



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2021 – 03:43 PM EDT

PDB ID : 2B76
Title : E. coli Quinol fumarate reductase FrdA E49Q mutation
Authors : Maklashina, E.; Iverson, T.M.; Sher, Y.; Kotlyar, V.; Mirza, O.; Andrell, J.;
Hudson, J.M.; Armstrong, F.A.; Cecchini, G.
Deposited on : 2005-10-03
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

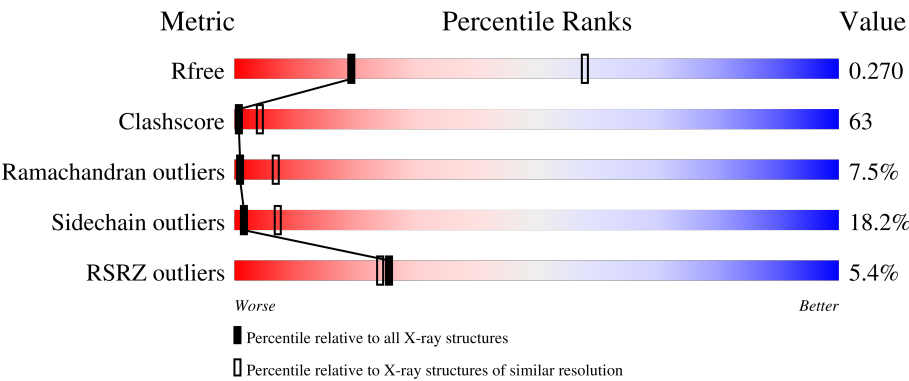
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	602	<div><div></div><div>28%41%21%5%.</div></div>
1	M	602	<div>16%</div> <div><div></div><div>24%56%13%. 5%</div></div>
2	B	243	<div>%</div> <div><div></div><div>35%54%9%.</div></div>
2	N	243	<div>5%</div> <div><div></div><div>21%59%19%.</div></div>
3	C	130	<div></div> <div><div></div><div>31%54%15%.</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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
10	MQ7	D	700	-	-	-	X
10	MQ7	P	800	-	-	-	X
5	FLC	A	702	-	-	X	-
5	FLC	M	802	-	-	-	X
9	SF4	N	246	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16840 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	803	839	31			
1	M	572	Total	C	N	O	S	0	0	0
			4414	2752	798	833	31			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	GLN	GLU	engineered mutation	GB P00363
M	49	GLN	GLU	engineered mutation	GB P00363

- Molecule 2 is a protein called Fumarate reductase iron-sulfur protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	19			
2	N	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	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
			1058	720	166	169	3			
3	O	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			

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

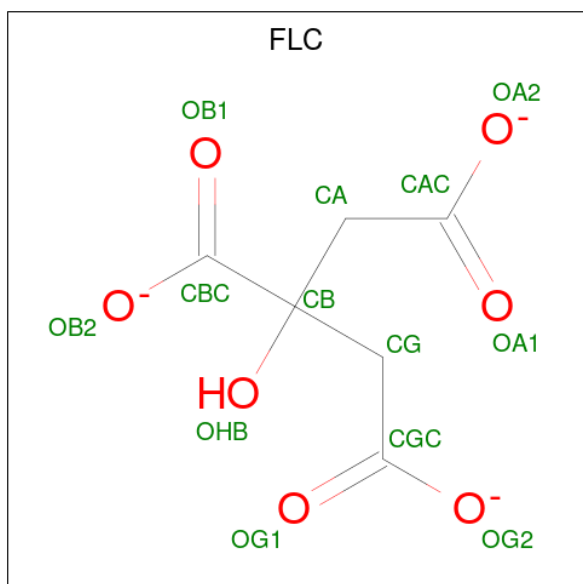
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

Continued on next page...

Continued from previous page...

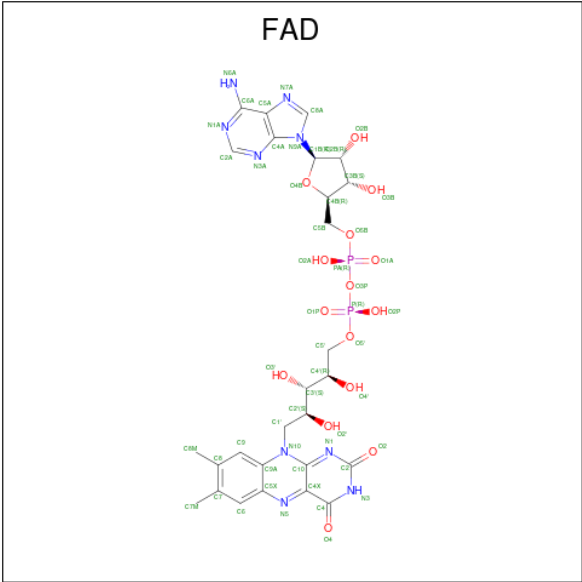
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

- Molecule 5 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7^-$).



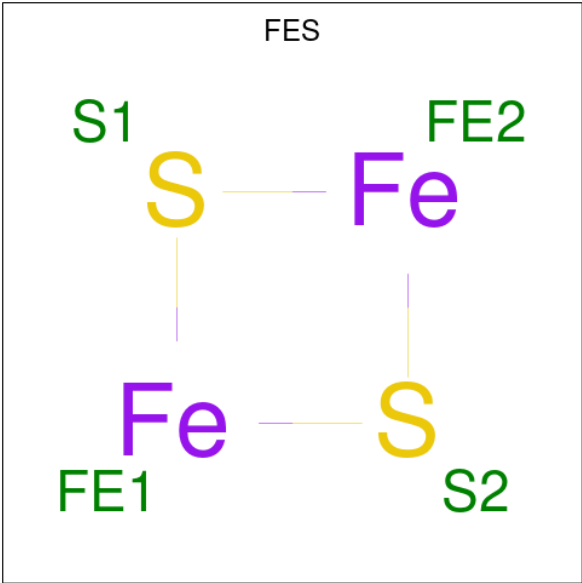
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		
5	M	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



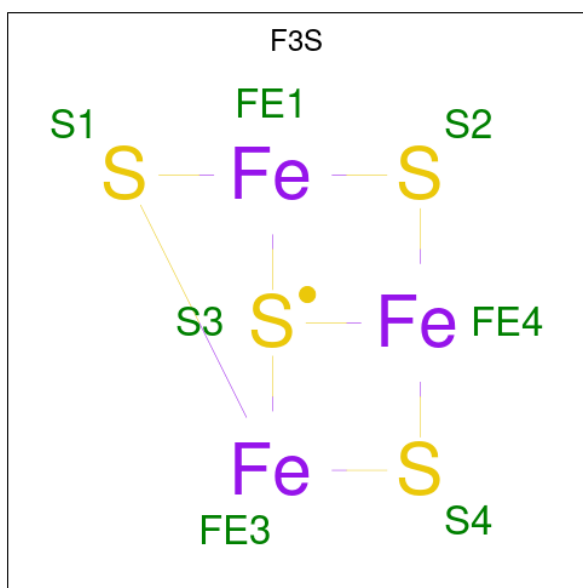
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 52	C 27	N 9	O 14	P 2	0	0
6	M	1	Total 52	C 27	N 9	O 14	P 2	0	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



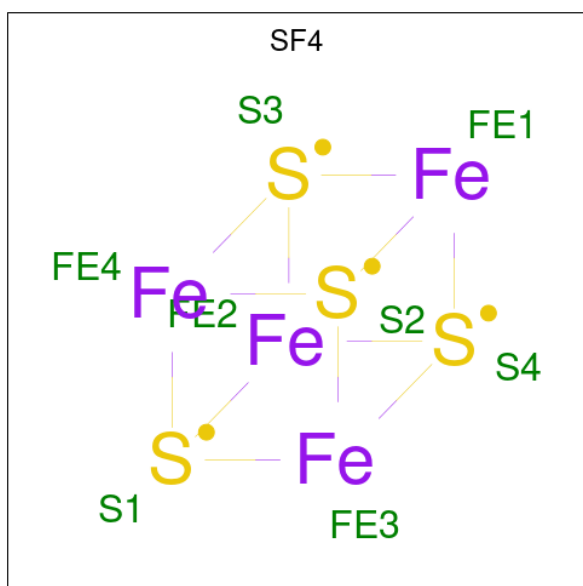
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



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

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



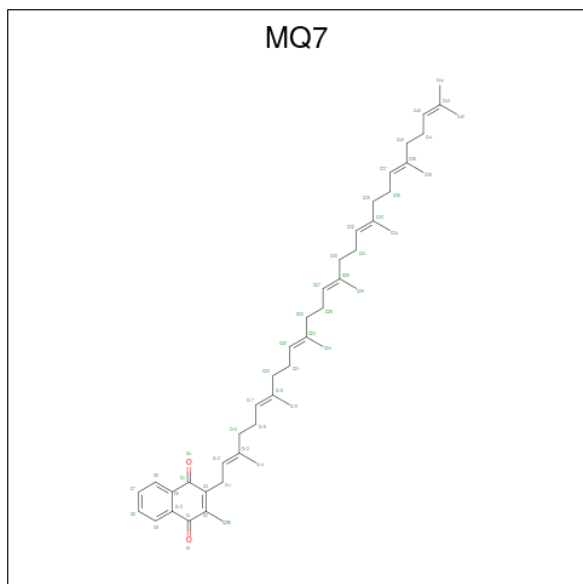
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		

Continued on next page...

Continued from previous page...

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

- Molecule 10 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).

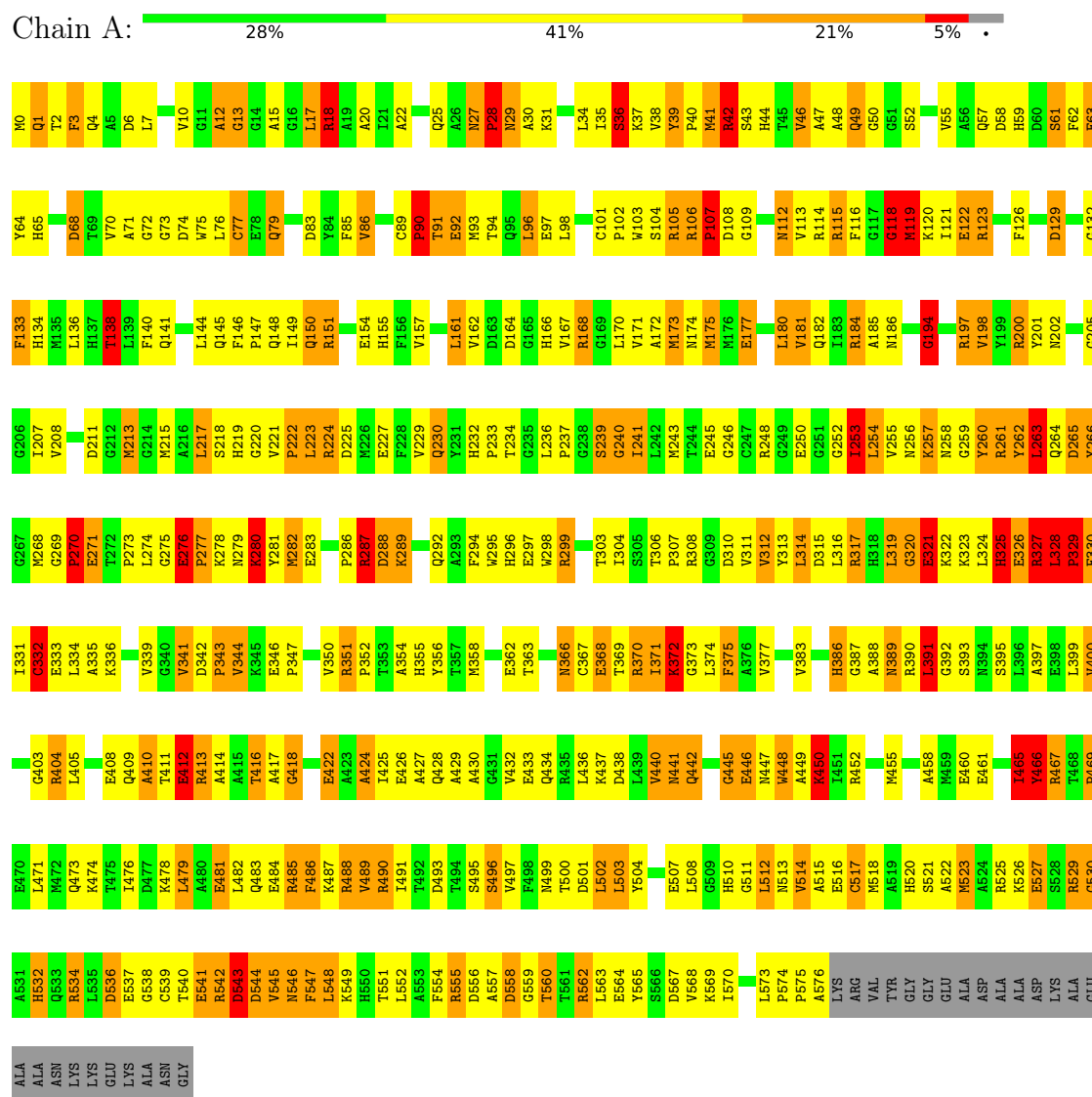


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	C	O	0	0
			33	31	2		
10	P	1	Total	C	O	0	0
			33	31	2		

3 Residue-property plots

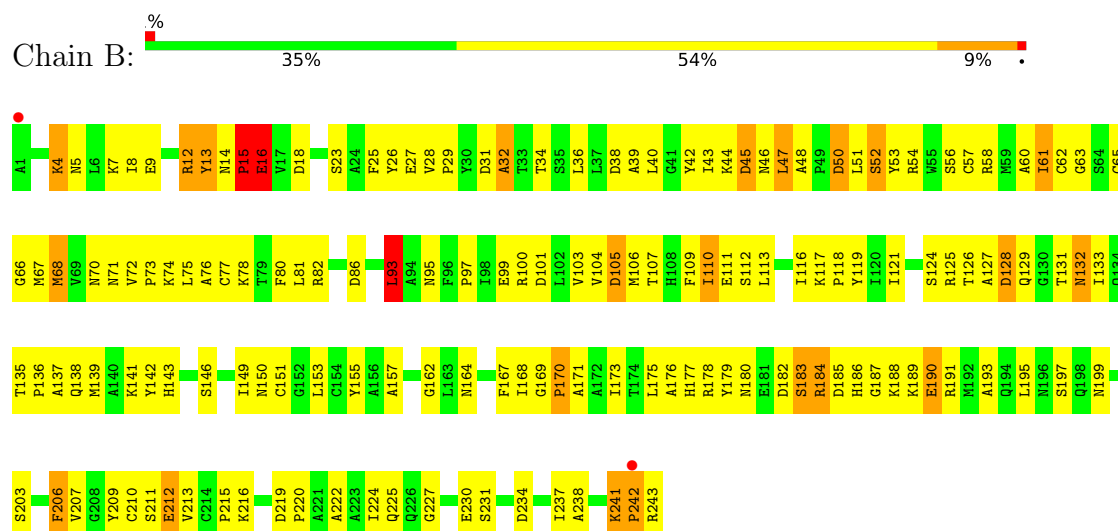
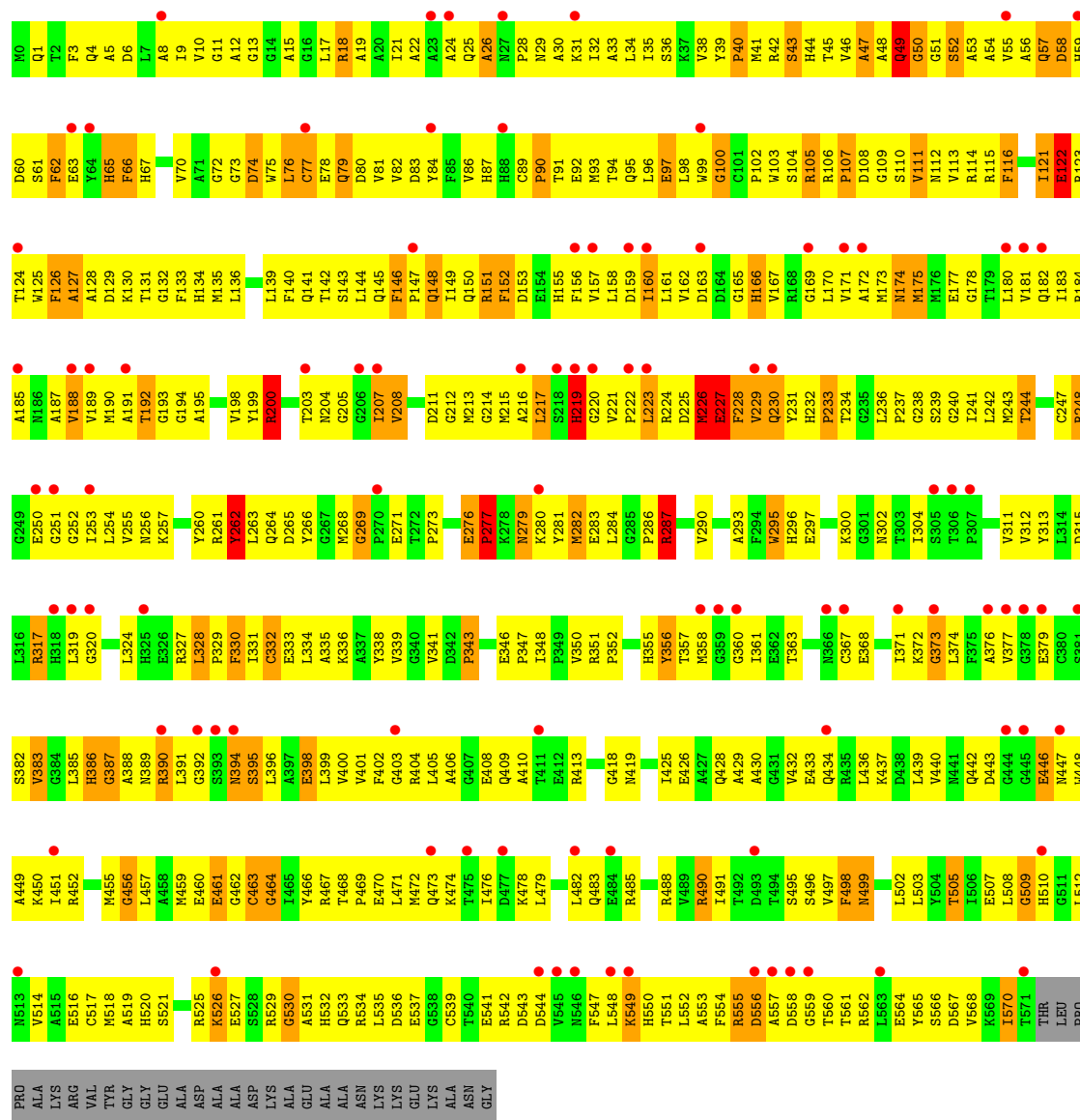
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

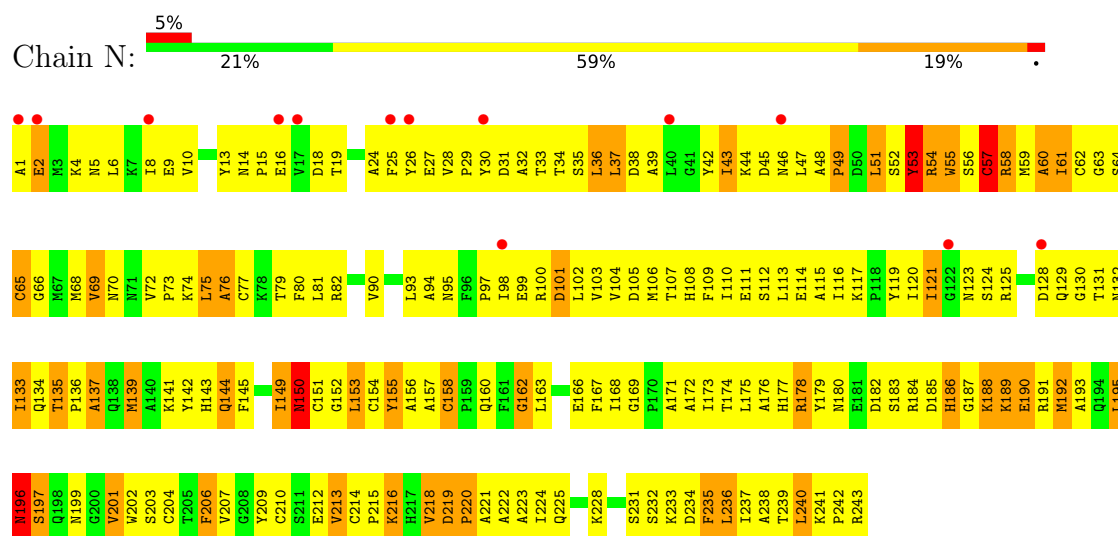


• Molecule 1: Fumarate reductase flavoprotein subunit

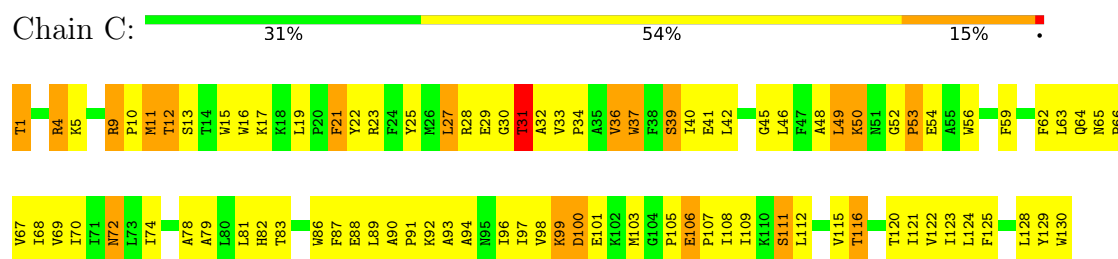




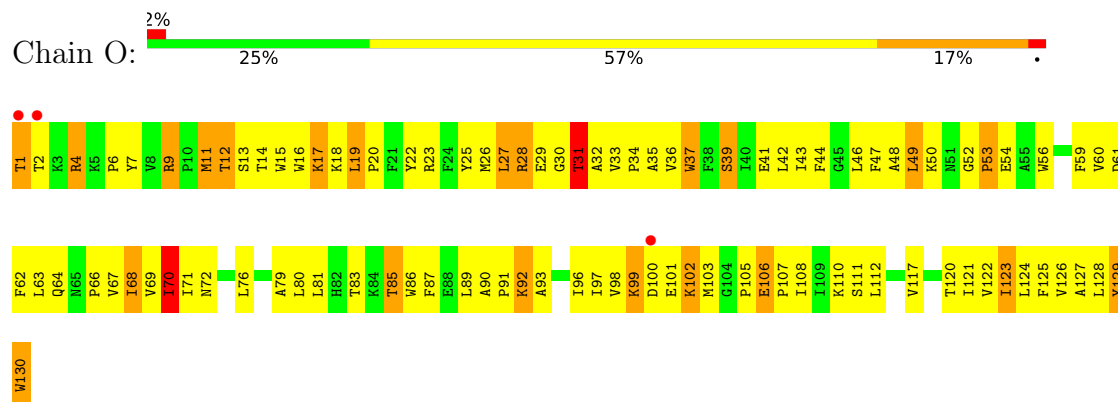
- Molecule 2: Fumarate reductase iron-sulfur protein



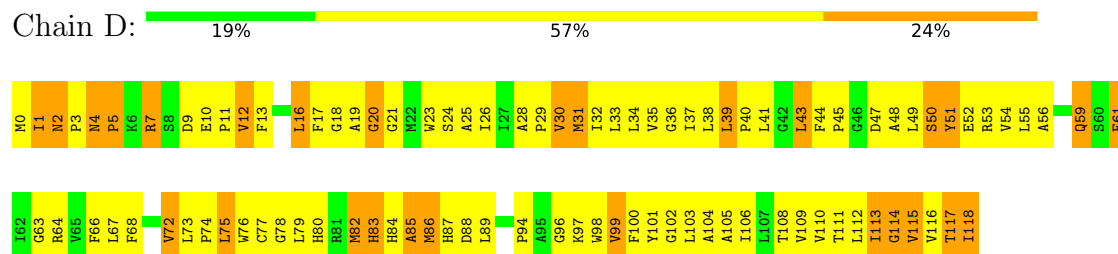
- Molecule 3: Fumarate reductase subunit C



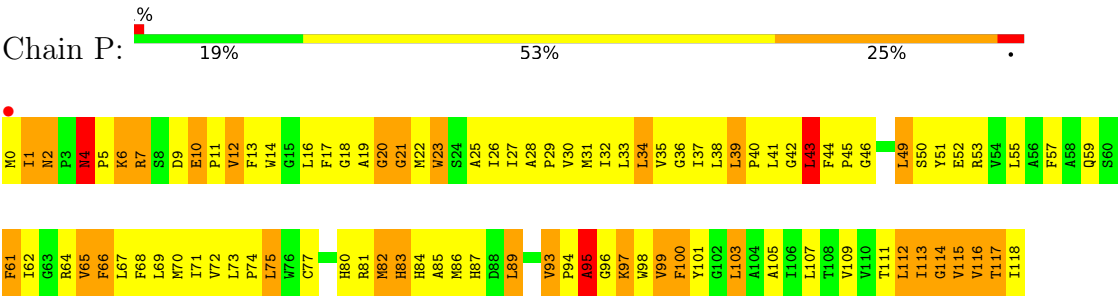
- Molecule 3: Fumarate reductase subunit C



- 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	96.80Å 139.53Å 273.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 39.53 – 3.30	Depositor EDS
% Data completeness (in resolution range)	83.5 (20.00-3.30) 83.4 (39.53-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.12 (at 3.32Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.248 , 0.284 0.237 , 0.270	Depositor DCC
R_{free} test set	1096 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	16840	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: FLC, FES, SF4, FAD, F3S, MQ7

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	1.71	79/4540 (1.7%)	1.81	109/6139 (1.8%)
1	M	0.36	0/4504	0.71	0/6087
2	B	1.01	2/1931 (0.1%)	1.15	8/2617 (0.3%)
2	N	0.41	0/1931	0.71	0/2617
3	C	0.98	0/1094	1.12	6/1496 (0.4%)
3	O	0.92	1/1094 (0.1%)	1.11	5/1496 (0.3%)
4	D	0.77	0/956	1.03	1/1303 (0.1%)
4	P	0.70	1/956 (0.1%)	1.06	3/1303 (0.2%)
All	All	1.06	83/17006 (0.5%)	1.22	132/23058 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	B	0	3
3	O	0	1
All	All	0	8

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	450	LYS	CD-CE	10.77	1.78	1.51
1	A	372	LYS	CB-CG	9.71	1.78	1.52
1	A	277	PRO	CA-C	9.18	1.71	1.52
1	A	484	GLU	CG-CD	8.83	1.65	1.51
1	A	240	GLY	C-O	-8.45	1.10	1.23

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	GLY	C-N-CD	-13.40	91.12	120.60
1	A	370	ARG	NE-CZ-NH1	-13.35	113.63	120.30
1	A	68	ASP	CB-CG-OD1	-10.64	108.72	118.30
1	A	68	ASP	CB-CG-OD2	10.35	127.61	118.30
1	A	501	ASP	CB-CG-OD2	10.22	127.50	118.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	GLY	Mainchain
1	A	276	GLU	Mainchain
1	A	341	VAL	Mainchain
1	A	422	GLU	Mainchain
2	B	15	PRO	Mainchain

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	4337	457	0
1	M	4414	0	4300	755	0
2	B	1888	0	1837	172	0
2	N	1888	0	1837	315	0
3	C	1058	0	1108	122	0
3	O	1058	0	1108	133	0
4	D	926	0	971	140	0
4	P	926	0	971	130	0
5	A	13	0	5	14	0
5	M	13	0	5	3	0
6	A	52	0	29	17	0
6	M	52	0	29	14	0
7	B	4	0	0	0	0
7	N	4	0	0	0	0
8	B	7	0	0	0	0
8	N	7	0	0	1	0
9	B	8	0	0	0	0
9	N	8	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	33	0	37	7	0
10	P	33	0	37	12	0
All	All	16840	0	16611	2099	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 63.

The worst 5 of 2099 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:207:ILE:CG1	1:A:207:ILE:CD1	1.79	1.57
1:A:450:LYS:CE	1:A:450:LYS:CD	1.78	1.57
1:A:372:LYS:CB	1:A:372:LYS:CG	1.78	1.56
1:A:173:MET:CE	1:A:173:MET:SD	2.06	1.43
1:M:44:HIS:NE2	6:M:803:FAD:HM82	1.13	1.42

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	575/602 (96%)	492 (86%)	69 (12%)	14 (2%)	6	28
1	M	570/602 (95%)	402 (70%)	103 (18%)	65 (11%)	0	2
2	B	241/243 (99%)	207 (86%)	30 (12%)	4 (2%)	9	35
2	N	241/243 (99%)	126 (52%)	79 (33%)	36 (15%)	0	1
3	C	128/130 (98%)	99 (77%)	25 (20%)	4 (3%)	4	23
3	O	128/130 (98%)	103 (80%)	18 (14%)	7 (6%)	2	11
4	D	117/119 (98%)	68 (58%)	35 (30%)	14 (12%)	0	2
4	P	117/119 (98%)	76 (65%)	26 (22%)	15 (13%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2117/2188 (97%)	1573 (74%)	385 (18%)	159 (8%)	1	7

5 of 159 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	GLY
1	A	270	PRO
1	A	321	GLU
2	B	242	PRO
3	C	31	THR

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	460/475 (97%)	349 (76%)	111 (24%)	0	2
1	M	456/475 (96%)	406 (89%)	50 (11%)	6	24
2	B	205/205 (100%)	171 (83%)	34 (17%)	2	10
2	N	205/205 (100%)	175 (85%)	30 (15%)	3	14
3	C	111/111 (100%)	89 (80%)	22 (20%)	1	5
3	O	111/111 (100%)	81 (73%)	30 (27%)	0	1
4	D	97/97 (100%)	79 (81%)	18 (19%)	1	7
4	P	97/97 (100%)	75 (77%)	22 (23%)	1	3
All	All	1742/1776 (98%)	1425 (82%)	317 (18%)	1	7

5 of 317 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	549	LYS
3	O	99	LYS
2	N	37	LEU
2	N	206	PHE
4	P	23	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	44	HIS
3	O	72	ASN
1	M	174	ASN
3	O	65	ASN
4	P	59	GLN

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](#)

12 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	FAD	A	703	-	51,57,58	3.82	26 (50%)	59,87,89	1.95	10 (16%)
8	F3S	B	245	2	0,9,9	-	-	-	-	-
10	MQ7	D	700	-	34,34,49	3.40	15 (44%)	42,45,63	2.34	14 (33%)
10	MQ7	P	800	-	34,34,49	3.42	16 (47%)	42,45,63	2.54	13 (30%)
9	SF4	N	246	2	0,12,12	-	-	-	-	-
9	SF4	B	246	2	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FAD	M	803	-	51,57,58	3.98	22 (43%)	59,87,89	1.86	9 (15%)
7	FES	N	244	2	0,4,4	-	-	-		
7	FES	B	244	2	0,4,4	-	-	-		
5	FLC	M	802	-	3,12,12	4.90	2 (66%)	3,17,17	5.77	2 (66%)
5	FLC	A	702	-	3,12,12	3.30	2 (66%)	3,17,17	8.57	2 (66%)
8	F3S	N	245	2	0,9,9	-	-	-		

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	FAD	A	703	-	-	9/30/46/50	0/6/6/6
10	MQ7	D	700	-	-	7/23/43/61	0/2/2/2
8	F3S	B	245	2	-	-	0/3/3/3
9	SF4	N	246	2	-	-	0/6/5/5
9	SF4	B	246	2	-	-	0/6/5/5
6	FAD	M	803	-	-	7/30/46/50	0/6/6/6
7	FES	N	244	2	-	-	0/1/1/1
7	FES	B	244	2	-	-	0/1/1/1
8	F3S	N	245	2	-	-	0/3/3/3
5	FLC	M	802	-	-	3/6/16/16	-
5	FLC	A	702	-	-	1/6/16/16	-
10	MQ7	P	800	-	-	9/23/43/61	0/2/2/2

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	703	FAD	C4X-N5	10.47	1.48	1.33
6	M	803	FAD	C10-N1	9.73	1.45	1.33
6	M	803	FAD	C4X-C10	9.71	1.48	1.38
6	M	803	FAD	C4X-N5	9.68	1.47	1.33
6	M	803	FAD	C9A-N10	9.52	1.51	1.38

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	702	FLC	CB-CA-CAC	14.66	138.46	114.98
10	P	800	MQ7	C16-C15-C13	9.16	143.11	112.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	802	FLC	CB-CA-CAC	8.36	128.37	114.98
10	D	700	MQ7	C12-C11-C3	6.94	130.77	112.05
10	D	700	MQ7	C16-C15-C13	6.82	135.43	112.98

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	802	FLC	CA-CB-CG-CGC
5	M	802	FLC	CBC-CB-CG-CGC
5	M	802	FLC	OHB-CB-CG-CGC
6	A	703	FAD	N10-C1'-C2'-O2'
6	A	703	FAD	N10-C1'-C2'-C3'

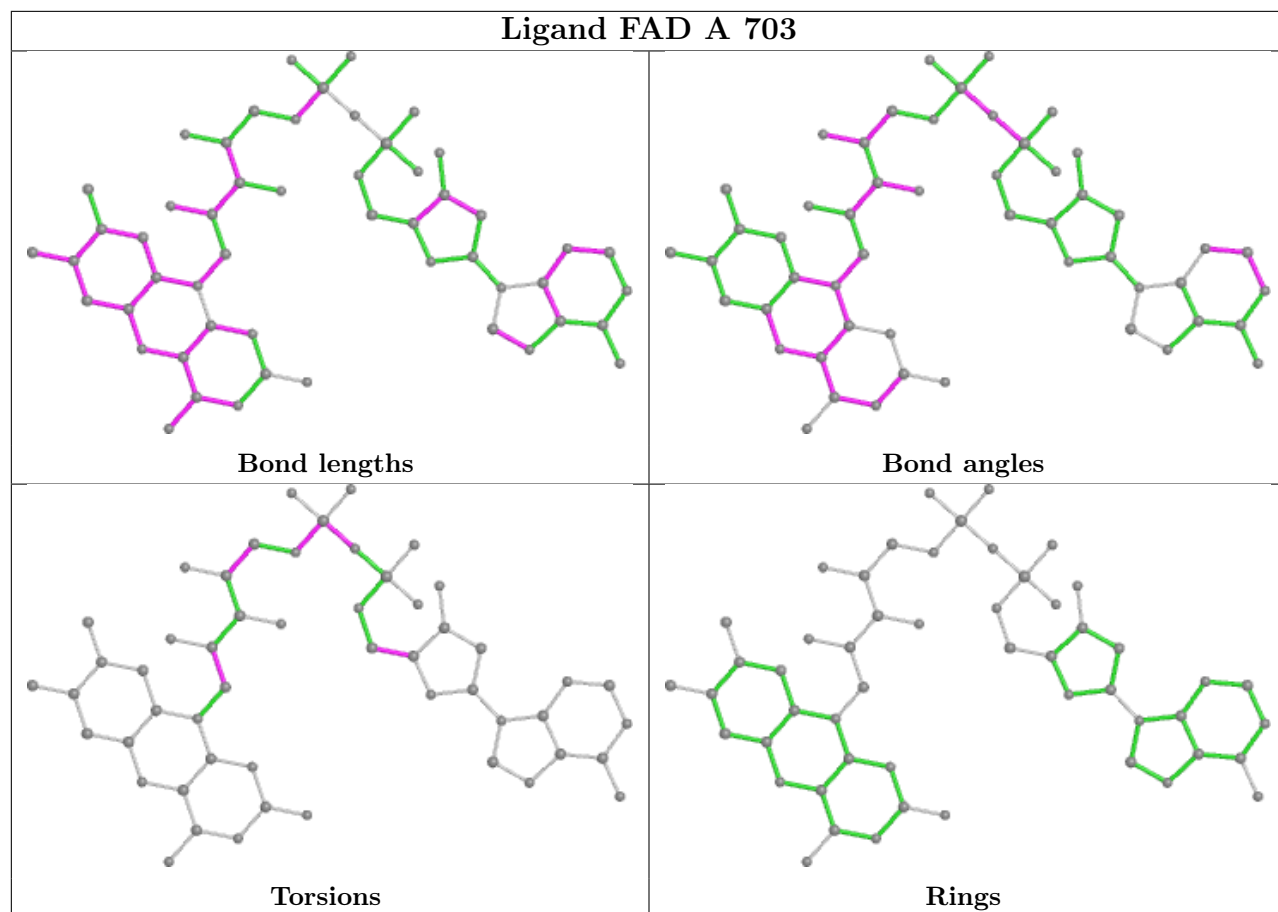
There are no ring outliers.

8 monomers are involved in 67 short contacts:

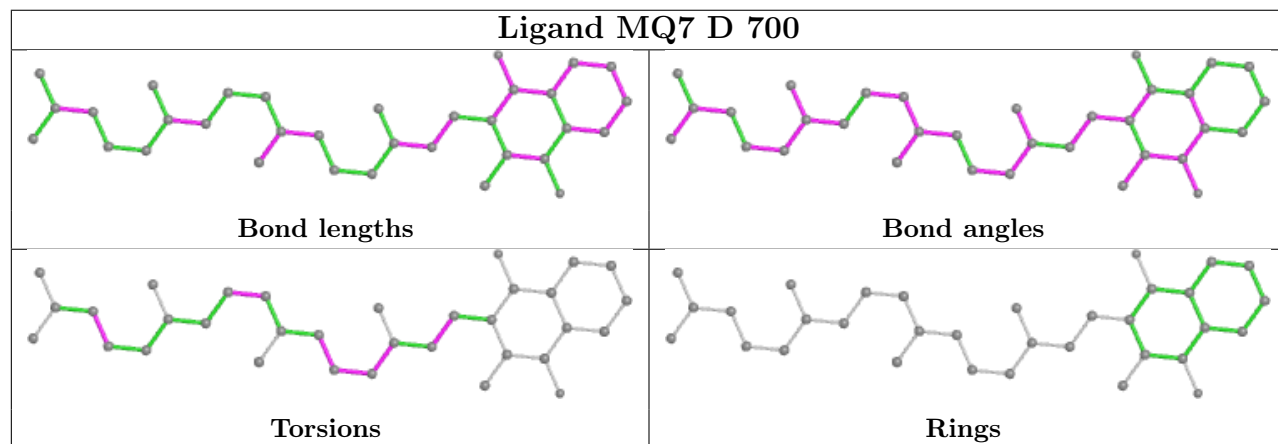
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	703	FAD	17	0
10	D	700	MQ7	7	0
10	P	800	MQ7	12	0
9	N	246	SF4	3	0
6	M	803	FAD	14	0
5	M	802	FLC	3	0
5	A	702	FLC	14	0
8	N	245	F3S	1	0

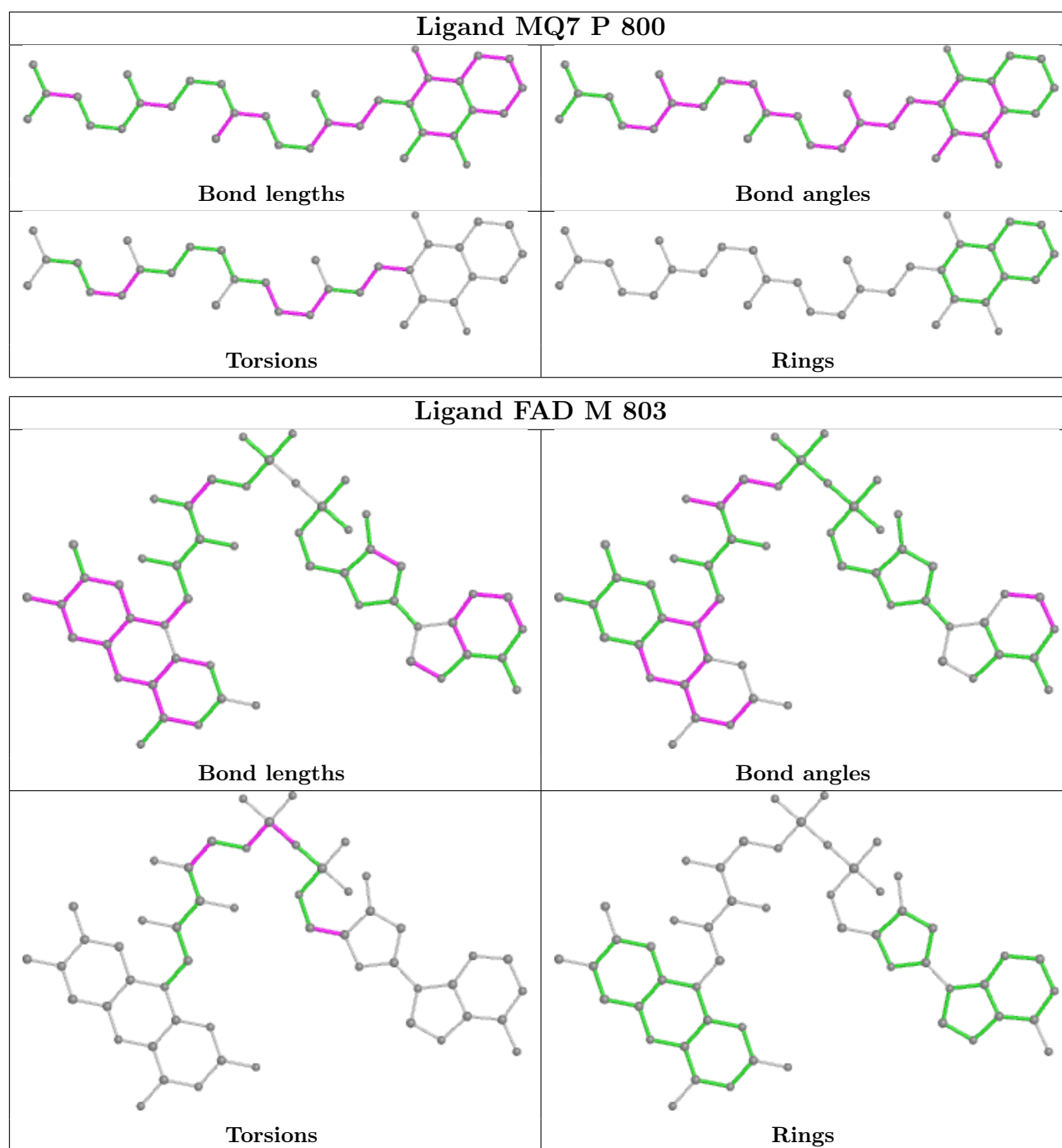
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand FAD A 703



Ligand MQ7 D 700





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	577/602 (95%)	-0.47	0 100 100	9, 14, 62, 85	0
1	M	572/602 (95%)	0.93	96 (16%) 1 1	30, 92, 127, 142	0
2	B	243/243 (100%)	-0.57	2 (0%) 86 86	9, 15, 36, 85	0
2	N	243/243 (100%)	0.28	13 (5%) 26 24	9, 62, 119, 147	0
3	C	130/130 (100%)	-0.47	0 100 100	10, 32, 59, 76	0
3	O	130/130 (100%)	-0.08	3 (2%) 60 59	24, 55, 106, 123	0
4	D	119/119 (100%)	-0.60	0 100 100	18, 36, 61, 70	0
4	P	119/119 (100%)	-0.34	1 (0%) 86 86	27, 49, 80, 118	0
All	All	2133/2188 (97%)	0.00	115 (5%) 25 24	9, 45, 114, 147	0

The worst 5 of 115 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	17	VAL	8.5
1	M	484	GLU	6.2
1	M	557	ALA	6.0
1	M	392	GLY	5.7
1	M	159	ASP	4.8

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

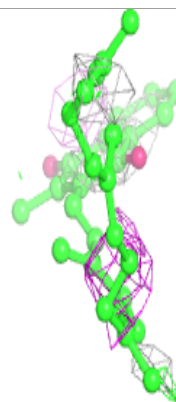
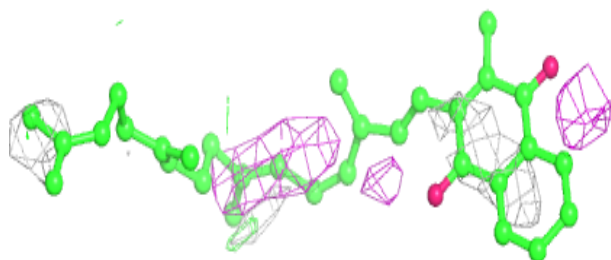
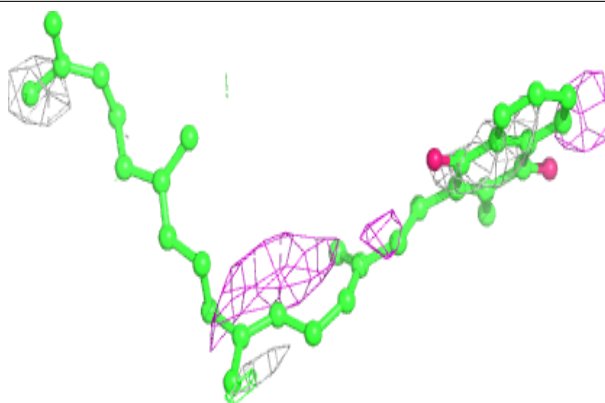
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	MQ7	P	800	33/48	0.60	1.16	83,106,120,123	0
10	MQ7	D	700	33/48	0.64	0.79	59,100,117,127	0
5	FLC	M	802	13/13	0.71	0.42	60,74,92,97	0
5	FLC	A	702	13/13	0.85	0.29	31,37,38,39	0
6	FAD	M	803	52/53	0.86	0.45	23,87,158,164	0
7	FES	N	244	4/4	0.96	0.14	21,24,44,53	0
6	FAD	A	703	52/53	0.97	0.21	0,1,17,36	0
9	SF4	N	246	8/8	0.97	0.15	20,29,49,53	0
7	FES	B	244	4/4	0.98	0.18	0,4,5,8	0
9	SF4	B	246	8/8	0.99	0.19	9,21,27,27	0
8	F3S	N	245	7/7	0.99	0.09	14,16,29,49	0
8	F3S	B	245	7/7	1.00	0.13	7,11,15,24	0

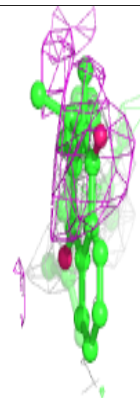
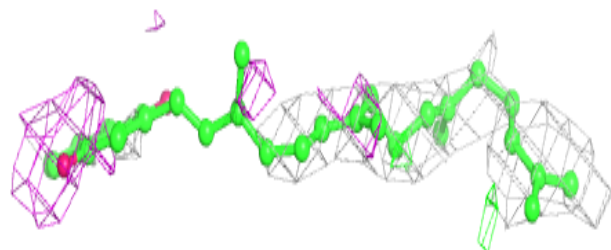
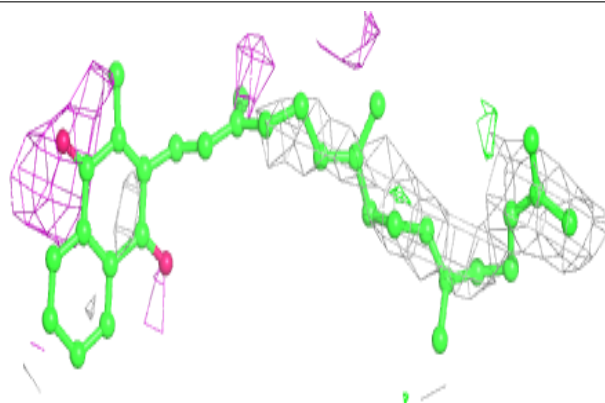
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MQ7 P 800:

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

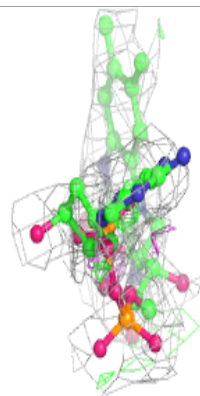
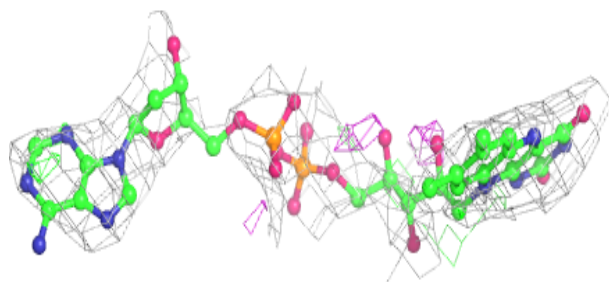
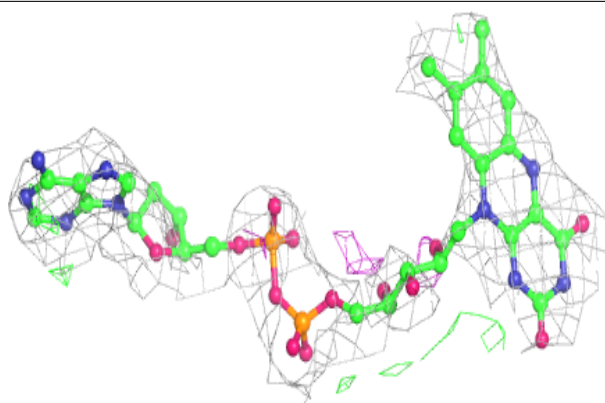
**Electron density around MQ7 D 700:**

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

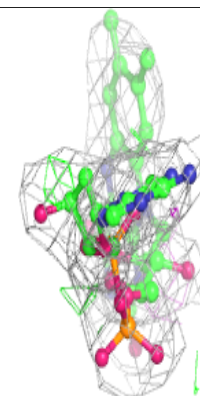
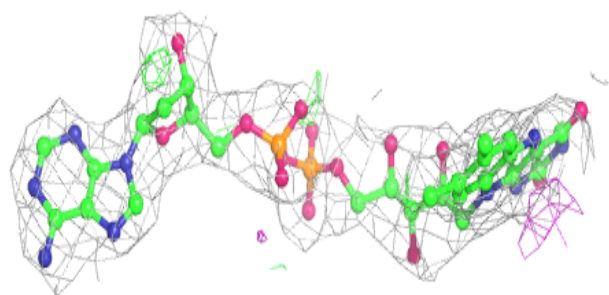
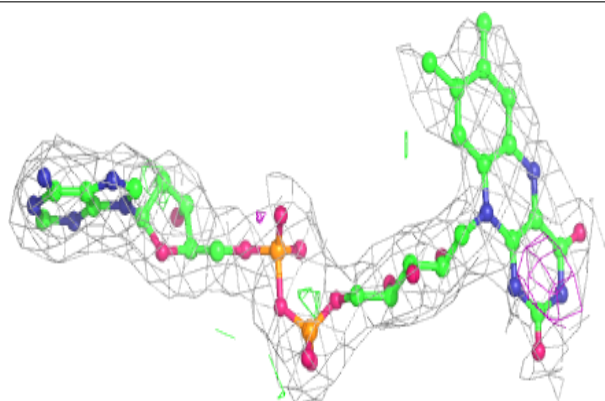


Electron density around FAD M 803:

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

**Electron density around FAD A 703:**

$2mF_o-DF_c$ (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.