wwPDB X-ray Structure Validation Summary Report (i)

May 2, 2023 – 10:35 am BST

PDB ID	:	8CDA
Title	:	Crystal structure of MAB_4123 from Mycobacterium abscessus
Authors	:	Ung, K.L.; Poussineau, C.; Couston, J.; Alsarraf, H.M.A.B.; Blaise, M.
Deposited on	:	2023-01-30
Resolution	:	2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

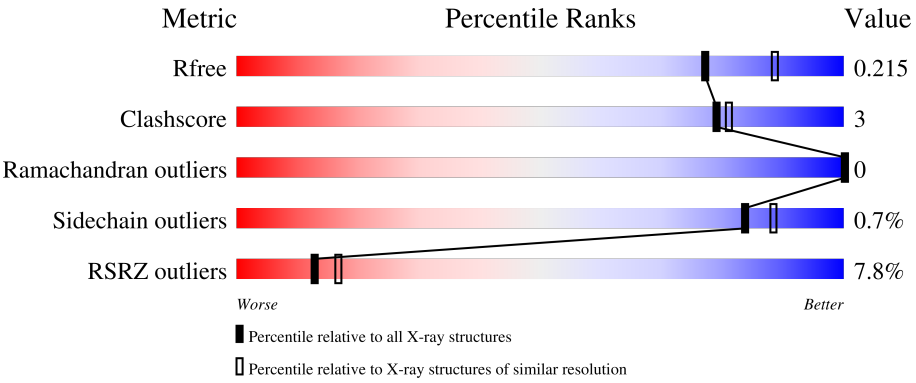
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 >=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 <=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	423	4% 88% 5% 6%
1	B	423	5% 87% 6% 6%
1	C	423	9% 87% 6% 6%
1	D	423	11% 83% 9% 8%
1	E	423	5% 86% 7% 6%

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Mol	Chain	Length	Quality of chain
1	F	423	4% 86% 7% 7%
1	G	423	7% 87% 7% 7%
1	H	423	7% 84% 8% 7%
1	I	423	9% 86% 8% 6%
1	J	423	9% 87% 6% 7%
1	K	423	3% 87% 7% 7%
1	L	423	13% 85% 8% 7%
1	M	423	7% 84% 9% 7%
1	N	423	11% 87% 6% 7%
1	O	423	9% 87% 7% 6%
1	P	423	4% 84% 8% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 51940 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.

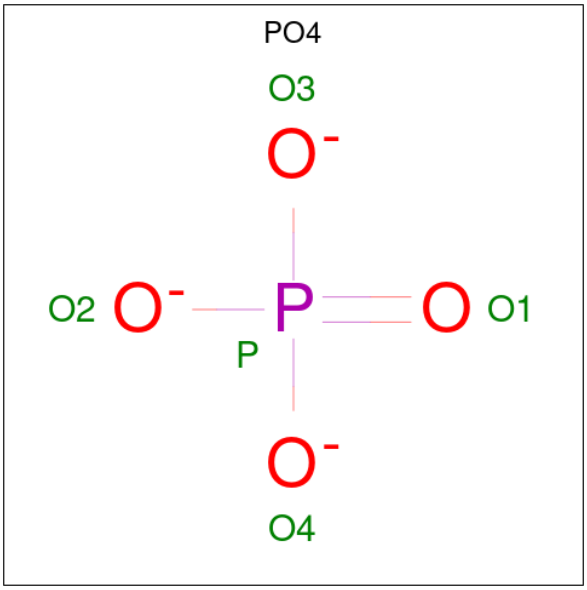
- Molecule 1 is a protein called Probable monooxygenase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	0	0	0
			3062	1916	556	590			
1	B	396	Total	C	N	O	0	1	0
			3068	1919	557	592			
1	C	396	Total	C	N	O	0	0	0
			3062	1916	556	590			
1	D	391	Total	C	N	O	0	0	0
			3017	1888	549	580			
1	E	396	Total	C	N	O	0	3	0
			3091	1932	563	596			
1	F	395	Total	C	N	O	0	0	0
			3052	1910	553	589			
1	G	395	Total	C	N	O	0	0	0
			3052	1910	553	589			
1	H	392	Total	C	N	O	0	0	0
			3029	1896	549	584			
1	I	396	Total	C	N	O	0	0	0
			3058	1913	554	591			
1	J	395	Total	C	N	O	0	1	0
			3061	1915	555	591			
1	K	395	Total	C	N	O	0	0	0
			3052	1910	553	589			
1	L	393	Total	C	N	O	0	0	0
			3038	1902	551	585			
1	M	394	Total	C	N	O	0	0	0
			3043	1905	552	586			
1	N	393	Total	C	N	O	0	1	0
			3045	1904	555	586			
1	O	397	Total	C	N	O	0	1	0
			3074	1922	558	594			
1	P	392	Total	C	N	O	0	0	0
			3029	1897	550	582			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP B1MIH5
B	0	GLY	-	expression tag	UNP B1MIH5
C	0	GLY	-	expression tag	UNP B1MIH5
D	0	GLY	-	expression tag	UNP B1MIH5
E	0	GLY	-	expression tag	UNP B1MIH5
F	0	GLY	-	expression tag	UNP B1MIH5
G	0	GLY	-	expression tag	UNP B1MIH5
H	0	GLY	-	expression tag	UNP B1MIH5
I	0	GLY	-	expression tag	UNP B1MIH5
J	0	GLY	-	expression tag	UNP B1MIH5
K	0	GLY	-	expression tag	UNP B1MIH5
L	0	GLY	-	expression tag	UNP B1MIH5
M	0	GLY	-	expression tag	UNP B1MIH5
N	0	GLY	-	expression tag	UNP B1MIH5
O	0	GLY	-	expression tag	UNP B1MIH5
P	0	GLY	-	expression tag	UNP B1MIH5

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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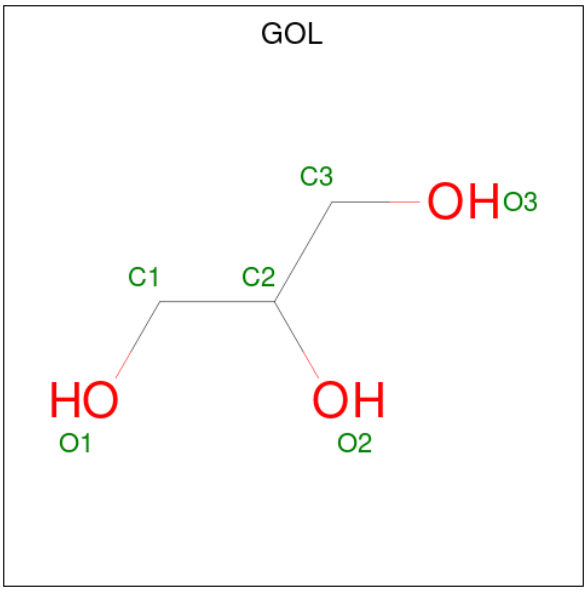
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	G	1	Total O P 5 4 1	0	0
2	H	1	Total O P 5 4 1	0	0
2	I	1	Total O P 5 4 1	0	0
2	J	1	Total O P 5 4 1	0	0
2	K	1	Total O P 5 4 1	0	0
2	L	1	Total O P 5 4 1	0	0
2	M	1	Total O P 5 4 1	0	0
2	N	1	Total O P 5 4 1	0	0
2	O	1	Total O P 5 4 1	0	0
2	P	1	Total O P 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 6 3 3	0	0
3	J	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	L	1	Total C O 6 3 3	0	0
3	M	1	Total C O 6 3 3	0	0
3	P	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	224	Total O 224 224	0	0
4	B	230	Total O 230 230	0	0
4	C	178	Total O 178 178	0	0
4	D	144	Total O 144 144	0	0
4	E	258	Total O 258 258	0	0
4	F	242	Total O 242 242	0	0

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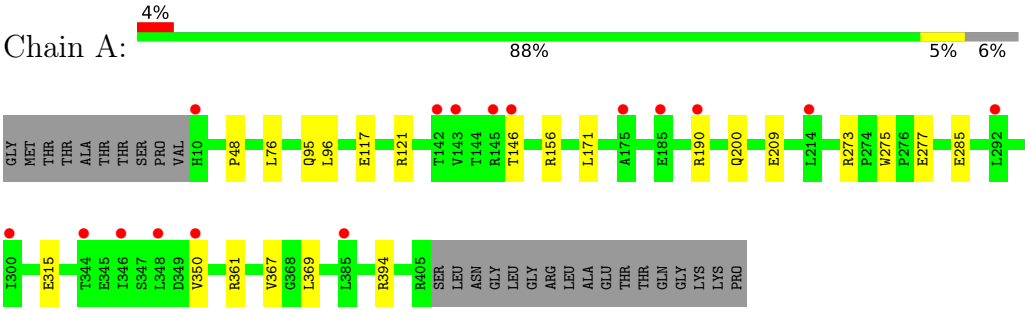
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	223	Total O 223 223	0	0
4	H	179	Total O 179 179	0	0
4	I	150	Total O 150 150	0	0
4	J	157	Total O 157 157	0	0
4	K	188	Total O 188 188	0	0
4	L	122	Total O 122 122	0	0
4	M	149	Total O 149 149	0	0
4	N	184	Total O 184 184	0	0
4	O	185	Total O 185 185	0	0
4	P	173	Total O 173 173	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.

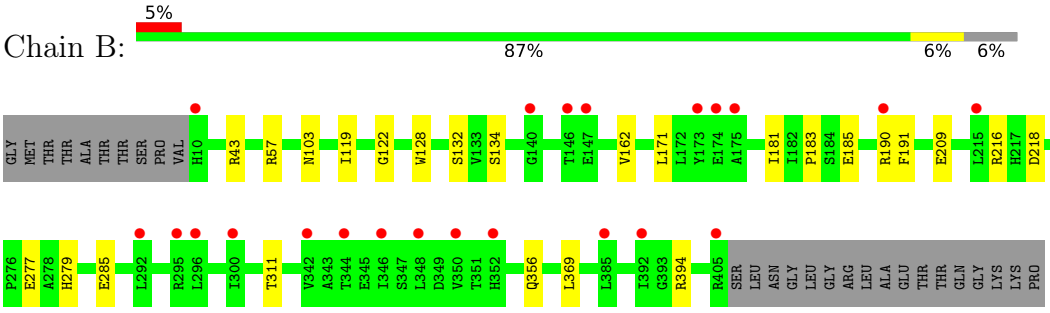
• Molecule 1: Probable monooxygenase

Chain A:



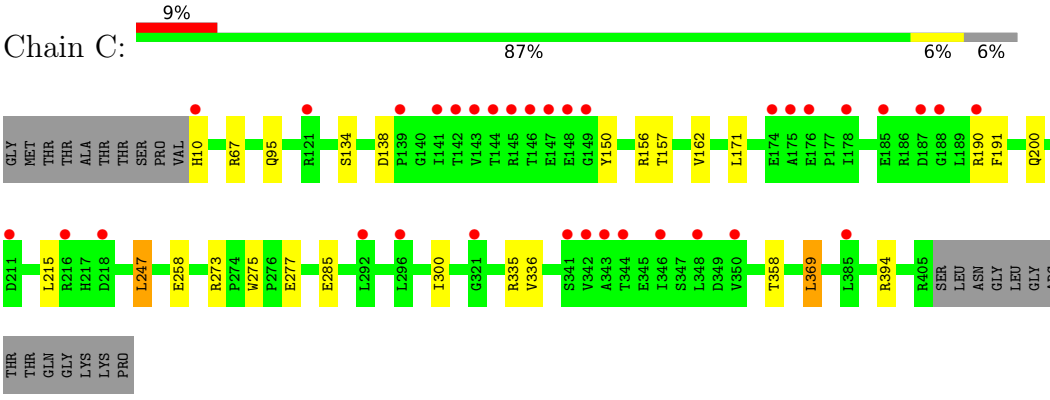
• Molecule 1: Probable monooxygenase

Chain B:



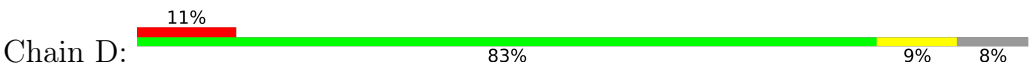
• Molecule 1: Probable monooxygenase

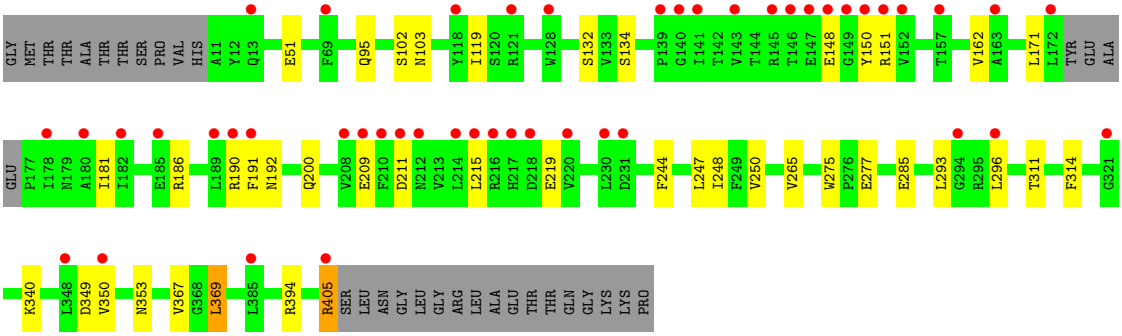
Chain C:



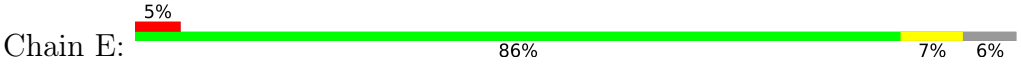
• Molecule 1: Probable monooxygenase

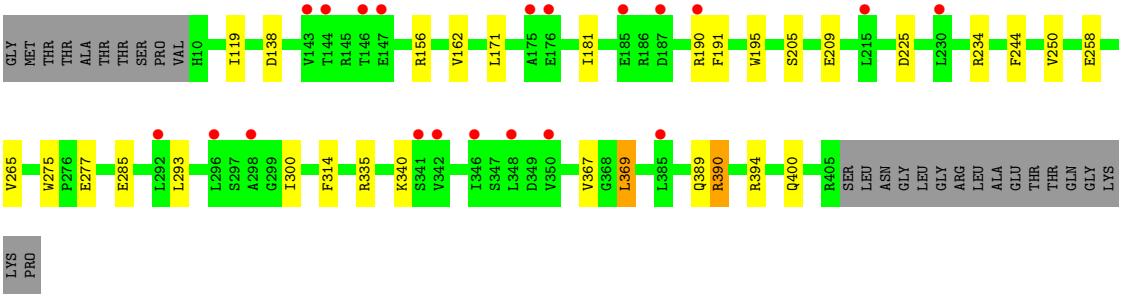
Chain D:



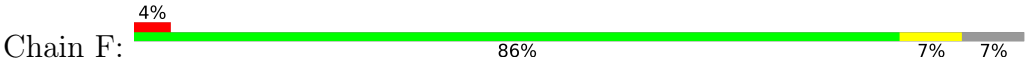


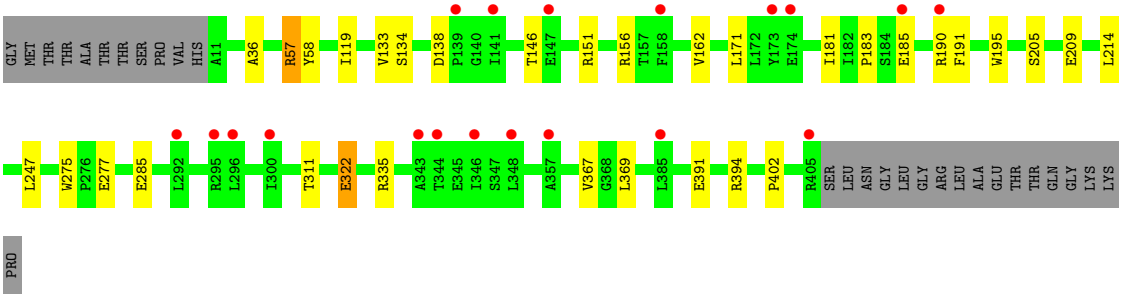
• Molecule 1: Probable monooxygenase



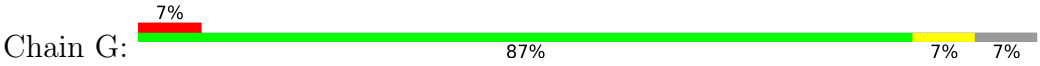


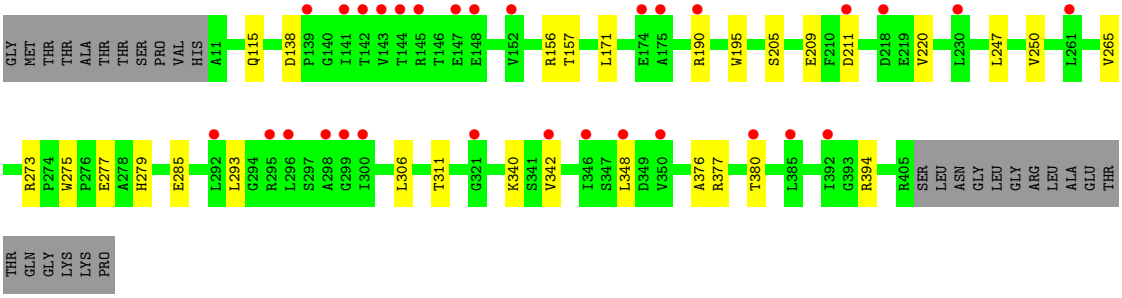
• Molecule 1: Probable monooxygenase





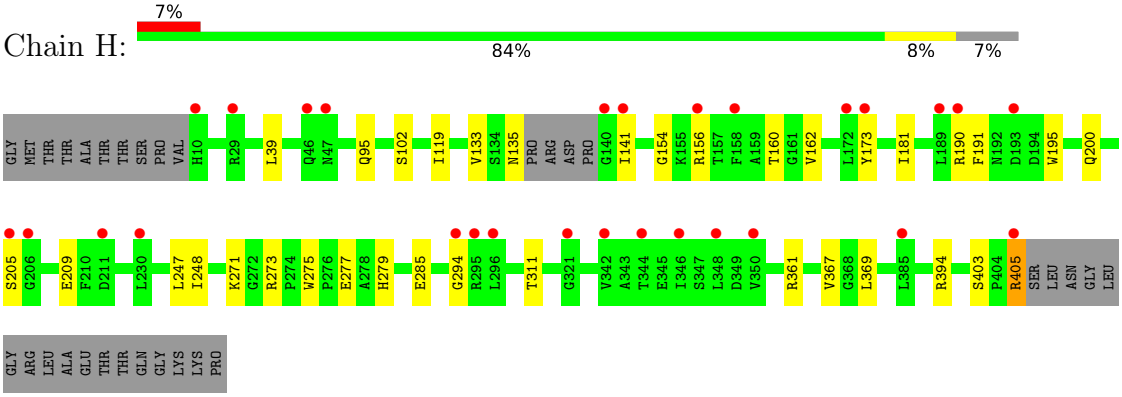
• Molecule 1: Probable monooxygenase





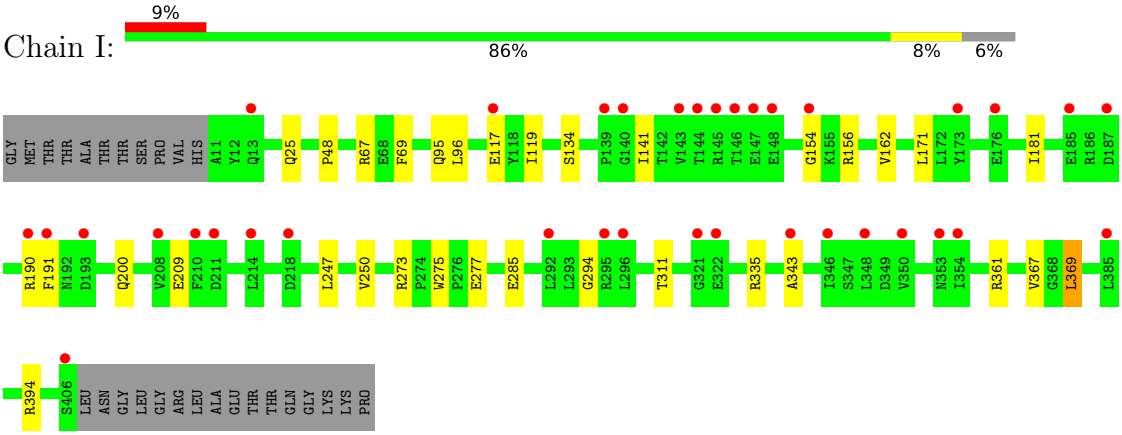
• Molecule 1: Probable monooxygenase

Chain H:



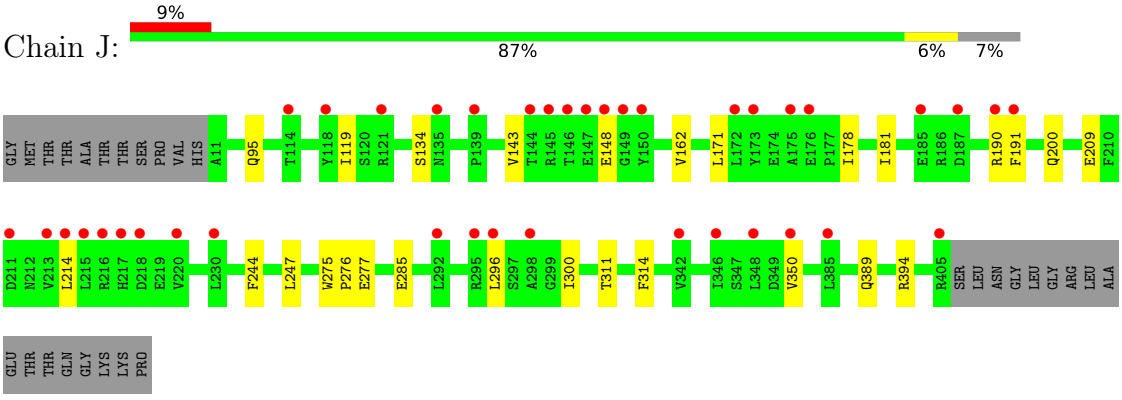
• Molecule 1: Probable monooxygenase

Chain I:



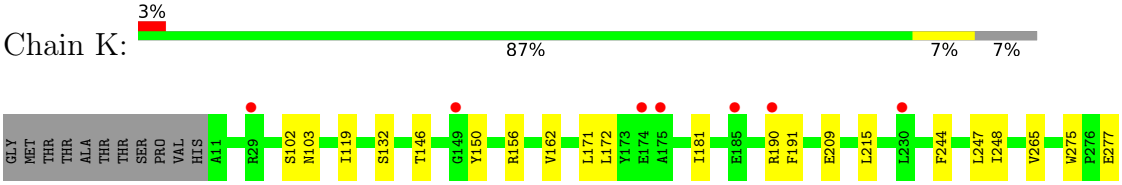
• Molecule 1: Probable monooxygenase

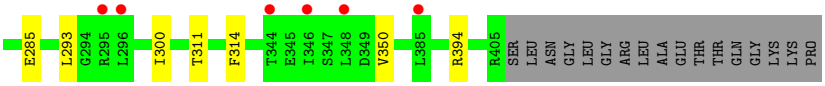
Chain J:



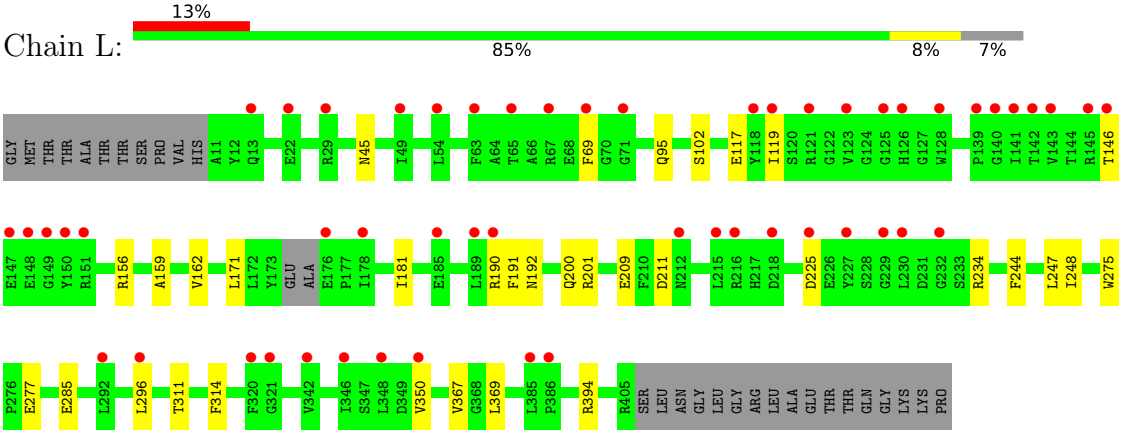
• Molecule 1: Probable monooxygenase

Chain K:

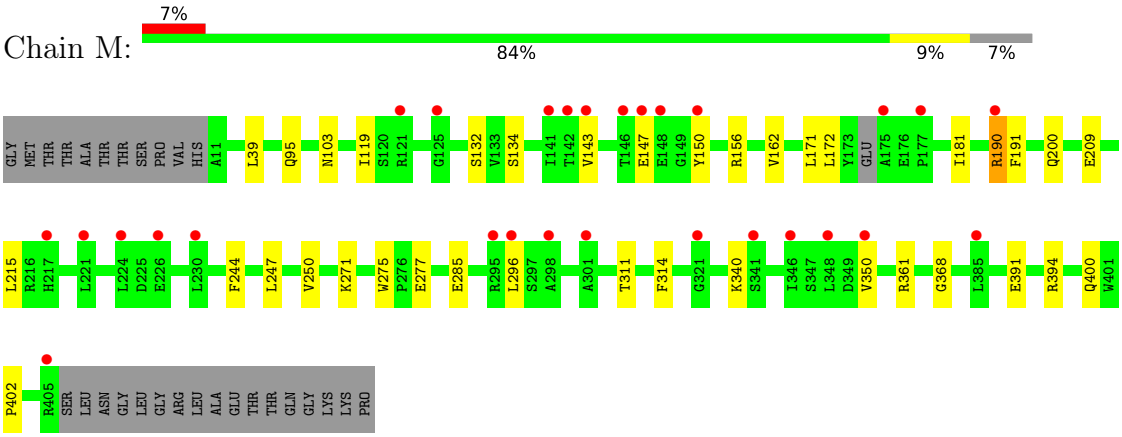




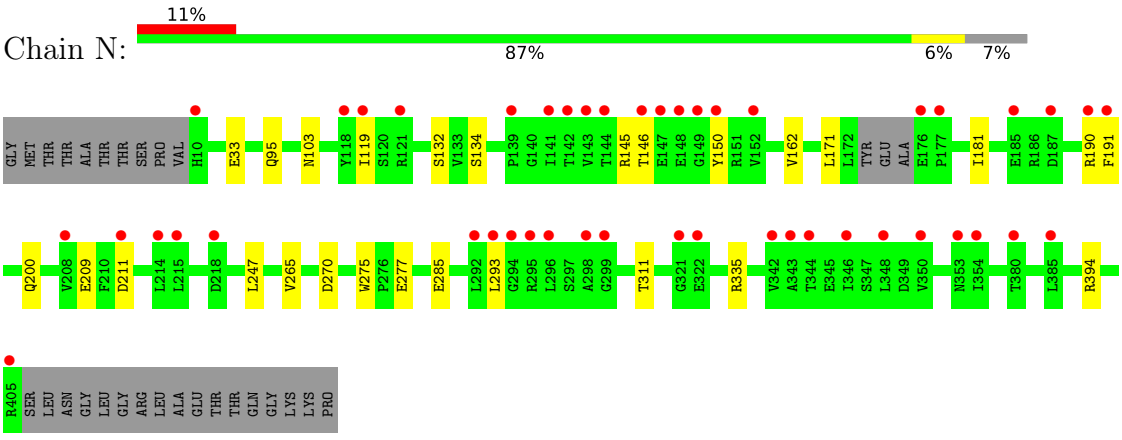
• Molecule 1: Probable monooxygenase



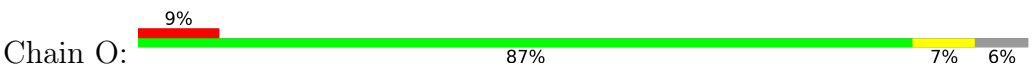
• Molecule 1: Probable monooxygenase

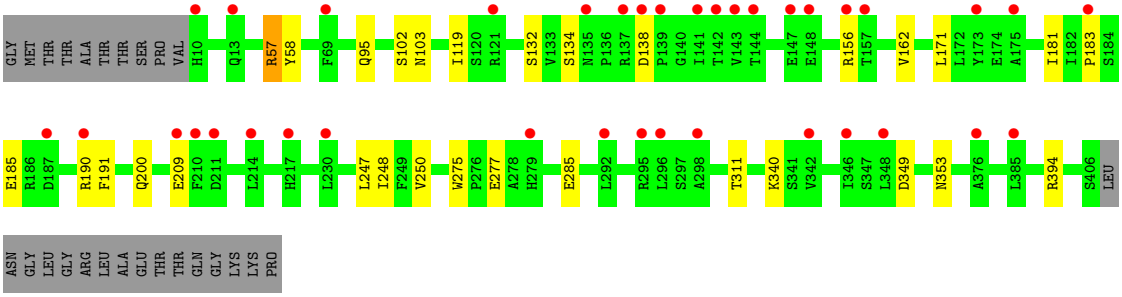


• Molecule 1: Probable monooxygenase

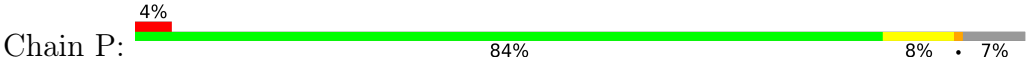


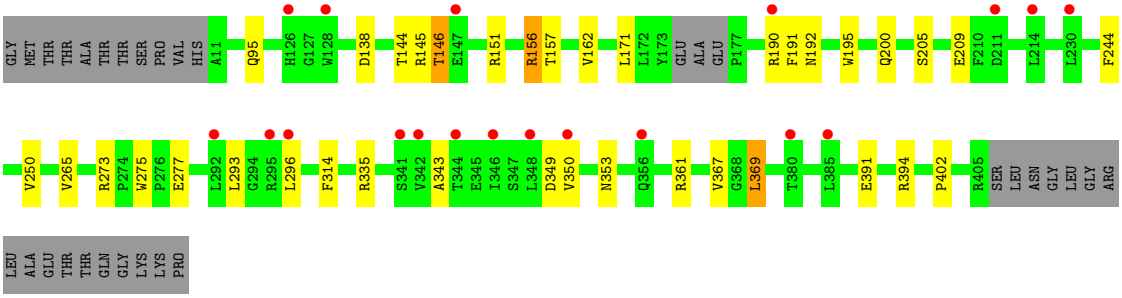
• Molecule 1: Probable monooxygenase





- Molecule 1: Probable monooxygenase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	131.91Å 134.18Å 206.80Å 90.00° 90.68° 90.00°	Depositor
Resolution (Å)	47.94 – 2.10 47.94 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.94-2.10) 98.8 (47.94-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.179 , 0.213 0.182 , 0.215	Depositor DCC
R_{free} test set	2016 reflections (0.49%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -k,-h,-l 0.013 for k,h,-l 0.074 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	51940	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, GOL

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	0.24	0/3128	0.50	0/4256
1	B	0.24	0/3134	0.50	0/4264
1	C	0.24	0/3128	0.50	0/4256
1	D	0.24	0/3080	0.49	0/4188
1	E	0.25	0/3157	0.51	0/4294
1	F	0.25	0/3117	0.51	0/4241
1	G	0.24	0/3117	0.51	0/4241
1	H	0.24	0/3092	0.50	0/4204
1	I	0.24	0/3123	0.50	0/4249
1	J	0.24	0/3126	0.50	0/4253
1	K	0.24	0/3117	0.51	0/4241
1	L	0.24	0/3102	0.49	0/4219
1	M	0.24	0/3107	0.49	0/4226
1	N	0.24	0/3109	0.50	0/4228
1	O	0.24	0/3140	0.50	0/4272
1	P	0.24	0/3093	0.50	0/4206
All	All	0.24	0/49870	0.50	0/67838

There are no bond length outliers.

There are no bond angle outliers.

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	3062	0	2960	12	0
1	B	3068	0	2962	15	0
1	C	3062	0	2960	16	0
1	D	3017	0	2927	24	0
1	E	3091	0	2984	19	0
1	F	3052	0	2953	18	0
1	G	3052	0	2953	17	0
1	H	3029	0	2928	21	0
1	I	3058	0	2958	19	0
1	J	3061	0	2960	16	0
1	K	3052	0	2953	15	0
1	L	3038	0	2941	19	0
1	M	3043	0	2946	20	0
1	N	3045	0	2946	15	0
1	O	3074	0	2967	17	0
1	P	3029	0	2936	20	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	10	0	0	0	0
2	G	5	0	0	1	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
2	M	5	0	0	0	0
2	N	5	0	0	0	0
2	O	5	0	0	0	0
2	P	5	0	0	0	0
3	D	6	0	8	0	0
3	J	6	0	8	0	0
3	K	6	0	8	0	0
3	L	6	0	8	0	0
3	M	6	0	8	0	0
3	P	6	0	8	0	0
4	A	224	0	0	0	0
4	B	230	0	0	2	0
4	C	178	0	0	1	0
4	D	144	0	0	1	0
4	E	258	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	242	0	0	1	0
4	G	223	0	0	0	0
4	H	179	0	0	0	0
4	I	150	0	0	2	0
4	J	157	0	0	0	0
4	K	188	0	0	0	0
4	L	122	0	0	0	0
4	M	149	0	0	0	0
4	N	184	0	0	1	0
4	O	185	0	0	1	0
4	P	173	0	0	0	0
All	All	51940	0	47282	265	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 3.

The worst 5 of 265 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:190:ARG:HB2	1:D:209:GLU:HB2	1.65	0.79
1:I:190:ARG:HB2	1:I:209:GLU:HB2	1.70	0.73
1:B:190:ARG:HB2	1:B:209:GLU:HB2	1.73	0.70
1:I:285:GLU:OE1	1:J:394:ARG:NH1	2.24	0.69
1:E:156:ARG:NH2	1:E:171:LEU:O	2.25	0.69

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	394/423 (93%)	391 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	395/423 (93%)	389 (98%)	6 (2%)	0	100	100
1	C	394/423 (93%)	391 (99%)	3 (1%)	0	100	100
1	D	387/423 (92%)	377 (97%)	10 (3%)	0	100	100
1	E	397/423 (94%)	394 (99%)	3 (1%)	0	100	100
1	F	393/423 (93%)	386 (98%)	7 (2%)	0	100	100
1	G	393/423 (93%)	389 (99%)	4 (1%)	0	100	100
1	H	388/423 (92%)	380 (98%)	8 (2%)	0	100	100
1	I	394/423 (93%)	391 (99%)	3 (1%)	0	100	100
1	J	394/423 (93%)	387 (98%)	7 (2%)	0	100	100
1	K	393/423 (93%)	386 (98%)	7 (2%)	0	100	100
1	L	389/423 (92%)	384 (99%)	5 (1%)	0	100	100
1	M	390/423 (92%)	384 (98%)	6 (2%)	0	100	100
1	N	390/423 (92%)	386 (99%)	4 (1%)	0	100	100
1	O	396/423 (94%)	390 (98%)	6 (2%)	0	100	100
1	P	388/423 (92%)	382 (98%)	6 (2%)	0	100	100
All	All	6275/6768 (93%)	6187 (99%)	88 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	310/331 (94%)	309 (100%)	1 (0%)	92	95
1	B	311/331 (94%)	308 (99%)	3 (1%)	76	82
1	C	310/331 (94%)	306 (99%)	4 (1%)	69	75
1	D	306/331 (92%)	304 (99%)	2 (1%)	84	88
1	E	313/331 (95%)	311 (99%)	2 (1%)	86	90
1	F	309/331 (93%)	305 (99%)	4 (1%)	69	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	309/331 (93%)	308 (100%)	1 (0%)	92 95
1	H	306/331 (92%)	302 (99%)	4 (1%)	69 75
1	I	310/331 (94%)	308 (99%)	2 (1%)	86 90
1	J	310/331 (94%)	310 (100%)	0	100 100
1	K	309/331 (93%)	308 (100%)	1 (0%)	92 95
1	L	308/331 (93%)	307 (100%)	1 (0%)	92 95
1	M	308/331 (93%)	306 (99%)	2 (1%)	86 90
1	N	309/331 (93%)	307 (99%)	2 (1%)	86 90
1	O	312/331 (94%)	311 (100%)	1 (0%)	92 95
1	P	307/331 (93%)	303 (99%)	4 (1%)	69 75
All	All	4947/5296 (93%)	4913 (99%)	34 (1%)	84 88

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	335	ARG
1	O	57	ARG
1	P	335	ARG
1	F	57	ARG
1	E	390	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	212	ASN
1	F	279	HIS

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)

23 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	F	502	-	4,4,4	0.92	0	6,6,6	0.40	0
2	PO4	F	501	-	4,4,4	0.94	0	6,6,6	0.45	0
3	GOL	D	501	-	5,5,5	0.90	0	5,5,5	1.00	0
2	PO4	P	502	-	4,4,4	0.93	0	6,6,6	0.44	0
2	PO4	G	501	-	4,4,4	0.93	0	6,6,6	0.41	0
2	PO4	A	501	-	4,4,4	0.92	0	6,6,6	0.41	0
2	PO4	H	501	-	4,4,4	0.92	0	6,6,6	0.42	0
3	GOL	J	501	-	5,5,5	0.89	0	5,5,5	0.99	0
2	PO4	N	501	-	4,4,4	0.97	0	6,6,6	0.45	0
2	PO4	M	502	-	4,4,4	0.95	0	6,6,6	0.42	0
2	PO4	B	501	-	4,4,4	0.97	0	6,6,6	0.44	0
2	PO4	K	502	-	4,4,4	0.92	0	6,6,6	0.44	0
3	GOL	K	501	-	5,5,5	0.91	0	5,5,5	0.98	0
2	PO4	J	502	-	4,4,4	0.97	0	6,6,6	0.43	0
3	GOL	M	501	-	5,5,5	0.91	0	5,5,5	1.02	0
2	PO4	L	502	-	4,4,4	0.92	0	6,6,6	0.45	0
2	PO4	C	501	-	4,4,4	0.92	0	6,6,6	0.43	0
2	PO4	O	501	-	4,4,4	0.90	0	6,6,6	0.46	0
2	PO4	I	501	-	4,4,4	0.91	0	6,6,6	0.42	0
3	GOL	L	501	-	5,5,5	0.93	0	5,5,5	0.99	0
2	PO4	D	502	-	4,4,4	0.98	0	6,6,6	0.48	0
3	GOL	P	501	-	5,5,5	0.90	0	5,5,5	0.96	0
2	PO4	E	501	-	4,4,4	0.95	0	6,6,6	0.41	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	K	501	-	-	0/4/4/4	-
3	GOL	J	501	-	-	2/4/4/4	-
3	GOL	M	501	-	-	1/4/4/4	-
3	GOL	L	501	-	-	0/4/4/4	-
3	GOL	P	501	-	-	2/4/4/4	-
3	GOL	D	501	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	501	GOL	O1-C1-C2-C3
3	P	501	GOL	O1-C1-C2-C3
3	P	501	GOL	O1-C1-C2-O2
3	J	501	GOL	O1-C1-C2-O2
3	M	501	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	501	PO4	1	0
2	C	501	PO4	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^{th} 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^2)	Q<0.9
1	A	396/423 (93%)	0.12	19 (4%) 30 36	30, 41, 70, 94	0
1	B	396/423 (93%)	0.14	22 (5%) 24 29	31, 42, 68, 110	0
1	C	396/423 (93%)	0.34	36 (9%) 9 12	31, 46, 88, 117	0
1	D	391/423 (92%)	0.53	47 (12%) 4 5	31, 52, 103, 149	0
1	E	396/423 (93%)	0.24	20 (5%) 28 33	26, 39, 70, 97	0
1	F	395/423 (93%)	0.24	19 (4%) 30 36	26, 37, 74, 107	0
1	G	395/423 (93%)	0.33	30 (7%) 13 18	28, 41, 79, 111	0
1	H	392/423 (92%)	0.32	28 (7%) 16 20	28, 45, 81, 106	0
1	I	396/423 (93%)	0.34	36 (9%) 9 12	33, 48, 85, 114	0
1	J	395/423 (93%)	0.39	39 (9%) 7 9	32, 48, 94, 129	0
1	K	395/423 (93%)	0.09	13 (3%) 46 53	31, 45, 74, 115	0
1	L	393/423 (92%)	0.65	53 (13%) 3 4	33, 57, 94, 136	0
1	M	394/423 (93%)	0.39	28 (7%) 16 20	33, 52, 87, 114	0
1	N	393/423 (92%)	0.52	46 (11%) 4 6	31, 45, 89, 127	0
1	O	397/423 (93%)	0.42	37 (9%) 8 11	31, 47, 88, 109	0
1	P	392/423 (92%)	0.34	19 (4%) 30 36	31, 48, 73, 101	0
All	All	6312/6768 (93%)	0.34	492 (7%) 13 17	26, 45, 85, 149	0

The worst 5 of 492 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	146	THR	6.0
1	D	147	GLU	5.9
1	L	321	GLY	5.8
1	M	321	GLY	5.8
1	H	156	ARG	5.8

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 monosaccharides 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^{th} 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^2)	Q<0.9
3	GOL	L	501	6/6	0.84	0.25	65,66,69,69	0
3	GOL	P	501	6/6	0.88	0.23	50,58,61,66	0
3	GOL	M	501	6/6	0.89	0.15	53,57,59,61	0
3	GOL	J	501	6/6	0.90	0.18	51,56,57,62	0
2	PO4	F	502	5/5	0.91	0.29	67,74,90,92	0
3	GOL	D	501	6/6	0.95	0.14	53,54,62,64	0
3	GOL	K	501	6/6	0.96	0.24	45,49,50,52	0
2	PO4	C	501	5/5	0.97	0.10	54,56,60,65	0
2	PO4	K	502	5/5	0.98	0.09	57,63,73,76	0
2	PO4	M	502	5/5	0.98	0.10	56,62,69,71	0
2	PO4	O	501	5/5	0.98	0.11	48,51,56,58	0
2	PO4	P	502	5/5	0.98	0.11	53,53,66,68	0
2	PO4	A	501	5/5	0.98	0.10	43,47,52,54	0
2	PO4	D	502	5/5	0.98	0.13	44,48,62,68	0
2	PO4	E	501	5/5	0.98	0.09	48,50,55,59	0
2	PO4	F	501	5/5	0.98	0.16	41,42,52,53	0
2	PO4	B	501	5/5	0.98	0.15	38,44,51,52	0
2	PO4	G	501	5/5	0.98	0.08	48,55,56,65	0
2	PO4	I	501	5/5	0.99	0.10	49,51,60,66	0
2	PO4	N	501	5/5	0.99	0.13	43,44,50,56	0
2	PO4	J	502	5/5	0.99	0.14	45,45,50,53	0
2	PO4	H	501	5/5	0.99	0.10	42,44,48,50	0
2	PO4	L	502	5/5	0.99	0.12	49,53,59,64	0

6.5 Other polymers (i)

There are no such residues in this entry.