Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 08:07 PM EST

PDB ID	:	4KX6
Title	:	Plasticity of the quinone-binding site of the complex II homolog quinol:fumarate reductase
Authors	:	Singh, P.K.; Sarwar, M.; Maklashina, E.; Kotlyar, V.; Rajagukguk, S.; Tomasiak, T.M.; Cecchini, G.; Iverson, T.M.
Deposited on	:	2013-05-24
Resolution	:	2.95 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 (i) 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 (i)) were used in the production of this report:

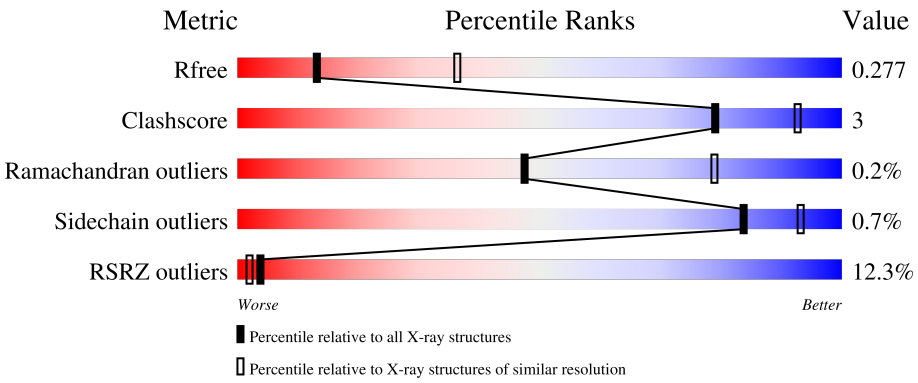
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 <=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	577	.% 93% 7%
1	M	577	31% 93% 7%
2	B	243	2% 92% 8%
2	N	243	17% 93% 6% •

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Mol	Chain	Length	Quality of chain
3	C	130	6% 88% 12%
3	O	130	15% 92% 8%
4	D	119	2% 97%
4	P	119	7% 93% 7%

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
9	MQ7	D	701	-	-	-	X
9	MQ7	N	304	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 16828 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 Fumarate reductase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	577	4448	2775	802	840	31	0	0	0
1	M	577	4448	2775	802	840	31	0	0	0

- Molecule 2 is a protein called Fumarate reductase (Anaerobic), Fe-S subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	243	1887	1189	323	356	19	0	0	0
2	N	243	1887	1189	323	356	19	0	0	0

- Molecule 3 is a protein called Fumarate reductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	130	1057	721	166	167	3	0	0	0
3	O	130	1057	721	166	167	3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	29	LEU	GLU	engineered mutation	UNP C9QU46
O	29	LEU	GLU	engineered mutation	UNP C9QU46

- Molecule 4 is a protein called Fumarate reductase subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	119	926	626	151	142	7	0	0	0

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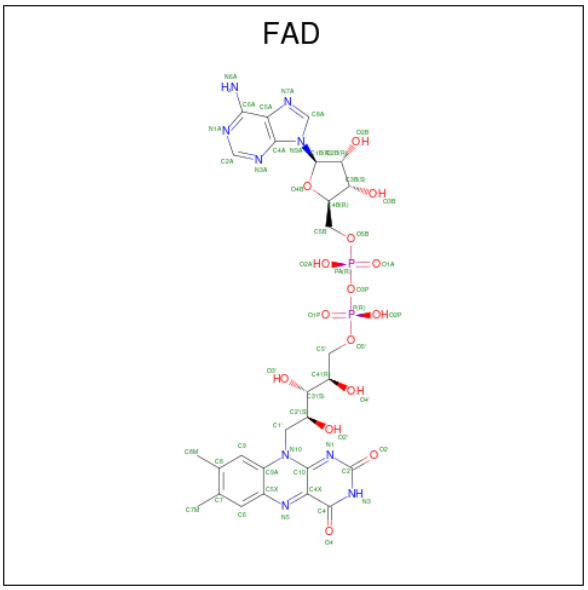
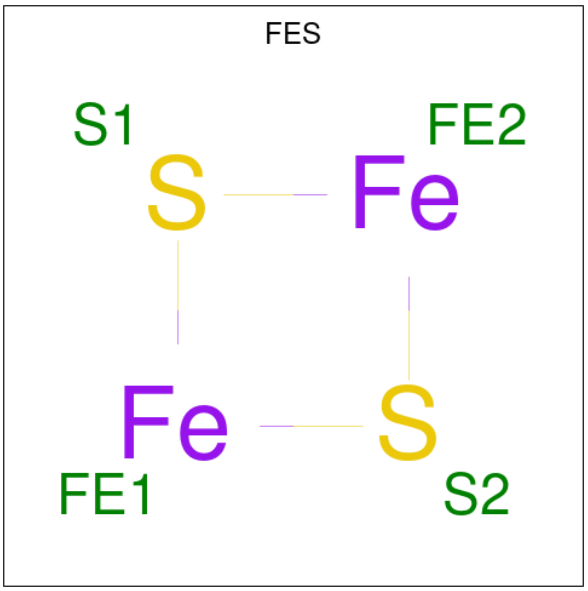
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	P	119	926	626	151	142	7	0	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



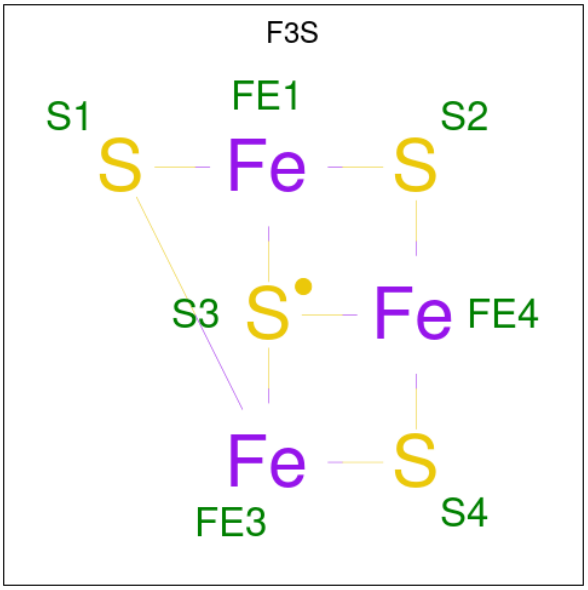
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
5	M	1	53	27	9	15	2	0	0

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



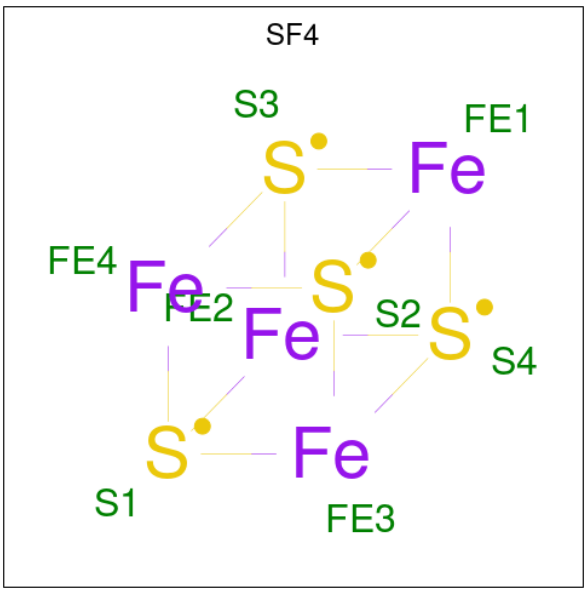
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
6	B	1	4	2	2	0	0
6	N	1	4	2	2	0	0

- Molecule 7 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



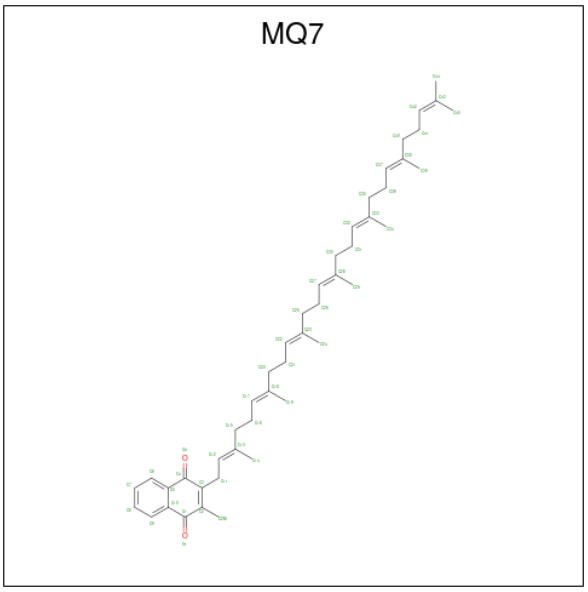
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
7	B	1	7	3	4	0	0
7	N	1	7	3	4	0	0

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
8	B	1	8	4	4	0	0
			Total	Fe	S		
8	N	1	8	4	4	0	0

- Molecule 9 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	D	1	24	22	2	0	0

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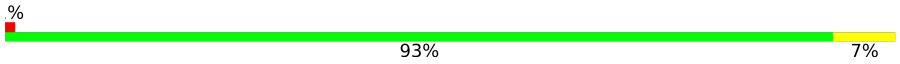
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	N	1	24	22	2	0	0

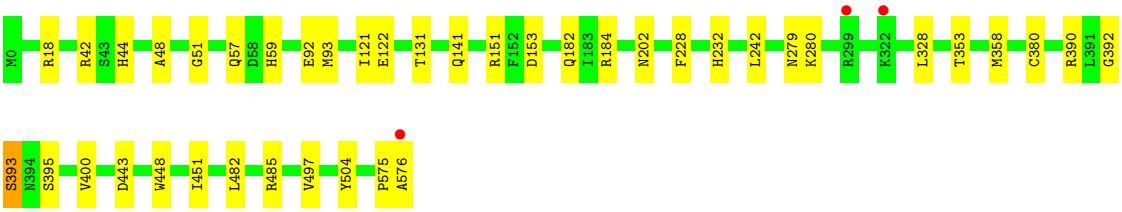
3 Residue-property plots (i)

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: Fumarate reductase flavoprotein subunit

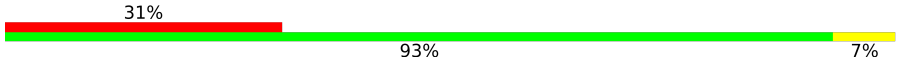
Chain A:

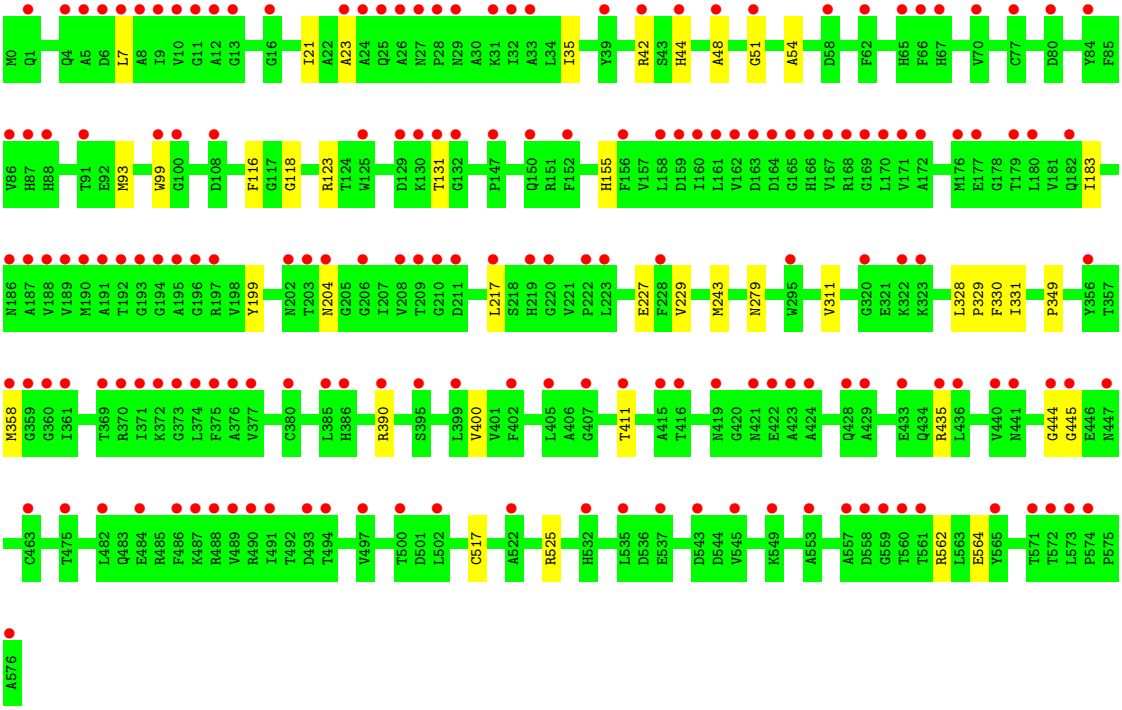




• Molecule 1: Fumarate reductase flavoprotein subunit

Chain M:



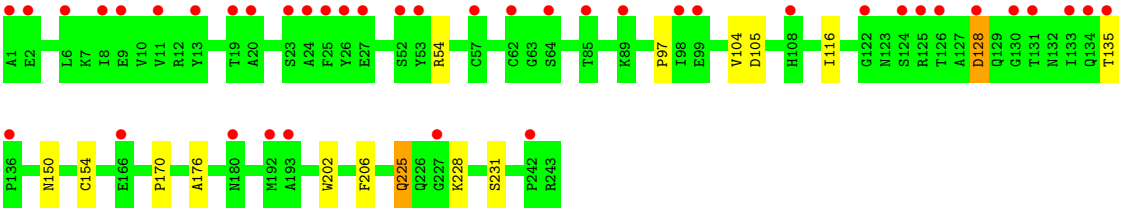


• Molecule 2: Fumarate reductase (Anaerobic), Fe-S subunit

Chain B: 2% 92% 8%

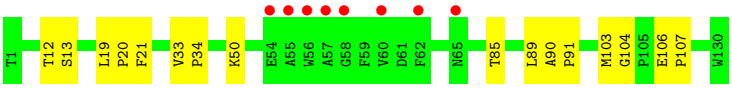
• Molecule 2: Fumarate reductase (Anaerobic), Fe-S subunit

Chain N: 17% 93% 6%



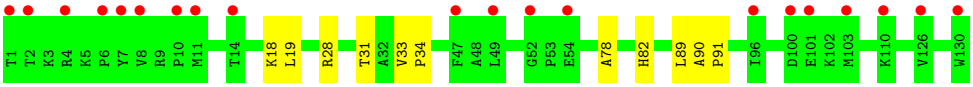
• Molecule 3: Fumarate reductase subunit C

Chain C: 6% 88% 12%



• Molecule 3: Fumarate reductase subunit C

Chain O: 15% 92% 8%

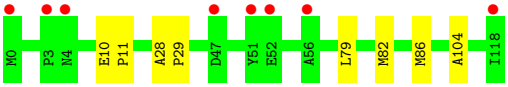


• Molecule 4: Fumarate reductase subunit D

Chain D: 2% 97%

• Molecule 4: Fumarate reductase subunit D

Chain P: 7% 93% 7%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.09Å 138.62Å 273.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.80 – 2.95 48.65 – 2.95	Depositor EDS
% Data completeness (in resolution range)	95.8 (47.80-2.95) 95.8 (48.65-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.51 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.7.0032, CNS	Depositor
R, R_{free}	0.240 , 0.280 0.243 , 0.277	Depositor DCC
R_{free} test set	1348 reflections (1.74%)	wwPDB-VP
Wilson B-factor (Å^2)	60.1	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	16828	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: FAD, MQ7, SF4, F3S, FES

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	0.33	0/4540	0.54	0/6139
1	M	0.32	0/4540	0.50	0/6139
2	B	0.32	0/1930	0.53	0/2617
2	N	0.33	0/1930	0.51	0/2617
3	C	0.31	0/1093	0.48	0/1495
3	O	0.31	0/1093	0.44	0/1495
4	D	0.29	0/956	0.42	0/1303
4	P	0.30	0/956	0.42	0/1303
All	All	0.32	0/17038	0.50	0/23108

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 (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	4448	0	4335	26	0
1	M	4448	0	4335	22	0
2	B	1887	0	1837	11	0
2	N	1887	0	1837	13	0
3	C	1057	0	1113	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	1057	0	1113	8	0
4	D	926	0	971	3	0
4	P	926	0	971	6	0
5	A	53	0	31	7	0
5	M	53	0	31	2	0
6	B	4	0	0	0	0
6	N	4	0	0	0	0
7	B	7	0	0	0	0
7	N	7	0	0	0	0
8	B	8	0	0	0	0
8	N	8	0	0	0	0
9	D	24	0	23	3	0
9	N	24	0	23	1	0
All	All	16828	0	16620	95	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 (95) 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:B:44:LYS:HA	2:B:48:ALA:O	1.83	0.77
9:D:701:MQ7:O4	9:D:701:MQ7:H12	1.84	0.76
3:O:31:THR:HG21	3:O:82:HIS:HB2	1.66	0.76
1:A:44:HIS:NE2	5:A:601:FAD:C8M	2.55	0.70
1:A:44:HIS:NE2	5:A:601:FAD:HM82	2.07	0.69
1:A:182:GLN:OE1	1:A:184:ARG:NH1	2.30	0.63
3:C:85:THR:O	3:C:89:LEU:HG	2.02	0.60
2:N:54:ARG:NH2	2:N:104:VAL:O	2.33	0.60
9:D:701:MQ7:O4	9:D:701:MQ7:C12	2.51	0.59
1:A:44:HIS:CE1	5:A:601:FAD:HM82	2.38	0.58
2:B:206:PHE:HE2	3:C:89:LEU:HD22	1.70	0.57
4:P:79:LEU:HD23	4:P:82:MET:HE3	1.86	0.56
2:B:62:CYS:SG	2:B:64:SER:OG	2.63	0.56
1:A:44:HIS:NE2	5:A:601:FAD:HM81	2.21	0.55
2:B:151:CYS:SG	2:B:153:LEU:HG	2.46	0.55
1:M:93:MET:CE	1:M:400:VAL:HG21	2.37	0.55
3:C:19:LEU:HD12	3:C:20:PRO:HD2	1.89	0.54
2:N:206:PHE:CE1	3:O:89:LEU:HG	2.43	0.54
1:A:151:ARG:NH1	1:A:153:ASP:OD2	2.40	0.54
3:C:50:LYS:HE3	4:D:117:THR:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:103:MET:HG2	3:C:104:GLY:N	2.24	0.53
1:A:390:ARG:HD2	1:A:395:SER:HB2	1.90	0.53
4:P:79:LEU:HD23	4:P:82:MET:CE	2.39	0.53
3:O:33:VAL:HB	3:O:34:PRO:HD3	1.91	0.53
1:M:227:GLU:OE2	1:M:525:ARG:NE	2.42	0.52
1:M:118:GLY:HA2	1:M:279:ASN:HD21	1.76	0.51
3:O:90:ALA:N	3:O:91:PRO:HD2	2.26	0.51
2:B:57:CYS:HB3	2:B:62:CYS:HB3	1.93	0.51
2:N:225:GLN:OE1	2:N:228:LYS:HD2	2.11	0.50
3:C:50:LYS:CE	4:D:117:THR:HG22	2.42	0.49
1:M:311:VAL:HG11	1:M:349:PRO:CB	2.43	0.49
1:M:51:GLY:HA2	1:M:131:THR:HG21	1.95	0.48
4:P:28:ALA:N	4:P:29:PRO:HD2	2.29	0.48
4:P:10:GLU:N	4:P:11:PRO:CD	2.76	0.48
2:N:154:CYS:SG	2:N:170:PRO:HG2	2.53	0.48
3:C:33:VAL:HB	3:C:34:PRO:HD3	1.95	0.48
2:N:116:ILE:CG2	2:N:176:ALA:HB2	2.44	0.48
4:D:20:GLY:HA2	4:D:73:LEU:HB3	1.97	0.47
2:N:206:PHE:O	2:N:206:PHE:HD1	1.97	0.47
2:N:202:TRP:HE1	2:N:231:SER:HG	1.62	0.47
1:A:141:GLN:HB3	2:B:118:PRO:O	2.13	0.47
1:M:44:HIS:NE2	5:M:601:FAD:HM82	2.29	0.47
1:M:183:ILE:N	1:M:183:ILE:HD12	2.29	0.47
1:M:243:MET:HE3	1:M:331:ILE:HG23	1.96	0.47
2:N:225:GLN:OE1	2:N:225:GLN:HA	2.15	0.47
1:A:51:GLY:HA2	1:A:131:THR:HG21	1.97	0.46
1:A:443:ASP:OD1	1:A:443:ASP:C	2.53	0.46
1:M:35:ILE:HD11	1:M:155:HIS:HB3	1.97	0.46
9:D:701:MQ7:H193	9:D:701:MQ7:H151	1.97	0.46
1:A:448:TRP:CH2	1:A:504:TYR:HB3	2.51	0.46
1:A:242:LEU:CD2	5:A:601:FAD:HM73	2.46	0.46
1:A:202:ASN:HA	1:A:353:THR:HG22	1.98	0.46
1:A:575:PRO:O	1:A:576:ALA:HB3	2.15	0.46
2:B:212:GLU:HG3	3:C:21:PHE:CE2	2.50	0.46
1:A:242:LEU:HD23	5:A:601:FAD:HM73	1.98	0.45
1:A:451:ILE:HG23	1:A:482:LEU:HD22	1.98	0.45
1:A:18:ARG:HG2	1:A:400:VAL:HA	1.98	0.45
2:N:206:PHE:O	2:N:206:PHE:CD1	2.70	0.45
1:A:232:HIS:CD2	1:A:242:LEU:CD1	3.00	0.44
1:M:7:LEU:HD12	1:M:23:ALA:HB1	1.98	0.44
1:M:42:ARG:NH2	2:N:150:ASN:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:79:LEU:HD13	4:P:104:ALA:HB2	1.99	0.44
1:M:48:ALA:HA	5:M:601:FAD:C6	2.48	0.44
3:O:18:LYS:HB3	3:O:19:LEU:HD23	2.00	0.43
1:A:497:VAL:HG21	2:B:15:PRO:HG2	2.00	0.43
2:B:167:PHE:CD1	2:B:203:SER:HB2	2.53	0.43
3:C:12:THR:HG22	3:C:13:SER:N	2.33	0.43
2:N:97:PRO:HG2	2:N:105:ASP:HB3	2.00	0.43
3:C:90:ALA:N	3:C:91:PRO:HD2	2.33	0.43
1:M:562:ARG:NH1	1:M:564:GLU:OE2	2.52	0.43
1:A:18:ARG:NH1	1:A:92:GLU:OE1	2.52	0.43
1:M:328:LEU:N	1:M:329:PRO:CD	2.81	0.43
1:M:21:ILE:HG21	1:M:99:TRP:CH2	2.53	0.43
3:O:31:THR:HG23	3:O:78:ALA:HB1	2.00	0.43
1:M:54:ALA:O	1:M:123:ARG:HB2	2.18	0.42
4:P:82:MET:O	4:P:86:MET:HG2	2.19	0.42
1:M:7:LEU:HD21	1:M:411:THR:HA	2.00	0.42
2:N:128:ASP:OD1	2:N:128:ASP:N	2.45	0.42
1:A:228:PHE:O	1:A:358:MET:HB2	2.20	0.42
3:O:31:THR:HG21	3:O:82:HIS:CB	2.45	0.42
3:C:106:GLU:N	3:C:107:PRO:CD	2.83	0.41
9:N:304:MQ7:H2M2	3:O:28:ARG:NH1	2.35	0.41
1:M:199:TYR:CE1	1:M:229:VAL:HG11	2.56	0.41
1:A:59:HIS:CE1	1:A:121:ILE:HG23	2.56	0.41
1:A:279:ASN:O	1:A:280:LYS:HB2	2.21	0.41
1:M:358:MET:SD	1:M:390:ARG:N	2.94	0.41
1:A:48:ALA:HA	5:A:601:FAD:C6	2.50	0.41
1:A:57:GLN:NE2	1:A:122:GLU:HG2	2.36	0.41
1:M:217:LEU:HD21	1:M:517:CYS:SG	2.61	0.41
2:N:116:ILE:HG21	2:N:176:ALA:HB2	2.02	0.41
1:A:392:GLY:O	1:A:393:SER:CB	2.69	0.41
1:M:44:HIS:NE2	1:M:204:ASN:HA	2.36	0.40
2:B:100:ARG:O	2:B:101:ASP:C	2.59	0.40
2:B:206:PHE:CD2	3:C:89:LEU:HD13	2.57	0.40
1:M:358:MET:HG2	1:M:390:ARG:HB2	2.03	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	575/577 (100%)	556 (97%)	17 (3%)	2 (0%)	41	73
1	M	575/577 (100%)	540 (94%)	33 (6%)	2 (0%)	41	73
2	B	241/243 (99%)	232 (96%)	8 (3%)	1 (0%)	34	69
2	N	241/243 (99%)	227 (94%)	14 (6%)	0	100	100
3	C	128/130 (98%)	125 (98%)	3 (2%)	0	100	100
3	O	128/130 (98%)	120 (94%)	8 (6%)	0	100	100
4	D	117/119 (98%)	112 (96%)	5 (4%)	0	100	100
4	P	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
All	All	2122/2138 (99%)	2023 (95%)	94 (4%)	5 (0%)	47	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	393	SER
1	M	444	GLY
2	B	56	SER
1	M	445	GLY
1	A	328	LEU

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	460/460 (100%)	456 (99%)	4 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	M	460/460 (100%)	457 (99%)	3 (1%)	84 93
2	B	205/205 (100%)	202 (98%)	3 (2%)	65 85
2	N	205/205 (100%)	202 (98%)	3 (2%)	65 85
3	C	111/111 (100%)	111 (100%)	0	100 100
3	O	111/111 (100%)	111 (100%)	0	100 100
4	D	97/97 (100%)	97 (100%)	0	100 100
4	P	97/97 (100%)	97 (100%)	0	100 100
All	All	1746/1746 (100%)	1733 (99%)	13 (1%)	84 93

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	93	MET
1	A	380	CYS
1	A	485	ARG
2	B	65	CYS
2	B	113	LEU
2	B	178	ARG
1	M	116	PHE
1	M	330	PHE
1	M	435	ARG
2	N	128	ASP
2	N	135	THR
2	N	225	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	87	HIS
1	A	141	GLN
1	A	232	HIS
1	A	279	ASN
1	A	292	GLN
1	A	409	GLN
2	B	134	GLN
2	B	194	GLN

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Mol	Chain	Res	Type
3	C	51	ASN
3	C	64	GLN
1	M	88	HIS
1	M	182	GLN
1	M	279	ASN
1	M	292	GLN
1	M	366	ASN
1	M	434	GLN
2	N	95	ASN
3	O	72	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	FES	B	301	2	0,4,4	-	-	-		
9	MQ7	N	304	-	25,25,49	2.04	2 (8%)	31,34,63	1.66	5 (16%)
6	FES	N	301	2	0,4,4	-	-	-		
7	F3S	N	302	2	0,9,9	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	FAD	A	601	-	53,58,58	1.30	6 (11%)	68,89,89	1.41	13 (19%)
8	SF4	N	303	2	0,12,12	-	-	-		
8	SF4	B	303	2	0,12,12	-	-	-		
5	FAD	M	601	-	53,58,58	1.32	6 (11%)	68,89,89	1.38	12 (17%)
7	F3S	B	302	2	0,9,9	-	-	-		
9	MQ7	D	701	-	25,25,49	2.03	2 (8%)	31,34,63	1.26	5 (16%)

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
9	MQ7	N	304	-	-	2/13/33/61	0/2/2/2
6	FES	B	301	2	-	-	0/1/1/1
6	FES	N	301	2	-	-	0/1/1/1
7	F3S	N	302	2	-	-	0/3/3/3
5	FAD	A	601	-	-	6/30/50/50	0/6/6/6
8	SF4	N	303	2	-	-	0/6/5/5
8	SF4	B	303	2	-	-	0/6/5/5
5	FAD	M	601	-	-	3/30/50/50	0/6/6/6
7	F3S	B	302	2	-	-	0/3/3/3
9	MQ7	D	701	-	-	7/13/33/61	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	701	MQ7	C3-C2	8.20	1.50	1.35
9	N	304	MQ7	C3-C2	8.08	1.50	1.35
5	A	601	FAD	C9A-C5X	5.35	1.50	1.41
5	M	601	FAD	C9A-C5X	5.30	1.50	1.41
9	N	304	MQ7	C10-C5	5.25	1.49	1.40
9	D	701	MQ7	C10-C5	5.17	1.49	1.40
5	M	601	FAD	C8-C7	3.32	1.49	1.40
5	A	601	FAD	C8-C7	2.68	1.47	1.40
5	M	601	FAD	C5A-C4A	2.45	1.47	1.40
5	M	601	FAD	C4-N3	-2.45	1.34	1.38
5	A	601	FAD	C4-N3	-2.36	1.34	1.38
5	A	601	FAD	C5X-N5	-2.27	1.35	1.39
5	M	601	FAD	C4X-N5	2.22	1.35	1.30
5	A	601	FAD	C5A-C4A	2.15	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	601	FAD	C5X-N5	-2.12	1.35	1.39
5	A	601	FAD	C4X-N5	2.11	1.34	1.30

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	304	MQ7	C14-C13-C15	5.42	124.38	115.27
5	A	601	FAD	N3A-C2A-N1A	-3.83	122.70	128.68
9	N	304	MQ7	C15-C13-C12	-3.62	113.80	121.12
5	M	601	FAD	N3A-C2A-N1A	-3.60	123.06	128.68
5	M	601	FAD	P-O3P-PA	-3.13	122.09	132.83
5	M	601	FAD	C4A-C5A-N7A	-3.02	106.25	109.40
9	N	304	MQ7	C2M-C2-C3	-3.01	119.49	124.40
9	D	701	MQ7	C19-C18-C20	2.98	119.39	115.98
5	A	601	FAD	C4A-C5A-N7A	-2.95	106.33	109.40
5	A	601	FAD	O4-C4-C4X	-2.85	119.03	126.60
5	M	601	FAD	C4X-C10-N1	-2.82	118.18	124.73
9	D	701	MQ7	C16-C17-C18	-2.72	121.12	127.66
9	D	701	MQ7	C2M-C2-C3	-2.69	120.01	124.40
5	A	601	FAD	C4X-C10-N1	-2.66	118.55	124.73
9	D	701	MQ7	C11-C12-C13	-2.60	122.46	126.79
5	M	601	FAD	C4-C4X-N5	2.58	121.91	118.23
5	A	601	FAD	O2-C2-N1	-2.54	117.62	121.83
5	M	601	FAD	C4X-C10-N10	2.40	119.99	116.48
5	M	601	FAD	C10-N1-C2	2.38	121.66	116.90
5	A	601	FAD	C10-N1-C2	2.37	121.64	116.90
9	N	304	MQ7	C2M-C2-C1	2.33	120.13	116.27
5	A	601	FAD	C9-C8-C7	2.28	122.94	119.67
9	N	304	MQ7	C19-C18-C20	2.27	118.58	115.98
5	A	601	FAD	C4X-C10-N10	2.26	119.78	116.48
5	A	601	FAD	C4-C4X-N5	2.26	121.45	118.23
5	A	601	FAD	C4X-C4-N3	2.24	118.88	113.19
5	M	601	FAD	O2-C2-N1	-2.22	118.14	121.83
5	A	601	FAD	C4-N3-C2	-2.16	121.65	125.64
5	A	601	FAD	P-O3P-PA	-2.13	125.51	132.83
9	D	701	MQ7	C2M-C2-C1	2.09	119.74	116.27
5	A	601	FAD	C1'-N10-C9A	2.08	123.98	120.51
5	M	601	FAD	C4X-C4-N3	2.07	118.46	113.19
5	M	601	FAD	O4-C4-C4X	-2.05	121.16	126.60
5	M	601	FAD	C1B-N9A-C4A	-2.03	123.07	126.64
5	M	601	FAD	C2A-N1A-C6A	2.02	122.20	118.75

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	FAD	N10-C1'-C2'-O2'
5	A	601	FAD	N10-C1'-C2'-C3'
5	A	601	FAD	PA-O3P-P-O5'
5	M	601	FAD	N10-C1'-C2'-O2'
5	M	601	FAD	N10-C1'-C2'-C3'
9	D	701	MQ7	C12-C11-C3-C2
9	D	701	MQ7	C12-C11-C3-C4
9	D	701	MQ7	C14-C13-C15-C16
9	D	701	MQ7	C12-C13-C15-C16
9	N	304	MQ7	C14-C13-C15-C16
9	N	304	MQ7	C12-C13-C15-C16
9	D	701	MQ7	C17-C18-C20-C21
5	A	601	FAD	P-O3P-PA-O1A
5	A	601	FAD	P-O3P-PA-O2A
9	D	701	MQ7	C13-C15-C16-C17
9	D	701	MQ7	C19-C18-C20-C21
5	A	601	FAD	O4B-C4B-C5B-O5B
5	M	601	FAD	O4B-C4B-C5B-O5B

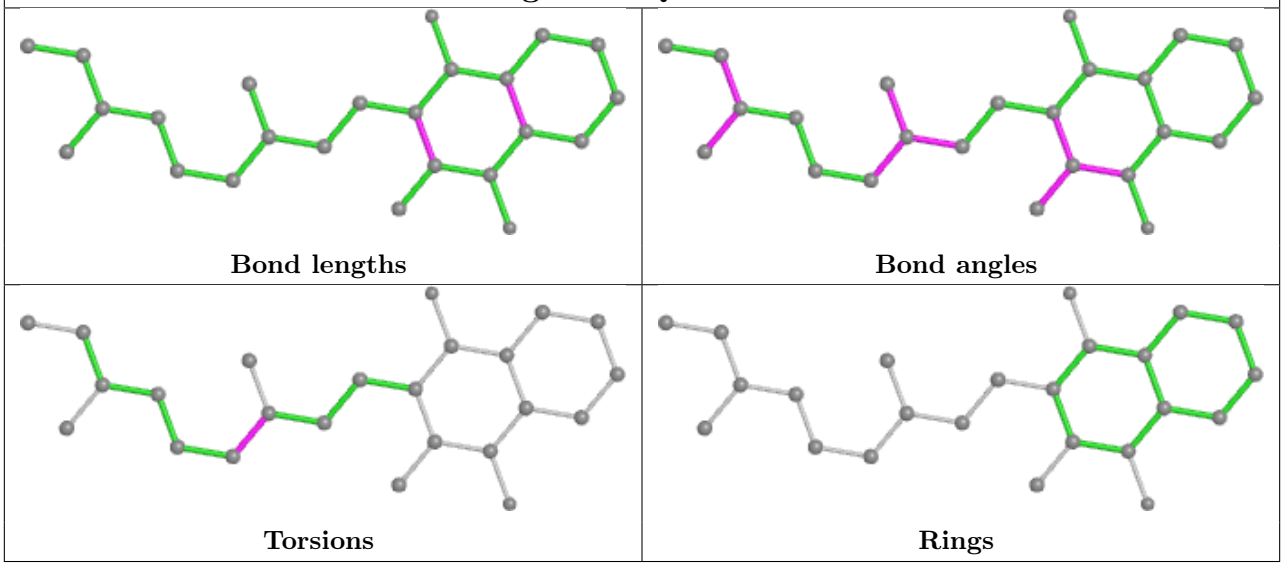
There are no ring outliers.

4 monomers are involved in 13 short contacts:

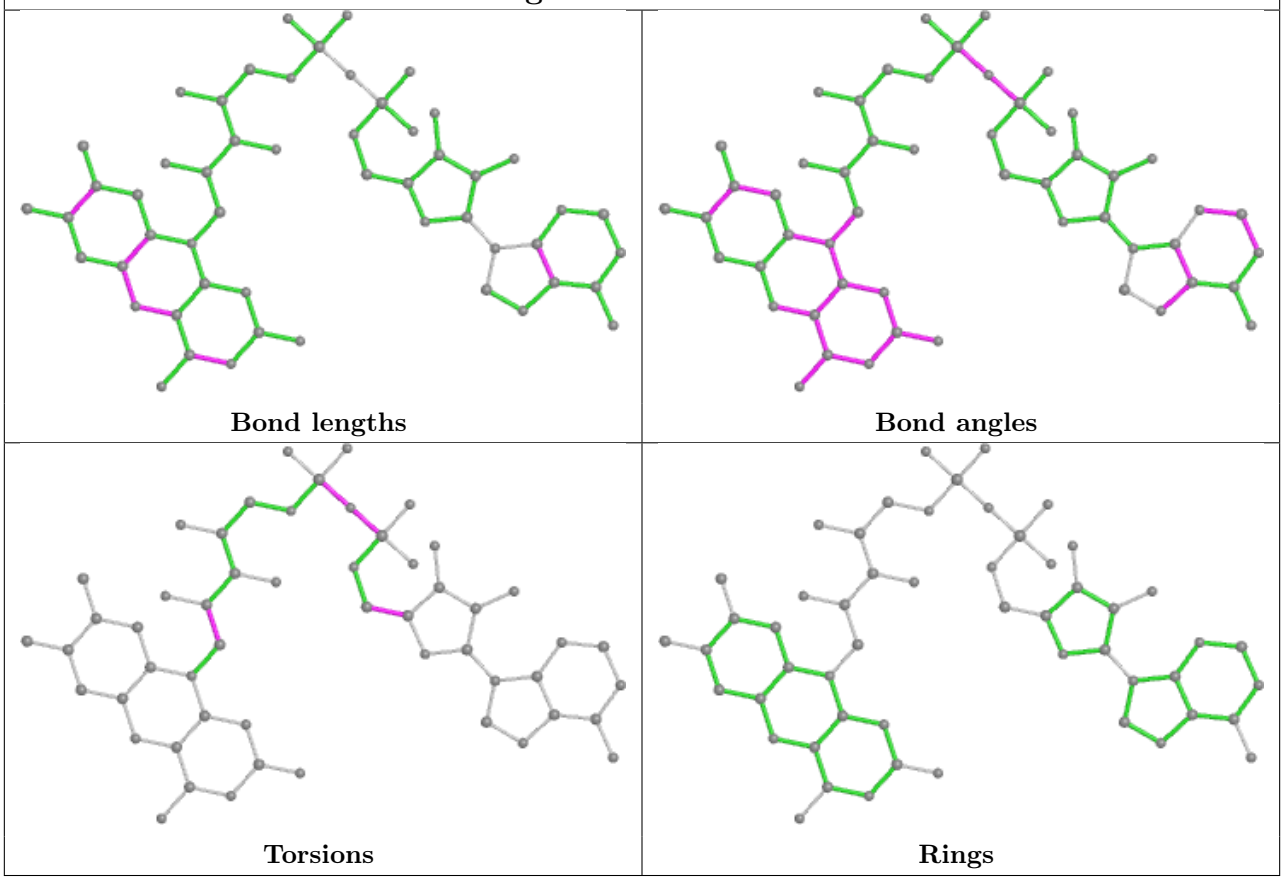
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	N	304	MQ7	1	0
5	A	601	FAD	7	0
5	M	601	FAD	2	0
9	D	701	MQ7	3	0

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 then 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.

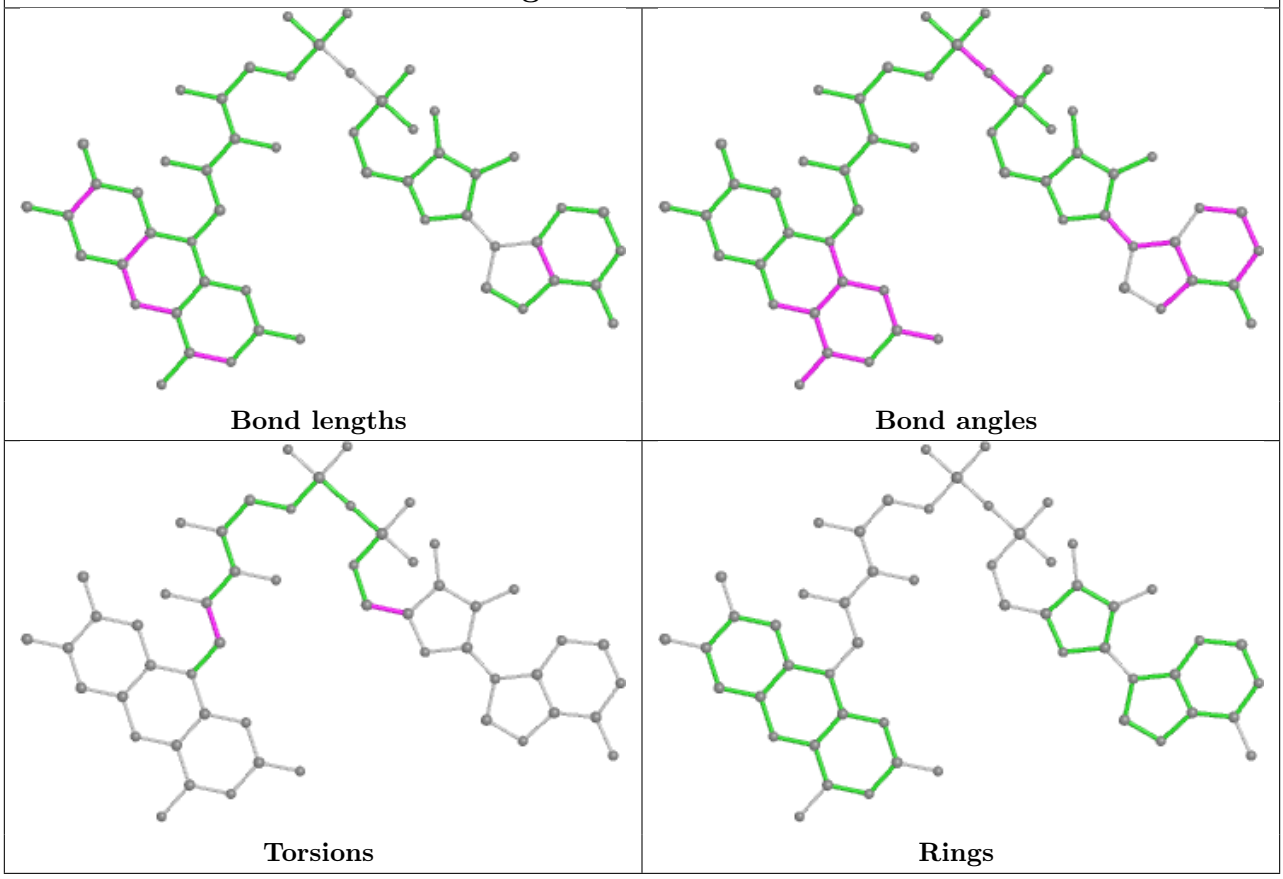
Ligand MQ7 N 304



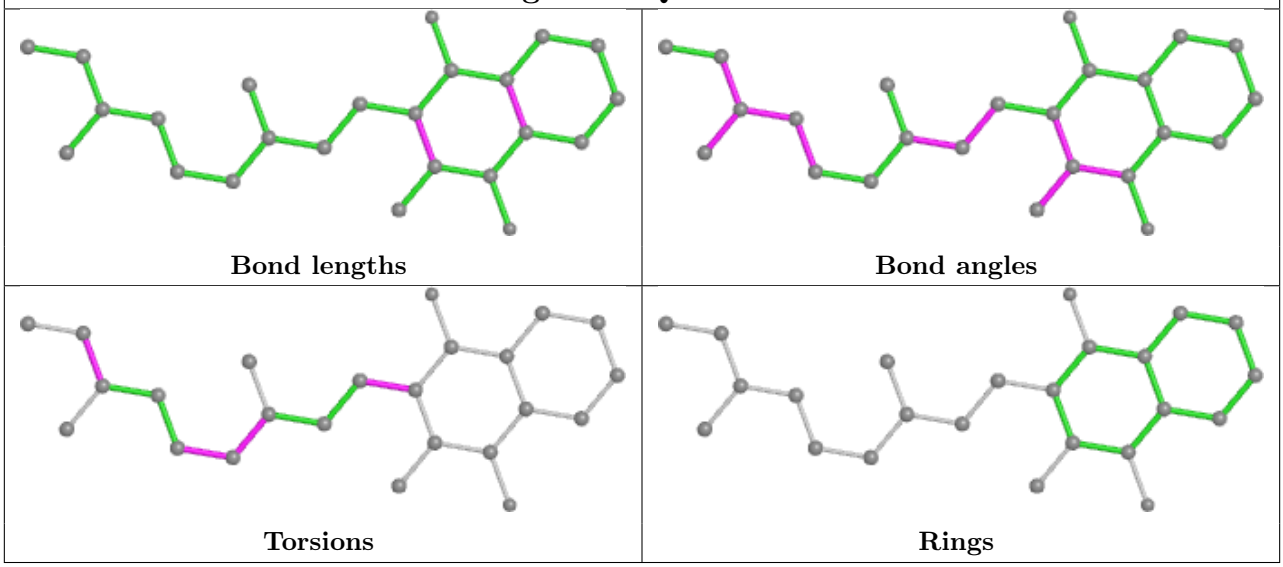
Ligand FAD A 601



Ligand FAD M 601



Ligand MQ7 D 701



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	577/577 (100%)	-0.08	3 (0%) 91 81	29, 40, 64, 95	0
1	M	577/577 (100%)	1.59	177 (30%) 0 0	72, 113, 147, 165	0
2	B	243/243 (100%)	-0.04	4 (1%) 72 55	30, 45, 64, 123	0
2	N	243/243 (100%)	1.03	41 (16%) 1 1	63, 97, 134, 141	0
3	C	130/130 (100%)	0.11	8 (6%) 20 12	50, 61, 92, 95	0
3	O	130/130 (100%)	0.61	20 (15%) 2 1	56, 79, 115, 145	0
4	D	119/119 (100%)	-0.23	2 (1%) 70 53	48, 63, 86, 95	0
4	P	119/119 (100%)	0.14	8 (6%) 17 10	63, 77, 101, 140	0
All	All	2138/2138 (100%)	0.56	263 (12%) 4 2	29, 71, 132, 165	0

All (263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	165	GLY	12.6
1	M	411	THR	8.5
1	M	163	ASP	7.3
3	O	1	THR	7.2
1	M	169	GLY	7.2
1	M	188	VAL	7.1
1	M	161	LEU	6.8
1	M	6	ASP	6.5
1	M	376	ALA	6.3
1	M	574	PRO	6.0
1	M	189	VAL	5.6
2	B	1	ALA	5.5
1	M	172	ALA	5.5
1	M	24	ALA	5.5
1	M	560	THR	5.4
1	M	162	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
2	N	20	ALA	5.3
1	M	170	LEU	5.3
1	M	77	CYS	5.2
1	M	159	ASP	5.2
1	M	380	CYS	5.2
1	M	8	ALA	5.2
1	M	375	PHE	5.1
2	N	19	THR	5.1
1	M	573	LEU	4.9
1	M	486	PHE	4.9
1	M	28	PRO	4.8
1	M	484	GLU	4.8
2	N	133	ILE	4.8
1	M	424	ALA	4.8
1	M	4	GLN	4.8
1	M	576	ALA	4.8
1	M	164	ASP	4.8
2	N	98	ILE	4.8
1	M	176	MET	4.6
1	M	160	ILE	4.6
2	N	126	THR	4.5
1	M	490	ARG	4.4
2	N	136	PRO	4.4
1	M	32	ILE	4.3
1	M	373	GLY	4.3
1	M	220	GLY	4.3
1	M	167	VAL	4.2
4	D	118	ILE	4.1
1	M	571	THR	4.0
1	M	84	TYR	4.0
1	M	219	HIS	3.9
1	M	386	HIS	3.9
1	M	180	LEU	3.9
1	M	370	ARG	3.8
2	N	1	ALA	3.8
1	M	489	VAL	3.8
1	M	405	LEU	3.8
1	M	11	GLY	3.8
1	M	419	ASN	3.8
1	M	192	THR	3.7
2	N	128	ASP	3.7
1	M	27	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	M	7	LEU	3.7
1	M	206	GLY	3.7
1	M	210	GLY	3.7
1	M	31	LYS	3.6
1	M	445	GLY	3.6
2	N	27	GLU	3.5
1	M	374	LEU	3.5
2	N	122	GLY	3.5
3	O	4	ARG	3.5
2	N	11	VAL	3.5
1	M	168	ARG	3.4
1	M	222	PRO	3.4
2	N	26	TYR	3.4
1	M	557	ALA	3.4
1	M	385	LEU	3.4
3	O	130	TRP	3.4
1	M	402	PHE	3.4
2	N	25	PHE	3.4
3	O	10	PRO	3.3
3	O	2	THR	3.3
4	P	3	PRO	3.3
1	M	44	HIS	3.3
2	B	243	ARG	3.3
1	M	66	PHE	3.3
1	M	360	GLY	3.3
1	M	395	SER	3.3
1	M	553	ALA	3.2
1	M	9	ILE	3.2
3	O	47	PHE	3.2
1	M	125	TRP	3.2
3	O	103	MET	3.2
1	M	187	ALA	3.2
1	M	191	ALA	3.2
4	P	56	ALA	3.2
1	M	422	GLU	3.2
1	M	493	ASP	3.2
3	O	100	ASP	3.2
3	C	58	GLY	3.2
2	N	52	SER	3.1
1	M	561	THR	3.1
1	A	322	LYS	3.1
4	P	51	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	M	190	MET	3.1
4	P	4	ASN	3.1
1	M	33	ALA	3.1
1	M	482	LEU	3.1
1	M	436	LEU	3.1
1	M	322	LYS	3.0
1	M	559	GLY	3.0
2	N	193	ALA	3.0
1	M	444	GLY	3.0
1	M	399	LEU	3.0
1	M	129	ASP	3.0
1	M	323	LYS	2.9
1	M	23	ALA	2.9
1	M	166	HIS	2.9
1	M	147	PRO	2.9
1	M	415	ALA	2.9
1	M	500	THR	2.9
1	M	204	ASN	2.9
2	B	2	GLU	2.9
1	M	25	GLN	2.9
2	N	2	GLU	2.9
3	C	65	ASN	2.9
1	M	535	LEU	2.9
1	M	65	HIS	2.8
3	O	126	VAL	2.8
3	C	54	GLU	2.8
1	M	10	VAL	2.8
1	M	377	VAL	2.8
1	M	549	LYS	2.8
1	M	428	GLN	2.8
1	M	152	PHE	2.8
1	M	223	LEU	2.8
1	M	491	ILE	2.8
1	M	572	THR	2.8
3	O	96	ILE	2.8
3	O	49	LEU	2.8
1	M	193	GLY	2.8
4	P	47	ASP	2.8
4	P	0	MET	2.7
3	O	6	PRO	2.7
1	M	211	ASP	2.7
2	N	99	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	447	ASN	2.7
2	N	8	ILE	2.7
1	M	203	THR	2.7
3	C	56	TRP	2.7
2	B	241	LYS	2.7
1	M	202	ASN	2.7
3	O	101	GLU	2.7
1	M	171	VAL	2.7
1	M	407	GLY	2.7
3	C	62	PHE	2.6
1	M	158	LEU	2.6
2	N	134	GLN	2.6
1	M	13	GLY	2.6
1	M	12	ALA	2.6
4	P	118	ILE	2.6
2	N	130	GLY	2.6
1	M	177	GLU	2.6
2	N	166	GLU	2.6
1	A	576	ALA	2.6
1	M	502	LEU	2.6
1	M	108	ASP	2.6
1	M	320	GLY	2.6
1	M	80	ASP	2.6
2	N	180	ASN	2.6
1	M	371	ILE	2.5
1	M	441	ASN	2.5
3	O	110	LYS	2.5
2	N	23	SER	2.5
1	M	558	ASP	2.5
1	M	62	PHE	2.5
2	N	62	CYS	2.5
1	M	390	ARG	2.5
2	N	64	SER	2.5
1	M	217	LEU	2.5
1	M	372	LYS	2.5
1	M	91	THR	2.5
1	M	475	THR	2.5
2	N	192	MET	2.5
3	O	11	MET	2.5
1	M	51	GLY	2.5
2	N	24	ALA	2.5
1	M	156	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	N	131	THR	2.5
1	M	361	ILE	2.5
1	M	433	GLU	2.4
1	M	39	TYR	2.4
1	M	86	VAL	2.4
1	M	194	GLY	2.4
1	M	87	HIS	2.4
3	O	14	THR	2.4
1	M	429	ALA	2.4
1	M	295	TRP	2.4
1	M	88	HIS	2.4
3	O	7	TYR	2.4
1	M	195	ALA	2.4
1	M	440	VAL	2.4
1	M	369	THR	2.4
1	M	197	ARG	2.4
2	N	125	ARG	2.4
4	D	0	MET	2.3
3	C	55	ALA	2.3
1	M	421	ASN	2.3
2	N	53	TYR	2.3
1	M	435	ARG	2.3
1	M	99	TRP	2.3
1	M	48	ALA	2.3
1	M	1	GLN	2.3
1	M	150	GLN	2.3
2	N	13	TYR	2.3
1	M	487	LYS	2.3
1	M	494	THR	2.3
1	M	488	ARG	2.3
1	M	423	ALA	2.3
1	M	209	THR	2.3
1	M	228	PHE	2.3
1	M	67	HIS	2.3
1	M	463	CYS	2.3
1	M	16	GLY	2.3
1	M	132	GLY	2.3
1	M	131	THR	2.3
3	O	54	GLU	2.3
1	M	100	GLY	2.3
2	N	9	GLU	2.3
1	M	545	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	358	MET	2.2
1	M	497	VAL	2.2
1	M	29	ASN	2.2
1	M	359	GLY	2.2
3	O	52	GLY	2.2
1	M	26	ALA	2.2
1	M	565	TYR	2.2
1	M	70	VAL	2.2
1	M	208	VAL	2.2
1	M	58	ASP	2.2
4	P	52	GLU	2.2
1	M	42	ARG	2.2
1	M	522	ALA	2.2
2	N	57	CYS	2.2
1	M	543	ASP	2.2
1	M	186	ASN	2.1
1	M	130	LYS	2.1
2	N	85	THR	2.1
2	N	89	LYS	2.1
1	M	537	GLU	2.1
1	M	179	THR	2.1
1	M	416	THR	2.1
1	M	196	GLY	2.1
2	N	108	HIS	2.1
3	C	60	VAL	2.1
2	N	242	PRO	2.1
2	N	6	LEU	2.1
1	M	182	GLN	2.1
1	M	532	HIS	2.0
1	A	299	ARG	2.0
2	N	124	SER	2.0
1	M	5	ALA	2.0
2	N	227	GLY	2.0
1	M	356	TYR	2.0
3	O	8	VAL	2.0
3	C	57	ALA	2.0
2	N	135	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

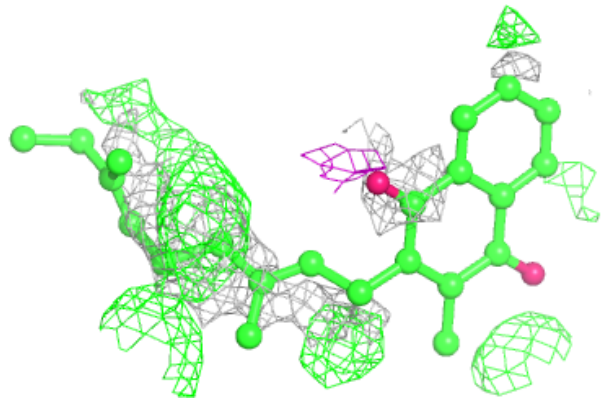
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

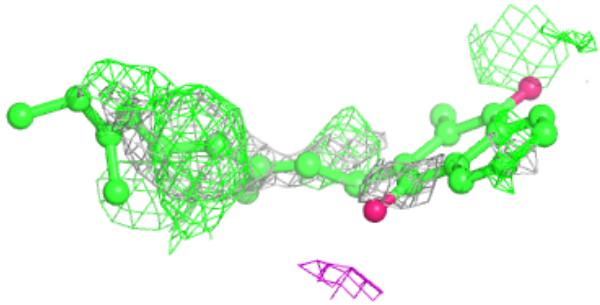
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MQ7	N	304	24/48	0.49	0.63	60,63,66,67	24
9	MQ7	D	701	24/48	0.69	0.56	43,45,46,47	24
5	FAD	M	601	53/53	0.84	0.29	41,61,89,91	0
8	SF4	N	303	8/8	0.95	0.12	40,42,43,44	0
7	F3S	N	302	7/7	0.96	0.10	48,50,55,55	0
7	F3S	B	302	7/7	0.97	0.11	27,28,29,30	0
5	FAD	A	601	53/53	0.97	0.18	17,19,22,22	0
8	SF4	B	303	8/8	0.97	0.15	23,24,24,25	0
6	FES	N	301	4/4	0.98	0.13	40,40,41,44	0
6	FES	B	301	4/4	0.99	0.16	19,20,20,20	0

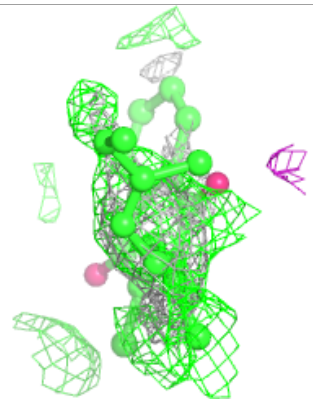
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MQ7 N 304:

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

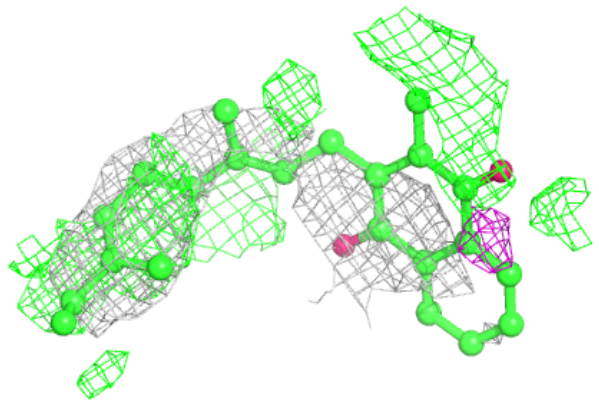


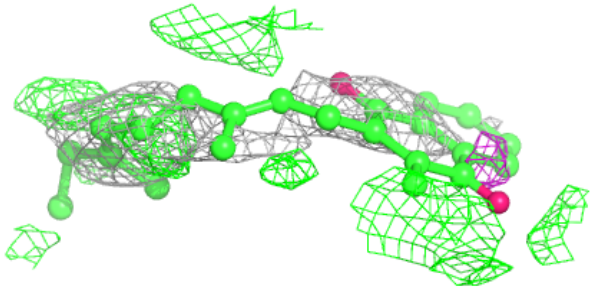


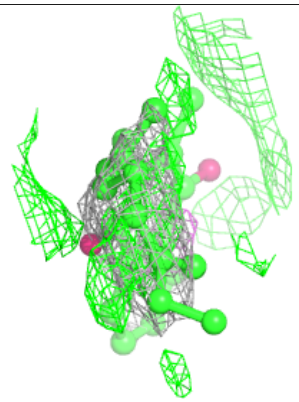


Electron density around MQ7 D 701:

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

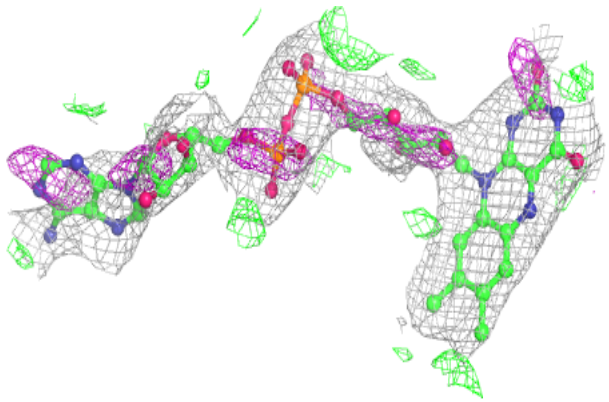


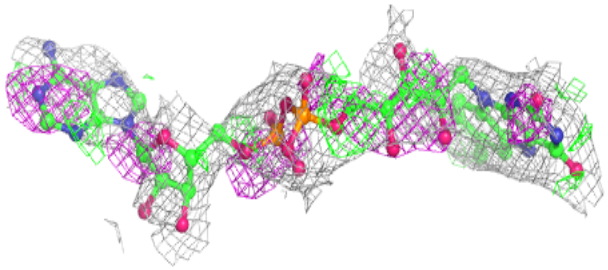


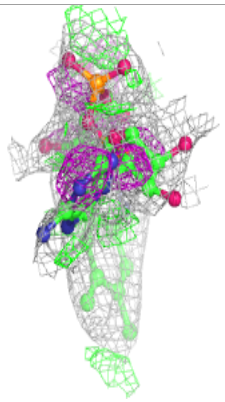


Electron density around FAD M 601:

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

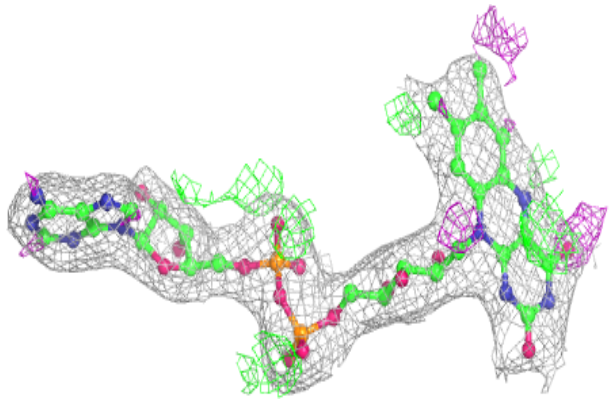


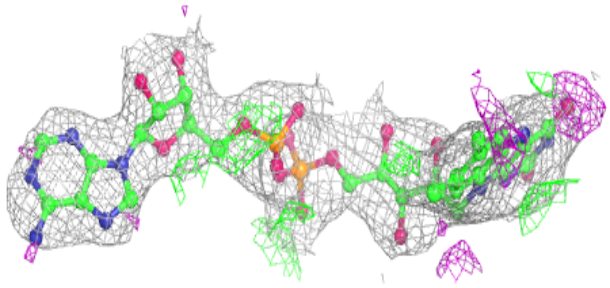


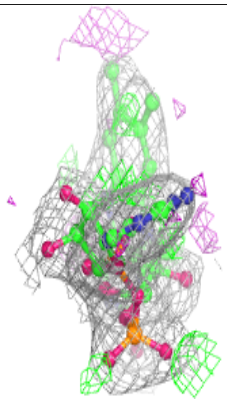


Electron density around FAD A 601:

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







6.5 Other polymers (i)

There are no such residues in this entry.