



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:16 PM UTC

PDB ID : 5OKM / pdb_00005okm
Title : Crystal structure of human SHIP2 Phosphatase-C2
Authors : Le Coq, J.; Lietha, D.
Deposited on : 2017-07-25
Resolution : 1.96 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

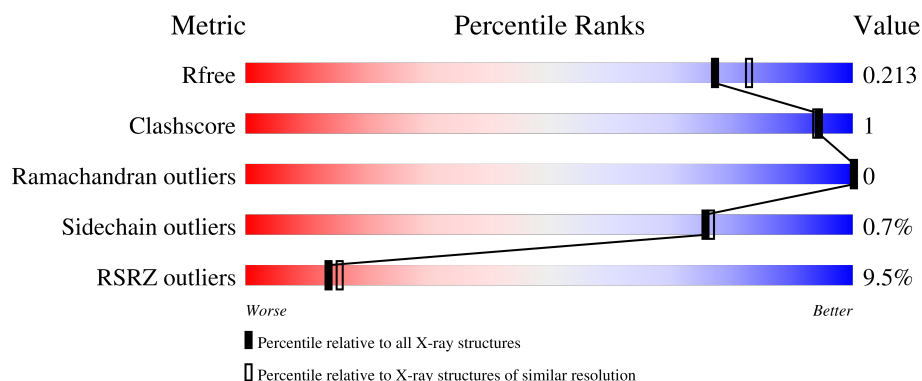
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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.



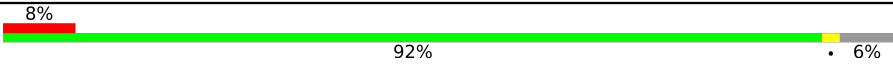
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	461	7% 88% 7% 6%
1	B	461	7% 93% • •
1	C	461	13% 91% • 7%
1	D	461	7% 91% • 5%
1	E	461	10% 91% •• 6%

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Mol	Chain	Length	Quality of chain
1	F	461	
1	G	461	
1	H	461	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29931 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	435	Total	C	N	O	S	0	3	0
			3529	2251	596	668	14			
1	B	442	Total	C	N	O	S	0	4	0
			3591	2290	607	680	14			
1	C	431	Total	C	N	O	S	0	0	0
			3488	2222	589	663	14			
1	D	436	Total	C	N	O	S	0	1	0
			3532	2252	598	668	14			
1	E	432	Total	C	N	O	S	0	5	0
			3525	2251	594	666	14			
1	F	433	Total	C	N	O	S	0	0	0
			3506	2236	595	661	14			
1	G	431	Total	C	N	O	S	0	2	0
			3497	2230	590	663	14			
1	H	427	Total	C	N	O	S	0	3	0
			3474	2218	584	658	14			

There are 16 discrepancies between the modelled and reference sequences:

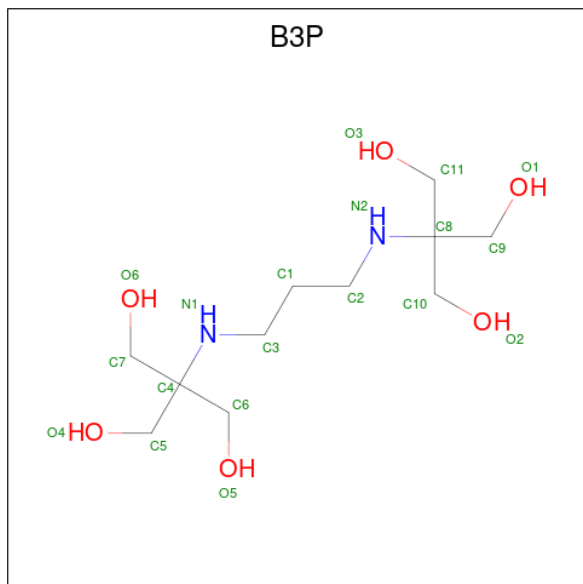
Chain	Residue	Modelled	Actual	Comment	Reference
A	418	GLY	-	expression tag	UNP O15357
A	419	PRO	-	expression tag	UNP O15357
B	418	GLY	-	expression tag	UNP O15357
B	419	PRO	-	expression tag	UNP O15357
C	418	GLY	-	expression tag	UNP O15357
C	419	PRO	-	expression tag	UNP O15357
D	418	GLY	-	expression tag	UNP O15357
D	419	PRO	-	expression tag	UNP O15357
E	418	GLY	-	expression tag	UNP O15357
E	419	PRO	-	expression tag	UNP O15357
F	418	GLY	-	expression tag	UNP O15357
F	419	PRO	-	expression tag	UNP O15357
G	418	GLY	-	expression tag	UNP O15357

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Chain	Residue	Modelled	Actual	Comment	Reference
G	419	PRO	-	expression tag	UNP O15357
H	418	GLY	-	expression tag	UNP O15357
H	419	PRO	-	expression tag	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		
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 NITRATE ION (CCD ID: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		
3	C	1	Total	N	O	0	0
			4	1	3		

- 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		

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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	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		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

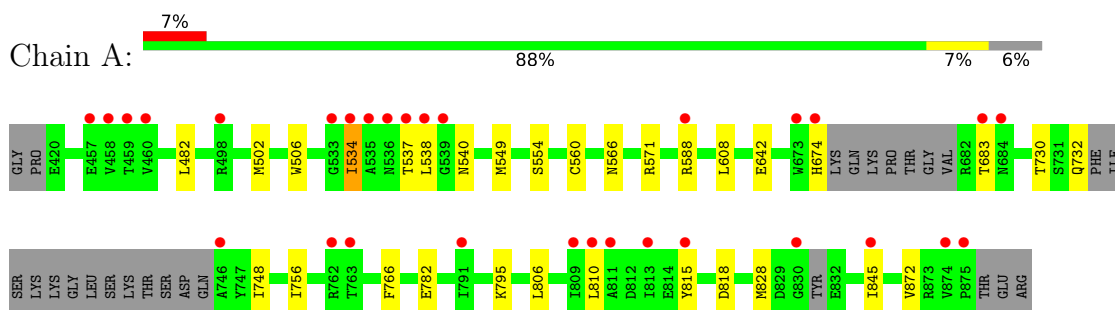
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	220	Total 220	O 220	0	0
5	B	232	Total 232	O 232	0	0
5	C	157	Total 157	O 157	0	0
5	D	187	Total 187	O 187	0	0
5	E	206	Total 206	O 206	0	0
5	F	190	Total 190	O 190	0	0
5	G	150	Total 150	O 150	0	0
5	H	222	Total 222	O 222	0	0

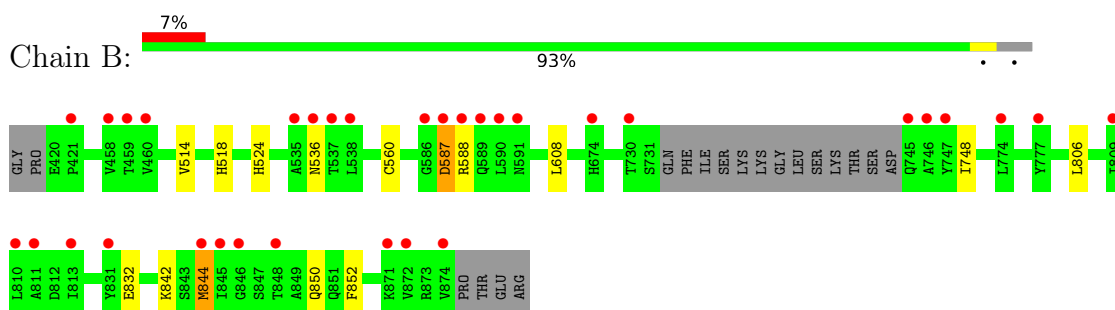
3 Residue-property plots [i](#)

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.

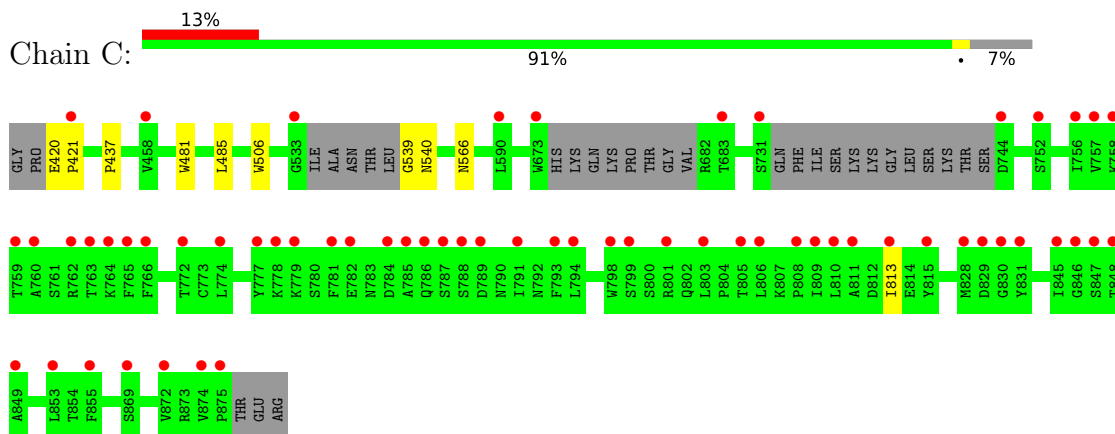
- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 5-phosphatase 2



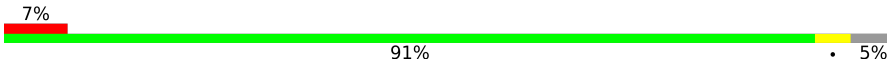
- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 5-phosphatase 2

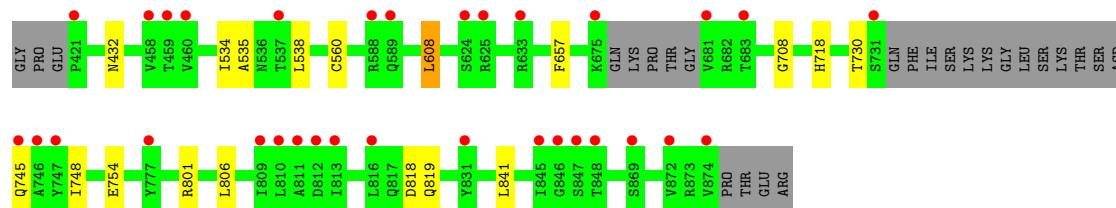


- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 5-phosphatase 2

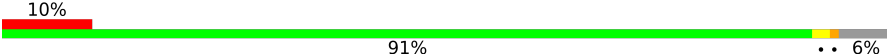


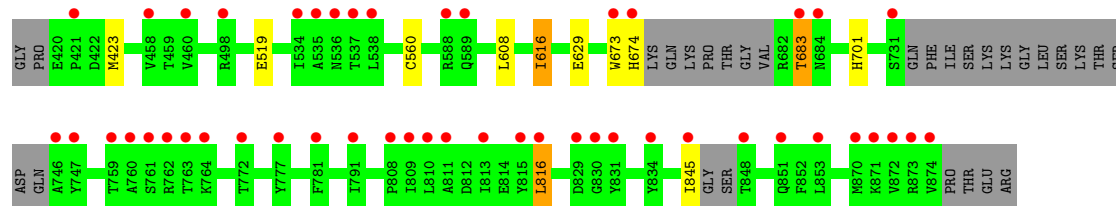
- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 5-phosphatase 2

Chain D: 

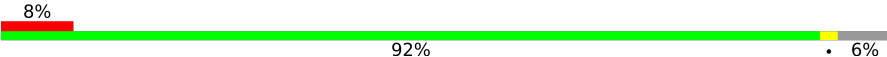


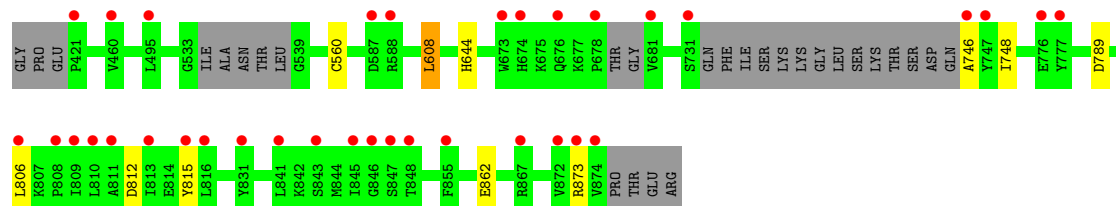
• Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 5-phosphatase 2

Chain E: 



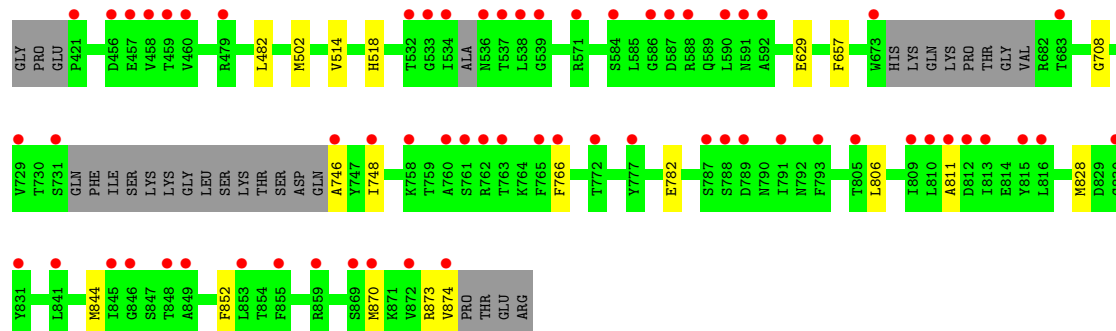
• Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 5-phosphatase 2

Chain F: 



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

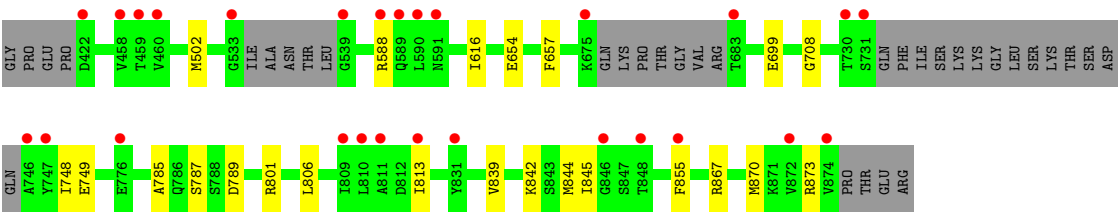
Chain G: 



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

Chain H: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	136.04Å 175.84Å 176.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.96 – 1.96 48.96 – 1.96	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.96-1.96) 100.0 (48.96-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.179 , 0.207 0.188 , 0.213	Depositor DCC
R_{free} test set	15180 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	29931	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.29% 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: B3P, NO3, EDO

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	0.65	0/3619	0.80	0/4900
1	B	0.67	0/3687	0.79	0/4993
1	C	0.60	0/3569	0.79	0/4831
1	D	0.63	0/3617	0.81	0/4896
1	E	0.63	0/3621	0.76	1/4903 (0.0%)
1	F	0.62	0/3588	0.78	0/4854
1	G	0.61	0/3583	0.75	0/4849
1	H	0.66	0/3564	0.78	1/4822 (0.0%)
All	All	0.64	0/28848	0.78	2/39048 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	616	ILE	N-CA-C	5.24	115.96	110.62
1	H	616	ILE	N-CA-C	5.24	115.86	110.36

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	3529	0	3459	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3591	0	3527	10	0
1	C	3488	0	3399	5	0
1	D	3532	0	3459	10	0
1	E	3525	0	3457	5	0
1	F	3506	0	3432	6	0
1	G	3497	0	3422	13	0
1	H	3474	0	3391	14	0
2	A	19	0	26	0	0
2	B	19	0	26	0	0
2	C	19	0	26	0	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	0	0	0
3	C	4	0	0	0	0
4	A	20	0	30	0	0
4	B	16	0	24	0	0
4	C	4	0	6	0	0
4	D	20	0	30	1	0
4	F	16	0	24	0	0
4	G	4	0	6	0	0
4	H	4	0	6	0	0
5	A	220	0	0	0	0
5	B	232	0	0	0	0
5	C	157	0	0	0	0
5	D	187	0	0	1	0
5	E	206	0	0	0	0
5	F	190	0	0	0	0
5	G	150	0	0	0	0
5	H	222	0	0	0	0
All	All	29931	0	27854	75	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 (75) 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:524:HIS:HB3	1:B:587:ASP:HB3	1.49	0.94
1:G:746:ALA:N	1:G:873:ARG:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:LEU:HB2	1:A:502:MET:HE1	1.73	0.70
1:G:782:GLU:HB3	1:G:828:MET:HE3	1.79	0.63
1:G:746:ALA:HB2	1:G:811:ALA:CB	2.32	0.60
1:E:423:MET:HE2	1:E:701:HIS:CD2	2.37	0.59
1:A:730:THR:HG21	1:A:818:ASP:HB3	1.85	0.59
1:G:748:ILE:HB	1:G:806:LEU:HB2	1.86	0.58
1:B:536:ASN:HD22	1:H:785:ALA:HA	1.69	0.56
1:C:437:PRO:HD3	1:H:502:MET:HG2	1.86	0.56
1:H:839:VAL:HG11	1:H:870:MET:HE1	1.90	0.54
1:C:506:TRP:CE3	1:C:540:ASN:HA	2.43	0.54
1:A:506:TRP:CE3	1:A:540:ASN:HA	2.42	0.54
1:G:746:ALA:HB2	1:G:811:ALA:HB1	1.90	0.54
1:D:560:CYS:SG	1:D:608:LEU:HD22	2.47	0.54
1:A:482:LEU:HD13	1:A:502:MET:HE3	1.91	0.53
1:A:549:MET:HE3	1:A:554:SER:HB3	1.91	0.52
1:D:748:ILE:HB	1:D:806:LEU:HB2	1.92	0.50
1:F:560:CYS:SG	1:F:608:LEU:HD22	2.51	0.50
1:A:845:ILE:HD13	1:A:872:VAL:HB	1.94	0.50
1:B:536:ASN:ND2	1:H:785:ALA:HA	2.26	0.50
1:H:813:ILE:HG23	1:H:845:ILE:HG21	1.94	0.49
1:H:749:GLU:OE2	1:H:873:ARG:NE	2.45	0.49
1:D:730:THR:HG21	1:D:818:ASP:HB3	1.94	0.48
1:B:844:MET:HE1	1:B:852:PHE:HB3	1.94	0.48
1:A:766:PHE:HB3	1:A:828:MET:HE2	1.96	0.48
1:G:746:ALA:HB2	1:G:811:ALA:HB2	1.96	0.48
1:H:844:MET:HE3	1:H:870:MET:HB3	1.94	0.48
1:A:766:PHE:HB3	1:A:828:MET:CE	2.44	0.48
1:A:748:ILE:HG12	1:A:872:VAL:HG22	1.96	0.47
1:A:782:GLU:CG	1:A:828:MET:HE3	2.43	0.47
1:B:588:ARG:O	1:B:588:ARG:HG2	2.15	0.47
1:C:420:GLU:CB	1:C:421:PRO:HD3	2.44	0.47
1:G:482:LEU:HD22	1:G:502:MET:HE2	1.97	0.47
1:D:819:GLN:HB2	1:D:841:LEU:HD12	1.97	0.47
1:E:816:LEU:HB3	1:E:845:ILE:HD11	1.97	0.47
1:G:657:PHE:CD1	1:G:708:GLY:HA2	2.50	0.47
1:G:844:MET:CE	1:G:852:PHE:HB3	2.45	0.46
1:B:560:CYS:SG	1:B:608:LEU:HD22	2.55	0.46
1:G:844:MET:HE3	1:G:870:MET:HG2	1.97	0.46
1:G:514:VAL:HG22	1:G:518:HIS:HB2	1.98	0.46
1:A:674:HIS:HB2	1:A:683:THR:OG1	2.14	0.46
1:D:534:ILE:HD11	1:F:789:ASP:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:801:ARG:NH1	5:D:1003:HOH:O	2.46	0.45
1:E:616:ILE:HD13	1:E:673:TRP:HB2	1.98	0.45
1:A:560:CYS:SG	1:A:608:LEU:HD22	2.56	0.45
1:B:844:MET:CG	1:B:850:GLN:HB2	2.47	0.45
1:B:748:ILE:HB	1:B:806:LEU:HB2	1.99	0.45
1:F:748:ILE:HB	1:F:806:LEU:HB2	1.99	0.44
1:A:534:ILE:HG23	1:A:537:THR:OG1	2.17	0.44
1:C:539:GLY:HA3	1:H:588:ARG:HD2	1.98	0.44
1:B:514:VAL:HG22	1:B:518:HIS:HB2	1.99	0.44
1:H:699:GLU:HB3	1:H:842:LYS:HE2	1.98	0.44
1:D:754:GLU:HB3	4:D:906:EDO:H21	2.00	0.44
1:A:588:ARG:HH21	1:H:801:ARG:HG3	1.82	0.43
1:F:746:ALA:HA	1:F:873:ARG:O	2.18	0.43
1:E:560:CYS:SG	1:E:608:LEU:HD22	2.59	0.43
1:G:766:PHE:HB3	1:G:828:MET:HE2	2.01	0.42
1:F:644:HIS:HD1	1:F:862:GLU:CD	2.27	0.42
1:H:657:PHE:CD1	1:H:708:GLY:HA2	2.54	0.42
1:A:534:ILE:CD1	1:A:571:ARG:HE	2.33	0.42
1:C:481:TRP:CZ2	1:C:485:LEU:HD11	2.54	0.42
1:A:756:ILE:HD11	1:A:795:LYS:HE2	2.01	0.42
1:D:535:ALA:HB3	1:D:538:LEU:HD12	2.02	0.42
1:A:810:LEU:HD23	1:A:815:TYR:CG	2.55	0.42
1:F:812:ASP:HB3	1:F:815:TYR:HB3	2.02	0.41
1:E:674:HIS:HB2	1:E:683:THR:OG1	2.20	0.41
1:B:844:MET:HG2	1:B:850:GLN:HB2	2.02	0.41
1:D:657:PHE:CD1	1:D:708:GLY:HA2	2.56	0.41
1:A:748:ILE:HB	1:A:806:LEU:HB2	2.03	0.41
1:G:844:MET:HE2	1:G:852:PHE:HB3	2.03	0.40
1:H:813:ILE:HD12	1:H:813:ILE:H	1.86	0.40
1:H:748:ILE:HB	1:H:806:LEU:HB2	2.03	0.40
1:D:432:ASN:HB3	1:D:718:HIS:CG	2.57	0.40
1:H:787:SER:OG	1:H:789:ASP:OD1	2.37	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	430/461 (93%)	423 (98%)	7 (2%)	0	100	100
1	B	442/461 (96%)	435 (98%)	7 (2%)	0	100	100
1	C	423/461 (92%)	416 (98%)	7 (2%)	0	100	100
1	D	431/461 (94%)	423 (98%)	8 (2%)	0	100	100
1	E	429/461 (93%)	418 (97%)	11 (3%)	0	100	100
1	F	425/461 (92%)	419 (99%)	6 (1%)	0	100	100
1	G	425/461 (92%)	418 (98%)	7 (2%)	0	100	100
1	H	422/461 (92%)	417 (99%)	5 (1%)	0	100	100
All	All	3427/3688 (93%)	3369 (98%)	58 (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	397/417 (95%)	392 (99%)	5 (1%)	61	58
1	B	404/417 (97%)	400 (99%)	4 (1%)	68	67
1	C	391/417 (94%)	389 (100%)	2 (0%)	81	82
1	D	396/417 (95%)	394 (100%)	2 (0%)	81	82
1	E	397/417 (95%)	393 (99%)	4 (1%)	68	67
1	F	393/417 (94%)	392 (100%)	1 (0%)	86	87
1	G	393/417 (94%)	391 (100%)	2 (0%)	81	82
1	H	390/417 (94%)	386 (99%)	4 (1%)	68	67
All	All	3161/3336 (95%)	3137 (99%)	24 (1%)	76	74

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	534	ILE
1	A	538	LEU
1	A	566	ASN
1	A	642	GLU
1	A	732	GLN
1	B	587	ASP
1	B	832	GLU
1	B	842	LYS
1	B	844	MET
1	C	566	ASN
1	C	813	ILE
1	D	608	LEU
1	D	745	GLN
1	E	519	GLU
1	E	629	GLU
1	E	683	THR
1	E	816	LEU
1	F	608	LEU
1	G	629	GLU
1	G	874	VAL
1	H	654	GLU
1	H	855[A]	PHE
1	H	855[B]	PHE
1	H	867	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	507	ASN
1	A	551	ASN
1	A	566	ASN
1	A	617	GLN
1	A	674	HIS
1	A	705	ASN
1	A	819	GLN
1	B	503	GLN
1	B	536	ASN
1	B	819	GLN
1	C	507	ASN
1	C	802	GLN
1	C	819	GLN
1	C	850	GLN
1	D	503	GLN

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Mol	Chain	Res	Type
1	D	589	GLN
1	D	591	ASN
1	D	674	HIS
1	D	819	GLN
1	E	507	ASN
1	E	621	ASN
1	E	705	ASN
1	E	851	GLN
1	F	503	GLN
1	F	674	HIS
1	F	705	ASN
1	F	792	ASN
1	F	802	GLN
1	F	819	GLN
1	G	705	ASN
1	H	503	GLN
1	H	705	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

30 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	B3P	E	901	-	18,18,18	1.03	1 (5%)	23,23,23	0.96	0
2	B3P	C	901	-	18,18,18	1.00	1 (5%)	23,23,23	0.83	0
4	EDO	F	903	-	3,3,3	0.50	0	2,2,2	0.19	0
4	EDO	B	902	-	3,3,3	0.47	0	2,2,2	0.25	0
4	EDO	D	905	-	3,3,3	0.40	0	2,2,2	0.28	0
4	EDO	F	902	-	3,3,3	0.69	0	2,2,2	0.57	0
4	EDO	C	903	-	3,3,3	0.45	0	2,2,2	0.29	0
4	EDO	B	903	-	3,3,3	0.51	0	2,2,2	0.29	0
3	NO3	A	902	-	1,3,3	0.27	0	0,3,3	-	-
4	EDO	A	904	-	3,3,3	0.42	0	2,2,2	0.49	0
4	EDO	D	903	-	3,3,3	0.45	0	2,2,2	0.33	0
4	EDO	A	905	-	3,3,3	0.48	0	2,2,2	0.37	0
4	EDO	D	904	-	3,3,3	0.52	0	2,2,2	0.25	0
2	B3P	A	901	-	18,18,18	1.00	1 (5%)	23,23,23	1.11	1 (4%)
4	EDO	A	907	-	3,3,3	0.48	0	2,2,2	0.05	0
4	EDO	B	904	-	3,3,3	0.43	0	2,2,2	0.10	0
4	EDO	A	903	-	3,3,3	0.39	0	2,2,2	0.39	0
2	B3P	D	901	-	18,18,18	0.87	0	23,23,23	0.89	0
4	EDO	H	902	-	3,3,3	0.47	0	2,2,2	0.21	0
4	EDO	D	902	-	3,3,3	0.47	0	2,2,2	0.21	0
4	EDO	A	906	-	3,3,3	0.51	0	2,2,2	0.17	0
2	B3P	H	901	-	18,18,18	0.90	0	23,23,23	0.85	0
4	EDO	F	905	-	3,3,3	0.42	0	2,2,2	0.40	0
4	EDO	F	904	-	3,3,3	0.43	0	2,2,2	0.13	0
4	EDO	G	901	-	3,3,3	0.49	0	2,2,2	0.35	0
2	B3P	B	901	-	18,18,18	1.32	2 (11%)	23,23,23	0.82	0
2	B3P	F	901	-	18,18,18	1.00	2 (11%)	23,23,23	0.80	0
4	EDO	B	905	-	3,3,3	0.43	0	2,2,2	0.33	0
3	NO3	C	902	-	1,3,3	0.36	0	0,3,3	-	-
4	EDO	D	906	-	3,3,3	0.42	0	2,2,2	0.25	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	E	901	-	-	0/28/28/28	-
2	B3P	C	901	-	-	2/28/28/28	-
4	EDO	F	903	-	-	1/1/1/1	-
4	EDO	B	902	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	905	-	-	0/1/1/1	-
4	EDO	F	902	-	-	0/1/1/1	-
4	EDO	C	903	-	-	0/1/1/1	-
4	EDO	B	903	-	-	0/1/1/1	-
4	EDO	A	904	-	-	0/1/1/1	-
4	EDO	D	903	-	-	0/1/1/1	-
4	EDO	A	905	-	-	0/1/1/1	-
4	EDO	D	904	-	-	0/1/1/1	-
2	B3P	A	901	-	-	0/28/28/28	-
4	EDO	A	907	-	-	0/1/1/1	-
4	EDO	B	904	-	-	1/1/1/1	-
4	EDO	A	903	-	-	1/1/1/1	-
2	B3P	D	901	-	-	3/28/28/28	-
4	EDO	H	902	-	-	0/1/1/1	-
4	EDO	D	902	-	-	0/1/1/1	-
4	EDO	A	906	-	-	0/1/1/1	-
2	B3P	H	901	-	-	4/28/28/28	-
4	EDO	F	905	-	-	0/1/1/1	-
4	EDO	F	904	-	-	1/1/1/1	-
4	EDO	G	901	-	-	0/1/1/1	-
2	B3P	B	901	-	-	9/28/28/28	-
2	B3P	F	901	-	-	0/28/28/28	-
4	EDO	B	905	-	-	0/1/1/1	-
4	EDO	D	906	-	-	0/1/1/1	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	B3P	C10-C8	3.37	1.57	1.53
2	B	901	B3P	C7-C4	2.68	1.56	1.53
2	E	901	B3P	C7-C4	2.59	1.56	1.53
2	C	901	B3P	C7-C4	2.51	1.56	1.53
2	F	901	B3P	C7-C4	2.43	1.56	1.53
2	A	901	B3P	C3-N1	2.23	1.49	1.46
2	F	901	B3P	C5-C4	2.02	1.55	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	B3P	C6-C4-C5	-2.52	104.50	110.02

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	901	B3P	N1-C4-C6-O5
2	H	901	B3P	C7-C4-C6-O5
2	H	901	B3P	C5-C4-C6-O5
2	D	901	B3P	C3-C1-C2-N2
2	C	901	B3P	C11-C8-N2-C2
2	B	901	B3P	O2-C10-C8-C9
2	H	901	B3P	C3-C1-C2-N2
2	B	901	B3P	N2-C8-C9-O1
2	D	901	B3P	N1-C4-C6-O5
2	B	901	B3P	O3-C11-C8-C10
2	B	901	B3P	C1-C2-N2-C8
2	B	901	B3P	C3-C1-C2-N2
2	C	901	B3P	C10-C8-N2-C2
2	B	901	B3P	O3-C11-C8-C9
4	A	903	EDO	O1-C1-C2-O2
2	B	901	B3P	O2-C10-C8-N2
2	B	901	B3P	O3-C11-C8-N2
4	B	904	EDO	O1-C1-C2-O2
4	F	903	EDO	O1-C1-C2-O2
4	F	904	EDO	O1-C1-C2-O2
2	B	901	B3P	O2-C10-C8-C11
2	D	901	B3P	N2-C8-C9-O1

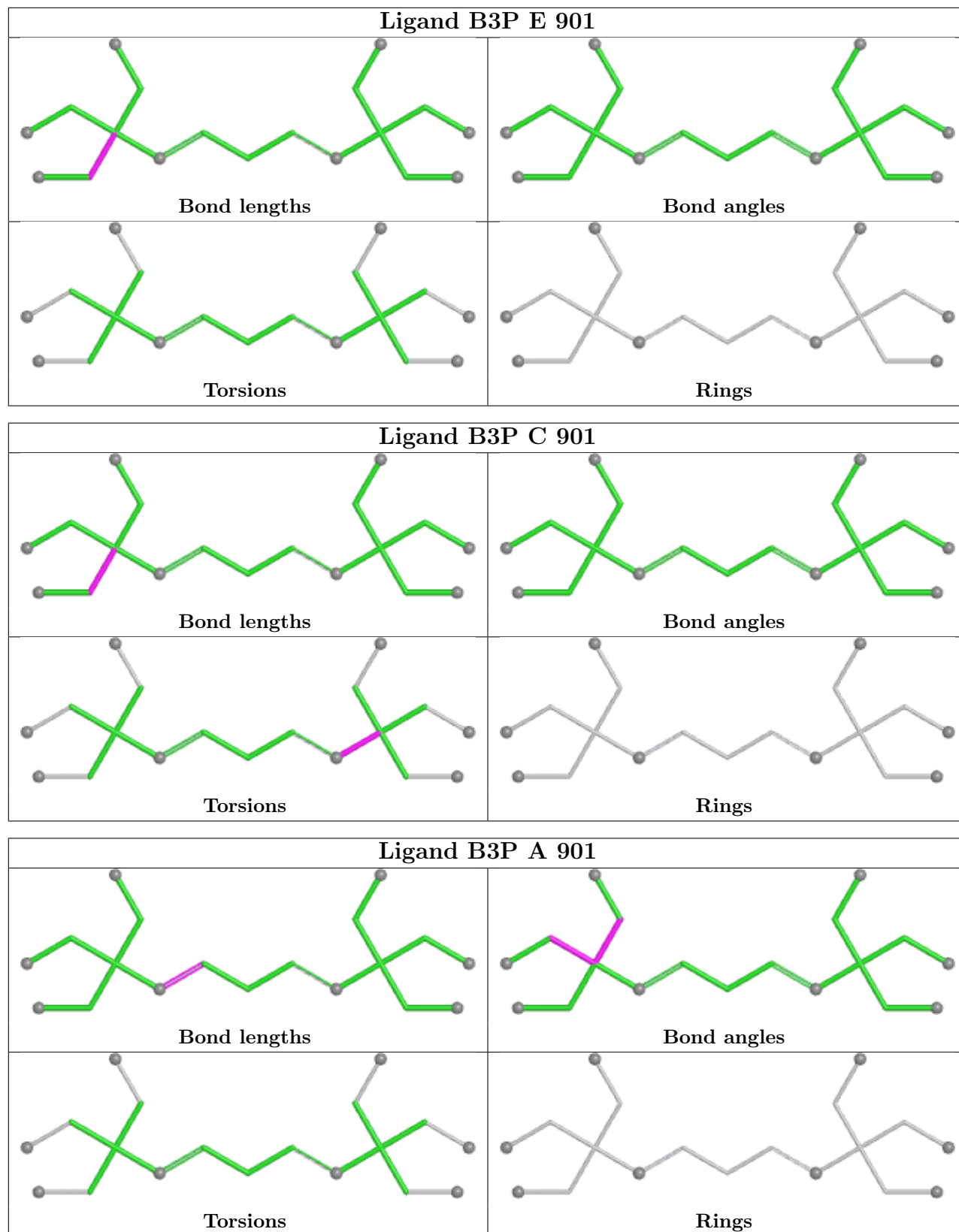
There are no ring outliers.

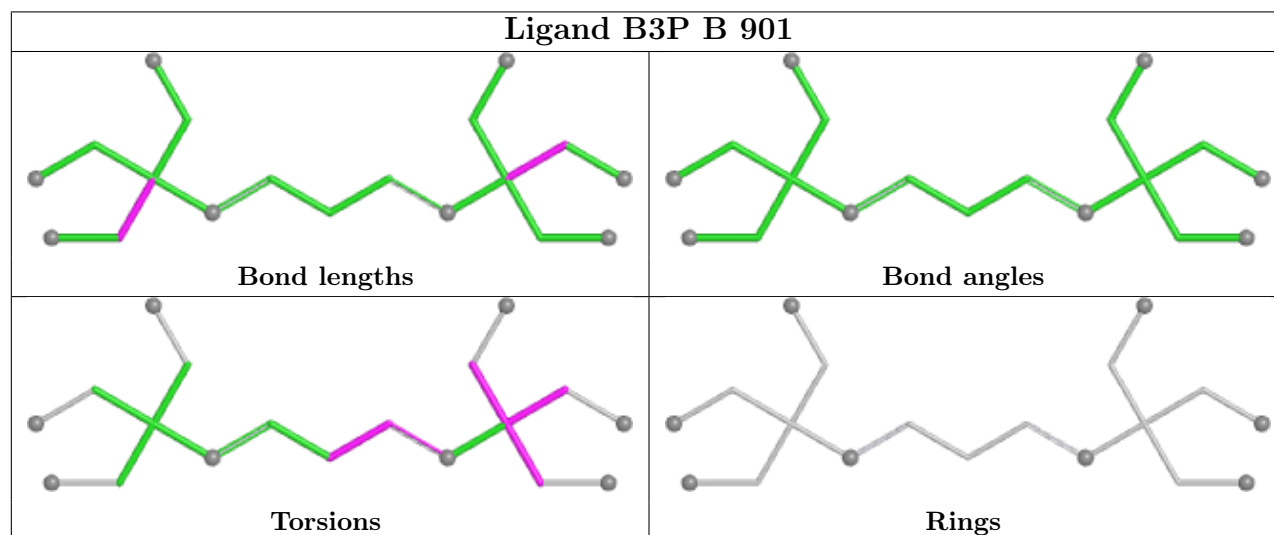
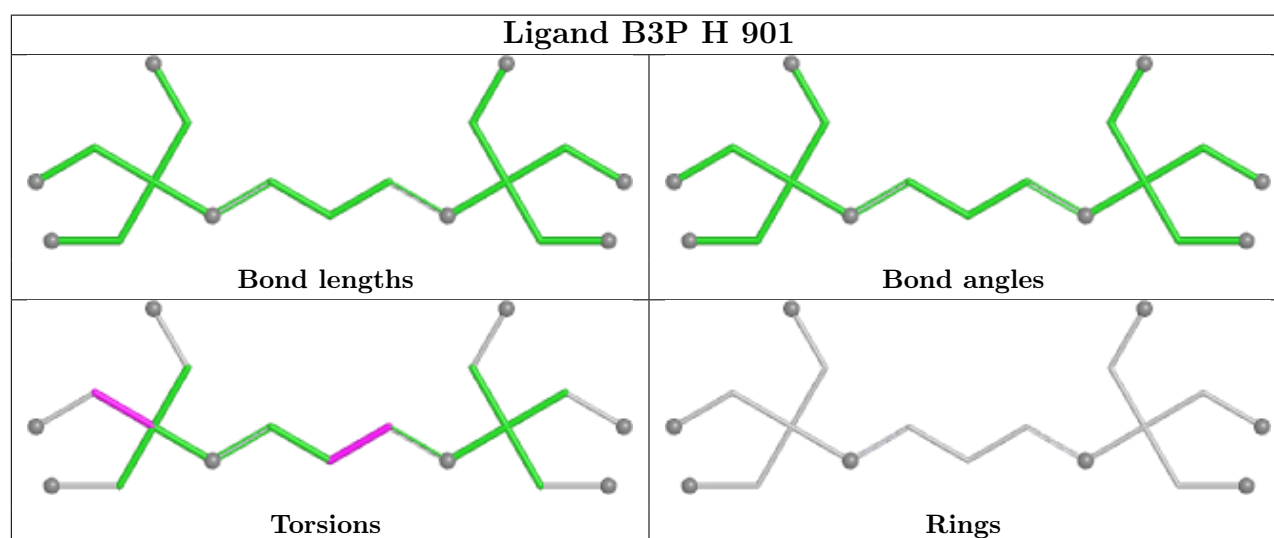
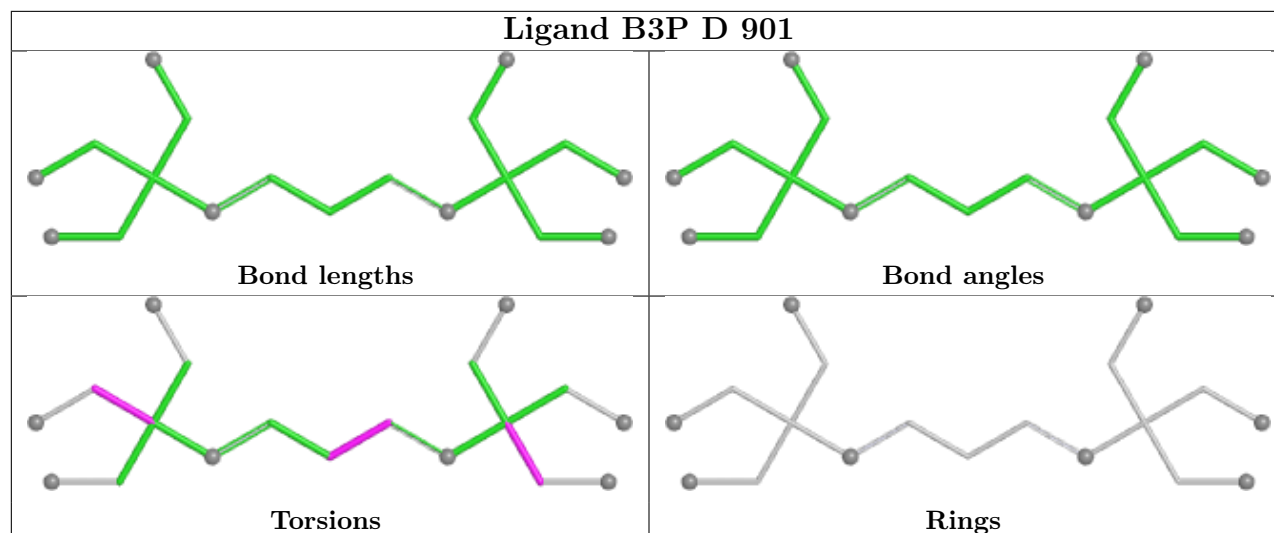
1 monomer is involved in 1 short contact:

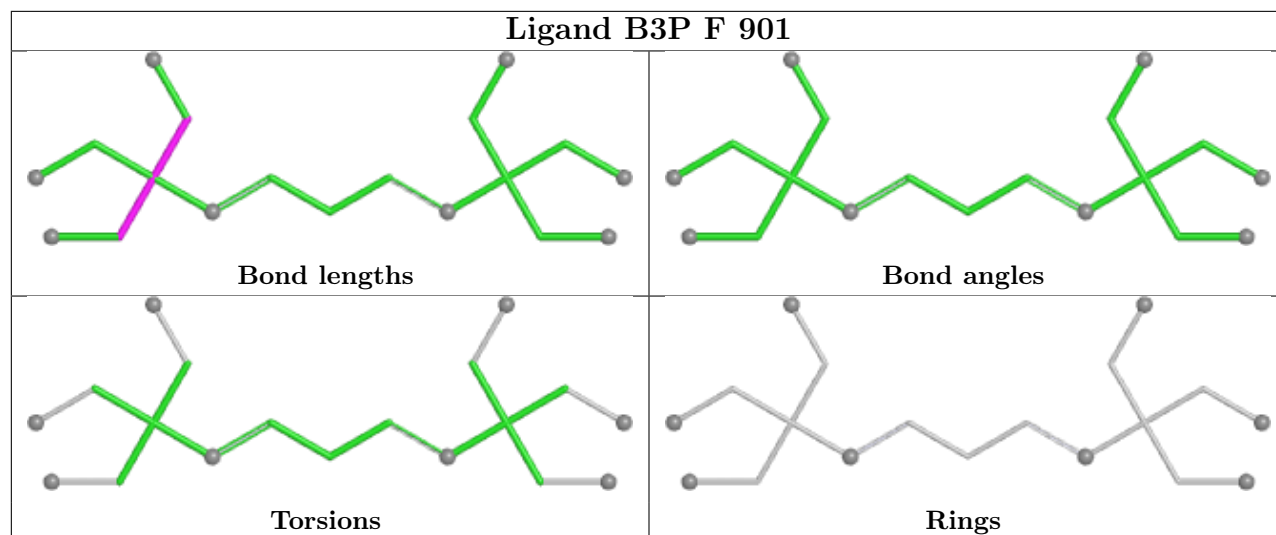
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	906	EDO	1	0

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.







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	435/461 (94%)	0.35	30 (6%) 23 26	17, 39, 72, 93	3 (0%)
1	B	442/461 (95%)	0.25	33 (7%) 20 23	19, 36, 75, 94	4 (0%)
1	C	431/461 (93%)	0.80	62 (14%) 6 6	25, 48, 113, 147	0
1	D	436/461 (94%)	0.42	32 (7%) 21 24	24, 42, 74, 93	1 (0%)
1	E	432/461 (93%)	0.53	48 (11%) 10 12	19, 43, 89, 130	5 (1%)
1	F	433/461 (93%)	0.43	35 (8%) 18 21	24, 41, 82, 113	0
1	G	431/461 (93%)	0.83	64 (14%) 5 6	27, 47, 107, 149	2 (0%)
1	H	427/461 (92%)	0.18	27 (6%) 26 30	19, 35, 65, 86	3 (0%)
All	All	3467/3688 (94%)	0.47	331 (9%) 14 15	17, 41, 88, 149	18 (0%)

All (331) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	874	VAL	7.9
1	G	791	ILE	6.5
1	G	538	LEU	6.4
1	G	537	THR	6.2
1	B	587	ASP	6.1
1	E	673	TRP	6.1
1	G	813	ILE	5.9
1	F	874	VAL	5.6
1	G	458	VAL	5.5
1	D	874	VAL	5.4
1	G	460	VAL	5.4
1	C	791	ILE	5.3
1	G	534	ILE	5.3
1	B	586	GLY	5.2
1	A	535	ALA	5.1
1	A	538	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	537	THR	4.9
1	B	874	VAL	4.9
1	E	534	ILE	4.8
1	E	845	ILE	4.8
1	F	810	LEU	4.8
1	C	673	TRP	4.7
1	F	746	ALA	4.7
1	A	830	GLY	4.6
1	H	588	ARG	4.6
1	C	794	LEU	4.5
1	G	810	LEU	4.5
1	G	746	ALA	4.5
1	D	681	VAL	4.5
1	E	791	ILE	4.3
1	E	811	ALA	4.3
1	G	590	LEU	4.3
1	A	791	ILE	4.3
1	F	845	ILE	4.3
1	G	809	ILE	4.3
1	E	746	ALA	4.3
1	E	809	ILE	4.2
1	F	678	PRO	4.2
1	F	587	ASP	4.2
1	H	874	VAL	4.1
1	H	590	LEU	4.1
1	A	875	PRO	4.1
1	B	590	LEU	4.0
1	E	874	VAL	4.0
1	H	460	VAL	4.0
1	C	831	TYR	4.0
1	G	673	TRP	3.9
1	B	588	ARG	3.9
1	B	810	LEU	3.9
1	F	813	ILE	3.9
1	E	815	TYR	3.8
1	G	816	LEU	3.8
1	F	811	ALA	3.8
1	C	801	ARG	3.8
1	C	874	VAL	3.8
1	F	872	VAL	3.8
1	E	848	THR	3.8
1	D	811	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	813	ILE	3.8
1	D	813	ILE	3.8
1	E	683	THR	3.7
1	B	538	LEU	3.7
1	C	810	LEU	3.7
1	A	674	HIS	3.7
1	C	809	ILE	3.7
1	E	810	LEU	3.6
1	E	813	ILE	3.6
1	C	781	PHE	3.6
1	A	536	ASN	3.6
1	B	872	VAL	3.6
1	E	674	HIS	3.6
1	F	816	LEU	3.6
1	A	673	TRP	3.5
1	E	537	THR	3.5
1	E	762	ARG	3.5
1	F	815	TYR	3.5
1	A	534	ILE	3.5
1	F	809	ILE	3.5
1	G	815	TYR	3.4
1	D	810	LEU	3.4
1	D	588	ARG	3.4
1	E	535	ALA	3.4
1	G	811	ALA	3.4
1	C	590	LEU	3.4
1	C	875	PRO	3.4
1	G	831	TYR	3.3
1	B	460	VAL	3.3
1	H	811	ALA	3.3
1	A	810	LEU	3.3
1	E	816	LEU	3.3
1	C	793	PHE	3.3
1	H	589	GLN	3.3
1	B	536	ASN	3.3
1	C	784	ASP	3.3
1	F	747	TYR	3.2
1	G	849	ALA	3.2
1	F	848	THR	3.2
1	H	810	LEU	3.2
1	E	536	ASN	3.2
1	H	746	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	533	GLY	3.2
1	G	459	THR	3.2
1	C	787	SER	3.2
1	G	731	SER	3.2
1	H	533	GLY	3.2
1	C	765	PHE	3.1
1	A	683	THR	3.1
1	C	731	SER	3.1
1	C	788	SER	3.1
1	G	845	ILE	3.1
1	E	588	ARG	3.1
1	B	777	TYR	3.1
1	C	774	LEU	3.1
1	E	851	GLN	3.1
1	E	498	ARG	3.1
1	G	683	THR	3.1
1	C	744	ASP	3.1
1	H	458	VAL	3.1
1	G	855	PHE	3.0
1	D	809	ILE	3.0
1	G	729	VAL	3.0
1	G	533	GLY	3.0
1	E	870	MET	3.0
1	G	872	VAL	2.9
1	G	777	TYR	2.9
1	C	764	LYS	2.9
1	C	782	GLU	2.9
1	C	785	ALA	2.9
1	G	761	SER	2.9
1	D	460	VAL	2.9
1	E	872	VAL	2.9
1	B	831	TYR	2.9
1	E	763	THR	2.9
1	C	760	ALA	2.9
1	H	459	THR	2.9
1	H	539	GLY	2.9
1	C	803	LEU	2.9
1	H	813	ILE	2.9
1	A	533	GLY	2.9
1	D	872	VAL	2.8
1	C	421	PRO	2.8
1	F	674	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	747	TYR	2.8
1	G	457	GLU	2.8
1	A	539	GLY	2.8
1	C	762	ARG	2.8
1	H	683	THR	2.8
1	E	421	PRO	2.8
1	A	537	THR	2.8
1	C	759	THR	2.8
1	G	853	LEU	2.8
1	G	456	ASP	2.8
1	D	745	GLN	2.7
1	C	766	PHE	2.7
1	B	459	THR	2.7
1	H	730	THR	2.7
1	C	786	GLN	2.7
1	E	460	VAL	2.7
1	C	798	TRP	2.7
1	E	747	TYR	2.7
1	E	831	TYR	2.7
1	G	793	PHE	2.7
1	C	779	LYS	2.7
1	E	538	LEU	2.7
1	F	777	TYR	2.6
1	A	459	THR	2.6
1	D	848	THR	2.6
1	G	763	THR	2.6
1	C	799	SER	2.6
1	F	731	SER	2.6
1	A	809	ILE	2.6
1	A	845	ILE	2.6
1	B	813	ILE	2.6
1	H	872	VAL	2.6
1	G	762	ARG	2.6
1	G	787	SER	2.6
1	F	421	PRO	2.6
1	F	873	ARG	2.6
1	G	812	ASP	2.6
1	G	846	GLY	2.6
1	H	422	ASP	2.6
1	D	458	VAL	2.6
1	D	537	THR	2.6
1	D	624	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	813	ILE	2.6
1	G	789	ASP	2.6
1	G	539	GLY	2.6
1	B	811	ALA	2.6
1	G	760	ALA	2.6
1	E	731	SER	2.6
1	F	847	SER	2.6
1	H	591	ASN	2.6
1	F	831	TYR	2.5
1	H	831	TYR	2.5
1	H	855[A]	PHE	2.5
1	B	846	GLY	2.5
1	G	788	SER	2.5
1	B	848	THR	2.5
1	F	867	ARG	2.5
1	G	586	GLY	2.5
1	D	845	ILE	2.5
1	G	748	ILE	2.5
1	G	588	ARG	2.5
1	C	853	LEU	2.5
1	D	816	LEU	2.5
1	F	588	ARG	2.5
1	C	869	SER	2.5
1	D	869	SER	2.5
1	H	731	SER	2.5
1	C	811	ALA	2.5
1	C	683	THR	2.5
1	C	763	THR	2.5
1	F	681	VAL	2.5
1	B	871	LYS	2.5
1	E	871	LYS	2.5
1	B	421	PRO	2.5
1	B	589	GLN	2.4
1	G	584	SER	2.4
1	B	809	ILE	2.4
1	C	805	THR	2.4
1	H	675	LYS	2.4
1	C	872	VAL	2.4
1	F	460	VAL	2.4
1	A	498	ARG	2.4
1	B	591	ASN	2.4
1	E	830	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	776	GLU	2.4
1	D	731	SER	2.4
1	G	765	PHE	2.4
1	G	848	THR	2.4
1	A	874	VAL	2.4
1	C	757	VAL	2.4
1	C	778	LYS	2.4
1	C	806	LEU	2.4
1	E	829	ASP	2.4
1	B	745	GLN	2.4
1	D	421	PRO	2.4
1	E	808	PRO	2.4
1	F	808	PRO	2.4
1	A	460	VAL	2.4
1	B	458	VAL	2.4
1	D	747	TYR	2.3
1	D	459	THR	2.3
1	G	772	THR	2.3
1	D	589	GLN	2.3
1	C	830	GLY	2.3
1	F	846	GLY	2.3
1	C	752	SER	2.3
1	G	859	ARG	2.3
1	D	831	TYR	2.3
1	E	759	THR	2.3
1	H	848	THR	2.3
1	C	828	MET	2.3
1	G	479	ARG	2.3
1	F	673	TRP	2.3
1	G	841	LEU	2.3
1	G	532	THR	2.3
1	G	536	ASN	2.3
1	G	766	PHE	2.3
1	B	535	ALA	2.3
1	B	746	ALA	2.3
1	C	845	ILE	2.3
1	E	873	ARG	2.3
1	C	789	ASP	2.3
1	D	812	ASP	2.3
1	A	458	VAL	2.3
1	E	458	VAL	2.3
1	G	758	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	811	ALA	2.2
1	C	808	PRO	2.2
1	E	760	ALA	2.2
1	A	457	GLU	2.2
1	F	841	LEU	2.2
1	G	592	ALA	2.2
1	C	777	TYR	2.2
1	B	730	THR	2.2
1	D	683	THR	2.2
1	F	806	LEU	2.2
1	A	746	ALA	2.2
1	D	777	TYR	2.2
1	E	781	PHE	2.2
1	E	834	TYR	2.2
1	A	684	ASN	2.2
1	A	762	ARG	2.2
1	E	684[A]	ASN	2.2
1	G	870	MET	2.2
1	D	625	ARG	2.2
1	D	675	LYS	2.2
1	C	855	PHE	2.1
1	H	776	GLU	2.1
1	E	589	GLN	2.1
1	D	847	SER	2.1
1	E	761	SER	2.1
1	G	830	GLY	2.1
1	F	495	LEU	2.1
1	C	849	ALA	2.1
1	C	756	ILE	2.1
1	A	763	THR	2.1
1	C	772	THR	2.1
1	A	588	ARG	2.1
1	E	764	LYS	2.1
1	E	853	LEU	2.1
1	F	855	PHE	2.1
1	C	815	TYR	2.1
1	E	777	TYR	2.1
1	G	587	ASP	2.1
1	H	809	ILE	2.1
1	C	847	SER	2.1
1	F	843	SER	2.1
1	C	846	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	674	HIS	2.1
1	D	746	ALA	2.1
1	A	815	TYR	2.0
1	B	844	MET	2.0
1	C	848	THR	2.0
1	H	846	GLY	2.0
1	F	676	GLN	2.0
1	C	458	VAL	2.0
1	G	421	PRO	2.0
1	B	774	LEU	2.0
1	C	829	ASP	2.0
1	D	633	ARG	2.0
1	G	571	ARG	2.0
1	C	758	LYS	2.0
1	G	869	SER	2.0
1	B	845	ILE	2.0
1	D	846	GLY	2.0
1	E	772	THR	2.0
1	G	805	THR	2.0
1	B	747	TYR	2.0
1	G	591	ASN	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
2	B3P	A	901	19/19	0.64	0.21	42,46,48,48	19
2	B3P	E	901	19/19	0.74	0.19	38,44,47,50	19

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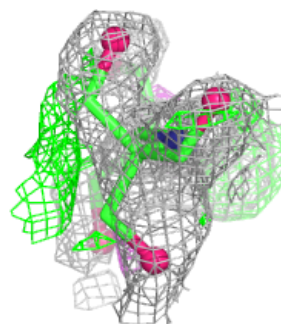
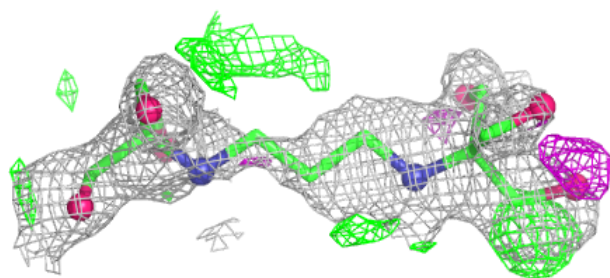
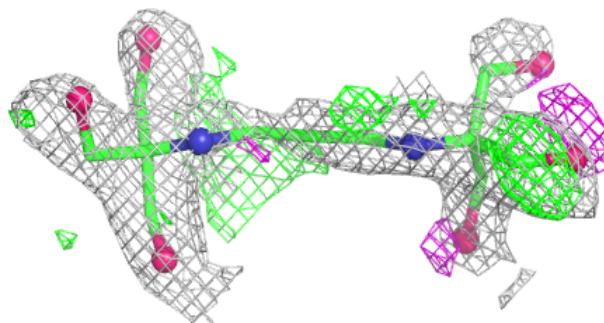
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	B3P	D	901	19/19	0.76	0.15	44,46,49,50	0
2	B3P	C	901	19/19	0.80	0.14	42,44,48,49	0
4	EDO	F	902	4/4	0.81	0.20	39,39,41,42	0
4	EDO	A	904	4/4	0.85	0.16	45,45,46,46	0
4	EDO	F	903	4/4	0.85	0.15	40,42,42,43	0
2	B3P	B	901	19/19	0.86	0.12	37,40,45,45	0
2	B3P	F	901	19/19	0.86	0.12	39,43,45,48	0
4	EDO	A	903	4/4	0.86	0.16	42,43,46,49	0
4	EDO	D	903	4/4	0.88	0.14	44,44,45,46	0
4	EDO	F	905	4/4	0.88	0.14	43,44,44,47	0
2	B3P	H	901	19/19	0.89	0.12	36,40,42,46	0
4	EDO	G	901	4/4	0.89	0.14	38,41,41,43	0
4	EDO	B	905	4/4	0.90	0.17	43,44,45,47	0
4	EDO	A	907	4/4	0.90	0.15	45,46,46,50	0
4	EDO	D	906	4/4	0.91	0.20	40,40,41,42	0
4	EDO	A	906	4/4	0.91	0.12	38,41,42,43	0
4	EDO	C	903	4/4	0.91	0.15	43,43,44,44	0
4	EDO	B	904	4/4	0.91	0.12	40,40,42,42	0
4	EDO	D	905	4/4	0.91	0.13	36,38,40,41	0
4	EDO	D	902	4/4	0.92	0.11	42,42,44,47	0
3	NO3	A	902	4/4	0.92	0.14	35,40,41,42	0
4	EDO	A	905	4/4	0.93	0.10	39,39,41,41	0
3	NO3	C	902	4/4	0.93	0.17	35,38,39,43	0
4	EDO	B	902	4/4	0.94	0.14	33,38,38,42	0
4	EDO	F	904	4/4	0.95	0.10	33,34,35,36	0
4	EDO	B	903	4/4	0.96	0.07	30,32,34,34	0
4	EDO	D	904	4/4	0.97	0.07	30,31,32,32	0
4	EDO	H	902	4/4	0.98	0.06	31,32,33,33	0

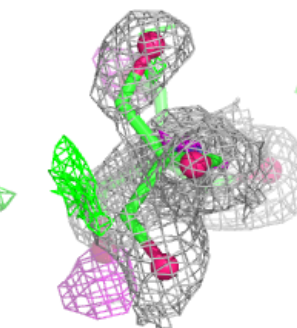
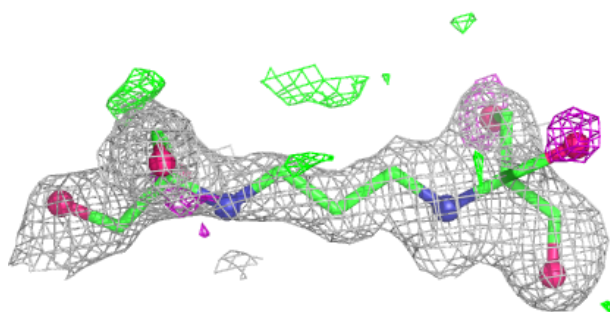
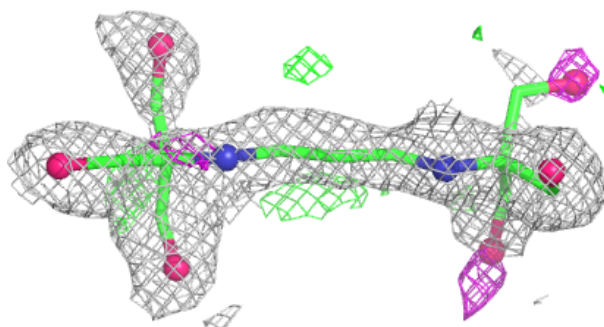
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B3P 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)

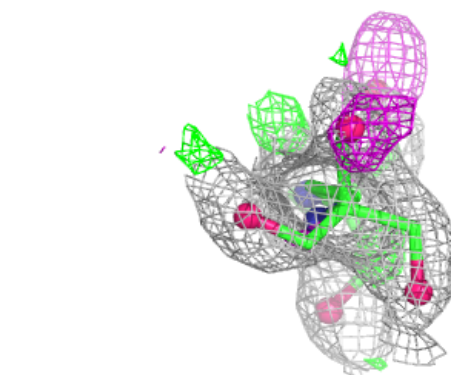
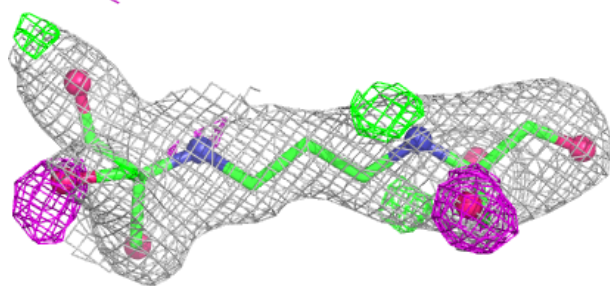
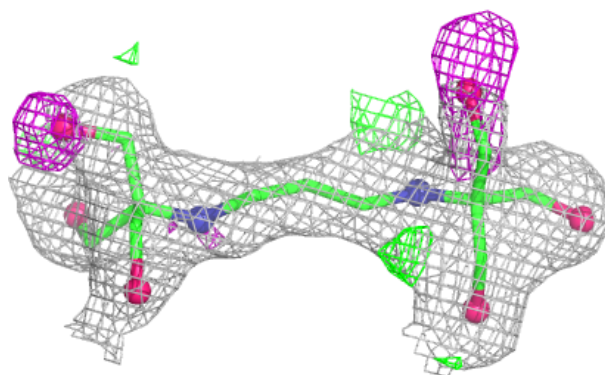
**Electron density around B3P E 901:**

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

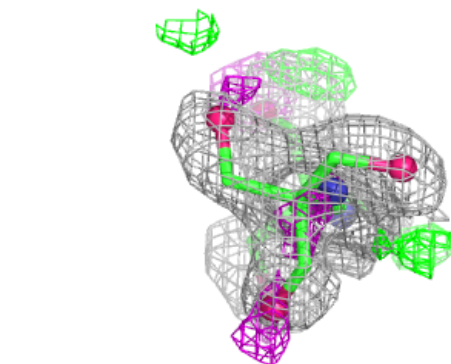
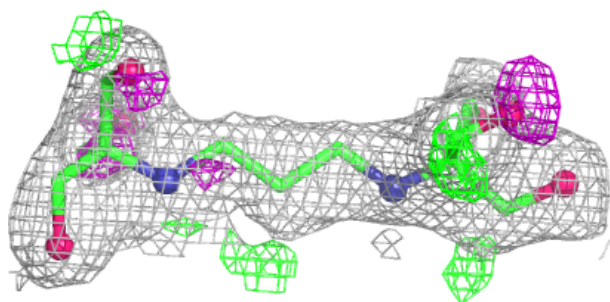
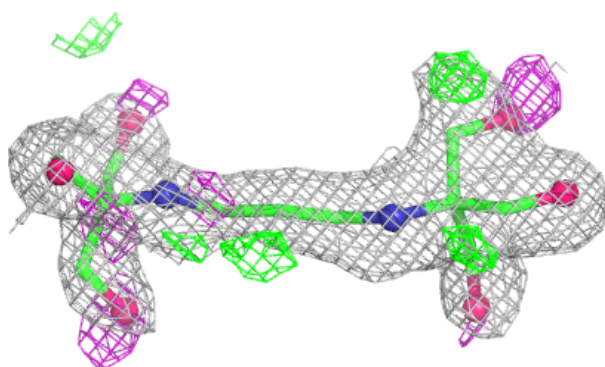


Electron density around B3P D 901:

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

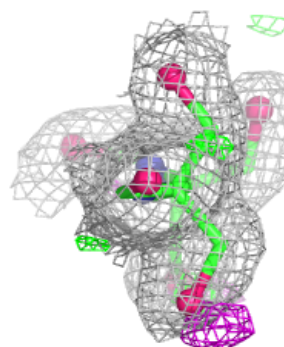
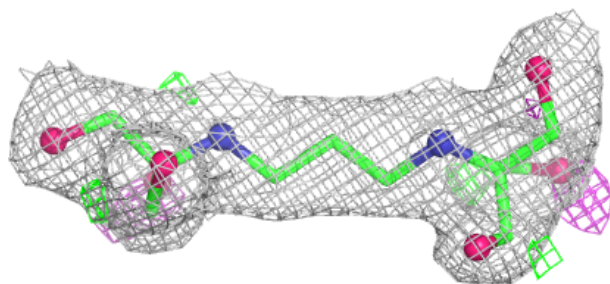
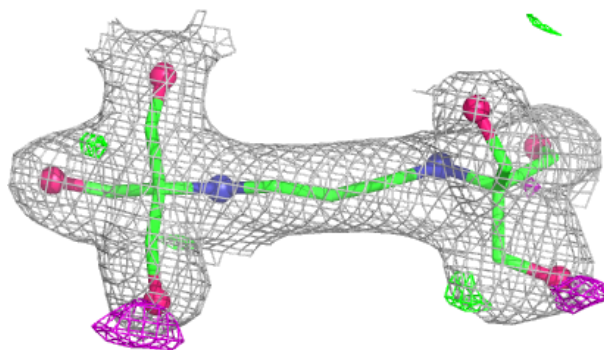
**Electron density around B3P C 901:**

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

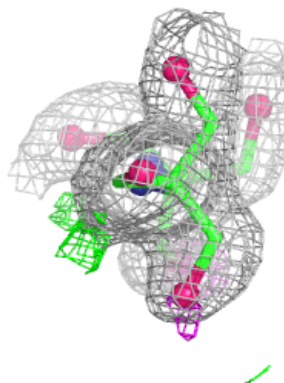
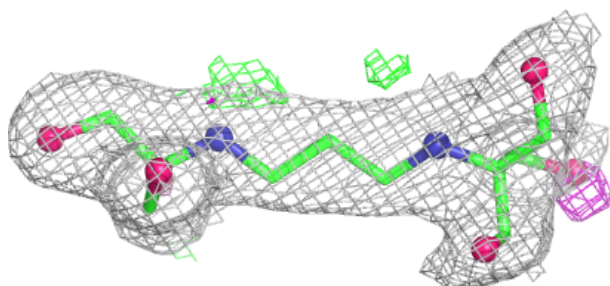
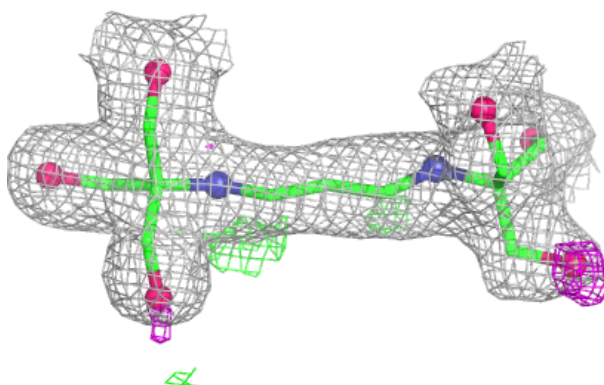


Electron density around B3P B 901:

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

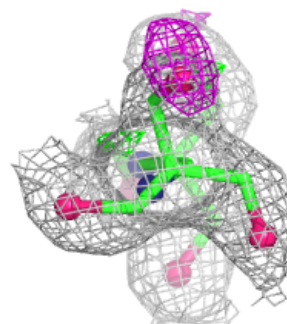
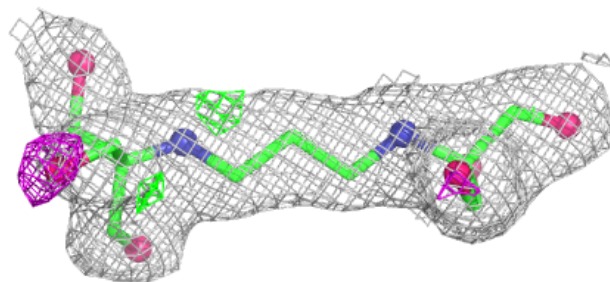
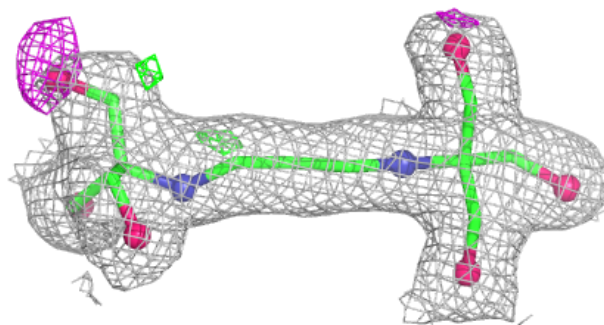
**Electron density around B3P F 901:**

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



Electron density around B3P H 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.