



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 02:14 AM EDT

PDB ID : 3LSM  
Title : Pyranose 2-oxidase H167A mutant with flavin N(5) sulfite adduct  
Authors : Tan, T.C.; Spadiut, O.; Divne, C.  
Deposited on : 2010-02-12  
Resolution : 1.70 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

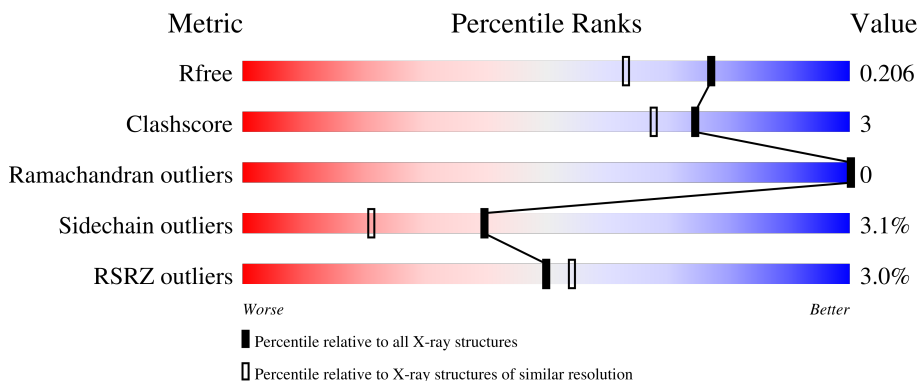
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	623	
1	B	623	

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
2	SFD	A	801	X	-	-	-
2	SFD	B	801	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10395 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.

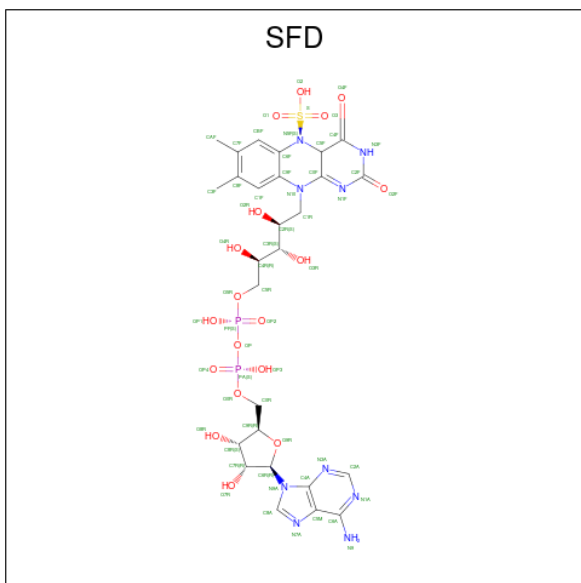
- Molecule 1 is a protein called Pyranose 2-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	574	Total 4521	C 2856	N 773	O 868	S 24	0	0	0
1	B	576	Total 4537	C 2865	N 775	O 872	S 25	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

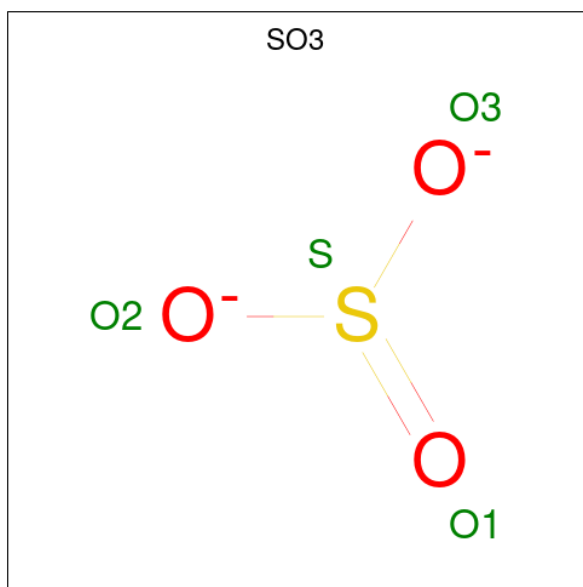
Chain	Residue	Modelled	Actual	Comment	Reference
A	167	ALA	HIS	engineered mutation	UNP Q7ZA32
B	167	ALA	HIS	engineered mutation	UNP Q7ZA32

- Molecule 2 is (S)-10-((2S,3S,4R)-5-((S)-((S)-(((2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3,4-DIHYDROXY-TETRAHYDROFURAN-2-YL)METHOXY)(HYDROXY)PHOSPHORYLOXY)(HYDROXY)PHOSPHORYLOXY)-2,3,4-TRIHYDROXYPENTYL)-7,8-DIMETHYL-2,4-DIOXO-2,3,4,4A-TETRAHYDROBENZO[G]PTERIDINE-5(10H)-SULFONIC ACID (three-letter code: SFD) (formula: C<sub>27</sub>H<sub>35</sub>N<sub>9</sub>O<sub>18</sub>P<sub>2</sub>S).



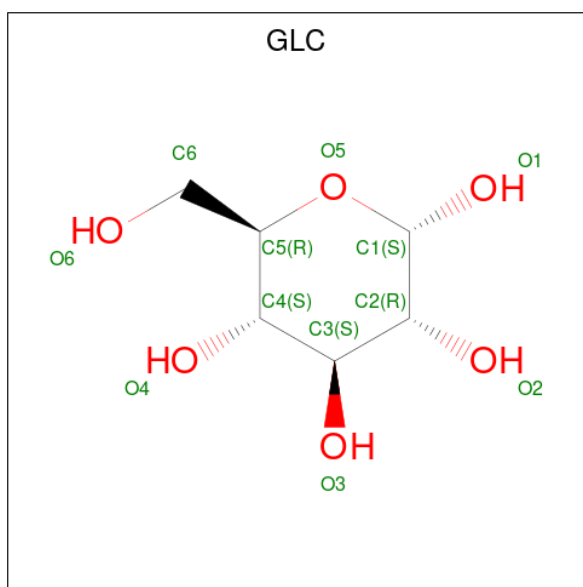
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	S	0	0
			57	27	9	18	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			57	27	9	18	2	1		

- Molecule 3 is SULFITE ION (three-letter code: SO3) (formula: O<sub>3</sub>S).



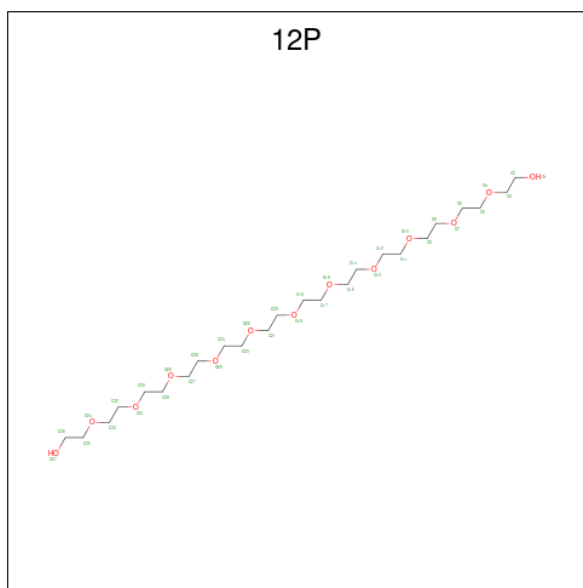
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			4	3 1		
3	A	1	Total	O S	0	0
			4	3 1		
3	B	1	Total	O S	0	0
			4	3 1		
3	B	1	Total	O S	0	0
			4	3 1		

- Molecule 4 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is DODECAETHYLENE GLYCOL (three-letter code: 12P) (formula:  $C_{24}H_{50}O_{13}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	8	4		
5	B	1	Total	C	O	0	0
			14	9	5		

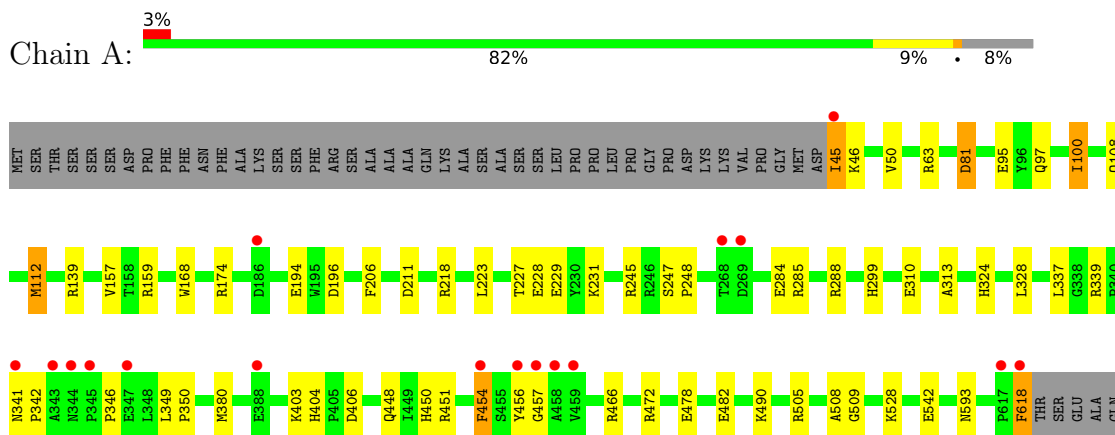
- Molecule 6 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	A	607	Total 607	O 607	0	0
6	B	562	Total 562	O 562	0	0

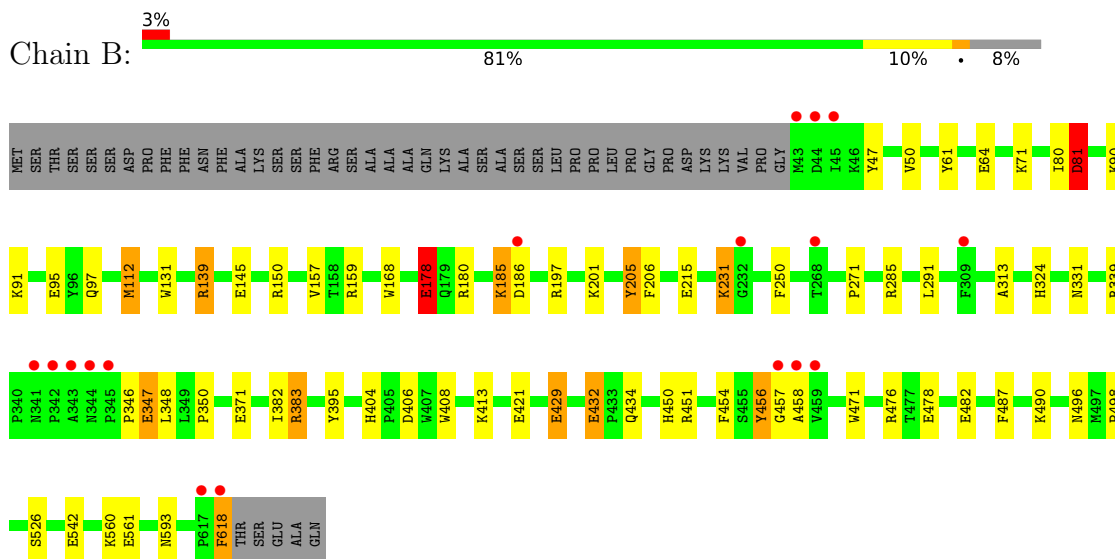
### 3 Residue-property plots [i](#)

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: Pyranose 2-oxidase



- Molecule 1: Pyranose 2-oxidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.57Å 101.57Å 249.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.20 – 1.70 29.18 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.20-1.70) 99.5 (29.18-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.160 , 0.195 0.174 , 0.206	Depositor DCC
$R_{free}$ test set	2871 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.0	Xtrriage
Anisotropy	0.255	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10395	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3927e-03.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, 12P, SFD, SO3

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	1.19	15/4636 (0.3%)	1.12	26/6304 (0.4%)
1	B	1.17	22/4652 (0.5%)	1.10	17/6325 (0.3%)
All	All	1.18	37/9288 (0.4%)	1.11	43/12629 (0.3%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	478	GLU	CD-OE1	8.10	1.34	1.25
1	A	310	GLU	CB-CG	-7.56	1.37	1.52
1	B	542	GLU	CD-OE1	7.02	1.33	1.25
1	A	482	GLU	CG-CD	6.98	1.62	1.51
1	B	432	GLU	CD-OE2	6.73	1.33	1.25
1	B	95	GLU	CB-CG	-6.46	1.39	1.52
1	B	178	GLU	CG-CD	6.39	1.61	1.51
1	B	81	ASP	CB-CG	-6.39	1.38	1.51
1	B	371	GLU	CG-CD	6.21	1.61	1.51
1	A	81	ASP	CB-CG	-6.13	1.38	1.51
1	A	211	ASP	CB-CG	6.10	1.64	1.51
1	B	215	GLU	CB-CG	-6.07	1.40	1.52
1	A	542	GLU	CD-OE1	5.91	1.32	1.25
1	A	112	MET	CB-CG	5.85	1.70	1.51
1	B	131	TRP	CE3-CZ3	5.83	1.48	1.38
1	A	95	GLU	CB-CG	-5.77	1.41	1.52
1	B	429	GLU	CG-CD	5.77	1.60	1.51
1	A	509	GLY	N-CA	-5.72	1.37	1.46
1	B	64	GLU	CD-OE1	5.62	1.31	1.25
1	B	395	TYR	CD2-CE2	5.58	1.47	1.39
1	A	63	ARG	CG-CD	-5.50	1.38	1.51
1	B	482	GLU	CG-CD	5.48	1.60	1.51
1	B	421	GLU	CB-CG	5.48	1.62	1.52
1	B	478	GLU	CD-OE1	5.41	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	560	LYS	CE-NZ	5.32	1.62	1.49
1	B	561	GLU	CG-CD	5.30	1.59	1.51
1	A	508	ALA	C-O	5.28	1.33	1.23
1	B	112	MET	CB-CG	5.25	1.68	1.51
1	B	61	TYR	CD1-CE1	5.23	1.47	1.39
1	A	194	GLU	CG-CD	5.23	1.59	1.51
1	A	482	GLU	CD-OE1	5.21	1.31	1.25
1	B	478	GLU	CG-CD	5.15	1.59	1.51
1	A	542	GLU	CG-CD	5.14	1.59	1.51
1	B	250	PHE	CE2-CZ	5.10	1.47	1.37
1	A	211	ASP	CG-OD1	5.10	1.37	1.25
1	B	205	TYR	CD1-CE1	5.08	1.47	1.39
1	B	91	LYS	CB-CG	-5.01	1.39	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ARG	NE-CZ-NH1	24.26	132.43	120.30
1	A	139	ARG	NE-CZ-NH1	23.88	132.24	120.30
1	B	139	ARG	NE-CZ-NH2	-20.09	110.25	120.30
1	A	139	ARG	NE-CZ-NH2	-13.71	113.45	120.30
1	B	383	ARG	NE-CZ-NH1	-12.37	114.11	120.30
1	A	211	ASP	CB-CG-OD1	10.86	128.07	118.30
1	A	196	ASP	CB-CG-OD1	10.64	127.87	118.30
1	B	451	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	A	380	MET	CG-SD-CE	-8.54	86.53	100.20
1	A	466	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	B	139	ARG	CD-NE-CZ	7.03	133.44	123.60
1	A	339	ARG	NE-CZ-NH1	-6.97	116.82	120.30
1	A	139	ARG	CD-NE-CZ	6.53	132.74	123.60
1	B	150	ARG	NE-CZ-NH1	-6.53	117.04	120.30
1	A	349	LEU	CB-CG-CD2	6.07	121.32	111.00
1	A	451	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	B	383	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	B	159	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	339	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	A	288	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	B	406	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	97	GLN	CA-CB-CG	-5.75	100.76	113.40
1	B	97	GLN	CA-CB-CG	-5.72	100.81	113.40
1	A	228	GLU	CB-CA-C	-5.69	99.02	110.40
1	A	196	ASP	CB-CG-OD2	-5.67	113.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	81	ASP	N-CA-C	5.60	126.11	111.00
1	A	228	GLU	CA-CB-CG	5.51	125.52	113.40
1	A	406	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	245	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	180	ARG	N-CA-CB	-5.38	100.91	110.60
1	B	159	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	B	150	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	A	505	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	339	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	A	174	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	288	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	197	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	B	80	ILE	C-N-CA	5.13	134.52	121.70
1	A	337	LEU	CB-CG-CD2	-5.13	102.28	111.00
1	A	81	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	A	81	ASP	CB-CA-C	-5.05	100.30	110.40
1	B	81	ASP	CB-CA-C	-5.00	100.40	110.40

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	4521	0	4373	27	0
1	B	4537	0	4386	30	0
2	A	57	0	32	0	0
2	B	57	0	32	0	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
4	A	12	0	12	0	0
5	A	12	0	14	0	0
5	B	14	0	16	0	0
6	A	607	0	0	8	0
6	B	562	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10395	0	8865	57	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.

All (57) 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:B:231:LYS:O	1:B:231:LYS:HG2	1.64	0.95
1:A:618:PHE:C	1:A:618:PHE:HD1	1.90	0.76
1:A:618:PHE:C	1:A:618:PHE:CD1	2.63	0.72
1:B:404:HIS:HE1	6:B:1489:HOH:O	1.79	0.66
1:A:218:ARG:HD2	6:A:1144:HOH:O	1.96	0.66
1:B:178:GLU:CD	1:B:476:ARG:HH12	2.00	0.64
1:B:456:TYR:HE1	6:B:2149:HOH:O	1.80	0.63
1:A:404:HIS:HE1	6:A:1488:HOH:O	1.83	0.62
1:B:458:ALA:HB2	6:B:2039:HOH:O	2.01	0.61
1:A:285:ARG:NH2	1:A:299:HIS:ND1	2.49	0.60
1:A:223:LEU:O	1:A:227:THR:HG23	2.03	0.59
1:B:618:PHE:CD1	1:B:618:PHE:C	2.75	0.56
1:B:383:ARG:NH1	6:B:1635:HOH:O	2.37	0.56
1:B:145:GLU:OE2	1:B:490:LYS:NZ	2.37	0.55
1:A:457:GLY:HA3	6:A:1555:HOH:O	2.06	0.55
1:B:347:GLU:HG3	1:B:348:LEU:N	2.20	0.55
1:A:50:VAL:HG13	1:A:313:ALA:HB2	1.88	0.55
1:B:456:TYR:CE1	6:B:2149:HOH:O	2.53	0.54
1:A:285:ARG:NH2	1:A:299:HIS:CE1	2.76	0.53
1:B:231:LYS:O	1:B:231:LYS:CG	2.46	0.53
1:B:231:LYS:HD3	1:B:231:LYS:H	1.76	0.50
1:B:618:PHE:C	1:B:618:PHE:HD1	2.15	0.50
1:B:81:ASP:O	1:B:90:LYS:HE2	2.12	0.50
1:A:229:GLU:O	1:A:231:LYS:HD3	2.12	0.49
1:B:457:GLY:HA3	6:B:1380:HOH:O	2.13	0.49
1:B:50:VAL:HG13	1:B:313:ALA:HB2	1.94	0.49
1:B:285:ARG:HD3	1:B:331:ASN:O	2.13	0.48
1:A:108:GLN:HG2	6:A:2068:HOH:O	2.12	0.47
1:B:157:VAL:HG21	1:B:324:HIS:HE1	1.78	0.47
1:B:346:PRO:HG2	1:B:350:PRO:HA	1.96	0.47
1:A:247:SER:HB2	1:A:248:PRO:CD	2.45	0.47
1:B:178:GLU:O	1:B:178:GLU:HG3	2.15	0.46
1:A:45:ILE:CG1	1:A:46:LYS:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ARG:CG	6:A:2057:HOH:O	2.64	0.46
1:A:100:ILE:HD11	6:A:2158:HOH:O	2.15	0.45
1:A:404:HIS:CE1	6:A:1488:HOH:O	2.64	0.45
1:A:157:VAL:HG21	1:A:324:HIS:HE1	1.82	0.45
1:A:454:PHE:CD1	1:A:456:TYR:CE2	3.06	0.44
1:A:284:GLU:C	1:A:328:LEU:CD1	2.85	0.44
1:A:346:PRO:HG2	1:A:350:PRO:HA	1.99	0.44
1:B:382:ILE:HD13	6:B:1570:HOH:O	2.18	0.44
1:B:471:TRP:CH2	1:B:526:SER:HA	2.52	0.44
1:A:285:ARG:HH22	1:A:299:HIS:CE1	2.35	0.44
1:A:284:GLU:O	1:A:328:LEU:CD1	2.66	0.43
1:A:448:GLN:NE2	1:A:472:ARG:HH21	2.16	0.43
1:A:285:ARG:HG2	6:A:2057:HOH:O	2.18	0.43
1:A:341:ASN:HA	1:A:342:PRO:HD2	1.87	0.43
1:B:487:PHE:HB3	1:B:498:PRO:HB2	2.01	0.43
1:A:247:SER:HB2	1:A:248:PRO:HD2	2.00	0.42
1:B:47:TYR:O	1:B:313:ALA:HA	2.20	0.42
1:B:271:PRO:HG3	6:B:1928:HOH:O	2.19	0.42
1:B:201:LYS:NZ	6:B:2083:HOH:O	2.44	0.41
1:B:201:LYS:HE2	1:B:205:TYR:OH	2.20	0.41
1:B:432:GLU:HG3	1:B:434:GLN:NE2	2.36	0.41
1:B:185:LYS:O	1:B:186:ASP:HB2	2.20	0.41
1:A:229:GLU:HB3	1:A:528:LYS:HD3	2.03	0.41
1:B:71:LYS:HE3	6:B:1971:HOH:O	2.22	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	572/623 (92%)	558 (98%)	14 (2%)	0	<a href="#">100</a> <a href="#">100</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	574/623 (92%)	561 (98%)	13 (2%)	0	100	100
All	All	1146/1246 (92%)	1119 (98%)	27 (2%)	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	501/541 (93%)	489 (98%)	12 (2%)	49	31
1	B	503/541 (93%)	484 (96%)	19 (4%)	33	14
All	All	1004/1082 (93%)	973 (97%)	31 (3%)	40	21

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ILE
1	A	81	ASP
1	A	100	ILE
1	A	112	MET
1	A	168	TRP
1	A	206	PHE
1	A	403	LYS
1	A	450	HIS
1	A	454	PHE
1	A	490	LYS
1	A	593	ASN
1	A	618	PHE
1	B	81	ASP
1	B	112	MET
1	B	139	ARG
1	B	168	TRP
1	B	178	GLU
1	B	185	LYS

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Mol	Chain	Res	Type
1	B	206	PHE
1	B	231	LYS
1	B	291	LEU
1	B	347	GLU
1	B	408	TRP
1	B	413	LYS
1	B	429	GLU
1	B	450	HIS
1	B	454	PHE
1	B	456	TYR
1	B	496	ASN
1	B	593	ASN
1	B	618	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	A	263	GLN
1	A	324	HIS
1	A	344	ASN
1	A	404	HIS
1	A	461	GLN
1	A	563	ASN
1	B	132	GLN
1	B	233	GLN
1	B	263	GLN
1	B	324	HIS
1	B	404	HIS
1	B	461	GLN

### 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](#)

9 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
5	12P	B	902	-	13,13,36	0.54	0	12,12,35	0.40	0
2	SFD	B	801	-	54,62,62	3.23	19 (35%)	64,97,97	1.90	15 (23%)
2	SFD	A	801	-	54,62,62	3.01	14 (25%)	64,97,97	2.02	16 (25%)
3	SO3	A	911	-	1,3,3	1.67	0	0,3,3	-	-
3	SO3	B	911	-	1,3,3	1.75	0	0,3,3	-	-
4	GLC	A	912	-	12,12,12	0.75	0	17,17,17	2.21	4 (23%)
3	SO3	B	910	-	1,3,3	0.19	0	0,3,3	-	-
5	12P	A	901	-	11,11,36	0.58	0	10,10,35	0.37	0
3	SO3	A	910	-	1,3,3	0.80	0	0,3,3	-	-

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	12P	B	902	-	-	1/11/11/34	-
2	SFD	B	801	-	1/1/16/17	1/34/88/88	0/5/6/6
2	SFD	A	801	-	1/1/16/17	4/34/88/88	0/5/6/6
4	GLC	A	912	-	-	0/2/22/22	0/1/1/1
5	12P	A	901	-	-	3/9/9/34	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	SFD	C6F-N5F	-12.62	1.32	1.44
2	A	801	SFD	C6F-N5F	-12.09	1.33	1.44
2	B	801	SFD	O3-S	10.53	1.54	1.42
2	A	801	SFD	O3-S	9.67	1.53	1.42
2	B	801	SFD	C5F-C4F	-8.13	1.45	1.52
2	A	801	SFD	C1R-C2R	7.79	1.63	1.52
2	A	801	SFD	C5F-C4F	-6.57	1.47	1.52
2	B	801	SFD	C1R-C2R	6.32	1.61	1.52
2	B	801	SFD	C0F-N1F	5.62	1.43	1.31
2	A	801	SFD	C9F-N10	4.70	1.49	1.41
2	B	801	SFD	O1-S	4.70	1.47	1.42
2	A	801	SFD	O9R-C6R	4.49	1.47	1.41
2	A	801	SFD	O1-S	4.19	1.46	1.42
2	B	801	SFD	C5F-N5F	-3.76	1.41	1.49
2	A	801	SFD	C1F-C8F	3.42	1.44	1.39
2	B	801	SFD	C9F-N10	3.36	1.47	1.41
2	B	801	SFD	O9R-C9R	-3.27	1.37	1.45
2	A	801	SFD	C5F-N5F	-3.18	1.42	1.49
2	B	801	SFD	C4F-N3F	3.10	1.42	1.37
2	B	801	SFD	C1F-C9F	3.10	1.44	1.39
2	B	801	SFD	C7R-C6R	2.85	1.58	1.53
2	B	801	SFD	CBF-C7F	2.79	1.43	1.39
2	B	801	SFD	C4R-C3R	2.68	1.58	1.53
2	B	801	SFD	C5R-C4R	2.63	1.55	1.51
2	A	801	SFD	C0F-N10	2.37	1.42	1.38
2	A	801	SFD	O5R-C5R	2.30	1.53	1.44
2	B	801	SFD	C0F-N10	-2.29	1.34	1.38
2	B	801	SFD	C2A-N3A	2.12	1.35	1.32
2	A	801	SFD	O4R-C4R	2.07	1.47	1.43
2	B	801	SFD	O5R-C5R	2.06	1.52	1.44
2	B	801	SFD	C5M-C4A	-2.04	1.35	1.40
2	A	801	SFD	C4F-N3F	2.03	1.40	1.37
2	A	801	SFD	C2F-N3F	-2.03	1.34	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	SFD	C5F-N5F-S	-7.00	104.91	117.50
2	A	801	SFD	C5F-N5F-S	-6.46	105.88	117.50
2	A	801	SFD	C1F-C9F-N10	-5.74	114.08	121.84
2	A	801	SFD	O1-S-N5F	5.72	121.96	109.91
2	A	801	SFD	O3-S-O1	-4.92	106.41	119.22
4	A	912	GLC	O5-C1-C2	4.88	119.00	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	SFD	CAF-C7F-CBF	-4.17	111.78	119.49
4	A	912	GLC	C1-C2-C3	-4.16	101.69	110.31
4	A	912	GLC	C1-O5-C5	-4.08	105.96	113.66
2	B	801	SFD	O5R-C5R-C4R	-4.07	98.49	109.36
4	A	912	GLC	O1-C1-C2	3.89	120.00	109.03
2	B	801	SFD	O3-S-N5F	-3.87	101.76	109.91
2	B	801	SFD	N3A-C2A-N1A	-3.68	122.92	128.68
2	B	801	SFD	C1R-N10-C9F	3.60	126.51	120.51
2	B	801	SFD	C5R-C4R-C3R	-3.54	105.36	112.20
2	B	801	SFD	O3-S-O1	-3.48	110.15	119.22
2	B	801	SFD	C1F-C9F-N10	-3.41	117.23	121.84
2	A	801	SFD	N3A-C2A-N1A	-3.23	123.63	128.68
2	B	801	SFD	O1-S-N5F	3.03	116.28	109.91
2	B	801	SFD	CAF-C7F-CBF	-2.84	114.24	119.49
2	B	801	SFD	CBF-C7F-C8F	2.79	123.67	119.67
2	A	801	SFD	C6F-C9F-N10	2.68	122.41	118.92
2	A	801	SFD	C9F-C1F-C8F	-2.44	114.40	119.30
2	A	801	SFD	CBF-C7F-C8F	2.39	123.10	119.67
2	A	801	SFD	C1F-C9F-C6F	2.23	123.50	120.11
2	A	801	SFD	O3-S-N5F	-2.22	105.24	109.91
2	B	801	SFD	C5M-C6A-N9	2.17	123.66	120.35
2	A	801	SFD	CAF-C7F-C8F	2.14	125.12	120.74
2	B	801	SFD	O9R-C6R-C7R	-2.09	103.87	106.93
2	A	801	SFD	O9R-C9R-C0R	-2.08	102.54	109.37
2	B	801	SFD	C7R-C8R-C9R	2.08	106.67	102.64
2	A	801	SFD	O9R-C6R-C7R	-2.07	103.90	106.93
2	A	801	SFD	C1R-N10-C9F	2.03	123.89	120.51
2	B	801	SFD	O9R-C9R-C0R	-2.02	102.72	109.37
2	A	801	SFD	C8R-C7R-C6R	2.02	104.02	100.98

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	801	SFD	C5F
2	B	801	SFD	C5F

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	901	12P	O13-C14-C15-O16
2	A	801	SFD	PA-OP-PF-O5R
2	A	801	SFD	C6F-N5F-S-O3

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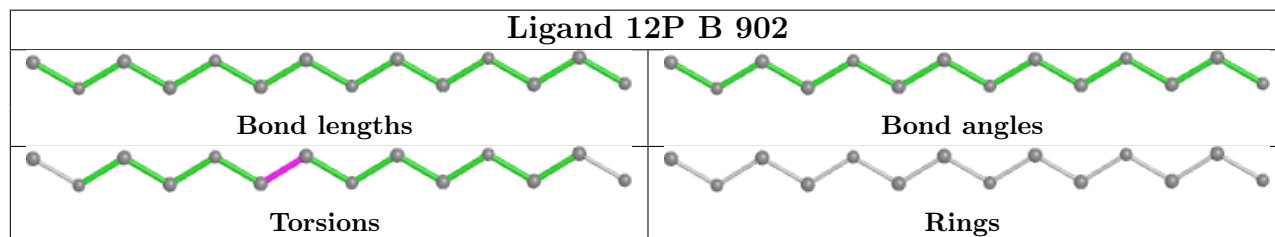
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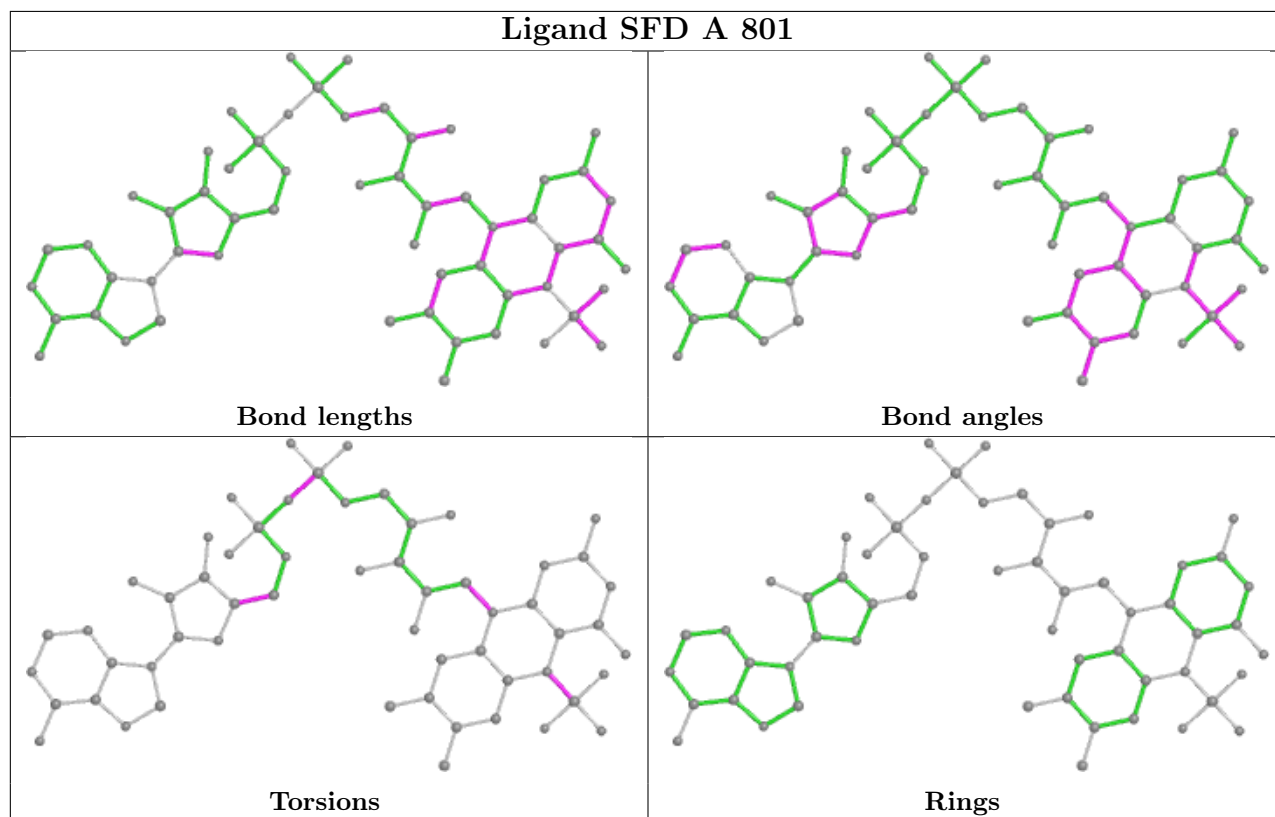
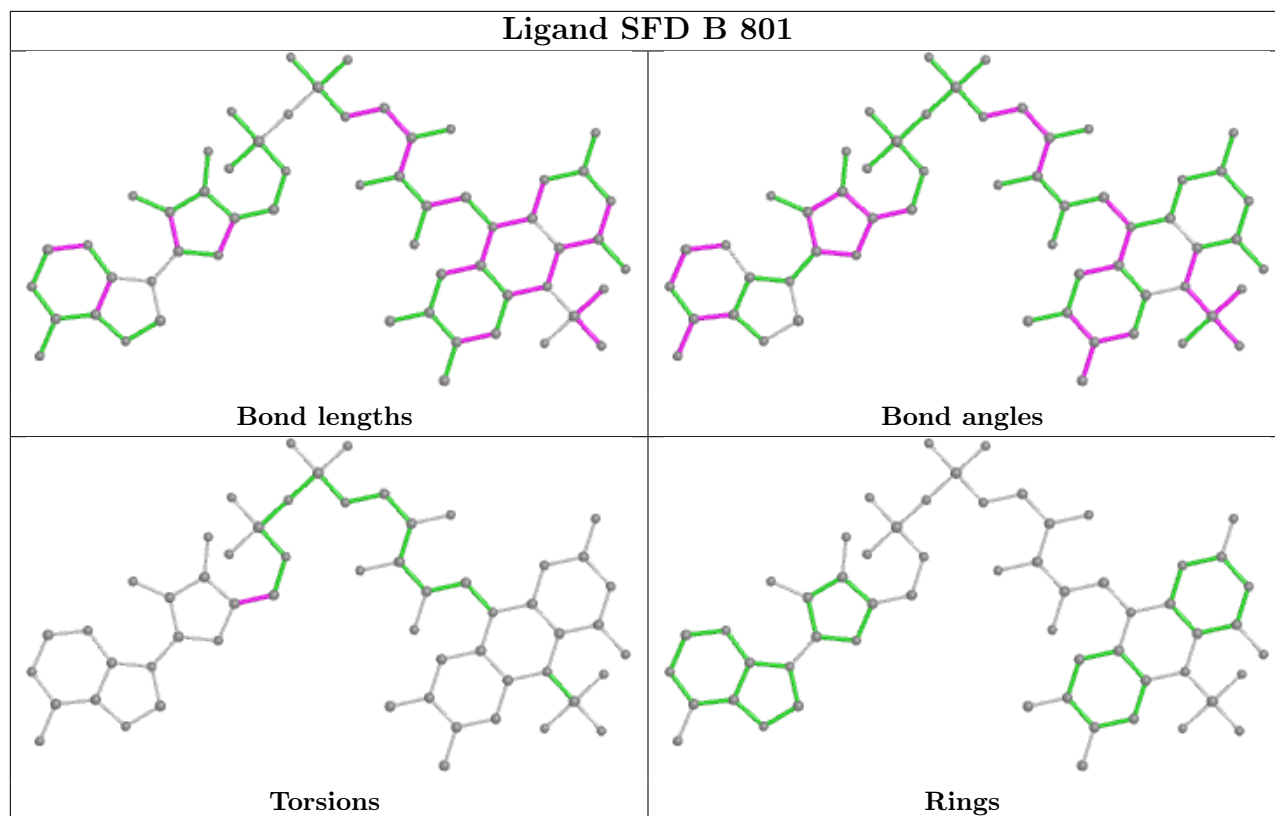
Mol	Chain	Res	Type	Atoms
5	B	902	12P	O7-C8-C9-O10
5	A	901	12P	O10-C11-C12-O13
5	A	901	12P	O7-C8-C9-O10
2	A	801	SFD	C2R-C1R-N10-C0F
2	A	801	SFD	O0R-C0R-C9R-O9R
2	B	801	SFD	O0R-C0R-C9R-O9R

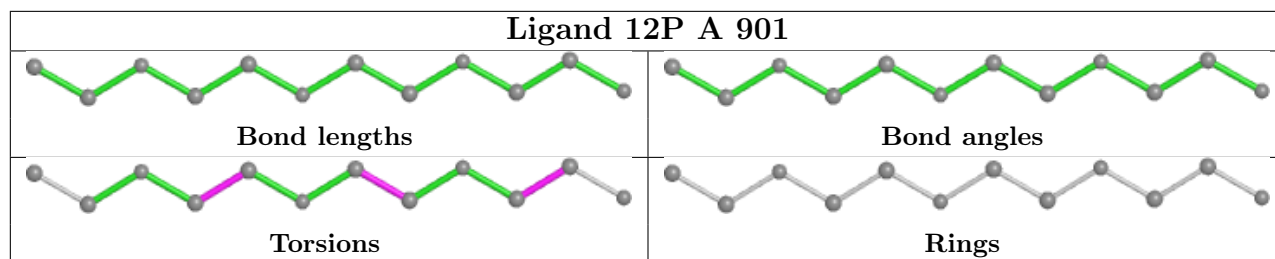
There are no ring outliers.

No monomer is involved in short contacts.

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 than 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.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	574/623 (92%)	-0.13	17 (2%) 50 54	11, 16, 32, 51	0
1	B	576/623 (92%)	-0.06	17 (2%) 50 54	11, 18, 34, 58	0
All	All	1150/1246 (92%)	-0.09	34 (2%) 50 54	11, 17, 34, 58	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	343	ALA	7.5
1	B	618	PHE	6.0
1	A	618	PHE	5.8
1	B	459	VAL	5.7
1	B	344	ASN	5.5
1	A	45	ILE	5.3
1	A	459	VAL	5.2
1	B	458	ALA	4.7
1	A	343	ALA	4.4
1	B	345	PRO	4.1
1	B	341	ASN	4.0
1	B	457	GLY	3.8
1	B	232	GLY	3.4
1	A	458	ALA	3.3
1	B	342	PRO	3.2
1	B	45	ILE	3.1
1	A	344	ASN	3.1
1	B	44	ASP	3.0
1	B	617	PRO	2.8
1	A	268	THR	2.7
1	B	43	MET	2.7
1	B	309	PHE	2.5
1	A	345	PRO	2.5
1	B	186	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	341	ASN	2.2
1	A	457	GLY	2.2
1	A	347	GLU	2.2
1	A	617	PRO	2.1
1	A	456	TYR	2.1
1	A	269	ASP	2.1
1	B	268	THR	2.1
1	A	186	ASP	2.0
1	A	388	GLU	2.0
1	A	454	PHE	2.0

## 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

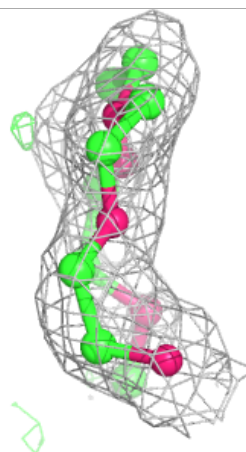
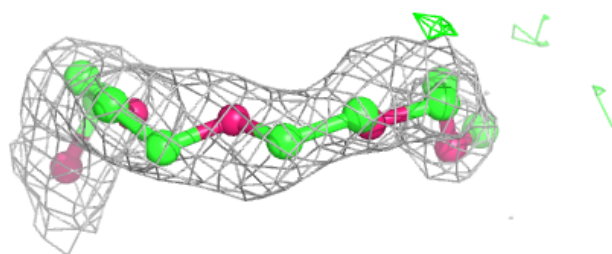
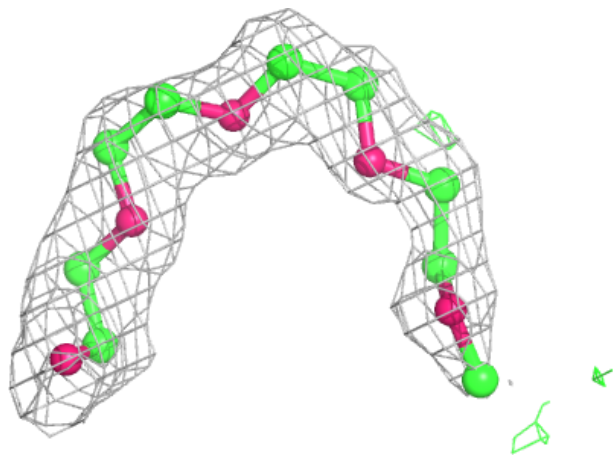
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GLC	A	912	12/12	0.82	0.14	28,35,37,38	0
5	12P	B	902	14/37	0.84	0.18	36,41,49,49	0
5	12P	A	901	12/37	0.90	0.13	33,36,40,45	0
3	SO3	A	910	4/4	0.94	0.09	29,34,37,39	0
3	SO3	B	910	4/4	0.96	0.07	28,38,38,40	0
2	SFD	A	801	57/57	0.97	0.09	9,12,28,30	0
2	SFD	B	801	57/57	0.97	0.08	10,14,30,32	0
3	SO3	B	911	4/4	0.97	0.07	23,32,35,37	0
3	SO3	A	911	4/4	0.98	0.14	35,35,39,39	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.



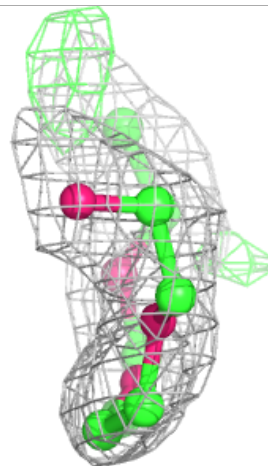
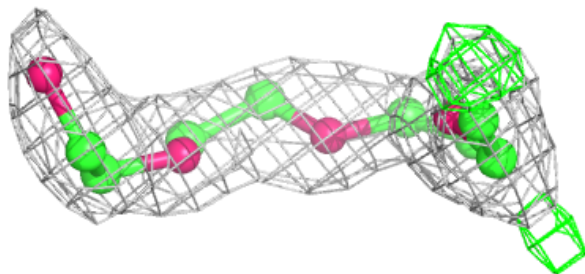
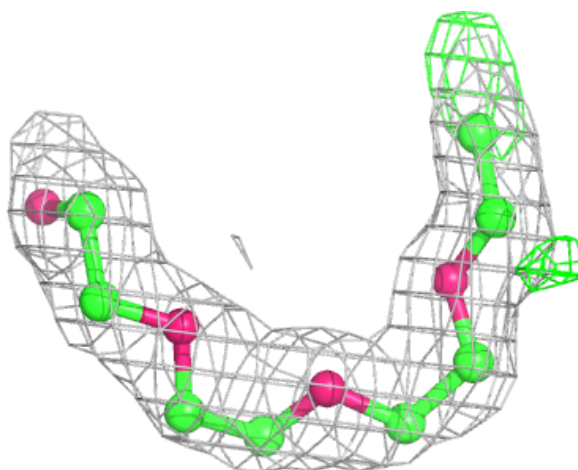
**Electron density around 12P B 902:**

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



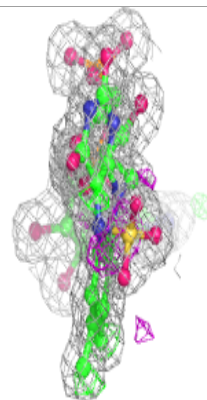
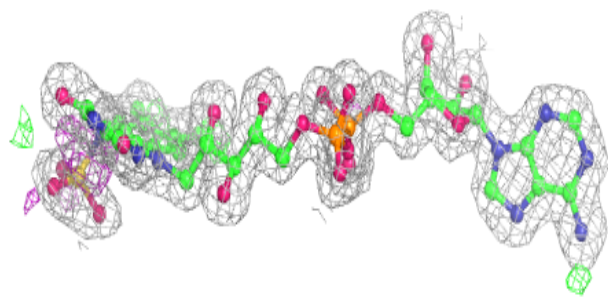
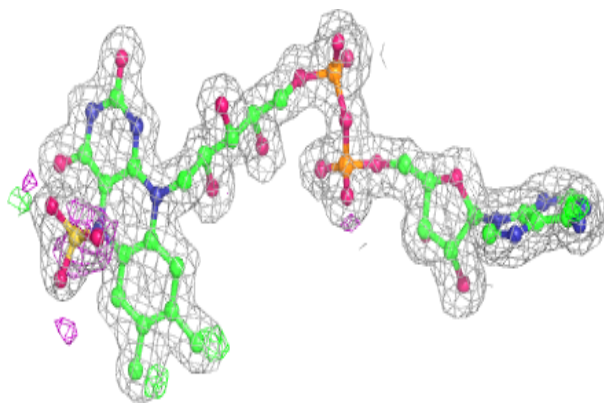
**Electron density around 12P A 901:**

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

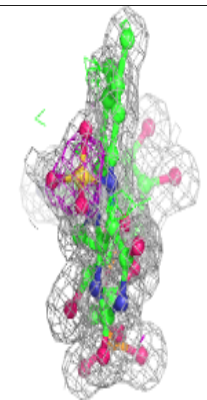
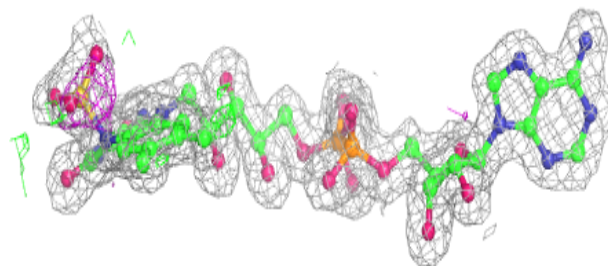
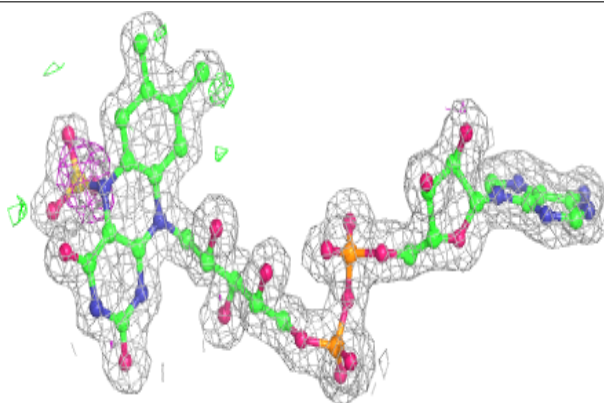


**Electron density around SFD A 801:**

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

**Electron density around SFD B 801:**

$2mF_o-DF_c$  (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.