



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:50 PM GMT

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 validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

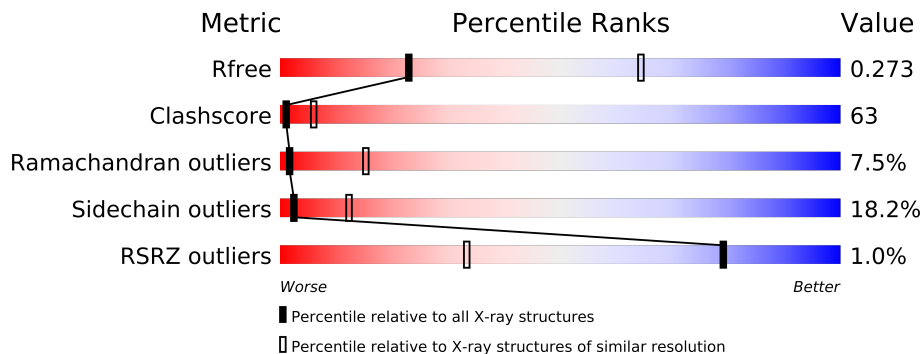
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	602	
1	M	602	
2	B	243	
2	N	243	
3	C	130	
3	O	130	
4	D	119	
4	P	119	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	MQ7	D	700	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
10	MQ7	P	800	-	X
5	FLC	A	702	-	X
8	SF4	B	246	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16840 atoms, of which 0 are hydrogen and 0 are deuterium.

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	GB P00363
M	49	GLN	GLU	ENGINEERED	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.

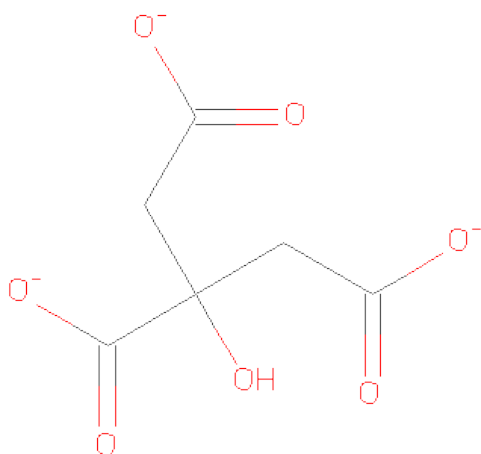
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

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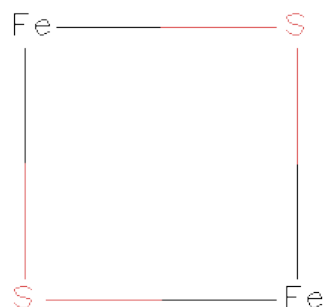
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

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



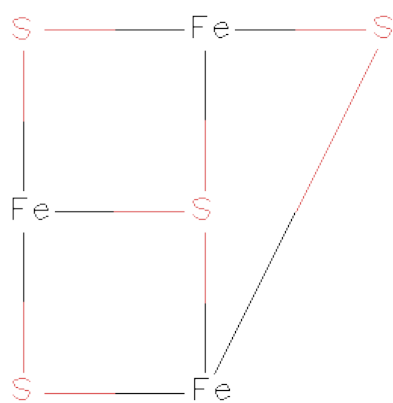
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		
5	M	1	Total	C	O	0	0
			13	6	7		

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



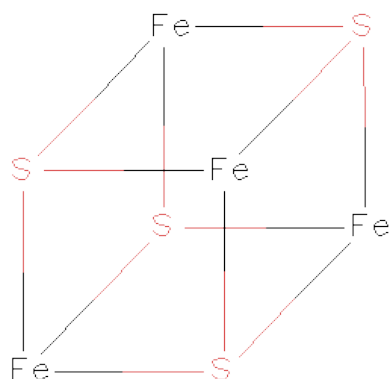
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			4	2	2		
6	N	1	Total	Fe	S	0	0
			4	2	2		

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



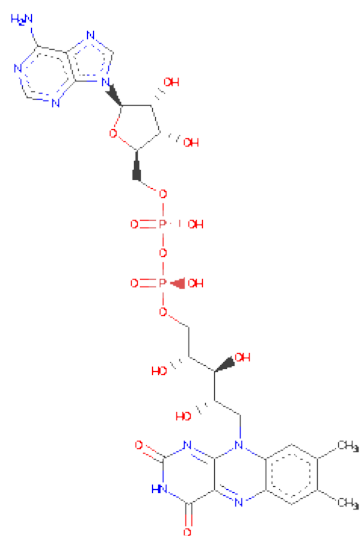
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			7	3	4		
7	N	1	Total	Fe	S	0	0
			7	3	4		

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



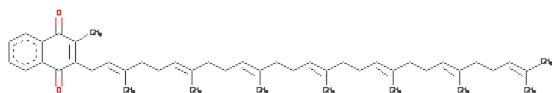
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		
8	N	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).

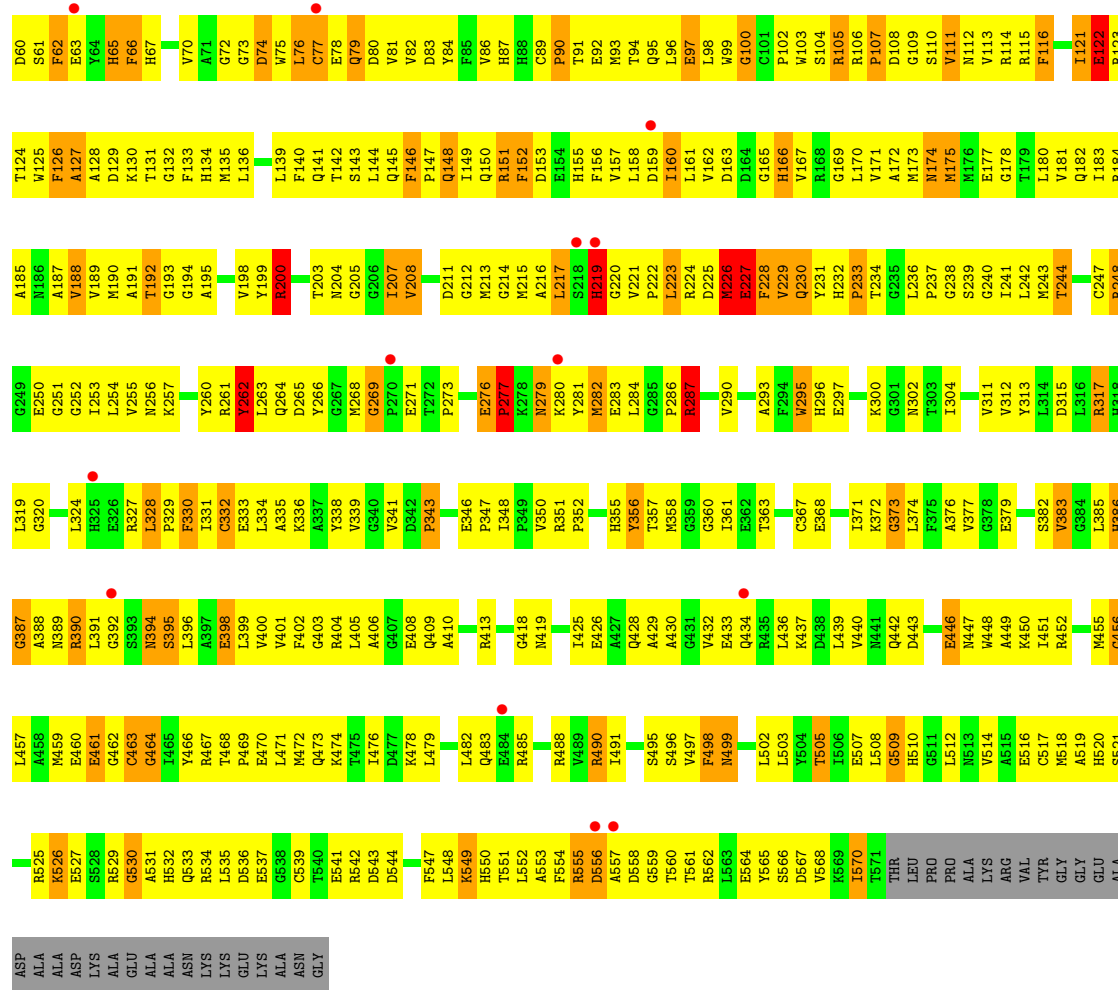


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			52	27	9	14	2		
9	M	1	Total	C	N	O	P	0	0
			52	27	9	14	2		

- Molecule 10 is MENAQUINONE-7 (three-letter code: MQ7) (formula: C₄₆H₆₄O₂).

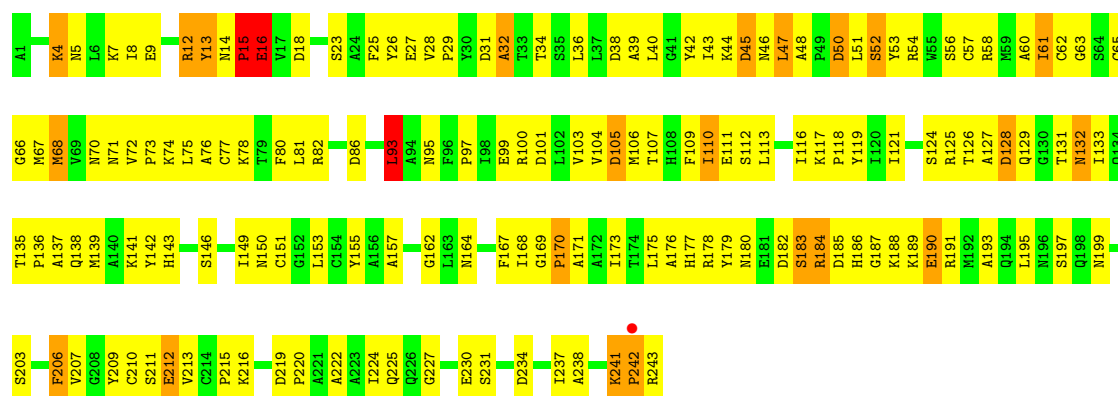


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	C	O	0	0
			33	31	2		
10	P	1	Total	C	O	0	0
			33	31	2		



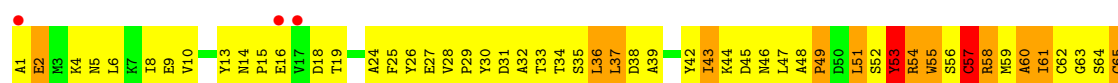
• Molecule 2: Fumarate reductase iron-sulfur protein

Chain B:



• Molecule 2: Fumarate reductase iron-sulfur protein

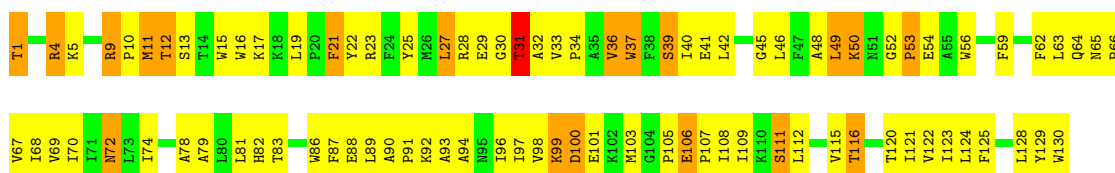
Chain N:





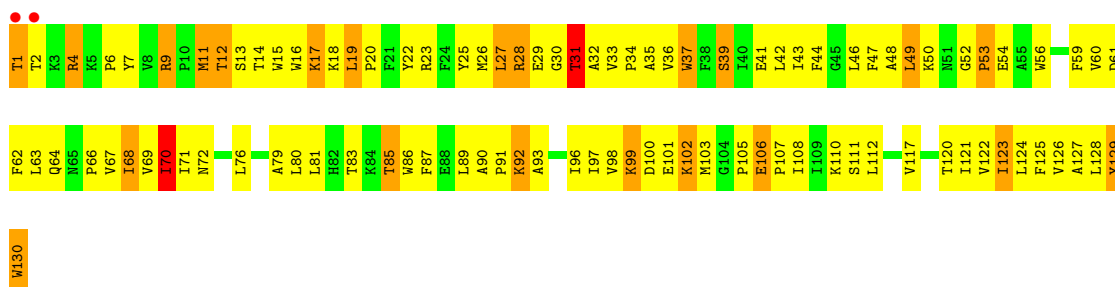
• Molecule 3: Fumarate reductase subunit C

Chain C:



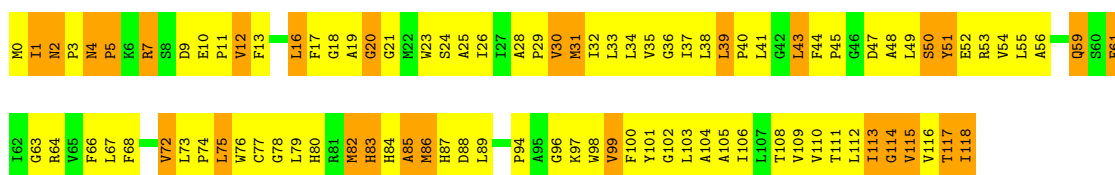
• Molecule 3: Fumarate reductase subunit C

Chain O:



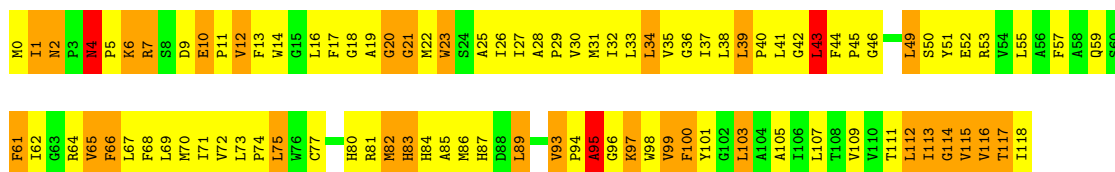
• Molecule 4: Fumarate reductase subunit D

Chain D:



• Molecule 4: Fumarate reductase subunit D

Chain P:



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 0.243 , 0.273	Depositor DCC
R_{free} test set	923 reflections (1.99%)	DCC
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 19.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 56072 reflections	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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4448	0	4337	456	0
1	M	4414	0	4300	754	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	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	1	0
8	B	8	0	0	0	0
8	N	8	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	52	0	29	16	0
9	M	52	0	29	13	0
10	D	33	0	37	7	0
10	P	33	0	37	12	0
All	All	16840	0	16611	2097	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 63.

The worst 5 of 2097 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:450:LYS:CE	1:A:450:LYS:CD	1.78	1.57
1:A:207:ILE:CD1	1:A:207:ILE:CG1	1.79	1.57
1:A:372:LYS:CG	1:A:372:LYS:CB	1.78	1.56
1:A:173:MET:CE	1:A:173:MET:SD	2.06	1.43
1:M:44:HIS:NE2	9:M:803:FAD:HM82	1.13	1.42

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	575/602 (96%)	492 (86%)	69 (12%)	14 (2%)	9	53
1	M	570/602 (95%)	402 (70%)	103 (18%)	65 (11%)	1	5
2	B	241/243 (99%)	207 (86%)	30 (12%)	4 (2%)	14	62
2	N	241/243 (99%)	126 (52%)	79 (33%)	36 (15%)	0	2
3	C	128/130 (98%)	99 (77%)	25 (20%)	4 (3%)	7	45
3	O	128/130 (98%)	103 (80%)	18 (14%)	7 (6%)	3	25
4	D	117/119 (98%)	68 (58%)	35 (30%)	14 (12%)	1	4
4	P	117/119 (98%)	76 (65%)	26 (22%)	15 (13%)	0	3
All	All	2117/2188 (97%)	1573 (74%)	385 (18%)	159 (8%)	2	15

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%)	1	4
1	M	456/475 (96%)	406 (89%)	50 (11%)	9	38
2	B	205/205 (100%)	171 (83%)	34 (17%)	3	16
2	N	205/205 (100%)	175 (85%)	30 (15%)	5	23
3	C	111/111 (100%)	89 (80%)	22 (20%)	2	9
3	O	111/111 (100%)	81 (73%)	30 (27%)	1	2
4	D	97/97 (100%)	79 (81%)	18 (19%)	2	11
4	P	97/97 (100%)	75 (77%)	22 (23%)	1	5
All	All	1742/1776 (98%)	1425 (82%)	317 (18%)	2	12

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

Mol	Chain	Res	Type
2	B	237	ILE
4	D	59	GLN
3	O	117	VAL
3	C	11	MET
3	C	72	ASN

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

Mol	Chain	Res	Type
4	D	59	GLN

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Mol	Chain	Res	Type
1	M	137	HIS
3	O	72	ASN
1	M	65	HIS
1	M	174	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
5	FLC	A	702	-	5,12,12	14.14	4 (80%)	7,17,17	6.06	2 (28%)
9	FAD	A	703	1	56,57,58	4.06	32 (57%)	79,87,89	2.18	16 (20%)
6	FES	B	244	2	0,4,4	0.00	-	0,4,4	0.00	-
7	F3S	B	245	2	3,9,9	13.24	3 (100%)	0,15,15	0.00	-
8	SF4	B	246	2	12,12,12	16.77	12 (100%)	0,24,24	0.00	-
10	MQ7	D	700	-	34,34,49	3.69	16 (47%)	43,45,63	2.32	14 (32%)
5	FLC	M	802	-	5,12,12	7.24	4 (80%)	7,17,17	4.10	2 (28%)
9	FAD	M	803	1	56,57,58	3.89	27 (48%)	79,87,89	2.17	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FES	N	244	2	0,4,4	0.00	-	0,4,4	0.00	-
7	F3S	N	245	2	3,9,9	7.26	3 (100%)	0,15,15	0.00	-
8	SF4	N	246	2	12,12,12	8.16	12 (100%)	0,24,24	0.00	-
10	MQ7	P	800	-	34,34,49	3.74	16 (47%)	43,45,63	2.54	16 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FLC	A	702	-	-	0/6/16/16	0/0/0/0
9	FAD	A	703	1	-	0/34/46/50	0/1/6/6
6	FES	B	244	2	-	0/0/4/4	0/0/1/1
7	F3S	B	245	2	-	0/0/24/24	0/0/3/3
8	SF4	B	246	2	-	0/0/48/48	0/0/5/5
10	MQ7	D	700	-	-	0/23/43/61	0/0/2/2
5	FLC	M	802	-	-	0/6/16/16	0/0/0/0
9	FAD	M	803	1	-	0/34/46/50	0/1/6/6
6	FES	N	244	2	-	0/0/4/4	0/0/1/1
7	F3S	N	245	2	-	0/0/24/24	0/0/3/3
8	SF4	N	246	2	-	0/0/48/48	0/0/5/5
10	MQ7	P	800	-	-	0/23/43/61	0/0/2/2

The worst 5 of 129 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	702	FLC	CG-CGC	-30.94	1.30	1.49
8	B	246	SF4	S3-FE2	-22.27	2.18	2.33
8	B	246	SF4	S4-FE1	-21.09	2.19	2.33
8	B	246	SF4	S1-FE4	-19.21	2.20	2.33
8	B	246	SF4	S3-FE4	-17.80	2.21	2.33

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	702	FLC	CB-CA-CAC	15.70	138.46	115.01
10	P	800	MQ7	C16-C15-C13	9.17	143.11	112.74
5	M	802	FLC	CB-CA-CAC	8.94	128.37	115.01
9	M	803	FAD	C8A-N9A-C4A	-8.92	100.09	106.90
9	A	703	FAD	C8A-N9A-C4A	-8.70	100.26	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.40	0 100 100	9, 14, 62, 85	0
1	M	572/602 (95%)	0.41	13 (2%) 57 15	30, 92, 127, 142	0
2	B	243/243 (100%)	-0.43	1 (0%) 90 57	9, 15, 36, 85	0
2	N	243/243 (100%)	-0.01	3 (1%) 75 29	9, 62, 119, 147	0
3	C	130/130 (100%)	-0.36	0 100 100	10, 32, 59, 76	0
3	O	130/130 (100%)	-0.17	2 (1%) 70 24	24, 55, 106, 123	0
4	D	119/119 (100%)	-0.42	0 100 100	18, 36, 61, 70	0
4	P	119/119 (100%)	-0.31	0 100 100	27, 49, 80, 118	0
All	All	2133/2188 (97%)	-0.12	19 (0%) 79 37	9, 45, 114, 147	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	17	VAL	4.0
1	M	484	GLU	3.6
1	M	392	GLY	3.1
1	M	557	ALA	3.0
1	M	219	HIS	2.9

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
10	MQ7	P	800	33/48	0.97	17.74	83,106,120,123	0
10	MQ7	D	700	33/48	0.74	12.18	59,100,117,127	0
5	FLC	A	702	13/13	0.31	4.26	31,37,38,39	0
8	SF4	B	246	8/8	0.18	2.25	9,21,27,27	0
5	FLC	M	802	13/13	0.43	1.09	60,74,92,97	0
9	FAD	M	803	52/53	0.43	0.95	23,87,158,164	0
9	FAD	A	703	52/53	0.19	-0.09	0,1,17,36	0
6	FES	B	244	4/4	0.17	-0.12	0,4,5,8	0
7	F3S	B	245	7/7	0.13	-0.64	7,11,15,24	0
8	SF4	N	246	8/8	0.14	-0.81	20,29,49,53	0
6	FES	N	244	4/4	0.12	-2.05	21,24,44,53	0
7	F3S	N	245	7/7	0.07	-2.70	14,16,29,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.