



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:39 AM 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 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

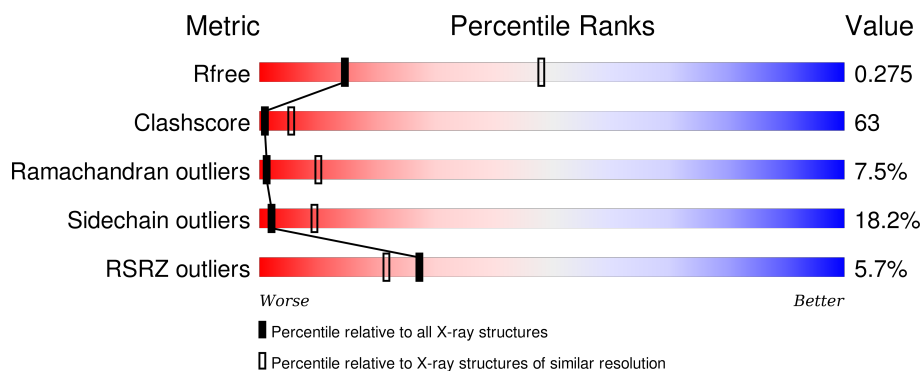
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (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. 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	
1	M	602	
2	B	243	
2	N	243	
3	C	130	

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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	X
5	FLC	M	802	-	-	-	X
8	SF4	N	246	-	-	X	-
9	FAD	M	803	-	-	-	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	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.

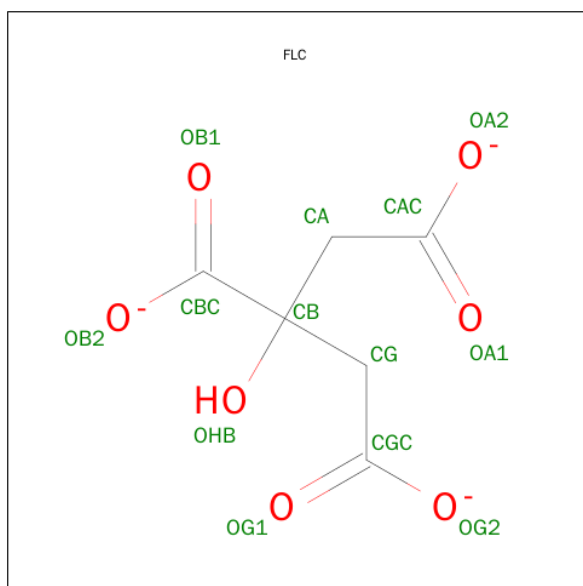
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

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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: $C_6H_5O_7$).



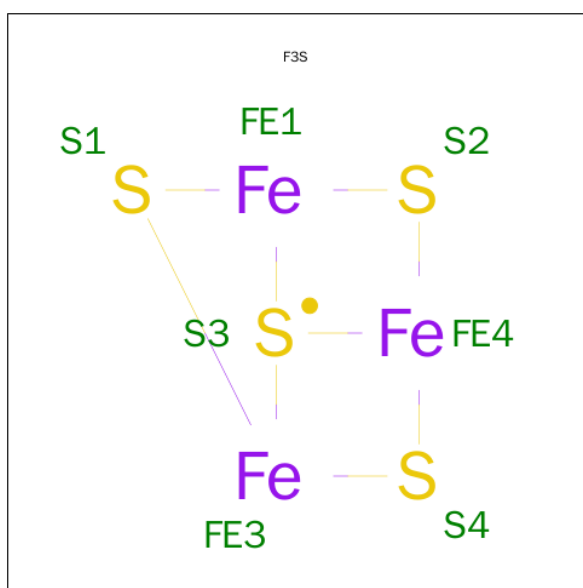
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		
5	M	1	Total	C	O	0	0
			13	6	7		

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



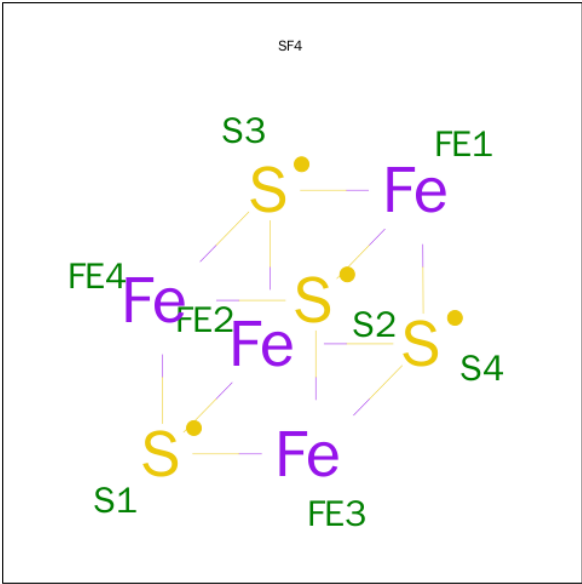
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			4	2	2		
6	N	1	Total	Fe	S	0	0
			4	2	2		

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



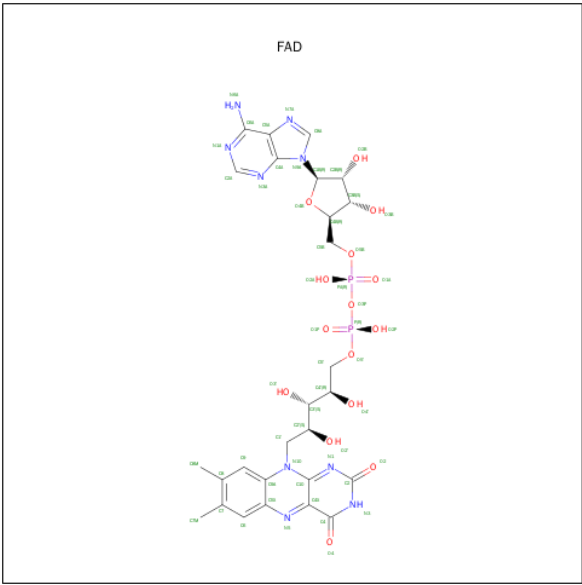
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			7	3	4		
7	N	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



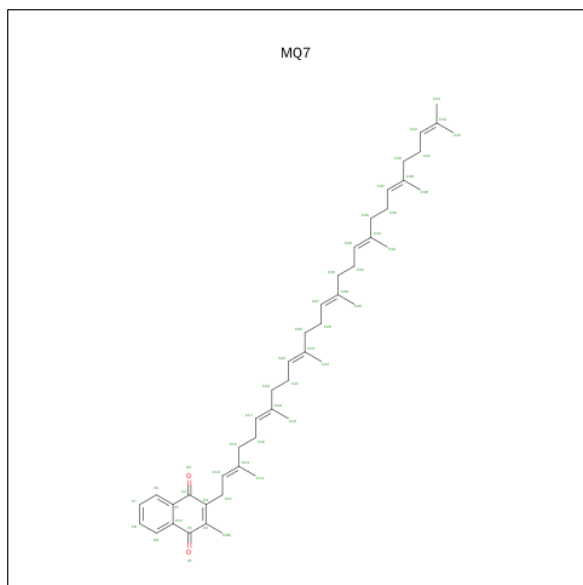
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		
8	N	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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: $C_{46}H_{64}O_2$).

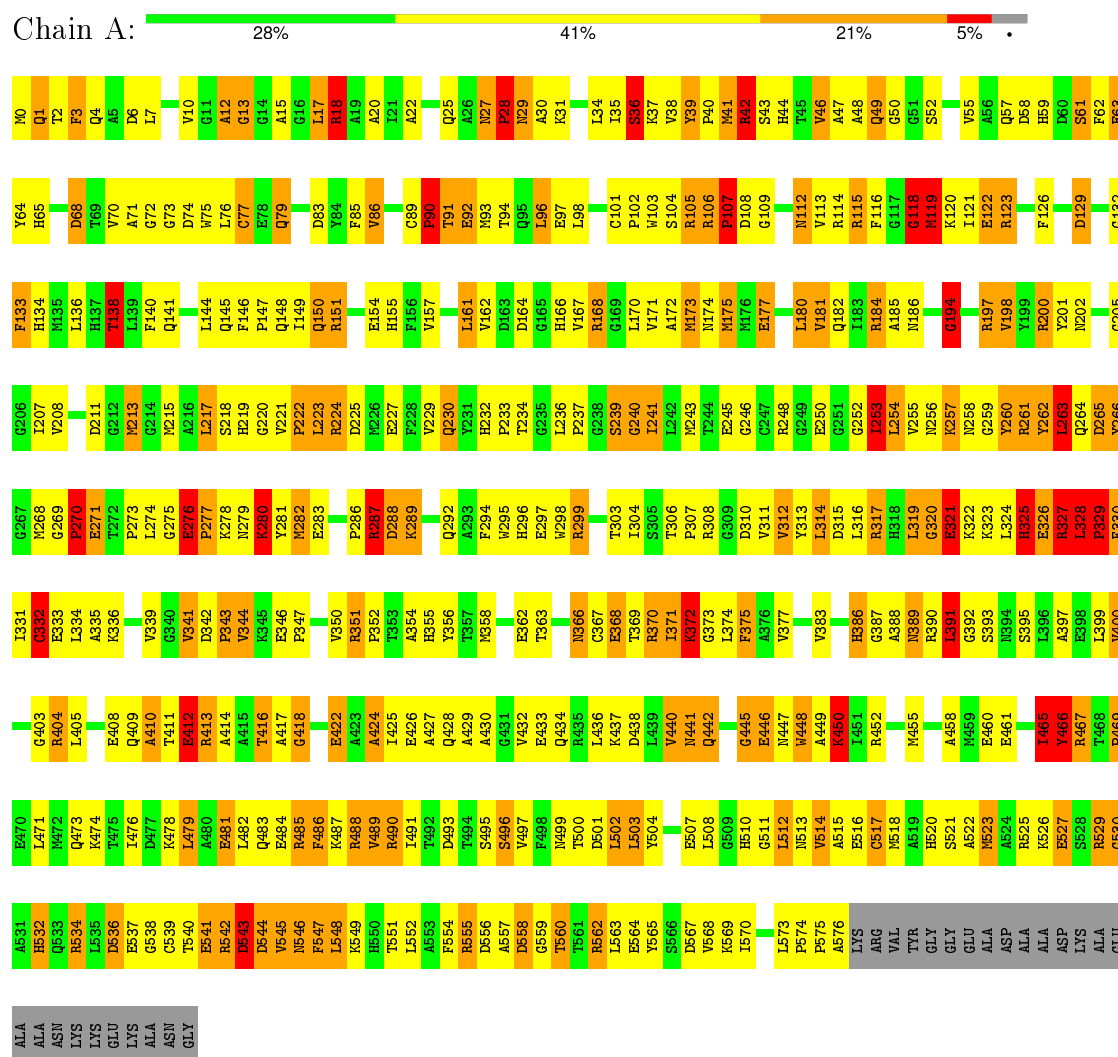


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	C	O	0	0
			33	31	2		
10	P	1	Total	C	O	0	0
			33	31	2		

3 Residue-property plots

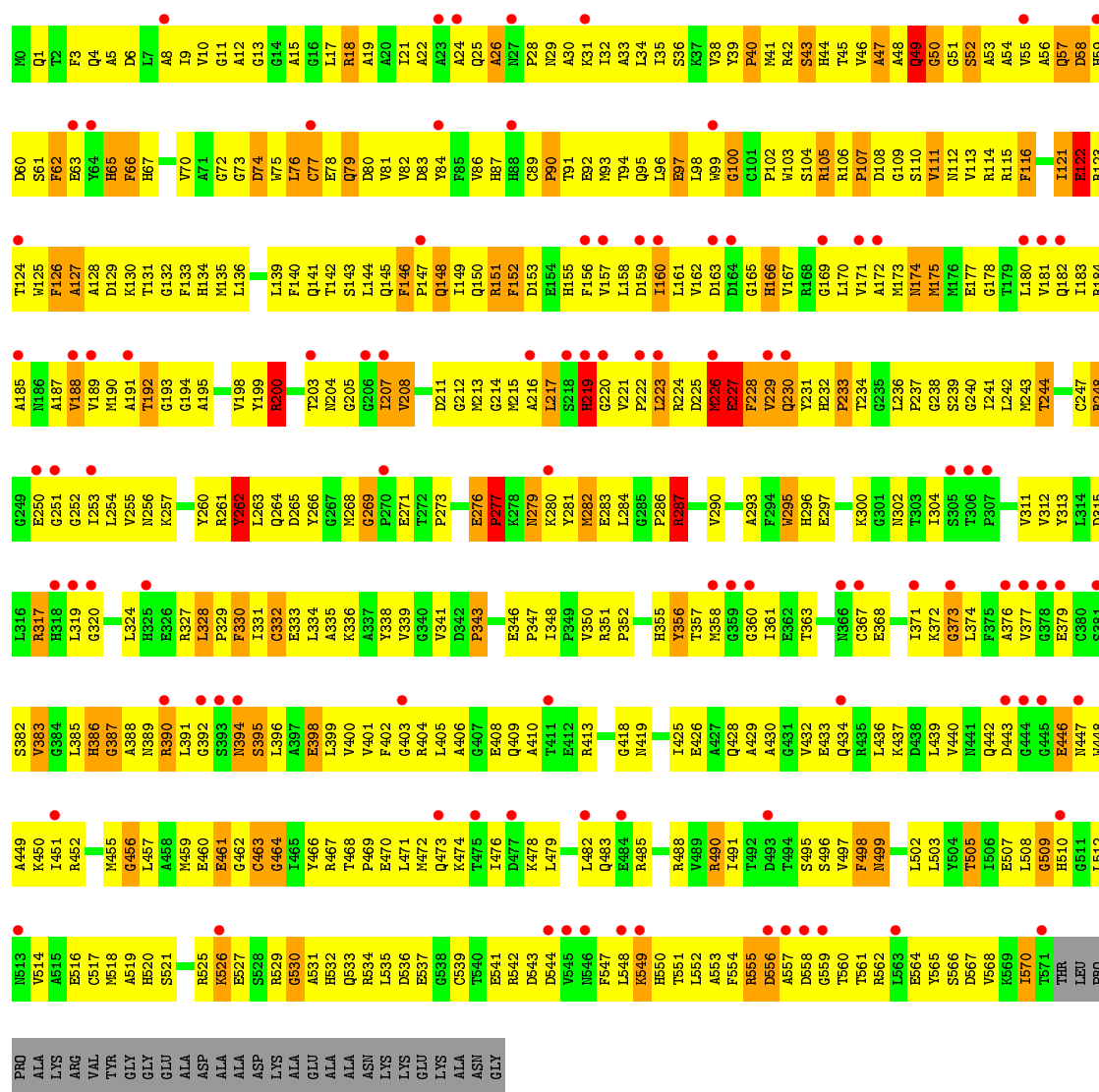
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

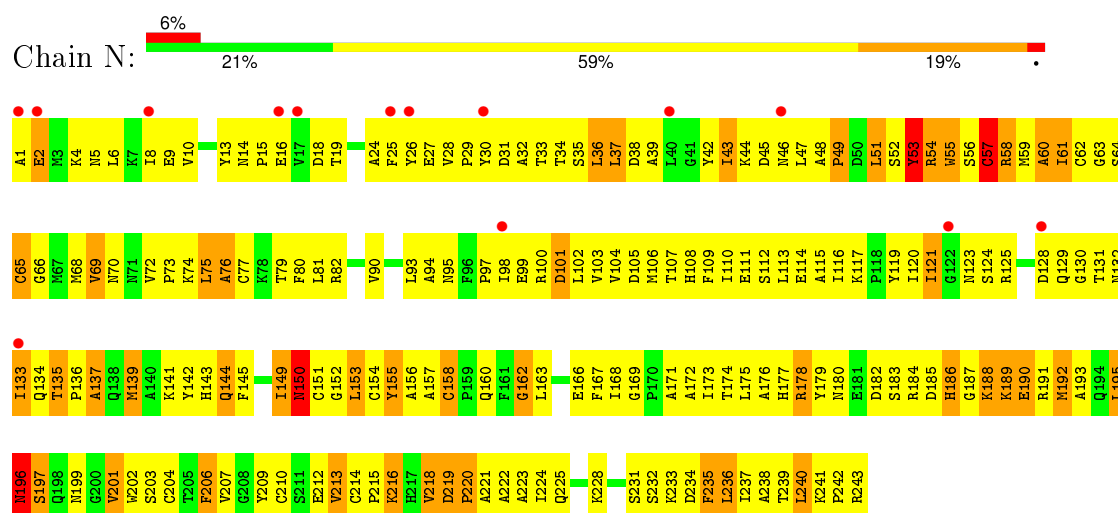
• Molecule 1: Fumarate reductase flavoprotein subunit

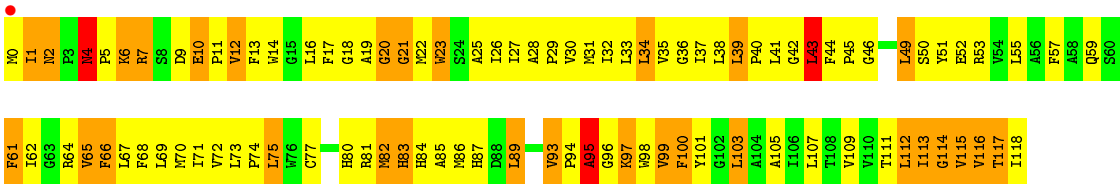


• Molecule 1: Fumarate reductase flavoprotein subunit









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 0.241 , 0.275	Depositor DCC
R_{free} test set	1094 reflections (2.37%)	DCC
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 59.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 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	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
9	A	52	0	29	16	0
9	M	52	0	29	13	0

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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	2097	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 2097 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: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 [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%)	7	38
1	M	570/602 (95%)	402 (70%)	103 (18%)	65 (11%)	0	3
2	B	241/243 (99%)	207 (86%)	30 (12%)	4 (2%)	11	47
2	N	241/243 (99%)	126 (52%)	79 (33%)	36 (15%)	0	1
3	C	128/130 (98%)	99 (77%)	25 (20%)	4 (3%)	5	32
3	O	128/130 (98%)	103 (80%)	18 (14%)	7 (6%)	2	16
4	D	117/119 (98%)	68 (58%)	35 (30%)	14 (12%)	0	3
4	P	117/119 (98%)	76 (65%)	26 (22%)	15 (13%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2117/2188 (97%)	1573 (74%)	385 (18%)	159 (8%)	1	10

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	3
1	M	456/475 (96%)	406 (89%)	50 (11%)	8	31
2	B	205/205 (100%)	171 (83%)	34 (17%)	3	13
2	N	205/205 (100%)	175 (85%)	30 (15%)	4	18
3	C	111/111 (100%)	89 (80%)	22 (20%)	1	7
3	O	111/111 (100%)	81 (73%)	30 (27%)	0	2
4	D	97/97 (100%)	79 (81%)	18 (19%)	2	9
4	P	97/97 (100%)	75 (77%)	22 (23%)	1	4
All	All	1742/1776 (98%)	1425 (82%)	317 (18%)	2	9

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
1	M	137	HIS
3	O	72	ASN
1	M	65	HIS
1	M	174	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z > 2$
5	FLC	A	702	-	3,12,12	3.17	2 (66%)	3,17,17	8.64	2 (66%)
9	FAD	A	703	1	48,57,58	3.69	25 (52%)	55,87,89	2.21	10 (18%)
6	FES	B	244	2	0,4,4	0.00	-	0,4,4	0.00	-
7	F3S	B	245	2	0,9,9	0.00	-	0,15,15	0.00	-
8	SF4	B	246	2	0,12,12	0.00	-	0,24,24	0.00	-
10	MQ7	D	700	-	34,34,49	3.69	15 (44%)	44,45,63	2.28	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FLC	M	802	-	3,12,12	4.65	2 (66%)	3,17,17	5.81	2 (66%)
9	FAD	M	803	1	48,57,58	3.88	23 (47%)	55,87,89	2.18	9 (16%)
6	FES	N	244	2	0,4,4	0.00	-	0,4,4	0.00	-
7	F3S	N	245	2	0,9,9	0.00	-	0,15,15	0.00	-
8	SF4	N	246	2	0,12,12	0.00	-	0,24,24	0.00	-
10	MQ7	P	800	-	34,34,49	3.73	15 (44%)	44,45,63	2.51	14 (31%)

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	-	0/30/46/50	0/6/6/6
6	FES	B	244	2	-	0/0/4/4	0/1/1/1
7	F3S	B	245	2	-	0/0/24/24	0/0/3/3
8	SF4	B	246	2	-	0/0/48/48	0/6/5/5
10	MQ7	D	700	-	-	0/23/43/61	0/2/2/2
5	FLC	M	802	-	-	0/6/16/16	0/0/0/0
9	FAD	M	803	1	-	0/30/46/50	0/6/6/6
6	FES	N	244	2	-	0/0/4/4	0/1/1/1
7	F3S	N	245	2	-	0/0/24/24	0/0/3/3
8	SF4	N	246	2	-	0/0/48/48	0/6/5/5
10	MQ7	P	800	-	-	0/23/43/61	0/2/2/2

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	700	MQ7	C11-C12	-4.40	1.43	1.50
9	A	703	FAD	C7M-C7	-3.99	1.43	1.51
9	A	703	FAD	C5A-C4A	-3.85	1.31	1.40
9	A	703	FAD	C2B-C3B	-3.73	1.42	1.52
10	P	800	MQ7	C11-C12	-3.67	1.45	1.50

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	803	FAD	N3A-C2A-N1A	-6.82	123.67	128.89
9	A	703	FAD	N3A-C2A-N1A	-6.76	123.72	128.89
9	A	703	FAD	C4-C4X-C10	-6.53	115.76	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	803	FAD	C4-C4X-C10	-5.85	116.20	119.94
9	M	803	FAD	C4X-C10-N10	-5.39	117.34	120.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	702	FLC	14	0
9	A	703	FAD	16	0
10	D	700	MQ7	7	0
5	M	802	FLC	3	0
9	M	803	FAD	13	0
7	N	245	F3S	1	0
8	N	246	SF4	3	0
10	P	800	MQ7	12	0

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%)	-0.46	0 100 100	9, 14, 62, 85	0
1	M	572/602 (95%)	0.97	99 (17%) 2 2	30, 92, 127, 142	0
2	B	243/243 (100%)	-0.56	3 (1%) 81 76	9, 15, 36, 85	0
2	N	243/243 (100%)	0.31	14 (5%) 26 21	9, 62, 119, 147	0
3	C	130/130 (100%)	-0.46	0 100 100	10, 32, 59, 76	0
3	O	130/130 (100%)	-0.06	3 (2%) 64 57	24, 55, 106, 123	0
4	D	119/119 (100%)	-0.59	1 (0%) 87 84	18, 36, 61, 70	0
4	P	119/119 (100%)	-0.32	1 (0%) 87 84	27, 49, 80, 118	0
All	All	2133/2188 (97%)	0.02	121 (5%) 27 22	9, 45, 114, 147	0

The worst 5 of 121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	17	VAL	8.7
1	M	484	GLU	6.2
1	M	557	ALA	6.0
1	M	392	GLY	5.9
1	M	218	SER	4.9

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 [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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
10	MQ7	P	800	33/48	0.61	1.16	15.76	83,106,120,123	0
10	MQ7	D	700	33/48	0.65	0.79	12.81	59,100,117,127	0
5	FLC	A	702	13/13	0.85	0.28	2.75	31,37,38,39	0
8	SF4	B	246	8/8	0.99	0.19	1.54	9,21,27,27	0
5	FLC	M	802	13/13	0.72	0.42	1.02	60,74,92,97	0
9	FAD	M	803	52/53	0.86	0.45	0.92	23,87,158,164	0
9	FAD	A	703	52/53	0.97	0.21	0.03	0,1,17,36	0
6	FES	B	244	4/4	0.98	0.18	-0.26	0,4,5,8	0
7	F3S	B	245	7/7	1.00	0.13	-0.89	7,11,15,24	0
8	SF4	N	246	8/8	0.97	0.14	-0.96	20,29,49,53	0
6	FES	N	244	4/4	0.96	0.14	-1.54	21,24,44,53	0
7	F3S	N	245	7/7	0.99	0.09	-2.70	14,16,29,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.