



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2020 – 12:30 am BST

PDB ID : 5LUN  
Title : Ethylene Forming Enzyme from *Pseudomonas syringae* pv. *phaseolicola* - P1 ultra-high resolution crystal form in complex with iron, N-oxalylglycine and arginine  
Authors : McDonough, M.A.; Zhang, Z.; Schofield, C.J.  
Deposited on : 2016-09-09  
Resolution : 1.08 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

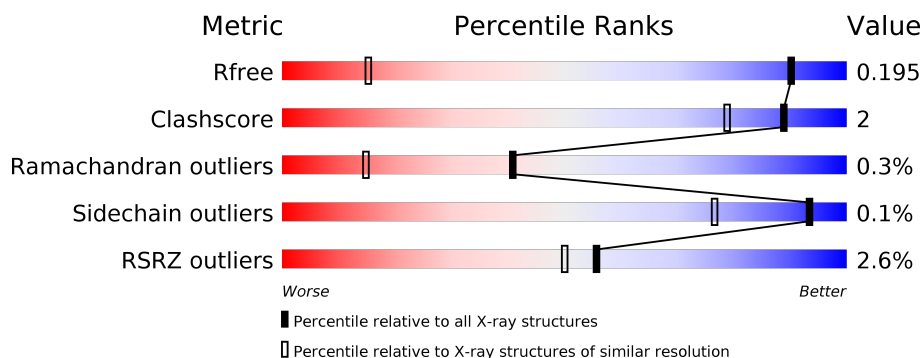
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.08 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	1386 (1.12-1.04)
Clashscore	141614	1021 (1.10-1.06)
Ramachandran outliers	138981	1381 (1.12-1.04)
Sidechain outliers	138945	1379 (1.12-1.04)
RSRZ outliers	127900	1359 (1.12-1.04)

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	352	<div> <div>%</div> <div> </div> <div>92%</div> <div>• •</div> </div>
1	B	352	<div> <div>3%</div> <div> </div> <div>92%</div> <div>• •</div> </div>
1	C	352	<div> <div>2%</div> <div> </div> <div>93%</div> <div>• •</div> </div>
1	D	352	<div> <div>4%</div> <div> </div> <div>93%</div> <div>• •</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13304 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 2-oxoglutarate-dependent ethylene/succinate-forming enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	13	0
			2744	1754	467	507	16			
1	B	339	Total	C	N	O	S	0	12	0
			2737	1749	464	509	15			
1	C	340	Total	C	N	O	S	0	11	0
			2735	1748	468	503	16			
1	D	341	Total	C	N	O	S	0	12	0
			2756	1757	471	512	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P32021
A	0	THR	-	expression tag	UNP P32021
A	1	ASN	-	expression tag	UNP P32021
B	-1	GLY	-	expression tag	UNP P32021
B	0	THR	-	expression tag	UNP P32021
B	1	ASN	-	expression tag	UNP P32021
C	-1	GLY	-	expression tag	UNP P32021
C	0	THR	-	expression tag	UNP P32021
C	1	ASN	-	expression tag	UNP P32021
D	-1	GLY	-	expression tag	UNP P32021
D	0	THR	-	expression tag	UNP P32021
D	1	ASN	-	expression tag	UNP P32021

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

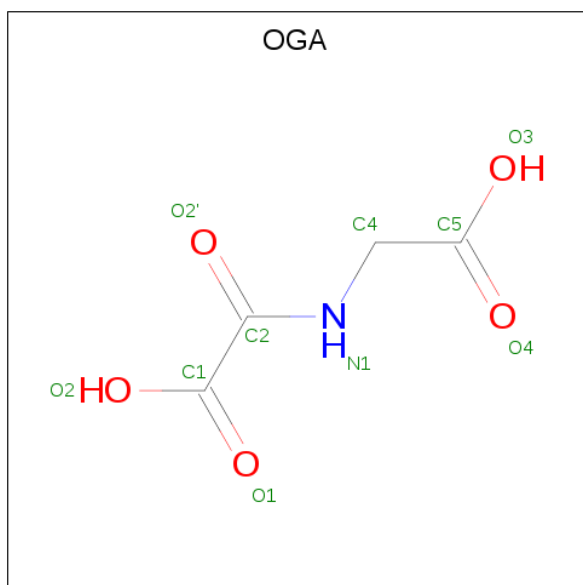
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		

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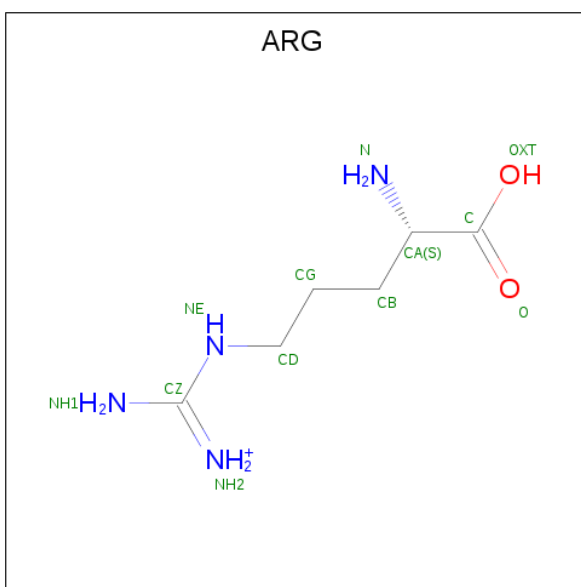
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

- Molecule 3 is N-OXALYLGLYCINE (three-letter code: OGA) (formula:  $C_4H_5NO_5$ ).



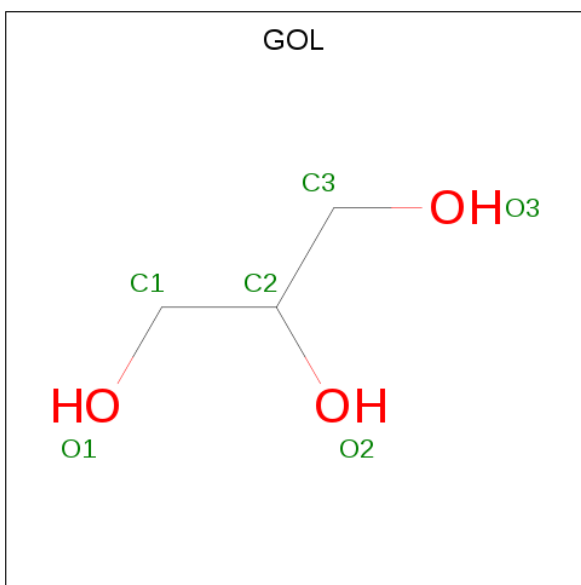
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			20	8	2	10		
3	B	1	Total	C	N	O	0	1
			20	8	2	10		
3	C	1	Total	C	N	O	0	1
			20	8	2	10		
3	D	1	Total	C	N	O	0	1
			20	8	2	10		

- Molecule 4 is ARGinine (three-letter code: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			24	12	8	4		
4	B	1	Total	C	N	O	0	1
			24	12	8	4		
4	C	1	Total	C	N	O	0	1
			24	12	8	4		
4	D	1	Total	C	N	O	0	1
			24	12	8	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

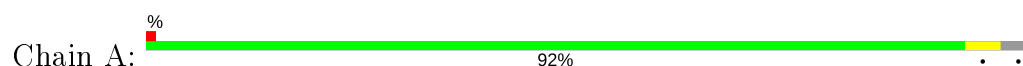
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	573	Total	O	0	31
			594	594		
6	B	491	Total	O	0	23
			510	510		
6	C	489	Total	O	0	28
			512	512		
6	D	497	Total	O	0	20
			512	512		

### 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.

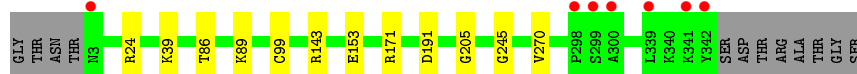
- Molecule 1: 2-oxoglutarate-dependent ethylene/succinate-forming enzyme



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.84Å 79.06Å 97.86Å 91.56° 93.42° 100.80°	Depositor
Resolution (Å)	77.60 – 1.08 77.60 – 1.08	Depositor EDS
% Data completeness (in resolution range)	92.1 (77.60-1.08) 92.4 (77.60-1.08)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 1.08Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.162 , 0.185 0.173 , 0.195	Depositor DCC
$R_{free}$ test set	29238 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.7	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	13304	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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, OGA, FE

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	0.61	0/2850	0.73	1/3867 (0.0%)
1	B	0.59	0/2848	0.71	3/3866 (0.1%)
1	C	0.55	0/2840	0.67	2/3855 (0.1%)
1	D	0.52	0/2864	0.67	0/3888
All	All	0.57	0/11402	0.70	6/15476 (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
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	143	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	143	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	253	ASP	CB-CG-OD1	5.88	123.59	118.30
1	C	143	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	72	ASP	CB-CG-OD1	5.25	123.02	118.30
1	B	91	ASP	CB-CG-OD2	-5.13	113.68	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191[A]	ASP	Peptide
1	B	191[A]	ASP	Peptide
1	C	191[A]	ASP	Peptide
1	D	191[A]	ASP	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	2744	0	2681	11	0
1	B	2737	0	2670	7	0
1	C	2735	0	2667	11	0
1	D	2756	0	2689	10	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	20	0	6	2	0
3	B	20	0	6	1	0
3	C	20	0	6	2	0
3	D	20	0	6	2	0
4	A	24	0	24	2	0
4	B	24	0	24	0	0
4	C	24	0	24	2	0
4	D	24	0	24	0	0
5	A	6	0	8	1	0
5	B	18	0	24	0	0
6	A	594	0	0	1	0
6	B	510	0	0	3	0
6	C	512	0	0	6	0
6	D	512	0	0	8	1
All	All	13304	0	10859	41	1

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 2.

All (41) 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:D:332:ARG:NH1	6:D:658[B]:HOH:O	2.24	0.68
1:C:153:GLU:OE2	6:C:501:HOH:O	2.15	0.65
1:B:161:ASP:O	6:B:501:HOH:O	2.15	0.64
1:A:76:SER:HG	1:A:99[A]:CYS:HG	1.36	0.64
1:C:86:THR:HG1	4:C:403[A]:ARG:N	2.00	0.60
1:A:86:THR:HG1	4:A:403[A]:ARG:N	1.99	0.60
1:C:86:THR:HG1	4:C:403[B]:ARG:N	1.98	0.60
1:A:27[A]:ILE:HD11	1:A:148:THR:HG23	1.85	0.59
1:A:86:THR:HG1	4:A:403[B]:ARG:N	2.00	0.57
1:D:28[B]:GLN:HG2	6:D:747:HOH:O	2.07	0.55
1:D:135:GLU:OE1	6:D:501:HOH:O	2.18	0.53
1:D:16[B]:CYS:HB2	6:D:891[B]:HOH:O	2.09	0.52
1:C:171:ARG:NE	3:C:402[B]:OGA:O2	2.31	0.51
1:A:74:THR:OG1	1:A:99[A]:CYS:SG	2.70	0.50
1:B:157:ASN:ND2	6:B:507:HOH:O	2.44	0.50
3:A:402[A]:OGA:H4C2	6:A:1533:HOH:O	2.11	0.49
1:B:24:ARG:NH2	1:B:153[A]:GLU:OE2	2.46	0.49
1:C:24:ARG:NH2	6:C:504[A]:HOH:O	2.34	0.48
3:D:402[A]:OGA:H4C2	6:D:623:HOH:O	2.13	0.48
1:D:28[B]:GLN:HG3	6:D:540:HOH:O	2.14	0.47
1:C:153:GLU:HG2	6:C:504[A]:HOH:O	2.15	0.47
1:A:191[B]:ASP:OD2	1:A:196:VAL:HG21	2.14	0.46
1:B:24:ARG:NH1	6:B:514:HOH:O	2.48	0.46
1:D:8[B]:GLU:OE2	1:D:39[B]:LYS:NZ	2.40	0.46
1:A:270:VAL:HG21	3:A:402[B]:OGA:H4C1	1.98	0.46
1:D:49:GLN:NE2	6:D:505:HOH:O	2.46	0.46
1:A:297:GLU:C	1:A:299:SER:HA	2.36	0.45
1:C:39[B]:LYS:HE2	1:C:245:GLY:O	2.16	0.45
1:A:76:SER:OG	1:A:99[A]:CYS:SG	2.55	0.45
1:B:174:ARG:NH2	1:B:276:GLU:OE1	2.46	0.45
1:C:270:VAL:HG21	3:C:402[B]:OGA:H4C1	2.00	0.44
1:C:99[B]:CYS:SG	6:C:604:HOH:O	2.61	0.44
1:C:24:ARG:NH1	6:C:505:HOH:O	2.50	0.42
1:B:336:LEU:O	1:B:340:LYS:HG3	2.19	0.42
1:D:270:VAL:HG21	3:D:402[B]:OGA:H4C1	2.02	0.41
1:D:75:TYR:HB2	6:D:553[B]:HOH:O	2.20	0.41
1:B:270:VAL:HG21	3:B:402[B]:OGA:H4C1	2.02	0.41
1:C:89[A]:LYS:NZ	6:C:506:HOH:O	2.39	0.41
1:A:120:PRO:CA	5:A:404:GOL:H31	2.50	0.41
1:D:287:ASN:OD1	1:D:289:GLU:HG2	2.21	0.40
1:A:255[A]:LEU:HD23	1:A:255[A]:LEU:HA	1.98	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:793:HOH:O	6:D:906:HOH:O[1_655]	2.01	0.19

## 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	347/352 (99%)	341 (98%)	5 (1%)	1 (0%)	41	15
1	B	348/352 (99%)	342 (98%)	5 (1%)	1 (0%)	41	15
1	C	349/352 (99%)	343 (98%)	5 (1%)	1 (0%)	41	15
1	D	351/352 (100%)	342 (97%)	8 (2%)	1 (0%)	41	15
All	All	1395/1408 (99%)	1368 (98%)	23 (2%)	4 (0%)	41	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	GLY
1	B	205	GLY
1	C	205	GLY
1	D	205	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/301 (99%)	297 (100%)	0	100	100
1	B	297/301 (99%)	297 (100%)	0	100	100
1	C	294/301 (98%)	294 (100%)	0	100	100
1	D	299/301 (99%)	298 (100%)	1 (0%)	92	75
All	All	1187/1204 (99%)	1186 (100%)	1 (0%)	93	76

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	336	LEU

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 ⓘ

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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	OGA	C	402[B]	2	3,9,9	3.42	2 (66%)	4,11,11	1.93	1 (25%)
5	GOL	A	404	-	5,5,5	0.31	0	5,5,5	0.71	0
3	OGA	B	402[A]	2	3,9,9	3.39	2 (66%)	4,11,11	2.10	1 (25%)
3	OGA	D	402[B]	2	3,9,9	3.23	1 (33%)	4,11,11	1.95	1 (25%)
3	OGA	B	402[B]	2	3,9,9	3.05	2 (66%)	4,11,11	1.21	0
5	GOL	B	405[A]	-	5,5,5	0.33	0	5,5,5	0.43	0
3	OGA	D	402[A]	2	3,9,9	3.38	2 (66%)	4,11,11	3.49	1 (25%)
5	GOL	B	405[B]	-	5,5,5	0.33	0	5,5,5	0.45	0
3	OGA	A	402[B]	2	3,9,9	2.86	1 (33%)	4,11,11	0.97	0
3	OGA	A	402[A]	2	3,9,9	3.25	2 (66%)	4,11,11	3.43	1 (25%)
3	OGA	C	402[A]	2	3,9,9	3.35	2 (66%)	4,11,11	3.04	1 (25%)
5	GOL	B	404	-	5,5,5	0.33	0	5,5,5	0.18	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
3	OGA	C	402[B]	2	-	1/3/9/9	-
5	GOL	A	404	-	-	4/4/4/4	-
3	OGA	B	402[A]	2	-	0/3/9/9	-
3	OGA	D	402[B]	2	-	1/3/9/9	-
3	OGA	B	402[B]	2	-	1/3/9/9	-
5	GOL	B	405[A]	-	-	1/4/4/4	-
3	OGA	D	402[A]	2	-	0/3/9/9	-
5	GOL	B	405[B]	-	-	0/4/4/4	-
3	OGA	A	402[B]	2	-	1/3/9/9	-
3	OGA	A	402[A]	2	-	0/3/9/9	-
3	OGA	C	402[A]	2	-	0/3/9/9	-
5	GOL	B	404	-	-	2/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402[B]	OGA	C2-N1	5.51	1.45	1.33
3	D	402[A]	OGA	C2-N1	5.39	1.45	1.33
3	B	402[A]	OGA	C2-N1	5.37	1.45	1.33
3	C	402[A]	OGA	C2-N1	5.25	1.45	1.33
3	D	402[B]	OGA	C2-N1	5.23	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402[A]	OGA	C2-N1	5.14	1.45	1.33
3	A	402[B]	OGA	C2-N1	4.57	1.43	1.33
3	B	402[B]	OGA	C2-N1	4.53	1.43	1.33
3	C	402[A]	OGA	O2'-C2	-2.44	1.18	1.23
3	B	402[A]	OGA	O2'-C2	-2.37	1.18	1.23
3	D	402[A]	OGA	O2'-C2	-2.31	1.18	1.23
3	A	402[A]	OGA	O2'-C2	-2.28	1.18	1.23
3	B	402[B]	OGA	O2'-C2	-2.16	1.18	1.23
3	C	402[B]	OGA	O2'-C2	-2.04	1.19	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402[A]	OGA	C1-C2-N1	6.70	122.26	115.60
3	A	402[A]	OGA	C1-C2-N1	6.53	122.09	115.60
3	C	402[A]	OGA	C1-C2-N1	5.70	121.26	115.60
3	B	402[A]	OGA	C1-C2-N1	3.91	119.48	115.60
3	D	402[B]	OGA	C1-C2-N1	3.74	119.32	115.60
3	C	402[B]	OGA	C1-C2-N1	3.72	119.30	115.60

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404	GOL	O1-C1-C2-O2
5	A	404	GOL	O1-C1-C2-C3
5	B	404	GOL	O1-C1-C2-C3
5	B	404	GOL	O1-C1-C2-O2
5	A	404	GOL	C1-C2-C3-O3
3	A	402[B]	OGA	C5-C4-N1-C2
3	B	402[B]	OGA	C5-C4-N1-C2
3	C	402[B]	OGA	C5-C4-N1-C2
3	D	402[B]	OGA	C5-C4-N1-C2
5	A	404	GOL	O2-C2-C3-O3
5	B	405[A]	GOL	O1-C1-C2-C3

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402[B]	OGA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	404	GOL	1	0
3	D	402[B]	OGA	1	0
3	B	402[B]	OGA	1	0
3	D	402[A]	OGA	1	0
3	A	402[B]	OGA	1	0
3	A	402[A]	OGA	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	338/352 (96%)	-0.31	4 (1%) 79 74	8, 13, 27, 56	0
1	B	339/352 (96%)	-0.16	10 (2%) 51 46	9, 16, 38, 63	0
1	C	340/352 (96%)	-0.24	7 (2%) 63 56	13, 18, 34, 73	0
1	D	341/352 (96%)	-0.06	14 (4%) 37 31	12, 19, 40, 65	0
All	All	1358/1408 (96%)	-0.19	35 (2%) 56 50	8, 17, 38, 73	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	THR	6.3
1	A	2	THR	6.1
1	C	341	LYS	6.0
1	C	298	PRO	6.0
1	D	298	PRO	5.9
1	B	339	LEU	5.4
1	D	1	ASN	5.1
1	D	299	SER	4.5
1	D	113	TRP	4.5
1	D	182	LEU	4.3
1	D	339	LEU	4.3
1	D	2	THR	4.2
1	B	331	ASN	4.1
1	D	336	LEU	3.8
1	A	3	ASN	3.7
1	B	1	ASN	3.6
1	D	104	VAL	3.6
1	C	299	SER	3.5
1	B	298	PRO	3.1
1	B	338	ASP	3.0
1	C	342	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	181	THR	2.9
1	B	301	ASN	2.9
1	D	338	ASP	2.8
1	A	223	PRO	2.8
1	A	299	SER	2.5
1	C	300	ALA	2.5
1	D	107	GLN	2.4
1	C	339	LEU	2.4
1	B	327	ILE	2.3
1	C	3	ASN	2.2
1	B	223	PRO	2.2
1	D	337	GLU	2.2
1	D	340	LYS	2.2
1	B	337	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
5	GOL	B	404	6/6	0.69	0.16	47,50,53,54	0
5	GOL	A	404	6/6	0.74	0.16	47,50,51,54	0
3	OGA	B	402[A]	10/10	0.91	0.16	14,19,21,22	10
3	OGA	B	402[B]	10/10	0.91	0.16	14,17,19,19	10
3	OGA	D	402[B]	10/10	0.91	0.12	22,24,25,25	10
3	OGA	D	402[A]	10/10	0.91	0.12	22,25,27,28	10
5	GOL	B	405[A]	6/6	0.92	0.14	18,26,28,32	6
5	GOL	B	405[B]	6/6	0.92	0.14	20,27,30,32	6
3	OGA	C	402[A]	10/10	0.93	0.11	20,21,23,23	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	OGA	C	402[B]	10/10	0.93	0.11	17,20,22,23	10
4	ARG	D	403[B]	12/12	0.95	0.09	20,22,24,25	12
4	ARG	D	403[A]	12/12	0.95	0.09	19,20,21,21	12
3	OGA	A	402[A]	10/10	0.96	0.10	12,15,17,18	10
4	ARG	B	403[B]	12/12	0.96	0.08	12,15,22,23	12
4	ARG	B	403[A]	12/12	0.96	0.08	10,12,15,15	12
4	ARG	C	403[B]	12/12	0.96	0.08	14,16,20,21	12
4	ARG	C	403[A]	12/12	0.96	0.08	12,13,14,15	12
3	OGA	A	402[B]	10/10	0.96	0.10	11,12,13,14	10
4	ARG	A	403[B]	12/12	0.98	0.06	10,12,15,15	12
4	ARG	A	403[A]	12/12	0.98	0.06	7,10,12,12	12
2	FE	B	401	1/1	1.00	0.03	13,13,13,13	0
2	FE	D	401	1/1	1.00	0.03	20,20,20,20	0
2	FE	A	401	1/1	1.00	0.03	11,11,11,11	0
2	FE	C	401	1/1	1.00	0.03	16,16,16,16	0

## 6.5 Other polymers

There are no such residues in this entry.