



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 05:42 AM GMT

PDB ID : 1KF6
Title : E. coli Quinol-Fumarate Reductase with Bound Inhibitor HQNO
Authors : Iverson, T.M.; Luna-Chavez, C.; Croal, L.R.; Cecchini, G.; Rees, D.C.
Deposited on : 2001-11-19
Resolution : 2.70 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>

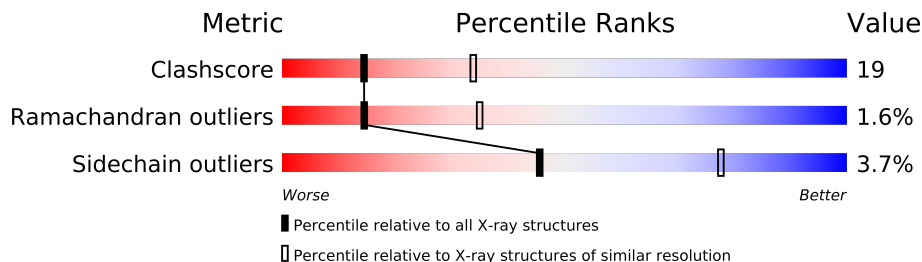
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
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 2.70 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))
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)

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.

Note EDS was not executed.

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	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 17071 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.

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 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 15 KDA HYDROPHOBIC PROTEIN.

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			

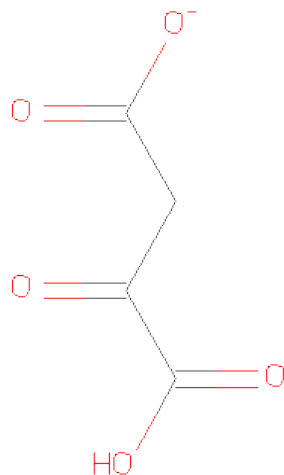
- Molecule 4 is a protein called FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN.

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

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

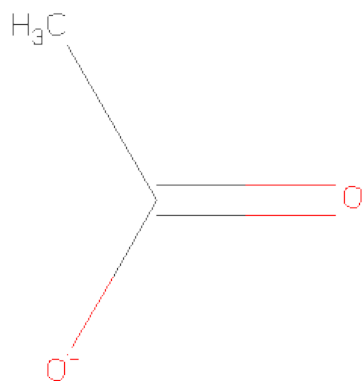
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		
5	M	1	Total	K	0	0
			1	1		

- Molecule 6 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).



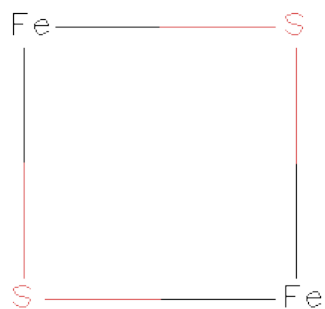
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	4	5		
6	M	1	Total	C	O	0	0
			9	4	5		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	N	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



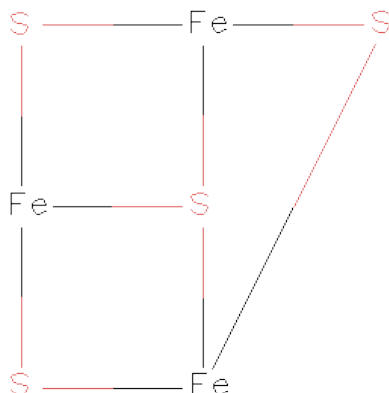
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			4	2	2		

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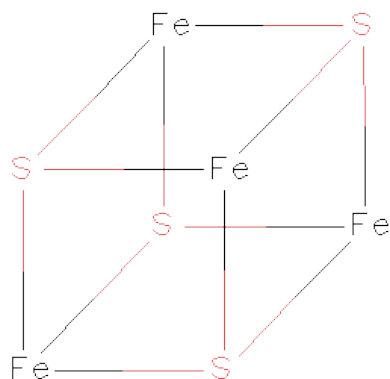
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 9 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



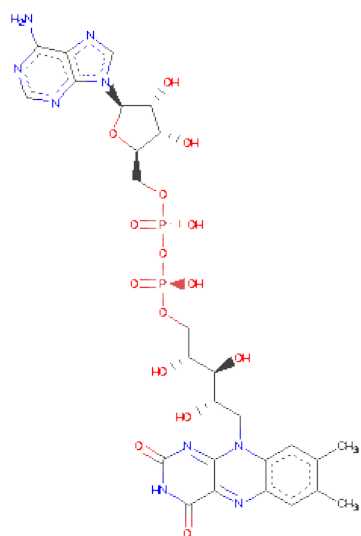
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		
9	N	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 10 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 11 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



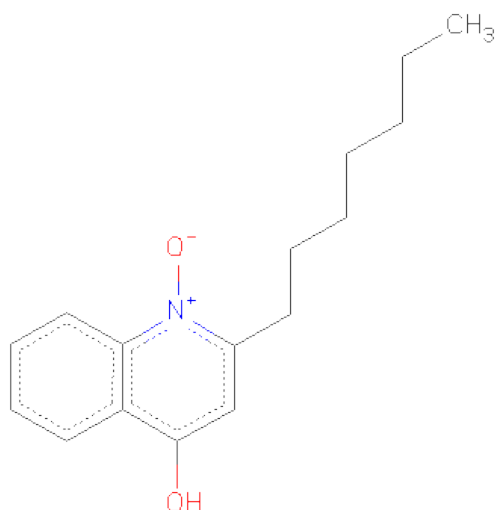
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			53	27	9	15		

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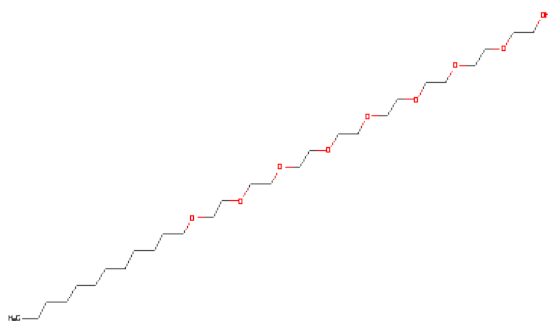
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	M	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 12 is 2-HEPTYL-4-HYDROXY QUINOLINE N-OXIDE (three-letter code: HQO) (formula: $C_{16}H_{21}NO_2$).



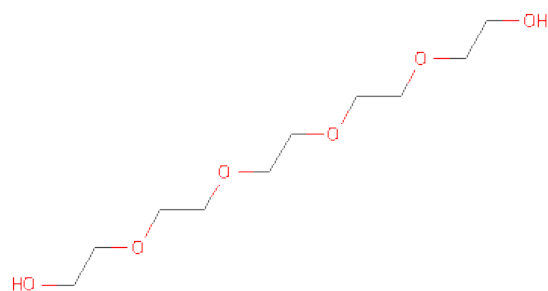
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	N	O	0	0
			19	16	1	2		
12	N	1	Total	C	N	O	0	0
			19	16	1	2		

- Molecule 13 is O-DODECANYL OCTAETHYLENE GLYCOL (three-letter code: CE1) (formula: $C_{28}H_{58}O_9$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	P	1	Total	C	O	0	0
			37	28	9		
13	P	1	Total	C	O	0	0
			37	28	9		
13	O	1	Total	C	O	0	0
			37	28	9		
13	O	1	Total	C	O	0	0
			37	28	9		
13	O	1	Total	C	O	0	0
			37	28	9		

- Molecule 14 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	10	Total	O	0	0
			10	10		
15	B	1	Total	O	0	0
			1	1		
15	M	4	Total	O	0	0
			4	4		
15	N	1	Total	O	0	0
			1	1		

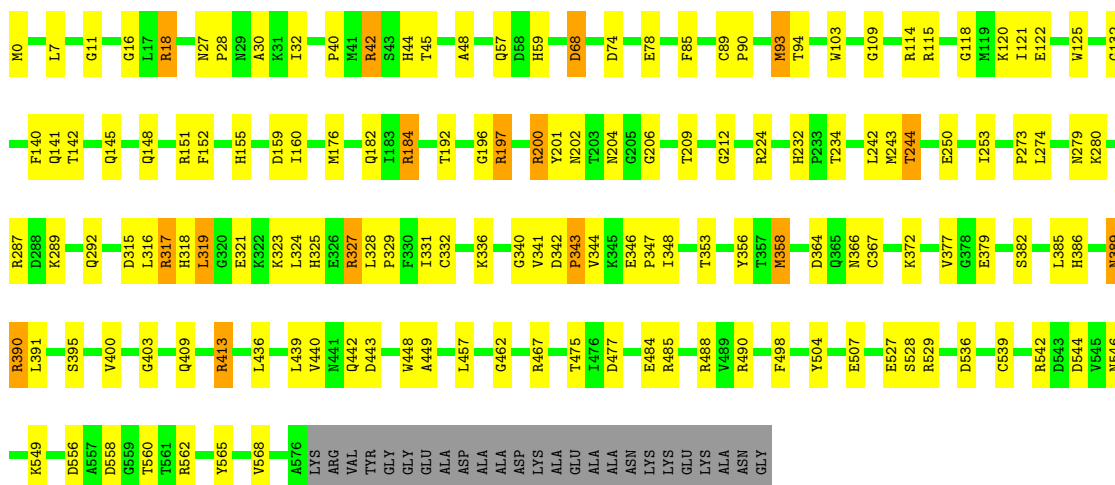
3 Residue-property plots

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.

Note EDS was not executed.

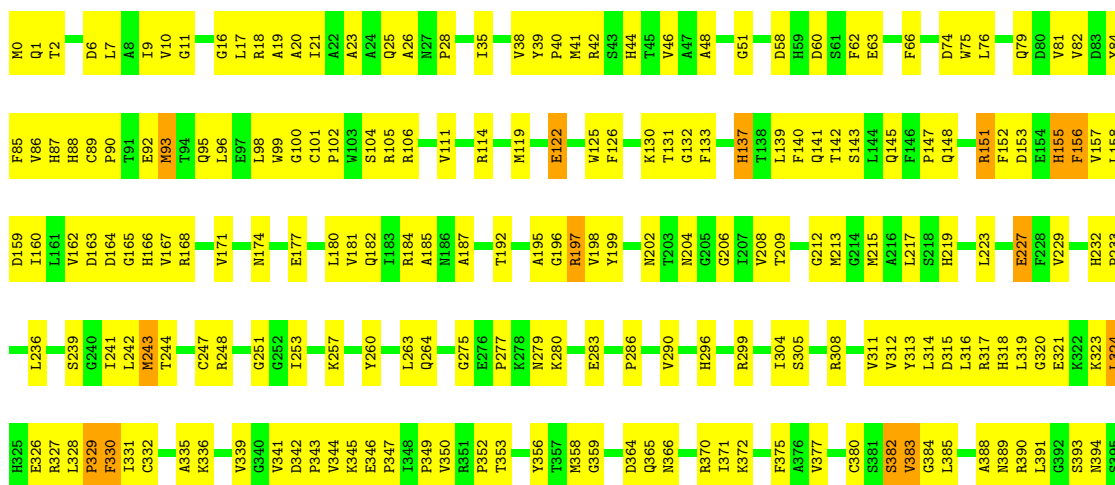
• Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN

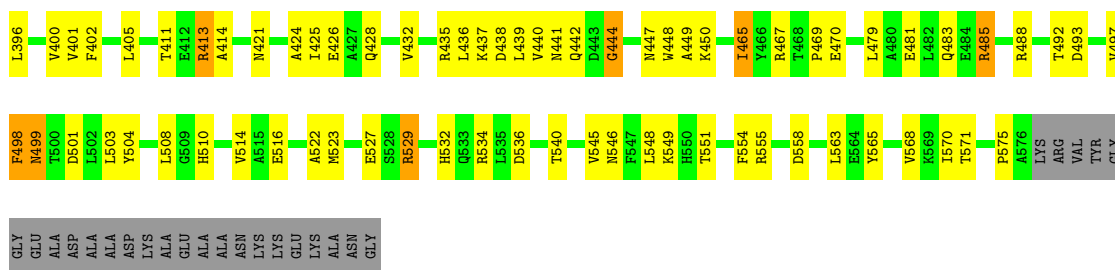
Chain A:



• Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN

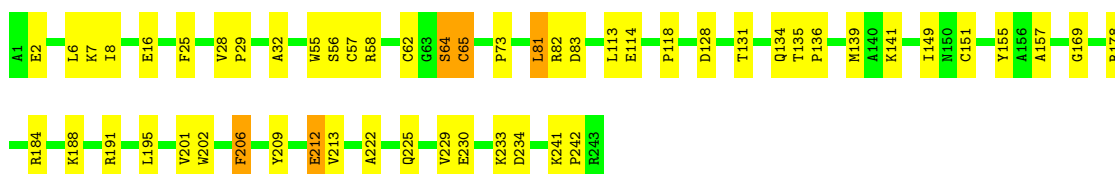
Chain M:





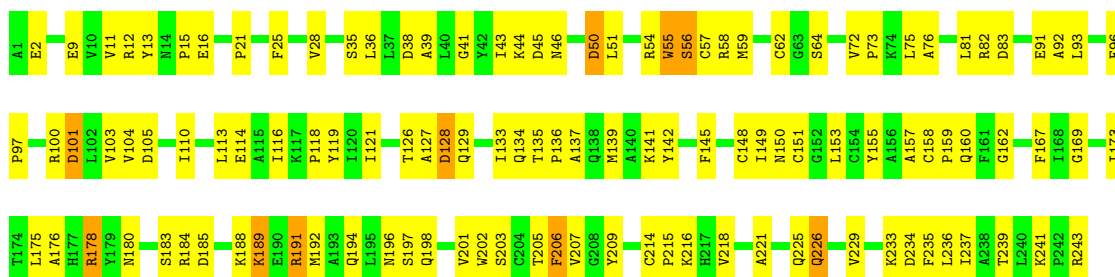
• Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN

Chain B:



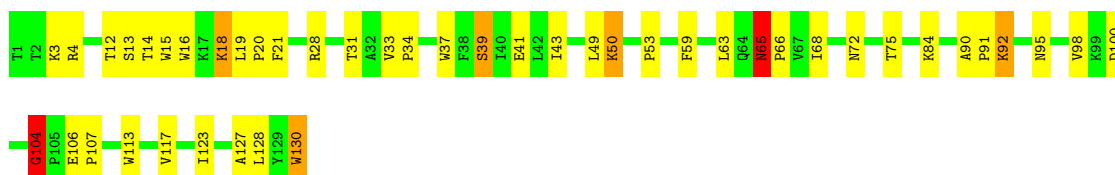
• Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN

Chain N:



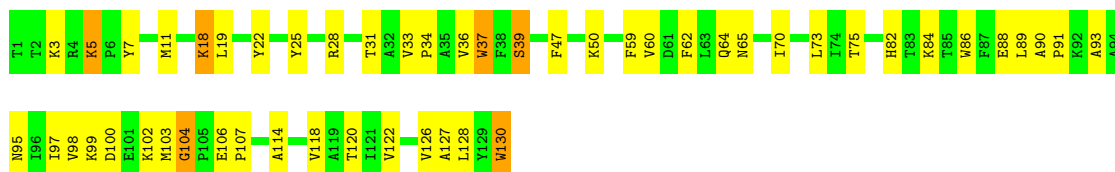
• Molecule 3: FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN

Chain C:



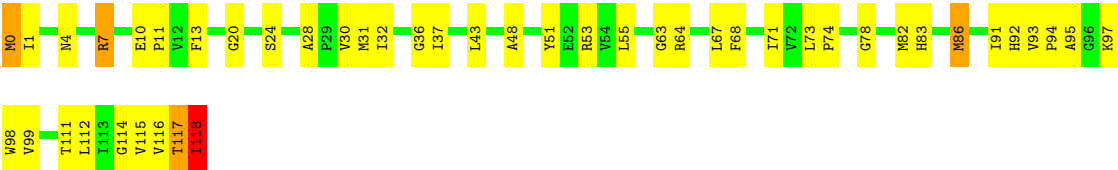
• Molecule 3: FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN

Chain O:



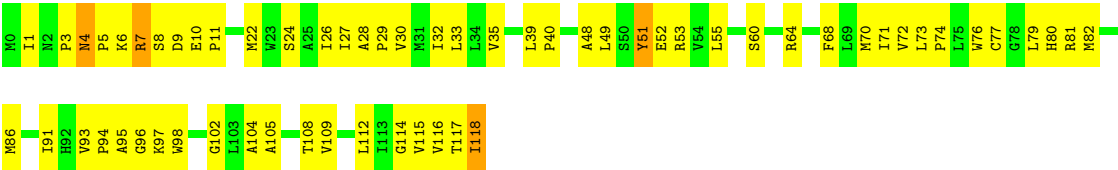
• Molecule 4: FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN

Chain D:



● Molecule 4: FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN

Chain P:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.50Å 137.84Å 273.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.231 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17071	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OAA, SF4, ACT, 1PE, F3S, FES, CE1, HQO, K, 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	0.81	0/4540	0.98	10/6139 (0.2%)
1	M	0.53	1/4540 (0.0%)	0.81	2/6139 (0.0%)
2	B	0.78	1/1931 (0.1%)	0.92	7/2617 (0.3%)
2	N	0.59	0/1931	0.81	1/2617 (0.0%)
3	C	0.77	3/1094 (0.3%)	0.87	2/1496 (0.1%)
3	O	0.68	3/1094 (0.3%)	0.79	1/1496 (0.1%)
4	D	0.78	1/956 (0.1%)	0.89	1/1303 (0.1%)
4	P	0.70	2/956 (0.2%)	0.82	0/1303
All	All	0.70	11/17042 (0.1%)	0.88	24/23110 (0.1%)

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
3	C	0	2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	118	ILE	C-OXT	11.65	1.45	1.23
4	P	118	ILE	C-OXT	8.01	1.38	1.23
2	B	65	CYS	CB-SG	-7.99	1.68	1.82
3	C	65	ASN	C-O	-7.42	1.09	1.23
3	O	104	GLY	C-O	-6.55	1.13	1.23

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ARG	NE-CZ-NH2	-7.24	116.68	120.30
4	D	7	ARG	NE-CZ-NH2	-7.24	116.68	120.30
2	B	191	ARG	NE-CZ-NH1	-6.88	116.86	120.30
3	C	28	ARG	NE-CZ-NH2	-6.71	116.95	120.30
2	B	65	CYS	N-CA-CB	-6.56	98.79	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	65	ASN	Mainchain,Peptide

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	4335	119	0
1	M	4448	0	4335	253	0
2	B	1888	0	1837	44	0
2	N	1888	0	1837	108	0
3	C	1058	0	1108	47	0
3	O	1058	0	1108	48	0
4	D	926	0	971	47	0
4	P	926	0	971	65	0
5	A	1	0	0	0	0
5	M	1	0	0	0	0
6	A	9	0	2	2	0
6	M	9	0	2	0	0
7	A	4	0	3	0	0
7	B	4	0	3	0	0
7	N	4	0	3	2	0
8	B	4	0	0	0	0
8	N	4	0	0	0	0
9	B	7	0	0	0	0
9	N	7	0	0	1	0
10	B	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	N	8	0	0	4	0
11	A	53	0	31	8	0
11	M	53	0	31	8	0
12	C	19	0	20	3	0
12	N	19	0	20	2	0
13	O	111	0	174	0	0
13	P	74	0	116	5	0
14	A	16	0	20	5	0
15	A	10	0	0	1	0
15	B	1	0	0	0	0
15	M	4	0	0	0	0
15	N	1	0	0	0	0
All	All	17071	0	16927	659	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 19.

The worst 5 of 659 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:44:HIS:NE2	11:A:721:FAD:HM82	1.21	1.44
1:M:44:HIS:NE2	11:M:821:FAD:HM82	1.18	1.42
1:A:44:HIS:NE2	11:A:721:FAD:C8M	1.89	1.33
1:M:44:HIS:NE2	11:M:821:FAD:C8M	1.98	1.27
1:A:44:HIS:CE1	11:A:721:FAD:HM82	1.86	1.08

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%)	541 (94%)	30 (5%)	4 (1%)	30 62
1	M	575/602 (96%)	487 (85%)	75 (13%)	13 (2%)	10 24
2	B	241/243 (99%)	224 (93%)	16 (7%)	1 (0%)	43 76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	241/243 (99%)	215 (89%)	20 (8%)	6 (2%)	9	21
3	C	128/130 (98%)	120 (94%)	4 (3%)	4 (3%)	7	14
3	O	128/130 (98%)	114 (89%)	12 (9%)	2 (2%)	14	35
4	D	117/119 (98%)	111 (95%)	3 (3%)	3 (3%)	8	20
4	P	117/119 (98%)	102 (87%)	14 (12%)	1 (1%)	25	55
All	All	2122/2188 (97%)	1914 (90%)	174 (8%)	34 (2%)	14	35

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	18	LYS
3	C	65	ASN
1	M	244	THR
1	M	382	SER
1	A	318	HIS

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%)	446 (97%)	14 (3%)	53	84
1	M	460/475 (97%)	437 (95%)	23 (5%)	34	66
2	B	205/205 (100%)	199 (97%)	6 (3%)	55	85
2	N	205/205 (100%)	195 (95%)	10 (5%)	35	67
3	C	111/111 (100%)	107 (96%)	4 (4%)	47	79
3	O	111/111 (100%)	108 (97%)	3 (3%)	57	87
4	D	97/97 (100%)	94 (97%)	3 (3%)	52	83
4	P	97/97 (100%)	95 (98%)	2 (2%)	66	91
All	All	1746/1776 (98%)	1681 (96%)	65 (4%)	45	78

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	122	GLU
1	M	164	ASP
3	O	5	LYS
1	M	126	PHE
1	M	155	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	174	ASN
1	M	409	GLN
2	N	186	HIS
1	M	292	GLN
1	M	421	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 ⓘ

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 for Mogul analysis.

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	OAA	A	702	-	6,8,8	1.34	1 (16%)	7,10,10	1.71	2 (28%)
7	ACT	A	703	-	1,3,3	1.68	0	0,3,3	0.00	-
14	1PE	A	705	-	15,15,15	1.62	0	14,14,14	2.18	8 (57%)
11	FAD	A	721	-	58,58,58	1.67	10 (17%)	85,89,89	2.04	14 (16%)
8	FES	B	244	2	0,4,4	0.00	-	0,4,4	0.00	-
9	F3S	B	245	2	3,9,9	14.65	3 (100%)	0,15,15	0.00	-
10	SF4	B	246	2	12,12,12	28.16	12 (100%)	0,24,24	0.00	-
7	ACT	B	704	-	1,3,3	2.86	1 (100%)	0,3,3	0.00	-
12	HQO	C	700	-	20,20,20	1.87	7 (35%)	26,26,26	1.02	1 (3%)
6	OAA	M	802	-	6,8,8	1.31	1 (16%)	7,10,10	1.72	2 (28%)
11	FAD	M	821	-	58,58,58	1.49	12 (20%)	85,89,89	2.08	11 (12%)
8	FES	N	244	2	0,4,4	0.00	-	0,4,4	0.00	-
9	F3S	N	245	2	3,9,9	11.71	2 (66%)	0,15,15	0.00	-
10	SF4	N	246	2	12,12,12	62.27	12 (100%)	0,24,24	0.00	-
12	HQO	N	800	-	20,20,20	1.87	7 (35%)	26,26,26	1.02	1 (3%)
7	ACT	N	803	-	1,3,3	2.65	1 (100%)	0,3,3	0.00	-
13	CE1	O	811	-	36,36,36	1.10	0	35,35,35	1.95	16 (45%)
13	CE1	O	812	-	36,36,36	1.10	0	35,35,35	1.87	16 (45%)
13	CE1	O	813	-	36,36,36	1.17	0	35,35,35	1.93	16 (45%)
13	CE1	P	710	-	36,36,36	1.09	0	35,35,35	1.89	16 (45%)
13	CE1	P	810	-	36,36,36	1.09	0	35,35,35	1.97	16 (45%)

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	OAA	A	702	-	-	0/6/8/8	0/0/0/0
7	ACT	A	703	-	-	0/0/0/0	0/0/0/0
14	1PE	A	705	-	-	0/13/13/13	0/0/0/0
11	FAD	A	721	-	-	0/34/50/50	0/1/6/6
8	FES	B	244	2	-	0/0/4/4	0/0/1/1
9	F3S	B	245	2	-	0/0/24/24	0/0/3/3
10	SF4	B	246	2	-	0/0/48/48	0/0/5/5
7	ACT	B	704	-	-	0/0/0/0	0/0/0/0
12	HQO	C	700	-	-	0/7/7/7	0/0/2/2
6	OAA	M	802	-	-	0/6/8/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	FAD	M	821	-	-	0/34/50/50	0/1/6/6
8	FES	N	244	2	-	0/0/4/4	0/0/1/1
9	F3S	N	245	2	-	0/0/24/24	0/0/3/3
10	SF4	N	246	2	-	0/0/48/48	0/0/5/5
12	HQO	N	800	-	-	0/7/7/7	0/0/2/2
7	ACT	N	803	-	-	0/0/0/0	0/0/0/0
13	CE1	O	811	-	-	0/34/34/34	0/0/0/0
13	CE1	O	812	-	-	0/34/34/34	0/0/0/0
13	CE1	O	813	-	-	0/34/34/34	0/0/0/0
13	CE1	P	710	-	-	0/34/34/34	0/0/0/0
13	CE1	P	810	-	-	0/34/34/34	0/0/0/0

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	246	SF4	S1-FE2	96.29	2.98	2.33
10	N	246	SF4	S2-FE3	-94.96	1.69	2.33
10	N	246	SF4	S2-FE1	93.86	2.96	2.33
10	N	246	SF4	S1-FE4	-82.38	1.77	2.33
10	N	246	SF4	S1-FE3	-58.80	1.93	2.33

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	821	FAD	N3A-C2A-N1A	-10.73	119.73	128.71
11	A	721	FAD	C2-N1-C10	8.02	123.06	114.98
11	M	821	FAD	C2-N1-C10	6.84	121.87	114.98
11	A	721	FAD	N3A-C2A-N1A	-6.62	123.17	128.71
11	A	721	FAD	C4X-N5-C5X	5.70	123.09	116.69

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.