



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:28 PM UTC

PDB ID : 4NMF / pdb_00004nmf
Title : Crystal structure of proline utilization A (PutA) from *Geobacter sulfurreducens* PCA inactivated by N-propargylglycine and complexed with menadione bisulfite
Authors : Singh, H.; Tanner, J.J.
Deposited on : 2013-11-14
Resolution : 1.95 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

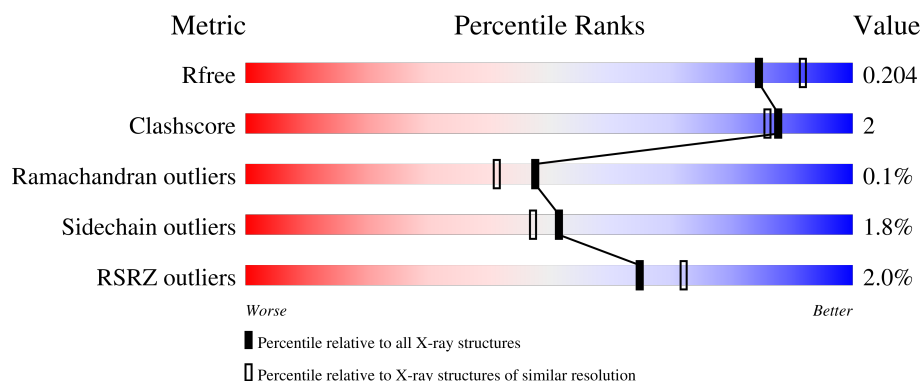
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	1005	3% 91% 5% .
1	B	1005	% 91% 6% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 16394 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.

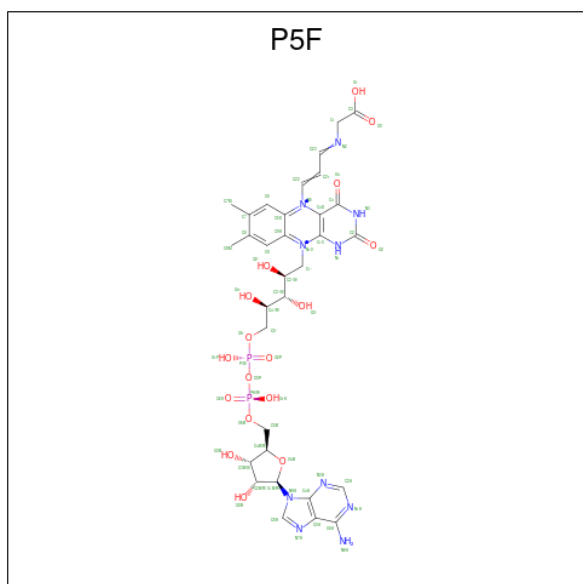
- Molecule 1 is a protein called Proline dehydrogenase and Delta-1-pyrroline-5-carboxylate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	973	Total	C	N	O	S	0	4	0
			7568	4837	1313	1379	39			
1	B	979	Total	C	N	O	S	0	2	0
			7624	4864	1323	1399	38			

There are 2 discrepancies between the modelled and reference sequences:

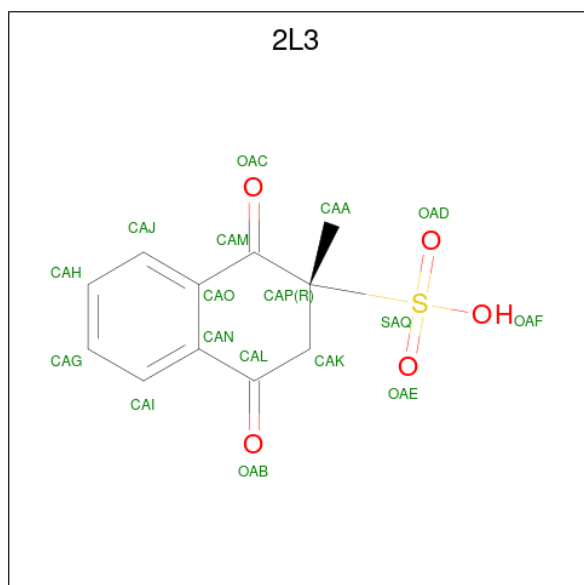
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q746X3
B	0	SER	-	expression tag	UNP Q746X3

- Molecule 2 is N-propargylglycine-modified flavin adenine dinucleotide (CCD ID: P5F) (formula: C₃₂H₄₀N₁₀O₁₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			56	30	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			56	30	9	15	2		

- Molecule 3 is (2R)-2-methyl-1,4-dioxo-1,2,3,4-tetrahydronaphthalene-2-sulfonic acid (CCD ID: 2L3) (formula: C₁₁H₁₀O₅S).



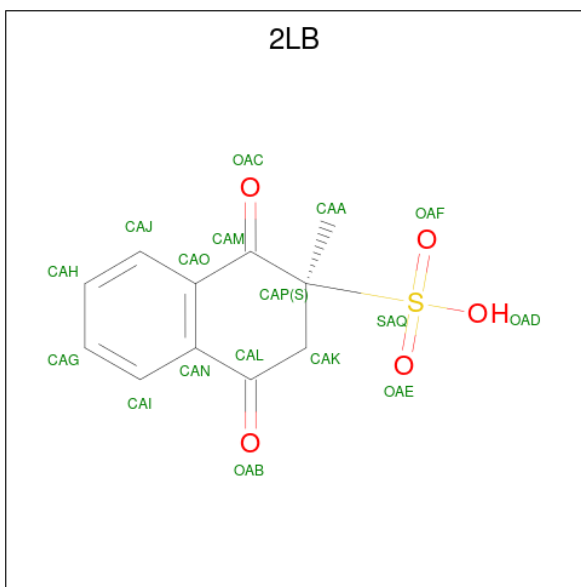
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			17	11	5	1		
3	B	1	Total	C	O	S	0	1
			17	11	5	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is (2S)-2-methyl-1,4-dioxo-1,2,3,4-tetrahydronaphthalene-2-sulfonic acid (CCD ID: 2LB) (formula: C₁₁H₁₀O₅S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	1
			17	11	5	1		

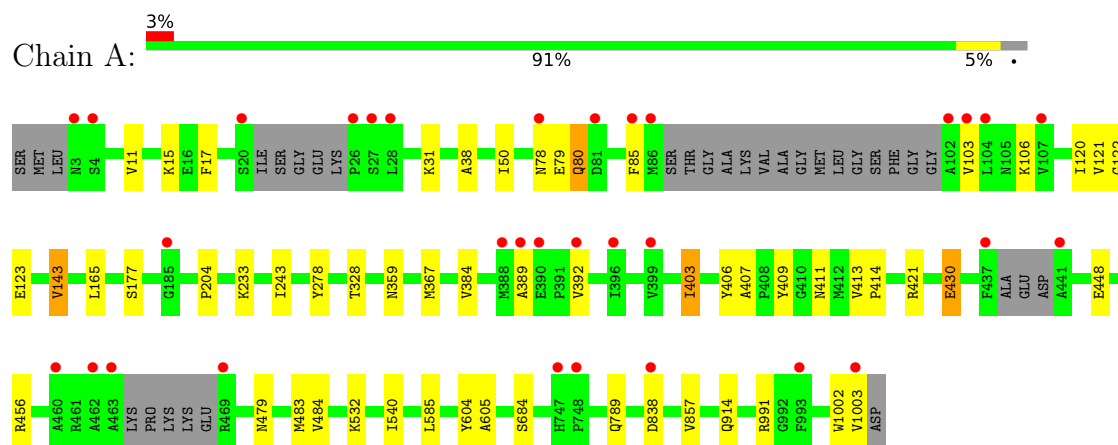
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	497	Total	O	0	0
			497	497		
6	B	510	Total	O	0	0
			510	510		

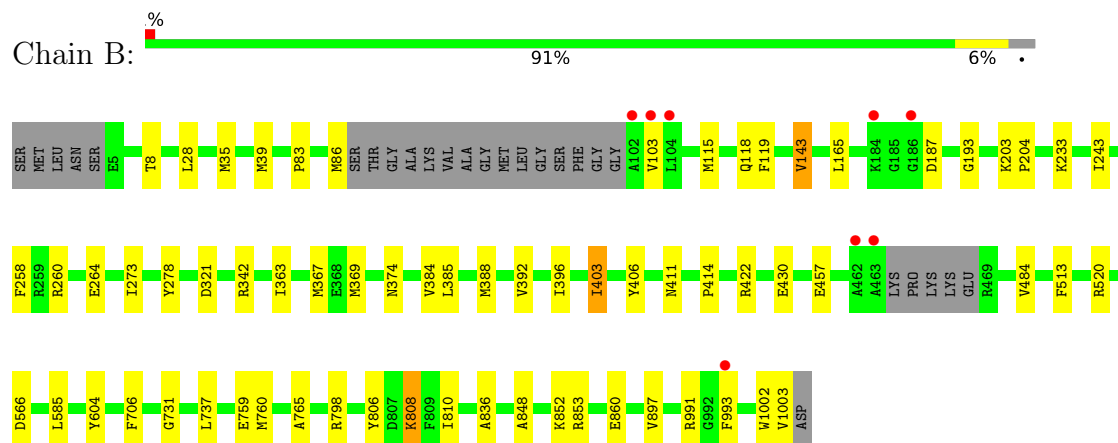
3 Residue-property plots [i](#)

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: Proline dehydrogenase and Delta-1-pyrroline-5-carboxylate dehydrogenase



- Molecule 1: Proline dehydrogenase and Delta-1-pyrroline-5-carboxylate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.59Å 151.74Å 176.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.60 – 1.95 47.60 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.60-1.95) 98.2 (47.60-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.173 , 0.203 0.175 , 0.204	Depositor DCC
R_{free} test set	9211 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16394	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, 2L3, 2LB, P5F

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	0.44	0/7751	0.75	3/10500 (0.0%)
1	B	0.44	0/7802	0.75	1/10570 (0.0%)
All	All	0.44	0/15553	0.75	4/21070 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	VAL	CA-C-N	-5.83	113.68	119.56
1	A	413	VAL	C-N-CA	-5.83	113.68	119.56
1	B	836	ALA	N-CA-C	5.36	117.12	111.28
1	A	789	GLN	CB-CA-C	-5.14	102.98	111.36

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	7568	0	7425	26	0
1	B	7624	0	7485	35	0
2	A	56	0	35	1	0
2	B	56	0	35	2	0
3	A	17	0	9	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	9	1	0
4	A	20	0	30	0	0
4	B	12	0	18	0	0
5	B	17	0	9	3	0
6	A	497	0	0	1	0
6	B	510	0	0	1	0
All	All	16394	0	15055	61	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 2.

All (61) 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:422:ARG:NH1	3:B:1102[A]:2L3:OAF	2.25	0.69
1:B:28:LEU:HD22	1:B:39:MET:HG3	1.77	0.66
1:A:389:ALA:HB1	1:A:392:VAL:HB	1.77	0.66
1:B:321:ASP:HB2	6:B:1649:HOH:O	2.00	0.62
1:B:143:VAL:HG13	1:B:406:TYR:HA	1.83	0.61
1:A:120:ILE:HG22	1:A:122:GLY:H	1.66	0.59
1:B:203:LYS:HE3	5:B:1103[B]:2LB:H5	1.85	0.58
1:B:35:MET:HE3	1:B:115:MET:HG2	1.84	0.58
1:B:810:ILE:HD11	1:B:897:VAL:HG11	1.86	0.56
1:B:852:LYS:NZ	1:B:860:GLU:OE2	2.39	0.54
2:B:1101:P5F:Cl'	5:B:1103[B]:2LB:H10	2.39	0.53
1:B:83:PRO:HD2	1:B:86:MET:HG3	1.90	0.53
1:A:359:ASN:HD22	2:A:1101:P5F:H1	1.56	0.52
1:B:187:ASP:O	1:B:193:GLY:HA2	2.10	0.52
1:A:78:ASN:O	1:A:80:GLN:N	2.43	0.51
1:B:1002:TRP:CG	1:B:1003:VAL:H	2.29	0.51
1:B:363:ILE:HG22	1:B:367:MET:HE2	1.92	0.51
1:A:384:VAL:HG22	1:A:403:ILE:HD11	1.92	0.51
1:B:808:LYS:NZ	1:B:808:LYS:HB2	2.25	0.50
1:A:121:VAL:HG11	1:A:407:ALA:HB1	1.93	0.49
1:A:448:GLU:OE2	1:A:456:ARG:NH1	2.45	0.49
1:B:731:GLY:O	1:B:760:MET:HA	2.14	0.48
1:A:143:VAL:HG13	1:A:406:TYR:HA	1.96	0.47
1:A:1002:TRP:CG	1:A:1003:VAL:H	2.33	0.46
1:A:430:GLU:H	1:A:430:GLU:CD	2.24	0.46
1:A:483[B]:MET:HE1	1:A:605:ALA:HA	1.99	0.45
1:A:50:ILE:HG12	1:B:993:PHE:HZ	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:GLN:NE2	6:A:1490:HOH:O	2.38	0.45
1:B:385:LEU:HD21	5:B:1103[B]:2LB:H9	2.00	0.44
1:A:484:VAL:HB	1:A:604:TYR:CG	2.53	0.44
1:B:806:TYR:O	1:B:810:ILE:HG12	2.18	0.43
1:A:120:ILE:HG23	1:A:409:TYR:HA	2.00	0.43
1:A:17:PHE:CE2	1:A:367:MET:HE1	2.54	0.43
1:B:848:ALA:O	1:B:852:LYS:HG3	2.18	0.43
1:A:421:ARG:NE	3:A:1102:2L3:OAF	2.43	0.43
1:B:484:VAL:HB	1:B:604:TYR:CG	2.54	0.43
1:B:258:PHE:HB2	1:B:273:ILE:HD13	2.01	0.43
1:B:991:ARG:HA	1:B:991:ARG:HD3	1.92	0.42
1:B:411:ASN:HB3	1:B:414:PRO:HD2	2.01	0.42
1:B:86:MET:HE3	1:B:86:MET:HB3	1.95	0.42
1:B:342:ARG:HB2	1:B:369:MET:SD	2.59	0.42
1:A:11:VAL:O	1:A:15:LYS:HG3	2.19	0.42
2:B:1101:P5F:C4	2:B:1101:P5F:H35	2.49	0.42
1:B:765:ALA:HA	1:B:798:ARG:O	2.20	0.42
1:A:328:THR:HG21	1:B:1003:VAL:HG11	2.02	0.42
1:B:165:LEU:HD22	1:B:233:LYS:HG3	2.01	0.42
1:A:411:ASN:HB3	1:A:414:PRO:HD2	2.02	0.41
1:A:165:LEU:HD22	1:A:233:LYS:HG3	2.01	0.41
1:B:384:VAL:HG22	1:B:403:ILE:HD11	2.02	0.41
1:A:204:PRO:HG3	1:A:243:ILE:HG23	2.02	0.41
1:A:484:VAL:HB	1:A:604:TYR:CD1	2.55	0.41
1:B:392:VAL:O	1:B:396:ILE:HG13	2.20	0.41
1:A:38:ALA:HA	1:A:85:PHE:CZ	2.56	0.41
1:A:540:ILE:HG13	1:A:684:SER:HB2	2.03	0.41
1:B:513:PHE:HB3	1:B:706:PHE:HB3	2.03	0.41
1:B:119:PHE:HE1	1:B:388:MET:HB3	1.87	0.41
1:A:991:ARG:HD3	1:A:991:ARG:HA	1.89	0.40
1:B:204:PRO:HG3	1:B:243:ILE:HG23	2.03	0.40
1:B:115:MET:O	1:B:118:GLN:HB3	2.21	0.40
1:B:737:LEU:HD23	1:B:737:LEU:HA	1.90	0.40
1:B:260:ARG:O	1:B:264:GLU:HG3	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	967/1005 (96%)	948 (98%)	17 (2%)	2 (0%)	43	36
1	B	975/1005 (97%)	953 (98%)	22 (2%)	0	100	100
All	All	1942/2010 (97%)	1901 (98%)	39 (2%)	2 (0%)	48	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	GLU
1	A	80	GLN

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	768/821 (94%)	754 (98%)	14 (2%)	51	47
1	B	777/821 (95%)	763 (98%)	14 (2%)	51	47
All	All	1545/1642 (94%)	1517 (98%)	28 (2%)	51	47

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	103	VAL
1	A	106	LYS
1	A	123	GLU

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Mol	Chain	Res	Type
1	A	143	VAL
1	A	177	SER
1	A	278	TYR
1	A	403	ILE
1	A	430	GLU
1	A	479	ASN
1	A	532	LYS
1	A	585	LEU
1	A	838	ASP
1	A	857	VAL
1	B	8	THR
1	B	103	VAL
1	B	143	VAL
1	B	278	TYR
1	B	374	ASN
1	B	403	ILE
1	B	430	GLU
1	B	457	GLU
1	B	520	ARG
1	B	566	ASP
1	B	585	LEU
1	B	759	GLU
1	B	808	LYS
1	B	853	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	479	ASN
1	A	542	GLN
1	A	752	ASN
1	A	856	HIS
1	B	111	ASN
1	B	429	ASN
1	B	522	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
2	P5F	A	1101	1	56,61,66	2.95	19 (33%)	74,93,99	2.15	22 (29%)
2	P5F	B	1101	1	56,61,66	2.78	19 (33%)	74,93,99	2.07	23 (31%)
5	2LB	B	1103[B]	-	14,18,18	4.43	5 (35%)	20,29,29	1.89	7 (35%)
4	EDO	A	1103	-	3,3,3	0.51	0	2,2,2	0.47	0
4	EDO	A	1107	-	3,3,3	0.60	0	2,2,2	0.39	0
4	EDO	B	1104	-	3,3,3	0.54	0	2,2,2	0.18	0
4	EDO	A	1106	-	3,3,3	0.53	0	2,2,2	0.32	0
3	2L3	B	1102[A]	-	14,18,18	4.47	5 (35%)	20,29,29	1.77	6 (30%)
4	EDO	B	1105	-	3,3,3	0.56	0	2,2,2	0.47	0
4	EDO	A	1104	-	3,3,3	0.60	0	2,2,2	0.38	0
4	EDO	B	1106	-	3,3,3	0.58	0	2,2,2	0.50	0
3	2L3	A	1102	-	14,18,18	4.41	5 (35%)	20,29,29	1.77	4 (20%)
4	EDO	A	1105	-	3,3,3	0.45	0	2,2,2	0.37	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
2	P5F	A	1101	1	-	2/34/53/58	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P5F	B	1101	1	-	5/34/53/58	0/6/6/6
5	2LB	B	1103[B]	-	-	6/6/28/28	0/2/2/2
4	EDO	A	1103	-	-	0/1/1/1	-
4	EDO	A	1107	-	-	1/1/1/1	-
4	EDO	B	1104	-	-	0/1/1/1	-
4	EDO	A	1106	-	-	1/1/1/1	-
3	2L3	B	1102[A]	-	-	5/6/28/28	0/2/2/2
4	EDO	B	1105	-	-	0/1/1/1	-
4	EDO	A	1104	-	-	1/1/1/1	-
4	EDO	B	1106	-	-	1/1/1/1	-
3	2L3	A	1102	-	-	0/6/28/28	0/2/2/2
4	EDO	A	1105	-	-	0/1/1/1	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1102[A]	2L3	OAC-CAM	10.60	1.37	1.21
5	B	1103[B]	2LB	OAC-CAM	10.51	1.37	1.21
3	A	1102	2L3	OAC-CAM	10.40	1.37	1.21
3	A	1102	2L3	OAB-CAL	8.87	1.37	1.22
5	B	1103[B]	2LB	OAB-CAL	8.80	1.37	1.22
3	B	1102[A]	2L3	OAB-CAL	8.76	1.37	1.22
2	A	1101	P5F	PA-O3P	-8.70	1.50	1.59
2	B	1101	P5F	PA-O3P	-7.82	1.51	1.59
2	A	1101	P5F	C6-C5X	7.81	1.49	1.40
2	B	1101	P5F	O4-C4	7.68	1.38	1.23
2	A	1101	P5F	O4-C4	7.58	1.37	1.23
2	B	1101	P5F	C6-C5X	7.01	1.48	1.40
2	B	1101	P5F	O2-C2	6.84	1.37	1.23
2	A	1101	P5F	O2-C2	6.63	1.37	1.23
2	A	1101	P5F	C9-C9A	6.61	1.48	1.40
3	B	1102[A]	2L3	CAI-CAN	6.09	1.49	1.39
2	B	1101	P5F	C9-C9A	5.96	1.47	1.40
5	B	1103[B]	2LB	CAI-CAN	5.95	1.49	1.39
3	A	1102	2L3	CAI-CAN	5.71	1.48	1.39
3	A	1102	2L3	CAJ-CAO	5.65	1.48	1.39
3	B	1102[A]	2L3	CAJ-CAO	5.58	1.48	1.39
5	B	1103[B]	2LB	CAJ-CAO	5.38	1.48	1.39
2	A	1101	P5F	C22-N5	-5.07	1.28	1.46
2	B	1101	P5F	C10-N1	4.93	1.44	1.36
2	A	1101	P5F	C10-N1	4.70	1.44	1.36
5	B	1103[B]	2LB	CAO-CAN	-4.35	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	P5F	C9A-N10	4.27	1.46	1.37
2	A	1101	P5F	C6A-N6A	4.13	1.44	1.34
3	B	1102[A]	2L3	CAO-CAN	-4.04	1.34	1.40
2	B	1101	P5F	C2-N1	4.03	1.44	1.37
2	B	1101	P5F	C6A-N6A	4.03	1.44	1.34
2	A	1101	P5F	P-O3P	3.89	1.63	1.59
3	A	1102	2L3	CAO-CAN	-3.73	1.34	1.40
2	B	1101	P5F	C9A-N10	3.72	1.45	1.37
2	A	1101	P5F	C2-N1	3.69	1.43	1.37
2	B	1101	P5F	C5X-C9A	-3.37	1.35	1.42
2	A	1101	P5F	C5X-C9A	-3.00	1.36	1.42
2	B	1101	P5F	P-O3P	2.98	1.62	1.59
2	B	1101	P5F	PA-O5B	-2.69	1.48	1.59
2	A	1101	P5F	PA-O5B	-2.54	1.49	1.59
2	B	1101	P5F	C5A-C4A	2.49	1.43	1.39
2	B	1101	P5F	C22-N5	-2.30	1.38	1.46
2	A	1101	P5F	C2-N3	2.30	1.41	1.37
2	B	1101	P5F	C4X-C4	2.25	1.49	1.43
2	B	1101	P5F	C2-N3	2.23	1.41	1.37
2	A	1101	P5F	C5A-C4A	2.22	1.43	1.39
2	A	1101	P5F	C4X-C4	2.13	1.49	1.43
2	B	1101	P5F	P-O2P	2.13	1.58	1.50
2	A	1101	P5F	P-O2P	2.12	1.58	1.50
2	A	1101	P5F	C9-C8	2.07	1.42	1.39
2	B	1101	P5F	C4A-N9A	2.06	1.42	1.37
2	A	1101	P5F	C2B-C3B	-2.03	1.47	1.53
2	B	1101	P5F	C2B-C3B	-2.03	1.47	1.53

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	P5F	N3A-C2A-N1A	-5.37	120.45	128.58
2	B	1101	P5F	C5A-C4A-N3A	-5.25	119.48	126.72
2	B	1101	P5F	O1P-P-O3P	5.11	121.08	107.27
2	A	1101	P5F	O3P-PA-O2A	-5.01	95.62	110.70
2	B	1101	P5F	N3A-C2A-N1A	-4.93	121.11	128.58
2	A	1101	P5F	C5A-C4A-N3A	-4.87	120.01	126.72
2	A	1101	P5F	O3P-P-O2P	-4.77	96.35	110.70
2	B	1101	P5F	N3A-C4A-N9A	4.58	134.96	127.17
2	A	1101	P5F	O1A-PA-O3P	4.54	119.55	107.27
2	A	1101	P5F	N3A-C4A-N9A	4.45	134.73	127.17
2	A	1101	P5F	C4-N3-C2	-4.42	120.28	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	P5F	O1P-P-O3P	4.34	119.00	107.27
2	B	1101	P5F	O3P-P-O2P	-4.31	97.74	110.70
3	A	1102	2L3	OAE-SAQ-CAP	4.14	116.30	107.79
2	B	1101	P5F	C5A-N7A-C8A	3.86	109.52	103.45
2	B	1101	P5F	C4-N3-C2	-3.77	121.18	126.37
3	A	1102	2L3	OAE-SAQ-OAD	-3.69	103.82	117.52
2	B	1101	P5F	O4-C4-C4X	-3.68	119.79	128.01
5	B	1103[B]	2LB	CAK-CAL-CAN	3.65	121.48	116.49
2	A	1101	P5F	C5A-N7A-C8A	3.60	109.11	103.45
2	A	1101	P5F	C4X-C4-N3	3.52	119.11	111.84
5	B	1103[B]	2LB	OAE-SAQ-CAP	3.39	114.75	107.79
2	A	1101	P5F	N9A-C8A-N7A	-3.36	109.17	113.94
2	A	1101	P5F	O4-C4-C4X	-3.34	120.56	128.01
2	B	1101	P5F	C4X-C4-N3	3.33	118.72	111.84
3	B	1102[A]	2L3	CAK-CAL-CAN	3.28	120.97	116.49
2	A	1101	P5F	C2A-N3A-C4A	3.27	119.82	111.83
2	A	1101	P5F	N3-C2-N1	3.25	120.85	115.74
2	B	1101	P5F	N3-C2-N1	3.23	120.82	115.74
2	B	1101	P5F	C2A-N3A-C4A	3.21	119.68	111.83
2	A	1101	P5F	C1'-N10-C9A	3.15	123.54	119.02
2	B	1101	P5F	N9A-C8A-N7A	-3.05	109.61	113.94
5	B	1103[B]	2LB	OAE-SAQ-OAF	-3.03	106.27	117.52
3	A	1102	2L3	OAF-SAQ-OAE	-3.02	102.97	112.83
3	B	1102[A]	2L3	OAE-SAQ-OAD	-2.99	106.42	117.52
2	B	1101	P5F	O3P-PA-O2A	-2.90	101.97	110.70
5	B	1103[B]	2LB	OAD-SAQ-OAE	-2.89	103.40	112.83
2	B	1101	P5F	C1'-N10-C9A	2.88	123.16	119.02
3	B	1102[A]	2L3	OAD-SAQ-CAP	2.82	113.58	107.79
2	B	1101	P5F	O5B-PA-O2A	-2.75	98.05	108.94
3	B	1102[A]	2L3	OAF-SAQ-OAD	-2.74	103.88	112.83
3	B	1102[A]	2L3	OAF-SAQ-OAE	-2.72	103.95	112.83
2	B	1101	P5F	C4A-C5A-N7A	-2.65	107.55	110.58
2	A	1101	P5F	C4A-N9A-C8A	2.61	108.48	105.74
2	A	1101	P5F	C10-N10-C9A	-2.55	115.99	120.93
2	B	1101	P5F	C7-C6-C5X	-2.54	117.83	121.30
2	B	1101	P5F	O1P-P-O5'	2.52	119.00	107.57
3	A	1102	2L3	CAK-CAL-CAN	2.46	119.85	116.49
2	B	1101	P5F	O3'-C3'-C4'	-2.46	103.35	108.93
5	B	1103[B]	2LB	OAC-CAM-CAO	-2.43	118.84	122.36
2	A	1101	P5F	O1P-P-O5'	2.36	118.27	107.57
2	A	1101	P5F	O5B-PA-O2A	-2.36	99.60	108.94
2	B	1101	P5F	O1A-PA-O3P	2.33	113.56	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1103[B]	2LB	OAD-SAQ-OAF	-2.31	105.27	112.83
2	A	1101	P5F	O5'-P-O2P	-2.29	99.85	108.94
5	B	1103[B]	2LB	OAB-CAL-CAN	-2.29	119.14	121.71
2	A	1101	P5F	C4A-C5A-N7A	-2.28	107.97	110.58
2	B	1101	P5F	O5'-C5'-C4'	-2.24	103.39	109.36
2	A	1101	P5F	C4'-C3'-C2'	2.16	117.17	113.57
2	B	1101	P5F	O1A-PA-O5B	2.15	117.30	107.57
2	B	1101	P5F	O5'-P-O2P	-2.07	100.72	108.94
3	B	1102[A]	2L3	OAE-SAQ-CAP	2.05	112.00	107.79

There are no chirality outliers.

All (22) torsion outliers are listed below:

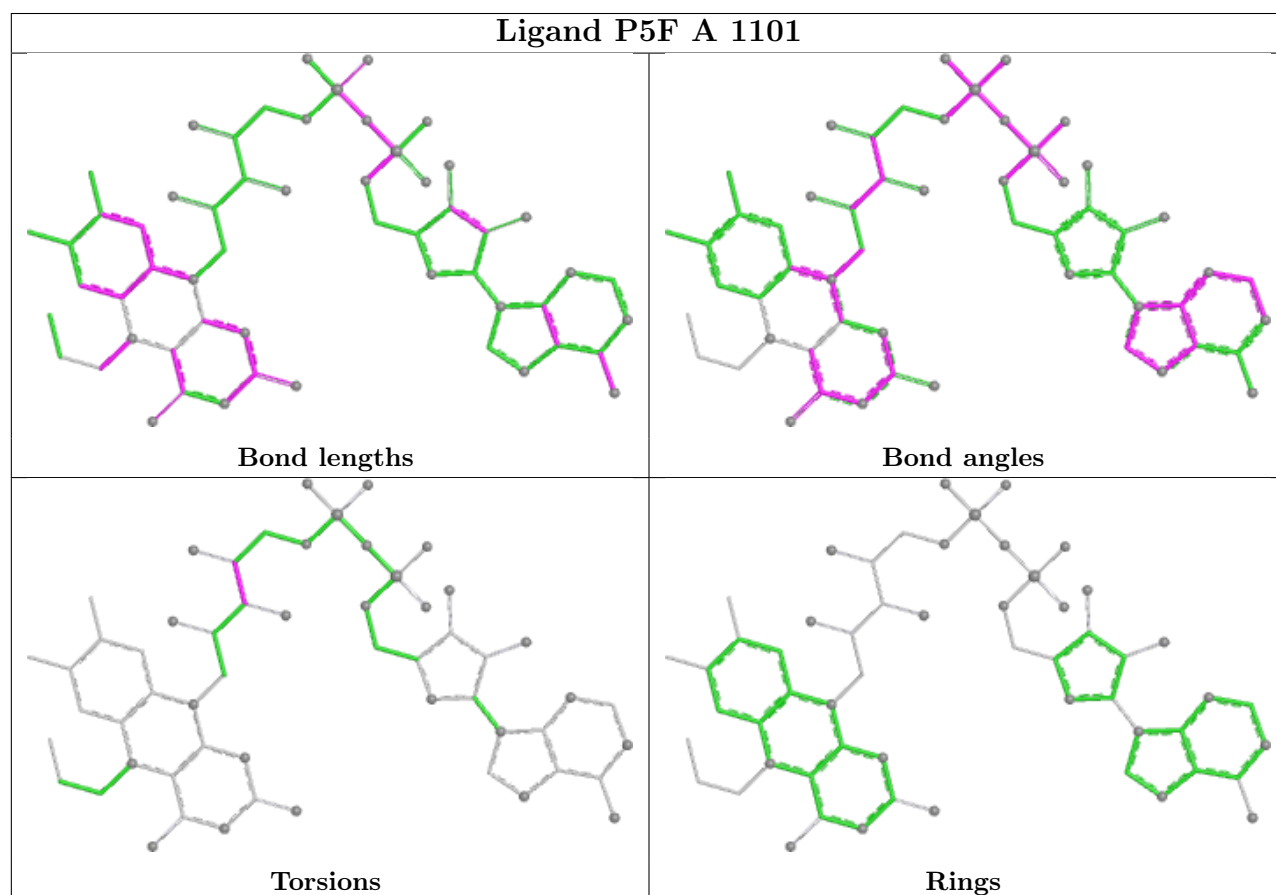
Mol	Chain	Res	Type	Atoms
2	B	1101	P5F	C5'-O5'-P-O2P
3	B	1102[A]	2L3	CAA-CAP-SAQ-OAD
3	B	1102[A]	2L3	CAM-CAP-SAQ-OAD
3	B	1102[A]	2L3	CAA-CAP-SAQ-OAE
5	B	1103[B]	2LB	CAA-CAP-SAQ-OAF
5	B	1103[B]	2LB	CAK-CAP-SAQ-OAF
5	B	1103[B]	2LB	CAM-CAP-SAQ-OAF
5	B	1103[B]	2LB	CAA-CAP-SAQ-OAE
5	B	1103[B]	2LB	CAK-CAP-SAQ-OAE
5	B	1103[B]	2LB	CAM-CAP-SAQ-OAE
4	B	1106	EDO	O1-C1-C2-O2
4	A	1106	EDO	O1-C1-C2-O2
2	A	1101	P5F	C2'-C3'-C4'-O4'
2	B	1101	P5F	P-O3P-PA-O5B
2	B	1101	P5F	C5'-O5'-P-O1P
2	B	1101	P5F	C5'-O5'-P-O3P
3	B	1102[A]	2L3	CAK-CAP-SAQ-OAD
3	B	1102[A]	2L3	CAK-CAP-SAQ-OAE
2	A	1101	P5F	O3'-C3'-C4'-O4'
2	B	1101	P5F	C3B-C4B-C5B-O5B
4	A	1107	EDO	O1-C1-C2-O2
4	A	1104	EDO	O1-C1-C2-O2

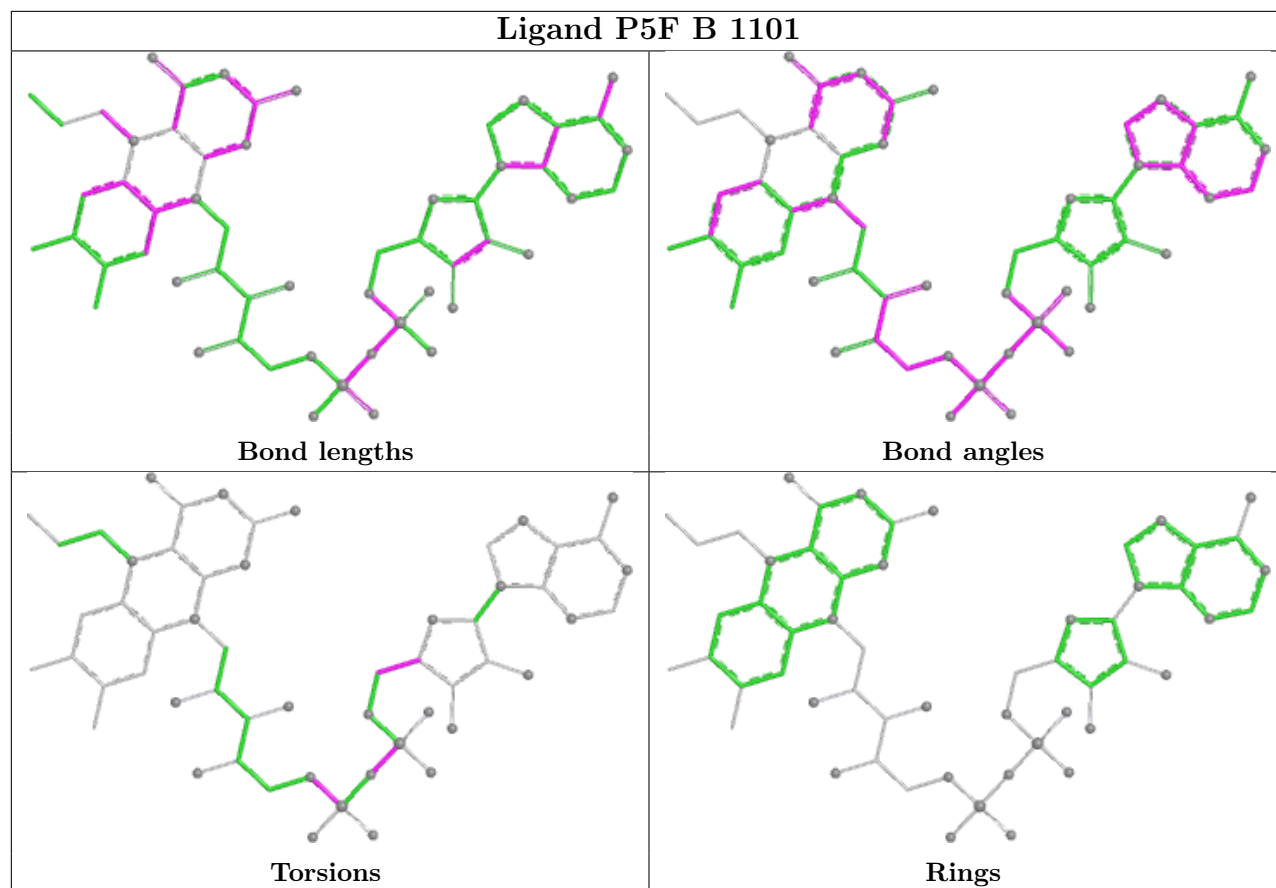
There are no ring outliers.

5 monomers are involved in 7 short contacts:

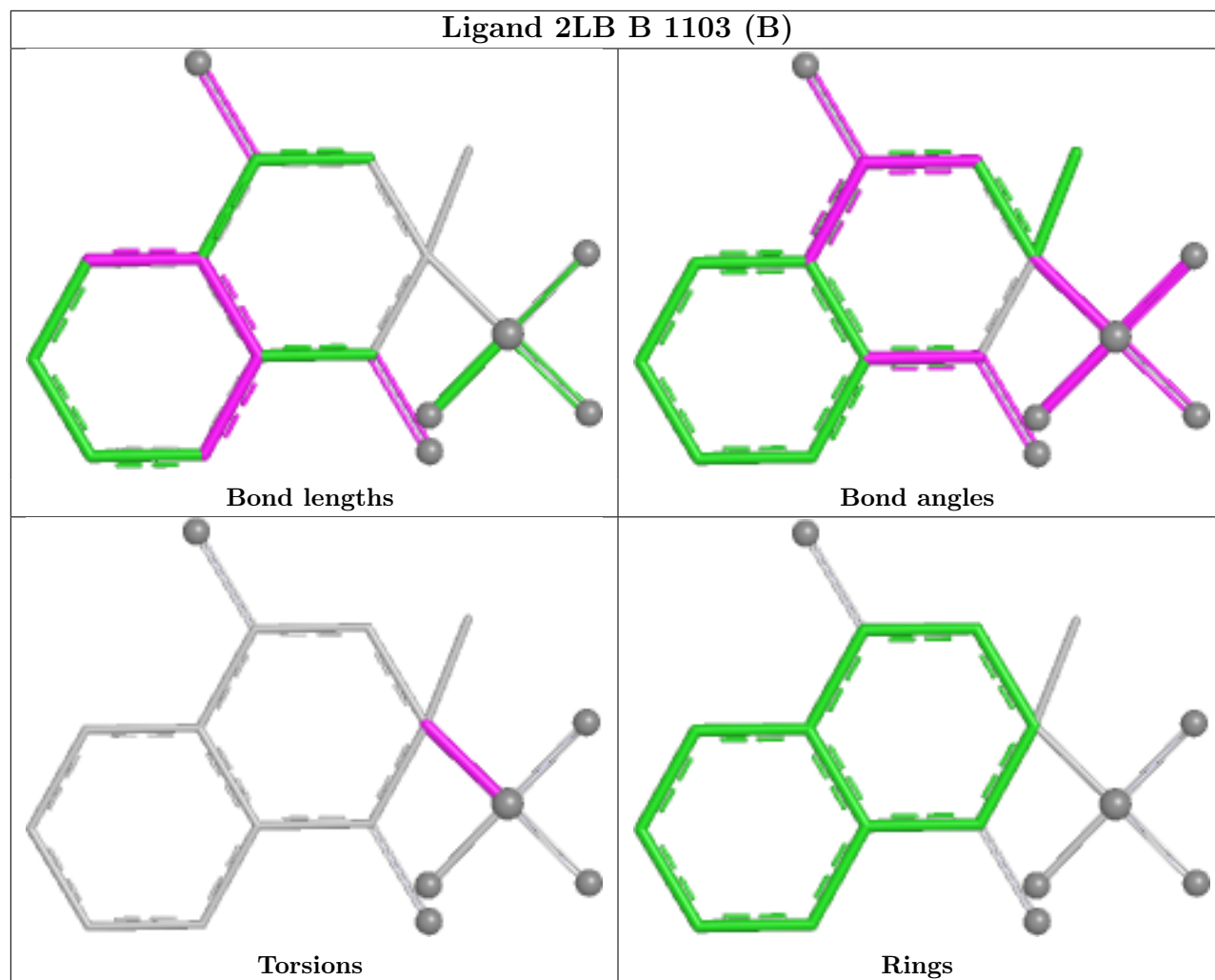
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	P5F	1	0
2	B	1101	P5F	2	0
5	B	1103[B]	2LB	3	0
3	B	1102[A]	2L3	1	0
3	A	1102	2L3	1	0

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 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.

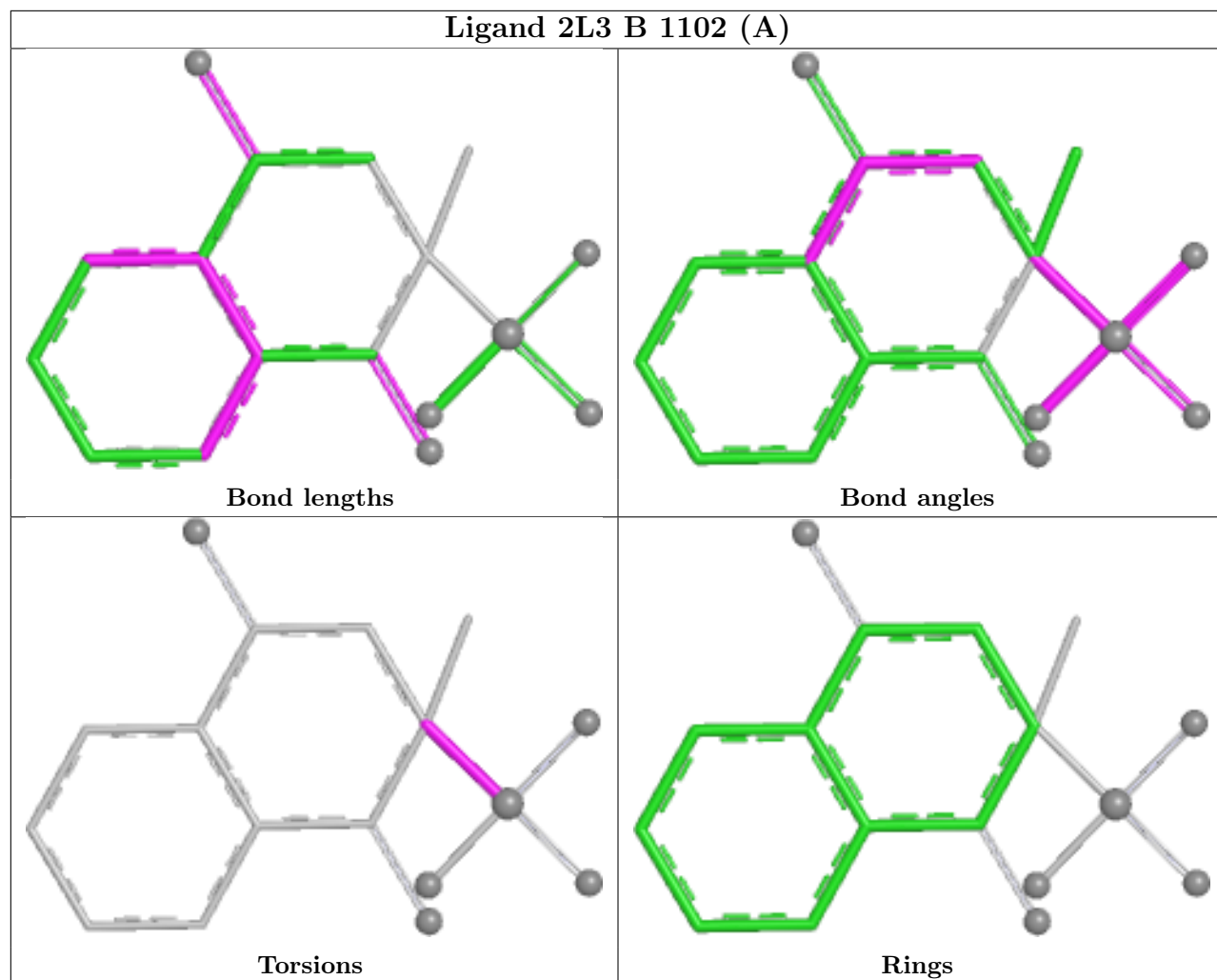


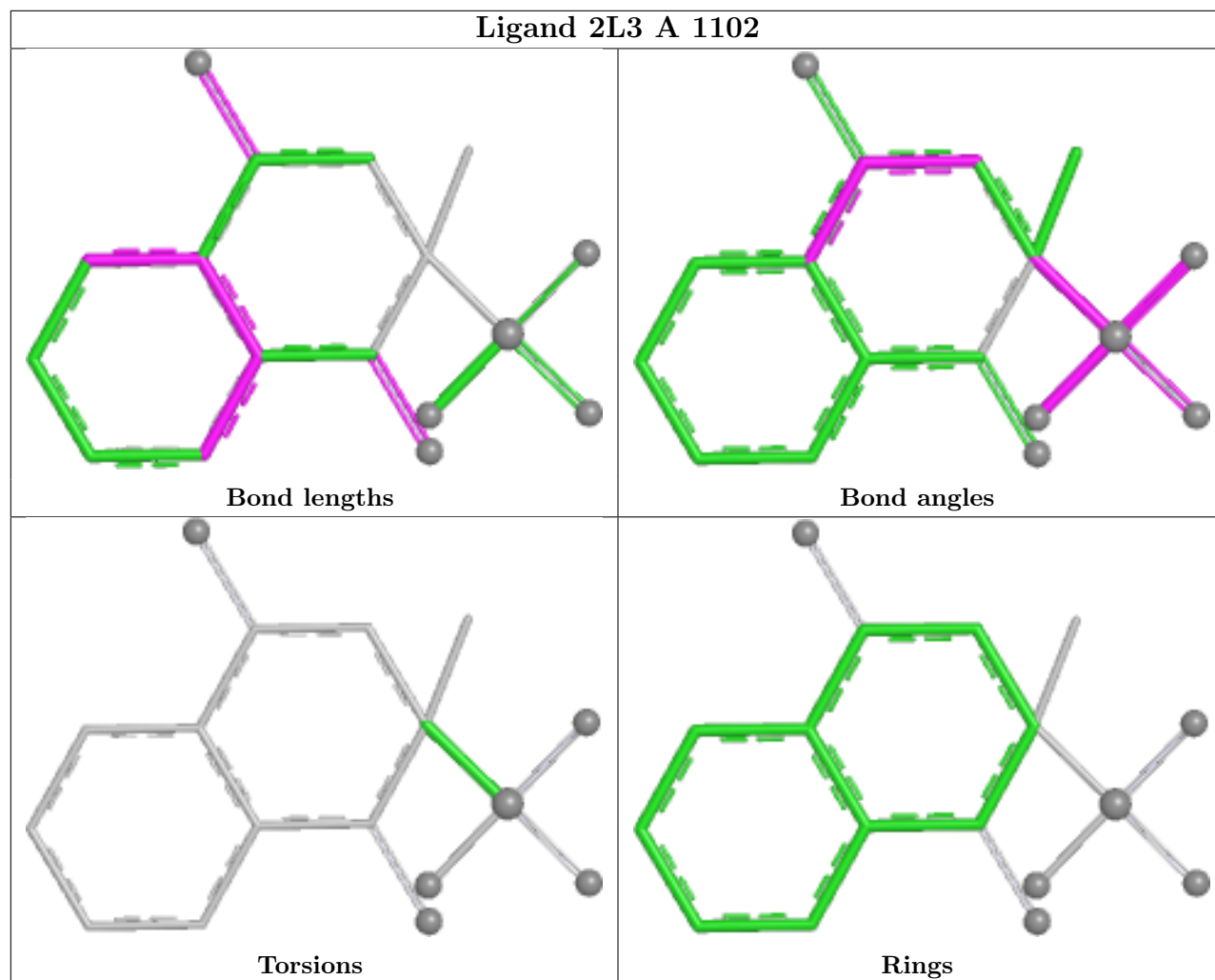


Ligand 2LB B 1103 (B)



Ligand 2L3 B 1102 (A)





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	973/1005 (96%)	-0.25	32 (3%)	49	55	10, 19, 47, 64	4 (0%)
1	B	979/1005 (97%)	-0.38	8 (0%)	82	86	9, 18, 37, 61	2 (0%)
All	All	1952/2010 (97%)	-0.32	40 (2%)	65	72	9, 19, 42, 64	6 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASN	5.9
1	A	103	VAL	4.9
1	A	463	ALA	4.5
1	B	463	ALA	4.4
1	A	26	PRO	4.3
1	A	389	ALA	4.0
1	A	748	PRO	4.0
1	A	102	ALA	3.9
1	A	437	PHE	3.6
1	A	441	ALA	3.5
1	A	85	PHE	3.5
1	A	4	SER	3.2
1	A	107	VAL	3.2
1	A	392	VAL	3.2
1	A	20	SER	3.2
1	B	102	ALA	3.1
1	A	81	ASP	3.1
1	B	993	PHE	2.9
1	A	396	ILE	2.9
1	A	388	MET	2.8
1	A	993[A]	PHE	2.8
1	A	78	ASN	2.8
1	A	185	GLY	2.8
1	A	390	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	27	SER	2.7
1	A	469	ARG	2.7
1	B	462	ALA	2.6
1	A	86	MET	2.6
1	A	104	LEU	2.5
1	A	462	ALA	2.5
1	A	28	LEU	2.4
1	B	103	VAL	2.4
1	B	186	GLY	2.3
1	B	184	LYS	2.3
1	A	399	VAL	2.2
1	A	838	ASP	2.1
1	B	104	LEU	2.1
1	A	747	HIS	2.0
1	A	1003	VAL	2.0
1	A	460	ALA	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(Å ²)	Q<0.9
3	2L3	B	1102[A]	17/17	0.85	0.13	26,28,33,36	17
3	2L3	A	1102	17/17	0.86	0.13	29,34,44,46	0
5	2LB	B	1103[B]	17/17	0.88	0.13	23,27,33,37	17
4	EDO	A	1105	4/4	0.91	0.09	19,19,20,23	0
4	EDO	A	1104	4/4	0.91	0.14	31,32,32,33	0
4	EDO	B	1106	4/4	0.93	0.09	18,28,29,30	0
4	EDO	B	1105	4/4	0.94	0.06	20,21,22,29	0

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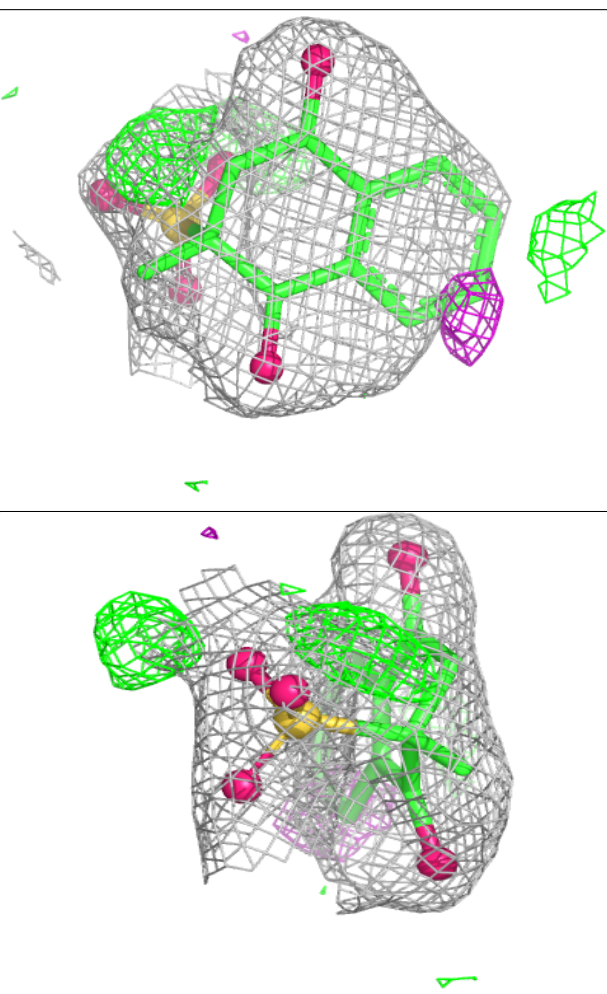
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	1106	4/4	0.97	0.07	14,21,25,29	0
4	EDO	A	1107	4/4	0.97	0.08	19,35,43,47	0
4	EDO	B	1104	4/4	0.97	0.05	20,26,27,28	0
4	EDO	A	1103	4/4	0.97	0.06	15,21,27,27	0
2	P5F	A	1101	56/61	0.97	0.06	8,15,27,30	0
2	P5F	B	1101	56/61	0.97	0.06	10,15,26,37	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.

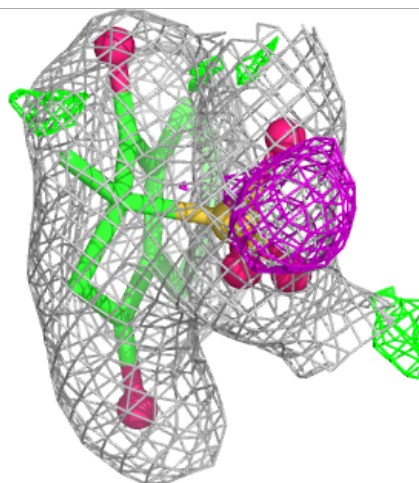
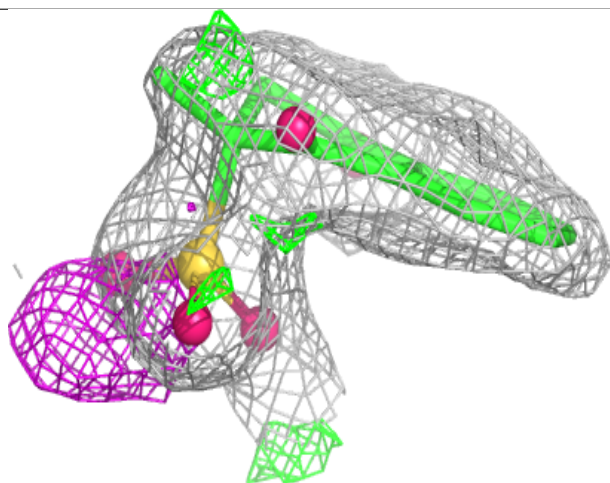
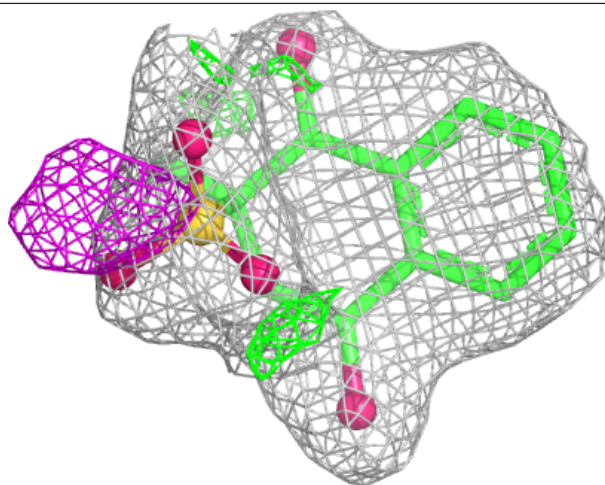
Electron density around 2L3 B 1102 (A):

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



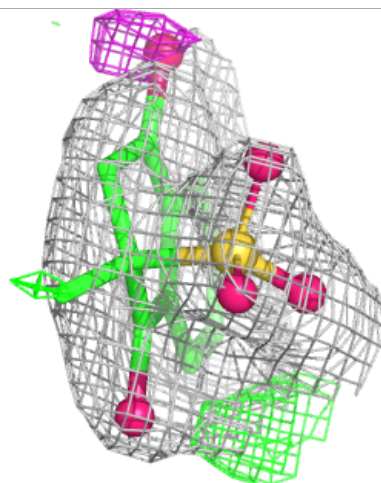
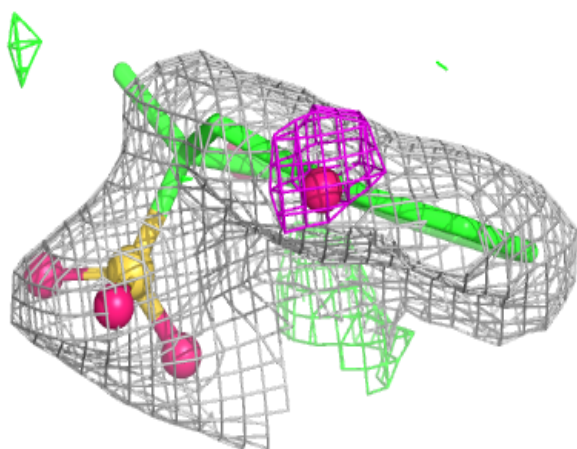
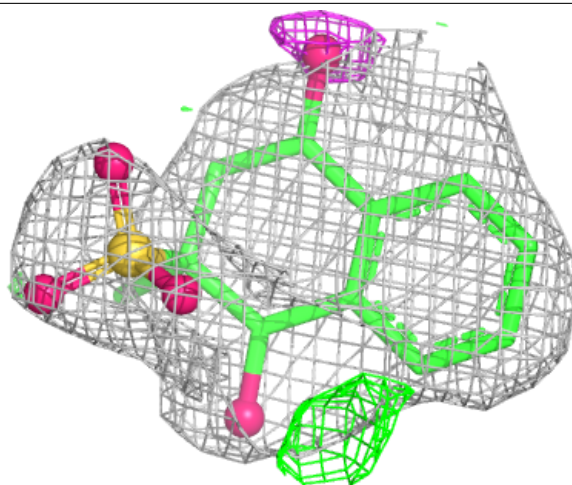
Electron density around 2L3 A 1102:

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



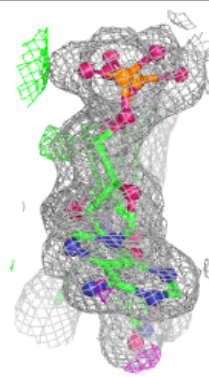
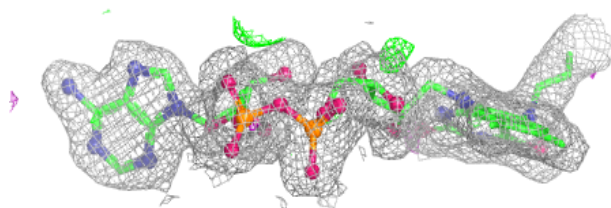
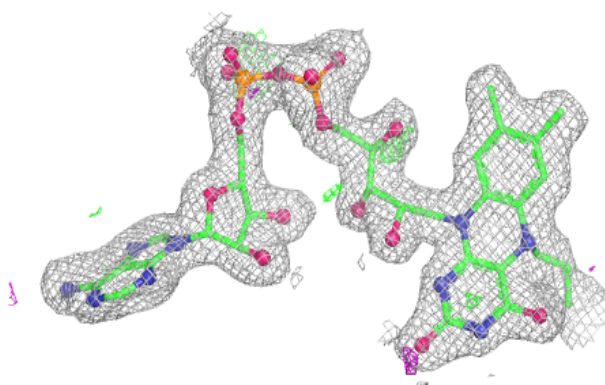
Electron density around 2LB B 1103 (B):

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

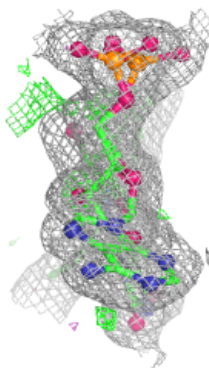
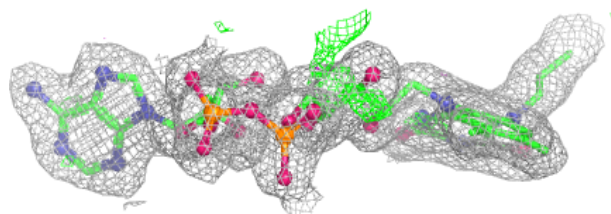
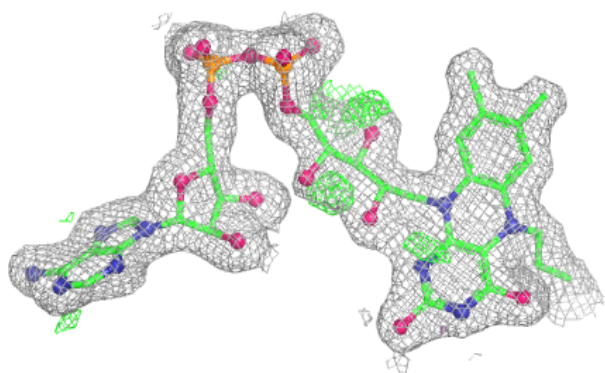


Electron density around P5F A 1101:

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

**Electron density around P5F B 1101:**

$2mF_o-DF_c$ (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.