



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:31 pm BST

PDB ID : 1W5P  
Title : Stepwise introduction of zinc binding site into porphobilinogen synthase of *Pseudomonas aeruginosa* (mutations A129C, D131C, D139C, P132E)  
Authors : Frere, F.; Reents, H.; Schubert, W.-D.; Heinz, D.W.; Jahn, D.  
Deposited on : 2004-08-09  
Resolution : 1.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

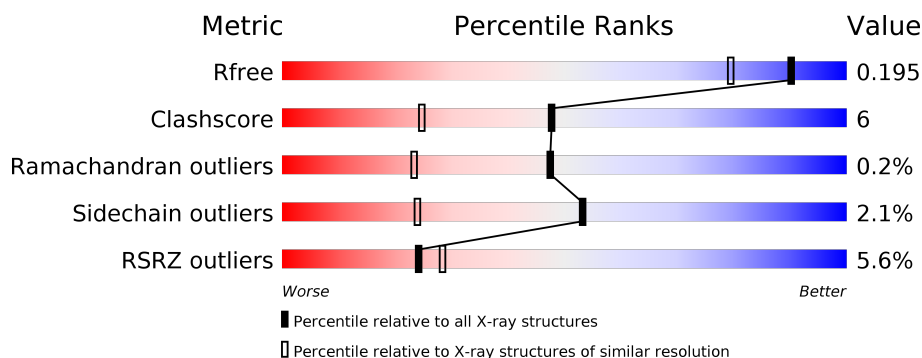
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.55 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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 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	337	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>• •</div> </div> </div>
1	B	337	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>• •</div> </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
3	FMT	A	1340	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5969 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 DELTA-AMINOLEVULINIC ACID DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	21	1
			2678	1675	477	509	17			
1	B	322	Total	C	N	O	S	0	21	1
			2676	1674	479	505	18			

There are 10 discrepancies between the modelled and reference sequences:

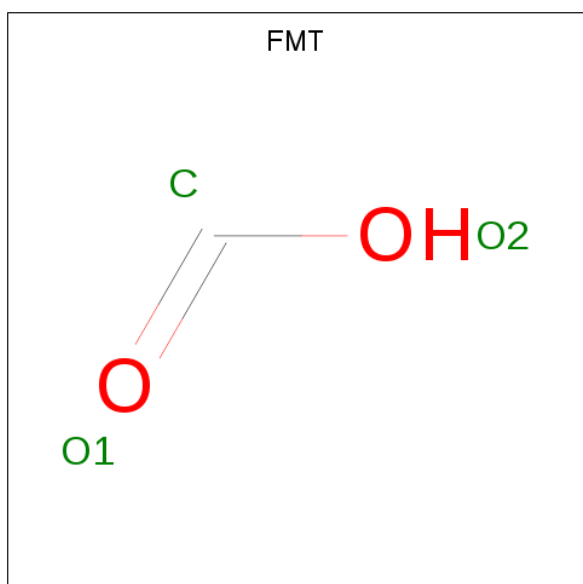
Chain	Residue	Modelled	Actual	Comment	Reference
A	129	CYS	ALA	engineered mutation	UNP Q59643
B	129	CYS	ALA	engineered mutation	UNP Q59643
A	131	CYS	ASP	engineered mutation	UNP Q59643
B	131	CYS	ASP	engineered mutation	UNP Q59643
A	132	GLU	PRO	engineered mutation	UNP Q59643
B	132	GLU	PRO	engineered mutation	UNP Q59643
A	139	CYS	ASP	engineered mutation	UNP Q59643
B	139	CYS	ASP	engineered mutation	UNP Q59643
A	199	VAL	ILE	SEE REMARK 999	UNP Q59643
B	199	VAL	ILE	SEE REMARK 999	UNP Q59643

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

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula:  $\text{CH}_2\text{O}_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0

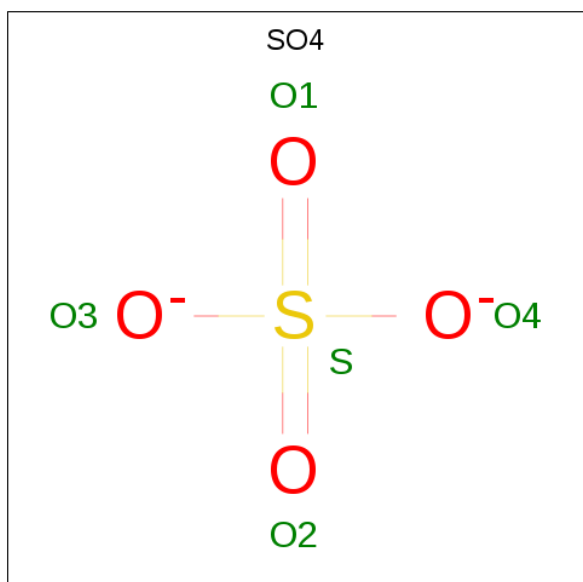
- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total K 1 1	0	0
4	A	1	Total K 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	1
			12	6	6		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Zn	0	0
			1	1		
8	A	1	Total	Zn	0	0
			1	1		

- Molecule 9 is water.

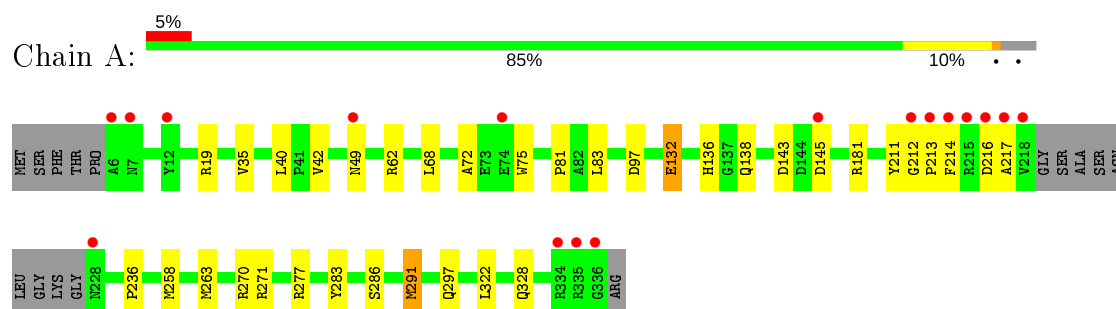
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	266	Total 266	O 266	0	0
9	B	265	Total 265	O 265	0	0



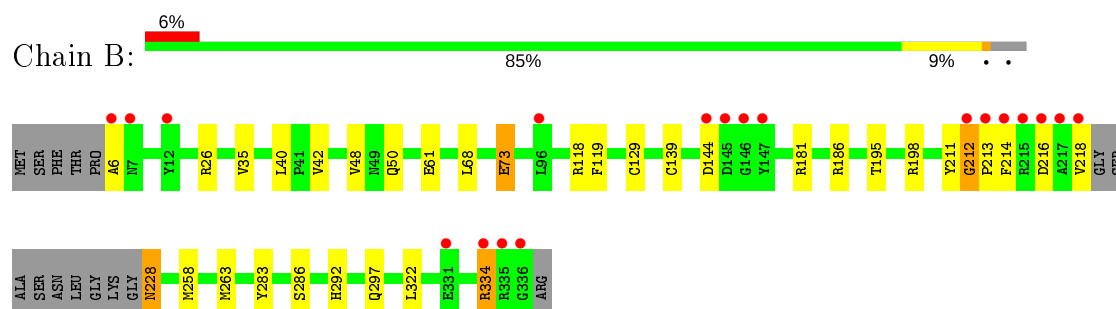
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: DELTA-AMINOLEVULINIC ACID DEHYDRATASE



#### • Molecule 1: DELTA-AMINOLEVULINIC ACID DEHYDRATASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.97Å 126.97Å 86.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.29 – 1.55 19.56 – 1.55	Depositor EDS
% Data completeness (in resolution range)	96.7 (91.29-1.55) 96.7 (19.56-1.55)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.95 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.157 , 0.185 0.170 , 0.195	Depositor DCC
$R_{free}$ test set	4950 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 57.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5969	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, FMT, ZN, EDO, SO4, K

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	0.67	0/2724	0.89	10/3690 (0.3%)
1	B	0.66	0/2721	0.88	4/3686 (0.1%)
All	All	0.67	0/5445	0.89	14/7376 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	19	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	291[A]	MET	CG-SD-CE	6.23	110.17	100.20
1	A	291[B]	MET	CG-SD-CE	6.23	110.17	100.20
1	B	144	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	216[A]	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	216[B]	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	186	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	271	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	277[A]	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	277[B]	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	143	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	270	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	145	ASP	CB-CG-OD2	5.09	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-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 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	2678	0	2625	37	0
1	B	2676	0	2636	35	0
2	A	12	0	18	2	0
2	B	8	0	12	0	0
3	A	3	0	1	2	0
3	B	3	0	1	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	1	0
7	A	6	0	8	1	0
7	B	36	0	48	2	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	266	0	0	10	0
9	B	265	0	0	14	0
All	All	5969	0	5349	66	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 6.

All (66) 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:216:ASP:HB3	9:A:2196:HOH:O	1.33	1.22
1:B:195[B]:THR:HG22	9:B:2191:HOH:O	1.07	1.21
1:B:73:GLU:OE2	9:B:2090:HOH:O	1.64	1.11
1:A:263[B]:MET:HE2	1:B:263[B]:MET:HE3	1.34	1.06
1:A:297[A]:GLN:OE1	9:A:2237:HOH:O	1.74	1.06
1:B:195[B]:THR:CG2	9:B:2191:HOH:O	1.73	1.01
1:B:40[A]:LEU:HD23	1:B:42[A]:VAL:HG13	1.43	1.01
1:B:214:PHE:CE1	9:B:2234:HOH:O	2.14	1.00
1:A:214:PHE:CE1	9:A:2233:HOH:O	2.18	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40[A]:LEU:HD23	1:A:42[A]:VAL:HG13	1.46	0.95
6:B:1342:SO4:O1	9:B:2259:HOH:O	1.89	0.90
1:A:328[B]:GLN:HG3	9:A:2256:HOH:O	1.74	0.86
1:B:40[A]:LEU:CD2	1:B:42[A]:VAL:HG13	2.05	0.86
1:B:40[A]:LEU:CD2	1:B:42[A]:VAL:CG1	2.53	0.86
1:A:263[B]:MET:HE2	1:B:263[B]:MET:CE	2.09	0.83
1:A:35[B]:VAL:HG21	9:A:2258:HOH:O	1.80	0.82
1:A:40[A]:LEU:CD2	1:A:42[A]:VAL:CG1	2.61	0.79
1:B:297:GLN:OE1	9:B:2237:HOH:O	2.02	0.77
1:A:40[A]:LEU:CD2	1:A:42[A]:VAL:HG13	2.14	0.77
1:A:132[B]:GLU:OE2	9:A:2137:HOH:O	2.03	0.77
1:B:334:ARG:NH2	9:B:2257:HOH:O	2.17	0.76
1:A:258[B]:MET:SD	1:A:322:LEU:HD13	2.26	0.76
1:A:263[B]:MET:CE	1:B:263[B]:MET:HE3	2.16	0.73
1:A:81:PRO:HA	2:A:1337:EDO:H21	1.69	0.73
1:B:258[B]:MET:SD	1:B:322:LEU:HD13	2.29	0.71
1:A:263[B]:MET:CE	1:B:263[B]:MET:CE	2.69	0.70
1:B:214:PHE:HE1	9:B:2234:HOH:O	1.62	0.69
1:A:236:PRO:HB2	2:A:1338:EDO:H12	1.76	0.67
1:A:40[A]:LEU:HD23	1:A:42[A]:VAL:CG1	2.22	0.65
1:B:35[B]:VAL:HG11	9:B:2096:HOH:O	1.98	0.63
1:A:40[A]:LEU:HD21	1:A:42[A]:VAL:CG1	2.29	0.62
1:B:40[A]:LEU:HD23	1:B:42[A]:VAL:CG1	2.19	0.61
1:B:334:ARG:CZ	9:B:2257:HOH:O	2.48	0.61
1:A:62:ARG:NH2	1:A:216:ASP:O	2.33	0.58
1:A:136[B]:HIS:HE1	9:A:2093:HOH:O	1.86	0.57
1:A:40[B]:LEU:HD11	7:A:1344:GOL:H32	1.89	0.55
1:B:61:GLU:OE2	9:B:2078:HOH:O	2.18	0.54
1:A:136[B]:HIS:HD2	1:A:138:GLN:H	1.55	0.54
1:B:129:CYS:SG	1:B:139:CYS:HB3	2.48	0.53
1:B:211:TYR:O	1:B:212:GLY:C	2.47	0.52
1:B:73:GLU:CD	1:B:118[B]:ARG:HH21	2.12	0.52
1:A:263[A]:MET:HG2	1:B:263[A]:MET:HG2	1.90	0.52
1:A:214:PHE:HE1	9:A:2233:HOH:O	1.76	0.51
1:B:40[A]:LEU:HD21	1:B:42[A]:VAL:CG1	2.37	0.50
1:B:40[B]:LEU:HD11	7:B:1344:GOL:H32	1.95	0.49
1:A:216:ASP:CB	9:A:2065:HOH:O	2.61	0.48
1:A:216:ASP:HB3	9:A:2065:HOH:O	2.13	0.48
1:B:118[B]:ARG:HG2	1:B:119:PHE:CE2	2.48	0.48
1:B:26[B]:ARG:CZ	9:B:2022:HOH:O	2.63	0.47
1:A:263[B]:MET:CE	1:B:263[B]:MET:HE2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ARG:NE	1:A:217:ALA:O	2.47	0.47
1:A:213:PRO:HB2	1:A:286:SER:HB2	1.98	0.45
1:A:214:PHE:CD1	3:A:1340:FMT:C	3.00	0.45
1:A:211:TYR:O	1:A:212:GLY:C	2.55	0.45
1:B:212:GLY:HA2	9:B:2083:HOH:O	2.17	0.43
1:B:6:ALA:HB1	9:B:2001:HOH:O	2.17	0.43
1:A:42[B]:VAL:HG11	1:A:68:LEU:HD13	2.01	0.43
1:B:48[B]:VAL:O	1:B:50:GLN:HG3	2.19	0.43
1:A:258[B]:MET:SD	1:A:322:LEU:CD1	3.04	0.42
1:A:214:PHE:CD1	3:A:1340:FMT:H	2.54	0.42
1:A:40[A]:LEU:HD22	1:A:83:LEU:HD22	2.02	0.41
1:B:42[B]:VAL:HG11	1:B:68:LEU:HD13	2.01	0.41
1:A:72:ALA:HA	1:A:75:TRP:CE3	2.56	0.41
1:B:213:PRO:HB2	1:B:286:SER:HB2	2.01	0.41
1:A:291[B]:MET:HE2	1:B:292:HIS:HA	2.01	0.40
1:B:228:ASN:HA	7:B:1347:GOL:O2	2.22	0.40

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	339/337 (101%)	334 (98%)	5 (2%)	0	100	100
1	B	339/337 (101%)	333 (98%)	5 (2%)	1 (0%)	41	19
All	All	678/674 (101%)	667 (98%)	10 (2%)	1 (0%)	47	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	212	GLY

### 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	280/270 (104%)	274 (98%)	6 (2%)	53	24
1	B	280/270 (104%)	273 (98%)	7 (2%)	47	18
All	All	560/540 (104%)	547 (98%)	13 (2%)	53	21

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49[A]	ASN
1	A	49[B]	ASN
1	A	132[A]	GLU
1	A	132[B]	GLU
1	A	181	ARG
1	A	283	TYR
1	B	73	GLU
1	B	181	ARG
1	B	198	ARG
1	B	218	VAL
1	B	228	ASN
1	B	283	TYR
1	B	334	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	ASN
1	A	298	ASN
1	A	332	GLN
1	B	228	ASN
1	B	298	ASN
1	B	332	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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	GOL	B	1343[A]	-	5,5,5	0.21	0	5,5,5	0.64	0
7	GOL	B	1343[B]	-	5,5,5	0.21	0	5,5,5	0.54	0
7	GOL	B	1344	-	5,5,5	0.20	0	5,5,5	0.63	0
2	EDO	B	1337	-	3,3,3	0.69	0	2,2,2	0.11	0
3	FMT	B	1339	-	0,2,2	0.00	-	0,1,1	0.00	-
7	GOL	B	1347	-	5,5,5	0.23	0	5,5,5	0.24	0
3	FMT	A	1340	-	0,2,2	0.00	-	0,1,1	0.00	-
2	EDO	A	1339	-	3,3,3	0.24	0	2,2,2	0.54	0
2	EDO	A	1338	-	3,3,3	0.57	0	2,2,2	0.34	0
7	GOL	A	1344	-	5,5,5	0.26	0	5,5,5	0.35	0
2	EDO	B	1338	-	3,3,3	0.42	0	2,2,2	0.33	0
7	GOL	B	1346	-	5,5,5	0.44	0	5,5,5	0.80	0
7	GOL	B	1345	4	5,5,5	0.28	0	5,5,5	0.69	0
2	EDO	A	1337	-	3,3,3	0.71	0	2,2,2	0.48	0
6	SO4	A	1343	-	4,4,4	0.19	0	6,6,6	0.52	0
6	SO4	B	1342	-	4,4,4	0.19	0	6,6,6	0.11	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
7	GOL	B	1343[A]	-	-	2/4/4/4	-
7	GOL	B	1343[B]	-	-	2/4/4/4	-
7	GOL	B	1344	-	-	0/4/4/4	-
2	EDO	B	1337	-	-	0/1/1/1	-
2	EDO	A	1337	-	-	1/1/1/1	-
7	GOL	B	1347	-	-	0/4/4/4	-
2	EDO	A	1339	-	-	1/1/1/1	-
2	EDO	A	1338	-	-	1/1/1/1	-
7	GOL	A	1344	-	-	0/4/4/4	-
2	EDO	B	1338	-	-	1/1/1/1	-
7	GOL	B	1346	-	-	4/4/4/4	-
7	GOL	B	1345	4	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1343[B]	GOL	O1-C1-C2-O2
7	B	1343[B]	GOL	O1-C1-C2-C3
7	B	1346	GOL	O1-C1-C2-C3
7	B	1346	GOL	O1-C1-C2-O2
7	B	1343[A]	GOL	O1-C1-C2-C3
7	B	1346	GOL	C1-C2-C3-O3
7	B	1343[A]	GOL	O1-C1-C2-O2
7	B	1346	GOL	O2-C2-C3-O3
2	A	1338	EDO	O1-C1-C2-O2
2	A	1337	EDO	O1-C1-C2-O2
2	A	1339	EDO	O1-C1-C2-O2
2	B	1338	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1344	GOL	1	0
7	B	1347	GOL	1	0
3	A	1340	FMT	2	0
2	A	1338	EDO	1	0
7	A	1344	GOL	1	0
2	A	1337	EDO	1	0
6	B	1342	SO4	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 ⓘ

### 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	322/337 (95%)	0.13	17 (5%)	26 31	12, 17, 30, 69	7 (2%)
1	B	322/337 (95%)	0.30	19 (5%)	22 26	12, 18, 31, 76	10 (3%)
All	All	644/674 (95%)	0.22	36 (5%)	24 28	12, 17, 31, 76	17 (2%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	GLY	28.2
1	B	335	ARG	8.6
1	B	214	PHE	8.0
1	B	215	ARG	7.6
1	A	214	PHE	7.1
1	A	215	ARG	6.9
1	B	212	GLY	6.8
1	B	216[A]	ASP	6.6
1	A	335	ARG	6.2
1	B	6	ALA	5.8
1	A	216	ASP	5.5
1	A	218	VAL	5.3
1	A	6	ALA	5.0
1	A	212	GLY	4.7
1	A	7	ASN	4.3
1	A	12	TYR	4.2
1	B	7	ASN	4.2
1	B	218	VAL	4.0
1	A	334	ARG	3.8
1	A	228	ASN	3.8
1	B	144	ASP	3.7
1	B	145	ASP	3.6
1	B	96	LEU	3.6
1	B	213	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	336	GLY	3.5
1	B	217	ALA	3.2
1	B	334	ARG	3.1
1	B	147	TYR	3.0
1	A	213	PRO	2.8
1	A	145	ASP	2.6
1	A	217	ALA	2.4
1	A	74[A]	GLU	2.4
1	B	146	GLY	2.3
1	B	12	TYR	2.2
1	A	49[A]	ASN	2.0
1	B	331	GLU	2.0

## 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 ⓘ

There are no carbohydrates in this entry.

## 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. 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	B	1337	4/4	0.47	0.18	38,40,41,41	0
7	GOL	B	1347	6/6	0.60	0.28	39,40,40,41	6
7	GOL	B	1346	6/6	0.69	0.23	27,34,36,37	6
2	EDO	A	1337	4/4	0.72	0.15	34,37,38,40	0
7	GOL	B	1343[A]	6/6	0.83	0.33	34,34,34,35	6
7	GOL	B	1343[B]	6/6	0.83	0.33	36,38,39,39	6
7	GOL	B	1345	6/6	0.83	0.24	39,41,42,42	0
2	EDO	B	1338	4/4	0.84	0.25	43,43,43,44	4
6	SO4	A	1343	5/5	0.85	0.20	31,32,33,33	5
2	EDO	A	1338	4/4	0.85	0.13	31,36,36,39	0
3	FMT	A	1340	3/3	0.88	0.10	19,19,21,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GOL	B	1344	6/6	0.88	0.12	23,26,27,28	0
2	EDO	A	1339	4/4	0.90	0.14	29,30,31,31	0
3	FMT	B	1339	3/3	0.91	0.10	20,20,22,26	0
7	GOL	A	1344	6/6	0.91	0.11	21,25,25,29	0
6	SO4	B	1342	5/5	0.93	0.17	47,47,48,48	5
4	K	A	1341	1/1	0.97	0.15	27,27,27,27	1
8	ZN	A	1345	1/1	0.98	0.03	17,17,17,17	1
5	MG	B	1341	1/1	0.99	0.08	14,14,14,14	0
8	ZN	B	1348	1/1	0.99	0.03	18,18,18,18	1
5	MG	A	1342	1/1	0.99	0.04	13,13,13,13	0
4	K	B	1340	1/1	1.00	0.08	25,25,25,25	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.