

# wwPDB X-ray Structure Validation Summary Report (i)

Dec 10, 2022 – 07:31 PM EST

PDB ID : 1QFF

Title : E. COLI FERRIC HYDROXAMATE UPTAKE RECEPTOR (FHUA) IN

COMPLEX WITH BOUND FERRICHROME-IRON

Authors: Ferguson, A.D.; Hofmann, E.; Coulton, J.W.; Diederichs, K.; Welte, W.

Deposited on : 1999-04-10

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

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED

EDS : NOT EXECUTED

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

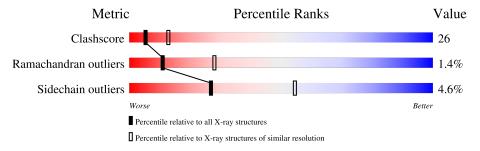
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain						
1	A	725	54%		40%				
2	В	9	33%	56%	11%				



# 2 Entry composition (i)

There are 11 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.

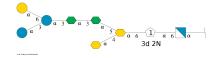
• Molecule 1 is a protein called FERRIC HYDROXAMATE UPTAKE RECEPTOR.

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

There are 11 discrepancies between the modelled and reference sequences:

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

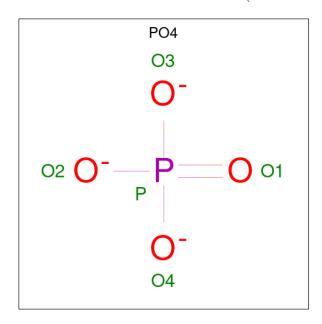
• Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-3)-[alpha-D-galactopyrano se-(1-6)]alpha-D-glucopyranose-(1-3)-L-glycero-alpha-D-manno-heptopyranose-(1-3)-L-glyce ro-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2,3-dideoxy-alpha-D-glucopyranose-(1-6)-2-amino-2-deoxy-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	В	9	Total 110	C 60	N 2	O 48	0	0	0

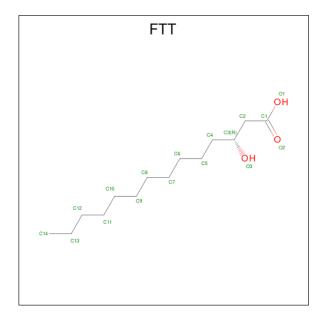


• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

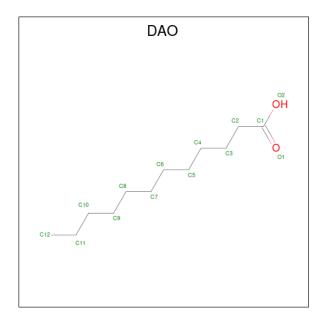
 $\bullet$  Molecule 4 is 3-HYDROXY-TETRADECANOIC ACID (three-letter code: FTT) (formula:  $C_{14}H_{28}O_3).$ 





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

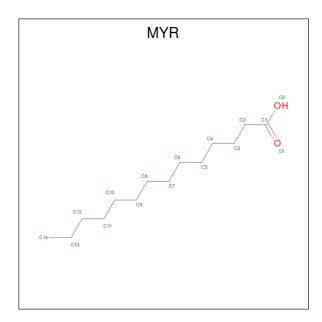
 $\bullet$  Molecule 5 is LAURIC ACID (three-letter code: DAO) (formula:  $\mathrm{C_{12}H_{24}O_{2}}).$ 



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

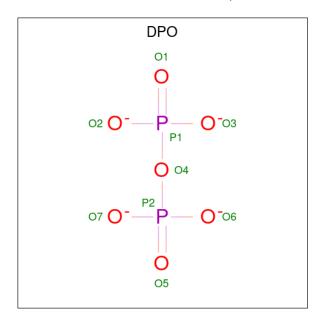
 $\bullet$  Molecule 6 is MYRISTIC ACID (three-letter code: MYR) (formula:  $\mathrm{C}_{14}\mathrm{H}_{28}\mathrm{O}_2).$ 





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

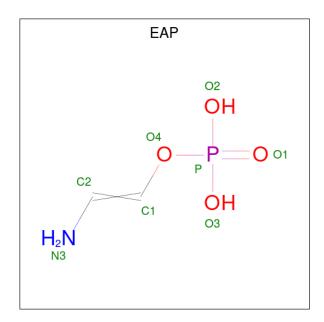
 $\bullet$  Molecule 7 is DIPHOSPHATE (three-letter code: DPO) (formula:  $\mathrm{O_7P_2}).$ 



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

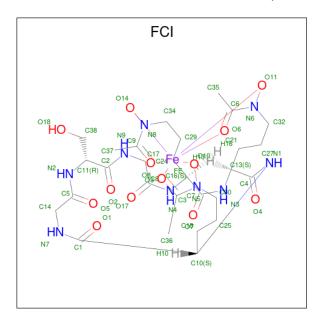
• Molecule 8 is 2-AMINO-VINYL-PHOSPHATE (three-letter code: EAP) (formula:  $C_2H_6NO_4P$ ).





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

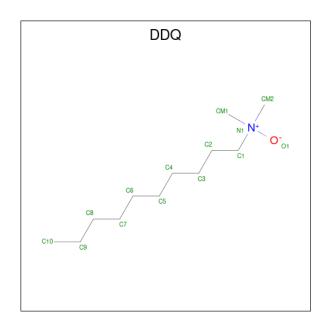
 $\bullet$  Molecule 9 is FERRICROCIN-IRON (three-letter code: FCI) (formula:  $\mathrm{C}_{28}\mathrm{H}_{44}\mathrm{FeN}_9\mathrm{O}_{13}).$ 



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

 $\bullet$  Molecule 10 is DECYLAMINE-N, N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula: C<sub>12</sub>H<sub>27</sub>NO).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
10	Λ	1	1 Total C N O		0	0			
10	A	1	14	12	1	1	0	0	
10	Λ	1	Total	С	N	О	0	0	
10	A	1	14	12	1	1	0	0	

• Molecule 11 is water.

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

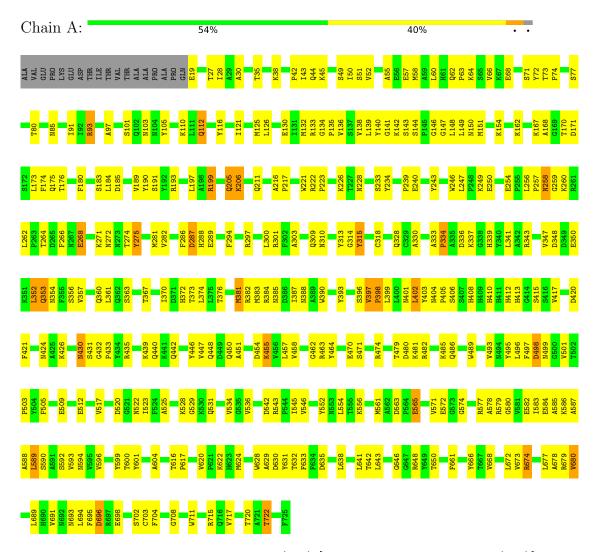


# 3 Residue-property plots (i)

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. 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. 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



• Molecule 2: alpha-D-glucopyranose-(1-3)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-L-glycero-alpha-D-manno-heptopyranose-(1-3)-L-glycero-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2,3-dideoxy-alpha-D-glucoyranose-(1-6)-2-amino-2-deoxy-alpha-D-glucopyranose



Chain B: 33% 56% 11%





# 4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 61	Depositor	
Cell constants	171.40Å 171.40Å 85.70Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor	
Resolution (Å)	30.00 - 2.70	Depositor	
% Data completeness	98.3 (30.00-2.70)	Depositor	
(in resolution range)	30.0 (80.00 2.10)	Беровног	
$R_{merge}$	(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 <sup>2</sup> )	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: GCN, DDQ, MYR, DPO, FTT, GLC, DAO, KDO, PO4, GLA, FCI, EAP, PA1, GMH

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	$\mathbf{lengths}$	Bond angles		
		Chain	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	В	110	0	84	5	0
3	A	8	0	0	1	0
4	A	56	0	83	4	0
5	A	13	0	23	0	0
6	A	15	0	27	0	0
7	A	8	0	0	0	0
8	A	7	0	4	2	0
9	A	51	0	44	2	0
10	A	28	0	54	1	0
11	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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	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%)	11 28	

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
1	A	589	LEU

#### 5.3.2 Protein sidechains (i)

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.

$\mathbf{Mol}$	Chain	Analysed	Analysed Rotameric		Percentiles	
1	A	587/591 (99%)	560 (95%)	27 (5%)	27 54	

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

Mol	Chain	Res	Type
1	A	354	ASN
1	A	402	LEU
1	A	674	ARG
1	A	397	VAL
1	A	430	ASN

Sometimes 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	410	HIS
1	A	438	ASN
1	A	686	ASN
1	A	522	ASN
1	A	430	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)

9 monosaccharides 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	Mol Type Chain Res Link		Вс	ond leng	ths	Bond angles				
MIOI	Type	Chain	Res	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PA1	В	1	4,7,2	11,11,12	0.64	0	14,15,17	0.77	1 (7%)
2	GCN	В	2	4,2,3	10,10,11	1.03	1 (10%)	13,13,15	2.64	2 (15%)
2	KDO	В	3	2	15,15,16	0.82	0	19,21,24	0.94	0
2	GMH	В	4	8,2	13,13,14	0.80	0	17,18,20	0.68	0
2	GMH	В	5	2,3	13,13,14	1.05	2 (15%)	17,18,20	1.35	2 (11%)
2	GLC	В	6	2	11,11,12	0.58	0	15,15,17	0.72	0
2	GLC	В	7	2	11,11,12	0.55	0	15,15,17	0.54	0
2	GLA	В	8	2	11,11,12	0.46	0	15,15,17	0.53	0
2	KDO	В	9	2	15,15,16	0.68	0	19,21,24	0.92	0

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	В	1	4,7,2	-	2/2/18/22	0/1/1/1
2	GCN	В	2	4,2,3	-	0/2/15/18	0/1/1/1
2	KDO	В	3	2	-	0/10/26/30	0/1/1/1
2	GMH	В	4	8,2	-	2/6/23/26	0/1/1/1
2	GMH	В	5	2,3	-	4/6/23/26	0/1/1/1
2	GLC	В	6	2	-	2/2/19/22	0/1/1/1
2	GLC	В	7	2	-	2/2/19/22	0/1/1/1
2	GLA	В	8	2	-	2/2/19/22	0/1/1/1
2	KDO	В	9	2	-	2/10/26/30	0/1/1/1

#### All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
2	В	2	GCN	C1-C2	2.70	1.55	1.52
2	В	5	GMH	O5-C5	2.31	1.46	1.43
2	В	5	GMH	O4-C4	2.07	1.47	1.43

#### All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	2	GCN	C3-C2-C1	8.73	116.91	109.82
2	В	5	GMH	C6-C5-C4	-3.42	108.36	114.03
2	В	5	GMH	C1-O5-C5	3.19	116.71	111.48
2	В	2	GCN	C1-O5-C5	2.55	115.64	112.19

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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	1	PA1	O5-C1-C2	2.28	112.17	109.51

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	4	GMH	O6-C6-C7-O7
2	В	5	GMH	C4-C5-C6-C7
2	В	5	GMH	C4-C5-C6-O6
2	В	5	GMH	O5-C5-C6-C7
2	В	5	GMH	O5-C5-C6-O6

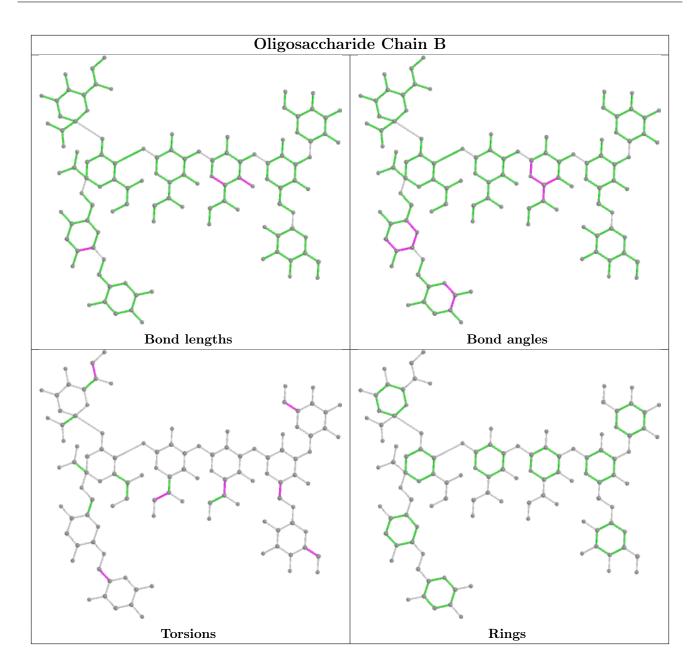
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	5	GMH	1	0
2	В	3	KDO	1	0
2	В	4	GMH	4	0
2	В	9	KDO	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 oligosaccharide.





## 5.6 Ligand geometry (i)

13 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	Bo	ond leng	ths	В	ond ang	les
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	A	2005	2	0,3,4	-	=	0,3,6	-	-
5	DAO	A	1012	4	12,12,13	1.05	1 (8%)	11,11,13	0.80	1 (9%)
10	DDQ	A	1101	-	10,13,13	0.60	0	12,15,15	0.61	0
4	FTT	A	1009	2	15,15,16	0.42	0	15,15,17	0.70	1 (6%)
10	DDQ	A	1102	-	10,13,13	0.56	0	12,15,15	0.60	0
8	EAP	A	2004	2	3,6,7	2.86	1 (33%)	0,6,9	_	_
4	FTT	A	1011	2,5	15,15,16	0.34	0	15,15,17	0.80	0
4	FTT	A	1013	6,2	16,16,16	0.90	1 (6%)	17,17,17	0.54	0
4	FTT	A	1010	2	6,6,16	1.31	1 (16%)	6,7,17	0.60	0
6	MYR	A	1014	4	14,14,15	1.00	1 (7%)	13,13,15	0.81	1 (7%)
3	PO4	A	2001	2	0,3,4	-	=	0,3,6	-	-
9	FCI	A	1050	-	56,56,56	1.39	4 (7%)	63,87,87	0.99	2 (3%)
7	DPO	A	2000	2	4,7,8	2.43	1 (25%)	5,10,13	0.95	0

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	DAO	A	1012	4	-	1/10/10/11	-
10	DDQ	A	1101	-	-	0/11/11/11	-
4	FTT	A	1009	2	-	0/14/14/15	-
10	DDQ	A	1102	-	-	0/11/11/11	-
8	EAP	A	2004	2	-	0/0/4/5	-
4	FTT	A	1011	2,5	-	3/14/14/15	-
4	FTT	A	1013	6,2	-	1/15/15/15	-
4	FTT	A	1010	2	-	0/4/4/15	-
6	MYR	A	1014	4	-	2/12/12/13	-
9	FCI	A	1050	-	-	11/62/116/116	0/4/6/6
7	DPO	A	2000	2	-	0/2/5/6	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
9	A	1050	FCI	O10-FE	5.97	2.12	1.99
9	A	1050	FCI	O3-FE	5.16	2.19	2.04
8	A	2004	EAP	P-O4	-4.57	1.49	1.63
7	A	2000	DPO	P1-O4	-4.34	1.50	1.63
6	A	1014	MYR	O2-C1	-3.69	1.23	1.42



All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
9	A	1050	FCI	C1-C10-N1	3.46	120.59	111.16
9	A	1050	FCI	O17-C8-N4	-2.16	119.31	122.95
4	A	1009	FTT	O2-C1-C2	-2.12	119.26	125.43
5	A	1012	DAO	O2-C1-C2	2.08	125.36	111.66
6	A	1014	MYR	O2-C1-C2	2.07	125.29	111.66

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1050	FCI	C2-C11-C38-O18
4	A	1011	FTT	O3-C3-C4-C5
9	A	1050	FCI	C24-C16-C7-N3
9	A	1050	FCI	C24-C16-C7-O7
9	A	1050	FCI	C38-C11-C2-O2

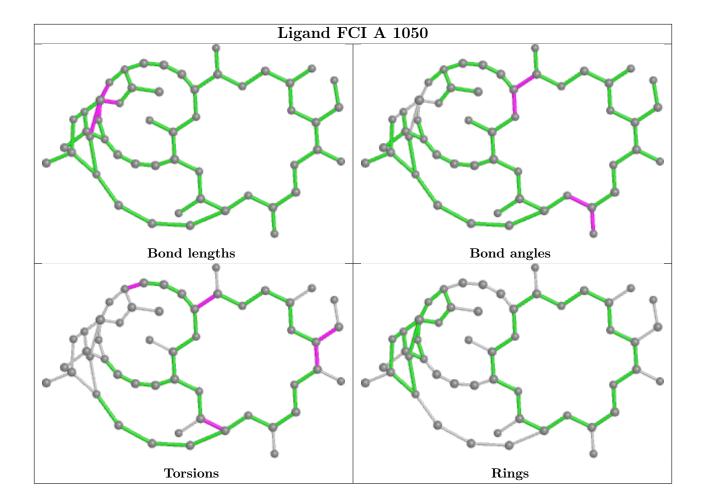
There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2005	PO4	1	0
10	A	1101	DDQ	1	0
4	A	1009	FTT	1	0
8	A	2004	EAP	2	0
4	A	1011	FTT	2	0
4	A	1013	FTT	3	0
9	A	1050	FCI	2	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 then 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.





# 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.

