



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 09:08 PM BST

PDB ID : 3GKE  
Title : Crystal Structure of Dicamba Monooxygenase  
Authors : Wilson, M.A.; Dumitru, R.; Jiang, W.Z.; Weeks, D.P.  
Deposited on : 2009-03-10  
Resolution : 1.75 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 : 2.13.1  
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) : 2.13.1

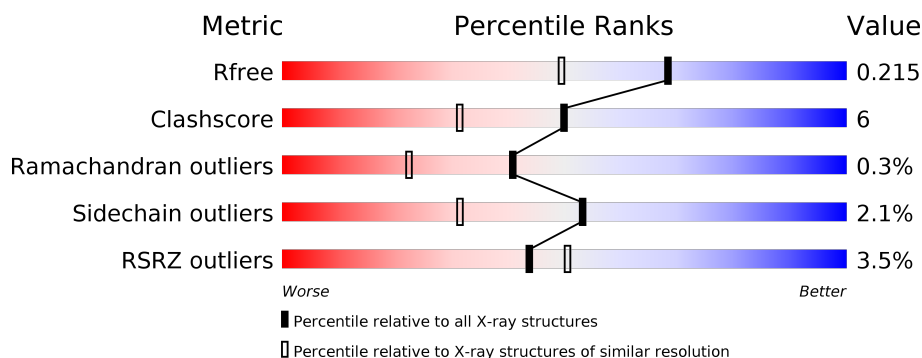
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	349	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>.</div> </div> </div>
1	B	349	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>.</div> </div> </div>
1	C	349	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>5%</div> <div>10%</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
4	EDO	B	352	-	-	X	-
5	ACT	A	353	-	-	X	-
5	ACT	B	700	-	-	X	-
5	ACT	C	353	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8593 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 DdmC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2633	1659	473	488	13			
1	B	334	Total	C	N	O	S	0	0	0
			2590	1634	463	480	13			
1	C	314	Total	C	N	O	S	0	3	0
			2451	1548	432	458	13			

There are 33 discrepancies between the modelled and reference sequences:

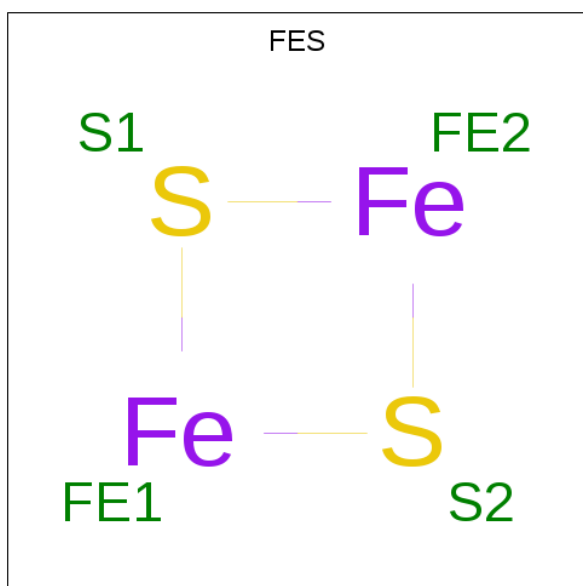
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INSERTION	UNP Q5S3I3
A	2	ALA	-	INSERTION	UNP Q5S3I3
A	341	ARG	-	INSERTION	UNP Q5S3I3
A	342	LEU	-	EXPRESSION TAG	UNP Q5S3I3
A	343	GLU	-	EXPRESSION TAG	UNP Q5S3I3
A	344	HIS	-	EXPRESSION TAG	UNP Q5S3I3
A	345	HIS	-	EXPRESSION TAG	UNP Q5S3I3
A	346	HIS	-	EXPRESSION TAG	UNP Q5S3I3
A	347	HIS	-	EXPRESSION TAG	UNP Q5S3I3
A	348	HIS	-	EXPRESSION TAG	UNP Q5S3I3
A	349	HIS	-	EXPRESSION TAG	UNP Q5S3I3
B	1	MET	-	INSERTION	UNP Q5S3I3
B	2	ALA	-	INSERTION	UNP Q5S3I3
B	341	ARG	-	INSERTION	UNP Q5S3I3
B	342	LEU	-	EXPRESSION TAG	UNP Q5S3I3
B	343	GLU	-	EXPRESSION TAG	UNP Q5S3I3
B	344	HIS	-	EXPRESSION TAG	UNP Q5S3I3
B	345	HIS	-	EXPRESSION TAG	UNP Q5S3I3
B	346	HIS	-	EXPRESSION TAG	UNP Q5S3I3
B	347	HIS	-	EXPRESSION TAG	UNP Q5S3I3
B	348	HIS	-	EXPRESSION TAG	UNP Q5S3I3
B	349	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	1	MET	-	INSERTION	UNP Q5S3I3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ALA	-	INSERTION	UNP Q5S3I3
C	341	ARG	-	INSERTION	UNP Q5S3I3
C	342	LEU	-	EXPRESSION TAG	UNP Q5S3I3
C	343	GLU	-	EXPRESSION TAG	UNP Q5S3I3
C	344	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	345	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	346	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	347	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	348	HIS	-	EXPRESSION TAG	UNP Q5S3I3
C	349	HIS	-	EXPRESSION TAG	UNP Q5S3I3

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Fe 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



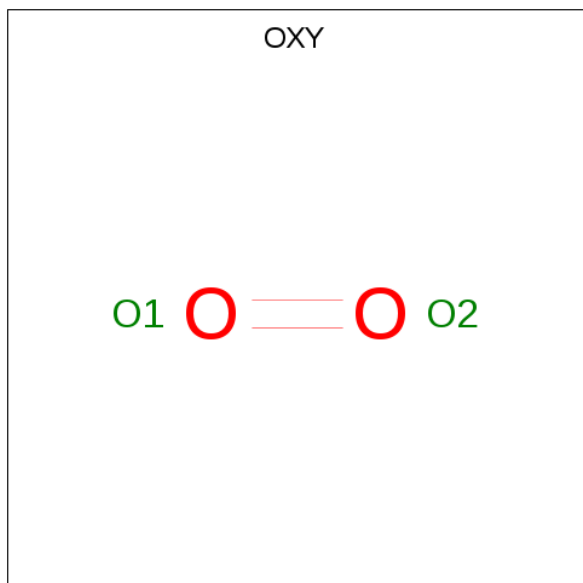
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 6 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 2	O 2	0	0

- Molecule 7 is water.

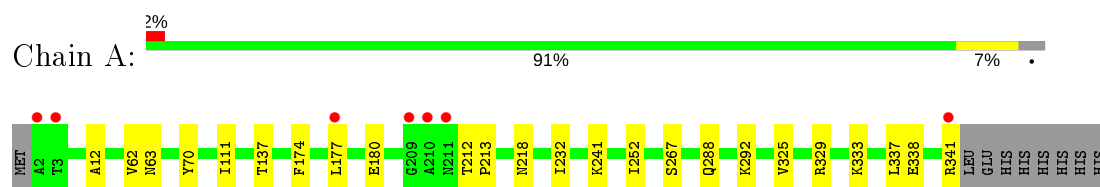
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	327	Total 327	O 327	0	0
7	B	256	Total 256	O 256	0	0
7	C	268	Total 268	O 268	0	0



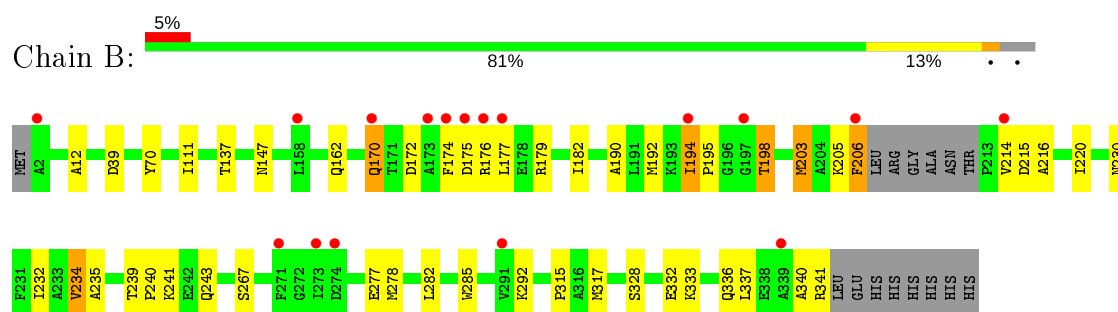
### 3 Residue-property plots [i](#)

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.

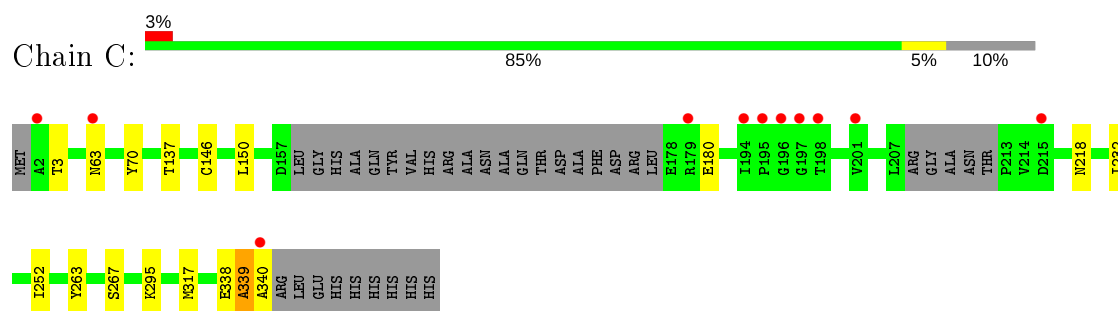
#### • Molecule 1: DdmC



#### • Molecule 1: DdmC



#### • Molecule 1: DdmC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.03Å 81.03Å 158.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.15 – 1.75 42.15 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.15-1.75) 99.3 (42.15-1.75)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.163 , 0.198 0.178 , 0.215	Depositor DCC
$R_{free}$ test set	5839 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.002 for -h,-k,l 0.032 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8593	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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: ACT, FE, OXY, FES, 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	0.47	0/2698	0.57	0/3674
1	B	0.48	0/2654	0.56	0/3612
1	C	0.48	0/2510	0.56	0/3416
All	All	0.47	0/7862	0.56	0/10702

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	194	ILE	Peptide
1	B	205	LYS	Peptide
1	C	339	ALA	Peptide

## 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	2633	0	2566	15	0
1	B	2590	0	2521	62	0
1	C	2451	0	2384	10	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	12	0	18	1	0
4	B	12	0	18	4	0
4	C	12	0	18	2	0
5	A	8	0	6	4	0
5	B	4	0	3	2	0
5	C	4	0	3	3	0
6	B	2	0	0	0	0
7	A	327	0	0	0	0
7	B	256	0	0	11	0
7	C	268	0	0	3	0
All	All	8593	0	7537	89	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 (89) 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:230:ASN:ND2	1:B:232:ILE:HD11	1.66	1.09
1:B:177:LEU:HG	1:B:192:MET:HE1	1.35	1.07
1:B:177:LEU:HG	1:B:192:MET:CE	1.87	1.04
1:C:63[B]:ASN:OD1	5:C:353:ACT:H2	1.57	1.03
1:B:174:PHE:O	1:B:177:LEU:HD13	1.58	1.02
1:A:232:ILE:HD12	5:A:353:ACT:H1	1.40	1.01
1:B:174:PHE:HA	1:B:177:LEU:CD1	2.01	0.91
1:B:292:LYS:HG2	7:B:734:HOH:O	1.71	0.89
1:B:230:ASN:ND2	1:B:232:ILE:CD1	2.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ASN:HD21	1:B:232:ILE:HD11	1.40	0.85
1:B:162:GLN:HG3	1:B:174:PHE:CD2	2.12	0.84
1:B:162:GLN:OE1	1:B:170:GLN:HA	1.85	0.77
1:B:337:LEU:HD21	1:B:341:ARG:HH21	1.51	0.75
1:B:203:MET:O	1:B:206:PHE:C	2.26	0.73
1:B:12:ALA:CB	1:B:111:ILE:HD12	2.18	0.73
1:B:203:MET:HE2	1:B:234:VAL:HG12	1.69	0.73
1:A:333:LYS:O	1:A:337:LEU:HD13	1.89	0.72
1:B:174:PHE:HA	1:B:177:LEU:HD11	1.70	0.72
1:B:174:PHE:O	1:B:177:LEU:CD1	2.36	0.71
1:C:63[B]:ASN:OD1	5:C:353:ACT:CH3	2.38	0.71
1:B:190:ALA:HB1	4:B:352:EDO:H21	1.72	0.70
1:B:239:THR:O	7:B:718:HOH:O	2.09	0.70
1:B:203:MET:CE	1:B:234:VAL:HG12	2.23	0.69
1:B:230:ASN:HD21	1:B:232:ILE:CD1	2.01	0.69
1:B:198:THR:OG1	7:B:442:HOH:O	2.11	0.68
1:B:336:GLN:HA	7:B:689:HOH:O	1.93	0.66
1:B:177:LEU:HG	1:B:192:MET:HE3	1.75	0.66
1:B:39:ASP:OD2	7:B:474:HOH:O	2.13	0.66
5:C:353:ACT:H3	7:C:376:HOH:O	1.96	0.65
1:A:232:ILE:CD1	5:A:353:ACT:H1	2.22	0.64
1:B:203:MET:HE1	1:B:206:PHE:HE1	1.63	0.63
1:B:190:ALA:CB	4:B:352:EDO:H21	2.29	0.63
1:B:190:ALA:HB3	4:B:352:EDO:H12	1.82	0.61
1:B:174:PHE:CA	1:B:177:LEU:CD1	2.78	0.60
1:B:177:LEU:CG	1:B:192:MET:HE1	2.23	0.59
1:A:252:ILE:HG23	4:A:350:EDO:H12	1.85	0.59
1:A:232:ILE:HD12	5:A:353:ACT:CH3	2.26	0.58
1:B:285:TRP:NE1	5:B:700:ACT:H1	2.18	0.58
1:A:218:ASN:OD1	1:A:232:ILE:HG12	2.04	0.57
1:B:340:ALA:O	1:B:341:ARG:HG3	2.05	0.56
1:B:174:PHE:CD2	1:B:177:LEU:HD11	2.41	0.56
1:C:317:MET:CE	1:C:317:MET:HA	2.37	0.55
1:B:12:ALA:HB2	1:B:111:ILE:HD12	1.90	0.54
1:C:252:ILE:HG23	4:C:350:EDO:H12	1.90	0.54
1:B:337:LEU:HD21	1:B:341:ARG:NH2	2.20	0.54
1:B:203:MET:HE1	1:B:206:PHE:CE1	2.43	0.54
1:B:203:MET:HG3	1:B:234:VAL:HB	1.90	0.54
1:B:220:ILE:HG22	4:B:352:EDO:H12	1.90	0.53
1:B:203:MET:CE	1:B:206:PHE:CE1	2.91	0.53
1:B:172:ASP:HB3	7:B:442:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ILE:HD12	1:B:216:ALA:O	2.09	0.52
1:B:174:PHE:HA	1:B:177:LEU:HD12	1.85	0.52
1:B:206:PHE:N	1:B:206:PHE:CD2	2.78	0.51
1:B:240:PRO:HG2	1:B:243:GLN:OE1	2.11	0.51
1:B:282:LEU:HD13	7:B:429:HOH:O	2.10	0.50
1:C:218[B]:ASN:ND2	1:C:232:ILE:HD12	2.27	0.50
1:C:146:CYS:HB2	1:C:150:LEU:HD12	1.93	0.50
1:B:172:ASP:CB	7:B:442:HOH:O	2.60	0.49
1:B:328:SER:O	1:B:332:GLU:HG2	2.13	0.48
1:A:137:THR:HA	1:A:267:SER:O	2.13	0.48
1:B:234:VAL:CG2	1:B:235:ALA:N	2.76	0.48
1:B:336:GLN:CA	7:B:689:HOH:O	2.59	0.47
1:A:325:VAL:O	1:A:329:ARG:HG3	2.15	0.47
1:B:195:PRO:HA	1:B:215:ASP:OD1	2.15	0.46
1:B:137:THR:HA	1:B:267:SER:O	2.16	0.46
4:C:350:EDO:H22	7:C:481:HOH:O	2.16	0.46
1:C:317:MET:HE2	1:C:317:MET:HA	1.96	0.46
1:B:333:LYS:O	1:B:337:LEU:HB2	2.16	0.46
1:A:174:PHE:O	1:A:177:LEU:HG	2.15	0.46
1:B:12:ALA:HB3	1:B:111:ILE:HD12	1.97	0.46
1:B:214:VAL:CG1	1:B:234:VAL:HG23	2.47	0.45
1:B:232:ILE:HD13	5:B:700:ACT:H2	1.97	0.45
1:B:147:ASN:ND2	7:B:756:HOH:O	2.49	0.44
1:B:175:ASP:HB2	1:B:176:ARG:HG3	2.00	0.44
1:A:212:THR:HB	1:A:213:PRO:CD	2.47	0.44
1:B:336:GLN:CB	7:B:689:HOH:O	2.66	0.44
1:B:203:MET:CE	1:B:234:VAL:CG1	2.95	0.44
1:C:137:THR:HA	1:C:267:SER:O	2.19	0.43
1:A:333:LYS:HE3	1:A:333:LYS:HB3	1.53	0.43
1:B:203:MET:HE3	1:B:206:PHE:CE1	2.54	0.43
1:A:12:ALA:CB	1:A:111:ILE:HD12	2.49	0.43
1:B:162:GLN:HG3	1:B:174:PHE:CE2	2.54	0.43
1:A:232:ILE:CD1	5:A:353:ACT:CH3	2.91	0.42
1:C:295:LYS:HE2	7:C:416:HOH:O	2.19	0.42
1:A:288:GLN:O	1:A:292:LYS:HB3	2.19	0.41
1:B:315:PRO:HB2	1:B:317:MET:CE	2.51	0.41
1:A:62:VAL:O	1:A:63:ASN:HB2	2.21	0.41
1:B:278:MET:O	1:B:278:MET:HE3	2.21	0.41
1:C:338:GLU:O	1:C:340:ALA:N	2.54	0.40

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	338/349 (97%)	324 (96%)	13 (4%)	1 (0%)	41	22
1	B	330/349 (95%)	314 (95%)	15 (4%)	1 (0%)	41	22
1	C	311/349 (89%)	300 (96%)	10 (3%)	1 (0%)	41	22
All	All	979/1047 (94%)	938 (96%)	38 (4%)	3 (0%)	41	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	LYS
1	C	339	ALA
1	B	241	LYS

### 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	275/284 (97%)	271 (98%)	4 (2%)	65	49
1	B	271/284 (95%)	262 (97%)	9 (3%)	38	15
1	C	259/284 (91%)	255 (98%)	4 (2%)	65	49
All	All	805/852 (94%)	788 (98%)	17 (2%)	53	31

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	TYR
1	A	180	GLU
1	A	338	GLU
1	A	341	ARG
1	B	70	TYR
1	B	170	GLN
1	B	179	ARG
1	B	182	ILE
1	B	198	THR
1	B	203	MET
1	B	206	PHE
1	B	234	VAL
1	B	277	GLU
1	C	3	THR
1	C	70	TYR
1	C	180	GLU
1	C	263	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	154	ASN

### 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 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	FES	B	500	1	0,4,4	0.00	-	-		
4	EDO	A	351	-	3,3,3	0.41	0	2,2,2	0.31	0
4	EDO	C	351	-	3,3,3	0.68	0	2,2,2	0.12	0
4	EDO	C	352	-	3,3,3	0.35	0	2,2,2	0.54	0
5	ACT	C	353	-	1,3,3	1.68	0	0,3,3	0.00	-
4	EDO	A	352	-	3,3,3	0.47	0	2,2,2	0.23	0
4	EDO	B	352	-	3,3,3	0.42	0	2,2,2	0.40	0
4	EDO	B	351	-	3,3,3	0.47	0	2,2,2	0.23	0
2	FES	A	500	1	0,4,4	0.00	-	-		
4	EDO	B	350	-	3,3,3	0.48	0	2,2,2	0.49	0
5	ACT	A	354	3	1,3,3	1.52	0	0,3,3	0.00	-
5	ACT	A	353	-	1,3,3	1.53	0	0,3,3	0.00	-
4	EDO	A	350	-	3,3,3	0.50	0	2,2,2	0.13	0
6	OXY	B	600	3	1,1,1	0.01	0	-		
4	EDO	C	350	-	3,3,3	0.35	0	2,2,2	0.57	0
2	FES	C	500	1	0,4,4	0.00	-	-		
5	ACT	B	700	-	1,3,3	1.69	0	0,3,3	0.00	-

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	FES	B	500	1	-	-	0/1/1/1
4	EDO	A	351	-	-	0/1/1/1	-
2	FES	C	500	1	-	-	0/1/1/1
4	EDO	C	352	-	-	0/1/1/1	-
4	EDO	A	352	-	-	1/1/1/1	-
4	EDO	B	352	-	-	1/1/1/1	-
4	EDO	B	351	-	-	0/1/1/1	-
2	FES	A	500	1	-	-	0/1/1/1
4	EDO	B	350	-	-	0/1/1/1	-
4	EDO	A	350	-	-	0/1/1/1	-
4	EDO	C	350	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	351	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	352	EDO	O1-C1-C2-O2
4	A	352	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	353	ACT	3	0
4	B	352	EDO	4	0
5	A	353	ACT	4	0
4	A	350	EDO	1	0
4	C	350	EDO	2	0
5	B	700	ACT	2	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	340/349 (97%)	-0.16	7 (2%) 63 71	20, 29, 56, 88	0
1	B	334/349 (95%)	0.30	17 (5%) 28 34	18, 32, 71, 91	0
1	C	314/349 (89%)	-0.10	11 (3%) 44 50	19, 28, 62, 83	0
All	All	988/1047 (94%)	0.01	35 (3%) 44 50	18, 30, 63, 91	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	4.9
1	C	2	ALA	4.6
1	B	339	ALA	4.0
1	C	198	THR	4.0
1	B	273	ILE	3.8
1	C	197	GLY	3.7
1	C	195	PRO	3.6
1	B	2	ALA	3.5
1	B	274	ASP	3.5
1	B	206	PHE	3.5
1	B	175	ASP	3.4
1	B	177	LEU	3.4
1	C	194	ILE	3.3
1	B	291	VAL	3.2
1	B	173	ALA	3.1
1	A	177	LEU	3.0
1	B	158	LEU	2.8
1	B	174	PHE	2.8
1	B	176	ARG	2.7
1	C	340	ALA	2.6
1	C	196	GLY	2.6
1	B	194	ILE	2.6
1	A	211	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	201	VAL	2.5
1	A	209	GLY	2.5
1	A	341	ARG	2.4
1	C	179	ARG	2.4
1	A	3	THR	2.3
1	B	214	VAL	2.2
1	C	215	ASP	2.2
1	B	197	GLY	2.1
1	B	170	GLN	2.0
1	B	271	PHE	2.0
1	C	63[A]	ASN	2.0
1	A	210	ALA	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 monosaccharides 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
4	EDO	C	351	4/4	0.80	0.14	35,44,45,54	0
5	ACT	C	353	4/4	0.80	0.17	55,62,64,66	0
5	ACT	B	700	4/4	0.89	0.12	40,48,52,55	0
6	OXY	B	600	2/2	0.94	0.12	41,41,41,42	0
4	EDO	B	351	4/4	0.94	0.10	26,27,28,31	0
4	EDO	B	352	4/4	0.95	0.14	32,33,48,56	0
4	EDO	A	352	4/4	0.96	0.08	31,34,37,37	0
4	EDO	A	351	4/4	0.96	0.10	31,31,31,33	0
4	EDO	C	352	4/4	0.96	0.09	34,35,40,41	0
4	EDO	A	350	4/4	0.98	0.11	24,24,29,29	0
5	ACT	A	354	4/4	0.98	0.08	26,27,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	C	350	4/4	0.98	0.12	19,29,30,33	0
5	ACT	A	353	4/4	0.98	0.10	29,32,32,42	0
4	EDO	B	350	4/4	0.99	0.14	22,22,23,24	0
3	FE	B	501	1/1	0.99	0.13	30,30,30,30	0
2	FES	B	500	4/4	1.00	0.10	19,21,21,22	0
2	FES	A	500	4/4	1.00	0.07	24,26,27,28	0
2	FES	C	500	4/4	1.00	0.10	21,21,22,23	0
3	FE	A	501	1/1	1.00	0.09	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.