Full wwPDB X-ray Structure Validation Report ⓘ

Aug 1, 2024 – 04:53 PM EDT

PDB ID	:	8W2D
Title	:	holo-PCP-Thioesterase di-domain structure from the sulfazecin biosynthetic nonribosomal peptide synthetase, SulM
Authors	:	Patel, K.D.; Gulick, A.M.
Deposited on	:	2024-02-20
Resolution	:	2.70 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*
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:

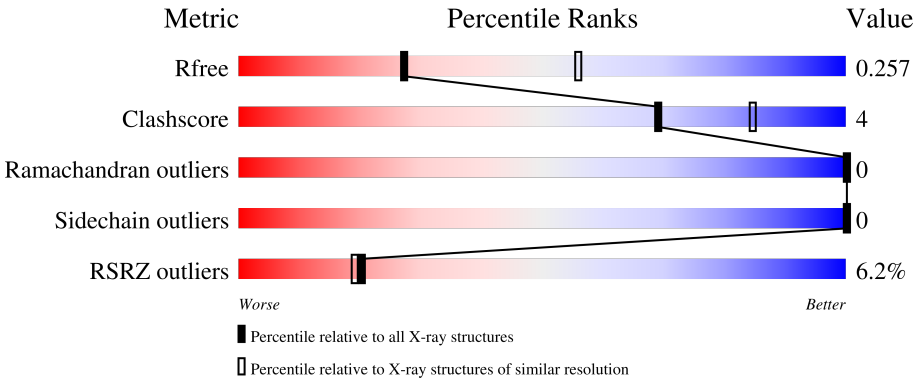
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	345	4% 87% 6% 7%
1	B	345	8% 87% 6% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	3004	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9536 atoms, of which 4680 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 Non-ribosomal peptide synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	322	Total	C	H	N	O	S	0	0	0
			4726	1526	2325	423	438	14			
1	B	320	Total	C	H	N	O	S	0	0	0
			4648	1501	2283	413	438	13			

There are 42 discrepancies between the modelled and reference sequences:

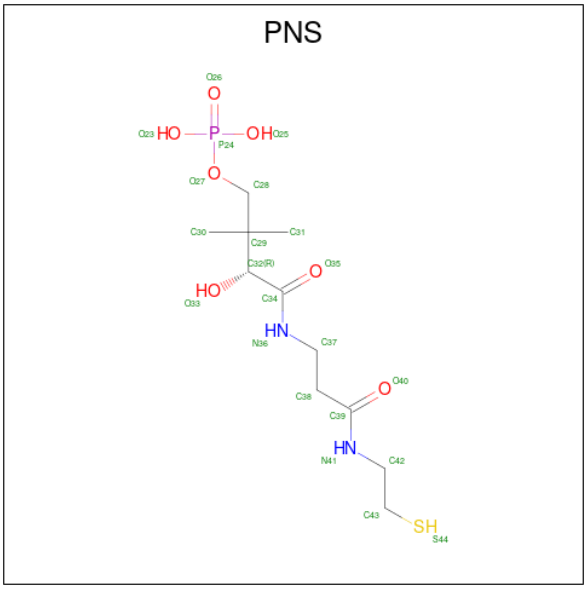
Chain	Residue	Modelled	Actual	Comment	Reference
A	2640	GLY	-	expression tag	UNP A0A1I9RH13
A	2641	SER	-	expression tag	UNP A0A1I9RH13
A	2642	SER	-	expression tag	UNP A0A1I9RH13
A	2643	HIS	-	expression tag	UNP A0A1I9RH13
A	2644	HIS	-	expression tag	UNP A0A1I9RH13
A	2645	HIS	-	expression tag	UNP A0A1I9RH13
A	2646	HIS	-	expression tag	UNP A0A1I9RH13
A	2647	HIS	-	expression tag	UNP A0A1I9RH13
A	2648	HIS	-	expression tag	UNP A0A1I9RH13
A	2649	SER	-	expression tag	UNP A0A1I9RH13
A	2650	SER	-	expression tag	UNP A0A1I9RH13
A	2651	GLY	-	expression tag	UNP A0A1I9RH13
A	2652	LEU	-	expression tag	UNP A0A1I9RH13
A	2653	VAL	-	expression tag	UNP A0A1I9RH13
A	2654	PRO	-	expression tag	UNP A0A1I9RH13
A	2655	ARG	-	expression tag	UNP A0A1I9RH13
A	2656	GLY	-	expression tag	UNP A0A1I9RH13
A	2657	SER	-	expression tag	UNP A0A1I9RH13
A	2658	HIS	-	expression tag	UNP A0A1I9RH13
A	2659	MET	-	expression tag	UNP A0A1I9RH13
A	2818	ALA	CYS	conflict	UNP A0A1I9RH13
B	2640	GLY	-	expression tag	UNP A0A1I9RH13
B	2641	SER	-	expression tag	UNP A0A1I9RH13
B	2642	SER	-	expression tag	UNP A0A1I9RH13
B	2643	HIS	-	expression tag	UNP A0A1I9RH13

Continued on next page...

Continued from previous page...

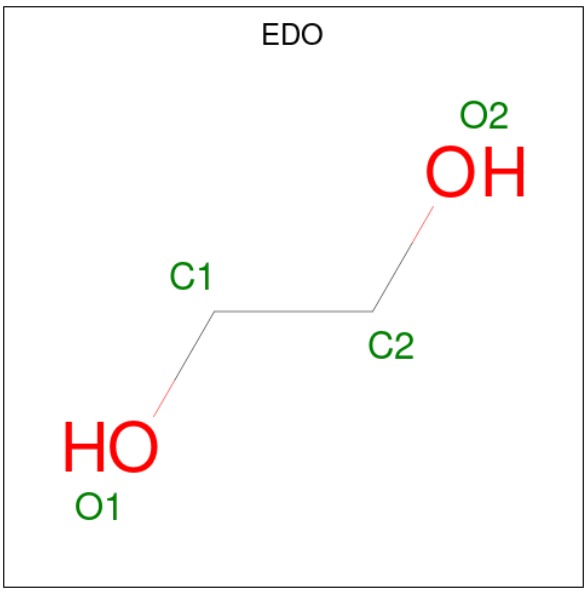
Chain	Residue	Modelled	Actual	Comment	Reference
B	2644	HIS	-	expression tag	UNP A0A1I9RH13
B	2645	HIS	-	expression tag	UNP A0A1I9RH13
B	2646	HIS	-	expression tag	UNP A0A1I9RH13
B	2647	HIS	-	expression tag	UNP A0A1I9RH13
B	2648	HIS	-	expression tag	UNP A0A1I9RH13
B	2649	SER	-	expression tag	UNP A0A1I9RH13
B	2650	SER	-	expression tag	UNP A0A1I9RH13
B	2651	GLY	-	expression tag	UNP A0A1I9RH13
B	2652	LEU	-	expression tag	UNP A0A1I9RH13
B	2653	VAL	-	expression tag	UNP A0A1I9RH13
B	2654	PRO	-	expression tag	UNP A0A1I9RH13
B	2655	ARG	-	expression tag	UNP A0A1I9RH13
B	2656	GLY	-	expression tag	UNP A0A1I9RH13
B	2657	SER	-	expression tag	UNP A0A1I9RH13
B	2658	HIS	-	expression tag	UNP A0A1I9RH13
B	2659	MET	-	expression tag	UNP A0A1I9RH13
B	2818	ALA	CYS	conflict	UNP A0A1I9RH13

- Molecule 2 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: $C_{11}H_{23}N_2O_7PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	0	0
			42	11	21	2	6	1	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			42	11	21	2	6	1	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0

- Molecule 4 is water.

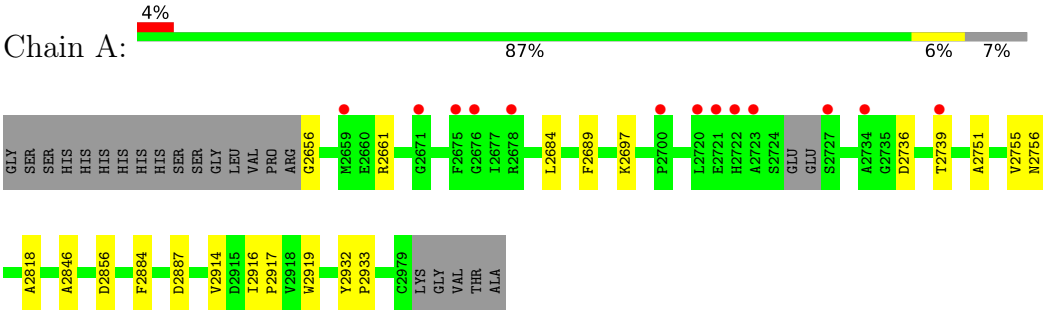
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	16	Total O 16 16	0	0
4	B	12	Total O 12 12	0	0

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.

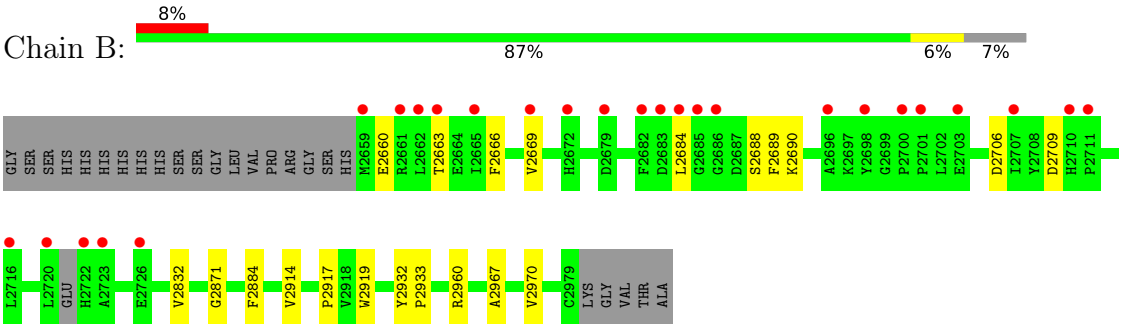
• Molecule 1: Non-ribosomal peptide synthetase

Chain A:



• Molecule 1: Non-ribosomal peptide synthetase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.12Å 79.07Å 70.48Å 90.00° 93.52° 90.00°	Depositor
Resolution (Å)	40.47 – 2.70 47.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.1 (40.47-2.70) 87.1 (47.80-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.35 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.221 , 0.257 0.221 , 0.257	Depositor DCC
R_{free} test set	1768 reflections (9.90%)	wwPDB-VP
Wilson B-factor (Å^2)	42.9	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 48.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9536	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.61% 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: EDO, PNS

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	0.26	0/2454	0.46	0/3345
1	B	0.29	0/2415	0.51	1/3296 (0.0%)
All	All	0.28	0/4869	0.48	1/6641 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2688	SER	N-CA-CB	-5.17	102.75	110.50

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	2401	2325	2340	17	0
1	B	2365	2283	2286	14	0
2	A	21	21	21	6	0
2	B	21	21	21	5	0
3	A	12	18	18	3	0
3	B	8	12	12	0	0
4	A	16	0	0	1	0
4	B	12	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4856	4680	4698	35	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 4.

All (35) 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:A:2656:GLY:O	1:A:2661:ARG:NH1	2.19	0.76
1:A:2689:PHE:CZ	2:A:3001:PNS:H302	2.36	0.61
2:A:3001:PNS:O35	2:A:3001:PNS:H303	2.03	0.58
1:A:2689:PHE:CE1	2:A:3001:PNS:H311	2.38	0.58
1:A:2856:ASP:HB3	4:A:3115:HOH:O	2.03	0.57
2:B:3001:PNS:O35	2:B:3001:PNS:H303	2.04	0.56
1:B:2689:PHE:O	1:B:2690:LYS:HB2	2.06	0.56
1:A:2736:ASP:OD1	1:A:2739:THR:OG1	2.24	0.55
1:A:2697:LYS:CD	3:A:3003:EDO:O2	2.55	0.54
1:B:2832:VAL:HG21	1:B:2914:VAL:HG11	1.93	0.50
2:B:3001:PNS:O35	2:B:3001:PNS:C30	2.59	0.50
1:A:2756:ASN:ND2	2:A:3001:PNS:O33	2.44	0.49
1:B:2689:PHE:CE1	2:B:3001:PNS:H311	2.48	0.49
2:A:3001:PNS:O35	2:A:3001:PNS:C30	2.59	0.49
1:A:2818:ALA:HA	1:A:2846:ALA:HB2	1.95	0.49
1:A:2914:VAL:HG11	1:A:2916:ILE:HD12	1.95	0.47
1:A:2932:TYR:N	1:A:2933:PRO:CD	2.77	0.47
1:A:2884:PHE:CE1	2:A:3001:PNS:H313	2.50	0.47
1:A:2697:LYS:HD2	3:A:3003:EDO:O2	2.15	0.47
1:A:2697:LYS:HD3	3:A:3003:EDO:O2	2.15	0.46
1:B:2871:GLY:O	1:B:2960:ARG:NH1	2.46	0.46
1:B:2917:PRO:HB2	1:B:2919:TRP:CZ3	2.51	0.46
1:B:2706:ASP:O	1:B:2709:ASP:O	2.33	0.45
1:A:2684:LEU:O	1:A:2684:LEU:HD12	2.16	0.45
1:B:2689:PHE:CZ	2:B:3001:PNS:H302	2.52	0.45
1:B:2967:ALA:O	1:B:2970:VAL:HG22	2.17	0.45
1:B:2666:PHE:O	1:B:2669:VAL:HG12	2.17	0.45
1:A:2917:PRO:HB2	1:A:2919:TRP:CZ3	2.54	0.42
1:B:2832:VAL:HG21	1:B:2914:VAL:CG1	2.49	0.42
1:A:2751:ALA:HA	1:A:2887:ASP:HB3	2.02	0.42
1:A:2755:VAL:O	1:A:2758:VAL:HG23	2.20	0.42
1:B:2884:PHE:CE1	2:B:3001:PNS:H313	2.55	0.41
1:B:2932:TYR:N	1:B:2933:PRO:CD	2.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2660:GLU:O	1:B:2663:THR:HG22	2.21	0.41
1:B:2684:LEU:HD12	1:B:2684:LEU:O	2.21	0.40

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	318/345 (92%)	309 (97%)	9 (3%)	0	100	100
1	B	316/345 (92%)	306 (97%)	10 (3%)	0	100	100
All	All	634/690 (92%)	615 (97%)	19 (3%)	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	242/275 (88%)	242 (100%)	0	100	100
1	B	236/275 (86%)	236 (100%)	0	100	100
All	All	478/550 (87%)	478 (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. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	2722	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

7 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	$\#\|Z\| > 2$
3	EDO	A	3003	-	3,3,3	0.82	0	2,2,2	0.39	0
2	PNS	B	3001	1	13,20,21	2.41	3 (23%)	18,26,29	1.59	4 (22%)
3	EDO	B	3002	-	3,3,3	0.48	0	2,2,2	0.36	0
2	PNS	A	3001	1	13,20,21	2.45	4 (30%)	18,26,29	1.57	3 (16%)
3	EDO	A	3004	-	3,3,3	0.85	0	2,2,2	0.40	0
3	EDO	B	3003	-	3,3,3	0.45	0	2,2,2	0.46	0
3	EDO	A	3002	-	3,3,3	0.47	0	2,2,2	0.31	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	EDO	A	3003	-	-	0/1/1/1	-
2	PNS	B	3001	1	-	13/24/26/27	-
3	EDO	B	3002	-	-	0/1/1/1	-
2	PNS	A	3001	1	-	13/24/26/27	-
3	EDO	A	3004	-	-	1/1/1/1	-
3	EDO	B	3003	-	-	1/1/1/1	-
3	EDO	A	3002	-	-	0/1/1/1	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	PNS	C34-N36	5.73	1.46	1.33
2	B	3001	PNS	C34-N36	5.57	1.45	1.33
2	A	3001	PNS	C39-N41	5.40	1.45	1.33
2	B	3001	PNS	C39-N41	5.34	1.45	1.33
2	B	3001	PNS	O35-C34	-2.49	1.18	1.23
2	A	3001	PNS	O35-C34	-2.48	1.18	1.23
2	A	3001	PNS	O40-C39	-2.12	1.19	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3001	PNS	O35-C34-N36	-3.28	115.96	122.99
2	A	3001	PNS	O35-C34-N36	-3.12	116.29	122.99
2	B	3001	PNS	C37-N36-C34	-2.41	118.28	122.59
2	A	3001	PNS	C37-N36-C34	-2.36	118.38	122.59
2	B	3001	PNS	C32-C34-N36	2.32	121.19	116.58
2	A	3001	PNS	C32-C34-N36	2.27	121.11	116.58
2	B	3001	PNS	C37-C38-C39	-2.15	108.77	112.36

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3001	PNS	O27-C28-C29-C32
2	A	3001	PNS	C28-C29-C32-O33
2	A	3001	PNS	C28-C29-C32-C34
2	A	3001	PNS	C30-C29-C32-O33
2	A	3001	PNS	C30-C29-C32-C34
2	A	3001	PNS	C31-C29-C32-O33
2	A	3001	PNS	C31-C29-C32-C34
2	A	3001	PNS	O33-C32-C34-O35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	3001	PNS	O33-C32-C34-N36
2	B	3001	PNS	C28-C29-C32-O33
2	B	3001	PNS	C28-C29-C32-C34
2	B	3001	PNS	C30-C29-C32-O33
2	B	3001	PNS	C30-C29-C32-C34
2	B	3001	PNS	C31-C29-C32-O33
2	B	3001	PNS	C31-C29-C32-C34
2	B	3001	PNS	O33-C32-C34-O35
2	B	3001	PNS	O33-C32-C34-N36
3	B	3003	EDO	O1-C1-C2-O2
2	A	3001	PNS	O27-C28-C29-C30
2	A	3001	PNS	O27-C28-C29-C31
2	B	3001	PNS	O27-C28-C29-C30
2	B	3001	PNS	O27-C28-C29-C31
3	A	3004	EDO	O1-C1-C2-O2
2	A	3001	PNS	C29-C32-C34-O35
2	B	3001	PNS	C29-C32-C34-O35
2	A	3001	PNS	C29-C32-C34-N36
2	B	3001	PNS	C29-C32-C34-N36
2	B	3001	PNS	O27-C28-C29-C32

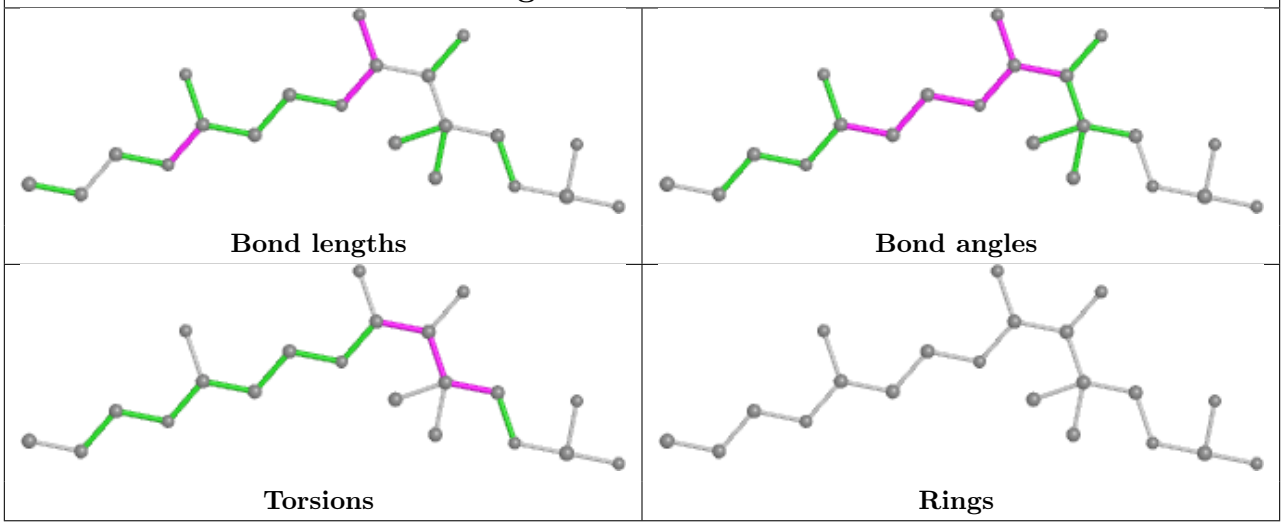
There are no ring outliers.

3 monomers are involved in 14 short contacts:

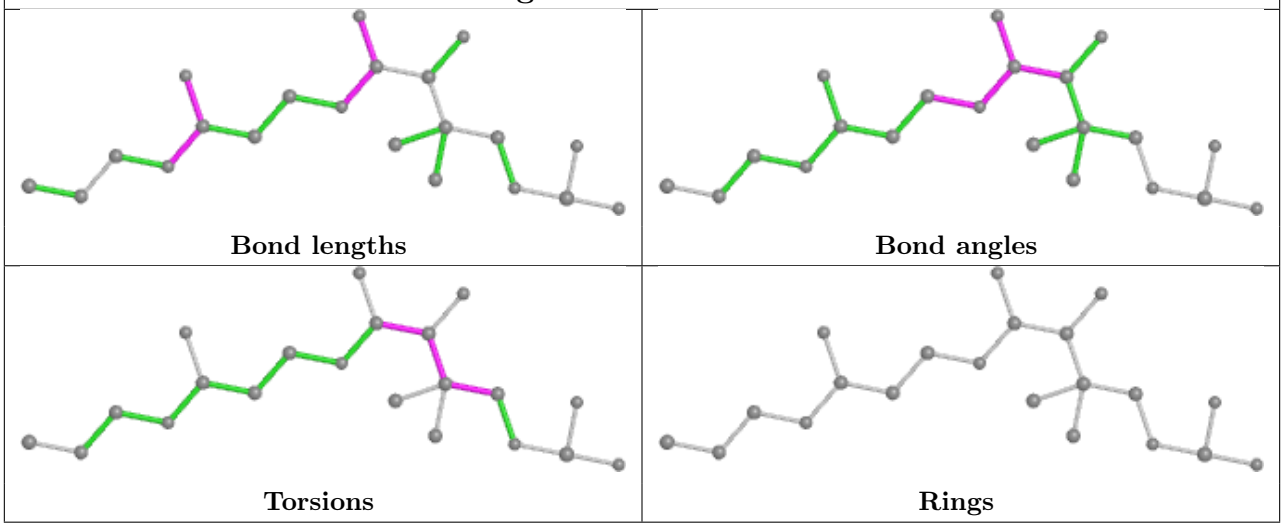
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3003	EDO	3	0
2	B	3001	PNS	5	0
2	A	3001	PNS	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PNS B 3001



Ligand PNS A 3001



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	322/345 (93%)	0.44	14 (4%)	35	33	30, 45, 71, 108	0
1	B	320/345 (92%)	0.53	26 (8%)	12	10	31, 48, 85, 106	0
All	All	642/690 (93%)	0.48	40 (6%)	20	19	30, 46, 81, 108	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2722	HIS	5.9
1	B	2661	ARG	4.2
1	A	2675	PHE	4.2
1	B	2665	ILE	4.0
1	B	2663	THR	3.9
1	B	2707	ILE	3.8
1	B	2669	VAL	3.8
1	B	2685	GLY	3.8
1	A	2700	PRO	3.6
1	B	2723	ALA	3.5
1	B	2711	PRO	3.4
1	B	2682	PHE	3.4
1	B	2710	HIS	3.2
1	B	2684	LEU	3.2
1	B	2679	ASP	3.1
1	B	2726	GLU	3.1
1	B	2722	HIS	2.9
1	A	2676	GLY	2.9
1	B	2672	HIS	2.9
1	B	2698	TYR	2.9
1	B	2700	PRO	2.9
1	A	2727	SER	2.8
1	A	2739	THR	2.8
1	B	2701	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	2723	ALA	2.6
1	B	2703	GLU	2.6
1	A	2659	MET	2.5
1	A	2721	GLU	2.4
1	A	2720	LEU	2.4
1	B	2662	LEU	2.4
1	A	2678	ARG	2.4
1	B	2686	GLY	2.3
1	A	2734	ALA	2.3
1	A	2802	ASP	2.3
1	B	2696	ALA	2.3
1	A	2671	GLY	2.3
1	B	2716	LEU	2.3
1	B	2720	LEU	2.2
1	B	2659	MET	2.1
1	B	2683	ASP	2.1

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)

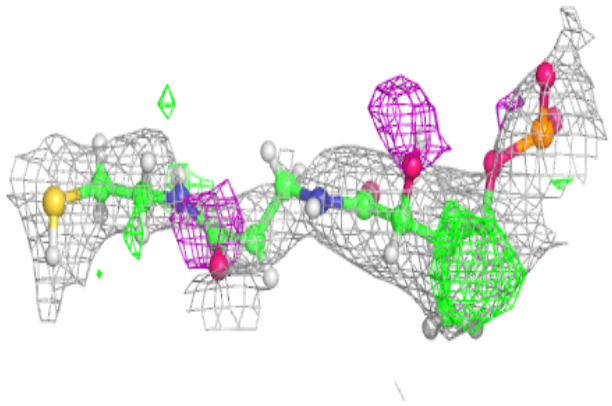
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

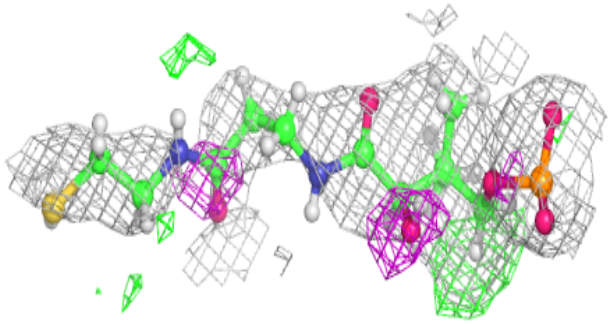
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	A	3004	4/4	0.52	0.46	46,61,65,73	0
3	EDO	B	3002	4/4	0.70	0.21	48,63,73,76	0
2	PNS	B	3001	21/22	0.79	0.33	47,64,82,108	0
3	EDO	A	3002	4/4	0.81	0.25	51,67,81,81	0
3	EDO	B	3003	4/4	0.86	0.42	49,59,86,86	0
2	PNS	A	3001	21/22	0.89	0.22	42,59,70,105	0
3	EDO	A	3003	4/4	0.91	0.11	51,61,67,70	0

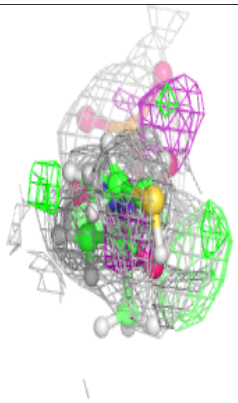
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PNS B 3001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

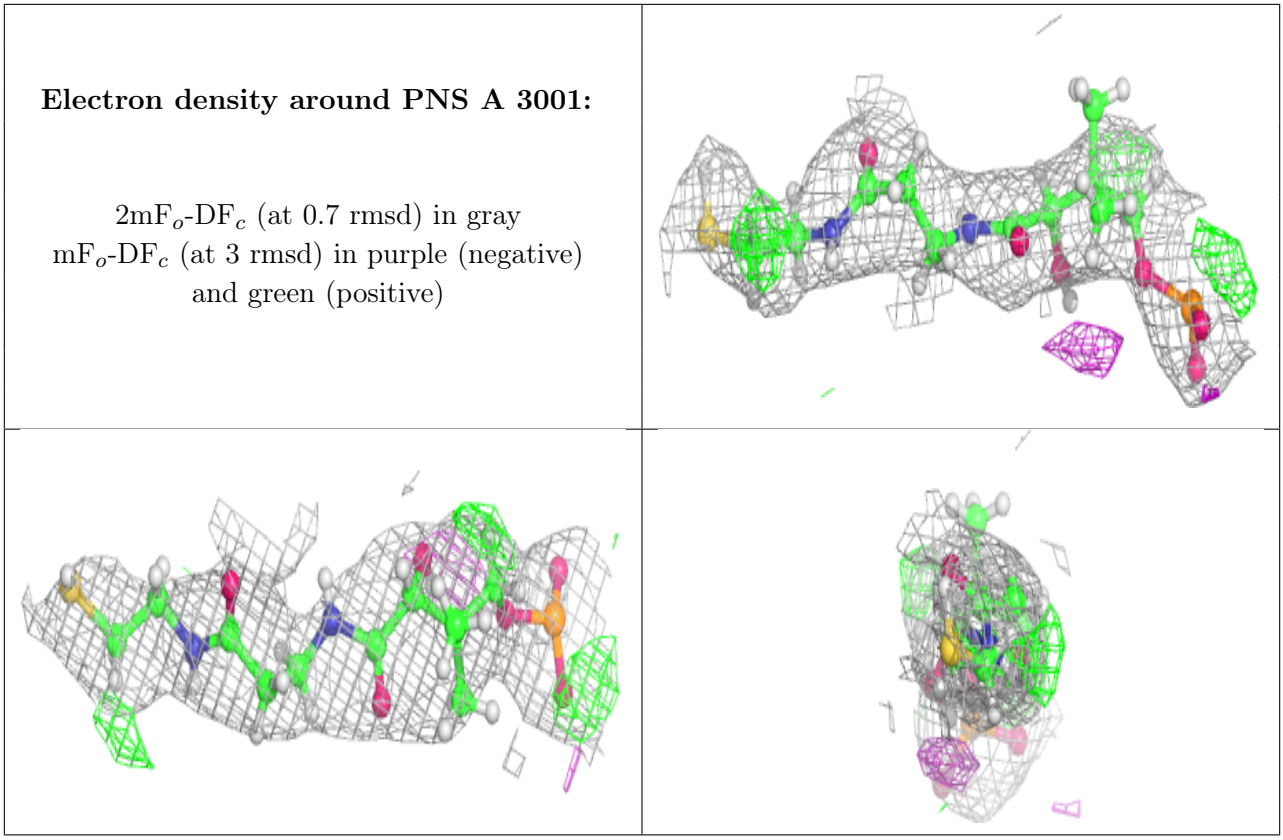






Electron density around PNS A 3001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.