



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:32 PM UTC

PDB ID : 3LSM / pdb_00003lsm
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

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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

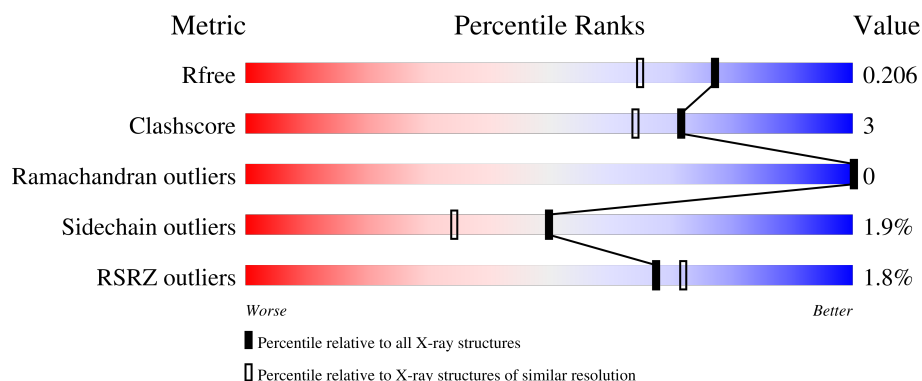
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

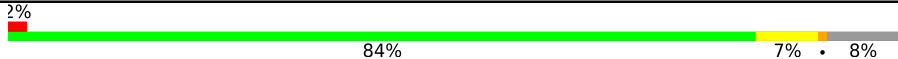
The reported resolution of this entry is 1.70 Å.

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 ≥ 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.

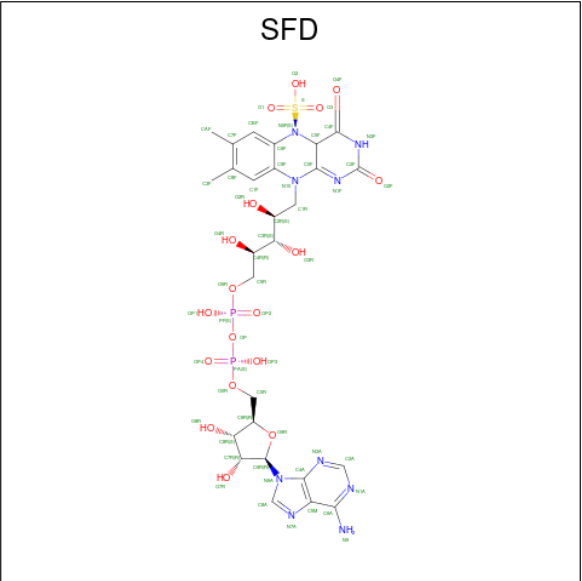
- Molecule 1 is a protein called Pyranose 2-oxidase.

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

There are 2 discrepancies between the modelled and reference sequences:

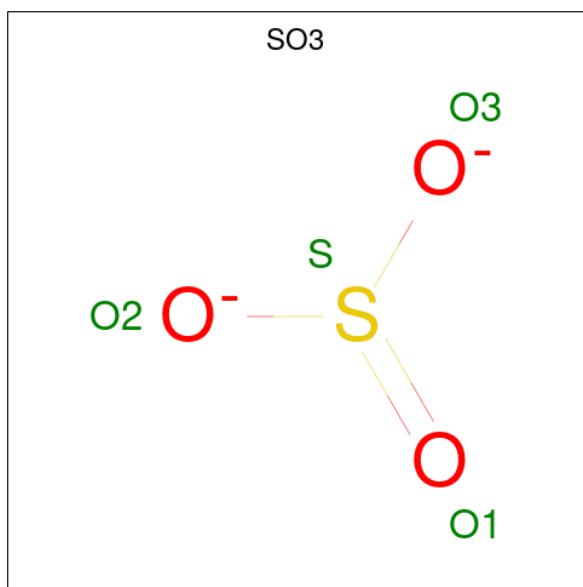
Chain	Residue	Modelled	Actual	Comment	Reference
A	167	ALA	HIS	engineered mutation	UNP Q7ZA32
B	167	ALA	HIS	engineered mutation	UNP Q7ZA32

- 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-TRIHIDROXYPENTYL)-7,8-DIMETHYL-2,4-DIOXO-2,3,4,4A-TETRAHYDROBENZO[G]PTERIDINE-5(10H)-SULFONIC ACID (CCD ID: SFD) (formula: C₂₇H₃₅N₉O₁₈P₂S).



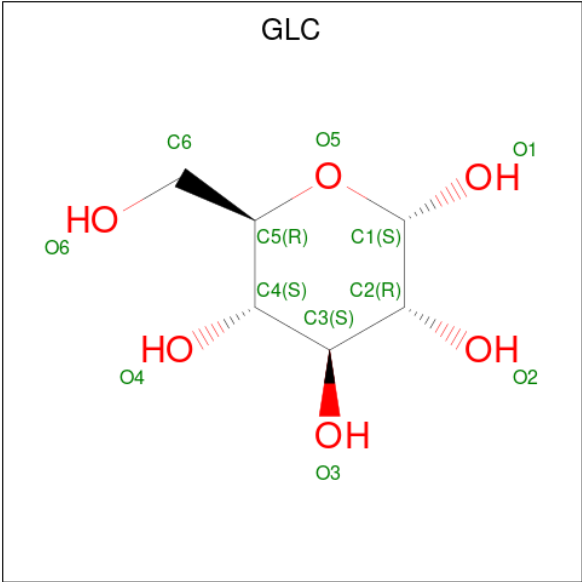
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			57	27	9	18	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			57	27	9	18	2	1		

- Molecule 3 is SULFITE ION (CCD ID: SO3) (formula: O₃S).



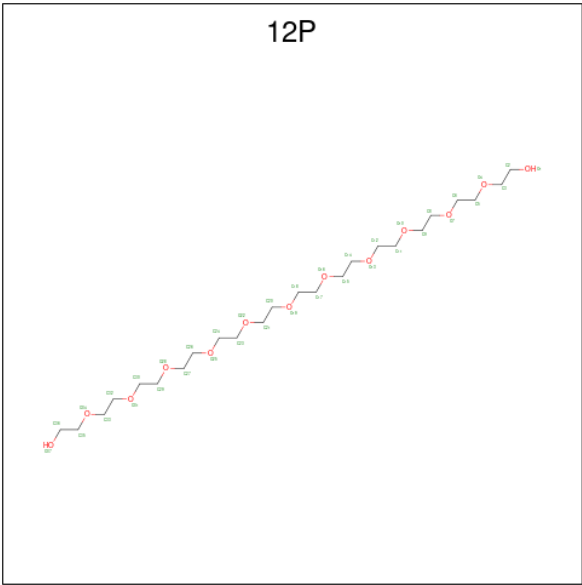
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			4	3	1		
3	A	1	Total	O	S	0	0
			4	3	1		
3	B	1	Total	O	S	0	0
			4	3	1		
3	B	1	Total	O	S	0	0
			4	3	1		

- Molecule 4 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



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

- Molecule 5 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: C₂₄H₅₀O₁₃).



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		

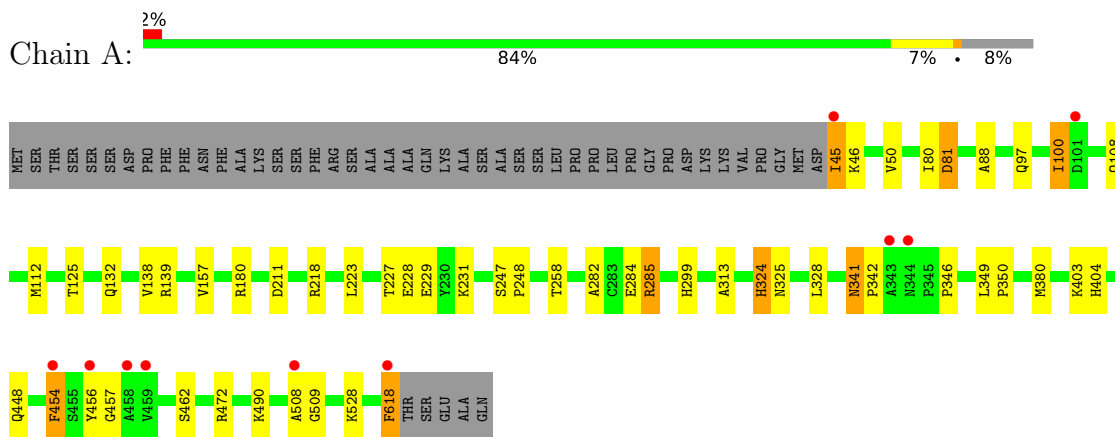
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	607	Total 607	O 607	0	0
6	B	562	Total 562	O 562	0	0

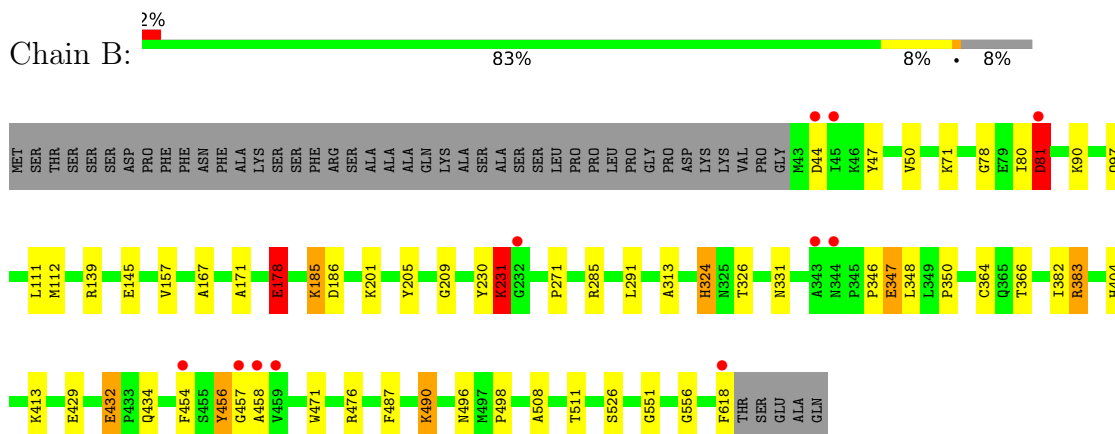
3 Residue-property plots [i](#)

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, α , β , γ	101.57Å 101.57Å 249.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.20 – 1.70 29.20 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.20-1.70) 99.5 (29.20-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 1.70Å)	Xtriage
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 (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10395	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage'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.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.44	16/4636 (0.3%)	1.21	18/6304 (0.3%)
1	B	1.40	15/4652 (0.3%)	1.22	17/6325 (0.3%)
All	All	1.42	31/9288 (0.3%)	1.21	35/12629 (0.3%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	ALA	CA-CB	-7.30	1.43	1.53
1	A	508	ALA	CA-C	6.83	1.62	1.53
1	A	508	ALA	C-O	6.77	1.33	1.23
1	B	171	ALA	CA-CB	-6.71	1.43	1.53
1	B	81	ASP	N-CA	6.45	1.52	1.46
1	A	211	ASP	CG-OD1	6.17	1.37	1.25
1	A	88	ALA	N-CA	6.08	1.53	1.45
1	B	551	GLY	C-O	-5.89	1.16	1.24
1	B	364	CYS	C-O	5.88	1.31	1.23
1	B	209	GLY	N-CA	5.88	1.51	1.45
1	A	112	MET	CB-CG	5.88	1.70	1.52
1	A	132	GLN	N-CA	5.71	1.53	1.46
1	B	167	ALA	CA-CB	-5.70	1.45	1.54
1	B	432	GLU	CA-CB	5.64	1.61	1.53
1	A	285	ARG	N-CA	5.60	1.52	1.46
1	A	258	THR	CA-C	5.55	1.59	1.52
1	A	132	GLN	C-O	5.54	1.30	1.24
1	B	556	GLY	N-CA	5.50	1.51	1.45
1	B	81	ASP	CB-CG	-5.49	1.38	1.52
1	B	81	ASP	CA-C	5.46	1.58	1.52
1	A	509	GLY	N-CA	-5.45	1.37	1.45
1	A	81	ASP	CB-CG	-5.27	1.38	1.52
1	B	112	MET	CB-CG	5.23	1.68	1.52
1	A	125	THR	N-CA	5.22	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	326	THR	N-CA	-5.21	1.40	1.46
1	A	325	ASN	CA-C	5.12	1.59	1.52
1	A	138	VAL	C-O	-5.10	1.19	1.24
1	B	111	LEU	N-CA	5.07	1.52	1.46
1	B	366	THR	N-CA	5.06	1.52	1.45
1	B	78	GLY	N-CA	5.02	1.50	1.45
1	A	211	ASP	CB-CG	5.00	1.64	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ARG	NE-CZ-NH1	10.93	132.43	121.50
1	A	139	ARG	NE-CZ-NH1	10.74	132.24	121.50
1	B	139	ARG	NE-CZ-NH2	-9.94	110.25	119.20
1	B	80	ILE	CA-C-N	9.32	134.52	120.17
1	B	80	ILE	C-N-CA	9.32	134.52	120.17
1	B	508	ALA	N-CA-C	7.77	122.02	112.54
1	A	81	ASP	N-CA-C	7.64	126.11	113.50
1	A	228	GLU	CB-CA-C	-7.55	99.02	110.88
1	B	178	GLU	CB-CG-CD	7.45	125.26	112.60
1	B	383	ARG	NE-CZ-NH1	-7.39	114.11	121.50
1	A	80	ILE	CA-C-N	7.36	131.51	120.17
1	A	80	ILE	C-N-CA	7.36	131.51	120.17
1	B	80	ILE	O-C-N	6.70	129.97	122.67
1	A	97	GLN	CA-CB-CG	-6.67	100.76	114.10
1	B	97	GLN	CA-CB-CG	-6.65	100.81	114.10
1	A	380	MET	CG-SD-CE	-6.53	86.53	100.90
1	B	139	ARG	CD-NE-CZ	6.46	133.44	124.40
1	A	139	ARG	NE-CZ-NH2	-6.39	113.45	119.20
1	B	81	ASP	N-CA-C	6.18	123.70	113.50
1	A	139	ARG	CD-NE-CZ	5.96	132.74	124.40
1	A	341	ASN	CA-C-N	5.94	125.61	119.56
1	A	341	ASN	C-N-CA	5.94	125.61	119.56
1	A	228	GLU	CA-CB-CG	5.71	125.52	114.10
1	A	80	ILE	O-C-N	5.66	128.84	122.67
1	A	324	HIS	CA-CB-CG	-5.58	108.22	113.80
1	B	44	ASP	CA-C-N	-5.34	115.44	122.16
1	B	44	ASP	C-N-CA	-5.34	115.44	122.16
1	A	462	SER	CA-CB-OG	-5.24	100.63	111.10
1	B	511	THR	N-CA-C	-5.20	105.70	111.36
1	B	324	HIS	N-CA-C	5.11	118.77	112.54
1	B	231	LYS	CA-C-N	-5.07	112.00	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	LYS	C-N-CA	-5.07	112.00	121.07
1	A	180	ARG	CA-C-N	5.06	125.05	119.89
1	A	180	ARG	C-N-CA	5.06	125.05	119.89
1	A	349	LEU	CB-CA-C	-5.02	106.63	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4521	0	4373	28	0
1	B	4537	0	4386	31	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
All	All	10395	0	8865	59	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 (59) 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	0.80
1:A:618:PHE:C	1:A:618:PHE:CD1	2.63	0.75
1:B:178:GLU:CD	1:B:476:ARG:HH12	2.00	0.69
1:B:404:HIS:HE1	6:B:1489:HOH:O	1.79	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:HD2	6:A:1144:HOH:O	1.96	0.66
1:B:456:TYR:HE1	6:B:2149:HOH:O	1.80	0.63
1:B:618:PHE:CD1	1:B:618:PHE:C	2.75	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: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:B:618:PHE:C	1:B:618:PHE:HD1	2.15	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:81:ASP:O	1:B:90:LYS:HE2	2.12	0.50
1:B:201:LYS:NZ	6:B:2083:HOH:O	2.44	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:A:284:GLU:C	1:A:328:LEU:CD1	2.85	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
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: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:284:GLU:C	1:A:328:LEU:HD11	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:230:TYR:O	1:B:231:LYS:C	2.64	0.40
1:B:71:LYS:HE3	6:B:1971:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	100	100
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 ⓘ

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%)	494 (99%)	7 (1%)	59	46
1	B	503/541 (93%)	491 (98%)	12 (2%)	43	26
All	All	1004/1082 (93%)	985 (98%)	19 (2%)	50	34

All (19) 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	403	LYS
1	A	454	PHE
1	A	490	LYS
1	A	618	PHE
1	B	81	ASP
1	B	178	GLU
1	B	185	LYS
1	B	231	LYS
1	B	291	LEU
1	B	347	GLU
1	B	413	LYS
1	B	429	GLU
1	B	454	PHE
1	B	456	TYR
1	B	490	LYS
1	B	496	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	A	257	ASN
1	A	263	GLN
1	A	276	ASN
1	A	324	HIS
1	A	344	ASN
1	A	404	HIS
1	A	419	HIS

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Mol	Chain	Res	Type
1	A	539	GLN
1	A	563	ASN
1	B	132	GLN
1	B	257	ASN
1	B	324	HIS
1	B	344	ASN
1	B	461	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	901	-	11,11,36	0.58	0	10,10,35	0.36	0
3	SO3	B	910	-	1,3,3	0.19	0	0,3,3	-	-
3	SO3	B	911	-	1,3,3	1.74	0	0,3,3	-	-
4	GLC	A	912	-	12,12,12	0.74	0	17,17,17	2.20	4 (23%)
3	SO3	A	911	-	1,3,3	1.66	0	0,3,3	-	-
5	12P	B	902	-	13,13,36	0.54	0	12,12,35	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SFD	B	801	-	61,62,62	3.18	19 (31%)	82,97,97	2.07	25 (30%)
2	SFD	A	801	-	61,62,62	3.05	15 (24%)	82,97,97	2.04	23 (28%)
3	SO3	A	910	-	1,3,3	0.79	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	A	901	-	-	3/9/9/34	-
4	GLC	A	912	-	-	0/2/22/22	0/1/1/1
5	12P	B	902	-	-	1/11/11/34	-
2	SFD	B	801	-	1/1/16/17	0/38/88/88	0/5/6/6
2	SFD	A	801	-	1/1/16/17	2/38/88/88	0/5/6/6

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	SFD	C6F-N5F	-13.35	1.32	1.44
2	A	801	SFD	C6F-N5F	-12.79	1.33	1.44
2	B	801	SFD	O3-S	10.59	1.54	1.42
2	A	801	SFD	O3-S	9.72	1.53	1.42
2	B	801	SFD	C5F-C4F	-8.13	1.45	1.52
2	A	801	SFD	C1R-C2R	7.88	1.63	1.52
2	A	801	SFD	PF-OP	6.76	1.66	1.59
2	A	801	SFD	C5F-C4F	-6.57	1.47	1.52
2	B	801	SFD	C1R-C2R	6.39	1.61	1.52
2	B	801	SFD	C0F-N1F	5.85	1.43	1.31
2	A	801	SFD	C9F-N10	4.77	1.49	1.41
2	B	801	SFD	O1-S	4.75	1.47	1.42
2	A	801	SFD	O1-S	4.24	1.46	1.42
2	B	801	SFD	C5F-N5F	-3.98	1.41	1.49
2	A	801	SFD	C1F-C8F	3.65	1.44	1.39
2	B	801	SFD	PF-OP	3.43	1.63	1.59
2	B	801	SFD	C9F-N10	3.41	1.47	1.41
2	A	801	SFD	C5F-N5F	-3.38	1.42	1.49
2	B	801	SFD	O9R-C9R	-3.29	1.37	1.45
2	B	801	SFD	C5M-N7A	-3.26	1.33	1.39
2	B	801	SFD	C1F-C9F	3.12	1.44	1.39
2	B	801	SFD	C4F-N3F	3.02	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	SFD	CBF-C7F	2.98	1.43	1.39
2	B	801	SFD	C4R-C3R	2.91	1.58	1.53
2	B	801	SFD	C5R-C4R	2.73	1.55	1.51
2	A	801	SFD	C4A-N9A	-2.55	1.32	1.37
2	B	801	SFD	C0F-N10	-2.52	1.34	1.38
2	A	801	SFD	C0F-N10	2.46	1.42	1.38
2	A	801	SFD	O5R-C5R	2.38	1.53	1.44
2	A	801	SFD	O9R-C6R	2.31	1.47	1.42
2	B	801	SFD	C2R-C3R	2.16	1.57	1.53
2	B	801	SFD	O5R-C5R	2.14	1.52	1.44
2	A	801	SFD	C2F-N3F	-2.13	1.34	1.39
2	A	801	SFD	O4R-C4R	2.10	1.47	1.43

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	SFD	C5F-N5F-S	-7.38	104.91	117.44
2	A	801	SFD	C5F-N5F-S	-6.81	105.88	117.44
2	A	801	SFD	C1F-C9F-N10	-5.78	114.08	121.85
2	A	801	SFD	O1-S-O3	-5.47	106.41	119.69
2	A	801	SFD	O1-S-N5F	5.27	121.96	109.98
2	B	801	SFD	C5M-C4A-N3A	-5.03	119.80	126.72
4	A	912	GLC	O5-C1-C2	4.95	119.00	110.30
2	A	801	SFD	CAF-C7F-CBF	-4.42	111.78	119.57
4	A	912	GLC	C1-C2-C3	-4.25	101.69	110.36
2	A	801	SFD	C5M-C4A-N3A	-4.20	120.93	126.72
2	B	801	SFD	N9A-C8A-N7A	-4.11	108.11	113.94
2	B	801	SFD	O5R-C5R-C4R	-4.07	98.49	109.36
4	A	912	GLC	C1-O5-C5	-3.98	105.96	113.65
2	B	801	SFD	O1-S-O3	-3.93	110.15	119.69
4	A	912	GLC	O1-C1-C2	3.80	120.00	108.98
2	B	801	SFD	N1A-C2A-N3A	-3.74	122.92	128.58
2	B	801	SFD	C5R-C4R-C3R	-3.64	105.36	112.22
2	B	801	SFD	O3-S-N5F	-3.61	101.76	109.98
2	B	801	SFD	C6F-N5F-C5F	3.56	119.23	114.73
2	B	801	SFD	C5M-N7A-C8A	3.53	109.00	103.45
2	B	801	SFD	C1F-C9F-N10	-3.44	117.23	121.85
2	A	801	SFD	N1A-C2A-N3A	-3.27	123.63	128.58
2	B	801	SFD	C6A-C5M-C4A	3.21	121.56	117.18
2	B	801	SFD	CAF-C7F-CBF	-3.03	114.24	119.57
2	B	801	SFD	C1R-N10-C9F	3.02	126.51	120.63
2	A	801	SFD	OP-PA-OP4	-2.88	102.05	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	SFD	OP1-PF-OP	2.85	114.99	107.27
2	A	801	SFD	N3A-C4A-N9A	2.83	131.98	127.17
2	B	801	SFD	OP-PF-OP2	-2.82	102.23	110.70
2	A	801	SFD	N9A-C8A-N7A	-2.81	109.95	113.94
2	B	801	SFD	O1-S-N5F	2.78	116.28	109.98
2	A	801	SFD	C6F-C9F-N10	2.76	122.41	119.03
2	B	801	SFD	N3A-C4A-N9A	2.75	131.85	127.17
2	B	801	SFD	C2A-N3A-C4A	2.75	118.54	111.83
2	B	801	SFD	CBF-C7F-C8F	2.71	123.67	119.69
2	A	801	SFD	C2A-N3A-C4A	2.40	117.70	111.83
2	A	801	SFD	C9F-C1F-C8F	-2.40	114.40	119.22
2	B	801	SFD	C5M-C4A-N9A	2.33	108.35	105.81
2	A	801	SFD	CBF-C7F-C8F	2.32	123.10	119.69
2	A	801	SFD	C4A-N9A-C8A	2.25	108.10	105.74
2	A	801	SFD	C1F-C9F-C6F	2.24	123.50	120.06
2	A	801	SFD	C6F-N5F-C5F	2.23	117.55	114.73
2	A	801	SFD	CAF-C7F-C8F	2.14	125.12	120.76
2	A	801	SFD	OP3-PA-OP	2.12	113.00	107.27
2	A	801	SFD	O9R-C9R-C0R	-2.12	102.54	109.33
2	B	801	SFD	OP-PA-OP4	-2.12	104.34	110.70
2	B	801	SFD	C7R-C8R-C9R	2.10	106.67	102.61
2	A	801	SFD	O3-S-N5F	-2.08	105.24	109.98
2	B	801	SFD	O9R-C9R-C0R	-2.07	102.72	109.33
2	A	801	SFD	OP1-PF-OP	2.06	112.83	107.27
2	A	801	SFD	C6A-C5M-C4A	2.04	119.96	117.18
2	B	801	SFD	C4R-C3R-C2R	-2.00	110.24	113.57

All (2) chirality outliers are listed below:

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

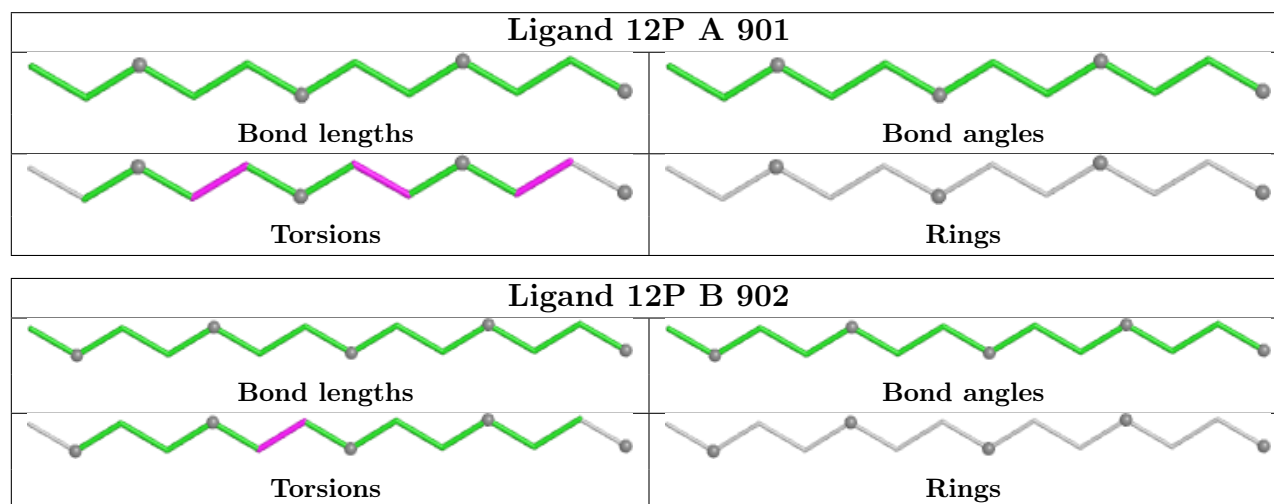
All (6) torsion outliers are listed below:

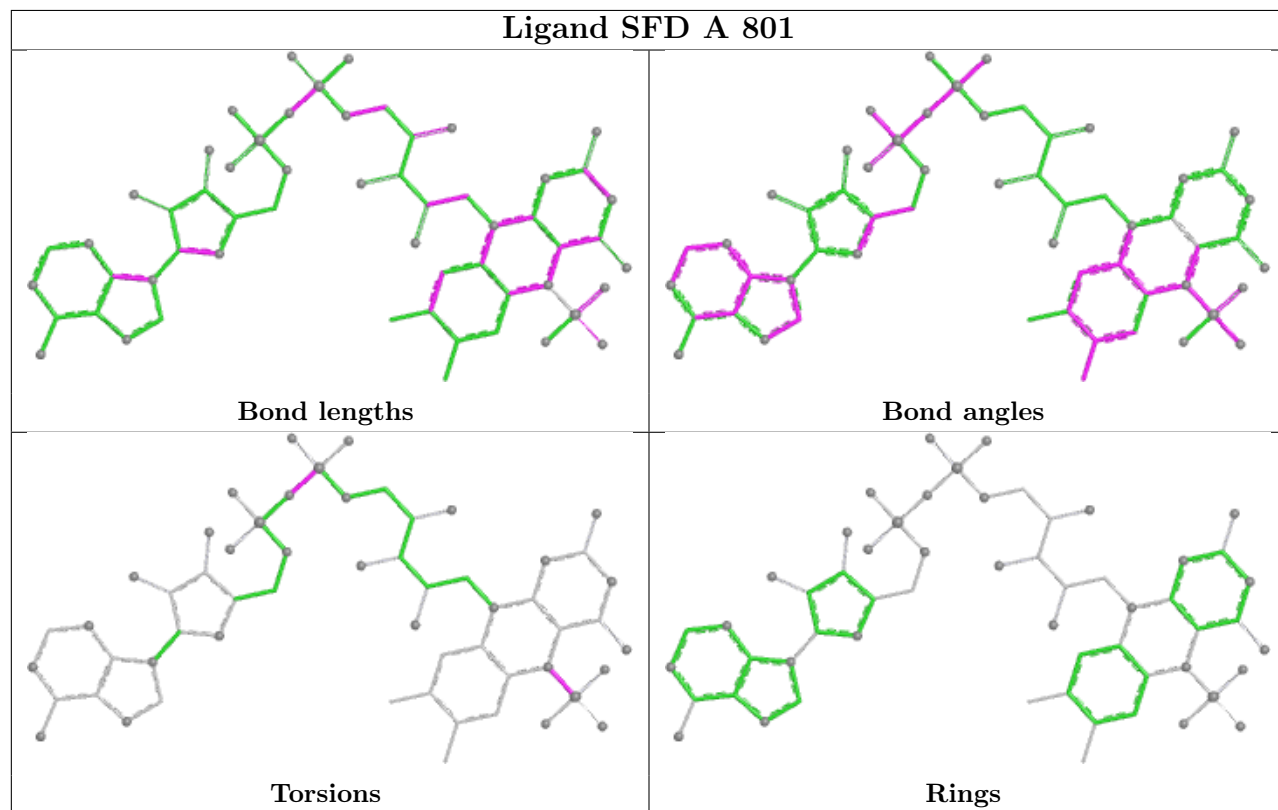
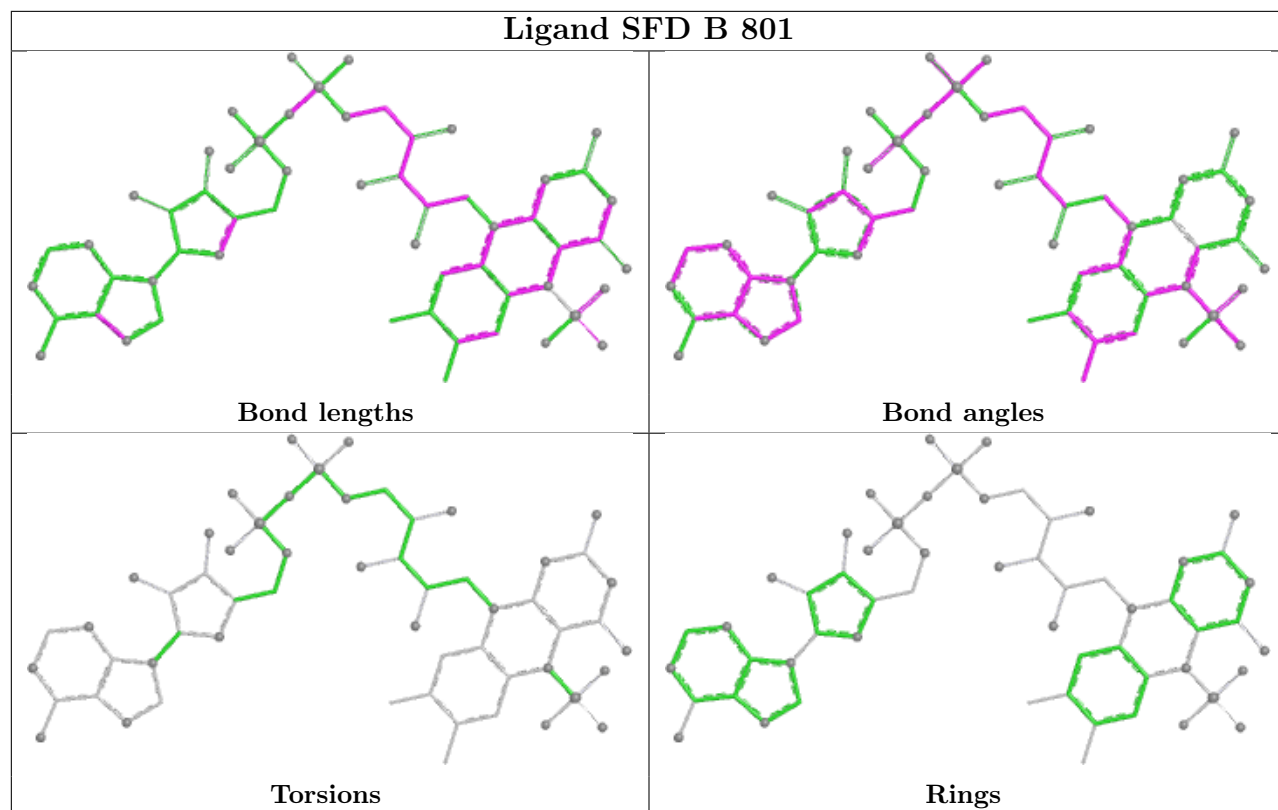
Mol	Chain	Res	Type	Atoms
5	A	901	12P	O13-C14-C15-O16
2	A	801	SFD	PA-OP-PF-O5R
2	A	801	SFD	C6F-N5F-S-O3
5	B	902	12P	O7-C8-C9-O10
5	A	901	12P	O7-C8-C9-O10
5	A	901	12P	O10-C11-C12-O13

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, 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	574/623 (92%)	-0.32	10 (1%) 69 73	11, 16, 32, 51	0
1	B	576/623 (92%)	-0.23	11 (1%) 66 71	11, 18, 34, 58	0
All	All	1150/1246 (92%)	-0.27	21 (1%) 67 72	11, 17, 34, 58	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	459	VAL	4.4
1	B	458	ALA	4.4
1	A	459	VAL	4.0
1	B	343	ALA	3.7
1	A	45	ILE	3.6
1	A	618	PHE	3.4
1	B	45	ILE	3.3
1	B	232	GLY	3.1
1	A	343	ALA	3.1
1	B	457	GLY	3.0
1	A	454	PHE	2.8
1	B	344	ASN	2.7
1	B	618	PHE	2.7
1	A	458	ALA	2.7
1	B	454	PHE	2.6
1	A	101	ASP	2.5
1	B	81	ASP	2.5
1	B	44	ASP	2.2
1	A	344	ASN	2.2
1	A	508	ALA	2.1
1	A	456	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

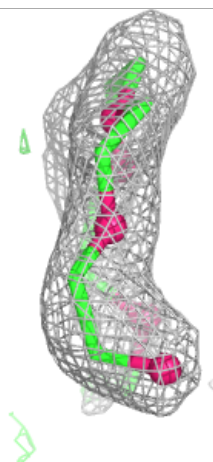
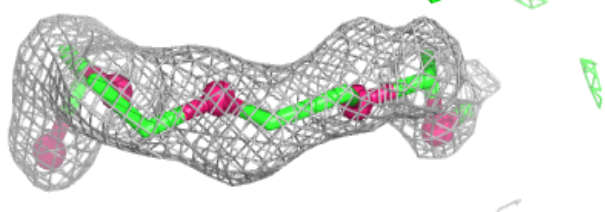
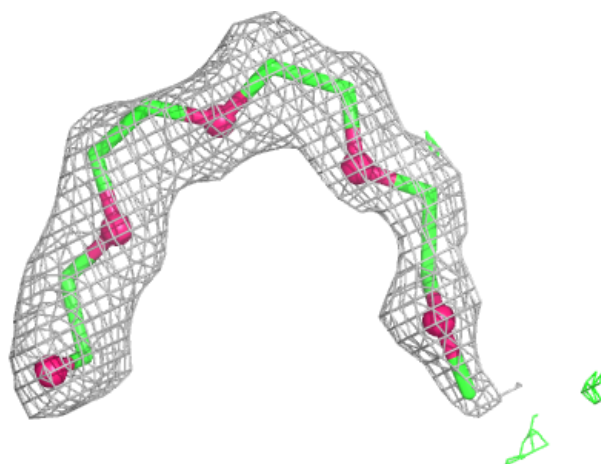
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	12P	B	902	14/37	0.84	0.15	36,41,49,49	0
5	12P	A	901	12/37	0.85	0.14	33,36,40,45	0
4	GLC	A	912	12/12	0.88	0.10	28,35,37,38	0
3	SO3	A	910	4/4	0.91	0.11	29,34,37,39	0
3	SO3	B	910	4/4	0.96	0.07	28,38,38,40	0
3	SO3	A	911	4/4	0.96	0.12	35,35,39,39	0
3	SO3	B	911	4/4	0.97	0.07	23,32,35,37	0
2	SFD	B	801	57/57	0.97	0.05	10,14,30,32	0
2	SFD	A	801	57/57	0.98	0.05	9,12,28,30	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.

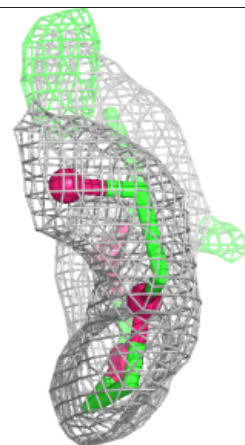
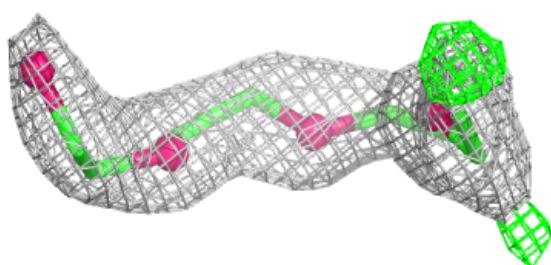
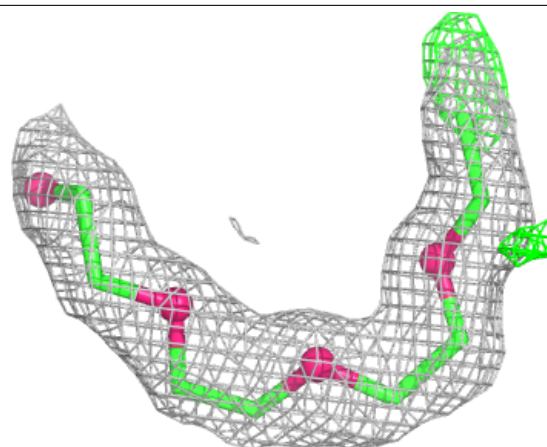
Electron density around 12P B 902:

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

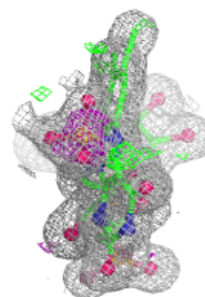
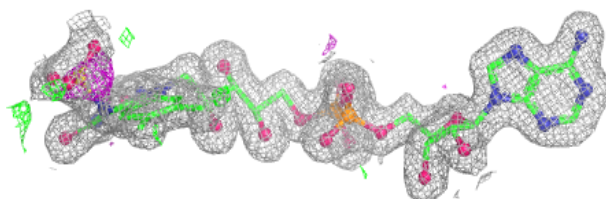
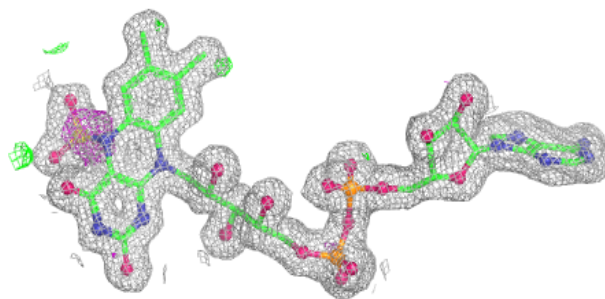


Electron density around 12P A 901:

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

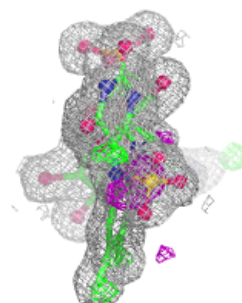
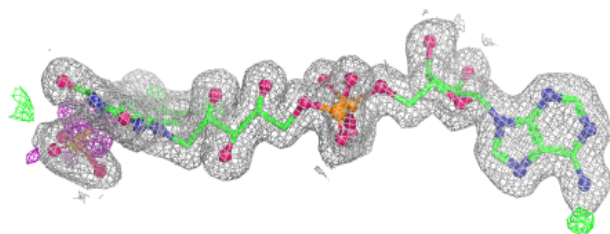
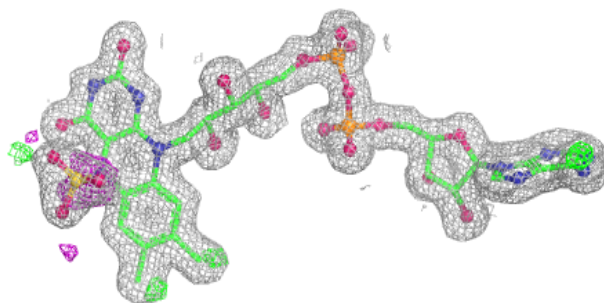
**Electron density around SFD B 801:**

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.