



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 10:30 PM UTC

PDB ID : 9UAE / pdb\_00009uae  
Title : Crystal structure of the OkaE-M71A mutant with coblat(II)  
Authors : Yu, J.J.; Yan, W.P.; Wang, X.Y.  
Deposited on : 2025-03-31  
Resolution : 2.40 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.

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

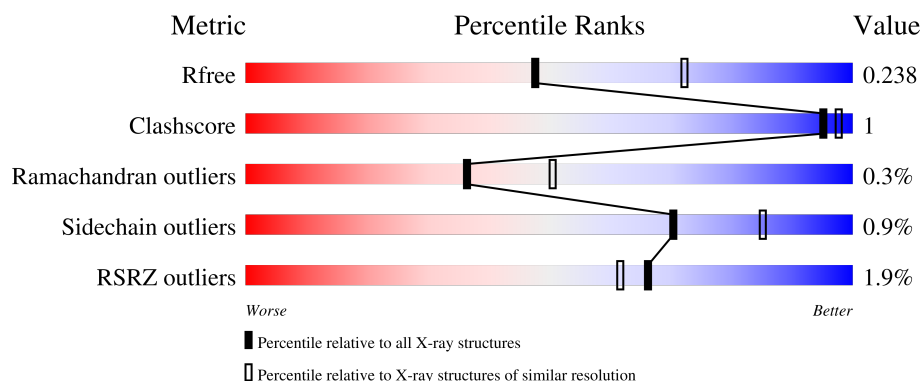
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	315	<div> <div>88%</div> <div>9%</div> </div>
1	B	315	<div> <div>90%</div> <div>8%</div> </div>
1	C	315	<div> <div>3%</div> <div>94%</div> <div>5%</div> </div>
1	D	315	<div> <div>2%</div> <div>86%</div> <div>5%</div> <div>9%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9758 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 Iron/ $\alpha$ -ketoglutarate-dependent dioxygenase okaE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	305	Total	C	N	O	S	0	0	0
			2380	1488	429	445	18			
1	D	288	Total	C	N	O	S	0	0	0
			2249	1410	406	417	16			
1	A	287	Total	C	N	O	S	0	0	0
			2250	1409	406	419	16			
1	B	289	Total	C	N	O	S	0	0	0
			2274	1424	411	422	17			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	MET	-	initiating methionine	UNP A0A2Z5U507
C	-5	GLY	-	expression tag	UNP A0A2Z5U507
C	-4	ASP	-	expression tag	UNP A0A2Z5U507
C	-3	ARG	-	expression tag	UNP A0A2Z5U507
C	-2	GLY	-	expression tag	UNP A0A2Z5U507
C	-1	PRO	-	expression tag	UNP A0A2Z5U507
C	0	GLU	-	expression tag	UNP A0A2Z5U507
C	1	PHE	-	expression tag	UNP A0A2Z5U507
C	71	ALA	MET	engineered mutation	UNP A0A2Z5U507
C	301	TRP	-	expression tag	UNP A0A2Z5U507
C	302	SER	-	expression tag	UNP A0A2Z5U507
C	303	HIS	-	expression tag	UNP A0A2Z5U507
C	304	PRO	-	expression tag	UNP A0A2Z5U507
C	305	GLN	-	expression tag	UNP A0A2Z5U507
C	306	PHE	-	expression tag	UNP A0A2Z5U507
C	307	GLU	-	expression tag	UNP A0A2Z5U507
C	308	LYS	-	expression tag	UNP A0A2Z5U507
D	-6	MET	-	initiating methionine	UNP A0A2Z5U507
D	-5	GLY	-	expression tag	UNP A0A2Z5U507
D	-4	ASP	-	expression tag	UNP A0A2Z5U507
D	-3	ARG	-	expression tag	UNP A0A2Z5U507

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP A0A2Z5U507
D	-1	PRO	-	expression tag	UNP A0A2Z5U507
D	0	GLU	-	expression tag	UNP A0A2Z5U507
D	1	PHE	-	expression tag	UNP A0A2Z5U507
D	71	ALA	MET	engineered mutation	UNP A0A2Z5U507
D	301	TRP	-	expression tag	UNP A0A2Z5U507
D	302	SER	-	expression tag	UNP A0A2Z5U507
D	303	HIS	-	expression tag	UNP A0A2Z5U507
D	304	PRO	-	expression tag	UNP A0A2Z5U507
D	305	GLN	-	expression tag	UNP A0A2Z5U507
D	306	PHE	-	expression tag	UNP A0A2Z5U507
D	307	GLU	-	expression tag	UNP A0A2Z5U507
D	308	LYS	-	expression tag	UNP A0A2Z5U507
A	-6	MET	-	initiating methionine	UNP A0A2Z5U507
A	-5	GLY	-	expression tag	UNP A0A2Z5U507
A	-4	ASP	-	expression tag	UNP A0A2Z5U507
A	-3	ARG	-	expression tag	UNP A0A2Z5U507
A	-2	GLY	-	expression tag	UNP A0A2Z5U507
A	-1	PRO	-	expression tag	UNP A0A2Z5U507
A	0	GLU	-	expression tag	UNP A0A2Z5U507
A	1	PHE	-	expression tag	UNP A0A2Z5U507
A	71	ALA	MET	engineered mutation	UNP A0A2Z5U507
A	301	TRP	-	expression tag	UNP A0A2Z5U507
A	302	SER	-	expression tag	UNP A0A2Z5U507
A	303	HIS	-	expression tag	UNP A0A2Z5U507
A	304	PRO	-	expression tag	UNP A0A2Z5U507
A	305	GLN	-	expression tag	UNP A0A2Z5U507
A	306	PHE	-	expression tag	UNP A0A2Z5U507
A	307	GLU	-	expression tag	UNP A0A2Z5U507
A	308	LYS	-	expression tag	UNP A0A2Z5U507
B	-6	MET	-	initiating methionine	UNP A0A2Z5U507
B	-5	GLY	-	expression tag	UNP A0A2Z5U507
B	-4	ASP	-	expression tag	UNP A0A2Z5U507
B	-3	ARG	-	expression tag	UNP A0A2Z5U507
B	-2	GLY	-	expression tag	UNP A0A2Z5U507
B	-1	PRO	-	expression tag	UNP A0A2Z5U507
B	0	GLU	-	expression tag	UNP A0A2Z5U507
B	1	PHE	-	expression tag	UNP A0A2Z5U507
B	71	ALA	MET	engineered mutation	UNP A0A2Z5U507
B	301	TRP	-	expression tag	UNP A0A2Z5U507
B	302	SER	-	expression tag	UNP A0A2Z5U507
B	303	HIS	-	expression tag	UNP A0A2Z5U507

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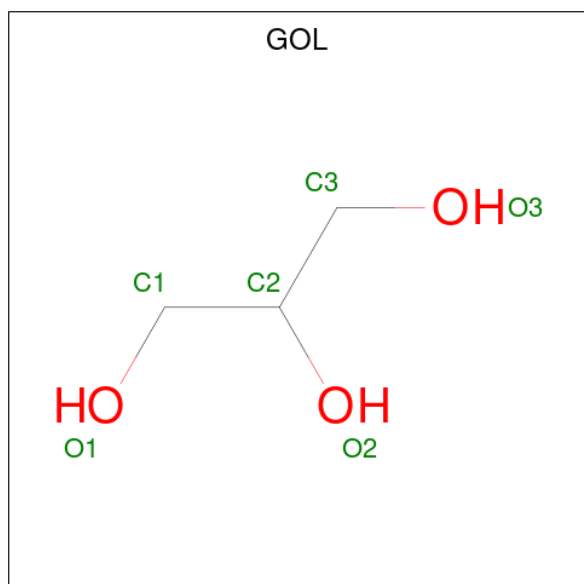
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Chain	Residue	Modelled	Actual	Comment	Reference
B	304	PRO	-	expression tag	UNP A0A2Z5U507
B	305	GLN	-	expression tag	UNP A0A2Z5U507
B	306	PHE	-	expression tag	UNP A0A2Z5U507
B	307	GLU	-	expression tag	UNP A0A2Z5U507
B	308	LYS	-	expression tag	UNP A0A2Z5U507

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Co 1 1	0	0
2	D	1	Total Co 1 1	0	0
2	A	1	Total Co 1 1	0	0
2	B	1	Total Co 1 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	144	Total	O	0	0
			144	144		
4	D	100	Total	O	0	0
			100	100		
4	A	137	Total	O	0	0
			137	137		
4	B	148	Total	O	0	0
			148	148		

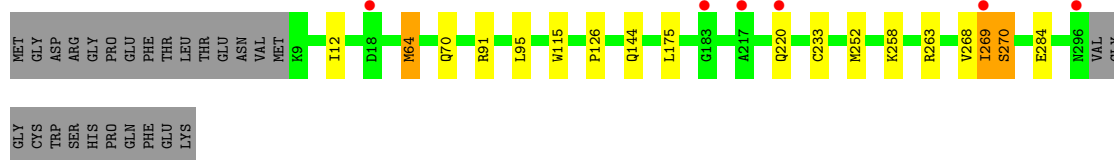
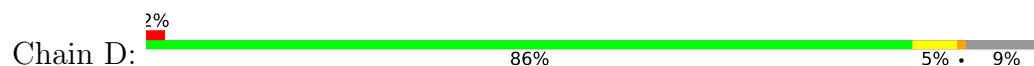
### 3 Residue-property plots [i](#)

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.

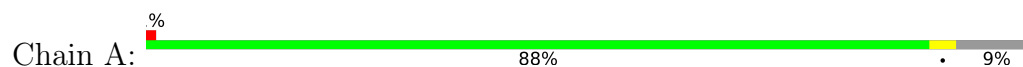
- Molecule 1: Iron/alpha-ketoglutarate-dependent dioxygenase okaE



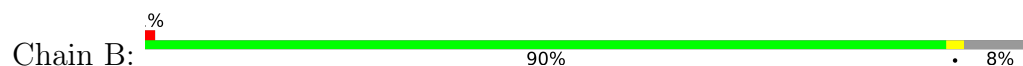
- Molecule 1: Iron/alpha-ketoglutarate-dependent dioxygenase okaE



- Molecule 1: Iron/alpha-ketoglutarate-dependent dioxygenase okaE



- Molecule 1: Iron/alpha-ketoglutarate-dependent dioxygenase okaE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.15Å 107.66Å 134.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.62 – 2.40 38.62 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.62-2.40) 99.9 (38.62-2.40)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.198 , 0.237 0.198 , 0.238	Depositor DCC
$R_{free}$ test set	2204 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 37.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9758	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4405e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, CO

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	0.11	0/2306	0.26	0/3143
1	B	0.09	0/2330	0.34	2/3172 (0.1%)
1	C	0.08	0/2438	0.28	0/3319
1	D	0.08	0/2304	0.26	0/3139
All	All	0.09	0/9378	0.29	2/12773 (0.0%)

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	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	ILE	CA-C-N	9.28	138.40	121.70
1	B	269	ILE	C-N-CA	9.28	138.40	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	ILE	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	2250	0	2195	5	0
1	B	2274	0	2232	3	0
1	C	2380	0	2319	4	0
1	D	2249	0	2202	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	18	0	24	0	0
3	B	36	0	48	0	0
3	C	6	0	8	0	0
3	D	12	0	16	1	0
4	A	137	0	0	2	0
4	B	148	0	0	1	0
4	C	144	0	0	0	0
4	D	100	0	0	1	0
All	All	9758	0	9044	21	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 1.

All (21) 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:C:164:PHE:HB2	1:C:196:LEU:H	1.58	0.69
1:A:164:PHE:HB2	1:A:196:LEU:H	1.60	0.65
1:B:8:MET:N	4:B:508:HOH:O	2.42	0.53
1:D:70:GLN:HB2	1:B:47:LYS:HD3	1.93	0.51
1:C:9:LYS:NZ	1:C:189:ASP:O	2.44	0.50
1:A:147:ARG:NH2	4:A:512:HOH:O	2.45	0.49
1:C:147:ARG:NH1	1:D:144:GLN:O	2.44	0.49
1:D:12:ILE:HG12	1:D:175:LEU:HD21	1.95	0.49
1:D:91:ARG:HA	1:D:95:LEU:HD12	1.94	0.48
1:A:91:ARG:HA	1:A:95:LEU:HD12	1.97	0.47
1:C:164:PHE:HZ	1:C:225:LEU:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:LYS:HZ1	3:D:403:GOL:H11	1.81	0.45
1:A:50:CYS:SG	4:A:620:HOH:O	2.53	0.44
1:D:269:ILE:O	1:D:270:SER:HB3	2.17	0.44
1:B:169:GLY:HA2	1:B:213:ALA:HB3	2.01	0.43
1:D:126:PRO:HG3	1:D:220:GLN:HA	2.01	0.43
1:D:91:ARG:HB2	1:D:252:MET:HE3	2.01	0.42
1:D:263:ARG:HG2	1:D:284:GLU:HB3	2.02	0.42
1:D:115:TRP:NE1	1:D:233:CYS:HA	2.34	0.41
1:A:263:ARG:HG2	1:A:284:GLU:HB3	2.03	0.41
1:D:258:LYS:NZ	4:D:507:HOH:O	2.48	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	285/315 (90%)	276 (97%)	9 (3%)	0	100	100
1	B	287/315 (91%)	280 (98%)	7 (2%)	0	100	100
1	C	303/315 (96%)	293 (97%)	9 (3%)	1 (0%)	36	50
1	D	286/315 (91%)	277 (97%)	6 (2%)	3 (1%)	12	20
All	All	1161/1260 (92%)	1126 (97%)	31 (3%)	4 (0%)	36	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	270	SER
1	D	270	SER
1	D	64	MET
1	D	268	VAL

### 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	247/274 (90%)	246 (100%)	1 (0%)	84	92
1	B	251/274 (92%)	249 (99%)	2 (1%)	73	86
1	C	260/274 (95%)	256 (98%)	4 (2%)	57	77
1	D	246/274 (90%)	244 (99%)	2 (1%)	73	86
All	All	1004/1096 (92%)	995 (99%)	9 (1%)	70	85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	64	MET
1	C	125	MET
1	C	269	ILE
1	C	270	SER
1	D	64	MET
1	D	269	ILE
1	A	64	MET
1	B	64	MET
1	B	125	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	135	ASN
1	D	19	HIS
1	D	135	ASN
1	D	144	GLN
1	A	11	GLN
1	A	144	GLN
1	A	292	ASN
1	B	135	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z  > 2$
3	GOL	B	404	-	5,5,5	0.91	0	5,5,5	1.07	0
3	GOL	D	402	-	5,5,5	0.96	0	5,5,5	1.08	0
3	GOL	B	407	-	5,5,5	0.92	0	5,5,5	1.05	0
3	GOL	B	402	-	5,5,5	0.92	0	5,5,5	1.07	0
3	GOL	A	403	-	5,5,5	0.93	0	5,5,5	1.04	0
3	GOL	B	403	-	5,5,5	0.91	0	5,5,5	1.09	0
3	GOL	A	402	-	5,5,5	0.95	0	5,5,5	1.08	0
3	GOL	D	403	-	5,5,5	0.97	0	5,5,5	1.04	0
3	GOL	A	404	-	5,5,5	0.98	0	5,5,5	1.03	0
3	GOL	B	405	-	5,5,5	0.93	0	5,5,5	1.08	0
3	GOL	B	406	-	5,5,5	0.92	0	5,5,5	1.10	0
3	GOL	C	402	-	5,5,5	0.94	0	5,5,5	1.09	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
3	GOL	B	404	-	-	3/4/4/4	-
3	GOL	D	402	-	-	0/4/4/4	-
3	GOL	B	407	-	-	2/4/4/4	-
3	GOL	B	402	-	-	0/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-
3	GOL	B	403	-	-	0/4/4/4	-
3	GOL	A	402	-	-	0/4/4/4	-
3	GOL	D	403	-	-	2/4/4/4	-
3	GOL	A	404	-	-	0/4/4/4	-
3	GOL	B	405	-	-	0/4/4/4	-
3	GOL	B	406	-	-	0/4/4/4	-
3	GOL	C	402	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	403	GOL	O1-C1-C2-C3
3	B	404	GOL	O1-C1-C2-C3
3	B	407	GOL	C1-C2-C3-O3
3	B	404	GOL	O1-C1-C2-O2
3	C	402	GOL	O1-C1-C2-O2
3	D	403	GOL	O1-C1-C2-O2
3	B	404	GOL	C1-C2-C3-O3
3	B	407	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	403	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	287/315 (91%)	-0.09	4 (1%) 73 69	23, 32, 48, 69	0
1	B	289/315 (91%)	-0.12	3 (1%) 79 76	21, 31, 45, 80	0
1	C	305/315 (96%)	-0.00	9 (2%) 52 48	23, 32, 49, 69	0
1	D	288/315 (91%)	0.19	6 (2%) 63 59	24, 38, 60, 86	0
All	All	1169/1260 (92%)	-0.01	22 (1%) 66 62	21, 33, 53, 86	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	ILE	5.3
1	B	296	ASN	3.2
1	C	-4	ASP	3.1
1	C	269	ILE	3.0
1	C	-2	GLY	3.0
1	A	288	GLU	2.9
1	D	269	ILE	2.8
1	C	270	SER	2.7
1	D	296	ASN	2.7
1	D	220	GLN	2.6
1	A	270	SER	2.6
1	C	42	HIS	2.5
1	D	18	ASP	2.5
1	D	217	ALA	2.5
1	C	70	GLN	2.4
1	C	43	GLU	2.3
1	C	166	GLU	2.3
1	B	70	GLN	2.2
1	C	217	ALA	2.2
1	B	295	LEU	2.1
1	A	42	HIS	2.1
1	D	183	GLY	2.0



## 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 oligosaccharides 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( $\text{\AA}^2$ )	Q<0.9
3	GOL	D	403	6/6	0.52	0.24	41,44,51,51	0
3	GOL	B	407	6/6	0.58	0.24	42,46,49,49	0
3	GOL	B	406	6/6	0.61	0.27	43,43,45,51	0
3	GOL	A	404	6/6	0.74	0.17	43,46,49,50	0
3	GOL	C	402	6/6	0.75	0.15	37,48,50,54	0
3	GOL	B	404	6/6	0.76	0.14	34,44,48,49	0
3	GOL	A	403	6/6	0.84	0.17	36,39,42,47	0
3	GOL	B	405	6/6	0.84	0.13	38,41,42,44	0
3	GOL	A	402	6/6	0.85	0.11	38,40,44,47	0
3	GOL	B	402	6/6	0.86	0.09	39,40,45,49	0
3	GOL	D	402	6/6	0.93	0.09	28,35,37,45	0
3	GOL	B	403	6/6	0.93	0.09	26,33,35,42	0
2	CO	D	401	1/1	0.98	0.15	73,73,73,73	0
2	CO	B	401	1/1	0.99	0.12	50,50,50,50	0
2	CO	A	401	1/1	1.00	0.01	31,31,31,31	0
2	CO	C	401	1/1	1.00	0.05	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.