



# wwPDB X-ray Structure Validation Summary Report

Nov 13, 2014 – 07:46 PM EST

PDB ID : 1FCP  
Title : FERRIC HYDROXAMATE UPTAKE RECEPTOR (FHUA) FROM E.COLI  
IN COMPLEX WITH BOUND FERRICHRONE-IRON  
Authors : Hofmann, E.; Ferguson, A.D.; Diederichs, K.; Welte, W.  
Deposited on : 1998-10-14  
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](mailto:validation@mail.wwpdb.org)

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

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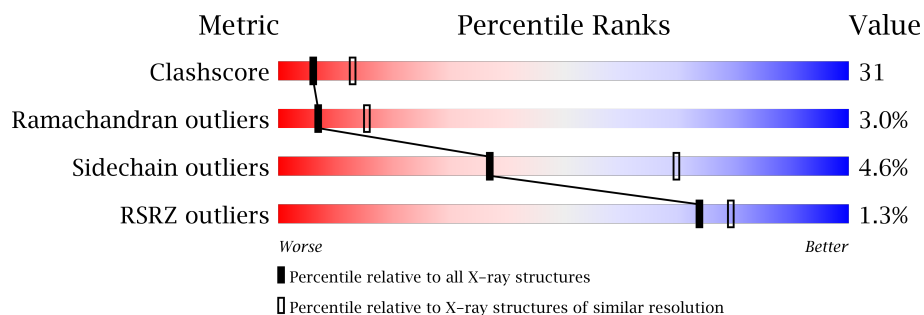
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable24195
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.1.3
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable24195

# 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)
RSRZ outliers	66119	1559 (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  $\geq 3$ , 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	705	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	LIL	A	903	-	X
4	LIL	A	904	-	X
6	LIM	A	906	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5832 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 PROTEIN (FERRIC HYDROXAMATE UPTAKE RECEPTOR).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	705	Total	C	N	O	S	Se	0	0	0
			5512	3469	942	1087	4	10			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	INSERTION	UNP P06971
A	407	HIS	-	INSERTION	UNP P06971
A	408	HIS	-	INSERTION	UNP P06971
A	409	HIS	-	INSERTION	UNP P06971
A	410	HIS	-	INSERTION	UNP P06971
A	411	HIS	-	INSERTION	UNP P06971
A	412	HIS	-	INSERTION	UNP P06971
A	413	GLY	-	INSERTION	UNP P06971
A	414	SER	-	INSERTION	UNP P06971
A	58	MSE	MET	MODIFIED RESIDUE	UNP P06971
A	125	MSE	MET	MODIFIED RESIDUE	UNP P06971
A	132	MSE	MET	MODIFIED RESIDUE	UNP P06971
A	151	MSE	MET	MODIFIED RESIDUE	UNP P06971
A	281	MSE	MET	MODIFIED RESIDUE	UNP P06971
A	381	MSE	MET	MODIFIED RESIDUE	UNP P06971
A	383	MSE	MET	MODIFIED RESIDUE	UNP P06971
A	559	MSE	MET	MODIFIED RESIDUE	UNP P06971
A	622	MSE	MET	MODIFIED RESIDUE	UNP P06971
A	680	MSE	MET	MODIFIED RESIDUE	UNP P06971

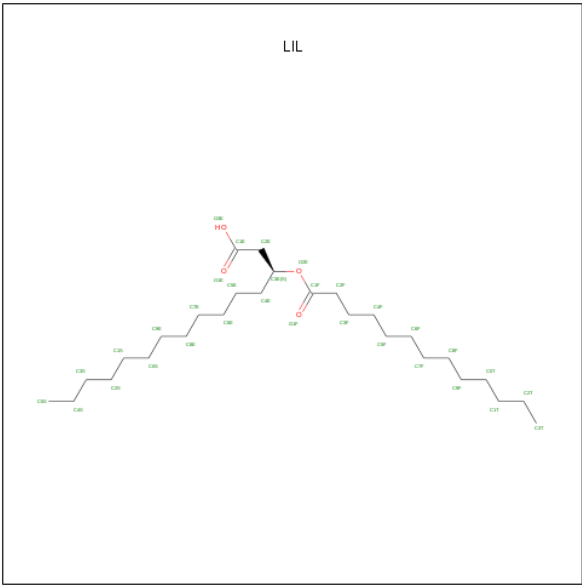
- Molecule 2 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	9	Total	C	N	O	P	0	0
			124	60	2	59	3		

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

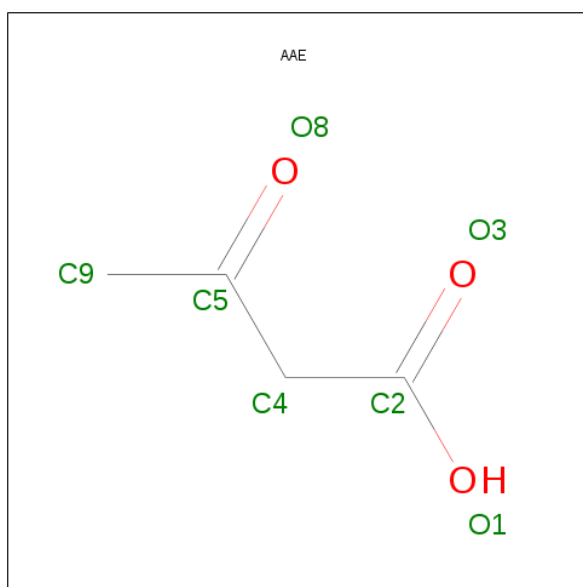
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ni	0	0
			2	2		

- Molecule 4 is 2-TRIDECANOYLOXY-PENTADECANOICACID (three-letter code: LIL) (formula: C<sub>28</sub>H<sub>54</sub>O<sub>4</sub>).



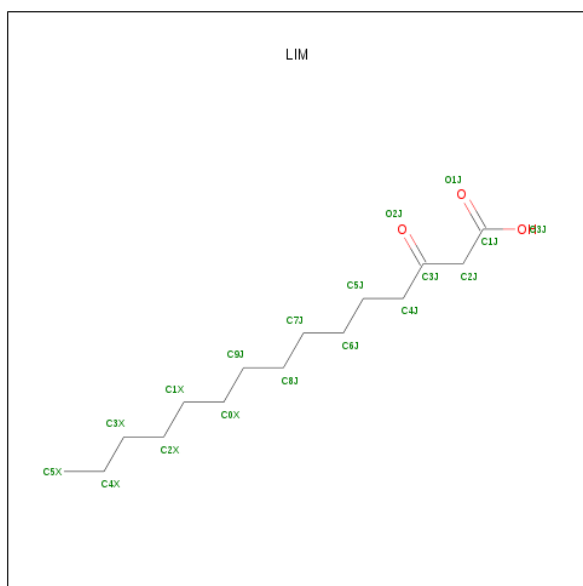
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			31	28	3		
4	A	1	Total	C	O	0	0
			31	28	3		

- Molecule 5 is ACETOACETIC ACID (three-letter code: AAE) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>3</sub>).



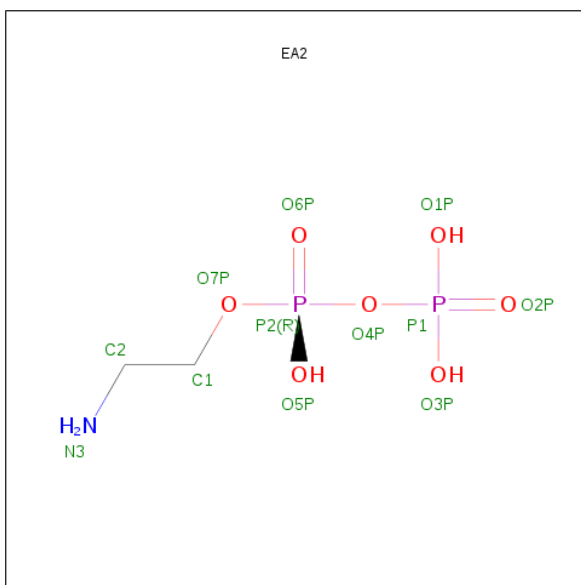
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 6 is 3-OXO-PENTADECANOIC ACID (three-letter code: LIM) (formula:  $C_{15}H_{28}O_3$ ).



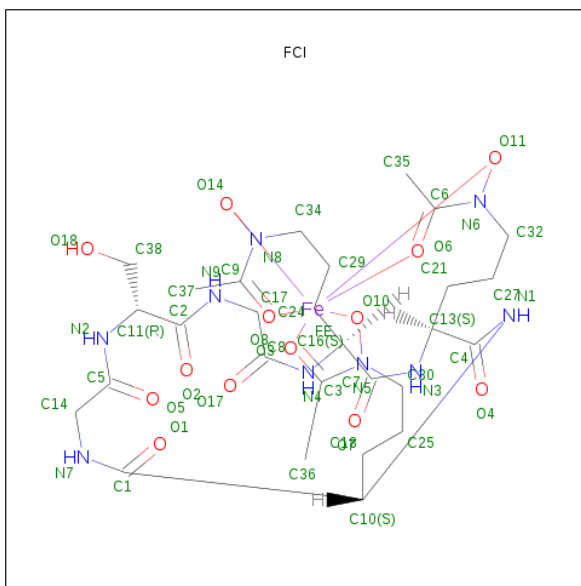
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			17	15	2		

- Molecule 7 is AMINOETHANOLPYROPHOSPHATE (three-letter code: EA2) (formula:  $C_2H_9NO_7P_2$ ).



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

- Molecule 8 is FERRICROCIN-IRON (three-letter code: FCI) (formula:  $C_{28}H_{44}FeN_9O_{13}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	Fe	N	O	0
			46	24	1	9	12	

- Molecule 9 is water.

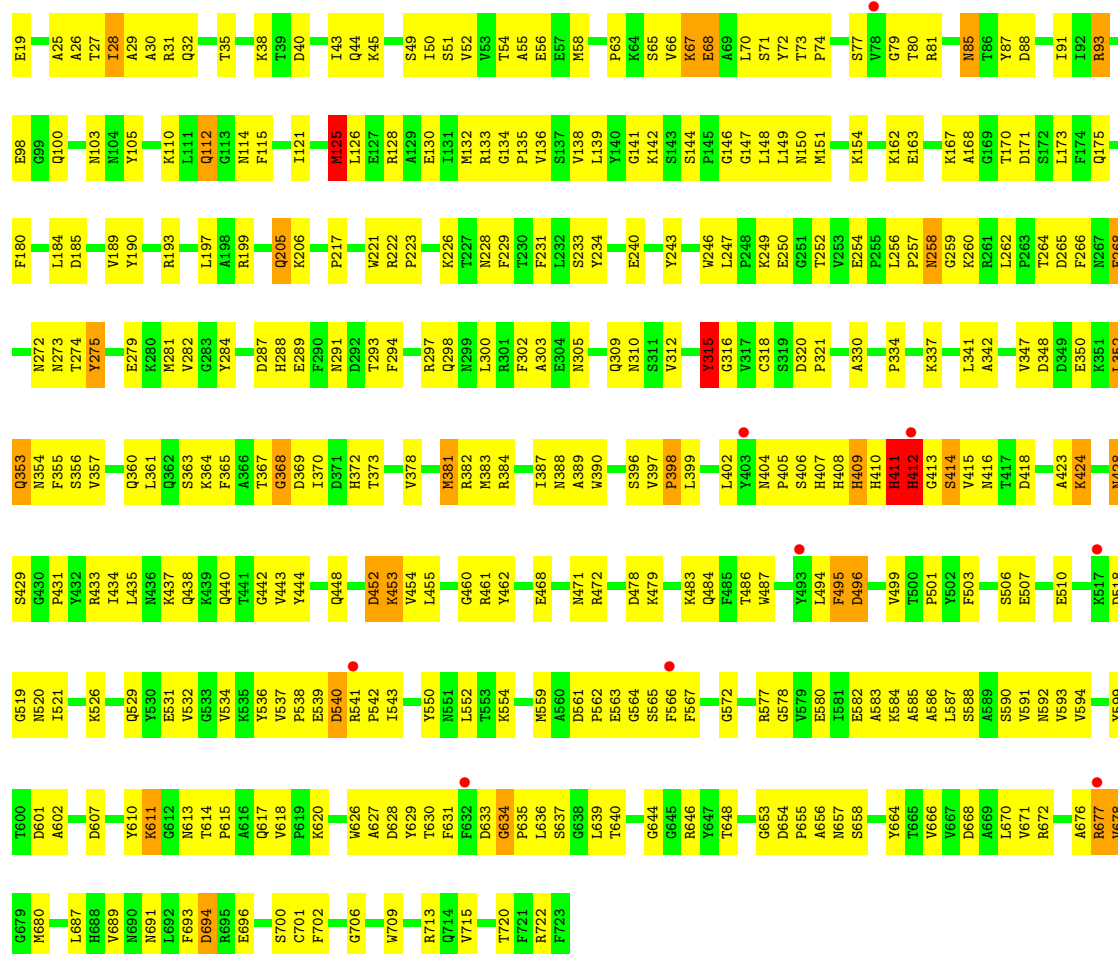
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	52	Total	O	0	0
			52	52		

### 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 ( $\text{RSRZ} > 2$ ). 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: PROTEIN (FERRIC HYDROXAMATE UPTAKE RECEPTOR)

Chain A: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.40Å 171.40Å 85.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 46.94 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.3 (40.00-2.70) 97.5 (46.94-2.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.69Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, $R_{free}$	0.232 , 0.281 0.231 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	58.6	Xtriage
Anisotropy	0.596	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 36.5	EDS
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 39633 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5832	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: AAE, NI, KDO, GPH, LIL, LIM, GLC, GAL, GP4, FCI, GMH, EA2, GP1

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	0.45	2/5642 (0.0%)	0.71	8/7650 (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
1	A	0	2
2	A	2	0
All	All	2	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	MSE	CG-SE	-5.73	1.75	1.95
1	A	680	MSE	CG-SE	-5.18	1.77	1.95

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	HIS	N-CA-C	15.24	152.14	111.00
1	A	412	HIS	CA-C-N	-9.20	97.79	116.20
1	A	409	HIS	N-CA-C	-7.00	92.10	111.00
1	A	411	HIS	N-CA-C	-6.74	92.82	111.00
1	A	412	HIS	CB-CA-C	-6.00	98.41	110.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1007	GAL	C1
2	A	1009	GAL	C1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	315	TYR	Sidechain
1	A	412	HIS	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	5512	0	5213	331	0
2	A	124	0	85	4	0
3	A	2	0	0	0	0
4	A	62	0	104	18	0
5	A	6	0	5	0	0
6	A	17	0	27	6	0
7	A	11	0	6	0	0
8	A	46	0	31	2	0
9	A	52	0	0	6	0
All	All	5832	0	5471	345	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 31.

The worst 5 of 345 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:410:HIS:HA	1:A:412:HIS:ND1	1.69	1.06
1:A:121:ILE:HB	1:A:151:MSE:HE1	1.40	1.01
1:A:28:ILE:HD12	1:A:28:ILE:H	1.24	1.00
1:A:410:HIS:H	1:A:412:HIS:HB3	1.27	0.97
1:A:410:HIS:CA	1:A:412:HIS:ND1	2.29	0.95

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	703/705 (100%)	624 (89%)	58 (8%)	21 (3%)	7 15

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	495	PHE
1	A	633	ASP
1	A	634	GLY
1	A	368	GLY
1	A	414	SER

### 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	585/575 (102%)	558 (95%)	27 (5%)	37 70

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

Mol	Chain	Res	Type
1	A	275	TYR
1	A	353	GLN
1	A	496	ASP
1	A	315	TYR
1	A	73	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	ASN
1	A	328	GLN
1	A	410	HIS
1	A	205	GLN
1	A	428	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 ⓘ

9 carbohydrates 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	KDO	A	1002	2	15,15,16	4.63	1 (6%)	16,21,24	2.90	4 (25%)
2	KDO	A	1003	2	15,15,16	4.73	1 (6%)	16,21,24	2.76	3 (18%)
2	GMH	A	1004	2,7	12,13,14	0.70	0	14,18,20	1.19	2 (14%)
2	GPH	A	1005	3,2	16,17,18	1.11	2 (12%)	21,25,27	1.40	2 (9%)
2	GLC	A	1006	2	10,11,12	0.65	0	11,15,17	1.07	0
2	GAL	A	1007	2	10,11,12	0.40	0	11,15,17	0.41	0
2	GAL	A	1009	2	10,11,12	0.56	0	11,15,17	0.66	0
2	GP4	A	901	2,4	13,15,16	1.26	1 (7%)	18,22,24	1.24	2 (11%)
2	GP1	A	902	3,2,5,6	16,16,16	1.21	1 (6%)	24,24,24	0.89	1 (4%)

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	KDO	A	1002	2	-	0/7/26/30	0/1/1/1
2	KDO	A	1003	2	-	0/7/26/30	0/1/1/1
2	GMH	A	1004	2,7	-	0/6/23/26	0/1/1/1
2	GPH	A	1005	3,2	-	0/11/28/31	0/1/1/1
2	GLC	A	1006	2	-	0/2/19/22	0/1/1/1
2	GAL	A	1007	2	1/1/4/5	0/2/19/22	0/1/1/1
2	GAL	A	1009	2	1/1/4/5	0/2/19/22	0/1/1/1
2	GP4	A	901	2,4	-	0/7/24/27	0/1/1/1
2	GP1	A	902	3,2,5,6	-	0/7/27/27	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	KDO	O6-C2	18.12	1.44	1.28
2	A	1002	KDO	O6-C2	17.60	1.44	1.28
2	A	901	GP4	P4A-O4A	-3.19	1.50	1.59
2	A	902	GP1	P4B-O1B	-2.99	1.50	1.59
2	A	1005	GPH	P1-O4	-2.26	1.52	1.59

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1002	KDO	O6-C2-C3	-10.57	111.10	124.91
2	A	1003	KDO	O6-C2-C3	-10.16	111.63	124.91
2	A	901	GP4	P4A-O4A-C4A	-4.04	112.45	121.77
2	A	1005	GPH	P1-O4-C4	-3.92	112.72	121.77
2	A	1004	GMH	O3-C3-C2	3.08	115.34	109.74

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1007	GAL	C1
2	A	1009	GAL	C1

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z  > 2$
7	EA2	A	1008	2	8,10,11	2.05	3 (37%)	9,13,16	1.02	1 (11%)
8	FCI	A	750	-	45,51,56	2.11	2 (4%)	44,78,87	0.46	0
4	LIL	A	903	2	30,30,31	3.19	2 (6%)	29,31,33	1.10	2 (6%)
4	LIL	A	904	2	30,30,31	23.77	5 (16%)	29,31,33	8.75	4 (13%)
5	AAE	A	905	2	3,5,6	3.78	2 (66%)	3,5,7	4.52	2 (66%)
6	LIM	A	906	2	16,16,17	5.44	3 (18%)	14,16,18	2.22	3 (21%)

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
7	EA2	A	1008	2	-	0/8/10/11	0/0/0/0
8	FCI	A	750	-	-	0/54/102/116	0/0/6/6
4	LIL	A	903	2	-	2/30/31/32	0/0/0/0
4	LIL	A	904	2	-	1/30/31/32	0/0/0/0
5	AAE	A	905	2	-	0/2/3/4	0/0/0/0
6	LIM	A	906	2	-	0/14/15/16	0/0/0/0

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	904	LIL	C2E-C3E	96.81	2.54	1.52
4	A	904	LIL	O1F-C1F	67.43	3.23	1.22
4	A	904	LIL	C2E-C1E	52.48	4.24	1.47
6	A	906	LIM	O1J-C1J	18.05	1.23	1.11
4	A	903	LIL	O1E-C1E	16.91	1.23	1.11

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	904	LIL	O2E-C1F-O1F	-29.65	44.55	123.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	904	LIL	C4E-C3E-C2E	28.44	149.92	114.40
4	A	904	LIL	O2E-C3E-C2E	-22.70	61.56	106.66
6	A	906	LIM	O2J-C3J-C2J	-6.80	109.68	120.86
5	A	905	AAE	O8-C5-C4	-5.93	109.64	122.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	903	LIL	C3E-O2E-C1F-O1F
4	A	904	LIL	C1F-O2E-C3E-C2E
4	A	903	LIL	C3E-O2E-C1F-C2F

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	705/705 (100%)	-0.20	9 (1%) 74 79	31, 62, 93, 113	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	412	HIS	6.0
1	A	566	PHE	3.3
1	A	677	ARG	2.9
1	A	517	LYS	2.4
1	A	493	TYR	2.4

### 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	GPH	A	1005	17/18	0.15	-0.41	55,82,120,120	0
2	GMH	A	1004	13/14	0.11	-1.01	43,59,80,83	0
2	KDO	A	1002	15/16	0.09	-2.14	45,59,70,92	0
2	GP1	A	902	16/16	0.08	-4.22	50,63,90,103	0
2	GP4	A	901	15/16	0.10	-4.91	32,46,71,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLC	A	1006	11/12	0.17	-	74,83,102,110	0
2	GAL	A	1009	11/12	0.22	-	81,91,107,107	0
2	KDO	A	1003	15/16	0.11	-	49,64,80,85	0
2	GAL	A	1007	11/12	0.28	-	74,96,110,120	0

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	LIL	A	903	31/32	0.37	12.49	48,78,93,96	0
6	LIM	A	906	17/18	0.41	11.08	54,65,82,97	0
4	LIL	A	904	31/32	0.30	6.92	48,59,76,83	0
8	FCI	A	750	46/51	0.16	-0.31	21,47,64,69	0
7	EA2	A	1008	11/12	0.16	-0.68	52,109,120,120	0
3	NI	A	1011	1/1	0.09	-2.17	98,98,98,98	0
5	AAE	A	905	6/7	0.19	-	75,80,86,107	0
3	NI	A	1012	1/1	0.10	-	113,113,113,113	0

## 6.5 Other polymers

There are no such residues in this entry.