



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2023 – 08:21 PM JST

PDB ID : 6A4U  
Title : The first crystal structure of crustacean ferritin that is a hybrid type of H and L ferritin  
Authors : Masuda, T.; Mikami, B.; Zang, J.; Zhao, G.  
Deposited on : 2018-06-21  
Resolution : 1.16 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](mailto:validation@mail.wwpdb.org)

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<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

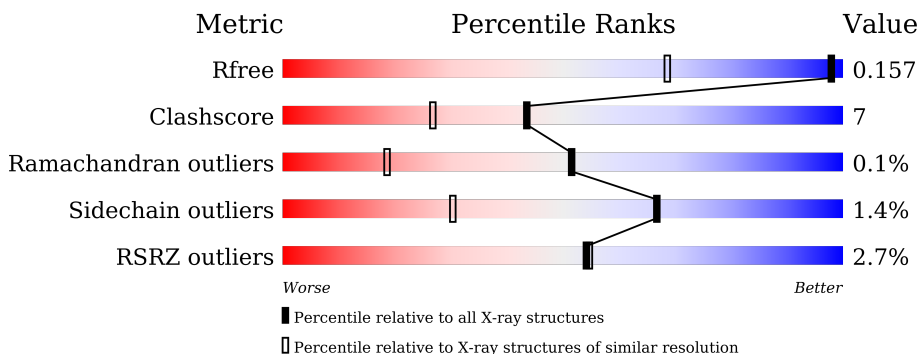
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.16 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))
$R_{free}$	130704	1758 (1.20-1.12)
Clashscore	141614	1832 (1.20-1.12)
Ramachandran outliers	138981	1768 (1.20-1.12)
Sidechain outliers	138945	1768 (1.20-1.12)
RSRZ outliers	127900	1724 (1.20-1.12)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	169	
1	B	169	
1	C	169	
1	D	169	
1	E	169	
1	F	169	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	EDO	A	207	-	-	-	X
2	EDO	A	209	-	-	-	X
2	EDO	E	211	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10626 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 Ferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	169	1566	1000	253	303	10	0	36	0
1	B	169	1577	1007	256	305	9	0	38	0
1	C	169	1547	987	250	301	9	0	33	0
1	D	169	1530	975	247	299	9	0	32	0
1	E	169	1593	1015	256	313	9	0	38	0
1	F	169	1535	978	251	297	9	0	32	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	ARG	GLN	engineered mutation	UNP T2B7E1
B	89	ARG	GLN	engineered mutation	UNP T2B7E1
C	89	ARG	GLN	engineered mutation	UNP T2B7E1
D	89	ARG	GLN	engineered mutation	UNP T2B7E1
E	89	ARG	GLN	engineered mutation	UNP T2B7E1
F	89	ARG	GLN	engineered mutation	UNP T2B7E1

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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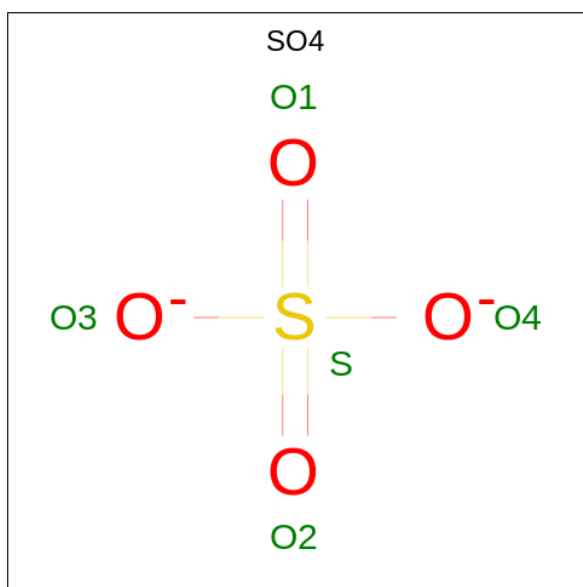
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	E	1	Total 4	C 2	O 2	0	0
2	E	1	Total 4	C 2	O 2	0	0
2	E	1	Total 4	C 2	O 2	0	0
2	E	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	2	Total Mg 2 2	0	0
5	D	2	Total Mg 2 2	0	0
5	F	1	Total Mg 1 1	0	0

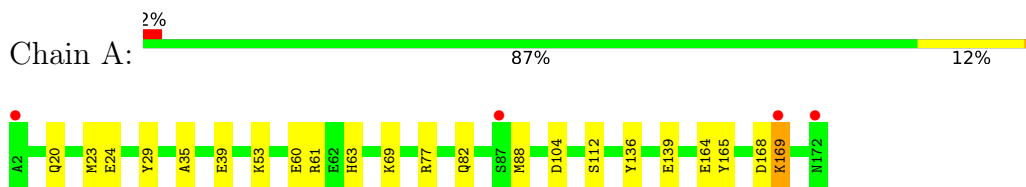
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	181	Total O 181 181	0	0
6	B	157	Total O 159 159	0	2
6	C	171	Total O 171 171	0	0
6	D	174	Total O 175 175	0	1
6	E	153	Total O 155 155	0	2
6	F	165	Total O 166 166	0	1

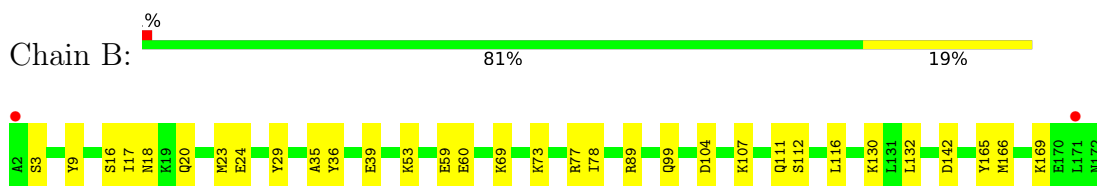
### 3 Residue-property plots [i](#)

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 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.

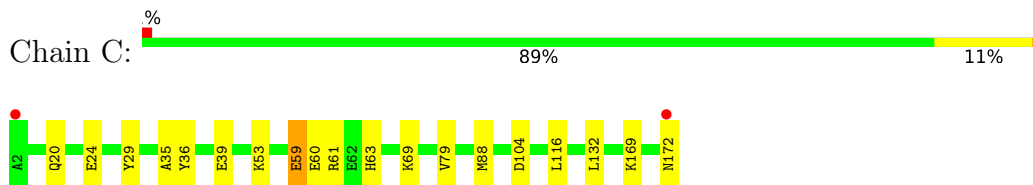
- Molecule 1: Ferritin



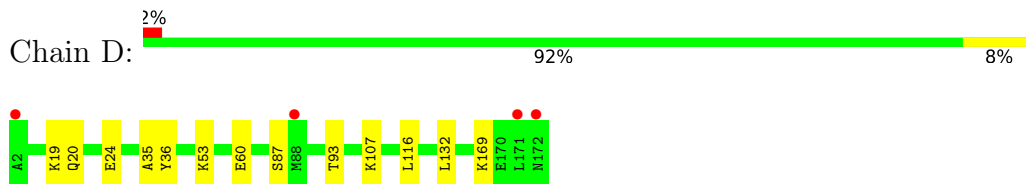
- Molecule 1: Ferritin



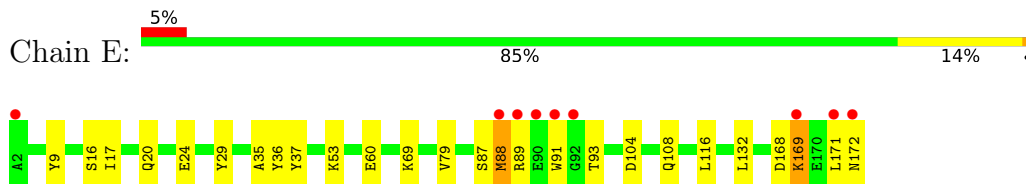
- Molecule 1: Ferritin



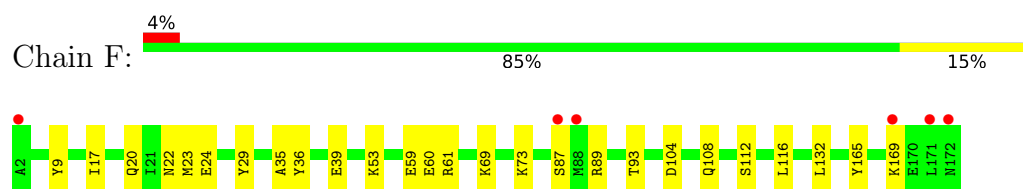
- Molecule 1: Ferritin



- Molecule 1: Ferritin



- Molecule 1: Ferritin



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.87Å 124.87Å 175.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.59 – 1.16 23.59 – 1.16	Depositor EDS
% Data completeness (in resolution range)	98.8 (23.59-1.16) 98.8 (23.59-1.16)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 1.16Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.138 , 0.157 0.138 , 0.157	Depositor DCC
$R_{free}$ test set	22868 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.6	Xtrriage
Anisotropy	0.095	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.004 for $-1/2^*h+1/2^*k-1/2^*l, 1/2^*h-1/2^*k-1/2^*l, -h-k$ 0.000 for $-1/2^*h+1/2^*k+1/2^*l, 1/2^*h-1/2^*k+1/2^*l, h+k$ 0.002 for $-1/2^*h-1/2^*k+1/2^*l, -1/2^*h-1/2^*k-1/2^*l, h-k$ 0.000 for $-1/2^*h-1/2^*k-1/2^*l, -1/2^*h-1/2^*k+1/2^*l, -h+k$ 0.011 for $-h, k, -l$	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	10626	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: EDO, CL, SO4, MG

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	0.31	0/1703	0.54	0/2278
1	B	0.32	0/1718	0.53	0/2298
1	C	0.32	0/1669	0.53	0/2233
1	D	0.31	0/1646	0.53	0/2204
1	E	0.32	0/1713	0.55	1/2292 (0.0%)
1	F	0.30	0/1651	0.52	0/2208
All	All	0.31	0/10100	0.53	1/13513 (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	E	169	LYS	CD-CE-NZ	-5.19	99.76	111.70

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	1566	0	1626	24	0
1	B	1577	0	1638	31	1
1	C	1547	0	1595	15	0
1	D	1530	0	1572	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1593	0	1630	25	0
1	F	1535	0	1580	34	1
2	A	36	0	50	3	0
2	B	28	0	42	1	0
2	C	40	0	59	0	0
2	D	20	0	30	1	1
2	E	48	0	71	3	0
2	F	28	0	42	2	1
3	A	15	0	0	0	0
3	B	15	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	1	0
4	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	F	1	0	0	0	0
6	A	181	0	0	13	0
6	B	159	0	0	13	0
6	C	171	0	0	7	1
6	D	175	0	0	3	0
6	E	155	0	0	7	1
6	F	166	0	0	12	0
All	All	10626	0	9935	131	3

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 7.

The worst 5 of 131 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:B:60[A]:GLU:OE1	6:B:301[A]:HOH:O	1.88	0.88
1:B:39[B]:GLU:OE1	6:B:302:HOH:O	1.91	0.86
1:A:82[B]:GLN:NE2	6:A:1004:HOH:O	2.08	0.86
1:E:60[A]:GLU:OE1	6:E:301:HOH:O	1.93	0.85
1:A:169:LYS:NZ	6:A:1003:HOH:O	2.07	0.84

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:345:HOH:O	6:E:302:HOH:O[3_655]	1.61	0.59
1:F:39[B]:GLU:OE2	2:F:202:EDO:O1[3_655]	1.87	0.33
1:B:39[B]:GLU:OE2	2:D:203:EDO:O1[6_555]	2.18	0.02

### 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	206/169 (122%)	202 (98%)	4 (2%)	0	100	100
1	B	208/169 (123%)	204 (98%)	4 (2%)	0	100	100
1	C	202/169 (120%)	198 (98%)	4 (2%)	0	100	100
1	D	200/169 (118%)	196 (98%)	4 (2%)	0	100	100
1	E	206/169 (122%)	201 (98%)	3 (2%)	2 (1%)	15	1
1	F	199/169 (118%)	197 (99%)	2 (1%)	0	100	100
All	All	1221/1014 (120%)	1198 (98%)	21 (2%)	2 (0%)	51	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	88[A]	MET
1	E	88[B]	MET

#### 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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/145 (126%)	179 (98%)	4 (2%)	52	13
1	B	185/145 (128%)	184 (100%)	1 (0%)	88	66
1	C	179/145 (123%)	173 (97%)	6 (3%)	37	5
1	D	177/145 (122%)	175 (99%)	2 (1%)	73	40
1	E	183/145 (126%)	181 (99%)	2 (1%)	73	40
1	F	176/145 (121%)	175 (99%)	1 (1%)	86	61
All	All	1083/870 (124%)	1067 (98%)	16 (2%)	67	28

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	172	ASN
1	E	29	TYR
1	C	88[A]	MET
1	D	19[B]	LYS
1	C	59[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 69 ligands modelled in this entry, 6 are monoatomic - leaving 63 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
2	EDO	A	203	-	3,3,3	0.44	0	2,2,2	0.31	0
2	EDO	B	206	-	3,3,3	0.46	0	2,2,2	0.28	0
2	EDO	B	203	-	3,3,3	0.46	0	2,2,2	0.35	0
3	SO4	E	213	-	4,4,4	0.15	0	6,6,6	0.06	0
2	EDO	A	205	-	3,3,3	0.49	0	2,2,2	0.23	0
2	EDO	A	209	-	3,3,3	0.42	0	2,2,2	0.42	0
2	EDO	E	209	-	3,3,3	0.46	0	2,2,2	0.30	0
2	EDO	C	207	-	3,3,3	0.42	0	2,2,2	0.40	0
2	EDO	A	204	1	3,3,3	0.48	0	2,2,2	0.64	0
2	EDO	C	204	-	3,3,3	0.41	0	2,2,2	0.43	0
2	EDO	D	204	-	3,3,3	0.45	0	2,2,2	0.38	0
2	EDO	E	201	-	3,3,3	0.48	0	2,2,2	0.21	0
2	EDO	E	204	-	3,3,3	0.46	0	2,2,2	0.30	0
2	EDO	E	208	-	3,3,3	0.44	0	2,2,2	0.29	0
2	EDO	C	210	-	3,3,3	0.41	0	2,2,2	0.49	0
2	EDO	F	207	-	3,3,3	0.45	0	2,2,2	0.31	0
3	SO4	A	212	-	4,4,4	0.14	0	6,6,6	0.08	0
2	EDO	C	206	-	3,3,3	0.46	0	2,2,2	0.23	0
2	EDO	D	205	-	3,3,3	0.46	0	2,2,2	0.27	0
2	EDO	C	203	-	3,3,3	0.46	0	2,2,2	0.24	0
2	EDO	E	206	-	3,3,3	0.45	0	2,2,2	0.28	0
2	EDO	B	207	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	E	203	-	3,3,3	0.43	0	2,2,2	0.34	0
3	SO4	A	211	-	4,4,4	0.14	0	6,6,6	0.05	0
2	EDO	D	201	-	3,3,3	0.39	0	2,2,2	0.28	0
2	EDO	A	201	-	3,3,3	0.50	0	2,2,2	0.11	0
2	EDO	A	208	-	3,3,3	0.46	0	2,2,2	0.28	0
2	EDO	B	204	-	3,3,3	0.43	0	2,2,2	0.38	0
2	EDO	E	207	-	3,3,3	0.49	0	2,2,2	0.35	0
3	SO4	D	206	-	4,4,4	0.14	0	6,6,6	0.04	0
2	EDO	C	209	-	3,3,3	0.44	0	2,2,2	0.32	0
3	SO4	B	208	-	4,4,4	0.13	0	6,6,6	0.05	0
3	SO4	E	214	-	4,4,4	0.14	0	6,6,6	0.06	0
2	EDO	F	205	-	3,3,3	0.49	0	2,2,2	0.25	0
2	EDO	A	206	-	3,3,3	0.43	0	2,2,2	0.41	0
2	EDO	F	204	-	3,3,3	0.45	0	2,2,2	0.36	0
2	EDO	B	202	-	3,3,3	0.50	0	2,2,2	0.30	0
3	SO4	F	208	-	4,4,4	0.14	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	A	202	-	3,3,3	0.48	0	2,2,2	0.32	0
2	EDO	E	212	-	3,3,3	0.44	0	2,2,2	0.23	0
3	SO4	F	209	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	B	209	-	4,4,4	0.14	0	6,6,6	0.05	0
2	EDO	C	201	-	3,3,3	0.47	0	2,2,2	0.23	0
2	EDO	E	210	-	3,3,3	0.43	0	2,2,2	0.36	0
2	EDO	E	205	-	3,3,3	0.45	0	2,2,2	0.25	0
2	EDO	F	202	1	3,3,3	0.52	0	2,2,2	0.22	0
2	EDO	D	203	-	3,3,3	0.53	0	2,2,2	0.16	0
2	EDO	D	202	-	3,3,3	0.47	0	2,2,2	0.15	0
2	EDO	B	205	-	3,3,3	0.47	0	2,2,2	0.24	0
2	EDO	A	207	1	3,3,3	0.41	0	2,2,2	0.26	0
2	EDO	C	205	1	3,3,3	0.46	0	2,2,2	0.23	0
2	EDO	C	208	-	3,3,3	0.48	0	2,2,2	0.34	0
2	EDO	E	211	1	3,3,3	0.44	0	2,2,2	0.12	0
2	EDO	F	201	-	3,3,3	0.49	0	2,2,2	0.14	0
2	EDO	E	202	-	3,3,3	0.46	0	2,2,2	0.43	0
3	SO4	B	210	-	4,4,4	0.14	0	6,6,6	0.05	0
2	EDO	B	201	-	3,3,3	0.49	0	2,2,2	0.25	0
3	SO4	A	210	-	4,4,4	0.14	0	6,6,6	0.18	0
3	SO4	C	211	-	4,4,4	0.13	0	6,6,6	0.07	0
2	EDO	F	206	-	3,3,3	0.42	0	2,2,2	0.38	0
2	EDO	F	203	-	3,3,3	0.42	0	2,2,2	0.31	0
2	EDO	C	202	-	3,3,3	0.44	0	2,2,2	0.35	0
3	SO4	D	207	-	4,4,4	0.14	0	6,6,6	0.12	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. <sup>1,2</sup> means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	203	-	-	0/1/1/1	-
2	EDO	B	206	-	-	1/1/1/1	-
2	EDO	B	203	-	-	0/1/1/1	-
2	EDO	A	205	-	-	0/1/1/1	-
2	EDO	A	209	-	-	1/1/1/1	-
2	EDO	E	209	-	-	1/1/1/1	-
2	EDO	C	207	-	-	1/1/1/1	-
2	EDO	A	204	1	-	0/1/1/1	-
2	EDO	C	204	-	-	0/1/1/1	-
2	EDO	D	204	-	-	0/1/1/1	-
2	EDO	E	201	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	E	204	-	-	1/1/1/1	-
2	EDO	E	208	-	-	0/1/1/1	-
2	EDO	C	210	-	-	0/1/1/1	-
2	EDO	F	207	-	-	0/1/1/1	-
2	EDO	C	206	-	-	0/1/1/1	-
2	EDO	D	205	-	-	0/1/1/1	-
2	EDO	C	203	-	-	0/1/1/1	-
2	EDO	E	206	-	-	0/1/1/1	-
2	EDO	B	207	-	-	0/1/1/1	-
2	EDO	E	203	-	-	0/1/1/1	-
2	EDO	D	201	-	-	0/1/1/1	-
2	EDO	A	201	-	-	0/1/1/1	-
2	EDO	A	208	-	-	0/1/1/1	-
2	EDO	B	204	-	-	0/1/1/1	-
2	EDO	E	207	-	-	0/1/1/1	-
2	EDO	C	209	-	-	1/1/1/1	-
2	EDO	F	205	-	-	0/1/1/1	-
2	EDO	A	206	-	-	0/1/1/1	-
2	EDO	F	204	-	-	0/1/1/1	-
2	EDO	B	202	-	-	0/1/1/1	-
2	EDO	A	202	-	-	0/1/1/1	-
2	EDO	E	212	-	-	0/1/1/1	-
2	EDO	C	201	-	-	0/1/1/1	-
2	EDO	E	210	-	-	0/1/1/1	-
2	EDO	E	205	-	-	0/1/1/1	-
2	EDO	F	202	1	-	0/1/1/1	-
2	EDO	D	203	-	-	1/1/1/1	-
2	EDO	D	202	-	-	0/1/1/1	-
2	EDO	B	205	-	-	0/1/1/1	-
2	EDO	A	207	1	-	0/1/1/1	-
2	EDO	C	205	1	-	0/1/1/1	-
2	EDO	C	208	-	-	1/1/1/1	-
2	EDO	E	211	1	-	1/1/1/1	-
2	EDO	F	201	-	-	0/1/1/1	-
2	EDO	E	202	-	-	0/1/1/1	-
2	EDO	B	201	-	-	0/1/1/1	-
2	EDO	F	206	-	-	1/1/1/1	-
2	EDO	F	203	-	-	0/1/1/1	-
2	EDO	C	202	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	204	EDO	O1-C1-C2-O2
2	C	207	EDO	O1-C1-C2-O2
2	D	203	EDO	O1-C1-C2-O2
2	C	208	EDO	O1-C1-C2-O2
2	E	211	EDO	O1-C1-C2-O2

There are no ring outliers.

13 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	206	EDO	1	0
2	A	209	EDO	1	0
2	F	207	EDO	1	0
2	D	205	EDO	1	0
2	E	206	EDO	1	0
2	A	206	EDO	1	0
3	F	208	SO4	1	0
2	A	202	EDO	1	0
2	E	212	EDO	1	0
2	F	202	EDO	0	1
2	D	203	EDO	0	1
2	E	211	EDO	1	0
2	F	206	EDO	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](#)

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	169/169 (100%)	-0.20	4 (2%) 59 58	7, 10, 17, 25	0
1	B	169/169 (100%)	-0.18	2 (1%) 79 79	8, 10, 18, 25	0
1	C	169/169 (100%)	-0.20	2 (1%) 79 79	8, 10, 17, 27	0
1	D	169/169 (100%)	-0.26	4 (2%) 59 58	7, 10, 17, 25	0
1	E	169/169 (100%)	-0.11	9 (5%) 26 27	7, 10, 15, 31	0
1	F	169/169 (100%)	-0.22	6 (3%) 42 44	7, 10, 17, 28	0
All	All	1014/1014 (100%)	-0.19	27 (2%) 54 55	7, 10, 17, 31	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	89[A]	ARG	5.5
1	E	88[A]	MET	4.9
1	C	2	ALA	4.8
1	A	2	ALA	4.7
1	B	2	ALA	4.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands i

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. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	EDO	E	211	4/4	-0.04	0.64	46,48,50,50	0
2	EDO	B	206	4/4	0.32	0.28	55,55,55,55	0
2	EDO	B	207	4/4	0.52	0.28	47,48,48,48	0
2	EDO	A	209	4/4	0.58	0.41	51,51,51,52	0
2	EDO	E	212	4/4	0.60	0.21	46,46,46,46	0
2	EDO	A	207	4/4	0.62	0.55	38,39,41,42	0
3	SO4	C	211	5/5	0.62	0.30	90,90,90,90	0
2	EDO	E	208	4/4	0.66	0.25	53,53,54,54	0
3	SO4	D	207	5/5	0.66	0.26	81,81,81,81	0
2	EDO	E	210	4/4	0.67	0.26	41,42,43,44	0
2	EDO	F	206	4/4	0.69	0.22	41,41,41,41	0
2	EDO	E	209	4/4	0.70	0.24	52,53,53,53	0
3	SO4	E	213	5/5	0.71	0.27	86,86,86,86	0
3	SO4	F	208	5/5	0.72	0.20	78,78,78,79	0
2	EDO	F	207	4/4	0.73	0.19	34,35,37,38	0
3	SO4	B	209	5/5	0.73	0.19	74,74,74,74	0
2	EDO	C	208	4/4	0.73	0.20	28,30,33,34	0
3	SO4	A	211	5/5	0.74	0.24	76,76,76,77	0
2	EDO	D	203	4/4	0.76	0.25	23,25,26,26	0
2	EDO	F	204	4/4	0.76	0.16	29,31,32,33	0
3	SO4	B	210	5/5	0.77	0.18	75,75,75,75	0
2	EDO	A	208	4/4	0.78	0.21	42,42,42,42	0
2	EDO	E	203	4/4	0.79	0.14	29,29,29,30	0
2	EDO	C	207	4/4	0.79	0.20	35,35,36,38	0
2	EDO	B	205	4/4	0.80	0.13	39,40,42,42	0
2	EDO	C	210	4/4	0.81	0.31	31,34,35,36	0
3	SO4	D	206	5/5	0.82	0.21	56,56,57,57	0
2	EDO	E	206	4/4	0.83	0.19	32,34,36,37	0
2	EDO	E	204	4/4	0.84	0.14	27,29,29,31	0
2	EDO	C	206	4/4	0.84	0.13	31,32,34,35	0
2	EDO	D	205	4/4	0.85	0.13	39,40,42,42	0
3	SO4	F	209	5/5	0.85	0.22	52,52,53,53	0
2	EDO	A	206	4/4	0.86	0.15	36,37,37,37	0
3	SO4	B	208	5/5	0.87	0.21	69,69,69,69	0
2	EDO	C	202	4/4	0.87	0.12	27,27,28,29	0
2	EDO	C	205	4/4	0.87	0.16	18,19,20,21	0
2	EDO	B	204	4/4	0.88	0.13	31,31,32,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	D	204	4/4	0.88	0.13	28,28,29,30	0
2	EDO	A	203	4/4	0.88	0.12	30,31,31,32	0
2	EDO	C	209	4/4	0.89	0.21	49,49,49,50	0
2	EDO	C	204	4/4	0.90	0.18	23,25,26,26	0
3	SO4	E	214	5/5	0.90	0.18	54,54,55,55	0
2	EDO	B	203	4/4	0.91	0.10	18,20,22,24	0
3	SO4	A	212	5/5	0.91	0.20	56,56,56,56	0
2	EDO	F	202	4/4	0.91	0.16	17,19,20,20	0
2	EDO	F	203	4/4	0.91	0.13	32,33,34,35	0
2	EDO	E	205	4/4	0.92	0.13	34,35,36,36	0
2	EDO	A	202	4/4	0.92	0.14	17,19,20,21	0
2	EDO	B	202	4/4	0.92	0.12	17,19,21,23	0
2	EDO	F	205	4/4	0.93	0.10	18,19,21,23	0
3	SO4	A	210	5/5	0.93	0.23	21,22,23,23	0
2	EDO	E	207	4/4	0.94	0.08	17,19,21,23	0
2	EDO	E	202	4/4	0.95	0.10	15,17,18,19	0
5	MG	F	210	1/1	0.95	0.04	35,35,35,35	0
2	EDO	F	201	4/4	0.96	0.09	17,17,18,18	0
2	EDO	A	201	4/4	0.96	0.13	18,18,19,19	0
5	MG	C	213	1/1	0.96	0.14	36,36,36,36	0
5	MG	D	209	1/1	0.96	0.09	36,36,36,36	0
2	EDO	A	205	4/4	0.96	0.11	15,16,19,21	0
2	EDO	C	201	4/4	0.97	0.09	18,19,19,19	0
2	EDO	E	201	4/4	0.97	0.06	17,17,18,18	0
2	EDO	A	204	4/4	0.97	0.12	9,12,13,13	0
2	EDO	C	203	4/4	0.97	0.07	12,14,15,16	4
5	MG	C	212	1/1	0.98	0.08	44,44,44,44	0
2	EDO	D	202	4/4	0.98	0.09	16,16,16,17	0
5	MG	D	208	1/1	0.98	0.17	28,28,28,28	0
2	EDO	B	201	4/4	0.98	0.06	16,16,16,17	0
2	EDO	D	201	4/4	0.98	0.10	8,11,11,11	0
4	CL	B	211	1/1	0.99	0.15	25,25,25,25	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.