-O2
7	E	3906	FZ2	C9'-C10-O3B-PB
5	E	3905	GOL	O1-C1-C2-C3
7	E	3906	FZ2	PA-O3A-PB-O2B
7	E	3906	FZ2	PA-O3A-PB-O1B
8	C	4931	FAD	PA-O3P-P-O1P
8	F	4932	FAD	PA-O3P-P-O1P
5	B	3906	GOL	O1-C1-C2-O2

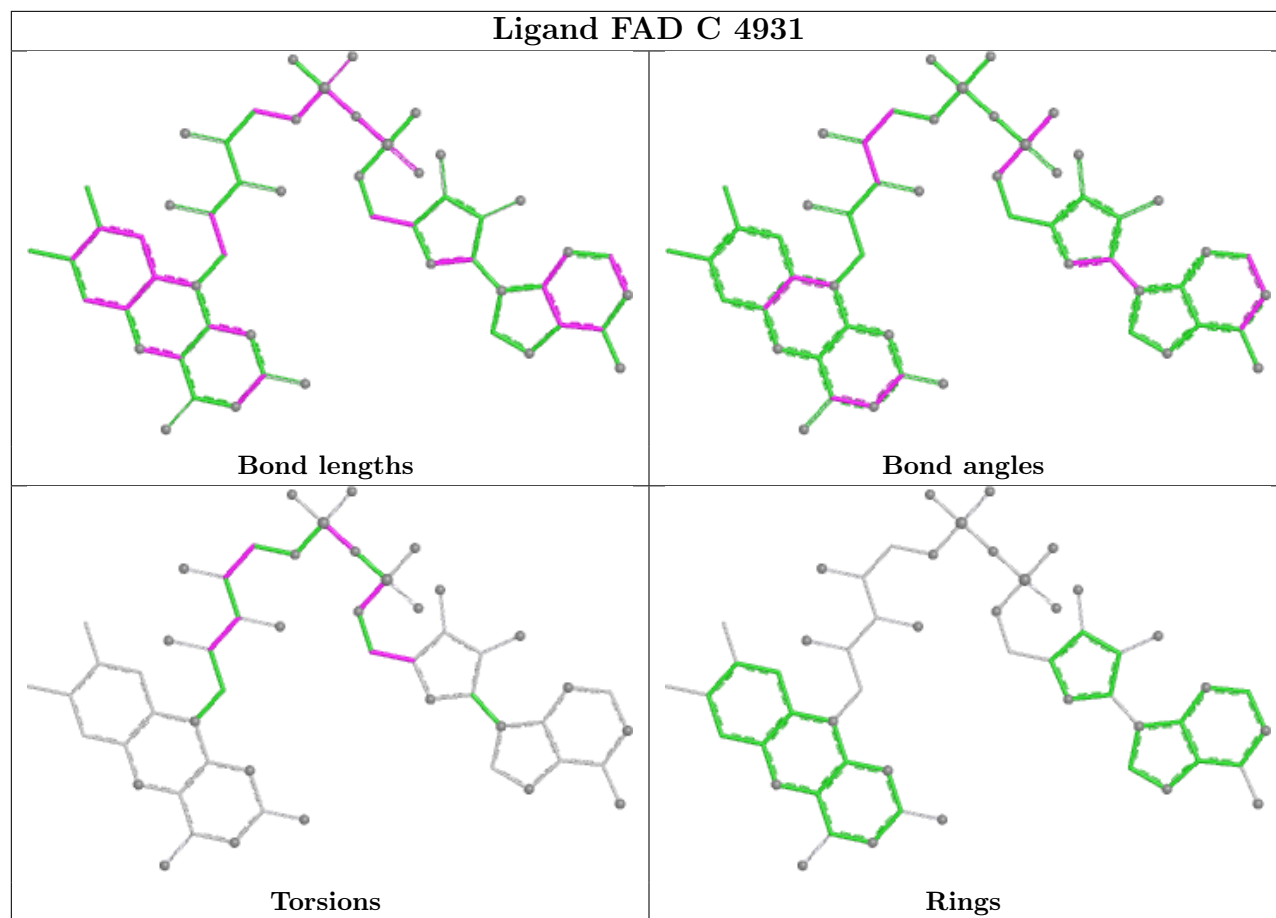
There are no ring outliers.

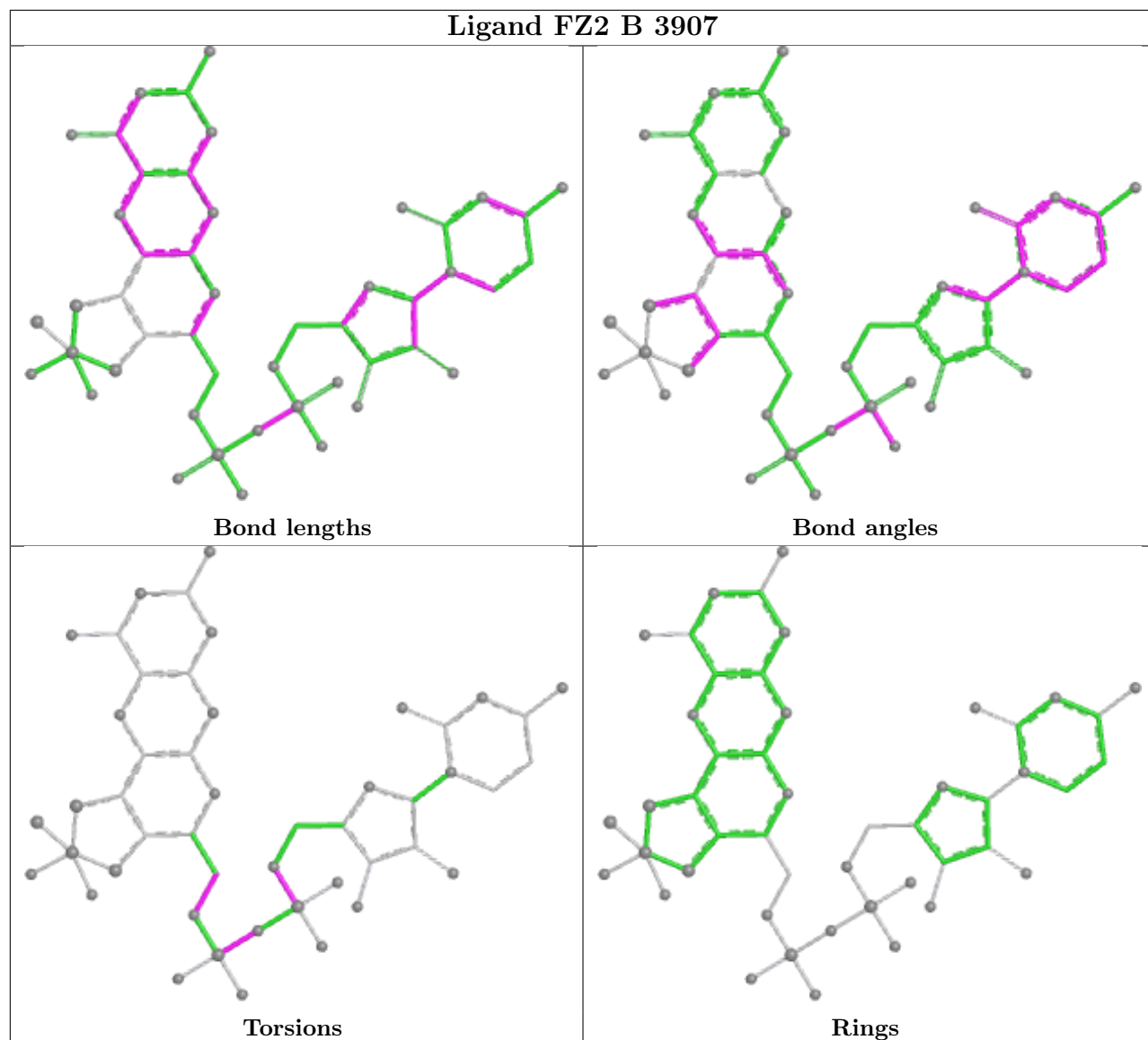
8 monomers are involved in 10 short contacts:

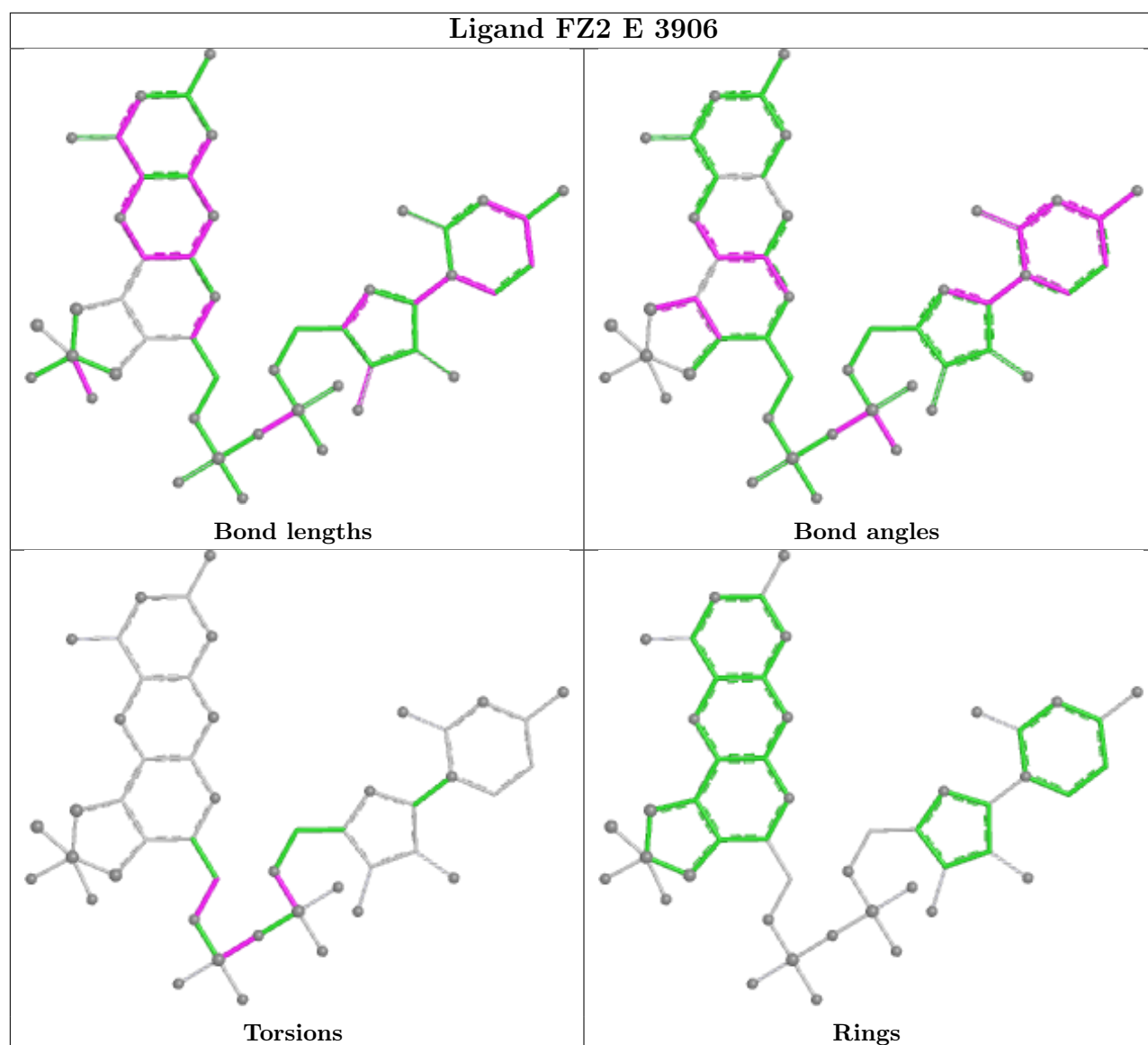
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3909	GOL	1	0
5	F	3903	GOL	2	0
5	B	3906	GOL	1	0
7	B	3907	FZ2	2	0
7	E	3906	FZ2	1	0
5	E	3904	GOL	1	0
6	B	3101	SO4	1	0
4	D	4910	FES	1	0

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 ⓘ

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	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%)

All (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
3	C	285	TYR	4.4
1	D	166	GLY	4.0
1	D	8	GLN	3.9
3	C	203	GLY	3.8
3	F	190	TYR	3.3
1	D	89	GLY	3.2
1	A	168	VAL	3.2
3	F	1	MET	3.1
2	E	594	GLY	3.1
2	E	595	VAL	2.9
1	A	89	GLY	2.7
3	C	204	GLY	2.6
3	F	185	ARG	2.5
1	A	9	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	187	LYS	2.5
3	C	190	TYR	2.5
3	C	1	MET	2.4
2	B	447	ALA	2.3
3	F	68	ILE	2.3
3	F	189	ASP	2.3
1	D	167	GLU	2.3
3	C	68	ILE	2.2
2	B	786	PRO	2.2
2	E	786	PRO	2.2
3	F	283	ALA	2.1
2	E	181	ALA	2.1
3	F	188	GLY	2.0
3	F	186	ARG	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
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

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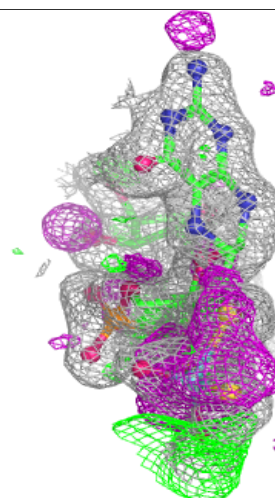
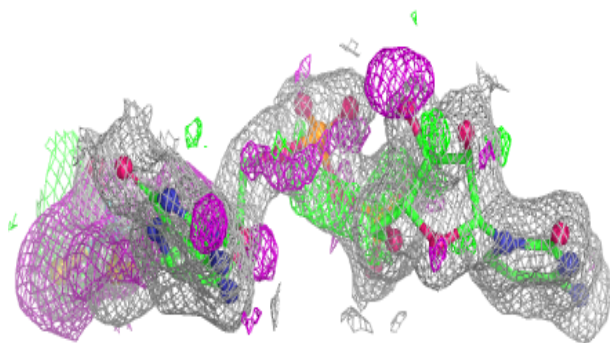
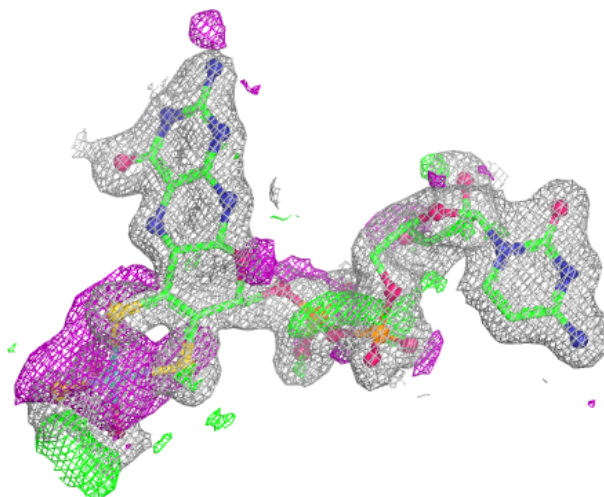
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	E	3103	5/5	0.84	0.16	73,74,74,74	0
5	GOL	B	3906	6/6	0.84	0.13	41,44,46,47	0
6	SO4	E	3104	5/5	0.87	0.10	68,68,69,69	0
5	GOL	E	3904	6/6	0.87	0.18	27,33,39,46	0
6	SO4	B	3101	5/5	0.88	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.

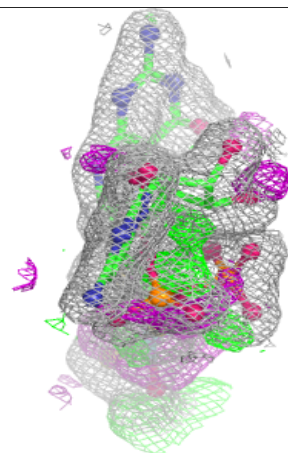
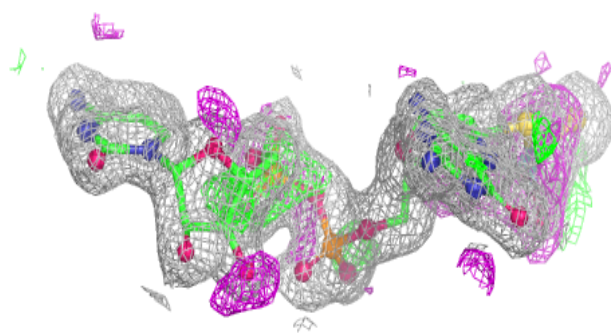
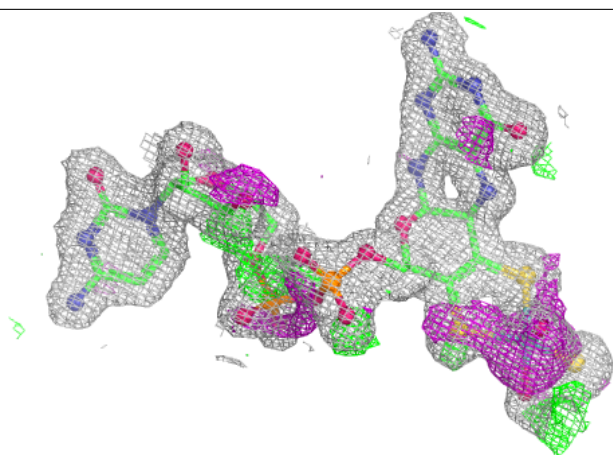
Electron density around FZ2 B 3907:

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

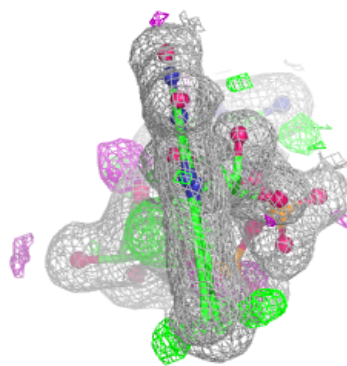
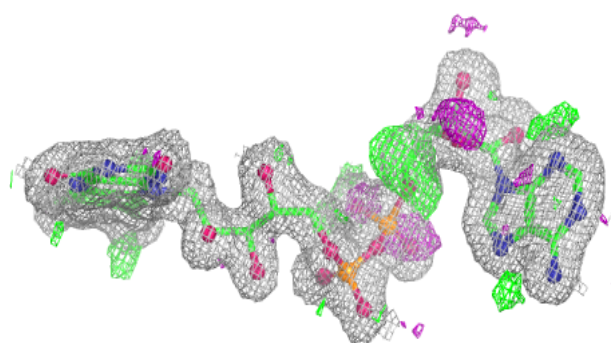
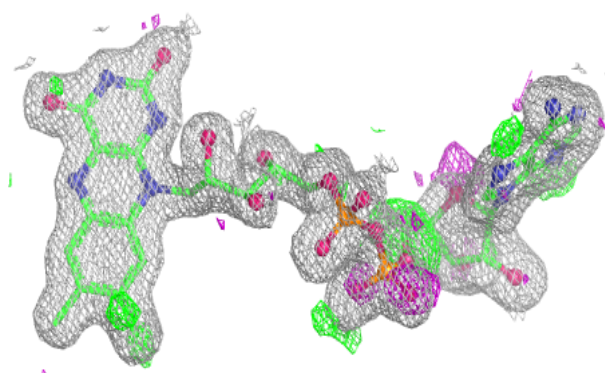


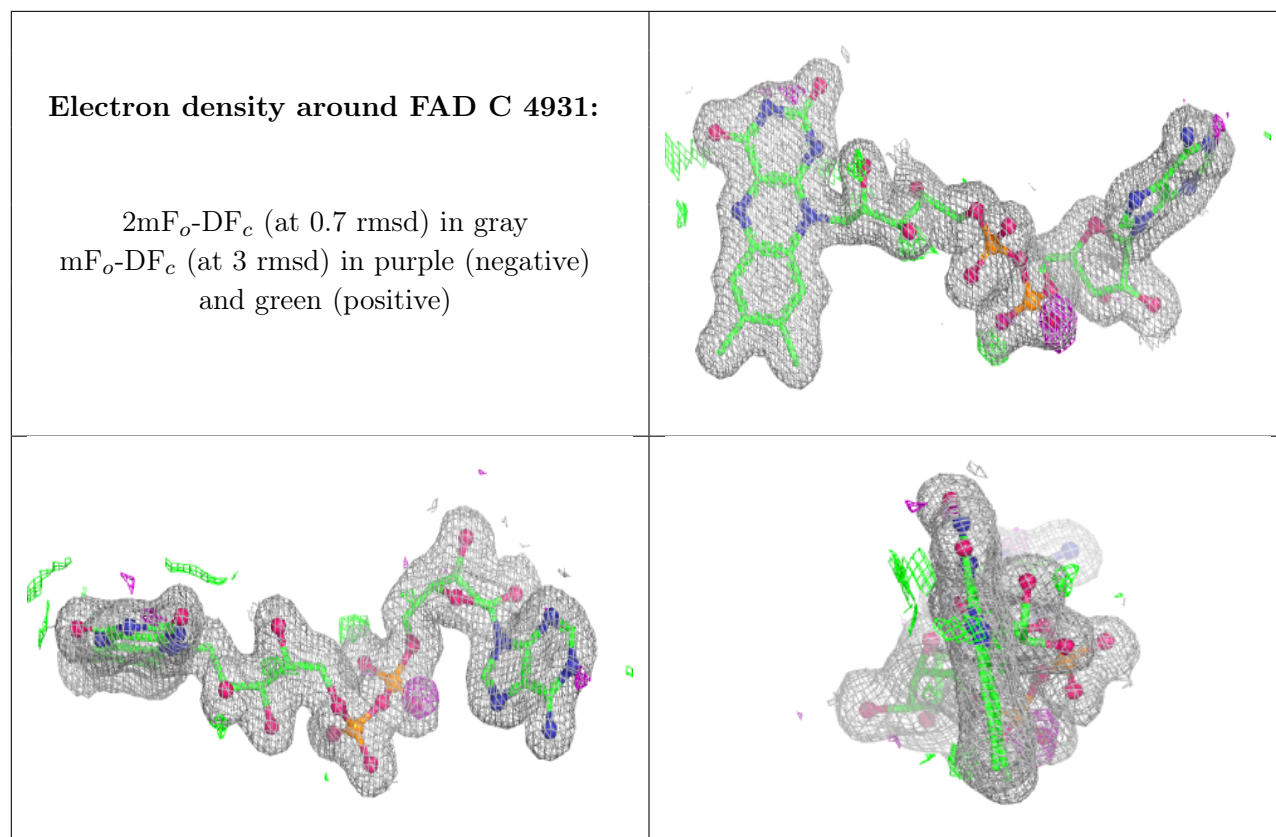
Electron density around FZ2 E 3906:

$2mF_o-DF_c$ (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.