



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:16 AM GMT

PDB ID : 3E04  
Title : Crystal structure of human fumarate hydratase  
Authors : Kavanagh, K.L.; Oppermann, U.; Structural Genomics Consortium (SGC)  
Deposited on : 2008-07-30  
Resolution : 1.95 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)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

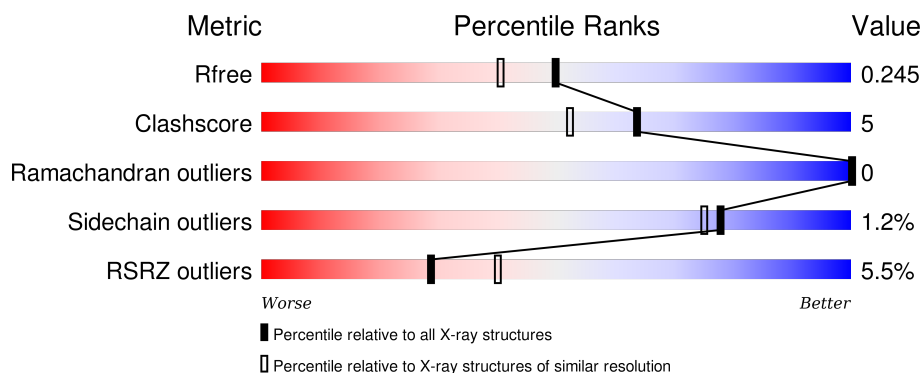
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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. 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	490	<div> <div>5%</div> <div>80% 12% 7%</div> </div>
1	B	490	<div> <div>6%</div> <div>82% 11% 7%</div> </div>
1	C	490	<div> <div>4%</div> <div>78% 7% 15%</div> </div>
1	D	490	<div> <div>6%</div> <div>84% 9% 6%</div> </div>

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	B	1	-	-	X	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13827 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 Fumarate hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	1	0
			3380	2133	587	639	21			
1	B	454	Total	C	N	O	S	0	1	0
			3350	2108	586	634	22			
1	C	415	Total	C	N	O	S	0	0	0
			3063	1929	533	579	22			
1	D	459	Total	C	N	O	S	0	1	1
			3367	2121	582	642	22			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	EXPRESSION TAG	UNP P07954
A	22	HIS	-	EXPRESSION TAG	UNP P07954
A	23	HIS	-	EXPRESSION TAG	UNP P07954
A	24	HIS	-	EXPRESSION TAG	UNP P07954
A	25	HIS	-	EXPRESSION TAG	UNP P07954
A	26	HIS	-	EXPRESSION TAG	UNP P07954
A	27	HIS	-	EXPRESSION TAG	UNP P07954
A	28	SER	-	EXPRESSION TAG	UNP P07954
A	29	SER	-	EXPRESSION TAG	UNP P07954
A	30	GLY	-	EXPRESSION TAG	UNP P07954
A	31	VAL	-	EXPRESSION TAG	UNP P07954
A	32	ASP	-	EXPRESSION TAG	UNP P07954
A	33	LEU	-	EXPRESSION TAG	UNP P07954
A	34	GLY	-	EXPRESSION TAG	UNP P07954
A	35	THR	-	EXPRESSION TAG	UNP P07954
A	36	GLU	-	EXPRESSION TAG	UNP P07954
A	37	ASN	-	EXPRESSION TAG	UNP P07954
A	38	LEU	-	EXPRESSION TAG	UNP P07954
A	39	TYR	-	EXPRESSION TAG	UNP P07954
A	40	PHE	-	EXPRESSION TAG	UNP P07954
A	41	GLN	-	EXPRESSION TAG	UNP P07954

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Chain	Residue	Modelled	Actual	Comment	Reference
A	42	SER	-	EXPRESSION TAG	UNP P07954
A	43	MET	-	EXPRESSION TAG	UNP P07954
B	21	MET	-	EXPRESSION TAG	UNP P07954
B	22	HIS	-	EXPRESSION TAG	UNP P07954
B	23	HIS	-	EXPRESSION TAG	UNP P07954
B	24	HIS	-	EXPRESSION TAG	UNP P07954
B	25	HIS	-	EXPRESSION TAG	UNP P07954
B	26	HIS	-	EXPRESSION TAG	UNP P07954
B	27	HIS	-	EXPRESSION TAG	UNP P07954
B	28	SER	-	EXPRESSION TAG	UNP P07954
B	29	SER	-	EXPRESSION TAG	UNP P07954
B	30	GLY	-	EXPRESSION TAG	UNP P07954
B	31	VAL	-	EXPRESSION TAG	UNP P07954
B	32	ASP	-	EXPRESSION TAG	UNP P07954
B	33	LEU	-	EXPRESSION TAG	UNP P07954
B	34	GLY	-	EXPRESSION TAG	UNP P07954
B	35	THR	-	EXPRESSION TAG	UNP P07954
B	36	GLU	-	EXPRESSION TAG	UNP P07954
B	37	ASN	-	EXPRESSION TAG	UNP P07954
B	38	LEU	-	EXPRESSION TAG	UNP P07954
B	39	TYR	-	EXPRESSION TAG	UNP P07954
B	40	PHE	-	EXPRESSION TAG	UNP P07954
B	41	GLN	-	EXPRESSION TAG	UNP P07954
B	42	SER	-	EXPRESSION TAG	UNP P07954
B	43	MET	-	EXPRESSION TAG	UNP P07954
C	21	MET	-	EXPRESSION TAG	UNP P07954
C	22	HIS	-	EXPRESSION TAG	UNP P07954
C	23	HIS	-	EXPRESSION TAG	UNP P07954
C	24	HIS	-	EXPRESSION TAG	UNP P07954
C	25	HIS	-	EXPRESSION TAG	UNP P07954
C	26	HIS	-	EXPRESSION TAG	UNP P07954
C	27	HIS	-	EXPRESSION TAG	UNP P07954
C	28	SER	-	EXPRESSION TAG	UNP P07954
C	29	SER	-	EXPRESSION TAG	UNP P07954
C	30	GLY	-	EXPRESSION TAG	UNP P07954
C	31	VAL	-	EXPRESSION TAG	UNP P07954
C	32	ASP	-	EXPRESSION TAG	UNP P07954
C	33	LEU	-	EXPRESSION TAG	UNP P07954
C	34	GLY	-	EXPRESSION TAG	UNP P07954
C	35	THR	-	EXPRESSION TAG	UNP P07954
C	36	GLU	-	EXPRESSION TAG	UNP P07954
C	37	ASN	-	EXPRESSION TAG	UNP P07954

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Chain	Residue	Modelled	Actual	Comment	Reference
C	38	LEU	-	EXPRESSION TAG	UNP P07954
C	39	TYR	-	EXPRESSION TAG	UNP P07954
C	40	PHE	-	EXPRESSION TAG	UNP P07954
C	41	GLN	-	EXPRESSION TAG	UNP P07954
C	42	SER	-	EXPRESSION TAG	UNP P07954
C	43	MET	-	EXPRESSION TAG	UNP P07954
D	21	MET	-	EXPRESSION TAG	UNP P07954
D	22	HIS	-	EXPRESSION TAG	UNP P07954
D	23	HIS	-	EXPRESSION TAG	UNP P07954
D	24	HIS	-	EXPRESSION TAG	UNP P07954
D	25	HIS	-	EXPRESSION TAG	UNP P07954
D	26	HIS	-	EXPRESSION TAG	UNP P07954
D	27	HIS	-	EXPRESSION TAG	UNP P07954
D	28	SER	-	EXPRESSION TAG	UNP P07954
D	29	SER	-	EXPRESSION TAG	UNP P07954
D	30	GLY	-	EXPRESSION TAG	UNP P07954
D	31	VAL	-	EXPRESSION TAG	UNP P07954
D	32	ASP	-	EXPRESSION TAG	UNP P07954
D	33	LEU	-	EXPRESSION TAG	UNP P07954
D	34	GLY	-	EXPRESSION TAG	UNP P07954
D	35	THR	-	EXPRESSION TAG	UNP P07954
D	36	GLU	-	EXPRESSION TAG	UNP P07954
D	37	ASN	-	EXPRESSION TAG	UNP P07954
D	38	LEU	-	EXPRESSION TAG	UNP P07954
D	39	TYR	-	EXPRESSION TAG	UNP P07954
D	40	PHE	-	EXPRESSION TAG	UNP P07954
D	41	GLN	-	EXPRESSION TAG	UNP P07954
D	42	SER	-	EXPRESSION TAG	UNP P07954
D	43	MET	-	EXPRESSION TAG	UNP P07954

- 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	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	152	Total	O	0	0
			152	152		
3	B	174	Total	O	0	0
			174	174		
3	C	161	Total	O	0	0
			161	161		
3	D	168	Total	O	0	0
			168	168		

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.

Chain A:

5% 80% 12% 7%

MET HIS HIS HIS HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET MET MET MET ALA SER GLN ASN S49 I52 F57 L60 T72 S75 G82 E86 T90 P91 D113 P114 K115 I116 A123 L138 N152 V153 N154

I157 G166 V181 S184 N188 F191 P192 M195 A217 F225 Q226 Q227 I231 G232 Q237 D238 A239 V240 P241 L244 M266 P267 T277 L283 M284 T285 V297 F305 A308 K311 S351 P359 E360 K361 E362 P363 G364 E500 V501 P509 LYS

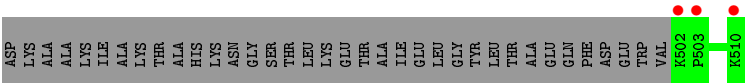
Chain B:

Sequence logo for Chain B. The y-axis represents information content in bits (0.00 to 0.10). The x-axis shows positions 1 to 300. A large green bar at the top indicates high conservation (82%) for the first 280 positions, with a yellow bar (11%) and grey bar (7%) for the last 20 positions. Amino acid labels are shown below the bar, with red dots indicating specific residues of interest.

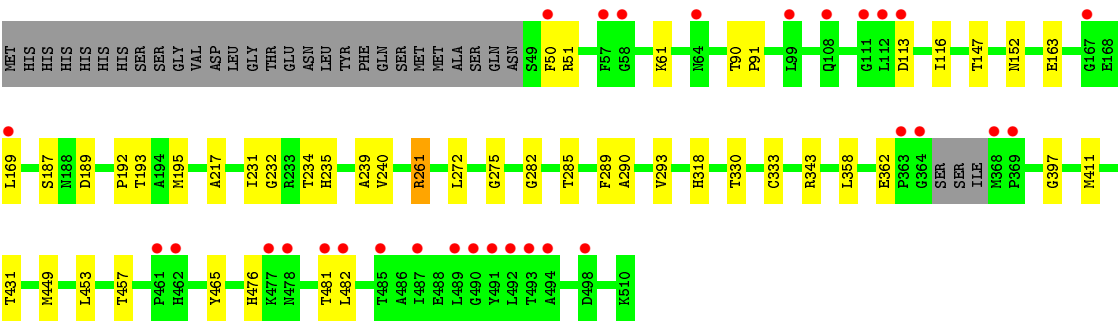
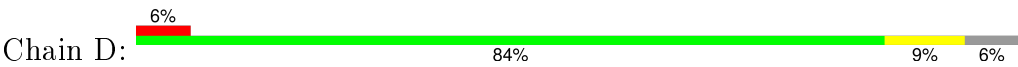
Position	Amino Acid
1	Met
2	His
3	His
4	His
5	His
6	His
7	His
8	His
9	Ser
10	Ser
11	Gly
12	Val
13	Asp
14	Leu
15	Gly
16	Thr
17	Glu
18	Asn
19	Leu
20	Tyr
21	Phe
22	Gln
23	Ser
24	Met
25	Met
26	Ala
27	Ser
28	Gln
29	Asn
30	S49
31	F50
32	R51
33	I52
34	E53
35	Y54
36	Asp
37	Thr
38	Phe
39	Gly
40	E59
41	V62
42	T72
43	V73
44	T76
45	V84
46	T85
47	D113
48	P114
49	K115
50	I116
51	A117
52	N118
53	T147
54	N152
55	G401
56	E404
57	K409
58	P410
59	M411
60	T431
61	M449
62	L455
63	P461
64	H462
65	I463
66	G464
67	Tyr
68	Asp
69	Lys
70	Ala
71	A469
72	K470
73	I471
74	A472
75	K476
76	G479
77	K483
78	A486
79	L487
80	E488
81	L489
82	G490
83	Y491
84	L492
85	T493
86	A494
87	E495
88	Q496
89	F497
90	D498
91	K510

Chain C:





● Molecule 1: Fumarate hydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	188.48Å 188.48Å 114.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 1.95 24.89 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (25.00-1.95) 99.3 (24.89-1.95)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.197 , 0.244 0.200 , 0.245	Depositor DCC
$R_{free}$ test set	1995 reflections (1.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 55.8	EDS
Estimated twinning fraction	0.245 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 168620 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13827	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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, 0.375 respectively for untwinned datasets, and 0.333, 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

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	0.69	0/3443	0.70	0/4672
1	B	0.70	0/3409	0.72	0/4623
1	C	0.68	0/3116	0.71	3/4226 (0.1%)
1	D	0.69	0/3429	0.70	5/4656 (0.1%)
All	All	0.69	0/13397	0.71	8/18177 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	261	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	C	189	ASP	CB-CG-OD1	5.34	123.10	118.30
1	D	51	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	261	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	411	MET	CG-SD-CE	-5.12	92.02	100.20

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	3380	0	3347	54	0
1	B	3350	0	3323	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3063	0	3041	26	0
1	D	3367	0	3305	35	0
2	A	8	0	12	0	0
2	B	4	0	6	7	0
3	A	152	0	0	1	0
3	B	174	0	0	1	0
3	C	161	0	0	0	0
3	D	168	0	0	2	0
All	All	13827	0	13034	137	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 5.

The worst 5 of 137 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HG12	1:A:454:MET:HE2	1.37	1.04
1:A:231:ILE:HG12	1:A:454:MET:CE	1.98	0.94
1:A:277:THR:HG21	1:A:285:THR:HG23	1.56	0.87
1:A:497:PHE:CE2	1:A:501:VAL:HG11	2.13	0.83
1:A:231:ILE:HD11	1:A:452:SER:HB3	1.61	0.82

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	453/490 (92%)	441 (97%)	12 (3%)	0	100	100
1	B	449/490 (92%)	434 (97%)	15 (3%)	0	100	100
1	C	411/490 (84%)	397 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	456/490 (93%)	443 (97%)	13 (3%)	0	100	100
All	All	1769/1960 (90%)	1715 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	346/396 (87%)	343 (99%)	3 (1%)	84	83
1	B	345/396 (87%)	335 (97%)	10 (3%)	50	38
1	C	317/396 (80%)	315 (99%)	2 (1%)	90	89
1	D	342/396 (86%)	341 (100%)	1 (0%)	94	94
All	All	1350/1584 (85%)	1334 (99%)	16 (1%)	78	75

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

Mol	Chain	Res	Type
1	B	186	SER
1	B	230	LYS
1	B	411	MET
1	B	152	ASN
1	C	152	ASN

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	EDO	A	1	-	3,3,3	0.52	0	2,2,2	0.21	0
2	EDO	A	511	-	3,3,3	0.53	0	2,2,2	0.06	0
2	EDO	B	1	-	3,3,3	0.17	0	2,2,2	1.18	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	EDO	A	1	-	-	0/1/1/1	0/0/0/0
2	EDO	A	511	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	EDO	7	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	456/490 (93%)	0.24	24 (5%) 30 41	18, 24, 34, 46	0
1	B	454/490 (92%)	0.14	27 (5%) 26 36	17, 22, 39, 48	0
1	C	415/490 (84%)	0.08	18 (4%) 39 50	18, 23, 38, 53	0
1	D	459/490 (93%)	0.24	30 (6%) 22 32	18, 24, 44, 51	0
All	All	1784/1960 (91%)	0.18	99 (5%) 29 40	17, 23, 38, 53	0

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	50	PHE	6.4
1	B	52	ILE	6.3
1	B	461	PRO	5.8
1	B	50	PHE	5.6
1	B	489	LEU	5.5

### 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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	B	1	4/4	0.83	0.23	10.63	32,32,32,35	0
2	EDO	A	1	4/4	0.89	0.25	1.74	40,42,42,44	0
2	EDO	A	511	4/4	0.92	0.16	1.39	43,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.