



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:55 PM UTC

PDB ID : 4KX6 / pdb_00004kx6
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

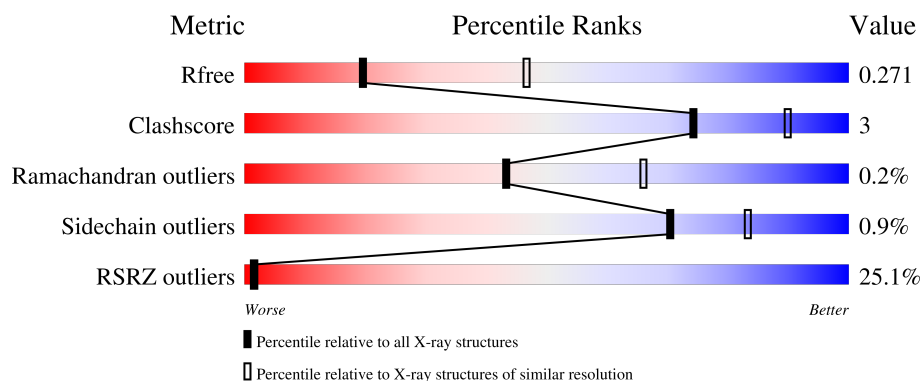
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	577	2% 92% 8%
1	M	577	63% 92% 8%
2	B	243	2% 92% 7%
2	N	243	43% 93% 7%

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Mol	Chain	Length	Quality of chain
3	C	130	
3	O	130	
4	D	119	
4	P	119	

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

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
1	A	577	Total	C	N	O	S	0	0	0
			4448	2775	802	840	31			
1	M	577	Total	C	N	O	S	0	0	0
			4448	2775	802	840	31			

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

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

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

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

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.

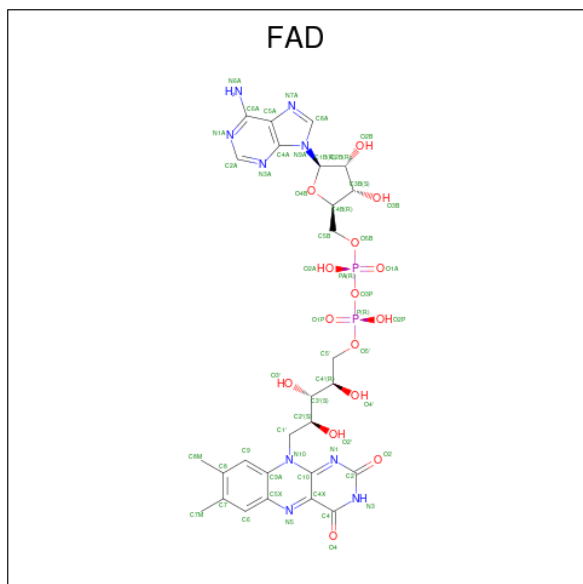
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

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

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



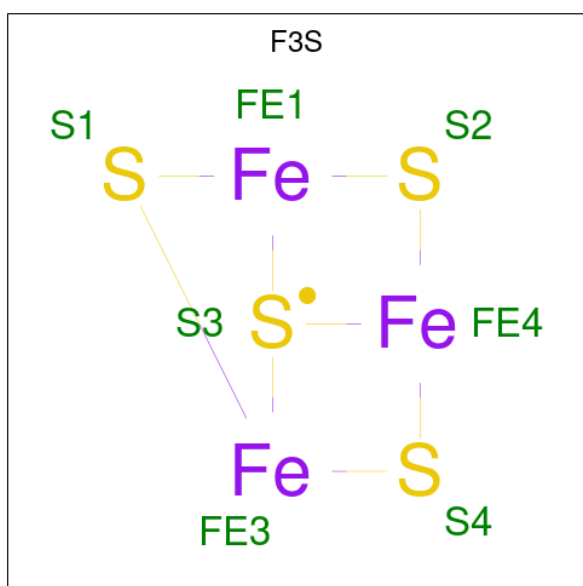
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	M	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



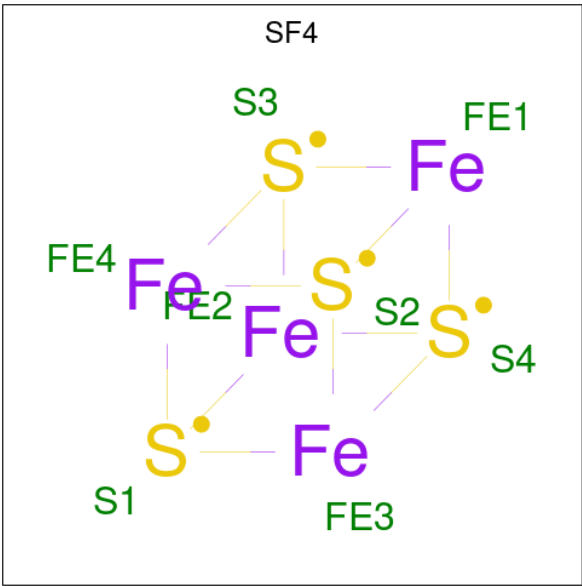
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			4	2	2		
6	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 7 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).



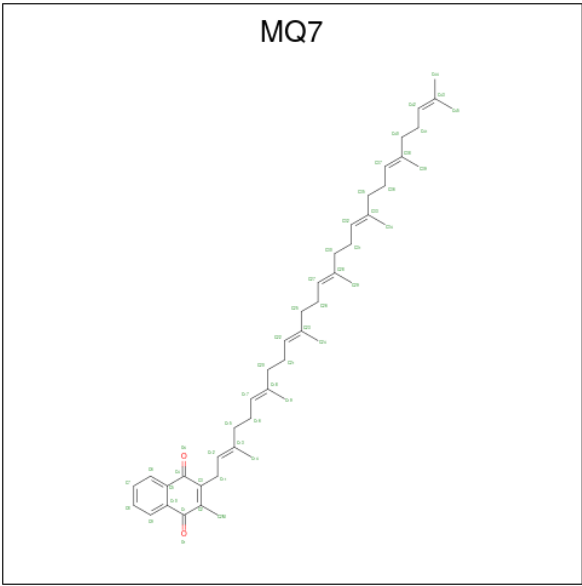
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			7	3	4		
7	N	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 9 is MENAQUINONE-7 (CCD ID: MQ7) (formula: C₄₆H₆₄O₂).



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

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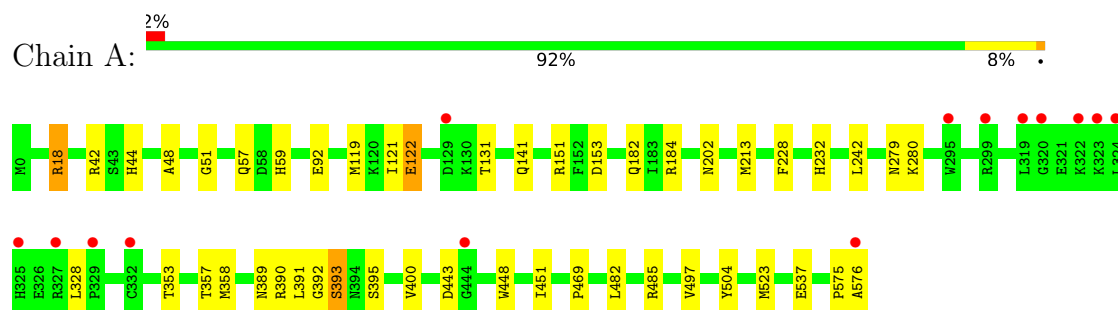
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	N	1	24	22	2	0	0

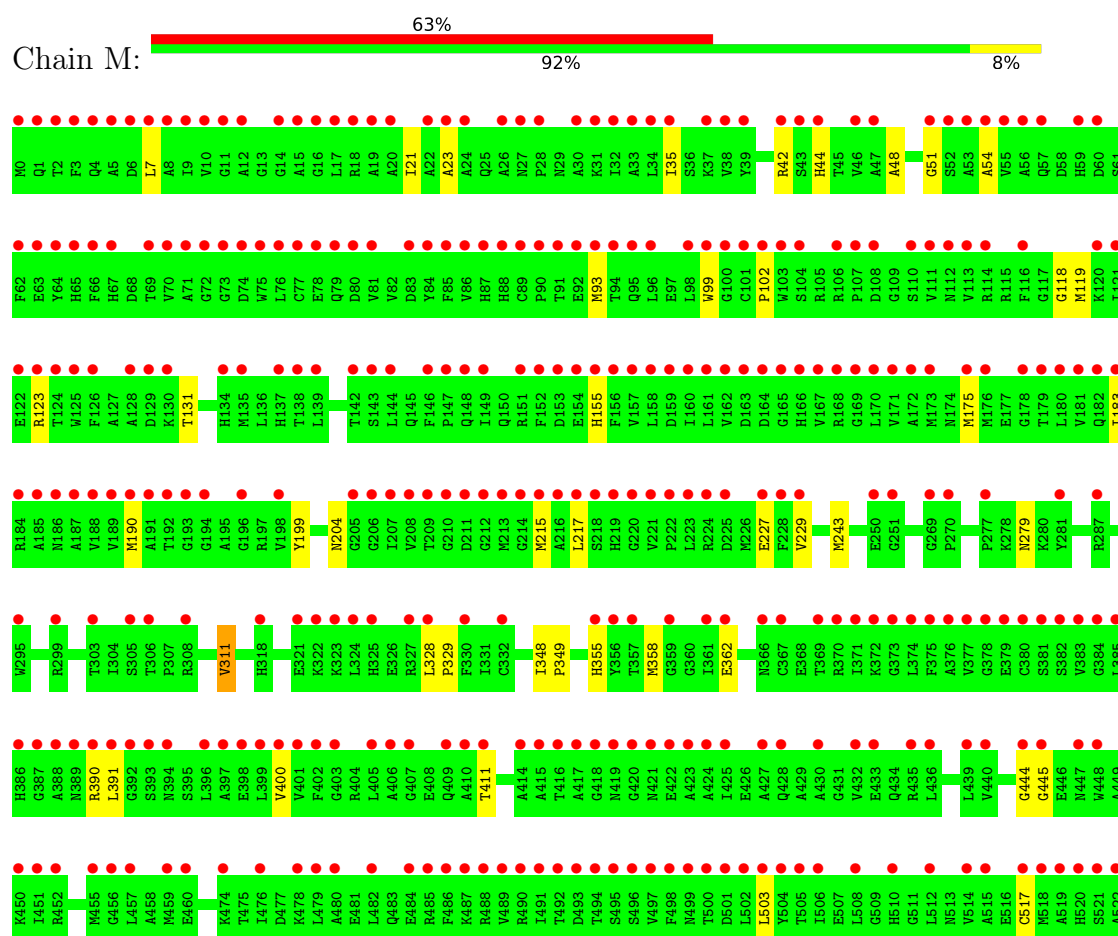
3 Residue-property plots

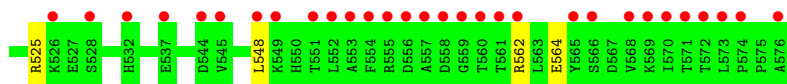
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

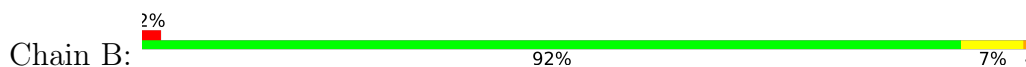


- Molecule 1: Fumarate reductase flavoprotein subunit

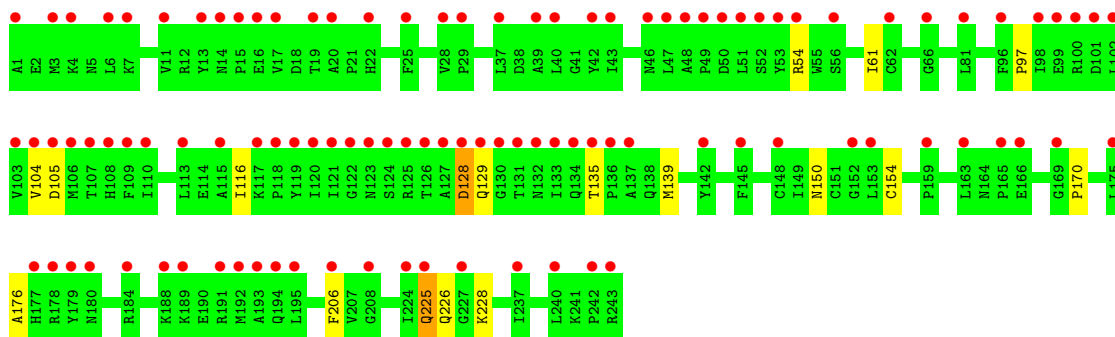
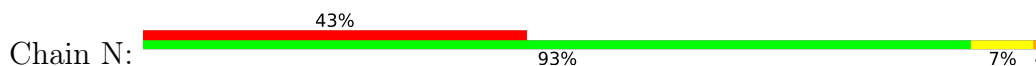




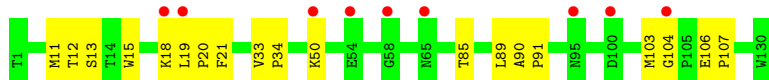
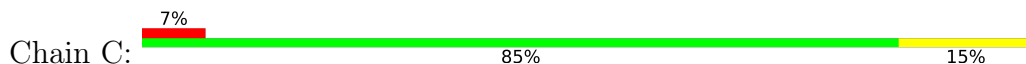
- Molecule 2: Fumarate reductase (Anaerobic), Fe-S subunit



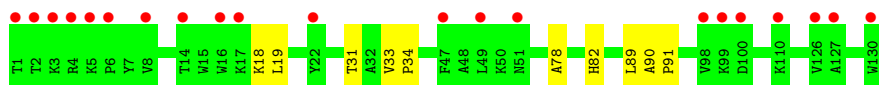
- Molecule 2: Fumarate reductase (Anaerobic), Fe-S subunit



- Molecule 3: Fumarate reductase subunit C



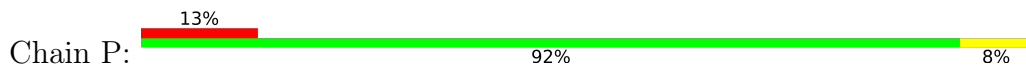
- Molecule 3: Fumarate reductase subunit C

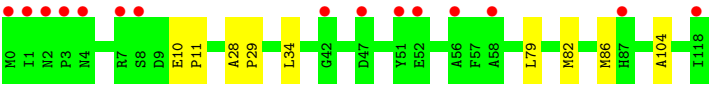


- Molecule 4: Fumarate reductase subunit D



- Molecule 4: Fumarate reductase subunit D





4 Data and refinement statistics

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 47.80 – 2.95	Depositor EDS
% Data completeness (in resolution range)	95.8 (47.80-2.95) 95.8 (47.80-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.7.0032, CNS	Depositor
R, R_{free}	0.240 , 0.280 (Not available) , 0.271	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)	0.32 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, MQ7, SF4, FES, F3S

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	0.48	0/4540	0.74	0/6139
1	M	0.48	0/4540	0.74	2/6139 (0.0%)
2	B	0.48	0/1930	0.76	3/2617 (0.1%)
2	N	0.49	0/1930	0.77	2/2617 (0.1%)
3	C	0.43	0/1093	0.77	1/1495 (0.1%)
3	O	0.46	0/1093	0.73	0/1495
4	D	0.42	0/956	0.75	0/1303
4	P	0.43	0/956	0.74	0/1303
All	All	0.47	0/17038	0.75	8/23108 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	17	VAL	N-CA-C	8.69	118.94	111.90
2	N	129	GLN	N-CA-C	7.65	122.92	112.90
3	C	18	LYS	N-CA-C	6.75	118.72	111.36
2	N	61	ILE	N-CA-C	6.35	117.05	111.90
2	B	65	CYS	N-CA-C	6.34	120.59	112.34
2	B	17	VAL	CB-CA-C	-6.26	105.29	111.30
1	M	355	HIS	N-CA-C	6.16	120.61	112.72
1	M	548	LEU	N-CA-C	-5.45	102.07	109.54

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	4448	0	4335	27	0
1	M	4448	0	4335	26	0
2	B	1887	0	1837	11	0
2	N	1887	0	1837	13	0
3	C	1057	0	1113	14	0
3	O	1057	0	1113	7	0
4	D	926	0	971	5	0
4	P	926	0	971	6	0
5	A	53	0	31	4	0
5	M	53	0	31	1	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	0	0
All	All	16828	0	16620	102	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 (102) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:HIS:NE2	5:A:601:FAD:HM83	1.82	0.94
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:119:MET:HE2	1:A:391:LEU:HD23	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:701:MQ7:O4	9:D:701:MQ7:C12	2.51	0.59
1:A:469:PRO:HB3	1:A:523:MET:HE1	1.86	0.58
2:B:206:PHE:HE2	3:C:89:LEU:HD22	1.70	0.57
2:B:62:CYS:SG	2:B:64:SER:OG	2.63	0.56
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
1:A:358:MET:HE3	1:A:389:ASN:HA	1.89	0.54
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
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
4:P:79:LEU:HD23	4:P:82:MET:HE3	1.93	0.51
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
1:A:443:ASP:OD1	1:A:443:ASP:C	2.53	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
1:A:141:GLN:HB3	2:B:118:PRO:O	2.13	0.47
1:M:183:ILE:N	1:M:183:ILE:HD12	2.29	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: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:M:190:MET:HE1	1:M:215:MET:HE3	1.97	0.46
1:A:448:TRP:CH2	1:A:504:TYR:HB3	2.51	0.46
1:M:243:MET:HE2	1:M:348:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:451:ILE:HG23	1:A:482:LEU:HD22	1.98	0.45
1:M:175:MET:HE3	1:M:503:LEU:HD13	1.98	0.45
2:B:100:ARG:O	2:B:101:ASP:C	2.59	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:M:102:PRO:HB2	2:N:139:MET:HE3	1.99	0.44
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
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:33:VAL:HG22	4:D:82:MET:HE2	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
4:D:57:PHE:O	4:D:60:SER:OG	2.33	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
1:M:119:MET:HE2	1:M:391:LEU:HD23	2.00	0.43
5:A:601:FAD:HM73	5:A:601:FAD:HM81	1.80	0.43
3:O:31:THR:HG23	3:O:78:ALA:HB1	2.00	0.43
1:A:213:MET:HE1	1:A:357:THR:HG21	2.01	0.42
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
1:A:392:GLY:O	1:A:393:SER:OG	2.30	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:11:MET:HE2	3:C:15:TRP:CG	2.54	0.41
1:M:243:MET:HE2	1:M:348:ILE:HD13	2.02	0.41
3:C:106:GLU:N	3:C:107:PRO:CD	2.83	0.41
1:M:199:TYR:CE1	1:M:229:VAL:HG11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

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	575/577 (100%)	556 (97%)	17 (3%)	2 (0%)	36	59
1	M	575/577 (100%)	540 (94%)	33 (6%)	2 (0%)	36	59
2	B	241/243 (99%)	232 (96%)	8 (3%)	1 (0%)	30	53
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%)	43	66

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 ⓘ

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%)	455 (99%)	5 (1%)	65	80
1	M	460/460 (100%)	458 (100%)	2 (0%)	84	92
2	B	205/205 (100%)	202 (98%)	3 (2%)	57	76
2	N	205/205 (100%)	201 (98%)	4 (2%)	48	71
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%)	96 (99%)	1 (1%)	68	82
All	All	1746/1746 (100%)	1731 (99%)	15 (1%)	70	83

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	42	ARG
1	A	122	GLU
1	A	485	ARG
1	A	537	GLU
2	B	64	SER
2	B	65	CYS
2	B	113	LEU
1	M	311	VAL
1	M	362	GLU
2	N	128	ASP

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Mol	Chain	Res	Type
2	N	135	THR
2	N	225	GLN
2	N	226	GLN
4	P	34	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	87	HIS
1	A	95	GLN
1	A	141	GLN
1	A	232	HIS
1	A	279	ASN
1	A	292	GLN
1	A	428	GLN
1	A	442	GLN
2	B	134	GLN
2	B	194	GLN
2	B	225	GLN
3	C	51	ASN
3	C	64	GLN
4	D	59	GLN
1	M	57	GLN
1	M	67	HIS
1	M	88	HIS
1	M	95	GLN
1	M	155	HIS
1	M	182	GLN
1	M	230	GLN
1	M	232	HIS
1	M	279	ASN
1	M	292	GLN
1	M	434	GLN
1	M	510	HIS
2	N	95	ASN
2	N	138	GLN
2	N	160	GLN
2	N	164	ASN
2	N	177	HIS
2	N	186	HIS
2	N	199	ASN

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Mol	Chain	Res	Type
2	N	226	GLN
3	O	72	ASN
4	P	59	GLN
4	P	83	HIS
4	P	84	HIS

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 oligosaccharides 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	N	301	2	0,4,4	-	-	-		
9	MQ7	D	701	-	25,25,49	2.07	2 (8%)	31,34,63	1.29	5 (16%)
8	SF4	N	303	2	0,12,12	-	-	-		
6	FES	B	301	2	0,4,4	-	-	-		
7	F3S	N	302	2	0,9,9	-	-	-		
9	MQ7	N	304	-	25,25,49	2.08	2 (8%)	31,34,63	1.63	5 (16%)
7	F3S	B	302	2	0,9,9	-	-	-		
8	SF4	B	303	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FAD	M	601	-	58,58,58	1.54	11 (18%)	85,89,89	1.59	20 (23%)
5	FAD	A	601	-	58,58,58	1.50	10 (17%)	85,89,89	1.64	18 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FES	N	301	2	-	-	0/1/1/1
9	MQ7	D	701	-	-	7/13/33/61	0/2/2/2
8	SF4	N	303	2	-	-	0/6/5/5
6	FES	B	301	2	-	-	0/1/1/1
7	F3S	N	302	2	-	-	0/3/3/3
9	MQ7	N	304	-	-	2/13/33/61	0/2/2/2
7	F3S	B	302	2	-	-	0/3/3/3
8	SF4	B	303	2	-	-	0/6/5/5
5	FAD	M	601	-	-	2/34/50/50	0/6/6/6
5	FAD	A	601	-	-	5/34/50/50	0/6/6/6

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	701	MQ7	C3-C2	8.35	1.50	1.35
9	N	304	MQ7	C3-C2	8.24	1.50	1.35
5	A	601	FAD	C9A-C5X	5.58	1.50	1.41
5	M	601	FAD	C9A-C5X	5.53	1.50	1.41
9	N	304	MQ7	C10-C5	5.35	1.49	1.40
9	D	701	MQ7	C10-C5	5.26	1.49	1.40
5	M	601	FAD	C5A-C4A	4.67	1.47	1.39
5	A	601	FAD	C5A-C4A	4.23	1.46	1.39
5	M	601	FAD	C8-C7	3.42	1.49	1.40
5	M	601	FAD	C5A-C6A	2.89	1.49	1.41
5	A	601	FAD	C8-C7	2.76	1.47	1.40
5	A	601	FAD	C8A-N7A	2.68	1.36	1.31
5	A	601	FAD	C5A-C6A	2.59	1.48	1.41
5	M	601	FAD	C8A-N7A	2.51	1.36	1.31
5	A	601	FAD	P-O3P	2.46	1.62	1.59
5	M	601	FAD	C4-N3	-2.43	1.34	1.38
5	A	601	FAD	C4A-N9A	-2.42	1.32	1.37
5	A	601	FAD	C5X-N5	-2.37	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	FAD	C4-N3	-2.35	1.34	1.38
5	A	601	FAD	C5A-N7A	-2.31	1.34	1.39
5	M	601	FAD	P-O3P	2.30	1.62	1.59
5	M	601	FAD	C5A-N7A	-2.23	1.35	1.39
5	M	601	FAD	PA-O3P	2.21	1.61	1.59
5	M	601	FAD	C5X-N5	-2.21	1.35	1.39
5	M	601	FAD	C4A-N9A	-2.10	1.33	1.37

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	FAD	C5A-C4A-N3A	-5.41	119.27	126.72
5	M	601	FAD	C5A-C4A-N3A	-5.32	119.39	126.72
9	N	304	MQ7	C14-C13-C15	5.27	124.38	115.23
5	M	601	FAD	N3A-C4A-N9A	4.01	133.98	127.17
5	A	601	FAD	N3A-C4A-N9A	3.93	133.85	127.17
5	A	601	FAD	C2A-N3A-C4A	3.90	121.34	111.83
5	A	601	FAD	N3A-C2A-N1A	-3.89	122.70	128.58
5	M	601	FAD	C4A-C5A-N7A	-3.79	106.25	110.58
5	M	601	FAD	C2A-N3A-C4A	3.74	120.96	111.83
5	A	601	FAD	C4A-C5A-N7A	-3.72	106.33	110.58
5	M	601	FAD	N3A-C2A-N1A	-3.65	123.06	128.58
9	N	304	MQ7	C15-C13-C12	-3.28	113.80	121.17
9	N	304	MQ7	C2M-C2-C3	-3.02	119.49	124.45
5	A	601	FAD	C4A-N9A-C8A	2.95	108.84	105.74
5	M	601	FAD	C4A-N9A-C8A	2.86	108.74	105.74
5	A	601	FAD	O4-C4-C4X	-2.84	119.03	126.53
9	D	701	MQ7	C16-C17-C18	-2.84	121.12	127.62
9	D	701	MQ7	C19-C18-C20	2.77	119.39	116.13
5	M	601	FAD	C5A-N7A-C8A	2.76	107.79	103.45
9	D	701	MQ7	C2M-C2-C3	-2.70	120.01	124.45
5	M	601	FAD	C4-C4X-N5	2.68	121.91	118.21
5	A	601	FAD	C6A-C5A-N7A	2.66	137.22	132.09
5	M	601	FAD	C4X-C10-N1	-2.62	118.18	124.59
5	A	601	FAD	C5A-N7A-C8A	2.58	107.51	103.45
5	M	601	FAD	C6A-C5A-N7A	2.55	137.01	132.09
9	D	701	MQ7	C11-C12-C13	-2.54	122.46	126.83
5	A	601	FAD	O2-C2-N1	-2.52	117.62	121.80
5	A	601	FAD	N9A-C8A-N7A	-2.46	110.44	113.94
5	A	601	FAD	C4X-C10-N1	-2.46	118.55	124.59
5	M	601	FAD	C4X-C10-N10	2.45	119.99	116.48
5	M	601	FAD	N9A-C8A-N7A	-2.36	110.58	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	FAD	C4-C4X-N5	2.35	121.45	118.21
5	A	601	FAD	C4X-C10-N10	2.31	119.78	116.48
5	A	601	FAD	C4-N3-C2	-2.25	121.65	125.64
5	M	601	FAD	C10-N1-C2	2.22	121.66	116.85
5	A	601	FAD	C9-C8-C7	2.21	122.94	119.69
5	A	601	FAD	C10-N1-C2	2.21	121.64	116.85
5	A	601	FAD	C4X-C4-N3	2.21	118.88	113.25
5	M	601	FAD	O2-C2-N1	-2.20	118.14	121.80
5	M	601	FAD	O4B-C1B-N9A	2.12	112.17	108.09
5	M	601	FAD	C2A-N1A-C6A	2.11	122.20	118.73
9	N	304	MQ7	C19-C18-C20	2.08	118.58	116.13
5	M	601	FAD	C4-N3-C2	-2.07	121.97	125.64
9	N	304	MQ7	C16-C17-C18	-2.07	122.89	127.62
5	M	601	FAD	C4X-C4-N3	2.05	118.46	113.25
5	M	601	FAD	O4-C4-C4X	-2.04	121.16	126.53
9	D	701	MQ7	C11-C3-C2	-2.03	121.41	124.89
5	M	601	FAD	C4'-C3'-C2'	-2.02	110.20	113.57

There are no chirality outliers.

All (16) torsion outliers are listed below:

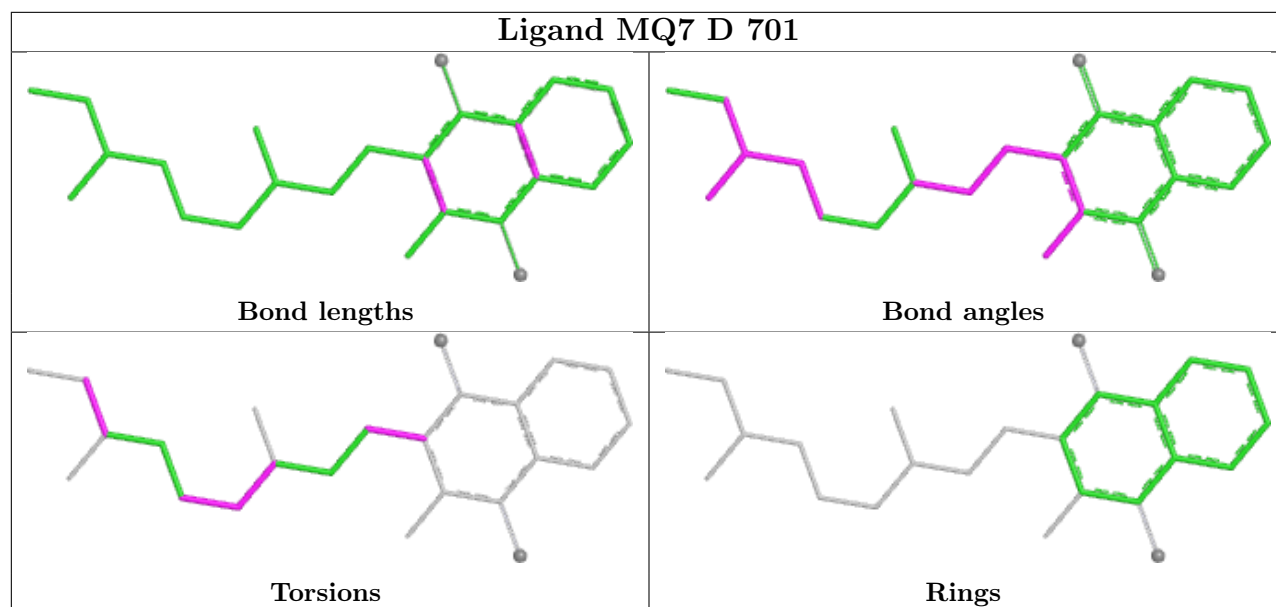
Mol	Chain	Res	Type	Atoms
5	A	601	FAD	N10-C1'-C2'-O2'
5	A	601	FAD	N10-C1'-C2'-C3'
5	A	601	FAD	PA-O3P-P-O5'
5	M	601	FAD	N10-C1'-C2'-O2'
5	M	601	FAD	N10-C1'-C2'-C3'
9	D	701	MQ7	C12-C11-C3-C2
9	D	701	MQ7	C12-C11-C3-C4
9	D	701	MQ7	C14-C13-C15-C16
9	N	304	MQ7	C14-C13-C15-C16
9	D	701	MQ7	C12-C13-C15-C16
9	N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

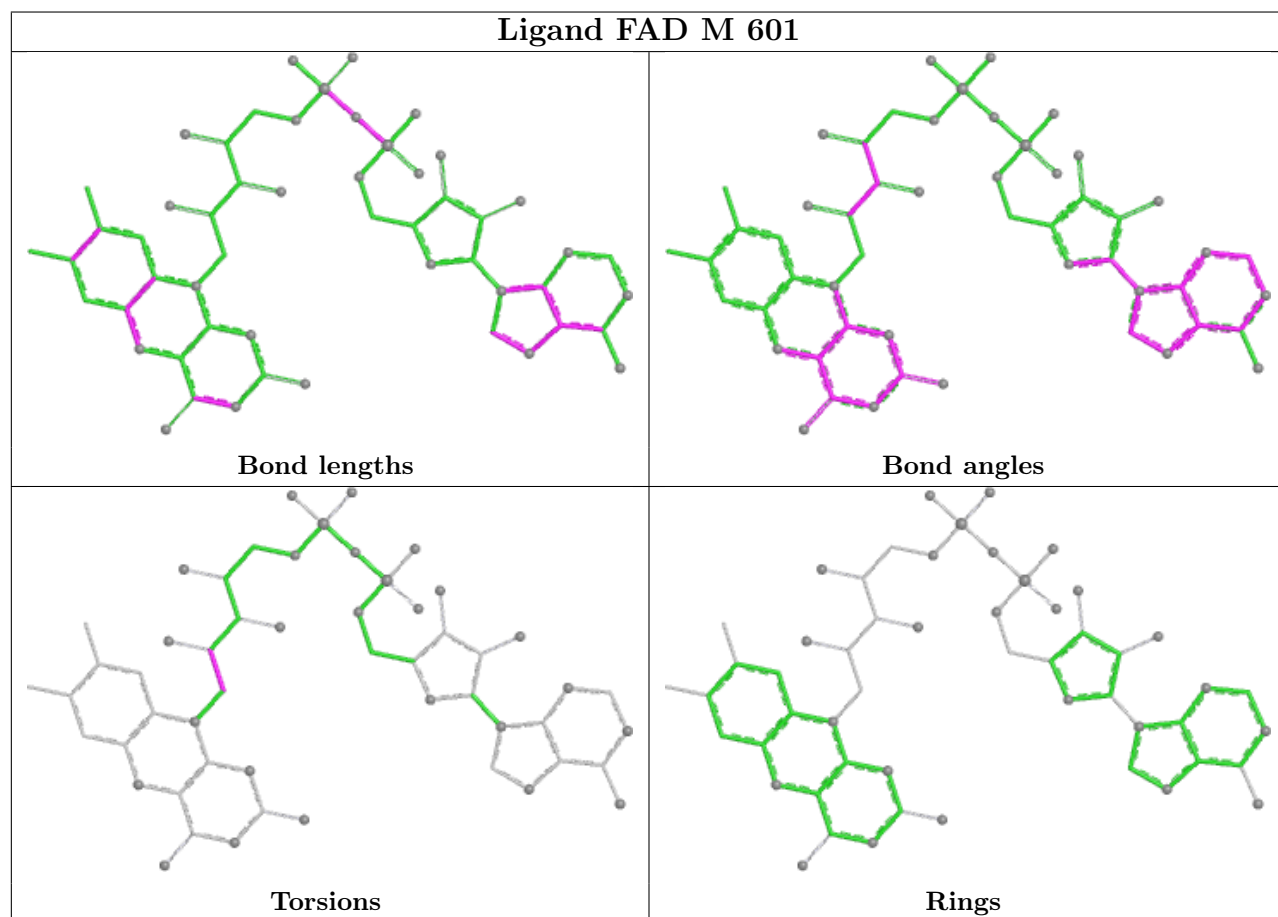
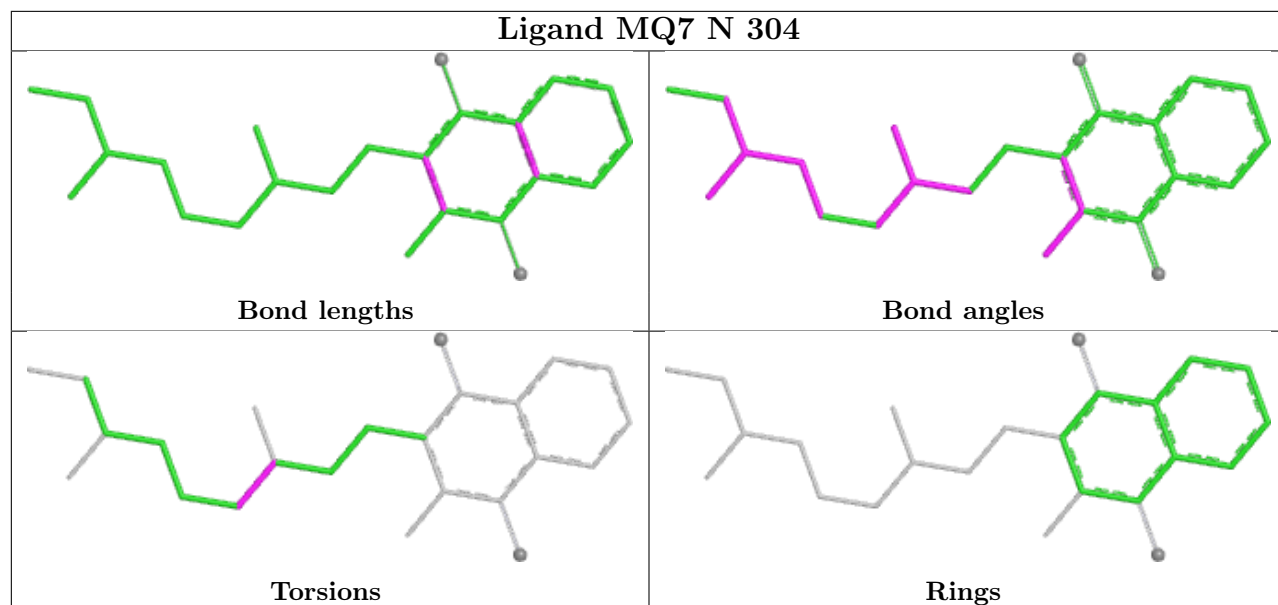
There are no ring outliers.

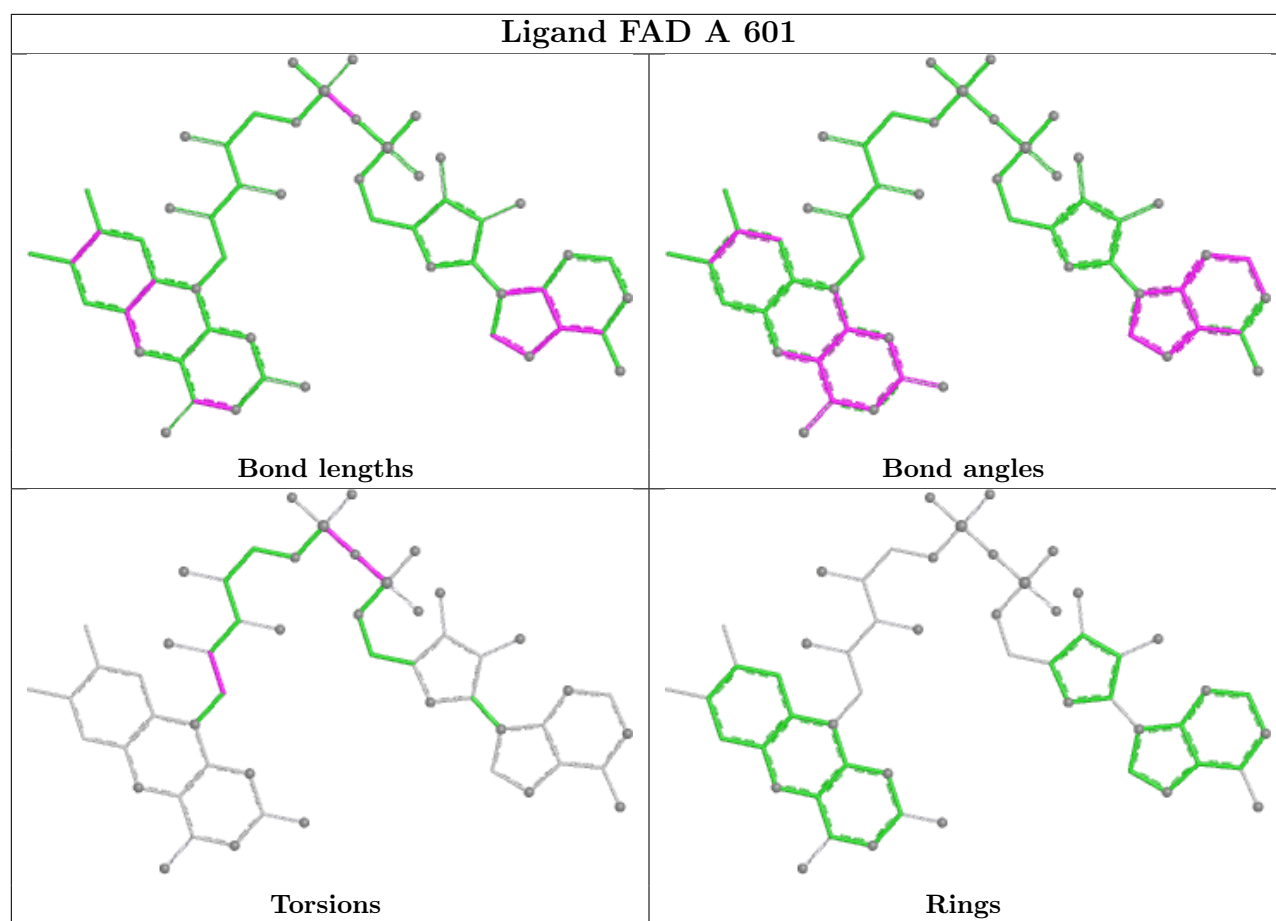
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	701	MQ7	3	0
5	M	601	FAD	1	0
5	A	601	FAD	4	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	577/577 (100%)	0.09	14 (2%) 59 51	29, 40, 64, 95	0
1	M	577/577 (100%)	2.58	362 (62%) 0 0	72, 113, 147, 165	0
2	B	243/243 (100%)	0.13	5 (2%) 63 55	30, 45, 64, 123	0
2	N	243/243 (100%)	2.05	104 (42%) 0 0	63, 97, 134, 141	0
3	C	130/130 (100%)	0.54	9 (6%) 23 19	50, 61, 92, 95	0
3	O	130/130 (100%)	0.99	21 (16%) 4 4	56, 79, 115, 145	0
4	D	119/119 (100%)	0.51	6 (5%) 34 28	48, 63, 86, 95	0
4	P	119/119 (100%)	0.98	15 (12%) 8 7	63, 77, 101, 140	0
All	All	2138/2138 (100%)	1.14	536 (25%) 1 1	29, 71, 132, 165	0

All (536) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	165	GLY	8.8
2	N	130	GLY	7.8
1	M	8	ALA	7.6
1	M	188	VAL	7.1
1	M	376	ALA	7.1
1	M	402	PHE	6.7
1	M	210	GLY	6.5
1	M	176	MET	6.5
1	M	189	VAL	6.5
1	M	557	ALA	6.4
1	M	560	THR	6.2
1	M	211	ASP	6.0
1	M	209	THR	6.0
1	M	411	THR	5.9
1	M	125	TRP	5.8
1	M	172	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
2	N	127	ALA	5.7
1	M	32	ILE	5.7
1	M	295	TRP	5.7
1	M	192	THR	5.7
1	M	576	ALA	5.6
4	D	118	ILE	5.6
1	M	170	LEU	5.6
1	M	55	VAL	5.5
1	M	77	CYS	5.5
1	M	163	ASP	5.5
1	M	193	GLY	5.4
1	M	375	PHE	5.4
1	M	573	LEU	5.4
1	M	56	ALA	5.4
1	M	380	CYS	5.4
1	M	223	LEU	5.3
1	M	377	VAL	5.3
1	M	405	LEU	5.3
1	M	161	LEU	5.2
1	M	222	PRO	5.2
1	M	12	ALA	5.2
1	M	99	TRP	5.2
1	M	169	GLY	5.1
1	M	491	ILE	5.1
4	P	1	ILE	5.1
1	M	386	HIS	5.0
1	M	10	VAL	5.0
1	M	207	ILE	5.0
1	M	180	LEU	5.0
1	A	576	ALA	5.0
1	M	498	PHE	5.0
1	M	574	PRO	5.0
1	M	9	ILE	4.9
1	M	6	ASP	4.9
1	M	187	ALA	4.9
1	M	221	VAL	4.9
1	M	486	PHE	4.9
1	M	553	ALA	4.8
1	M	23	ALA	4.8
4	P	51	TYR	4.8
1	M	156	PHE	4.8
1	M	492	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	M	11	GLY	4.7
2	N	102	LEU	4.7
2	N	240	LEU	4.7
1	M	497	VAL	4.7
1	M	500	THR	4.6
1	M	502	LEU	4.6
2	N	6	LEU	4.6
1	M	519	ALA	4.6
1	M	162	VAL	4.6
2	N	98	ILE	4.6
2	N	133	ILE	4.6
1	M	440	VAL	4.6
1	M	167	VAL	4.5
1	M	98	LEU	4.5
1	M	212	GLY	4.5
1	M	86	VAL	4.5
1	M	299	ARG	4.5
1	M	171	VAL	4.4
1	M	96	LEU	4.4
1	M	43	SER	4.4
1	M	17	LEU	4.4
1	M	214	GLY	4.4
1	M	385	LEU	4.4
1	M	374	LEU	4.4
1	M	436	LEU	4.4
1	M	390	ARG	4.3
1	M	7	LEU	4.3
1	M	447	ASN	4.3
1	M	379	GLU	4.3
1	M	160	ILE	4.2
2	N	52	SER	4.2
2	N	120	ILE	4.2
2	N	131	THR	4.2
1	M	66	PHE	4.2
1	M	166	HIS	4.2
1	M	372	LYS	4.2
3	O	6	PRO	4.2
1	M	406	ALA	4.2
2	N	49	PRO	4.2
2	N	99	GLU	4.2
1	M	399	LEU	4.1
1	M	152	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	M	493	ASP	4.1
2	N	180	ASN	4.1
1	M	424	ALA	4.1
1	M	129	ASP	4.1
1	M	217	LEU	4.1
2	N	137	ALA	4.1
1	M	487	LYS	4.1
2	N	101	ASP	4.0
1	M	361	ILE	4.0
1	M	504	TYR	4.0
1	M	378	GLY	4.0
1	M	33	ALA	4.0
1	M	124	THR	4.0
2	N	184	ARG	4.0
1	M	84	TYR	4.0
1	M	24	ALA	3.9
1	M	191	ALA	3.9
4	P	52	GLU	3.9
1	M	100	GLY	3.9
2	N	242	PRO	3.9
1	M	59	HIS	3.9
1	M	324	LEU	3.8
1	M	482	LEU	3.8
1	M	164	ASP	3.8
2	N	225	GLN	3.8
2	N	126	THR	3.8
1	M	130	LYS	3.8
2	N	17	VAL	3.8
2	N	47	LEU	3.8
2	N	166	GLU	3.8
1	M	81	VAL	3.8
1	M	370	ARG	3.8
2	N	11	VAL	3.8
3	O	130	TRP	3.8
1	M	173	MET	3.8
1	M	121	ILE	3.7
1	A	323	LYS	3.7
1	M	323	LYS	3.7
2	N	108	HIS	3.7
2	N	136	PRO	3.7
1	M	89	CYS	3.7
2	N	132	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	M	107	PRO	3.7
1	M	428	GLN	3.7
1	M	168	ARG	3.7
4	P	3	PRO	3.7
1	M	65	HIS	3.7
1	M	158	LEU	3.7
1	M	93	MET	3.7
1	M	126	PHE	3.7
2	N	109	PHE	3.7
1	M	371	ILE	3.7
1	M	410	ALA	3.7
1	M	116	PHE	3.6
1	M	205	GLY	3.6
1	M	398	GLU	3.6
1	M	70	VAL	3.6
1	M	181	VAL	3.6
1	M	87	HIS	3.6
1	M	190	MET	3.6
1	M	401	VAL	3.6
1	M	34	LEU	3.6
1	M	53	ALA	3.6
1	M	427	ALA	3.6
1	M	478	LYS	3.6
2	N	107	THR	3.6
2	N	192	MET	3.6
1	M	445	GLY	3.5
1	M	85	PHE	3.5
1	M	506	ILE	3.5
1	M	139	LEU	3.5
1	M	31	LYS	3.5
1	M	91	THR	3.5
1	M	208	VAL	3.5
1	M	383	VAL	3.5
1	M	448	TRP	3.5
1	M	565	TYR	3.5
1	M	415	ALA	3.5
2	N	123	ASN	3.5
4	P	56	ALA	3.5
1	M	367	CYS	3.4
1	M	373	GLY	3.4
2	N	122	GLY	3.4
1	M	80	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	M	108	ASP	3.4
2	N	20	ALA	3.4
1	M	508	LEU	3.4
1	M	28	PRO	3.4
1	M	183	ILE	3.4
2	N	119	TYR	3.4
2	N	134	GLN	3.4
2	N	25	PHE	3.4
2	N	103	VAL	3.4
1	M	19	ALA	3.4
1	M	369	THR	3.4
1	M	561	THR	3.4
4	D	0	MET	3.4
1	M	488	ARG	3.3
1	M	62	PHE	3.3
2	N	153	LEU	3.3
3	O	3	LYS	3.3
1	M	213	MET	3.3
1	M	480	ALA	3.3
1	M	518	MET	3.3
2	B	1	ALA	3.3
1	M	123	ARG	3.3
1	M	220	GLY	3.3
1	M	407	GLY	3.3
2	N	106	MET	3.3
2	N	237	ILE	3.3
2	N	22	HIS	3.3
1	M	450	LYS	3.3
2	N	193	ALA	3.3
1	A	299	ARG	3.3
1	M	46	VAL	3.3
1	M	182	GLN	3.3
1	A	129	ASP	3.2
1	M	120	LYS	3.2
2	N	14	ASN	3.2
1	M	15	ALA	3.2
1	M	229	VAL	3.2
1	M	206	GLY	3.2
1	M	83	ASP	3.2
1	M	396	LEU	3.2
2	N	178	ARG	3.2
1	M	251	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
4	P	0	MET	3.2
1	M	451	ILE	3.2
1	M	476	ILE	3.2
1	M	38	VAL	3.2
2	N	28	VAL	3.2
1	M	35	ILE	3.2
1	M	435	ARG	3.2
1	M	57	GLN	3.2
1	A	320	GLY	3.2
1	M	503	LEU	3.1
2	N	179	TYR	3.1
2	N	56	SER	3.1
2	N	125	ARG	3.1
1	M	128	ALA	3.1
1	M	499	ASN	3.1
1	M	322	LYS	3.1
1	M	400	VAL	3.1
3	O	1	THR	3.1
1	A	324	LEU	3.1
1	M	37	LYS	3.1
1	M	52	SER	3.1
1	M	101	CYS	3.1
1	M	423	ALA	3.1
1	M	330	PHE	3.1
1	M	444	GLY	3.1
1	M	92	GLU	3.1
2	N	1	ALA	3.1
1	M	3	PHE	3.1
2	N	175	LEU	3.1
1	M	216	ALA	3.1
1	A	325	HIS	3.1
2	N	145	PHE	3.1
1	M	27	ASN	3.1
1	M	421	ASN	3.1
1	M	384	GLY	3.1
1	M	416	THR	3.1
1	M	569	LYS	3.1
1	M	571	THR	3.1
1	M	392	GLY	3.0
1	M	403	GLY	3.0
2	N	54	ARG	3.0
1	M	147	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	M	2	THR	3.0
2	N	128	ASP	3.0
3	C	65	ASN	3.0
3	C	100	ASP	3.0
2	N	16	GLU	3.0
1	M	134	HIS	3.0
1	M	219	HIS	3.0
1	M	228	PHE	3.0
1	M	510	HIS	3.0
3	O	16	TRP	3.0
2	N	142	TYR	3.0
2	B	197	SER	3.0
1	M	555	ARG	3.0
2	N	53	TYR	3.0
1	M	552	LEU	3.0
2	N	208	GLY	3.0
1	M	532	HIS	3.0
1	A	295	TRP	2.9
1	M	114	ARG	2.9
1	M	559	GLY	2.9
1	M	90	PRO	2.9
1	M	417	ALA	2.9
3	O	8	VAL	2.9
1	M	425	ILE	2.9
1	M	26	ALA	2.9
1	M	551	THR	2.9
1	M	359	GLY	2.9
1	M	4	GLN	2.9
1	M	356	TYR	2.9
1	M	218	SER	2.9
2	N	4	LYS	2.9
2	N	206	PHE	2.9
1	M	490	ARG	2.9
1	M	185	ALA	2.9
1	M	501	ASP	2.9
4	D	9	ASP	2.9
1	M	179	THR	2.9
1	M	144	LEU	2.9
1	M	135	MET	2.8
1	M	78	GLU	2.8
1	M	430	ALA	2.8
1	M	514	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	51	GLY	2.8
2	N	169	GLY	2.8
1	M	39	TYR	2.8
1	M	545	VAL	2.8
1	M	391	LEU	2.8
1	M	439	LEU	2.8
2	N	113	LEU	2.8
2	N	13	TYR	2.8
1	M	325	HIS	2.8
1	M	102	PRO	2.8
2	N	118	PRO	2.8
1	M	328	LEU	2.8
1	M	418	GLY	2.8
1	M	76	LEU	2.7
1	M	149	ILE	2.7
1	M	548	LEU	2.7
2	N	3	MET	2.7
1	M	186	ASN	2.7
4	P	4	ASN	2.7
2	N	105	ASP	2.7
1	M	42	ARG	2.7
1	M	30	ALA	2.7
1	M	517	CYS	2.7
2	N	110	ILE	2.7
1	M	44	HIS	2.7
2	N	117	LYS	2.7
1	M	558	ASP	2.7
3	C	104	GLY	2.7
3	O	100	ASP	2.7
2	N	37	LEU	2.7
1	M	0	MET	2.7
3	O	22	TYR	2.7
1	M	389	ASN	2.7
1	M	184	ARG	2.7
1	M	572	THR	2.7
1	M	113	VAL	2.7
1	M	157	VAL	2.7
1	M	484	GLU	2.7
1	M	22	ALA	2.7
1	M	397	ALA	2.7
2	B	243	ARG	2.7
1	M	270	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	153	ASP	2.7
1	M	111	VAL	2.7
4	P	7	ARG	2.6
1	M	94	THR	2.6
1	M	60	ASP	2.6
1	M	549	LYS	2.6
2	N	194	GLN	2.6
1	M	71	ALA	2.6
1	M	215	MET	2.6
1	M	112	ASN	2.6
2	N	104	VAL	2.6
3	O	51	ASN	2.6
4	P	118	ILE	2.6
1	M	388	ALA	2.6
1	M	496	SER	2.6
2	N	66	GLY	2.6
1	M	570	ILE	2.6
1	M	95	GLN	2.6
3	C	95	ASN	2.6
4	P	2	ASN	2.6
1	M	515	ALA	2.6
2	N	188	LYS	2.6
2	N	135	THR	2.6
1	M	122	GLU	2.6
1	M	20	ALA	2.6
3	O	47	PHE	2.6
4	D	117	THR	2.5
1	M	63	GLU	2.5
2	N	129	GLN	2.5
1	A	327	ARG	2.5
1	M	151	ARG	2.5
1	M	137	HIS	2.5
2	N	51	LEU	2.5
1	M	196	GLY	2.5
2	N	227	GLY	2.5
3	C	58	GLY	2.5
3	O	126	VAL	2.5
1	M	409	GLN	2.5
1	M	494	THR	2.5
2	N	96	PHE	2.5
1	M	327	ARG	2.5
2	N	100	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	155	HIS	2.5
2	N	177	HIS	2.5
1	M	479	LEU	2.5
1	M	16	GLY	2.5
1	M	420	GLY	2.5
3	O	98	VAL	2.5
1	M	321	GLU	2.5
1	M	520	HIS	2.5
1	M	366	ASN	2.5
2	N	148	CYS	2.5
1	M	566	SER	2.4
1	M	308	ARG	2.4
1	M	522	ALA	2.4
2	N	48	ALA	2.4
2	N	19	THR	2.4
1	M	74	ASP	2.4
1	M	556	ASP	2.4
1	M	198	VAL	2.4
1	M	64	TYR	2.4
1	M	88	HIS	2.4
4	D	84	HIS	2.4
3	C	19	LEU	2.4
1	M	460	GLU	2.4
1	M	1	GLN	2.4
1	M	505	THR	2.4
1	M	512	LEU	2.4
2	N	29	PRO	2.4
1	A	322	LYS	2.4
1	M	387	GLY	2.4
1	A	332	CYS	2.4
3	C	50	LYS	2.4
3	O	5	LYS	2.4
2	N	124	SER	2.4
1	M	277	PRO	2.4
1	M	18	ARG	2.3
1	M	432	VAL	2.3
2	N	191	ARG	2.3
2	N	243	ARG	2.3
1	M	554	PHE	2.3
1	M	250	GLU	2.3
1	M	110	SER	2.3
1	M	306	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	485	ARG	2.3
1	M	489	VAL	2.3
1	M	332	CYS	2.3
2	N	62	CYS	2.3
1	M	148	GLN	2.3
1	M	382	SER	2.3
1	M	138	THR	2.3
1	M	394	ASN	2.3
2	N	39	ALA	2.3
1	M	159	ASP	2.3
1	M	544	ASP	2.3
1	M	318	HIS	2.3
1	M	104	SER	2.3
1	M	526	LYS	2.3
3	O	99	LYS	2.3
1	M	287	ARG	2.3
2	N	152	GLY	2.3
1	M	69	THR	2.3
1	M	143	SER	2.3
1	M	224	ARG	2.3
1	M	305	SER	2.3
3	O	14	THR	2.3
1	M	14	GLY	2.3
2	B	71	ASN	2.2
1	M	67	HIS	2.2
2	N	159	PRO	2.2
1	M	154	GLU	2.2
4	D	1	ILE	2.2
1	M	355	HIS	2.2
1	M	452	ARG	2.2
2	N	165	PRO	2.2
1	M	194	GLY	2.2
1	M	175	MET	2.2
1	A	319	LEU	2.2
2	N	163	LEU	2.2
2	N	189	LYS	2.2
3	O	49	LEU	2.2
2	N	43	ILE	2.2
1	M	225	ASP	2.2
1	A	329	PRO	2.2
1	M	455	MET	2.2
4	P	8	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	146	PHE	2.2
3	C	18	LYS	2.2
2	N	81	LEU	2.2
1	M	433	GLU	2.2
4	P	47	ASP	2.2
1	M	459	MET	2.2
1	M	72	GLY	2.2
1	M	73	GLY	2.2
1	M	75	TRP	2.2
1	M	457	LEU	2.2
1	M	227	GLU	2.2
4	P	87	HIS	2.1
2	N	7	LYS	2.1
1	A	444	GLY	2.1
3	O	2	THR	2.1
1	M	103	TRP	2.1
1	M	5	ALA	2.1
1	M	393	SER	2.1
1	M	414	ALA	2.1
1	M	521	SER	2.1
1	M	422	GLU	2.1
3	C	54	GLU	2.1
3	O	4	ARG	2.1
1	M	178	GLY	2.1
2	N	40	LEU	2.1
1	M	381	SER	2.1
2	N	121	ILE	2.1
2	N	224	ILE	2.1
1	M	474	LYS	2.1
2	N	15	PRO	2.1
1	M	269	GLY	2.1
2	N	195	LEU	2.1
1	M	562	ARG	2.1
2	N	42	TYR	2.1
2	N	46	ASN	2.1
1	M	106	ARG	2.1
1	M	357	THR	2.1
1	M	54	ALA	2.1
3	O	127	ALA	2.1
1	M	281	TYR	2.1
1	M	528	SER	2.0
2	B	146	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	79	GLN	2.0
1	M	419	ASN	2.0
1	M	456	GLY	2.0
1	M	303	THR	2.0
1	M	47	ALA	2.0
2	N	50	ASP	2.0
1	M	362	GLU	2.0
3	O	17	LYS	2.0
3	O	110	LYS	2.0
1	M	495	SER	2.0
1	M	568	VAL	2.0
4	P	42	GLY	2.0
1	M	142	THR	2.0
2	N	115	ALA	2.0
4	P	58	ALA	2.0
1	M	537	GLU	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.

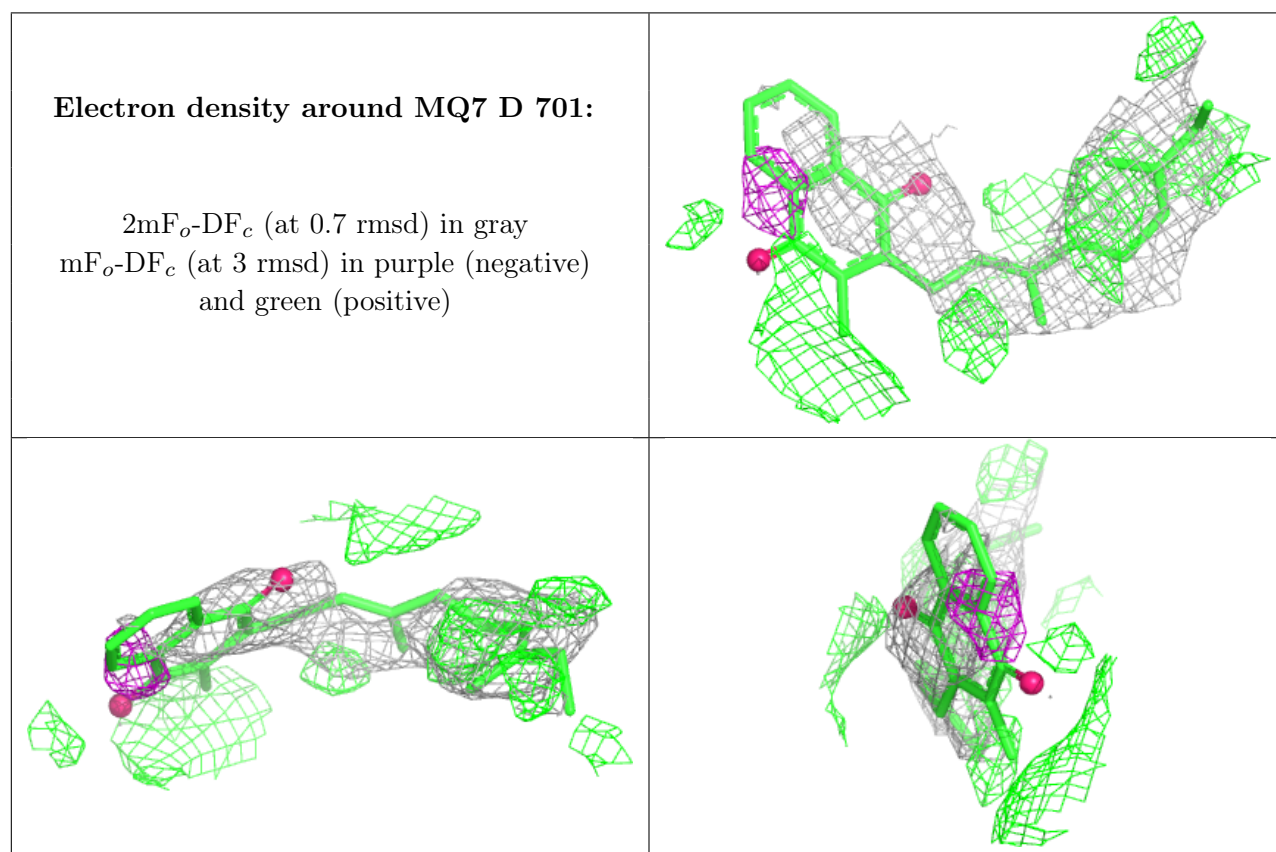
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	MQ7	D	701	24/48	0.65	0.42	43,45,46,47	24
9	MQ7	N	304	24/48	0.67	0.49	60,63,66,67	24
5	FAD	M	601	53/53	0.80	0.16	41,61,89,91	0
7	F3S	N	302	7/7	0.94	0.09	48,50,55,55	0
8	SF4	N	303	8/8	0.94	0.08	40,42,43,44	0
5	FAD	A	601	53/53	0.96	0.08	17,19,22,22	0
7	F3S	B	302	7/7	0.96	0.07	27,28,29,30	0

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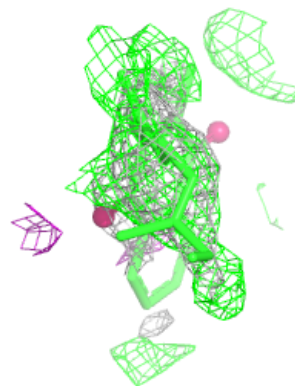
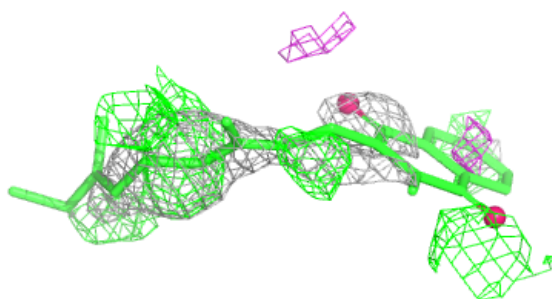
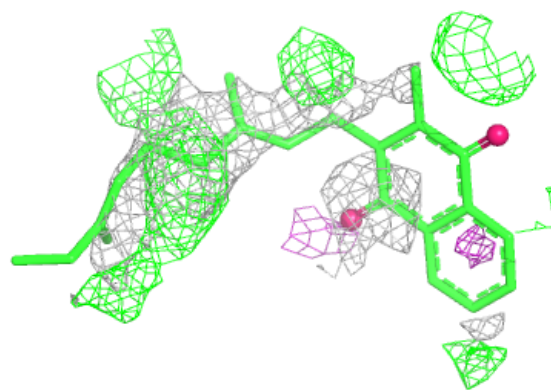
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SF4	B	303	8/8	0.97	0.05	23,24,24,25	0
6	FES	B	301	4/4	0.99	0.03	19,20,20,20	0
6	FES	N	301	4/4	0.99	0.07	40,40,41,44	0

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.

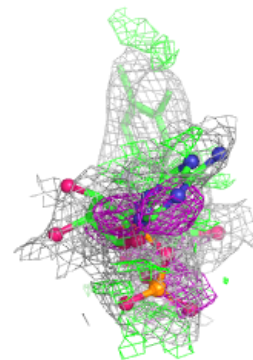
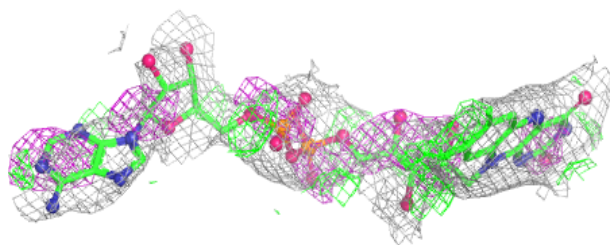
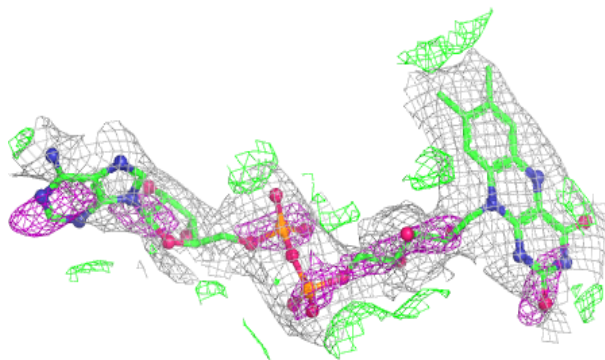


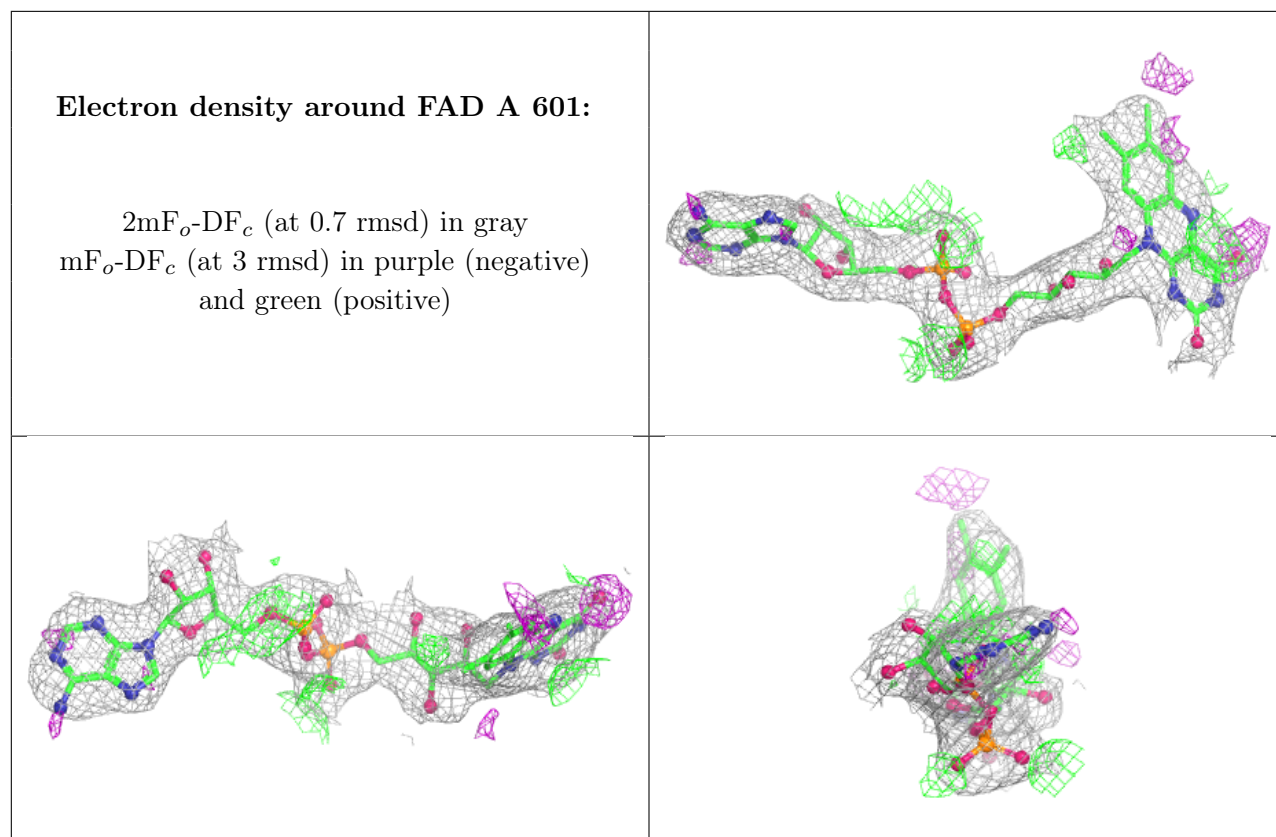
Electron density around MQ7 N 304:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.