



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:56 PM UTC

PDB ID : 5OKN / pdb_00005okn
Title : Crystal structure of human SHIP2 Phosphatase-C2 D607A mutant
Authors : Le Coq, J.; Lietha, D.
Deposited on : 2017-07-25
Resolution : 2.65 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

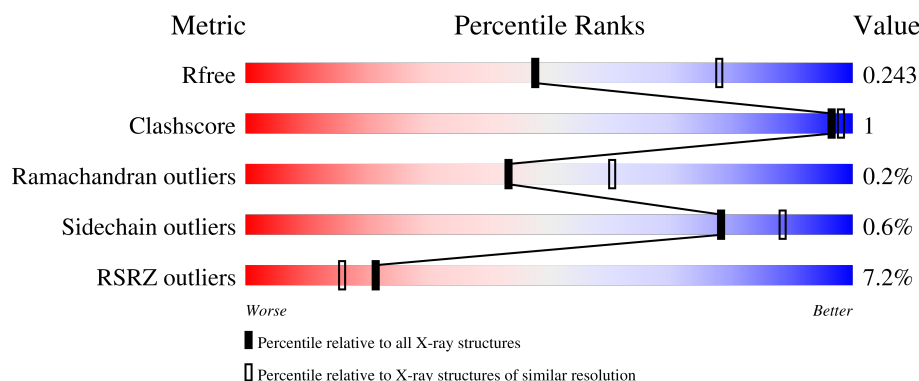
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	461	5% 89% 6%
1	B	461	4% 90% 7%
1	C	461	12% 90% 9%
1	D	461	3% 91% 6%
1	E	461	5% 90% 7%

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Mol	Chain	Length	Quality of chain
1	F	461	4% 90% 7%
1	G	461	16% 85% 13%
1	H	461	4% 91% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28076 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 Phosphatidylinositol 3,4,5-trisphosphate 5-phosphatase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	1	0
			3509	2239	593	663	14			
1	B	431	Total	C	N	O	S	0	0	0
			3482	2223	588	657	14			
1	C	421	Total	C	N	O	S	0	0	0
			3412	2178	575	645	14			
1	D	433	Total	C	N	O	S	0	0	0
			3501	2233	591	663	14			
1	E	427	Total	C	N	O	S	0	0	0
			3460	2207	585	654	14			
1	F	427	Total	C	N	O	S	0	0	0
			3461	2208	586	653	14			
1	G	402	Total	C	N	O	S	0	0	0
			3253	2082	548	611	12			
1	H	430	Total	C	N	O	S	0	0	0
			3477	2219	588	656	14			

There are 24 discrepancies between the modelled and reference sequences:

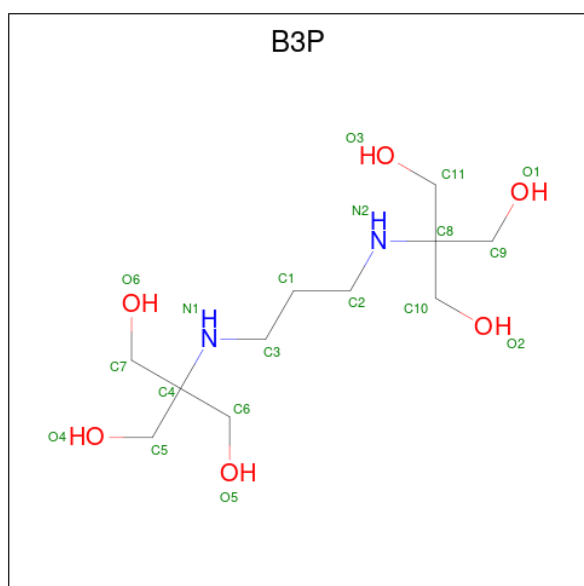
Chain	Residue	Modelled	Actual	Comment	Reference
A	418	GLY	-	expression tag	UNP O15357
A	419	PRO	-	expression tag	UNP O15357
A	607	ALA	ASP	engineered mutation	UNP O15357
B	418	GLY	-	expression tag	UNP O15357
B	419	PRO	-	expression tag	UNP O15357
B	607	ALA	ASP	engineered mutation	UNP O15357
C	418	GLY	-	expression tag	UNP O15357
C	419	PRO	-	expression tag	UNP O15357
C	607	ALA	ASP	engineered mutation	UNP O15357
D	418	GLY	-	expression tag	UNP O15357
D	419	PRO	-	expression tag	UNP O15357
D	607	ALA	ASP	engineered mutation	UNP O15357
E	418	GLY	-	expression tag	UNP O15357

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Chain	Residue	Modelled	Actual	Comment	Reference
E	419	PRO	-	expression tag	UNP O15357
E	607	ALA	ASP	engineered mutation	UNP O15357
F	418	GLY	-	expression tag	UNP O15357
F	419	PRO	-	expression tag	UNP O15357
F	607	ALA	ASP	engineered mutation	UNP O15357
G	418	GLY	-	expression tag	UNP O15357
G	419	PRO	-	expression tag	UNP O15357
G	607	ALA	ASP	engineered mutation	UNP O15357
H	418	GLY	-	expression tag	UNP O15357
H	419	PRO	-	expression tag	UNP O15357
H	607	ALA	ASP	engineered mutation	UNP O15357

- Molecule 2 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: $C_{11}H_{26}N_2O_6$).



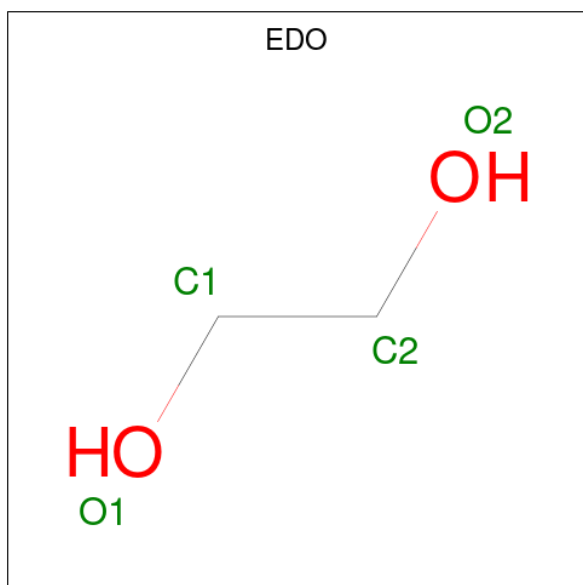
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	11	2	6		
2	B	1	Total	C	N	O	0	0
			19	11	2	6		
2	C	1	Total	C	N	O	0	0
			19	11	2	6		
2	D	1	Total	C	N	O	0	0
			19	11	2	6		
2	E	1	Total	C	N	O	0	0
			19	11	2	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total	C	N	O	0	0
			19	11	2	6		
2	H	1	Total	C	N	O	0	0
			19	11	2	6		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



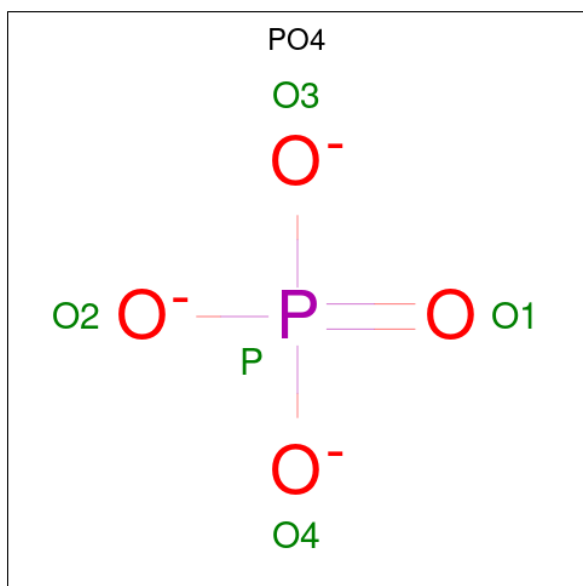
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0
4	E	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	O	P	0	0
			5	4	1		
4	G	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		
5	G	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		

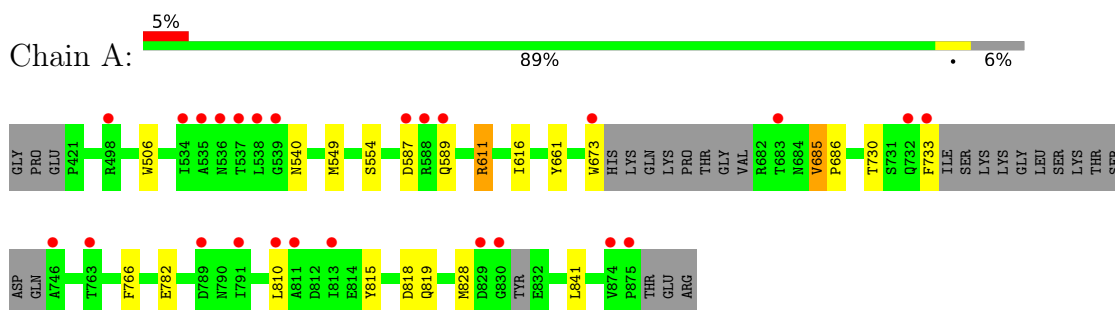
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	47	Total	O	0	0
			47	47		
6	B	51	Total	O	0	0
			51	51		
6	C	15	Total	O	0	0
			15	15		
6	D	40	Total	O	0	0
			40	40		
6	E	33	Total	O	0	0
			33	33		
6	F	34	Total	O	0	0
			34	34		
6	G	11	Total	O	0	0
			11	11		
6	H	53	Total	O	0	0
			53	53		

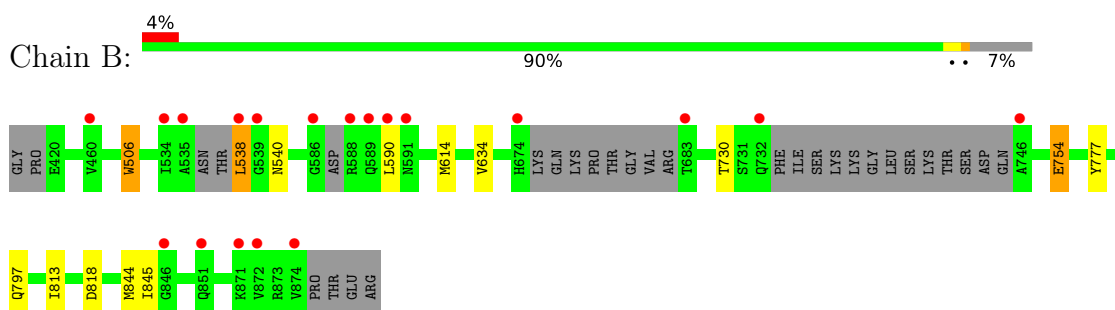
3 Residue-property plots [i](#)

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.

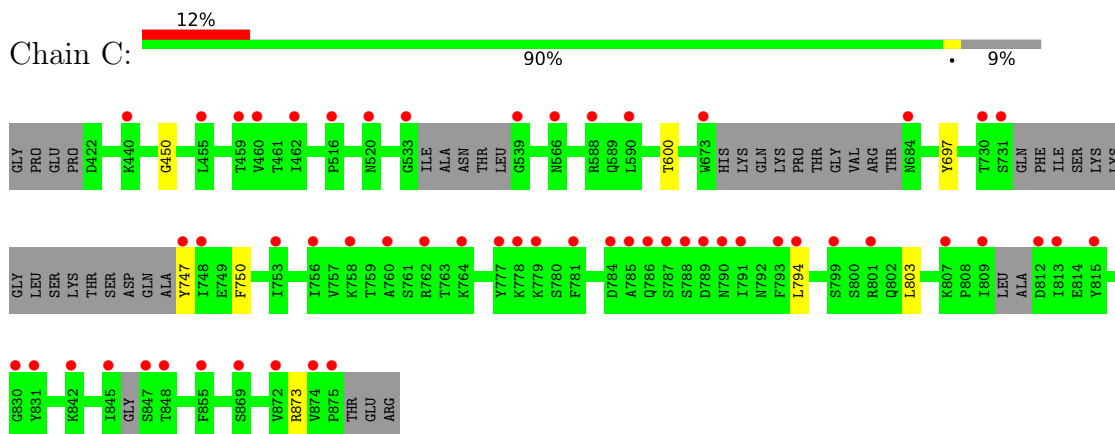
- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 5-phosphatase 2



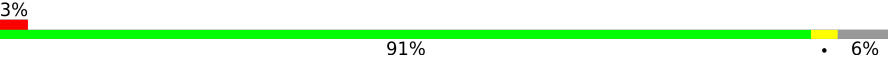
- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 5-phosphatase 2

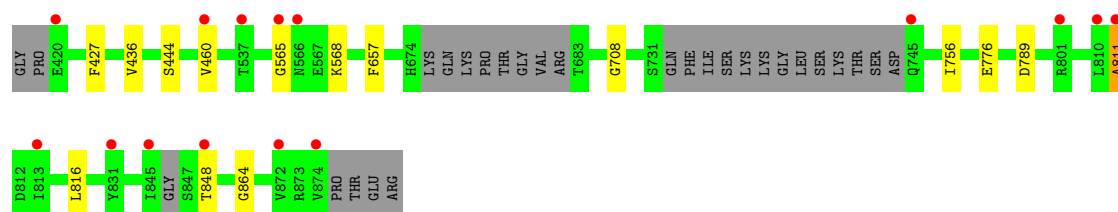


- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 5-phosphatase 2

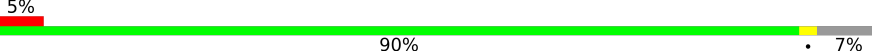


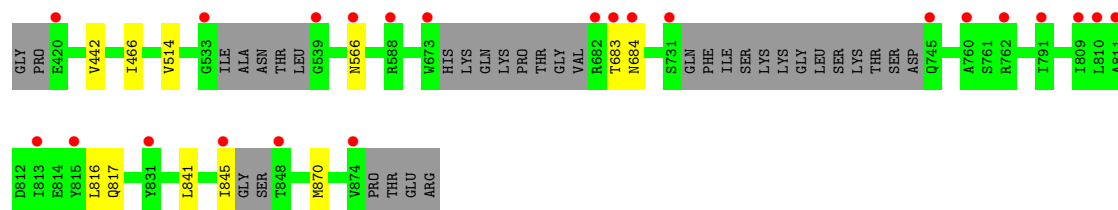
- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 5-phosphatase 2

Chain D:  3% 91% 6%



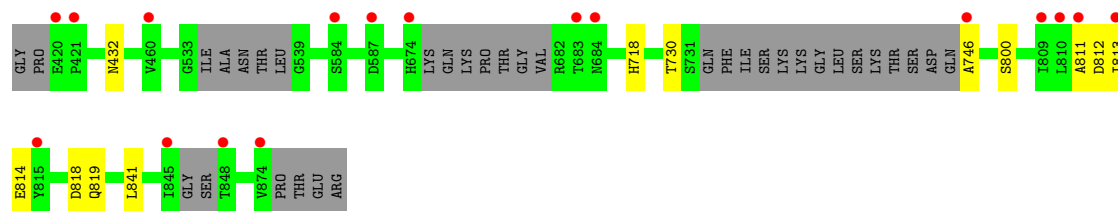
- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 5-phosphatase 2

Chain E:  5% 90% 7%



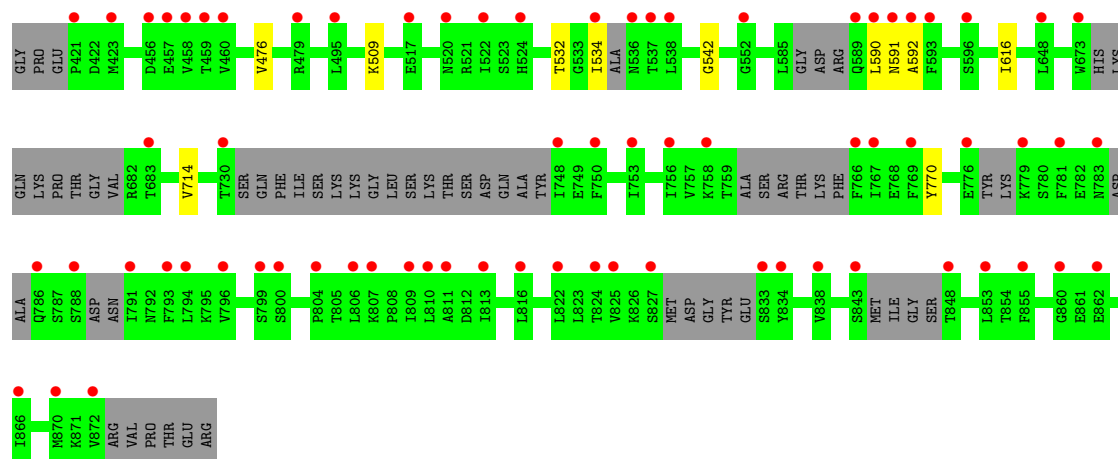
- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 5-phosphatase 2

Chain F:  4% 90% 7%

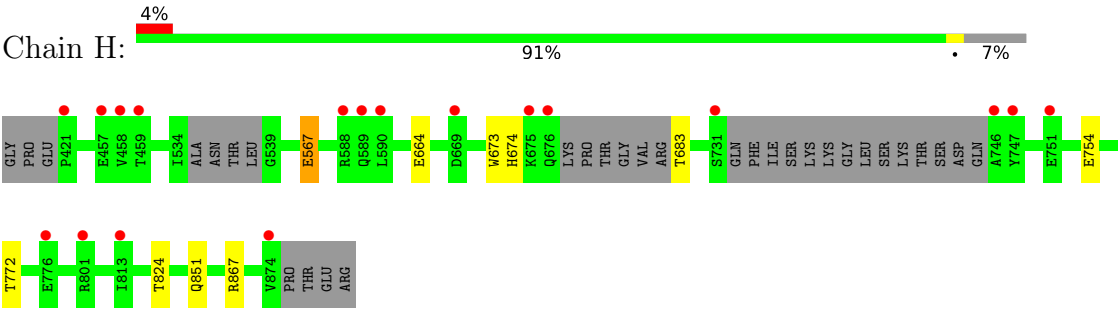


- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 5-phosphatase 2

Chain G:  16% 85% 13%



- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 5-phosphatase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.06Å 177.14Å 177.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.17 – 2.65 49.17 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.17-2.65) 99.9 (49.17-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.206 , 0.245 0.208 , 0.243	Depositor DCC
R_{free} test set	6370 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28076	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, B3P, MG, PO4

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	0.64	0/3593	0.81	1/4863 (0.0%)
1	B	0.66	0/3562	0.81	0/4820
1	C	0.62	0/3490	0.77	0/4720
1	D	0.64	0/3582	0.82	0/4850
1	E	0.64	0/3539	0.78	0/4788
1	F	0.65	0/3541	0.81	0/4791
1	G	0.64	0/3322	0.79	2/4489 (0.0%)
1	H	0.63	0/3558	0.81	0/4814
All	All	0.64	0/28187	0.80	3/38135 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	714	VAL	N-CA-C	6.92	118.80	112.43
1	A	685	VAL	N-CA-CB	6.20	115.85	110.08
1	G	616	ILE	N-CA-C	5.33	115.54	110.42

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	3509	0	3437	13	0
1	B	3482	0	3405	7	0
1	C	3412	0	3329	4	0
1	D	3501	0	3420	5	0
1	E	3460	0	3380	8	0
1	F	3461	0	3379	6	0
1	G	3253	0	3191	6	0
1	H	3477	0	3402	6	0
2	A	19	0	26	0	0
2	B	19	0	26	0	0
2	C	19	0	26	1	0
2	D	19	0	26	0	0
2	E	19	0	26	0	0
2	F	19	0	26	0	0
2	H	19	0	26	0	0
3	A	4	0	6	0	0
3	B	20	0	30	0	0
3	D	12	0	18	0	0
3	E	8	0	12	2	0
3	F	16	0	24	0	0
3	G	4	0	6	0	0
3	H	4	0	6	1	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	47	0	0	0	0
6	B	51	0	0	0	0
6	C	15	0	0	0	0
6	D	40	0	0	0	0
6	E	33	0	0	0	0
6	F	34	0	0	0	0
6	G	11	0	0	0	0
6	H	53	0	0	1	0
All	All	28076	0	27227	55	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 1.

All (55) 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:E:442:VAL:HG21	3:E:904:EDO:H22	1.62	0.79
1:G:590:LEU:HD21	1:G:770:TYR:CG	2.30	0.66
1:B:538:LEU:HD12	1:B:538:LEU:N	2.12	0.65
1:A:587:ASP:OD2	1:A:589:GLN:HG2	2.03	0.58
1:C:450:GLY:O	2:C:903:B3P:N1	2.37	0.57
1:E:683:THR:HG22	1:E:684:ASN:H	1.70	0.57
1:D:565:GLY:HA3	1:D:568:LYS:HG3	1.87	0.56
1:G:590:LEU:HD21	1:G:770:TYR:CD2	2.40	0.55
1:B:506:TRP:CZ3	1:B:540:ASN:HB3	2.42	0.55
1:A:733:PHE:CD1	1:A:815:TYR:HD1	2.24	0.55
1:E:683:THR:HG22	1:E:684:ASN:N	2.22	0.55
1:A:730:THR:HG21	1:A:818:ASP:HB3	1.90	0.52
1:A:733:PHE:CD1	1:A:815:TYR:CD1	2.98	0.51
1:H:673:TRP:CE3	1:H:674:HIS:HB2	2.46	0.51
1:F:746:ALA:HB2	1:F:811:ALA:HB2	1.93	0.51
1:E:566:ASN:ND2	1:E:683:THR:O	2.44	0.51
1:D:811:ALA:O	1:D:816:LEU:HD13	2.10	0.50
1:C:750:PHE:HB3	1:C:803:LEU:HD13	1.94	0.50
1:F:746:ALA:HB2	1:F:811:ALA:CB	2.43	0.49
1:B:538:LEU:N	1:B:538:LEU:CD1	2.78	0.47
1:A:506:TRP:CE3	1:A:540:ASN:HA	2.50	0.46
1:A:766:PHE:HB3	1:A:828:MET:HE2	1.97	0.46
1:E:442:VAL:CG2	3:E:904:EDO:H22	2.38	0.46
1:G:590:LEU:O	1:G:590:LEU:HG	2.15	0.46
1:E:817:GLN:HG3	1:E:845:ILE:HD12	1.97	0.46
1:D:657:PHE:CD1	1:D:708:GLY:HA2	2.51	0.46
1:A:549:MET:HE3	1:A:554:SER:HB3	1.98	0.46
1:H:567:GLU:OE1	1:H:567:GLU:N	2.44	0.46
1:H:683:THR:N	6:H:1002:HOH:O	2.49	0.46
1:A:733:PHE:HB3	1:A:810:LEU:HD22	1.99	0.45
1:A:611:ARG:NH1	1:A:685:VAL:O	2.49	0.45
1:B:730:THR:HG21	1:B:818:ASP:HB3	1.99	0.45
1:G:532:THR:HG23	1:G:542:GLY:HA2	1.97	0.45
1:A:616:ILE:HG12	1:A:673:TRP:CE3	2.52	0.45
1:F:730:THR:HG21	1:F:818:ASP:HB3	1.99	0.44
1:F:812:ASP:O	1:F:814:GLU:N	2.50	0.44
1:H:851:GLN:OE1	1:H:867:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:476:VAL:O	1:G:509:LYS:NZ	2.50	0.44
1:E:466:ILE:HG12	1:E:514:VAL:HG12	2.00	0.43
1:D:427:PHE:CD1	1:D:427:PHE:C	2.95	0.43
1:A:661:TYR:O	1:A:686:PRO:HA	2.19	0.43
1:B:754:GLU:HG2	1:B:797:GLN:HG3	2.01	0.43
1:F:819:GLN:HB2	1:F:841:LEU:HD12	2.01	0.43
1:H:673:TRP:CZ3	1:H:674:HIS:HB2	2.53	0.43
1:C:747:TYR:HB2	1:C:873:ARG:HB3	2.02	0.42
1:A:819:GLN:HB2	1:A:841:LEU:HD12	2.02	0.42
1:E:841:LEU:HD22	1:E:870:MET:HE1	2.00	0.42
1:B:614:MET:HE3	1:B:634:VAL:HG21	2.02	0.41
1:C:600:THR:HA	1:C:697:TYR:CD2	2.56	0.41
1:F:432:ASN:HB3	1:F:718:HIS:CG	2.55	0.41
1:A:782:GLU:HG2	1:A:828:MET:HE3	2.02	0.40
1:D:756:ILE:O	1:D:864:GLY:HA3	2.22	0.40
1:B:813:ILE:HG23	1:B:845:ILE:HG21	2.03	0.40
1:H:772:THR:HG23	3:H:904:EDO:O1	2.21	0.40
1:G:590:LEU:O	1:G:592:ALA:N	2.55	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	427/461 (93%)	415 (97%)	12 (3%)	0	100	100
1	B	421/461 (91%)	414 (98%)	6 (1%)	1 (0%)	43	60
1	C	409/461 (89%)	397 (97%)	12 (3%)	0	100	100
1	D	425/461 (92%)	409 (96%)	13 (3%)	3 (1%)	18	30
1	E	417/461 (90%)	404 (97%)	13 (3%)	0	100	100
1	F	417/461 (90%)	401 (96%)	15 (4%)	1 (0%)	43	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	380/461 (82%)	365 (96%)	14 (4%)	1 (0%)	36	52
1	H	422/461 (92%)	413 (98%)	9 (2%)	0	100	100
All	All	3318/3688 (90%)	3218 (97%)	94 (3%)	6 (0%)	43	60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	811	ALA
1	F	813	ILE
1	G	591	ASN
1	B	506	TRP
1	D	460	VAL
1	D	848	THR

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	393/416 (94%)	392 (100%)	1 (0%)	86	94
1	B	389/416 (94%)	384 (99%)	5 (1%)	61	77
1	C	383/416 (92%)	382 (100%)	1 (0%)	86	94
1	D	392/416 (94%)	388 (99%)	4 (1%)	68	81
1	E	387/416 (93%)	386 (100%)	1 (0%)	86	94
1	F	387/416 (93%)	386 (100%)	1 (0%)	86	94
1	G	367/416 (88%)	366 (100%)	1 (0%)	86	94
1	H	389/416 (94%)	385 (99%)	4 (1%)	68	81
All	All	3087/3328 (93%)	3069 (99%)	18 (1%)	78	88

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	611	ARG

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Mol	Chain	Res	Type
1	B	538	LEU
1	B	590	LEU
1	B	754	GLU
1	B	777	TYR
1	B	844	MET
1	C	794	LEU
1	D	436	VAL
1	D	444	SER
1	D	776	GLU
1	D	789	ASP
1	E	816	LEU
1	F	800	SER
1	G	534	ILE
1	H	567	GLU
1	H	664	GLU
1	H	754	GLU
1	H	824	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	551	ASN
1	A	705	ASN
1	A	817	GLN
1	A	819	GLN
1	B	566	ASN
1	B	701	HIS
1	B	792	ASN
1	B	797	GLN
1	C	566	ASN
1	C	684	ASN
1	C	705	ASN
1	C	802	GLN
1	C	850	GLN
1	C	865	ASN
1	D	819	GLN
1	E	591	ASN
1	E	705	ASN
1	E	865	ASN
1	F	524	HIS
1	F	674	HIS
1	F	792	ASN

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Mol	Chain	Res	Type
1	F	851	GLN
1	G	551	ASN
1	G	705	ASN
1	G	792	ASN
1	G	797	GLN
1	G	819	GLN
1	H	705	ASN

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 ⓘ

Of 36 ligands modelled in this entry, 6 are monoatomic - leaving 30 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	B3P	C	903	-	18,18,18	0.93	0	23,23,23	1.07	2 (8%)
4	PO4	H	901	5	4,4,4	1.02	0	6,6,6	0.46	0
3	EDO	E	905	-	3,3,3	0.39	0	2,2,2	0.43	0
3	EDO	F	907	-	3,3,3	0.46	0	2,2,2	0.21	0
4	PO4	G	901	5	4,4,4	0.98	0	6,6,6	0.52	0
2	B3P	H	903	-	18,18,18	0.73	0	23,23,23	1.08	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	B3P	D	903	-	18,18,18	0.88	0	23,23,23	1.19	2 (8%)
3	EDO	D	905	-	3,3,3	0.53	0	2,2,2	0.06	0
3	EDO	F	906	-	3,3,3	0.45	0	2,2,2	0.26	0
2	B3P	B	901	-	18,18,18	1.00	1 (5%)	23,23,23	1.38	4 (17%)
3	EDO	B	902	-	3,3,3	0.35	0	2,2,2	0.36	0
3	EDO	H	904	-	3,3,3	0.41	0	2,2,2	0.34	0
3	EDO	B	906	-	3,3,3	0.48	0	2,2,2	0.14	0
2	B3P	E	903	-	18,18,18	0.76	0	23,23,23	1.35	1 (4%)
3	EDO	A	902	-	3,3,3	0.44	0	2,2,2	0.39	0
4	PO4	F	901	5	4,4,4	1.00	0	6,6,6	0.57	0
4	PO4	E	901	5	4,4,4	0.89	0	6,6,6	0.51	0
3	EDO	B	905	-	3,3,3	0.46	0	2,2,2	0.13	0
3	EDO	D	906	-	3,3,3	0.39	0	2,2,2	0.30	0
3	EDO	B	903	-	3,3,3	0.46	0	2,2,2	0.22	0
3	EDO	D	904	-	3,3,3	0.50	0	2,2,2	0.15	0
3	EDO	G	903	-	3,3,3	0.42	0	2,2,2	0.33	0
4	PO4	C	901	5	4,4,4	0.98	0	6,6,6	0.43	0
2	B3P	F	903	-	18,18,18	0.80	0	23,23,23	1.13	1 (4%)
4	PO4	D	901	5	4,4,4	0.91	0	6,6,6	0.63	0
3	EDO	F	905	-	3,3,3	0.49	0	2,2,2	0.12	0
2	B3P	A	901	-	18,18,18	1.07	2 (11%)	23,23,23	1.32	3 (13%)
3	EDO	B	904	-	3,3,3	0.52	0	2,2,2	0.12	0
3	EDO	F	904	-	3,3,3	0.49	0	2,2,2	0.20	0
3	EDO	E	904	-	3,3,3	0.38	0	2,2,2	0.24	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	B3P	C	903	-	-	0/28/28/28	-
3	EDO	E	905	-	-	0/1/1/1	-
3	EDO	F	907	-	-	1/1/1/1	-
2	B3P	H	903	-	-	0/28/28/28	-
2	B3P	D	903	-	-	3/28/28/28	-
3	EDO	D	905	-	-	0/1/1/1	-
3	EDO	F	906	-	-	1/1/1/1	-
2	B3P	B	901	-	-	1/28/28/28	-
3	EDO	B	902	-	-	1/1/1/1	-
3	EDO	H	904	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	906	-	-	0/1/1/1	-
2	B3P	E	903	-	-	0/28/28/28	-
3	EDO	A	902	-	-	0/1/1/1	-
3	EDO	B	905	-	-	0/1/1/1	-
3	EDO	D	906	-	-	0/1/1/1	-
3	EDO	B	903	-	-	1/1/1/1	-
3	EDO	D	904	-	-	1/1/1/1	-
3	EDO	G	903	-	-	0/1/1/1	-
2	B3P	F	903	-	-	0/28/28/28	-
3	EDO	F	905	-	-	0/1/1/1	-
2	B3P	A	901	-	-	7/28/28/28	-
3	EDO	B	904	-	-	1/1/1/1	-
3	EDO	F	904	-	-	0/1/1/1	-
3	EDO	E	904	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	B3P	C3-N1	2.54	1.49	1.46
2	A	901	B3P	C6-C4	-2.17	1.51	1.53
2	B	901	B3P	C5-C4	-2.01	1.51	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	903	B3P	C2-N2-C8	-3.74	110.69	116.17
2	B	901	B3P	O5-C6-C4	-2.82	105.94	111.68
2	F	903	B3P	C2-N2-C8	-2.67	112.25	116.17
2	A	901	B3P	C2-N2-C8	-2.66	112.27	116.17
2	B	901	B3P	O3-C11-C8	-2.65	106.30	111.68
2	D	903	B3P	C6-C4-C5	-2.62	104.27	110.02
2	A	901	B3P	C7-C4-C6	-2.59	104.34	110.02
2	A	901	B3P	O5-C6-C4	-2.53	106.53	111.68
2	D	903	B3P	C2-N2-C8	-2.48	112.54	116.17
2	B	901	B3P	C2-N2-C8	-2.46	112.56	116.17
2	C	903	B3P	O4-C5-C4	-2.36	106.89	111.68
2	B	901	B3P	O4-C5-C4	-2.30	107.01	111.68
2	H	903	B3P	C2-N2-C8	-2.17	112.99	116.17
2	C	903	B3P	C2-N2-C8	-2.17	113.00	116.17

There are no chirality outliers.

All (17) torsion outliers are listed below:

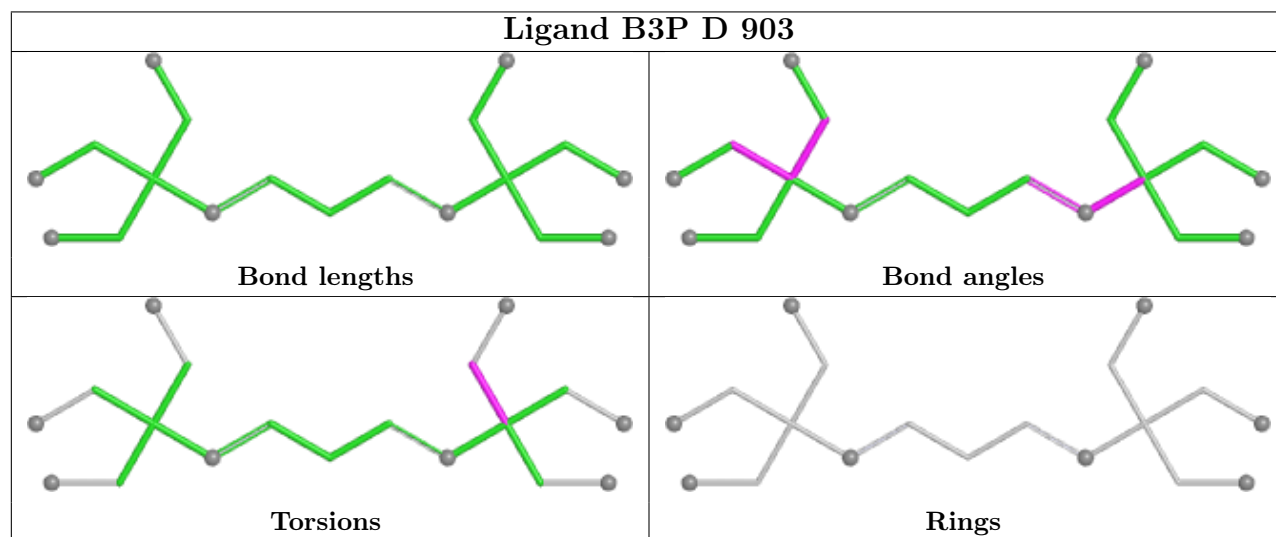
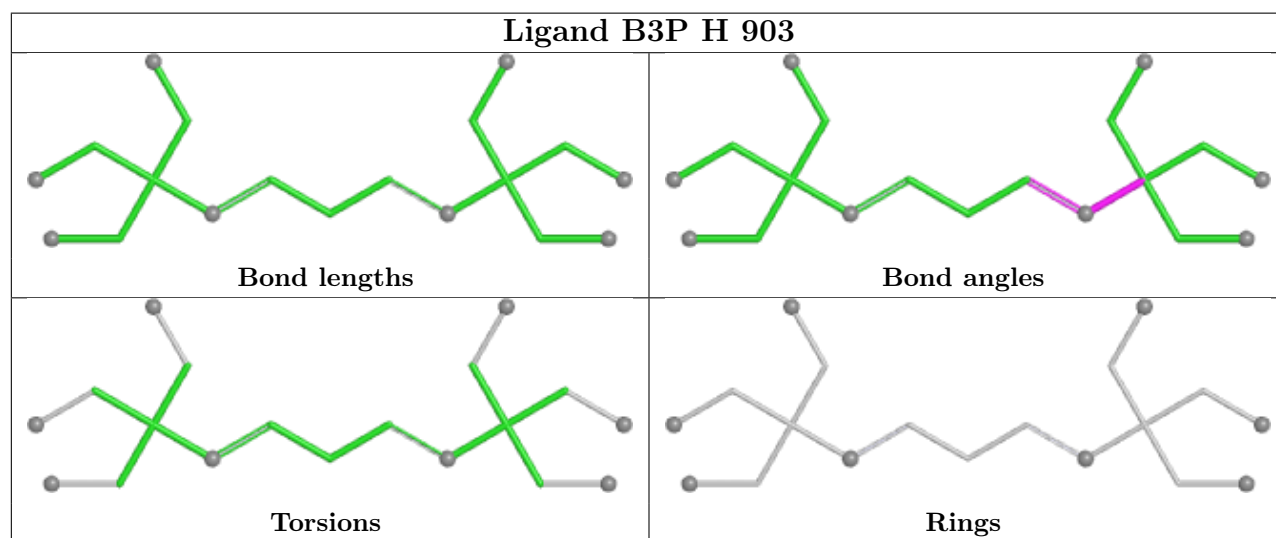
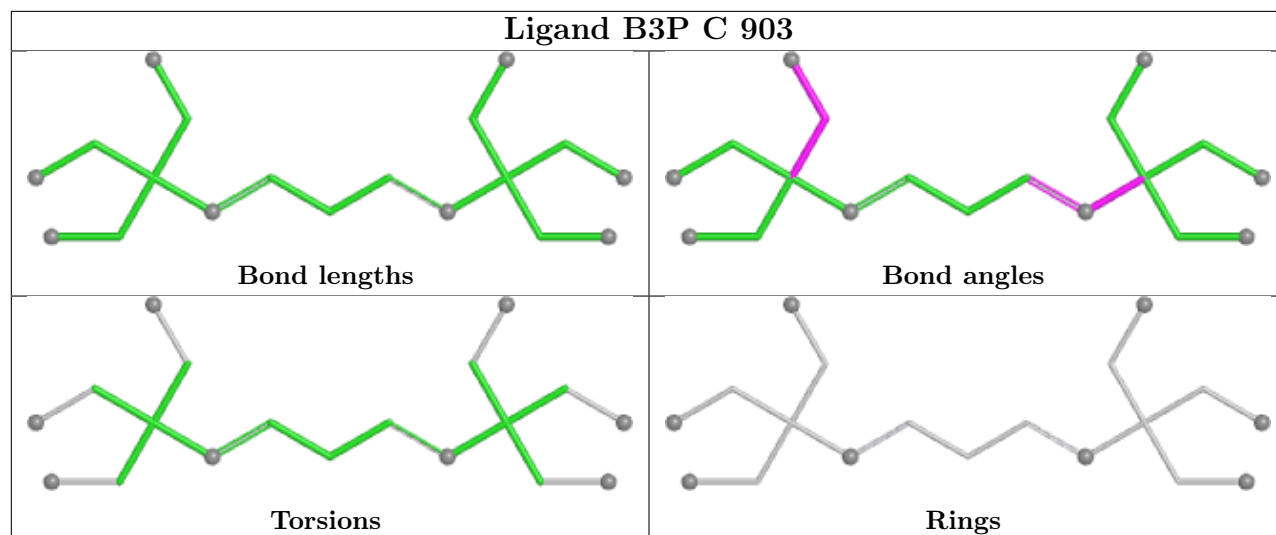
Mol	Chain	Res	Type	Atoms
2	A	901	B3P	C7-C4-C5-O4
2	D	903	B3P	O3-C11-C8-N2
2	D	903	B3P	O3-C11-C8-C9
2	D	903	B3P	O3-C11-C8-C10
2	A	901	B3P	N1-C4-C5-O4
2	A	901	B3P	C9-C8-N2-C2
2	A	901	B3P	C11-C8-N2-C2
3	D	904	EDO	O1-C1-C2-O2
2	A	901	B3P	N2-C8-C9-O1
2	A	901	B3P	C6-C4-C5-O4
3	B	903	EDO	O1-C1-C2-O2
3	B	902	EDO	O1-C1-C2-O2
2	A	901	B3P	C2-C1-C3-N1
2	B	901	B3P	N1-C4-C7-O6
3	F	907	EDO	O1-C1-C2-O2
3	B	904	EDO	O1-C1-C2-O2
3	F	906	EDO	O1-C1-C2-O2

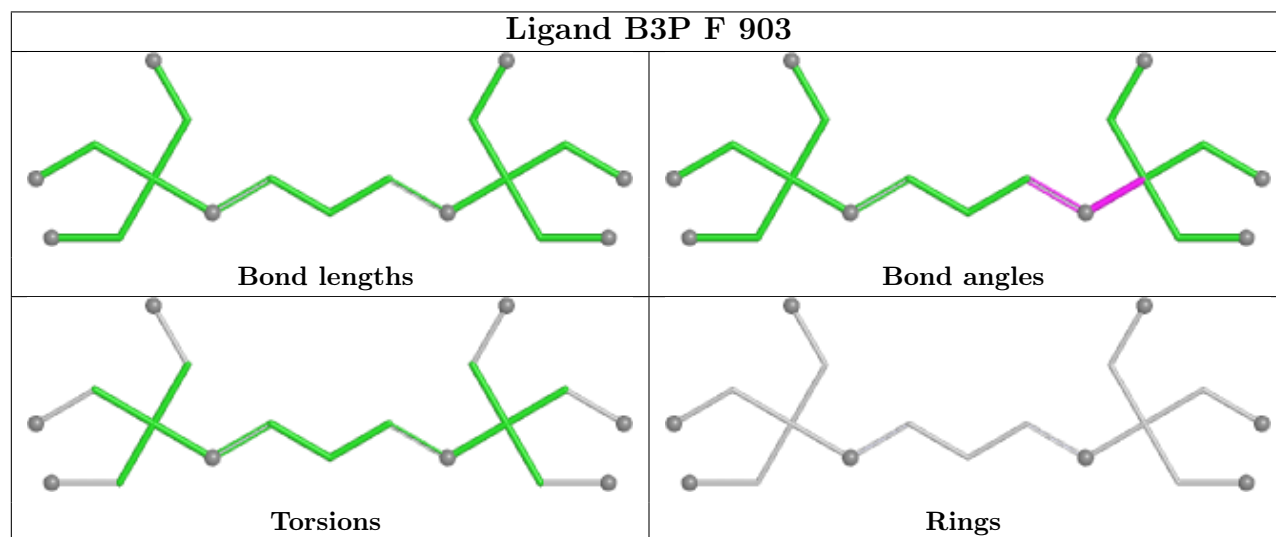
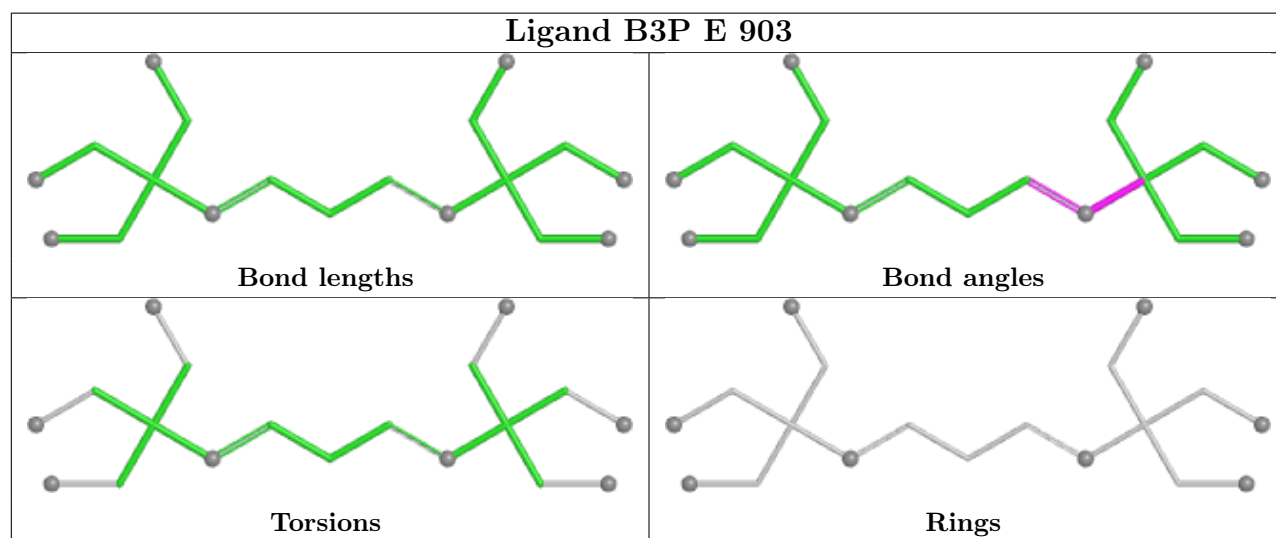
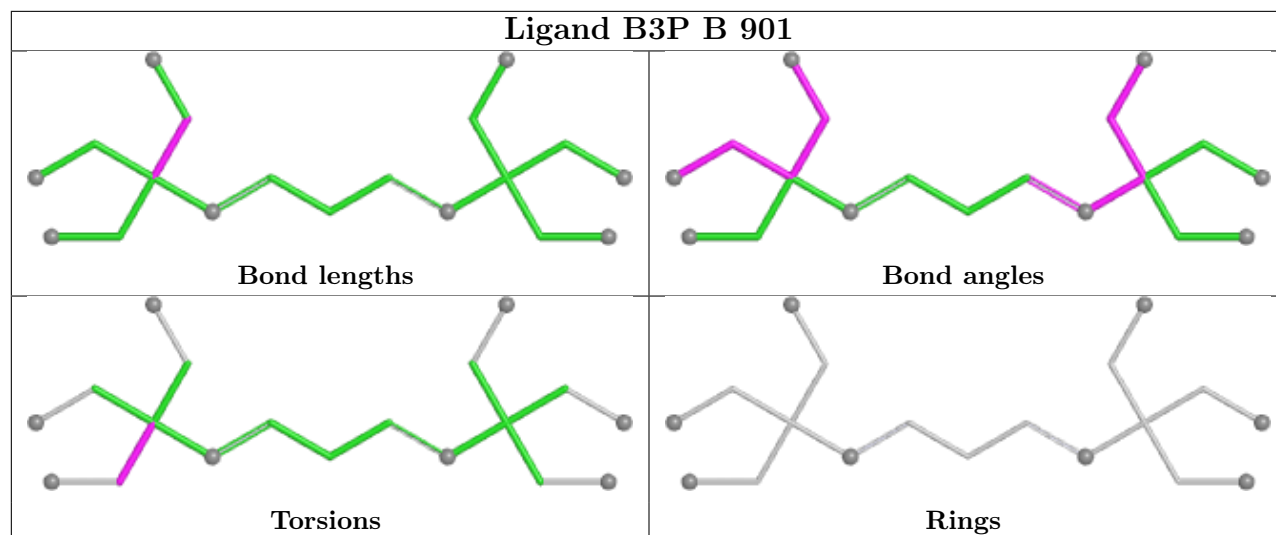
There are no ring outliers.

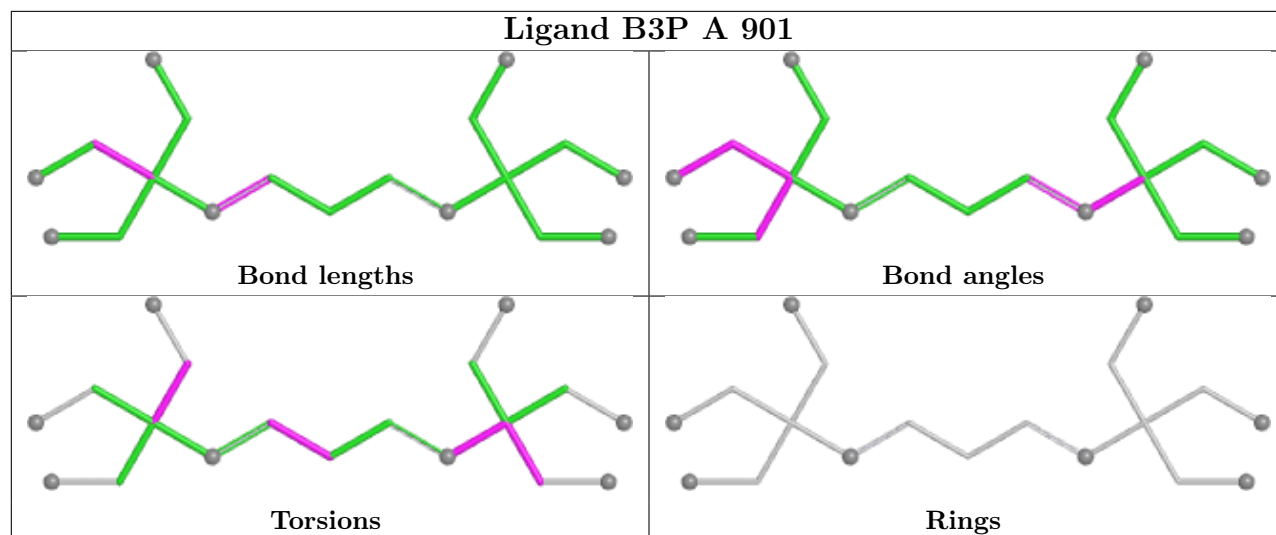
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	903	B3P	1	0
3	H	904	EDO	1	0
3	E	904	EDO	2	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.







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	434/461 (94%)	0.27	25 (5%)	29	22	23, 52, 97, 133	1 (0%)
1	B	431/461 (93%)	0.14	19 (4%)	39	31	32, 48, 82, 102	0
1	C	421/461 (91%)	0.85	56 (13%)	7	6	40, 70, 134, 156	0
1	D	433/461 (93%)	0.14	15 (3%)	47	38	32, 49, 87, 117	0
1	E	427/461 (92%)	0.28	23 (5%)	31	25	32, 54, 98, 127	0
1	F	427/461 (92%)	0.16	17 (3%)	42	34	33, 49, 88, 134	0
1	G	402/461 (87%)	1.01	72 (17%)	3	2	39, 75, 135, 157	0
1	H	430/461 (93%)	0.23	18 (4%)	40	32	33, 52, 90, 112	0
All	All	3405/3688 (92%)	0.38	245 (7%)	21	16	23, 55, 112, 157	1 (0%)

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	534	ILE	6.3
1	H	874	VAL	5.7
1	A	538	LEU	5.7
1	A	535	ALA	5.6
1	C	533	GLY	5.3
1	A	875	PRO	5.3
1	F	874	VAL	5.3
1	C	875	PRO	5.2
1	B	538	LEU	5.1
1	G	791	ILE	5.0
1	G	537	THR	4.8
1	B	588	ARG	4.8
1	C	791	ILE	4.7
1	D	874	VAL	4.6
1	E	874	VAL	4.5
1	G	590	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	874	VAL	4.3
1	G	794	LEU	4.2
1	D	845	ILE	4.2
1	C	731	SER	4.0
1	G	813	ILE	4.0
1	E	810	LEU	4.0
1	F	813	ILE	3.9
1	A	539	GLY	3.9
1	B	535	ALA	3.9
1	A	830	GLY	3.9
1	B	534	ILE	3.8
1	B	674	HIS	3.8
1	A	673	TRP	3.8
1	D	811	ALA	3.8
1	A	536	ASN	3.8
1	H	588	ARG	3.8
1	G	421	PRO	3.8
1	F	848	THR	3.7
1	F	845	ILE	3.7
1	A	588	ARG	3.7
1	G	460	VAL	3.6
1	G	673	TRP	3.6
1	D	537	THR	3.6
1	E	683	THR	3.5
1	C	784	ASP	3.5
1	F	683	THR	3.5
1	H	589	GLN	3.5
1	B	872	VAL	3.5
1	C	809	ILE	3.4
1	C	673	TRP	3.4
1	G	872	VAL	3.4
1	G	589	GLN	3.4
1	G	748	ILE	3.3
1	C	747	TYR	3.3
1	G	848	THR	3.3
1	G	538	LEU	3.3
1	C	872	VAL	3.3
1	G	456	ASP	3.3
1	G	860	GLY	3.3
1	F	746	ALA	3.2
1	A	589	GLN	3.2
1	A	534	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	462	ILE	3.2
1	E	809	ILE	3.2
1	G	459	THR	3.1
1	G	767	ILE	3.1
1	C	801	ARG	3.1
1	E	762	ARG	3.1
1	C	590	LEU	3.1
1	D	848	THR	3.1
1	C	831	TYR	3.1
1	G	827	SER	3.1
1	B	591	ASN	3.1
1	G	806	LEU	3.1
1	G	683	THR	3.1
1	E	588	ARG	3.1
1	G	769	PHE	3.1
1	G	811	ALA	3.0
1	C	787	SER	3.0
1	H	675	LYS	3.0
1	E	731	SER	3.0
1	G	834	TYR	3.0
1	B	683	THR	3.0
1	G	730	THR	3.0
1	A	811	ALA	3.0
1	C	785	ALA	3.0
1	E	760	ALA	3.0
1	G	458	VAL	3.0
1	G	810	LEU	2.9
1	C	460	VAL	2.9
1	G	766	PHE	2.9
1	G	781	PHE	2.9
1	C	789	ASP	2.9
1	H	746	ALA	2.9
1	C	874	VAL	2.9
1	G	793	PHE	2.9
1	E	745	GLN	2.9
1	C	777	TYR	2.9
1	B	586	GLY	2.8
1	G	855	PHE	2.8
1	C	847	SER	2.8
1	G	809	ILE	2.8
1	G	796	VAL	2.8
1	A	791	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	756	ILE	2.8
1	C	799	SER	2.8
1	C	762	ARG	2.8
1	G	479	ARG	2.7
1	G	520	ASN	2.7
1	A	874	VAL	2.7
1	D	813	ILE	2.7
1	D	872	VAL	2.7
1	H	421	PRO	2.7
1	E	831	TYR	2.6
1	B	539	GLY	2.6
1	G	591	ASN	2.6
1	G	779	LYS	2.6
1	A	732	GLN	2.6
1	C	778	LYS	2.6
1	C	520	ASN	2.6
1	G	750	PHE	2.6
1	G	457	GLU	2.6
1	E	848	THR	2.6
1	G	853	LEU	2.6
1	C	815	TYR	2.6
1	C	566	ASN	2.6
1	H	676	GLN	2.6
1	H	590	LEU	2.5
1	G	776	GLU	2.5
1	F	460	VAL	2.5
1	C	730	THR	2.5
1	G	824	THR	2.5
1	G	552	GLY	2.5
1	D	745	GLN	2.5
1	F	811	ALA	2.5
1	G	843	SER	2.5
1	G	866	ILE	2.5
1	C	794	LEU	2.5
1	C	539	GLY	2.5
1	A	733	PHE	2.5
1	G	536	ASN	2.5
1	E	673	TRP	2.5
1	D	565	GLY	2.5
1	F	421	PRO	2.5
1	A	810	LEU	2.4
1	E	791	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	813	ILE	2.4
1	F	809	ILE	2.4
1	G	862	GLU	2.4
1	H	457	GLU	2.4
1	G	804	PRO	2.4
1	A	813	ILE	2.4
1	E	533	GLY	2.4
1	B	732	GLN	2.4
1	G	816	LEU	2.4
1	D	420	GLU	2.4
1	C	781	PHE	2.4
1	A	537	THR	2.4
1	A	789	ASP	2.4
1	G	807	LYS	2.4
1	D	801	ARG	2.4
1	H	813	ILE	2.3
1	H	459	THR	2.3
1	C	869	SER	2.3
1	G	825	VAL	2.3
1	A	746	ALA	2.3
1	G	822	LEU	2.3
1	A	683	THR	2.3
1	F	684	ASN	2.3
1	C	788	SER	2.3
1	G	833	SER	2.3
1	B	846	GLY	2.3
1	C	756	ILE	2.3
1	E	811	ALA	2.3
1	H	751	GLU	2.3
1	H	776	GLU	2.3
1	D	566	ASN	2.3
1	F	584	SER	2.3
1	D	460	VAL	2.3
1	C	793	PHE	2.3
1	C	760	ALA	2.2
1	G	592	ALA	2.2
1	E	684	ASN	2.2
1	H	801	ARG	2.2
1	B	746	ALA	2.2
1	E	845	ILE	2.2
1	G	517	GLU	2.2
1	C	786	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	587	ASP	2.2
1	C	812	ASP	2.2
1	G	800	SER	2.2
1	C	845	ILE	2.2
1	C	588	ARG	2.2
1	D	831	TYR	2.2
1	C	440	LYS	2.2
1	D	810	LEU	2.2
1	E	539	GLY	2.2
1	G	648	LEU	2.2
1	G	593	PHE	2.2
1	B	871	LYS	2.2
1	C	758	LYS	2.2
1	C	807	LYS	2.2
1	G	423	MET	2.2
1	G	799	SER	2.2
1	G	838	VAL	2.2
1	B	589	GLN	2.1
1	G	783	ASN	2.1
1	A	829	ASP	2.1
1	C	748	ILE	2.1
1	A	498	ARG	2.1
1	C	779	LYS	2.1
1	G	786	GLN	2.1
1	C	455	LEU	2.1
1	F	810	LEU	2.1
1	H	747	TYR	2.1
1	F	674	HIS	2.1
1	F	587	ASP	2.1
1	H	669	ASP	2.1
1	E	566	ASN	2.1
1	F	815	TYR	2.1
1	C	855	PHE	2.1
1	G	596	SER	2.1
1	C	848	THR	2.1
1	G	522	ILE	2.1
1	G	753	ILE	2.1
1	B	460	VAL	2.1
1	H	458	VAL	2.1
1	E	420	GLU	2.0
1	H	731	SER	2.0
1	C	764	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	842	LYS	2.0
1	G	758	LYS	2.0
1	C	459	THR	2.0
1	C	516	PRO	2.0
1	G	495	LEU	2.0
1	C	684	ASN	2.0
1	C	813	ILE	2.0
1	C	830	GLY	2.0
1	E	815	TYR	2.0
1	F	420	GLU	2.0
1	G	788	SER	2.0
1	A	763	THR	2.0
1	G	870	MET	2.0
1	B	590	LEU	2.0
1	B	851	GLN	2.0
1	G	524	HIS	2.0
1	C	753	ILE	2.0
1	C	790	ASN	2.0
1	E	682	ARG	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
2	B3P	C	903	19/19	0.69	0.18	65,69,72,74	0
2	B3P	A	901	19/19	0.77	0.21	69,74,78,78	0
2	B3P	E	903	19/19	0.77	0.22	58,61,64,65	19
5	MG	F	902	1/1	0.78	0.17	58,58,58,58	0

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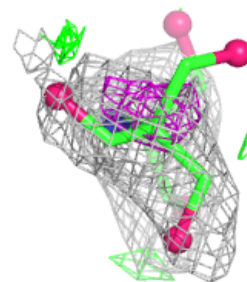
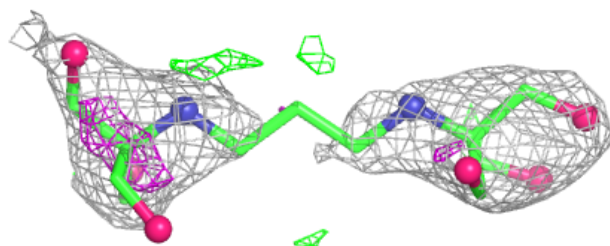
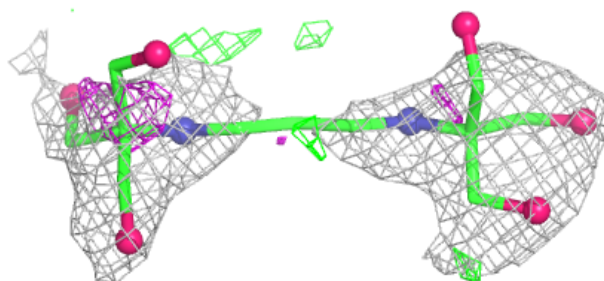
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	B3P	D	903	19/19	0.79	0.18	64,70,81,83	0
5	MG	C	902	1/1	0.80	0.24	83,83,83,83	0
2	B3P	H	903	19/19	0.80	0.15	58,62,66,69	0
5	MG	E	902	1/1	0.82	0.26	78,78,78,78	0
2	B3P	F	903	19/19	0.83	0.15	57,59,63,64	0
2	B3P	B	901	19/19	0.85	0.14	64,67,70,73	0
3	EDO	H	904	4/4	0.86	0.20	39,40,40,40	0
5	MG	G	902	1/1	0.86	0.17	75,75,75,75	0
3	EDO	A	902	4/4	0.87	0.19	67,67,68,73	0
4	PO4	E	901	5/5	0.87	0.16	109,110,112,112	0
3	EDO	F	906	4/4	0.87	0.17	63,65,65,65	0
5	MG	H	902	1/1	0.87	0.09	60,60,60,60	0
3	EDO	B	902	4/4	0.88	0.20	55,56,58,63	0
4	PO4	G	901	5/5	0.88	0.14	113,114,115,117	0
3	EDO	B	904	4/4	0.88	0.19	69,71,71,72	0
5	MG	D	902	1/1	0.88	0.11	50,50,50,50	0
3	EDO	B	906	4/4	0.89	0.15	69,70,71,71	0
4	PO4	F	901	5/5	0.91	0.15	82,83,85,85	0
3	EDO	F	904	4/4	0.91	0.15	52,55,55,57	0
4	PO4	C	901	5/5	0.92	0.12	108,109,109,110	0
3	EDO	G	903	4/4	0.92	0.13	59,59,59,60	0
3	EDO	F	905	4/4	0.93	0.15	57,61,62,62	0
3	EDO	E	905	4/4	0.93	0.15	38,39,39,40	0
3	EDO	B	905	4/4	0.94	0.11	51,51,51,53	0
4	PO4	H	901	5/5	0.94	0.10	71,71,74,74	0
3	EDO	B	903	4/4	0.94	0.12	53,54,55,56	0
3	EDO	E	904	4/4	0.94	0.15	35,36,37,38	0
3	EDO	F	907	4/4	0.95	0.12	57,58,58,58	0
3	EDO	D	905	4/4	0.96	0.09	44,45,45,46	0
3	EDO	D	906	4/4	0.96	0.08	43,43,44,45	0
3	EDO	D	904	4/4	0.96	0.08	47,49,49,50	0
4	PO4	D	901	5/5	0.97	0.08	60,61,61,62	0

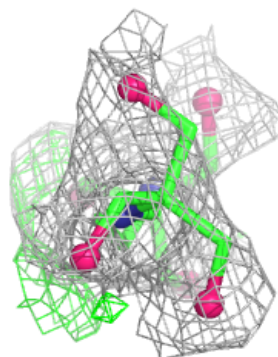
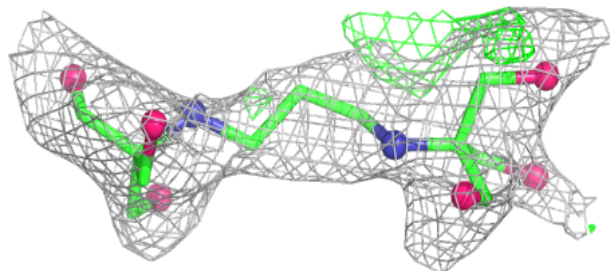
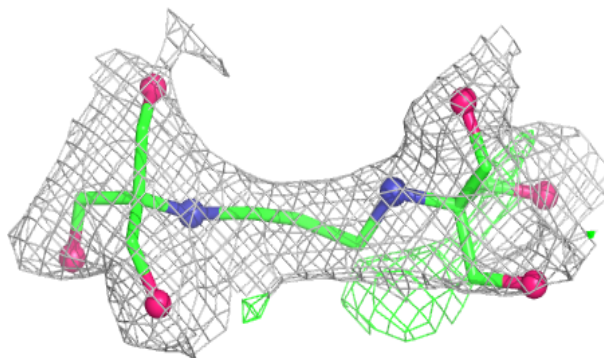
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B3P C 903:

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

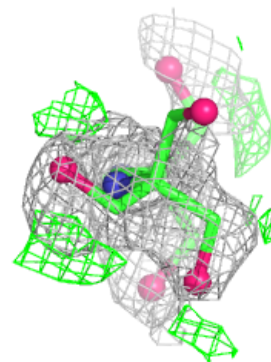
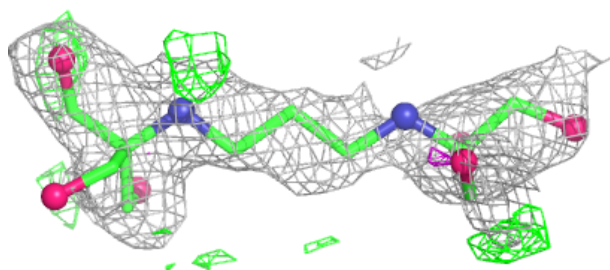
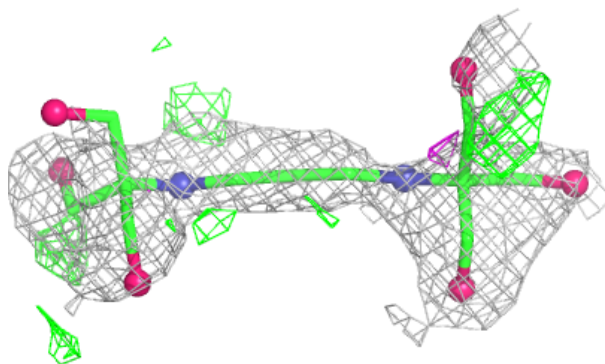
**Electron density around B3P A 901:**

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

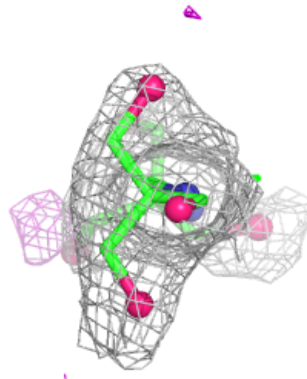
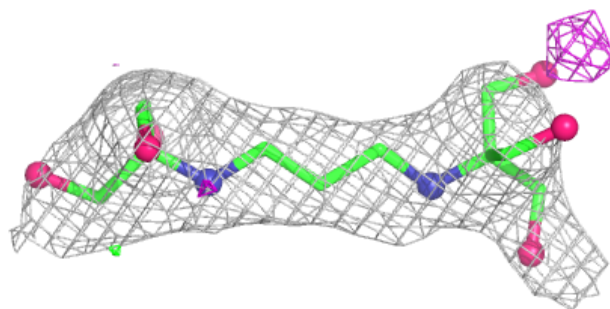
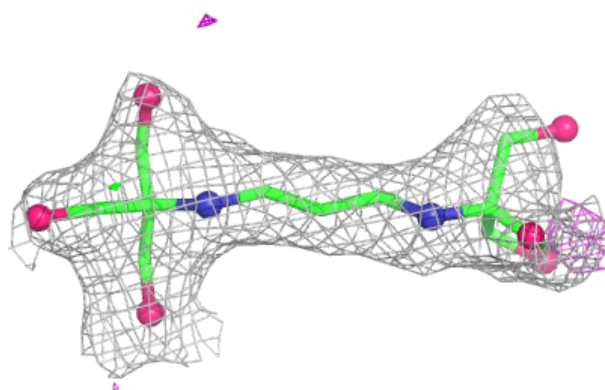


Electron density around B3P E 903:

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

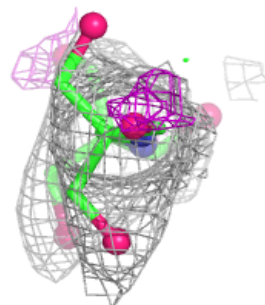
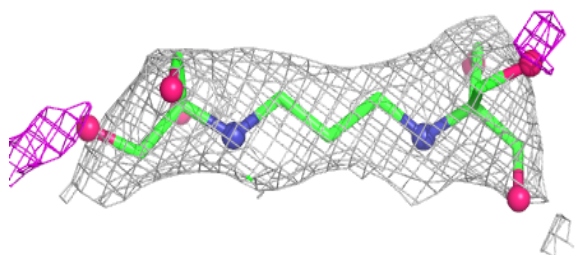
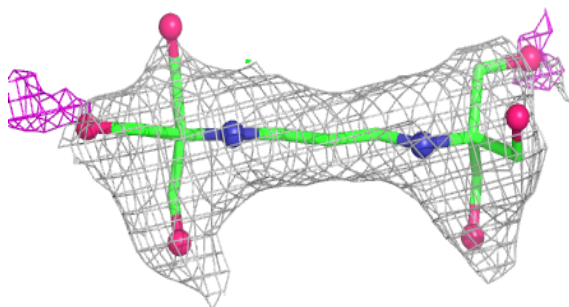
**Electron density around B3P D 903:**

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

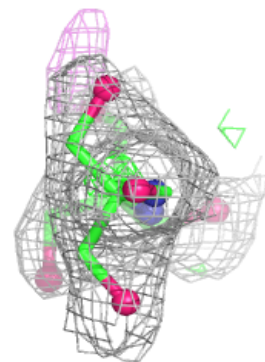
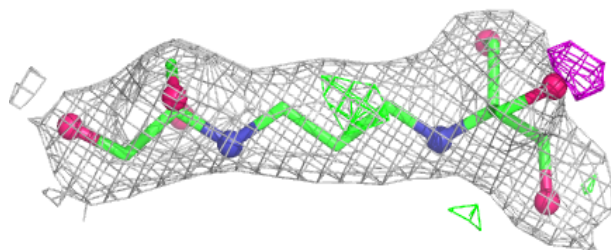
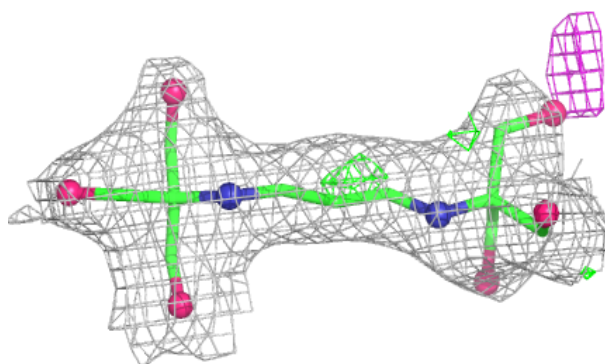


Electron density around B3P H 903:

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

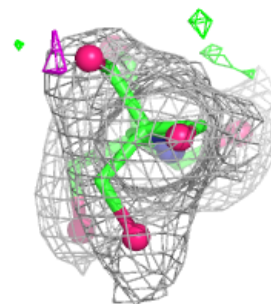
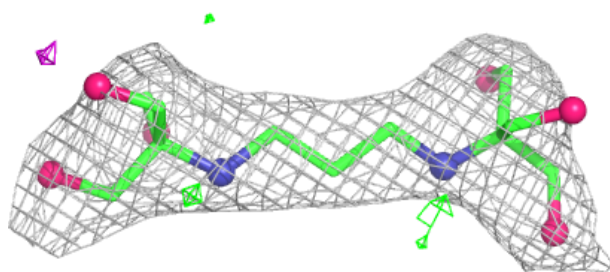
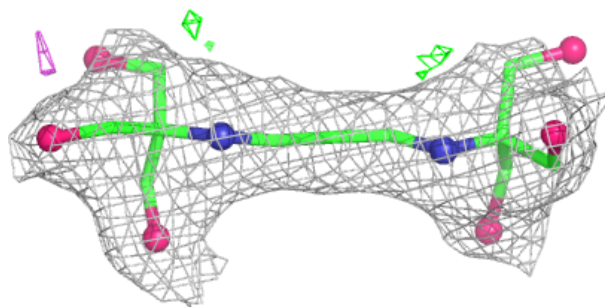
**Electron density around B3P F 903:**

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



Electron density around B3P B 901:

$2mF_o-DF_c$ (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.