



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:04 PM UTC

PDB ID : 3GYR / pdb_00003gyr
Title : Structure of Phenoxazinone synthase from Streptomyces antibioticus reveals a new type 2 copper center.
Authors : Smith, A.W.; Camara-Artigas, A.; Wang, M.; Francisco, W.A.; Allen, J.P.
Deposited on : 2009-04-05
Resolution : 2.30 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 ⓘ 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 ⓘ](#)) 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

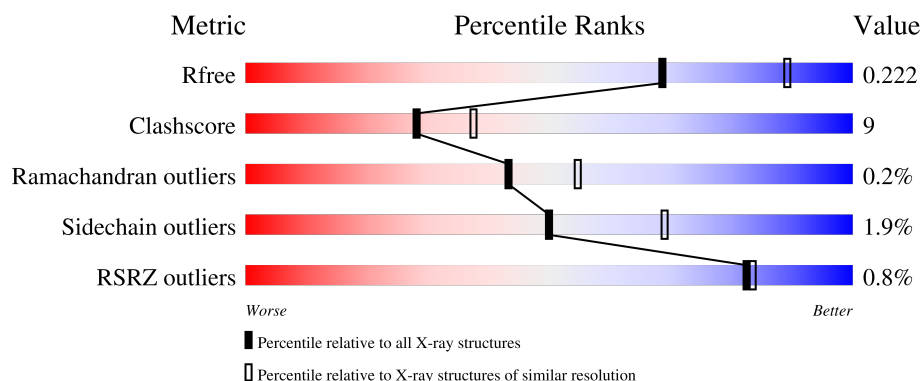
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	612	% 76% 19% • •
1	B	612	% 80% 16% •
1	C	612	84% 11% • •
1	D	612	81% 15% •
1	E	612	% 82% 13% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	612	 79% 16% . .
1	G	612	 79% 16% . .
1	H	612	 77% 17% . .
1	I	612	 75% 20% . .
1	J	612	 79% 15% . .
1	K	612	 77% 18% .
1	L	612	 78% 17% . .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 59241 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 Phenoxazinone synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	B	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	C	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	D	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	E	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	F	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	G	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	H	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	I	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	J	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	K	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	L	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	496	ARG	ALA	engineered mutation	UNP Q53692
B	496	ARG	ALA	engineered mutation	UNP Q53692
C	496	ARG	ALA	engineered mutation	UNP Q53692
D	496	ARG	ALA	engineered mutation	UNP Q53692
E	496	ARG	ALA	engineered mutation	UNP Q53692

Continued on next page...

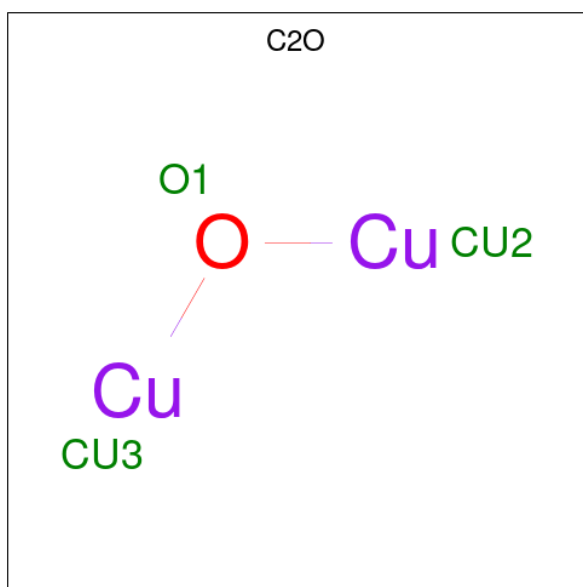
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	496	ARG	ALA	engineered mutation	UNP Q53692
G	496	ARG	ALA	engineered mutation	UNP Q53692
H	496	ARG	ALA	engineered mutation	UNP Q53692
I	496	ARG	ALA	engineered mutation	UNP Q53692
J	496	ARG	ALA	engineered mutation	UNP Q53692
K	496	ARG	ALA	engineered mutation	UNP Q53692
L	496	ARG	ALA	engineered mutation	UNP Q53692

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

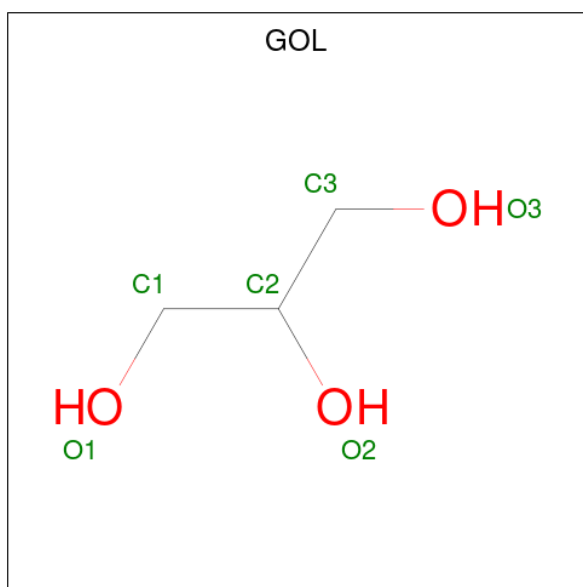
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Cu 3 3	0	0
2	B	3	Total Cu 3 3	0	0
2	C	3	Total Cu 3 3	0	0
2	D	3	Total Cu 3 3	0	0
2	E	3	Total Cu 3 3	0	0
2	F	3	Total Cu 3 3	0	0
2	G	3	Total Cu 3 3	0	0
2	H	3	Total Cu 3 3	0	0
2	I	3	Total Cu 3 3	0	0
2	J	3	Total Cu 3 3	0	0
2	K	3	Total Cu 3 3	0	0
2	L	3	Total Cu 3 3	0	0

- Molecule 3 is CU-O-CU LINKAGE (CCD ID: C2O) (formula: Cu₂O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Cu	O	0	0
			3	2	1		
3	B	1	Total	Cu	O	0	0
			3	2	1		
3	C	1	Total	Cu	O	0	0
			3	2	1		
3	D	1	Total	Cu	O	0	0
			3	2	1		
3	E	1	Total	Cu	O	0	0
			3	2	1		
3	F	1	Total	Cu	O	0	0
			3	2	1		
3	G	1	Total	Cu	O	0	0
			3	2	1		
3	H	1	Total	Cu	O	0	0
			3	2	1		
3	I	1	Total	Cu	O	0	0
			3	2	1		
3	J	1	Total	Cu	O	0	0
			3	2	1		
3	K	1	Total	Cu	O	0	0
			3	2	1		
3	L	1	Total	Cu	O	0	0
			3	2	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

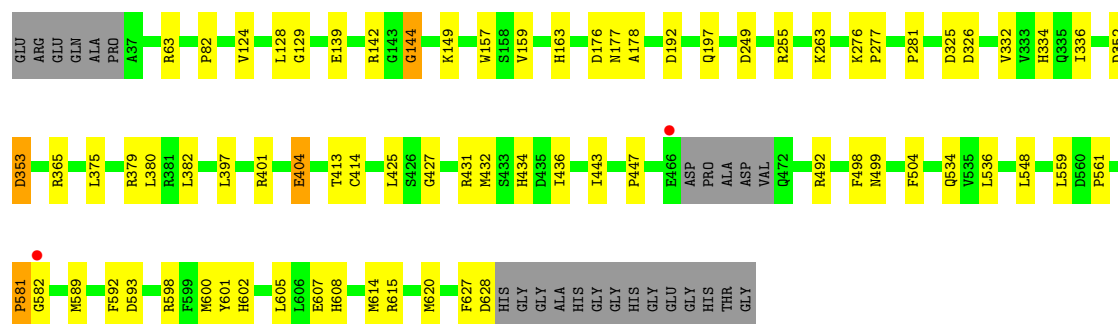


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		
4	K	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

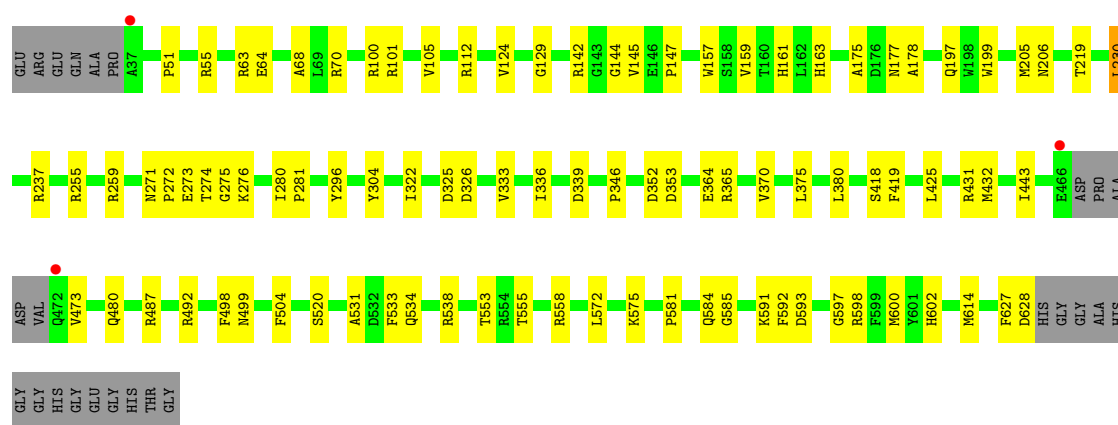
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	354	Total 354	O 354	0	0
5	B	362	Total 362	O 362	0	0
5	C	398	Total 398	O 398	0	0
5	D	386	Total 386	O 386	0	0
5	E	357	Total 357	O 357	0	0
5	F	361	Total 361	O 361	0	0
5	G	359	Total 359	O 359	0	0
5	H	376	Total 376	O 376	0	0
5	I	330	Total 330	O 330	0	0
5	J	388	Total 388	O 388	0	0
5	K	359	Total 359	O 359	0	0
5	L	347	Total 347	O 347	0	0

Chain C:  84% 11% . .



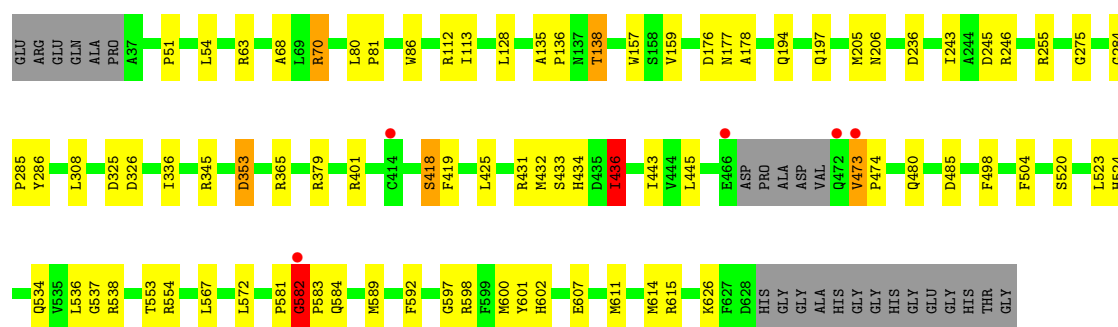
• Molecule 1: Phenoxazinone synthase

Chain D:  81% 15% .



• Molecule 1: Phenoxazinone synthase

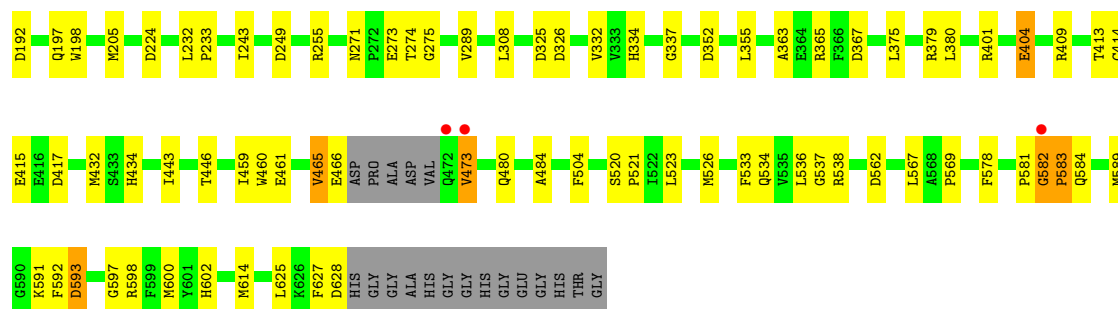
Chain E:  82% 13% . .



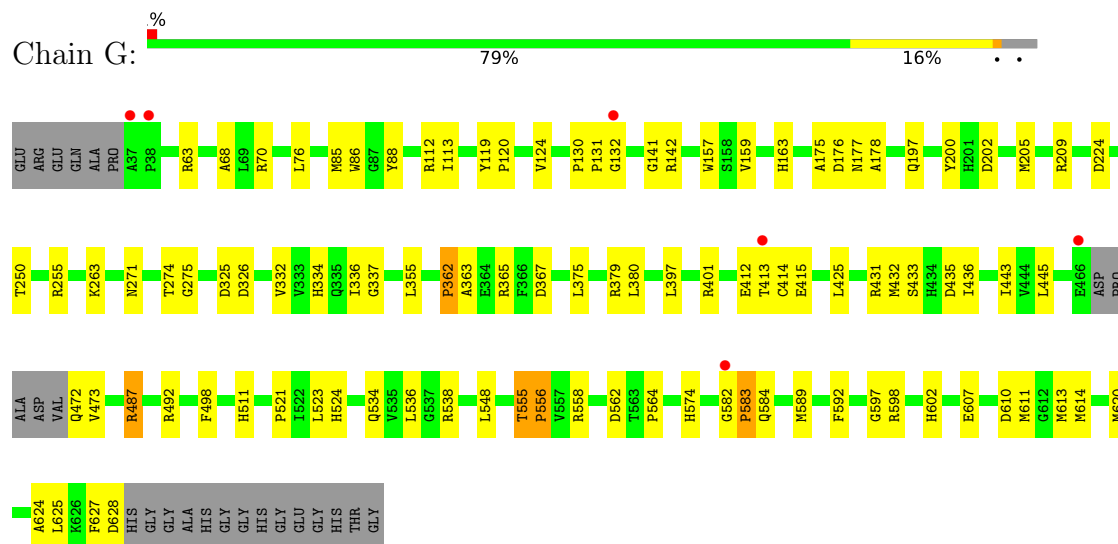
• Molecule 1: Phenoxazinone synthase

Chain F:  79% 16% . .

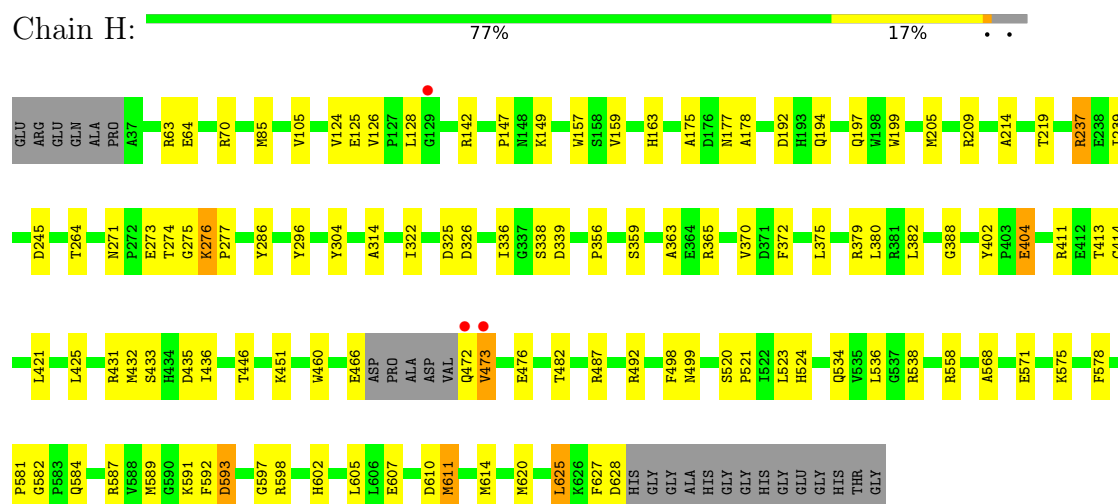




• Molecule 1: Phenoxazinone synthase

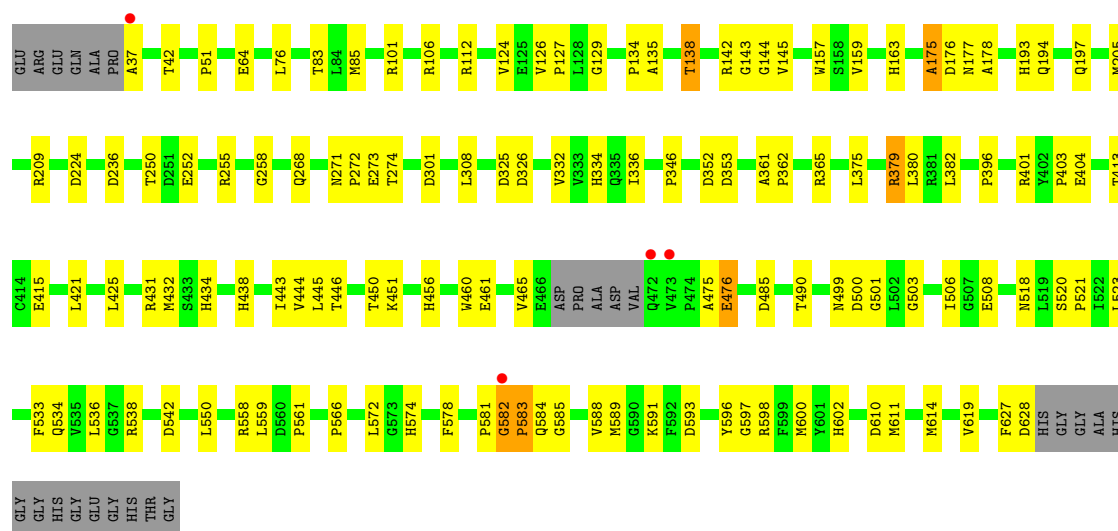


• Molecule 1: Phenoxazinone synthase

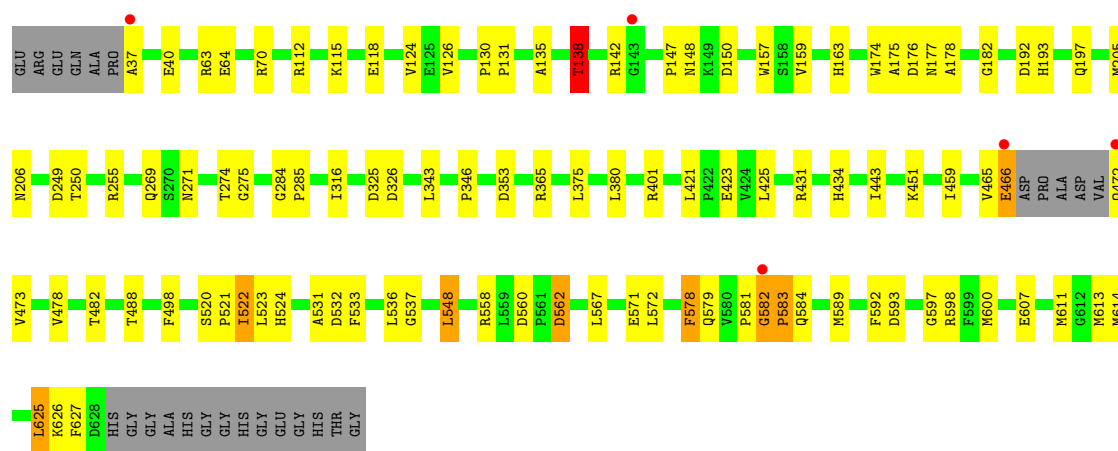
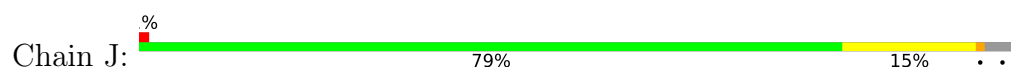


• Molecule 1: Phenoxazinone synthase

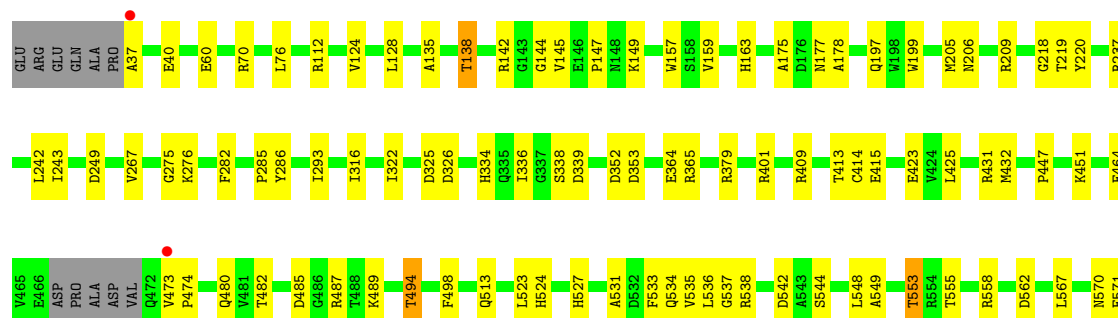
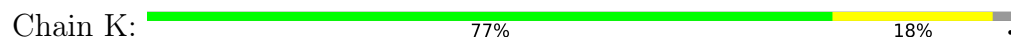


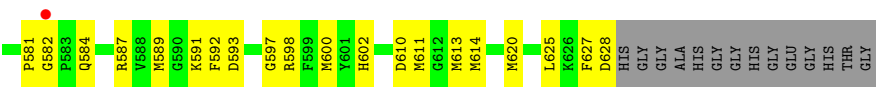


● Molecule 1: Phenoxazinone synthase

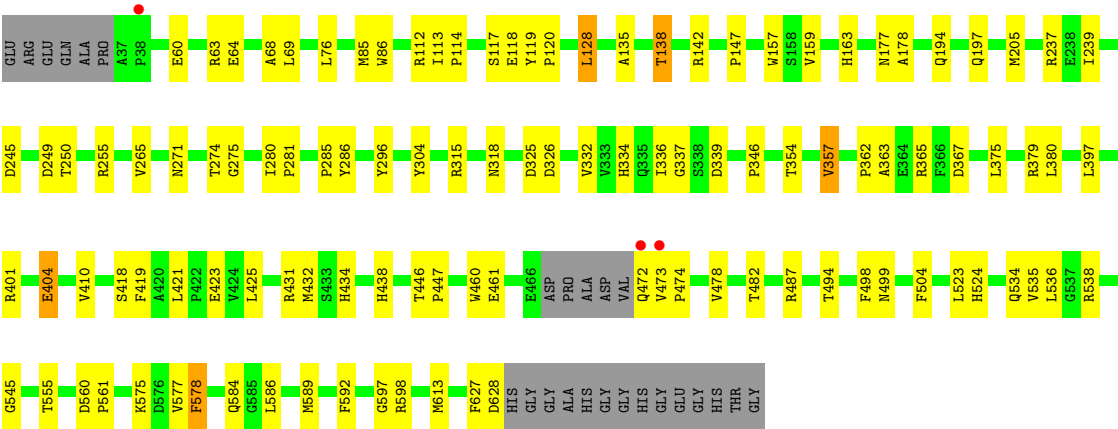
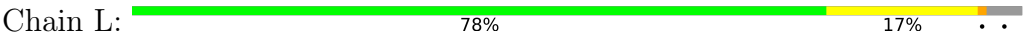


● Molecule 1: Phenoxazinone synthase





● Molecule 1: Phenoxazinone synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	109.49Å 163.46Å 164.35Å 117.04° 95.74° 107.23°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	86.3 (20.00-2.30) 86.2 (20.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.5.0072, CNS	Depositor
R, R_{free}	0.165 , 0.222 0.165 , 0.222	Depositor DCC
R_{free} test set	17920 reflections (4.33%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for -h,h+k+l,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	59241	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: C2O, GOL, CU

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	0.81	0/4697	0.97	6/6423 (0.1%)
1	B	0.83	0/4697	0.96	3/6423 (0.0%)
1	C	0.86	0/4697	0.97	4/6423 (0.1%)
1	D	0.86	1/4697 (0.0%)	0.95	5/6423 (0.1%)
1	E	0.83	0/4697	0.97	10/6423 (0.2%)
1	F	0.84	0/4697	0.96	4/6423 (0.1%)
1	G	0.84	0/4697	0.98	2/6423 (0.0%)
1	H	0.84	1/4697 (0.0%)	0.96	5/6423 (0.1%)
1	I	0.84	2/4697 (0.0%)	0.96	6/6423 (0.1%)
1	J	0.84	0/4697	0.97	9/6423 (0.1%)
1	K	0.82	0/4697	0.95	3/6423 (0.0%)
1	L	0.82	2/4697 (0.0%)	0.97	3/6423 (0.0%)
All	All	0.84	6/56364 (0.0%)	0.96	60/77076 (0.1%)

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	2
1	B	0	4
1	C	0	5
1	D	0	5
1	E	0	2
1	F	0	4
1	G	0	2
1	H	0	2
1	I	0	1
1	J	0	3
1	K	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
All	All	0	37

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	421	LEU	C-O	-5.61	1.19	1.25
1	H	239	ILE	CA-CB	5.52	1.58	1.54
1	I	51	PRO	CA-C	5.52	1.54	1.51
1	D	51	PRO	CA-C	5.33	1.54	1.51
1	L	421	LEU	C-O	-5.11	1.20	1.25

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	LEU	N-CA-C	8.07	119.71	111.07
1	B	128	LEU	N-CA-C	7.70	120.34	111.11
1	E	284	GLY	CA-C-N	7.68	127.40	119.64
1	E	284	GLY	C-N-CA	7.68	127.40	119.64
1	K	128	LEU	N-CA-C	7.45	120.05	111.11

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	GLY	Peptide
1	A	592	PHE	Peptide
1	B	275	GLY	Peptide
1	B	581	PRO	Peptide
1	B	592	PHE	Peptide

5.2 Too-close contacts [i](#)

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	4560	0	4408	99	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4560	0	4408	76	0
1	C	4560	0	4408	63	0
1	D	4560	0	4408	89	0
1	E	4560	0	4408	73	0
1	F	4560	0	4408	79	0
1	G	4560	0	4408	89	0
1	H	4560	0	4408	87	0
1	I	4560	0	4408	107	0
1	J	4560	0	4408	76	0
1	K	4560	0	4408	92	0
1	L	4560	0	4408	100	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	3	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	3	0	0	0	0
3	J	3	0	0	0	0
3	K	3	0	0	0	0
3	L	3	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	1	0
4	E	6	0	8	0	0
4	F	6	0	8	0	0
4	G	6	0	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	6	0	8	1	0
4	I	6	0	8	0	0
4	J	6	0	8	0	0
4	K	6	0	8	2	0
4	L	6	0	8	0	0
5	A	354	0	0	10	0
5	B	362	0	0	11	0
5	C	398	0	0	11	0
5	D	386	0	0	8	0
5	E	357	0	0	10	0
5	F	361	0	0	9	0
5	G	359	0	0	10	0
5	H	376	0	0	12	0
5	I	330	0	0	15	0
5	J	388	0	0	12	0
5	K	359	0	0	10	0
5	L	347	0	0	10	0
All	All	59241	0	52992	957	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 9.

The worst 5 of 957 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:L:138:THR:HG22	1:L:401:ARG:NH1	1.42	1.32
1:L:138:THR:CG2	1:L:401:ARG:NH1	2.04	1.20
1:L:555:THR:HG22	5:L:3298:HOH:O	1.49	1.12
1:K:494:THR:HG22	5:K:684:HOH:O	1.52	1.07
1:C:536:LEU:HD11	1:C:589:MET:HE3	1.26	1.07

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	583/612 (95%)	558 (96%)	23 (4%)	2 (0%)	36	46
1	B	583/612 (95%)	560 (96%)	22 (4%)	1 (0%)	43	55
1	C	583/612 (95%)	557 (96%)	26 (4%)	0	100	100
1	D	583/612 (95%)	561 (96%)	22 (4%)	0	100	100
1	E	583/612 (95%)	558 (96%)	23 (4%)	2 (0%)	36	46
1	F	583/612 (95%)	556 (95%)	24 (4%)	3 (0%)	24	31
1	G	583/612 (95%)	556 (95%)	24 (4%)	3 (0%)	24	31
1	H	583/612 (95%)	564 (97%)	18 (3%)	1 (0%)	43	55
1	I	583/612 (95%)	546 (94%)	34 (6%)	3 (0%)	24	31
1	J	583/612 (95%)	552 (95%)	29 (5%)	2 (0%)	36	46
1	K	583/612 (95%)	560 (96%)	23 (4%)	0	100	100
1	L	583/612 (95%)	558 (96%)	25 (4%)	0	100	100
All	All	6996/7344 (95%)	6686 (96%)	293 (4%)	17 (0%)	43	55

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	582	GLY
1	G	555	THR
1	G	556	PRO
1	G	583	PRO
1	H	473	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	484/499 (97%)	473 (98%)	11 (2%)	44	63
1	B	484/499 (97%)	471 (97%)	13 (3%)	39	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	484/499 (97%)	478 (99%)	6 (1%)	63	79
1	D	484/499 (97%)	480 (99%)	4 (1%)	73	86
1	E	484/499 (97%)	476 (98%)	8 (2%)	53	72
1	F	484/499 (97%)	474 (98%)	10 (2%)	47	66
1	G	484/499 (97%)	474 (98%)	10 (2%)	47	66
1	H	484/499 (97%)	471 (97%)	13 (3%)	39	58
1	I	484/499 (97%)	473 (98%)	11 (2%)	44	63
1	J	484/499 (97%)	476 (98%)	8 (2%)	53	72
1	K	484/499 (97%)	477 (99%)	7 (1%)	59	76
1	L	484/499 (97%)	474 (98%)	10 (2%)	47	66
All	All	5808/5988 (97%)	5697 (98%)	111 (2%)	50	69

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	445	LEU
1	L	578	PHE
1	H	472	GLN
1	L	431	ARG
1	K	553	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	534	GLN
1	L	191	ASN
1	H	480	GLN
1	L	177	ASN
1	L	513	GLN

5.3.3 RNA ⓘ

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 60 ligands modelled in this entry, 36 are monoatomic - leaving 24 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	C2O	D	1002	1	0,2,2	-	-	-		
3	C2O	G	1002	1	0,2,2	-	-	-		
4	GOL	I	5009	-	5,5,5	0.27	0	5,5,5	0.95	0
3	C2O	H	1002	1	0,2,2	-	-	-		
4	GOL	L	5012	-	5,5,5	0.51	0	5,5,5	1.00	0
4	GOL	C	5003	-	5,5,5	0.50	0	5,5,5	1.11	0
4	GOL	D	5004	-	5,5,5	0.41	0	5,5,5	0.85	0
4	GOL	G	5007	-	5,5,5	0.21	0	5,5,5	0.64	0
3	C2O	J	1002	1	0,2,2	-	-	-		
4	GOL	K	5011	-	5,5,5	0.39	0	5,5,5	1.25	1 (20%)
4	GOL	B	5002	-	5,5,5	0.39	0	5,5,5	0.77	0
4	GOL	J	5010	-	5,5,5	0.28	0	5,5,5	0.58	0
3	C2O	C	1002	1	0,2,2	-	-	-		
4	GOL	A	5001	-	5,5,5	0.47	0	5,5,5	0.99	0
4	GOL	E	5005	-	5,5,5	0.39	0	5,5,5	0.75	0
3	C2O	F	1002	1	0,2,2	-	-	-		
4	GOL	H	5008	-	5,5,5	0.40	0	5,5,5	0.82	0
3	C2O	I	1002	1	0,2,2	-	-	-		
3	C2O	K	1002	1	0,2,2	-	-	-		
3	C2O	B	1002	1	0,2,2	-	-	-		
4	GOL	F	5006	-	5,5,5	0.25	0	5,5,5	0.84	0
3	C2O	A	1002	1	0,2,2	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	C2O	L	1002	1	0,2,2	-	-	-		
3	C2O	E	1002	1	0,2,2	-	-	-		

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
4	GOL	H	5008	-	-	3/4/4/4	-
4	GOL	K	5011	-	-	0/4/4/4	-
4	GOL	F	5006	-	-	4/4/4/4	-
4	GOL	B	5002	-	-	2/4/4/4	-
4	GOL	I	5009	-	-	2/4/4/4	-
4	GOL	J	5010	-	-	2/4/4/4	-
4	GOL	A	5001	-	-	4/4/4/4	-
4	GOL	L	5012	-	-	3/4/4/4	-
4	GOL	C	5003	-	-	2/4/4/4	-
4	GOL	D	5004	-	-	0/4/4/4	-
4	GOL	G	5007	-	-	3/4/4/4	-
4	GOL	E	5005	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	5011	GOL	O2-C2-C1	2.08	117.79	109.18

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	5002	GOL	O2-C2-C3-O3
4	C	5003	GOL	O1-C1-C2-C3
4	G	5007	GOL	O1-C1-C2-C3
4	E	5005	GOL	O1-C1-C2-O2
4	F	5006	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5004	GOL	1	0
4	K	5011	GOL	2	0
4	H	5008	GOL	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	587/612 (95%)	-0.62	7 (1%) 76 77	6, 26, 50, 68	2 (0%)
1	B	587/612 (95%)	-0.60	7 (1%) 76 77	5, 24, 46, 69	4 (0%)
1	C	587/612 (95%)	-0.78	2 (0%) 90 90	14, 22, 46, 67	0
1	D	587/612 (95%)	-0.81	3 (0%) 87 87	14, 22, 44, 66	0
1	E	587/612 (95%)	-0.71	5 (0%) 81 82	5, 23, 47, 71	1 (0%)
1	F	587/612 (95%)	-0.63	5 (0%) 81 82	5, 23, 47, 69	3 (0%)
1	G	587/612 (95%)	-0.70	6 (1%) 79 80	14, 24, 47, 70	1 (0%)
1	H	587/612 (95%)	-0.67	3 (0%) 87 87	5, 24, 45, 70	2 (0%)
1	I	587/612 (95%)	-0.59	4 (0%) 84 85	6, 25, 53, 74	2 (0%)
1	J	587/612 (95%)	-0.72	5 (0%) 81 82	4, 23, 45, 61	2 (0%)
1	K	587/612 (95%)	-0.65	3 (0%) 87 87	5, 24, 49, 68	1 (0%)
1	L	587/612 (95%)	-0.67	3 (0%) 87 87	5, 25, 49, 71	1 (0%)
All	All	7044/7344 (95%)	-0.68	53 (0%) 82 83	4, 24, 48, 74	19 (0%)

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	473	VAL	31.0
1	F	473	VAL	29.4
1	L	472	GLN	29.4
1	H	473	VAL	29.3
1	F	472	GLN	28.3

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 ⓘ

There are no oligosaccharides 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, 95th 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
4	GOL	B	5002	6/6	0.91	0.12	33,39,42,42	0
4	GOL	D	5004	6/6	0.92	0.10	34,36,38,38	0
4	GOL	K	5011	6/6	0.92	0.12	29,41,42,43	0
4	GOL	L	5012	6/6	0.92	0.09	34,37,39,39	0
4	GOL	C	5003	6/6	0.93	0.09	26,28,32,34	0
4	GOL	H	5008	6/6	0.93	0.09	26,33,35,36	0
4	GOL	I	5009	6/6	0.94	0.09	28,36,39,40	0
4	GOL	F	5006	6/6	0.94	0.08	38,39,41,43	0
4	GOL	E	5005	6/6	0.94	0.10	35,40,43,43	0
3	C2O	G	1002	3/3	0.95	0.06	41,41,42,49	0
3	C2O	K	1002	3/3	0.95	0.07	42,42,45,46	0
4	GOL	A	5001	6/6	0.95	0.09	25,32,38,39	0
3	C2O	A	1002	3/3	0.95	0.07	41,41,44,52	0
3	C2O	B	1002	3/3	0.95	0.06	40,40,41,48	0
3	C2O	F	1002	3/3	0.95	0.07	38,38,39,48	0
3	C2O	H	1002	3/3	0.96	0.06	38,38,40,45	0
3	C2O	I	1002	3/3	0.96	0.06	37,37,46,47	0
3	C2O	J	1002	3/3	0.96	0.06	29,29,38,43	0
4	GOL	J	5010	6/6	0.96	0.06	27,35,35,37	0
3	C2O	C	1002	3/3	0.96	0.06	29,29,39,41	0
3	C2O	L	1002	3/3	0.96	0.06	39,39,41,46	0
4	GOL	G	5007	6/6	0.97	0.07	30,39,41,42	0
3	C2O	E	1002	3/3	0.97	0.06	32,32,40,40	0
3	C2O	D	1002	3/3	0.97	0.06	30,30,39,41	0
2	CU	E	1005	1/1	0.98	0.06	42,42,42,42	0
2	CU	A	1005	1/1	0.99	0.05	43,43,43,43	0
2	CU	B	1000	1/1	0.99	0.02	43,43,43,43	0
2	CU	B	1004	1/1	0.99	0.02	40,40,40,40	0
2	CU	B	1005	1/1	0.99	0.03	37,37,37,37	0
2	CU	C	1005	1/1	0.99	0.05	37,37,37,37	0
2	CU	D	1004	1/1	0.99	0.03	38,38,38,38	0
2	CU	D	1005	1/1	0.99	0.04	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CU	E	1000	1/1	0.99	0.04	45,45,45,45	0
2	CU	E	1004	1/1	0.99	0.02	41,41,41,41	0
2	CU	A	1000	1/1	0.99	0.02	50,50,50,50	0
2	CU	F	1000	1/1	0.99	0.03	42,42,42,42	0
2	CU	F	1005	1/1	0.99	0.04	38,38,38,38	0
2	CU	G	1004	1/1	0.99	0.03	43,43,43,43	0
2	CU	G	1005	1/1	0.99	0.04	39,39,39,39	0
2	CU	H	1000	1/1	0.99	0.03	49,49,49,49	0
2	CU	I	1005	1/1	0.99	0.04	42,42,42,42	0
2	CU	J	1000	1/1	0.99	0.02	40,40,40,40	0
2	CU	J	1005	1/1	0.99	0.06	39,39,39,39	0
2	CU	K	1000	1/1	0.99	0.02	43,43,43,43	0
2	CU	K	1004	1/1	0.99	0.02	40,40,40,40	0
2	CU	K	1005	1/1	0.99	0.04	42,42,42,42	0
2	CU	L	1005	1/1	0.99	0.06	41,41,41,41	0
2	CU	A	1004	1/1	0.99	0.03	41,41,41,41	0
2	CU	I	1000	1/1	1.00	0.02	46,46,46,46	0
2	CU	I	1004	1/1	1.00	0.02	43,43,43,43	0
2	CU	C	1004	1/1	1.00	0.02	39,39,39,39	0
2	CU	G	1000	1/1	1.00	0.02	43,43,43,43	0
2	CU	J	1004	1/1	1.00	0.02	41,41,41,41	0
2	CU	C	1000	1/1	1.00	0.03	43,43,43,43	0
2	CU	D	1000	1/1	1.00	0.03	37,37,37,37	0
2	CU	F	1004	1/1	1.00	0.02	42,42,42,42	0
2	CU	H	1004	1/1	1.00	0.02	43,43,43,43	0
2	CU	L	1000	1/1	1.00	0.03	43,43,43,43	0
2	CU	L	1004	1/1	1.00	0.02	43,43,43,43	0
2	CU	H	1005	1/1	1.00	0.06	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.