



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 26, 2017 – 05:36 AM EDT

PDB ID : 1QFF
Title : E. COLI FERRIC HYDROXAMATE UPTAKE RECEPTOR (FHUA) IN
COMPLEX WITH BOUND FERRICHRONE-IRON
Authors : Ferguson, A.D.; Hofmann, E.; Coulton, J.W.; Diederichs, K.; Welte, W.
Deposited on : unknown
Resolution : 2.70 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

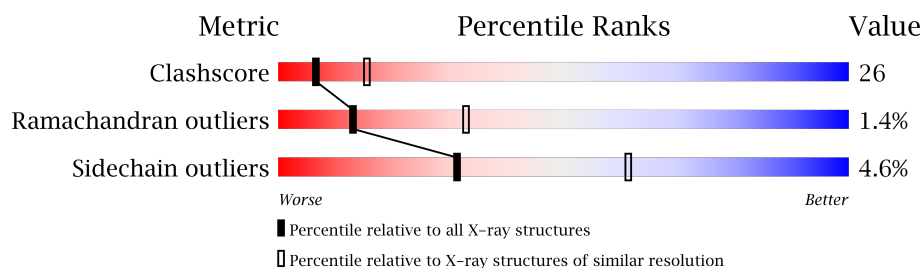
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	725	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 5972 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.

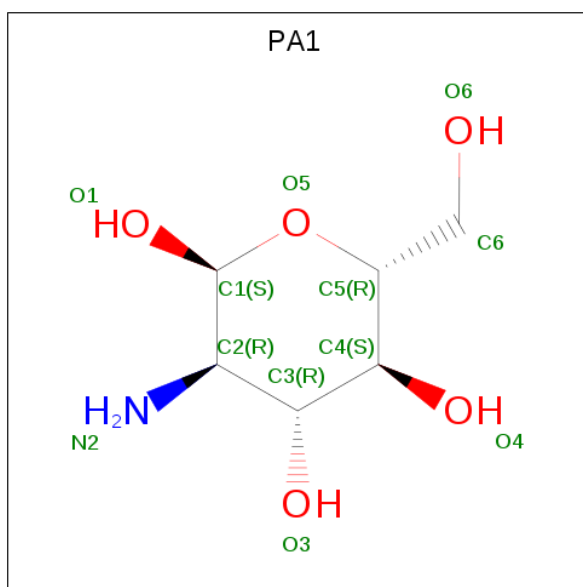
- Molecule 1 is a protein called FERRIC HYDROXAMATE UPTAKE RECEPTOR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	707	Total	C	N	O	S	Se	0	0	0
			5524	3475	944	1091	4	10			

There are 11 discrepancies between the modelled and reference sequences:

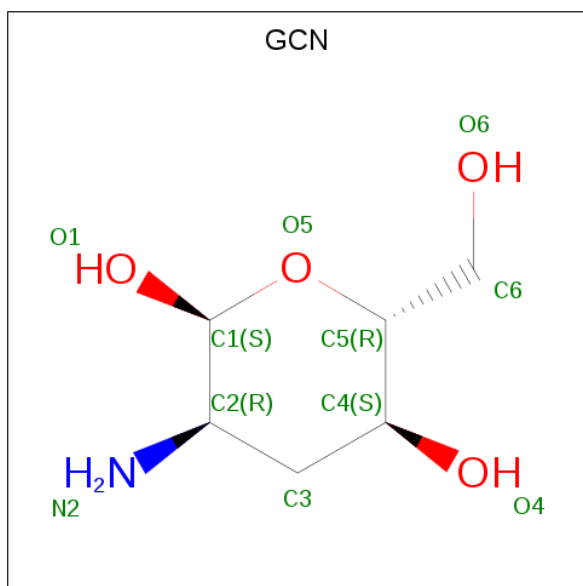
Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	INTRACHAIN HIS TAG	UNP P06971
A	407	SER	-	INTRACHAIN HIS TAG	UNP P06971
A	408	HIS	-	INTRACHAIN HIS TAG	UNP P06971
A	409	HIS	-	INTRACHAIN HIS TAG	UNP P06971
A	410	HIS	-	INTRACHAIN HIS TAG	UNP P06971
A	411	HIS	-	INTRACHAIN HIS TAG	UNP P06971
A	412	HIS	-	INTRACHAIN HIS TAG	UNP P06971
A	413	HIS	-	INTRACHAIN HIS TAG	UNP P06971
A	414	GLY	-	INTRACHAIN HIS TAG	UNP P06971
A	415	SER	-	INTRACHAIN HIS TAG	UNP P06971
A	416	SER	-	INTRACHAIN HIS TAG	UNP P06971

- Molecule 2 is 2-amino-2-deoxy-alpha-D-glucopyranose (three-letter code: PA1) (formula: C₆H₁₃NO₅).



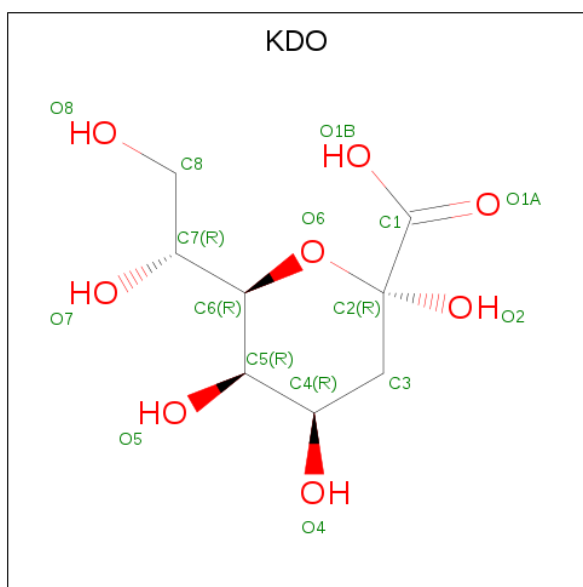
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 3 is 3-DEOXY-D-GLUCOSAMINE (three-letter code: GCN) (formula: $C_6H_{13}NO_4$).



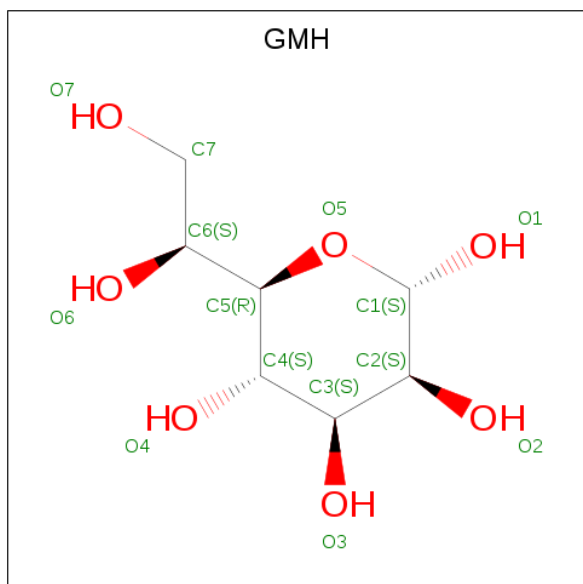
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 4 is 3-DEOXY-D-MANNO-OCT-2-ULOSONIC ACID (three-letter code: KDO) (formula: $C_8H_{14}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			15	8	7		
4	A	1	Total	C	O	0	0
			15	8	7		

- Molecule 5 is L-GLYCERO-D-MANNO-HEPTOPYRANOSE (three-letter code: GMH) (formula: $C_7H_{14}O_7$).



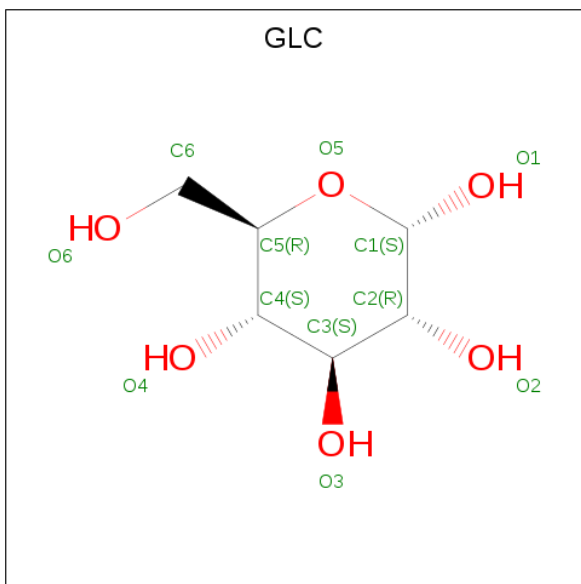
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	7	6		

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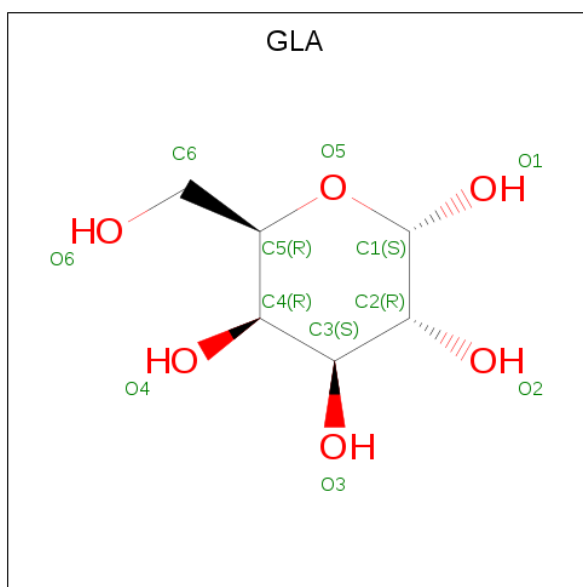
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	7	6		

- Molecule 6 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is ALPHA D-GALACTOSE (three-letter code: GLA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		

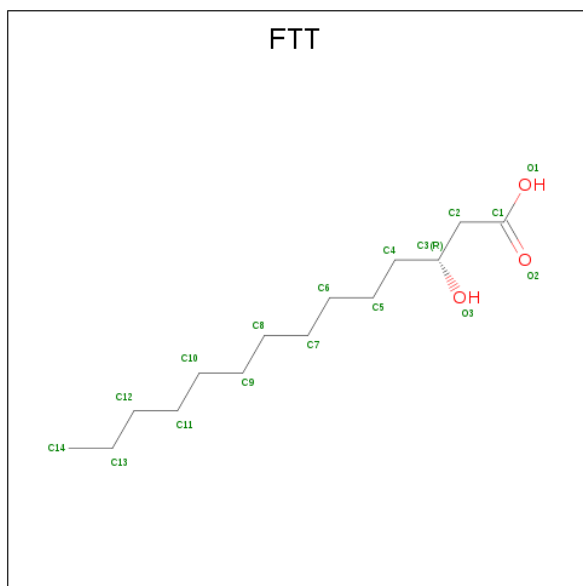
- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	P	0	0
			4	3	1		
8	A	1	Total	O	P	0	0
			4	3	1		

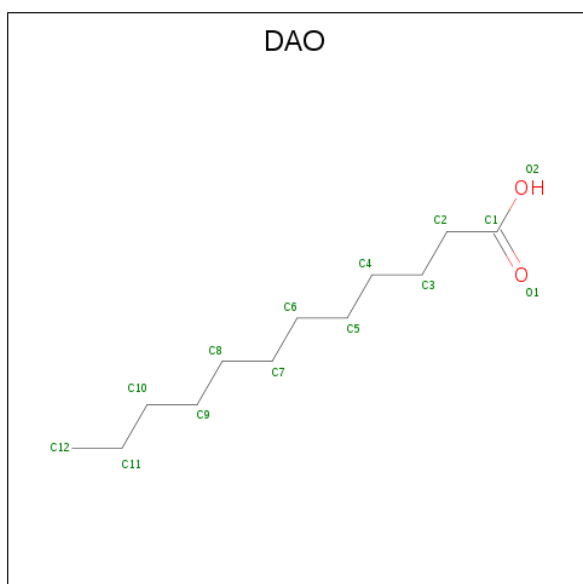
- Molecule 9 is 3-HYDROXY-TETRADECANOIC ACID (three-letter code: FTT) (formula:

$C_{14}H_{28}O_3$).



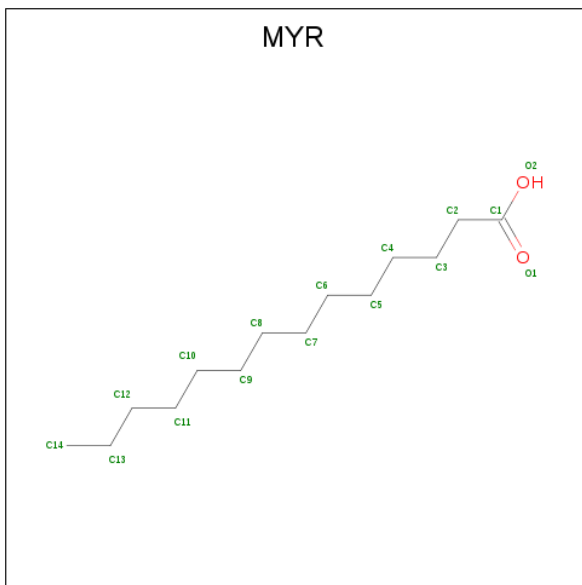
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			16	14	2		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			16	14	2		
9	A	1	Total	C	O	0	0
			17	14	3		

- Molecule 10 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$).



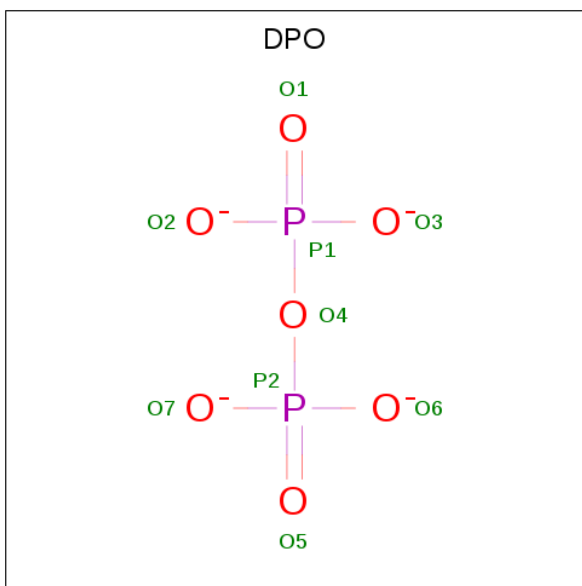
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			13	12	1		

- Molecule 11 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



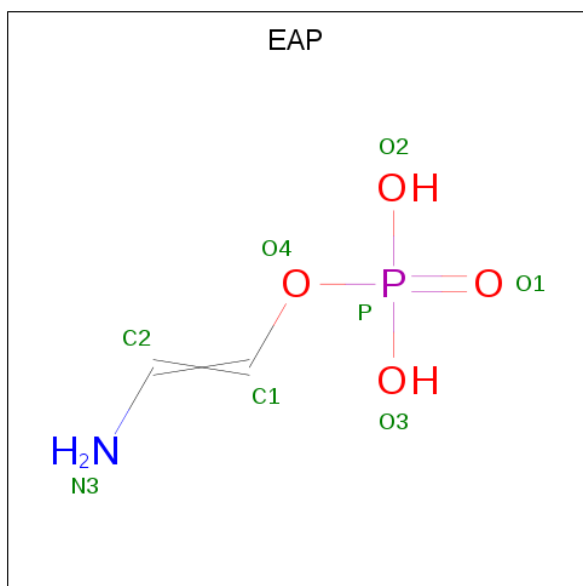
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			15	14	1		

- Molecule 12 is DIPHOSPHATE (three-letter code: DPO) (formula: O_7P_2).



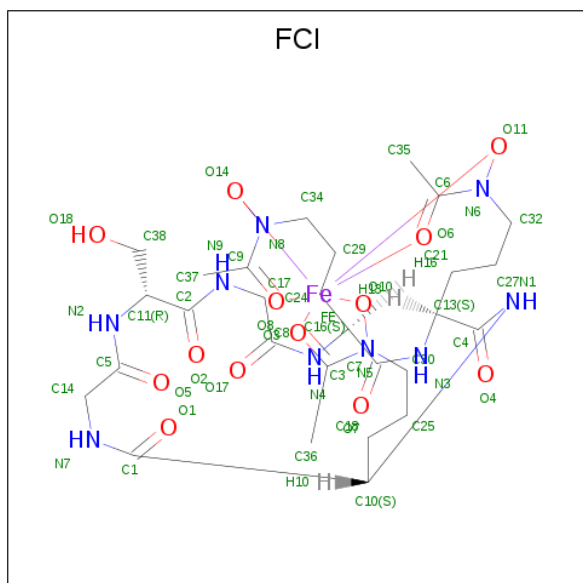
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	O	P	0	0
			8	6	2		

- Molecule 13 is 2-AMINO-VINYL-PHOSPHATE (three-letter code: EAP) (formula: $C_2H_6NO_4P$).



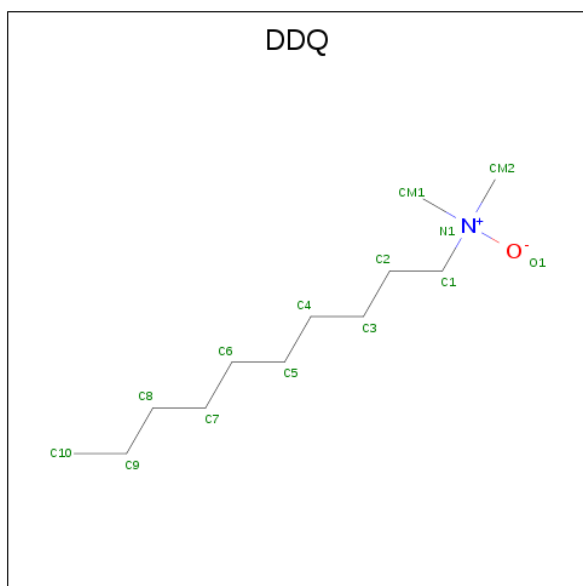
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	N	O	P	0	0
			7	2	1	3	1		

- Molecule 14 is FERRICROCIN-IRON (three-letter code: FCI) (formula: $C_{28}H_{44}FeN_9O_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	Fe	N	O	
			51	28	1	9	13	
							0	0

- Molecule 15 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula: $C_{12}H_{27}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	A	1	Total	C	N	O		
			14	12	1	1		
15	A	1	Total	C	N	O		
			14	12	1	1		
							0	0

- Molecule 16 is water.

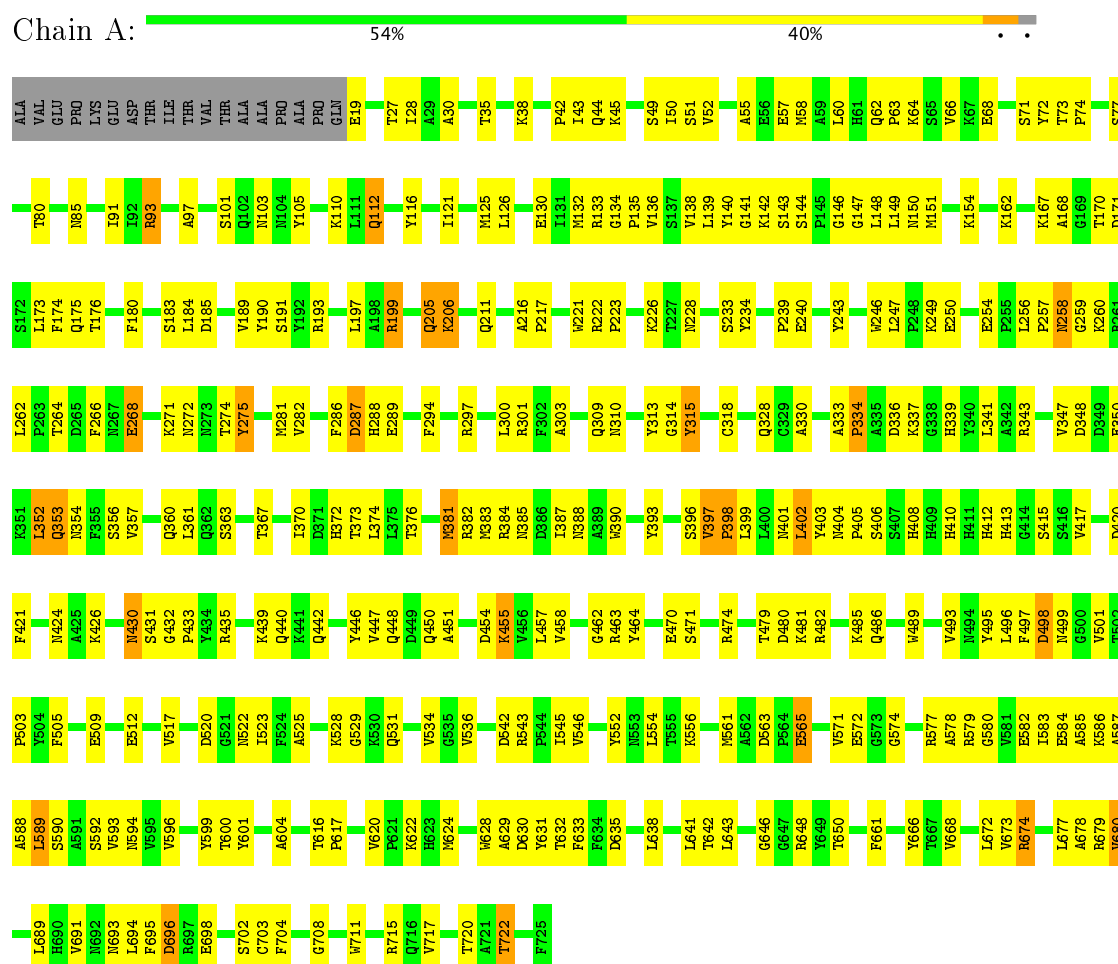
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	152	Total	O		
			152	152		
					0	0

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 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.

Note EDS was not executed.

• Molecule 1: FERRIC HYDROXAMATE UPTAKE RECEPTOR



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	171.40 Å 171.40 Å 85.70 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	98.3 (30.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5972	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PA1, DAO, FTT, GLA, PO4, MYR, GCN, DPO, KDO, EAP, GLC, FCI, GMH, DDQ

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	0.34	0/5654	0.62	0/7666

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5524	0	5223	290	0
2	A	11	0	8	0	0
3	A	10	0	6	0	0
4	A	30	0	22	2	0
5	A	26	0	20	5	0
6	A	22	0	18	0	0
7	A	11	0	10	0	0
8	A	8	0	0	1	0
9	A	56	0	83	4	0
10	A	13	0	23	0	0
11	A	15	0	27	0	0
12	A	8	0	0	0	0
13	A	7	0	4	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	51	0	44	2	0
15	A	28	0	54	1	0
16	A	152	0	0	11	0
All	All	5972	0	5542	299	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 26.

The worst 5 of 299 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:121:ILE:HB	1:A:151:MSE:HE1	1.33	1.10
1:A:28:ILE:HD12	1:A:28:ILE:H	1.25	0.97
1:A:381:MSE:HE1	1:A:383:MSE:HB2	1.48	0.96
1:A:126:LEU:HD11	1:A:151:MSE:HE3	1.50	0.92
1:A:126:LEU:HD21	1:A:151:MSE:HE2	1.52	0.91

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	705/725 (97%)	637 (90%)	58 (8%)	10 (1%)	13 33

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	PRO
1	A	679	ARG
1	A	334	PRO
1	A	498	ASP

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Mol	Chain	Res	Type
1	A	589	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	587/591 (99%)	560 (95%)	27 (5%)	31 61

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	352	LEU
1	A	381	MSE
1	A	674	ARG
1	A	353	GLN
1	A	199	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	ASN
1	A	388	ASN
1	A	438	ASN
1	A	328	GLN
1	A	522	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

22 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	$\# Z > 2$
2	PA1	A	1000	9,3,12	11,11,12	0.67	0	12,15,17	0.81	1 (8%)
3	GCN	A	1001	9,8,2,4	10,10,11	1.01	1 (10%)	9,13,15	1.09	1 (11%)
4	KDO	A	1002	3,5,4	12,15,16	0.73	0	13,21,24	0.73	0
4	KDO	A	1003	4	12,15,16	0.45	0	13,21,24	0.73	0
5	GMH	A	1004	13,5,4	13,13,14	0.81	0	16,18,20	0.69	0
5	GMH	A	1005	8,5,6	13,13,14	1.05	2 (15%)	16,18,20	1.15	1 (6%)
6	GLC	A	1006	5,7,6	11,11,12	0.58	0	13,15,17	0.77	0
6	GLC	A	1007	6	11,11,12	0.55	0	13,15,17	0.58	0
7	GLA	A	1008	6	11,11,12	0.45	0	13,15,17	0.56	0
9	FTT	A	1009	2	15,15,16	0.39	0	15,15,17	0.65	0
9	FTT	A	1010	2	3,6,16	0.30	0	4,7,17	0.71	0
9	FTT	A	1011	10,3	15,15,16	0.31	0	15,15,17	0.77	0
10	DAO	A	1012	9	12,12,13	1.03	1 (8%)	11,11,13	0.80	1 (9%)
9	FTT	A	1013	11,3	13,16,16	0.36	0	13,17,17	0.59	0
11	MYR	A	1014	9	14,14,15	0.98	1 (7%)	13,13,15	0.81	1 (7%)
14	FCI	A	1050	-	56,56,56	1.39	4 (7%)	63,87,87	1.00	2 (3%)
15	DDQ	A	1101	-	11,13,13	0.62	0	12,15,15	0.66	0
15	DDQ	A	1102	-	11,13,13	0.57	0	12,15,15	0.64	0
12	DPO	A	2000	2	5,7,8	3.28	2 (40%)	4,10,13	0.33	0
8	PO4	A	2001	3	0,3,4	0.00	-	0,3,6	0.00	-
13	EAP	A	2004	5	3,6,7	3.50	2 (66%)	0,6,9	0.00	-
8	PO4	A	2005	5	0,3,4	0.00	-	0,3,6	0.00	-

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
2	PA1	A	1000	9,3,12	-	0/2/18/22	0/1/1/1
3	GCN	A	1001	9,8,2,4	-	0/2/15/18	0/1/1/1
4	KDO	A	1002	3,5,4	-	0/6/26/30	0/1/1/1
4	KDO	A	1003	4	-	0/6/26/30	0/1/1/1
5	GMH	A	1004	13,5,4	-	0/6/23/26	0/1/1/1
5	GMH	A	1005	8,5,6	-	0/6/23/26	0/1/1/1
6	GLC	A	1006	5,7,6	-	0/2/19/22	0/1/1/1
6	GLC	A	1007	6	-	0/2/19/22	0/1/1/1
7	GLA	A	1008	6	-	0/2/19/22	0/1/1/1
9	FTT	A	1009	2	-	0/14/14/15	0/0/0/0
9	FTT	A	1010	2	-	0/2/4/15	0/0/0/0
9	FTT	A	1011	10,3	-	0/14/14/15	0/0/0/0
10	DAO	A	1012	9	-	0/10/10/11	0/0/0/0
9	FTT	A	1013	11,3	-	0/13/15/15	0/0/0/0
11	MYR	A	1014	9	-	0/12/12/13	0/0/0/0
14	FCI	A	1050	-	-	0/62/116/116	0/0/6/6
15	DDQ	A	1101	-	-	0/11/11/11	0/0/0/0
15	DDQ	A	1102	-	-	0/11/11/11	0/0/0/0
12	DPO	A	2000	2	-	0/2/5/6	0/0/0/0
8	PO4	A	2001	3	-	0/0/0/0	0/0/0/0
13	EAP	A	2004	5	-	0/0/4/5	0/0/0/0
8	PO4	A	2005	5	-	0/0/0/0	0/0/0/0

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	2000	DPO	P2-O4	-5.62	1.50	1.60
13	A	2004	EAP	P-O4	-4.46	1.49	1.63
12	A	2000	DPO	P1-O4	-4.26	1.50	1.63
11	A	1014	MYR	O2-C1	-3.61	1.23	1.42
10	A	1012	DAO	O2-C1	-3.51	1.23	1.42

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1050	FCI	O17-C8-N4	-2.12	119.31	122.97
11	A	1014	MYR	O2-C1-C2	2.06	125.29	111.65
10	A	1012	DAO	O2-C1-C2	2.08	125.36	111.65
2	A	1000	PA1	O5-C1-C2	2.28	112.17	109.51
3	A	1001	GCN	C1-O5-C5	2.52	115.64	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	KDO	1	0
4	A	1003	KDO	1	0
5	A	1004	GMH	4	0
5	A	1005	GMH	1	0
9	A	1009	FTT	1	0
9	A	1011	FTT	2	0
9	A	1013	FTT	3	0
14	A	1050	FCI	2	0
15	A	1101	DDQ	1	0
13	A	2004	EAP	2	0
8	A	2005	PO4	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.