



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:51 AM UTC

PDB ID : 5MG5 / pdb_00005mg5
Title : A multi-component acyltransferase PhlABC from *Pseudomonas protegens* soaked with the monoacetylphloroglucinol (MAPG)
Authors : Pavkov-Keller, T.; Schmidt, N.G.; Kroutil, W.; Gruber, K.
Deposited on : 2016-11-20
Resolution : 3.44 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

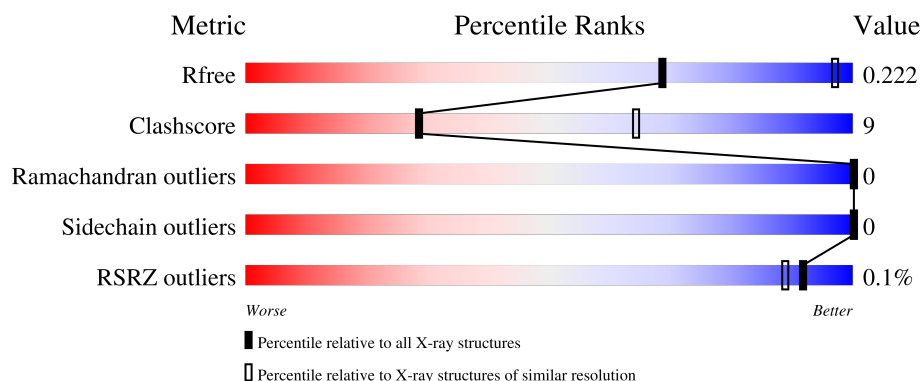
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.44 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	1736 (3.50-3.38)
Clashscore	190562	1808 (3.50-3.38)
Ramachandran outliers	187476	1776 (3.50-3.38)
Sidechain outliers	187428	1777 (3.50-3.38)
RSRZ outliers	180081	1736 (3.50-3.38)

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	362	
1	D	362	
1	G	362	
1	J	362	
1	M	362	

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Mol	Chain	Length	Quality of chain
1	P	362	 78% 21% .
1	S	362	 78% 20% .
1	V	362	 81% 17% .
2	B	146	 84% 16% .
2	E	146	 78% 21% .
2	H	146	 79% 21% .
2	K	146	 77% 23% .
2	N	146	 82% 17% .
2	Q	146	 84% 15% .
2	T	146	 74% 25% .
2	W	146	 70% 29% .
3	C	398	 84% 15% .
3	F	398	 76% 23% .
3	I	398	 % 72% 27% .
3	L	398	 76% 24% .
3	O	398	 76% 23% .
3	R	398	 74% 25% .
3	U	398	 78% 21% .
3	X	398	 82% 17% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 54522 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 Hydroxymethylglutaryl-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2677	1687	452	529	9			
1	D	359	Total	C	N	O	S	0	0	0
			2686	1693	454	530	9			
1	G	359	Total	C	N	O	S	0	0	0
			2686	1693	454	530	9			
1	J	359	Total	C	N	O	S	0	0	0
			2686	1693	454	530	9			
1	M	359	Total	C	N	O	S	0	0	0
			2686	1693	454	530	9			
1	P	358	Total	C	N	O	S	0	0	0
			2677	1687	452	529	9			
1	S	358	Total	C	N	O	S	0	1	0
			2687	1693	455	530	9			
1	V	359	Total	C	N	O	S	0	0	0
			2686	1693	454	530	9			

- Molecule 2 is a protein called 2,4-diacetylphloroglucinol biosynthesis protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	0	0
			1150	721	208	207	14			
2	E	145	Total	C	N	O	S	0	0	0
			1150	721	208	207	14			
2	H	145	Total	C	N	O	S	0	0	0
			1150	721	208	207	14			
2	K	145	Total	C	N	O	S	0	0	0
			1150	721	208	207	14			
2	N	145	Total	C	N	O	S	0	0	0
			1150	721	208	207	14			
2	Q	145	Total	C	N	O	S	0	0	0
			1150	721	208	207	14			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	145	Total	C	N	O	S	0	0	0
			1150	721	208	207	14			
2	W	145	Total	C	N	O	S	0	0	0
			1150	721	208	207	14			

- Molecule 3 is a protein called 2,4-diacetylphloroglucinol biosynthesis protein PhlC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	395	Total	C	N	O	S	0	0	0
			2965	1862	512	571	20			
3	F	395	Total	C	N	O	S	0	0	0
			2965	1862	512	571	20			
3	I	396	Total	C	N	O	S	0	0	0
			2970	1865	513	572	20			
3	L	396	Total	C	N	O	S	0	0	0
			2970	1865	513	572	20			
3	O	396	Total	C	N	O	S	0	0	0
			2970	1865	513	572	20			
3	R	395	Total	C	N	O	S	0	0	0
			2965	1862	512	571	20			
3	U	396	Total	C	N	O	S	0	0	0
			2970	1865	513	572	20			
3	X	396	Total	C	N	O	S	0	0	0
			2970	1865	513	572	20			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

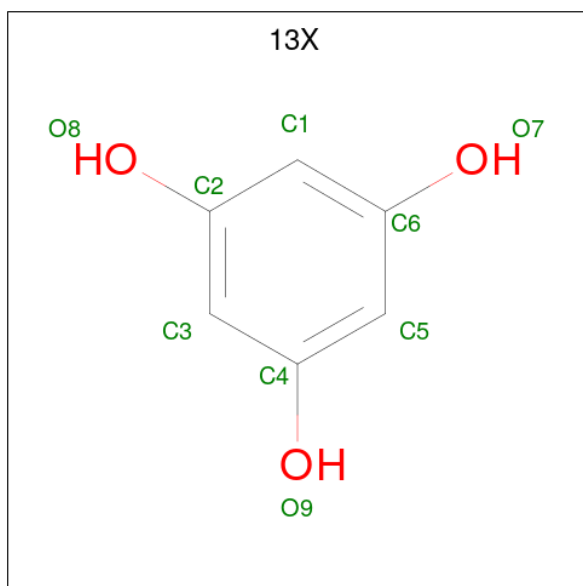
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		
4	K	1	Total	Zn	0	0
			1	1		
4	N	1	Total	Zn	0	0
			1	1		
4	Q	1	Total	Zn	0	0
			1	1		
4	T	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	W	1	Total	Zn	0	0
			1	1		

- Molecule 5 is benzene-1,3,5-triol (CCD ID: 13X) (formula: C₆H₆O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			9	6	3		
5	L	1	Total	C	O	0	0
			9	6	3		
5	O	1	Total	C	O	0	0
			9	6	3		
5	R	1	Total	C	O	0	0
			9	6	3		

- Molecule 6 is water.

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

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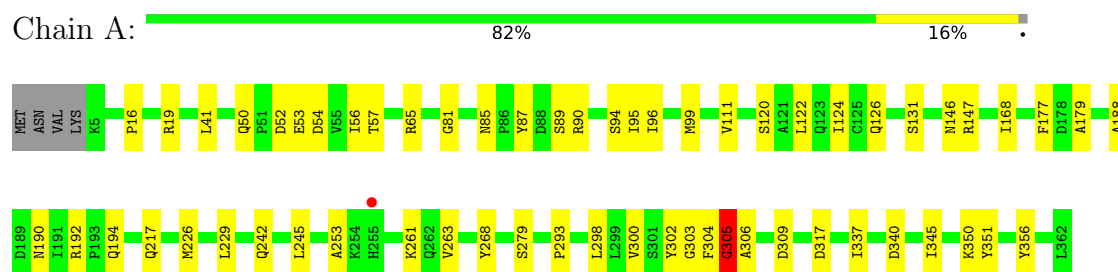
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	2	Total 2	O 2	0	0
6	F	2	Total 2	O 2	0	0
6	G	2	Total 2	O 2	0	0
6	H	3	Total 3	O 3	0	0
6	I	2	Total 2	O 2	0	0
6	J	5	Total 5	O 5	0	0
6	K	1	Total 1	O 1	0	0
6	L	1	Total 1	O 1	0	0
6	M	4	Total 4	O 4	0	0
6	N	3	Total 3	O 3	0	0
6	O	1	Total 1	O 1	0	0
6	P	1	Total 1	O 1	0	0
6	Q	2	Total 2	O 2	0	0
6	R	3	Total 3	O 3	0	0
6	S	2	Total 2	O 2	0	0
6	T	1	Total 1	O 1	0	0
6	U	1	Total 1	O 1	0	0
6	V	6	Total 6	O 6	0	0
6	X	4	Total 4	O 4	0	0

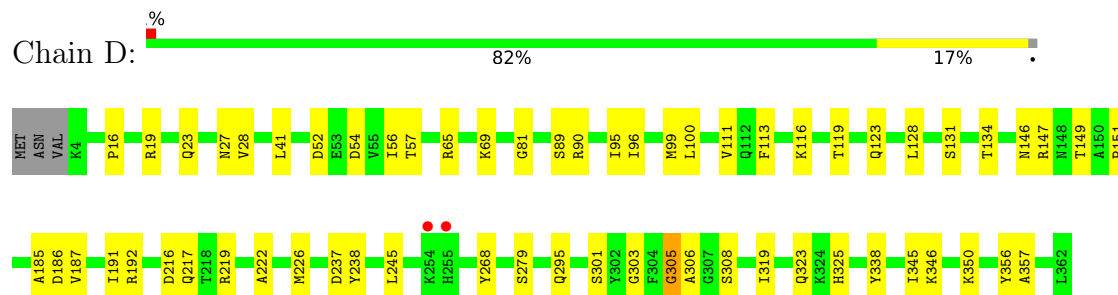
3 Residue-property plots

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.

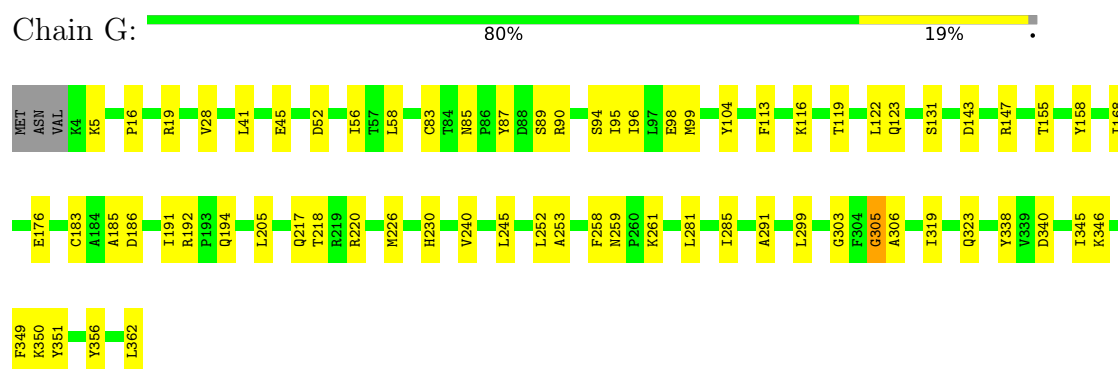
- Molecule 1: Hydroxymethylglutaryl-CoA synthase



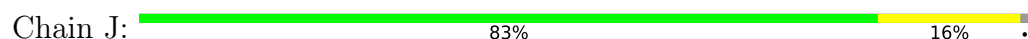
- Molecule 1: Hydroxymethylglutaryl-CoA synthase

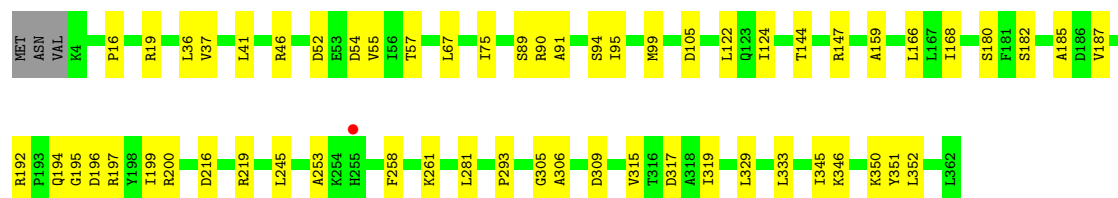


- Molecule 1: Hydroxymethylglutaryl-CoA synthase



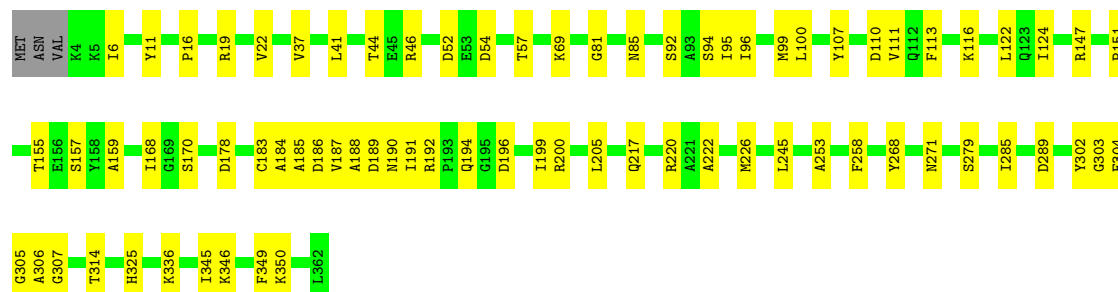
- Molecule 1: Hydroxymethylglutaryl-CoA synthase





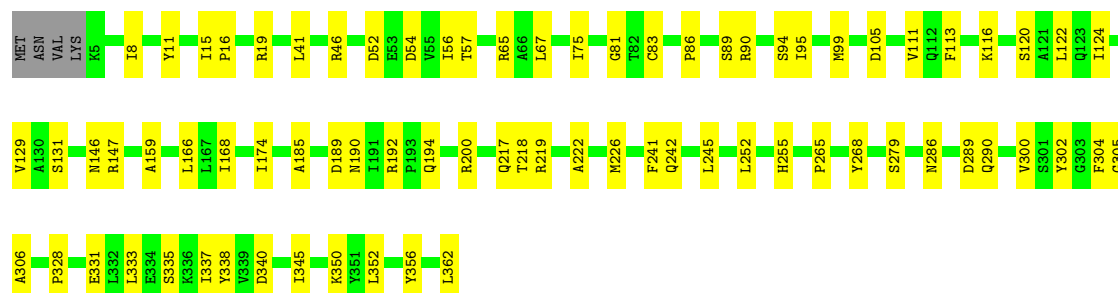
• Molecule 1: Hydroxymethylglutaryl-CoA synthase

Chain M: 78% 21%



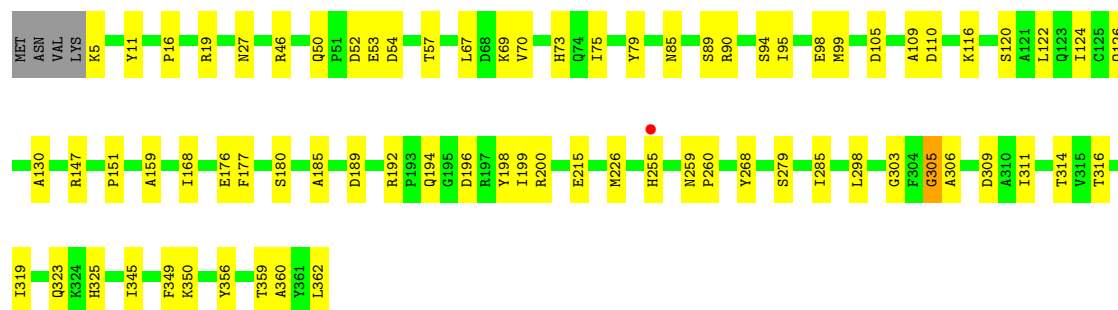
• Molecule 1: Hydroxymethylglutaryl-CoA synthase

Chain P: 78% 21%



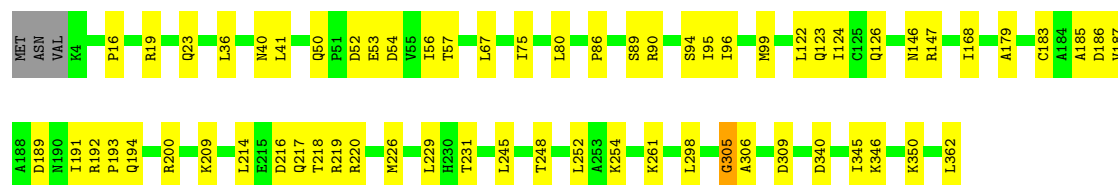
• Molecule 1: Hydroxymethylglutaryl-CoA synthase

Chain S: 78% 20%



• Molecule 1: Hydroxymethylglutaryl-CoA synthase

Chain V: 81% 17%



- Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein

Chain B: 84% 16%



- Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein

Chain E: 78% 21%



- Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein

Chain H: 79% 21%



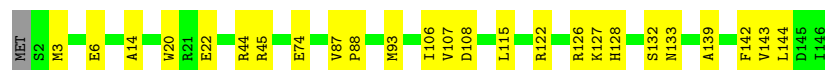
- Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein

Chain K: 77% 23%



- Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein

Chain N: 82% 17%

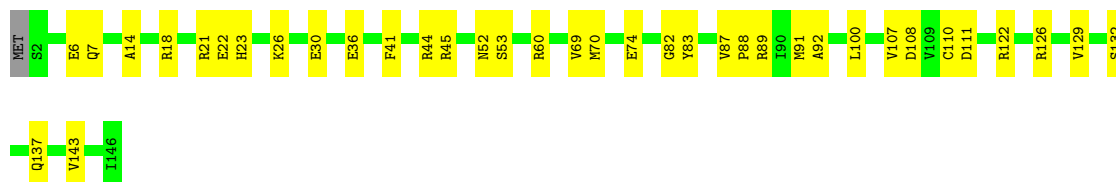


- Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein

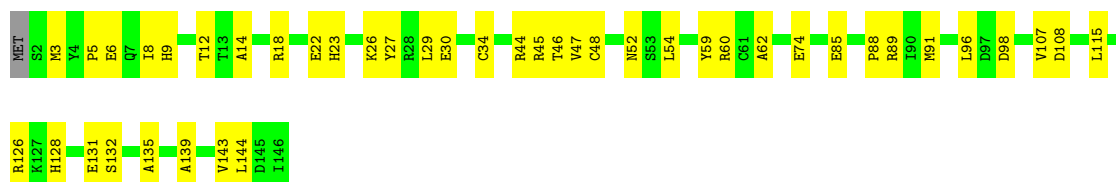
Chain Q: 84% 15%



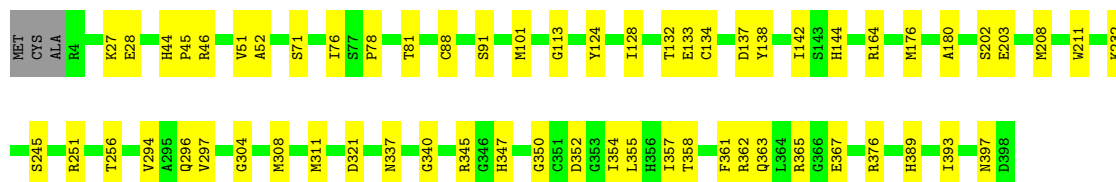
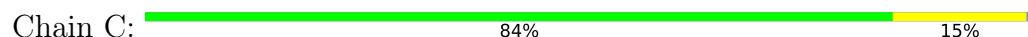
- Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein



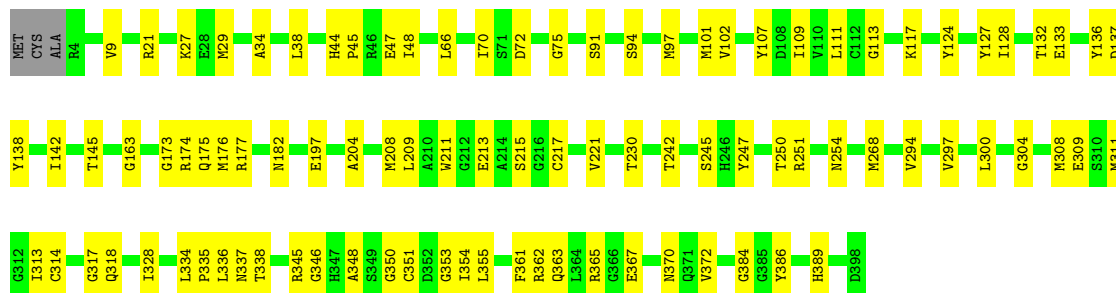
- Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein



- Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein PhlC

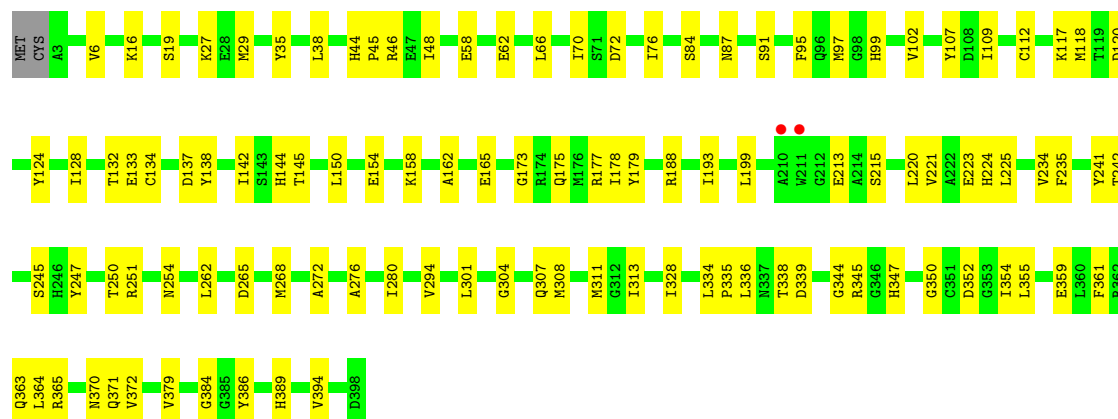


- Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein PhlC



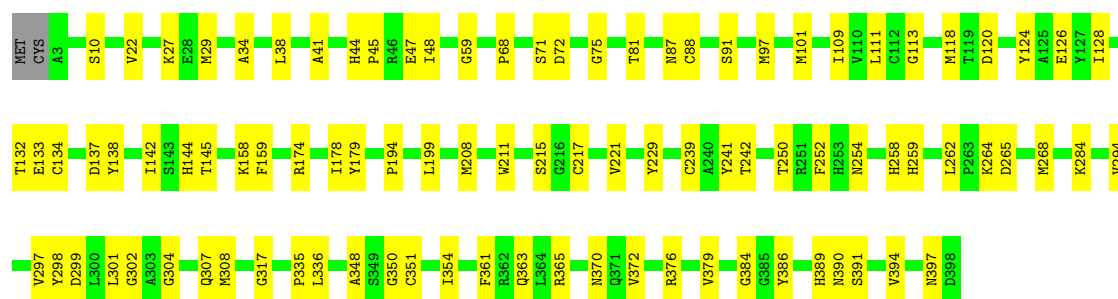
- Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein PhlC





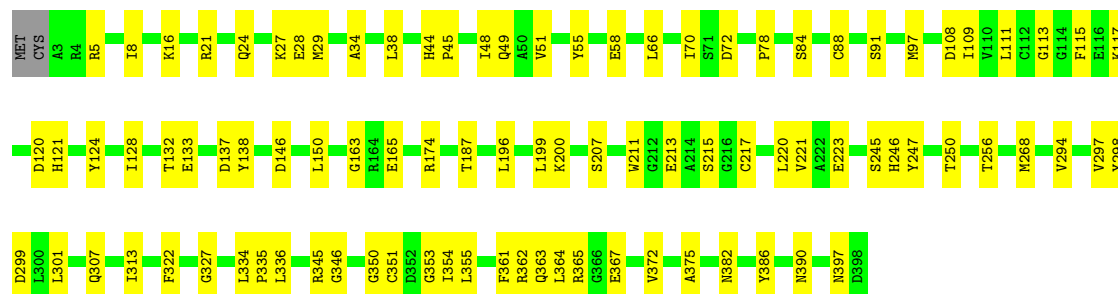
• Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein PhlC

Chain L: 76% 24%



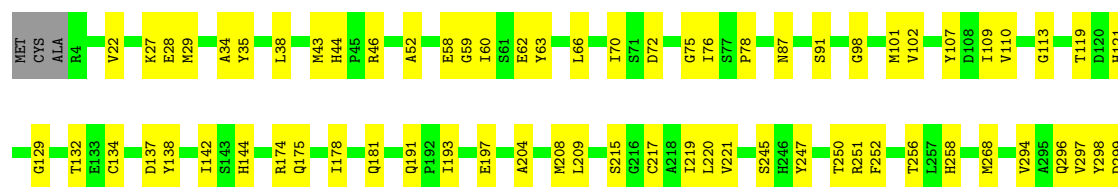
• Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein PhlC

Chain O: 76% 23%



• Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein PhlC

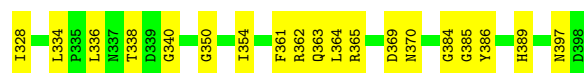
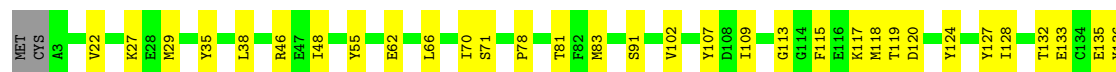
Chain R: 74% 25%





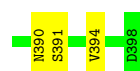
• Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein PhlC

Chain U: 78% 21%



• Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein PhlC

Chain X: 82% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.79Å 229.78Å 311.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 3.44 49.73 – 3.44	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.73-3.44) 99.1 (49.73-3.44)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.165 , 0.221 0.168 , 0.222	Depositor DCC
R_{free} test set	4986 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtriage
Anisotropy	0.743	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	54522	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: ZN, 13X, SCY

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	0.13	0/2721	0.34	1/3695 (0.0%)
1	D	0.13	0/2730	0.33	0/3706
1	G	0.13	0/2730	0.35	1/3706 (0.0%)
1	J	0.13	0/2730	0.34	0/3706
1	M	0.13	0/2730	0.35	0/3706
1	P	0.13	0/2721	0.34	0/3695
1	S	0.12	0/2732	0.35	0/3710
1	V	0.13	0/2730	0.37	0/3706
2	B	0.13	0/1172	0.35	0/1580
2	E	0.13	0/1172	0.34	0/1580
2	H	0.13	0/1172	0.35	0/1580
2	K	0.13	0/1172	0.34	0/1580
2	N	0.12	0/1172	0.33	0/1580
2	Q	0.14	0/1172	0.36	0/1580
2	T	0.13	0/1172	0.33	0/1580
2	W	0.14	0/1172	0.35	0/1580
3	C	0.13	0/3019	0.32	0/4082
3	F	0.12	0/3019	0.32	0/4082
3	I	0.12	0/3024	0.32	1/4089 (0.0%)
3	L	0.13	0/3024	0.33	0/4089
3	O	0.13	0/3024	0.32	0/4089
3	R	0.12	0/3019	0.31	0/4082
3	U	0.13	0/3024	0.32	0/4089
3	X	0.14	0/3024	0.34	0/4089
All	All	0.13	0/55377	0.34	3/74961 (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	D	0	1
1	G	0	1
1	M	0	1
1	P	0	1
1	S	0	1
1	V	0	1
All	All	0	7

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	301	LEU	CB-CA-C	-5.19	110.57	116.54
1	G	305	GLY	N-CA-C	-5.08	101.13	113.18
1	A	305	GLY	N-CA-C	-5.03	101.26	113.18

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	GLY	Peptide
1	D	305	GLY	Peptide
1	G	305	GLY	Peptide
1	M	305	GLY	Peptide
1	P	305	GLY	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	2677	0	2662	47	0
1	D	2686	0	2675	53	0
1	G	2686	0	2675	51	0
1	J	2686	0	2675	47	0
1	M	2686	0	2675	59	0
1	P	2677	0	2662	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S	2687	0	2668	57	0
1	V	2686	0	2675	50	0
2	B	1150	0	1149	22	0
2	E	1150	0	1149	24	0
2	H	1150	0	1149	24	0
2	K	1150	0	1149	24	0
2	N	1150	0	1149	20	0
2	Q	1150	0	1149	18	0
2	T	1150	0	1149	31	0
2	W	1150	0	1149	33	0
3	C	2965	0	2869	49	0
3	F	2965	0	2869	71	0
3	I	2970	0	2874	82	0
3	L	2970	0	2874	70	0
3	O	2970	0	2874	62	0
3	R	2965	0	2869	72	0
3	U	2970	0	2874	62	0
3	X	2970	0	2874	52	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
4	N	1	0	0	0	0
4	Q	1	0	0	0	0
4	T	1	0	0	0	0
4	W	1	0	0	0	0
5	C	9	0	6	2	0
5	L	9	0	6	2	0
5	O	9	0	6	1	0
5	R	9	0	6	0	0
6	A	5	0	0	0	0
6	B	3	0	0	0	0
6	C	5	0	0	0	0
6	D	3	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	3	0	0	0	0
6	I	2	0	0	0	0
6	J	5	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	4	0	0	0	0
6	N	3	0	0	0	0
6	O	1	0	0	1	0
6	P	1	0	0	0	0
6	Q	2	0	0	0	0
6	R	3	0	0	0	0
6	S	2	0	0	0	0
6	T	1	0	0	0	0
6	U	1	0	0	0	0
6	V	6	0	0	0	0
6	X	4	0	0	0	0
All	All	54522	0	53560	949	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 949 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)
3:U:132:THR:HG22	3:U:133:GLU:H	1.21	1.04
1:D:238:TYR:OH	1:D:295:GLN:OE1	1.76	1.03
3:L:132:THR:HG22	3:L:133:GLU:H	1.24	1.02
3:C:132:THR:HG22	3:C:133:GLU:H	1.25	0.99
3:X:132:THR:HG22	3:X:133:GLU:H	1.27	0.98

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	356/362 (98%)	345 (97%)	11 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	357/362 (99%)	345 (97%)	12 (3%)	0	100	100
1	G	357/362 (99%)	340 (95%)	17 (5%)	0	100	100
1	J	357/362 (99%)	347 (97%)	10 (3%)	0	100	100
1	M	357/362 (99%)	347 (97%)	10 (3%)	0	100	100
1	P	356/362 (98%)	345 (97%)	11 (3%)	0	100	100
1	S	357/362 (99%)	347 (97%)	10 (3%)	0	100	100
1	V	357/362 (99%)	346 (97%)	11 (3%)	0	100	100
2	B	143/146 (98%)	139 (97%)	4 (3%)	0	100	100
2	E	143/146 (98%)	138 (96%)	5 (4%)	0	100	100
2	H	143/146 (98%)	138 (96%)	5 (4%)	0	100	100
2	K	143/146 (98%)	140 (98%)	3 (2%)	0	100	100
2	N	143/146 (98%)	139 (97%)	4 (3%)	0	100	100
2	Q	143/146 (98%)	140 (98%)	3 (2%)	0	100	100
2	T	143/146 (98%)	140 (98%)	3 (2%)	0	100	100
2	W	143/146 (98%)	139 (97%)	4 (3%)	0	100	100
3	C	392/398 (98%)	376 (96%)	16 (4%)	0	100	100
3	F	392/398 (98%)	377 (96%)	15 (4%)	0	100	100
3	I	393/398 (99%)	380 (97%)	13 (3%)	0	100	100
3	L	393/398 (99%)	381 (97%)	12 (3%)	0	100	100
3	O	393/398 (99%)	382 (97%)	11 (3%)	0	100	100
3	R	392/398 (98%)	378 (96%)	14 (4%)	0	100	100
3	U	393/398 (99%)	378 (96%)	15 (4%)	0	100	100
3	X	393/398 (99%)	381 (97%)	12 (3%)	0	100	100
All	All	7139/7248 (98%)	6908 (97%)	231 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	279/283 (99%)	279 (100%)	0	100	100
1	D	280/283 (99%)	280 (100%)	0	100	100
1	G	280/283 (99%)	280 (100%)	0	100	100
1	J	280/283 (99%)	280 (100%)	0	100	100
1	M	280/283 (99%)	280 (100%)	0	100	100
1	P	279/283 (99%)	279 (100%)	0	100	100
1	S	280/283 (99%)	280 (100%)	0	100	100
1	V	280/283 (99%)	280 (100%)	0	100	100
2	B	124/125 (99%)	124 (100%)	0	100	100
2	E	124/125 (99%)	124 (100%)	0	100	100
2	H	124/125 (99%)	124 (100%)	0	100	100
2	K	124/125 (99%)	124 (100%)	0	100	100
2	N	124/125 (99%)	124 (100%)	0	100	100
2	Q	124/125 (99%)	124 (100%)	0	100	100
2	T	124/125 (99%)	124 (100%)	0	100	100
2	W	124/125 (99%)	124 (100%)	0	100	100
3	C	303/305 (99%)	303 (100%)	0	100	100
3	F	303/305 (99%)	303 (100%)	0	100	100
3	I	303/305 (99%)	303 (100%)	0	100	100
3	L	303/305 (99%)	303 (100%)	0	100	100
3	O	303/305 (99%)	303 (100%)	0	100	100
3	R	303/305 (99%)	303 (100%)	0	100	100
3	U	303/305 (99%)	303 (100%)	0	100	100
3	X	303/305 (99%)	303 (100%)	0	100	100
All	All	5654/5704 (99%)	5654 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	255	HIS
1	P	64	GLN
2	W	137	GLN

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Mol	Chain	Res	Type
1	M	271	ASN
2	N	9	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
3	SCY	C	88	3	7,8,9	0.89	0	4,9,11	0.87	0
3	SCY	U	88	3	7,8,9	0.94	0	4,9,11	0.68	0
3	SCY	F	88	3	7,8,9	0.91	0	4,9,11	0.77	0
3	SCY	I	88	3	7,8,9	0.89	0	4,9,11	0.78	0
3	SCY	R	88	3	7,8,9	0.86	0	4,9,11	0.90	0
3	SCY	O	88	3	7,8,9	0.89	0	4,9,11	0.84	0
3	SCY	L	88	3	7,8,9	0.90	0	4,9,11	0.87	0
3	SCY	X	88	3	7,8,9	0.91	0	4,9,11	0.78	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	SCY	C	88	3	-	2/5/7/9	-
3	SCY	U	88	3	-	2/5/7/9	-
3	SCY	F	88	3	-	2/5/7/9	-
3	SCY	I	88	3	-	2/5/7/9	-
3	SCY	R	88	3	-	2/5/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SCY	O	88	3	-	2/5/7/9	-
3	SCY	L	88	3	-	2/5/7/9	-
3	SCY	X	88	3	-	2/5/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	88	SCY	OCD-CD-SG-CB
3	C	88	SCY	CE-CD-SG-CB
3	F	88	SCY	OCD-CD-SG-CB
3	F	88	SCY	CE-CD-SG-CB
3	I	88	SCY	OCD-CD-SG-CB

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	88	SCY	2	0
3	O	88	SCY	1	0
3	L	88	SCY	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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
5	13X	O	500	-	9,9,9	0.93	0	12,12,12	0.37	0
5	13X	C	500	-	9,9,9	0.92	0	12,12,12	0.39	0
5	13X	R	500	-	9,9,9	0.93	0	12,12,12	0.37	0
5	13X	L	500	-	9,9,9	0.91	0	12,12,12	0.39	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
5	13X	O	500	-	-	-	0/1/1/1
5	13X	C	500	-	-	-	0/1/1/1
5	13X	R	500	-	-	-	0/1/1/1
5	13X	L	500	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	500	13X	1	0
5	C	500	13X	2	0
5	L	500	13X	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	358/362 (98%)	-0.43	1 (0%) 90 80	25, 37, 57, 169	0
1	D	359/362 (99%)	-0.48	2 (0%) 85 69	27, 38, 55, 213	0
1	G	359/362 (99%)	-0.33	0 100 100	36, 53, 71, 93	0
1	J	359/362 (99%)	-0.46	1 (0%) 90 80	27, 39, 59, 153	0
1	M	359/362 (99%)	-0.43	0 100 100	30, 39, 57, 87	0
1	P	358/362 (98%)	-0.34	0 100 100	34, 49, 65, 84	0
1	S	358/362 (98%)	-0.43	1 (0%) 90 80	29, 41, 57, 74	1 (0%)
1	V	359/362 (99%)	-0.39	0 100 100	34, 46, 64, 116	0
2	B	145/146 (99%)	-0.44	0 100 100	30, 44, 67, 87	0
2	E	145/146 (99%)	-0.40	0 100 100	32, 45, 69, 79	0
2	H	145/146 (99%)	-0.32	0 100 100	32, 48, 70, 96	0
2	K	145/146 (99%)	-0.46	0 100 100	30, 45, 65, 74	0
2	N	145/146 (99%)	-0.36	0 100 100	33, 46, 72, 92	0
2	Q	145/146 (99%)	-0.33	0 100 100	35, 48, 78, 90	0
2	T	145/146 (99%)	-0.38	0 100 100	33, 47, 72, 85	0
2	W	145/146 (99%)	-0.26	0 100 100	38, 55, 88, 95	0
3	C	394/398 (98%)	-0.40	0 100 100	32, 47, 59, 75	0
3	F	394/398 (98%)	-0.37	0 100 100	37, 49, 65, 88	0
3	I	395/398 (99%)	-0.29	2 (0%) 87 72	40, 56, 71, 155	0
3	L	395/398 (99%)	-0.33	0 100 100	36, 51, 69, 88	0
3	O	395/398 (99%)	-0.36	0 100 100	37, 50, 64, 81	0
3	R	394/398 (98%)	-0.36	0 100 100	38, 52, 66, 94	0
3	U	395/398 (99%)	-0.36	0 100 100	33, 48, 63, 88	0
3	X	395/398 (99%)	-0.25	0 100 100	42, 57, 76, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	7186/7248 (99%)	-0.37	7 (0%) 92 89	25, 48, 68, 213	1 (0%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	255[A]	HIS	4.5
1	D	255	HIS	3.5
1	J	255	HIS	3.1
1	A	255	HIS	3.1
3	I	211	TRP	2.8

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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(Å ²)	Q<0.9
3	SCY	U	88	9/10	0.82	0.15	37,48,62,64	0
3	SCY	F	88	9/10	0.87	0.14	41,44,70,77	0
3	SCY	I	88	9/10	0.91	0.13	51,53,69,75	0
3	SCY	C	88	9/10	0.91	0.11	44,45,56,57	0
3	SCY	X	88	9/10	0.91	0.11	48,51,59,63	0
3	SCY	O	88	9/10	0.93	0.10	37,44,52,53	0
3	SCY	R	88	9/10	0.94	0.10	48,52,58,58	0
3	SCY	L	88	9/10	0.95	0.10	40,44,54,57	0

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
5	13X	C	500	9/9	0.84	0.13	42,56,59,61	0
5	13X	O	500	9/9	0.84	0.16	50,56,60,63	0
5	13X	R	500	9/9	0.85	0.16	52,56,61,63	0
5	13X	L	500	9/9	0.86	0.17	50,56,58,60	0
4	ZN	T	200	1/1	0.97	0.05	132,132,132,132	0
4	ZN	W	200	1/1	0.97	0.08	135,135,135,135	0
4	ZN	H	200	1/1	0.99	0.03	81,81,81,81	0
4	ZN	K	200	1/1	0.99	0.04	104,104,104,104	0
4	ZN	N	200	1/1	0.99	0.05	97,97,97,97	0
4	ZN	Q	200	1/1	0.99	0.06	162,162,162,162	0
4	ZN	B	200	1/1	0.99	0.03	116,116,116,116	0
4	ZN	E	200	1/1	1.00	0.02	96,96,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.