



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:34 AM GMT

PDB ID : 2FCP
Title : FERRIC HYDROXAMATE UPTAKE RECEPTOR (FHUA) FROM E.COLI
Authors : Hofmann, E.; Ferguson, A.D.; Diederichs, K.; Welte, W.
Deposited on : 1998-10-15
Resolution : 2.50 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>

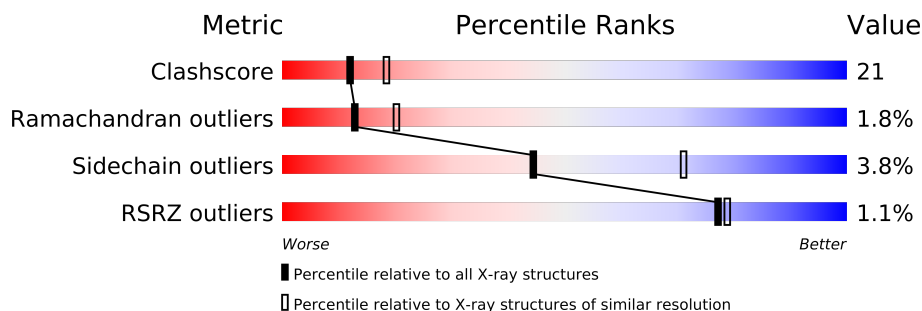
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
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 2.50 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	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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.

Mol	Chain	Length	Quality of chain
1	A	723	

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

Mol	Type	Chain	Res	Geometry	Electron density
6	LIL	A	903	-	X
7	AAE	A	905	X	-
8	LIM	A	906	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5833 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	0	0	0
			5512	3469	942	1087	14			

There are 9 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

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	5	Total	C	N	O	P	0	0
			74	35	2	35	2		

There are 9 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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	412	HIS	-	INSERTION	UNP P06971
A	413	GLY	-	INSERTION	UNP P06971
A	414	SER	-	INSERTION	UNP P06971

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	3	Total	C	O	0	0
			33	18	15		

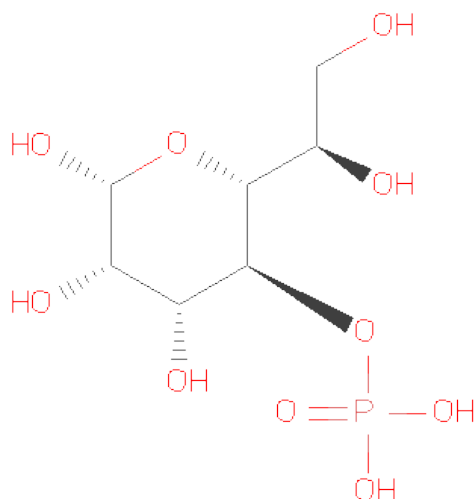
There are 9 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

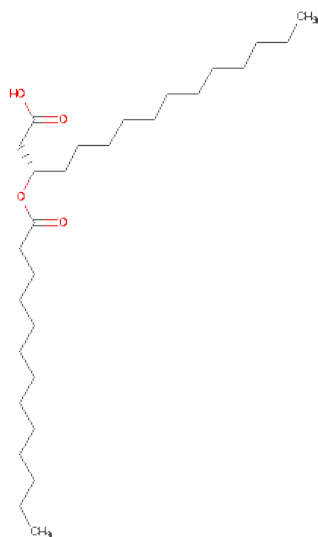
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ni	0	0
			2	2		

- Molecule 5 is 4-O-PHOSPHONO-D-GLYCERO-BETA-D-MANNO-HEPTOPYRANOSE (three-letter code: GPO) (formula: C₇H₁₅O₁₀P).



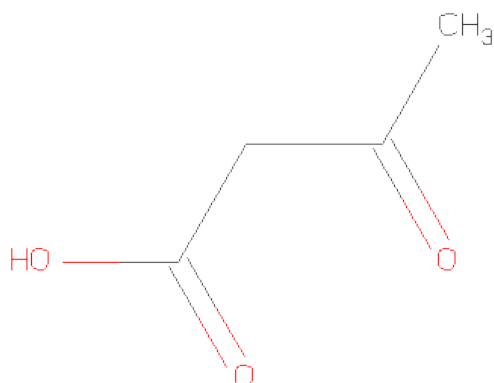
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			17	7	9	1		

- Molecule 6 is 2-TRIDECANOYLOXY-PENTADECANOICACID (three-letter code: LIL) (formula: $C_{28}H_{54}O_4$).



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

- Molecule 7 is ACETOACETIC ACID (three-letter code: AAE) (formula: $C_4H_6O_3$).



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

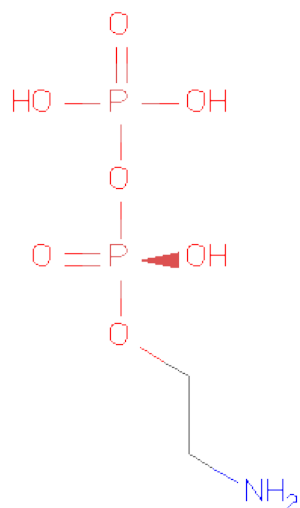
- Molecule 8 is 3-OXO-PENTADECANOIC ACID (three-letter code: LIM) (formula: $C_{15}H_{28}O_3$).



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

- Molecule 9 is AMINOETHANOLPYROPHOSPHATE (three-letter code: EA2) (formula:

C₂H₉NO₇P₂).



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

- Molecule 10 is water.

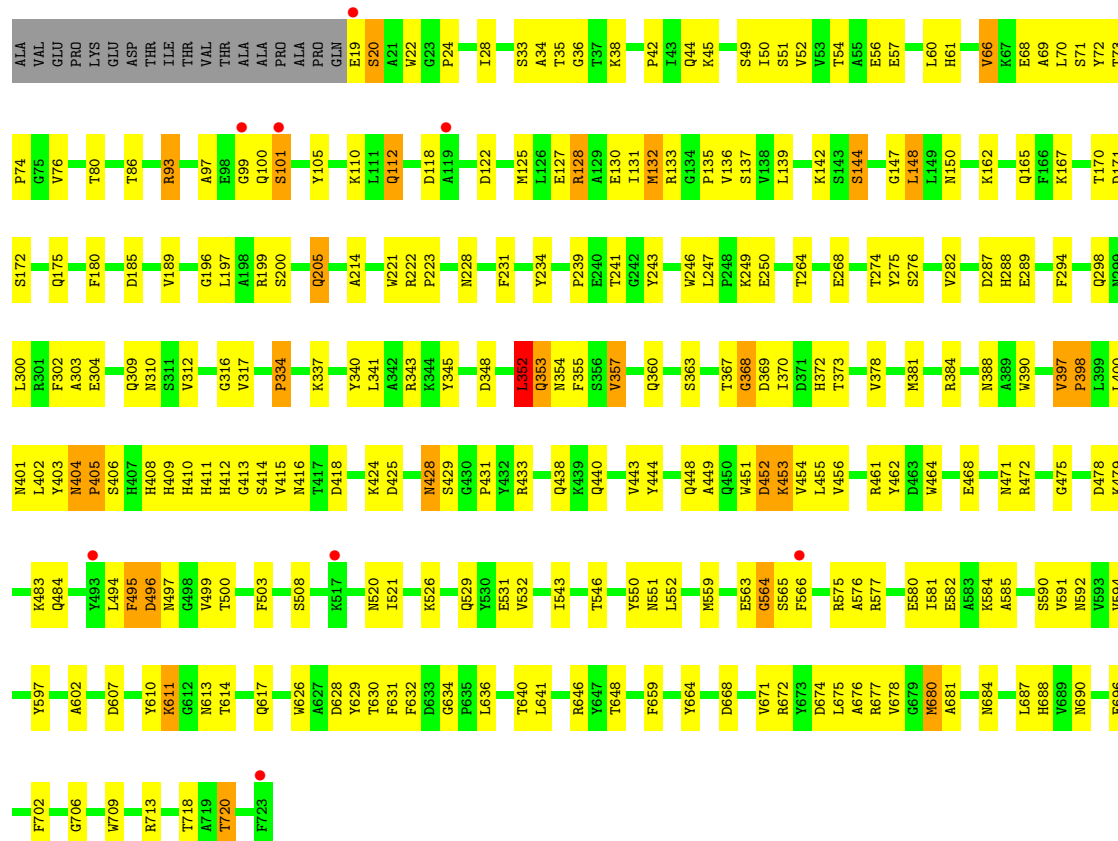
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	99	Total	O	0	0
			99	99		

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: 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, α , β , γ	171.55Å 171.55Å 87.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50 43.12 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.50) 98.8 (43.12-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.45Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.242 , 0.283 0.245 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.9	EDS
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 53749 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5833	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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, GMH, LIL, GLA, GLC, KDO, GPO, LIM, GP4, 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	0.40	0/5652	0.66	1/7680 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	LEU	CA-CB-CG	5.59	128.16	115.30

There are no chirality outliers.

There are no planarity outliers.

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	221	0
2	A	74	0	46	3	0
3	A	33	0	28	6	0
4	A	2	0	0	0	0
5	A	17	0	10	0	0
6	A	62	0	106	14	0
7	A	6	0	5	1	0
8	A	17	0	27	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	11	0	6	1	0
10	A	99	0	0	12	0
All	All	5833	0	5441	240	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 21.

The worst 5 of 240 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:86:THR:HG23	1:A:241:THR:HG21	1.35	1.04
1:A:70:LEU:HD13	1:A:131:ILE:HD11	1.32	1.04
1:A:132:MET:HG2	1:A:136:VAL:HG11	1.50	0.93
1:A:408:HIS:O	1:A:411:HIS:HB3	1.69	0.92
1:A:274:THR:HG22	1:A:310:ASN:HB2	1.57	0.83

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	703/723 (97%)	633 (90%)	57 (8%)	13 (2%)	13 20

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	A	452	ASP
1	A	564	GLY
1	A	634	GLY
1	A	418	ASP

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	585/599 (98%)	563 (96%)	22 (4%)	44 71

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	LEU
1	A	352	LEU
1	A	496	ASP
1	A	205	GLN
1	A	275	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	ASN
1	A	388	ASN
1	A	520	ASN
1	A	328	GLN
1	A	353	GLN

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 ⓘ

8 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	4.70	2 (13%)	16,21,24	2.85	3 (18%)
2	KDO	A	1003	2	15,15,16	4.56	2 (13%)	16,21,24	2.81	2 (12%)
2	GMH	A	1004	9,2	12,13,14	1.12	1 (8%)	14,18,20	1.40	2 (14%)
3	GLC	A	1006	3	10,11,12	0.67	0	11,15,17	0.90	1 (9%)
3	GLA	A	1007	3	10,11,12	0.45	0	11,15,17	0.37	0
3	GLA	A	1009	3	10,11,12	0.39	0	11,15,17	0.32	0
2	GP4	A	901	2,6	13,15,16	1.27	1 (7%)	18,22,24	1.34	1 (5%)
2	GP1	A	902	8,2,4,7	16,16,16	1.28	2 (12%)	24,24,24	1.12	2 (8%)

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	9,2	-	0/6/23/26	0/1/1/1
3	GLC	A	1006	3	-	0/2/19/22	0/1/1/1
3	GLA	A	1007	3	-	0/2/19/22	1/1/1/1
3	GLA	A	1009	3	-	0/2/19/22	0/1/1/1
2	GP4	A	901	2,6	-	0/7/24/27	0/1/1/1
2	GP1	A	902	8,2,4,7	-	0/7/27/27	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1002	KDO	O6-C2	17.78	1.44	1.28
2	A	1003	KDO	O6-C2	17.37	1.44	1.28
2	A	901	GP4	P4A-O4A	-3.11	1.50	1.59
2	A	902	GP1	P4B-O1B	-2.84	1.51	1.59
2	A	902	GP1	C3B-C2B	2.54	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1003	KDO	O6-C2-C3	-10.75	110.87	124.91
2	A	1002	KDO	O6-C2-C3	-10.46	111.25	124.91
2	A	901	GP4	P4A-O4A-C4A	-4.64	112.19	121.96
2	A	1004	GMH	O3-C3-C2	2.71	114.89	109.94
2	A	902	GP1	C4B-C3B-C2B	-2.64	106.46	111.31

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1007	GLA	C1-C2-C3-C4-C5-O5

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
5	GPO	A	1005	4	16,17,18	1.21	1 (6%)	21,25,27	1.57	1 (4%)
9	EA2	A	1008	2	8,10,11	2.10	2 (25%)	9,13,16	0.79	0
6	LIL	A	903	2	30,30,31	3.09	2 (6%)	29,31,33	1.03	2 (6%)
6	LIL	A	904	2	30,30,31	3.09	2 (6%)	29,31,33	1.01	1 (3%)
7	AAE	A	905	2	5,5,6	10.30	4 (80%)	3,5,7	2.89	2 (66%)
8	LIM	A	906	2	16,16,17	5.42	2 (12%)	14,16,18	2.20	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
5	GPO	A	1005	4	-	0/11/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EA2	A	1008	2	-	0/8/10/11	0/0/0/0
6	LIL	A	903	2	-	2/30/31/32	0/0/0/0
6	LIL	A	904	2	1/1/2/3	0/30/31/32	0/0/0/0
7	AAE	A	905	2	-	0/2/3/4	0/0/0/0
8	LIM	A	906	2	-	0/14/15/16	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)
7	A	905	AAE	O3-C2	21.24	1.26	1.11
8	A	906	LIM	O1J-C1J	18.11	1.23	1.11
6	A	904	LIL	O1E-C1E	16.39	1.22	1.11
6	A	903	LIL	O1E-C1E	16.38	1.22	1.11
8	A	906	LIM	O2J-C3J	11.70	1.43	1.21

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	906	LIM	O2J-C3J-C2J	-6.53	109.36	120.75
5	A	1005	GPO	P-O4-C4	-4.54	112.41	121.96
7	A	905	AAE	O8-C5-C9	-4.05	110.27	121.34
6	A	903	LIL	O2E-C1F-O1F	-3.90	113.21	123.65
6	A	904	LIL	O2E-C1F-O1F	-3.66	113.85	123.65

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	904	LIL	C3E

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	903	LIL	C3E-O2E-C1F-O1F
6	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, 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	705/723 (97%)	-0.15	8 (1%) 77 79	35, 64, 99, 119	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	19	GLU	4.1
1	A	517	LYS	3.6
1	A	723	PHE	3.2
1	A	566	PHE	2.9
1	A	493	TYR	2.2

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GP4	A	901	15/16	0.11	-2.71	35,53,71,81	0
2	GMH	A	1004	13/14	0.11	-3.10	44,58,75,81	0
2	KDO	A	1002	15/16	0.09	-4.27	49,60,76,92	0
2	KDO	A	1003	15/16	0.14	-5.00	69,78,84,87	0
2	GP1	A	902	16/16	0.10	-8.17	53,65,80,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GLA	A	1007	11/12	0.25	-	97,110,116,117	0
3	GLC	A	1006	11/12	0.23	-	80,98,107,114	0
3	GLA	A	1009	11/12	0.29	-	101,111,120,120	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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	LIL	A	903	31/32	0.28	8.03	65,82,92,95	0
8	LIM	A	906	17/18	0.24	5.46	57,69,86,97	0
6	LIL	A	904	31/32	0.19	1.96	46,65,74,84	0
9	EA2	A	1008	11/12	0.14	-0.76	59,102,120,120	0
5	GPO	A	1005	17/18	0.15	-1.08	52,84,106,113	0
4	NI	A	1011	1/1	0.05	-3.94	100,100,100,100	0
7	AAE	A	905	6/7	0.20	-	82,95,101,105	0
4	NI	A	1012	1/1	0.10	-	120,120,120,120	0

6.5 Other polymers

There are no such residues in this entry.