



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:45 PM UTC

PDB ID : 9GRO / pdb_00009gro
Title : Crystal structure of the engineered C-terminal phosphatase domain from *Saccharomyces cerevisiae* Vip1 in complex with 1,5-InsP8 (phosphatase dead mutant, loop deletion residues 848-918)
Authors : Raia, P.; Hothorn, M.
Deposited on : 2024-09-11
Resolution : 2.36 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

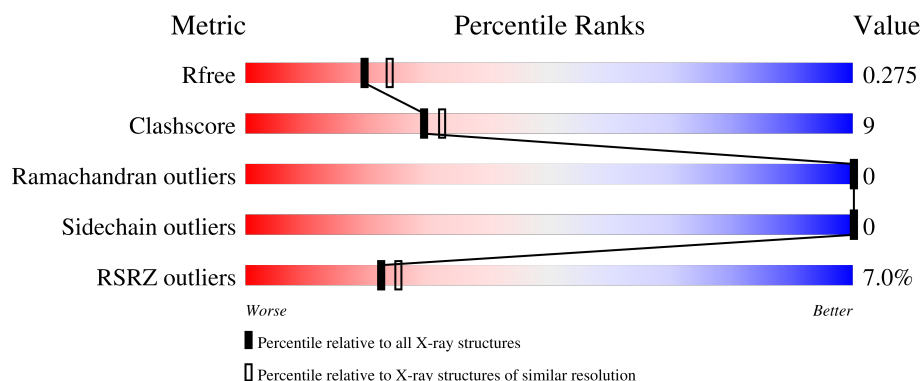
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	507	6% 81% 14% 5%
1	B	507	7% 76% 18% 6%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 16377 atoms, of which 8266 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 Inositol hexakisphosphate and diphosphoinositol-pentakisphosphate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	482	Total	C	H	N	O	S	0	3	0
			7962	2525	4027	675	718	17			
1	B	477	Total	C	H	N	O	S	0	3	0
			7862	2495	3978	665	707	17			

There are 146 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	534	GLY	-	expression tag	UNP Q06685
A	535	ALA	-	expression tag	UNP Q06685
A	547	ALA	ARG	conflict	UNP Q06685
A	548	ALA	HIS	conflict	UNP Q06685
A	551	ALA	ARG	conflict	UNP Q06685
A	?	-	LEU	deletion	UNP Q06685
A	?	-	PRO	deletion	UNP Q06685
A	?	-	ASN	deletion	UNP Q06685
A	?	-	GLU	deletion	UNP Q06685
A	?	-	ALA	deletion	UNP Q06685
A	?	-	ILE	deletion	UNP Q06685
A	?	-	ALA	deletion	UNP Q06685
A	?	-	ASP	deletion	UNP Q06685
A	?	-	GLU	deletion	UNP Q06685
A	?	-	LEU	deletion	UNP Q06685
A	?	-	GLY	deletion	UNP Q06685
A	?	-	SER	deletion	UNP Q06685
A	?	-	HIS	deletion	UNP Q06685
A	?	-	SER	deletion	UNP Q06685
A	?	-	LEU	deletion	UNP Q06685
A	?	-	VAL	deletion	UNP Q06685
A	?	-	ASP	deletion	UNP Q06685
A	?	-	ARG	deletion	UNP Q06685
A	?	-	TYR	deletion	UNP Q06685

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP Q06685
A	?	-	ILE	deletion	UNP Q06685
A	?	-	ASN	deletion	UNP Q06685
A	?	-	VAL	deletion	UNP Q06685
A	?	-	LEU	deletion	UNP Q06685
A	?	-	ALA	deletion	UNP Q06685
A	?	-	LYS	deletion	UNP Q06685
A	?	-	ASN	deletion	UNP Q06685
A	?	-	ASN	deletion	UNP Q06685
A	?	-	PHE	deletion	UNP Q06685
A	?	-	LYS	deletion	UNP Q06685
A	?	-	ILE	deletion	UNP Q06685
A	?	-	ILE	deletion	UNP Q06685
A	?	-	ASP	deletion	UNP Q06685
A	?	-	SER	deletion	UNP Q06685
A	?	-	HIS	deletion	UNP Q06685
A	?	-	SER	deletion	UNP Q06685
A	?	-	MET	deletion	UNP Q06685
A	?	-	ASN	deletion	UNP Q06685
A	?	-	ASN	deletion	UNP Q06685
A	?	-	SER	deletion	UNP Q06685
A	?	-	GLY	deletion	UNP Q06685
A	?	-	LYS	deletion	UNP Q06685
A	?	-	ASN	deletion	UNP Q06685
A	?	-	SER	deletion	UNP Q06685
A	?	-	SER	deletion	UNP Q06685
A	?	-	ASN	deletion	UNP Q06685
A	?	-	SER	deletion	UNP Q06685
A	?	-	VAL	deletion	UNP Q06685
A	?	-	GLY	deletion	UNP Q06685
A	?	-	SER	deletion	UNP Q06685
A	?	-	LEU	deletion	UNP Q06685
A	?	-	GLY	deletion	UNP Q06685
A	?	-	TRP	deletion	UNP Q06685
A	?	-	VAL	deletion	UNP Q06685
A	?	-	LEU	deletion	UNP Q06685
A	?	-	GLU	deletion	UNP Q06685
A	?	-	SER	deletion	UNP Q06685
A	?	-	GLY	deletion	UNP Q06685
A	?	-	LYS	deletion	UNP Q06685
A	?	-	THR	deletion	UNP Q06685
A	?	-	SER	deletion	UNP Q06685

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP Q06685
A	?	-	ALA	deletion	UNP Q06685
A	?	-	ARG	deletion	UNP Q06685
A	?	-	ASN	deletion	UNP Q06685
A	?	-	PRO	deletion	UNP Q06685
A	?	-	LYS	deletion	UNP Q06685
A	918	GLY	SER	conflict	UNP Q06685
B	534	GLY	-	expression tag	UNP Q06685
B	535	ALA	-	expression tag	UNP Q06685
B	547	ALA	ARG	conflict	UNP Q06685
B	548	ALA	HIS	conflict	UNP Q06685
B	551	ALA	ARG	conflict	UNP Q06685
B	?	-	LEU	deletion	UNP Q06685
B	?	-	PRO	deletion	UNP Q06685
B	?	-	ASN	deletion	UNP Q06685
B	?	-	GLU	deletion	UNP Q06685
B	?	-	ALA	deletion	UNP Q06685
B	?	-	ILE	deletion	UNP Q06685
B	?	-	ALA	deletion	UNP Q06685
B	?	-	ASP	deletion	UNP Q06685
B	?	-	GLU	deletion	UNP Q06685
B	?	-	LEU	deletion	UNP Q06685
B	?	-	GLY	deletion	UNP Q06685
B	?	-	SER	deletion	UNP Q06685
B	?	-	HIS	deletion	UNP Q06685
B	?	-	SER	deletion	UNP Q06685
B	?	-	LEU	deletion	UNP Q06685
B	?	-	VAL	deletion	UNP Q06685
B	?	-	ASP	deletion	UNP Q06685
B	?	-	ARG	deletion	UNP Q06685
B	?	-	TYR	deletion	UNP Q06685
B	?	-	PRO	deletion	UNP Q06685
B	?	-	ILE	deletion	UNP Q06685
B	?	-	ASN	deletion	UNP Q06685
B	?	-	VAL	deletion	UNP Q06685
B	?	-	LEU	deletion	UNP Q06685
B	?	-	ALA	deletion	UNP Q06685
B	?	-	LYS	deletion	UNP Q06685
B	?	-	ASN	deletion	UNP Q06685
B	?	-	ASN	deletion	UNP Q06685
B	?	-	PHE	deletion	UNP Q06685
B	?	-	LYS	deletion	UNP Q06685

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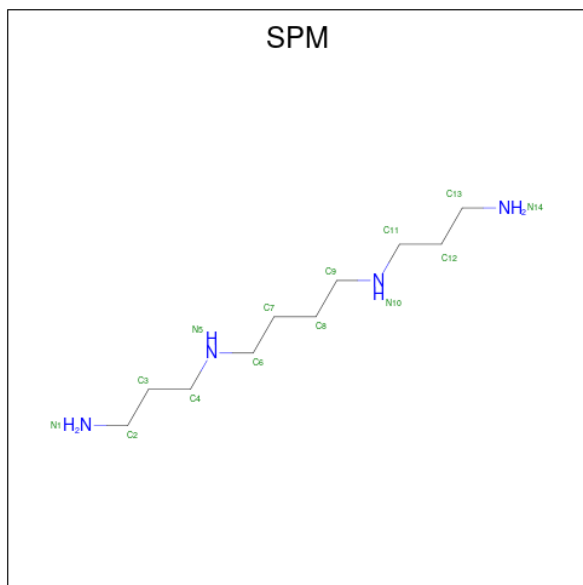
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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ILE	deletion	UNP Q06685
B	?	-	ILE	deletion	UNP Q06685
B	?	-	ASP	deletion	UNP Q06685
B	?	-	SER	deletion	UNP Q06685
B	?	-	HIS	deletion	UNP Q06685
B	?	-	SER	deletion	UNP Q06685
B	?	-	MET	deletion	UNP Q06685
B	?	-	ASN	deletion	UNP Q06685
B	?	-	ASN	deletion	UNP Q06685
B	?	-	SER	deletion	UNP Q06685
B	?	-	GLY	deletion	UNP Q06685
B	?	-	LYS	deletion	UNP Q06685
B	?	-	ASN	deletion	UNP Q06685
B	?	-	SER	deletion	UNP Q06685
B	?	-	SER	deletion	UNP Q06685
B	?	-	ASN	deletion	UNP Q06685
B	?	-	SER	deletion	UNP Q06685
B	?	-	VAL	deletion	UNP Q06685
B	?	-	GLY	deletion	UNP Q06685
B	?	-	SER	deletion	UNP Q06685
B	?	-	LEU	deletion	UNP Q06685
B	?	-	GLY	deletion	UNP Q06685
B	?	-	TRP	deletion	UNP Q06685
B	?	-	VAL	deletion	UNP Q06685
B	?	-	LEU	deletion	UNP Q06685
B	?	-	GLU	deletion	UNP Q06685
B	?	-	SER	deletion	UNP Q06685
B	?	-	GLY	deletion	UNP Q06685
B	?	-	LYS	deletion	UNP Q06685
B	?	-	THR	deletion	UNP Q06685
B	?	-	SER	deletion	UNP Q06685
B	?	-	THR	deletion	UNP Q06685
B	?	-	ALA	deletion	UNP Q06685
B	?	-	ARG	deletion	UNP Q06685
B	?	-	ASN	deletion	UNP Q06685
B	?	-	PRO	deletion	UNP Q06685
B	?	-	LYS	deletion	UNP Q06685
B	918	GLY	SER	conflict	UNP Q06685

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

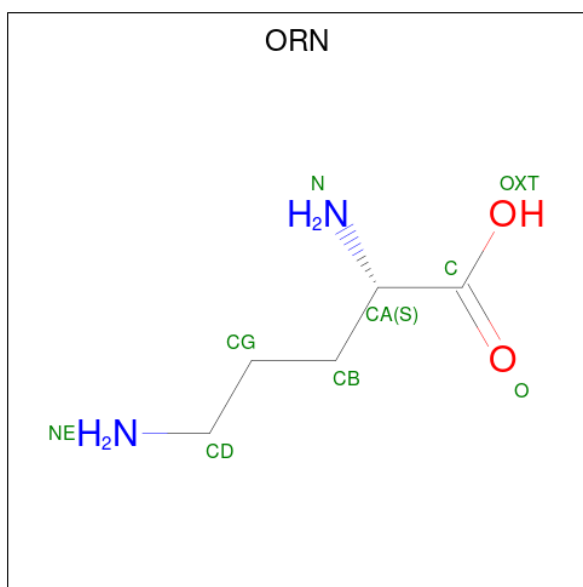
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



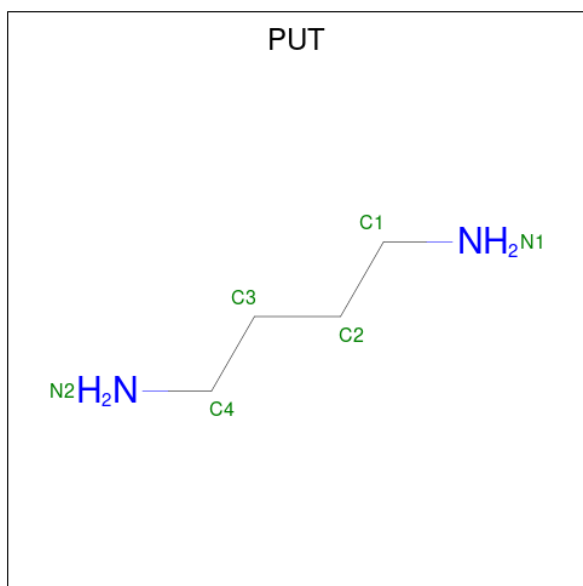
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			38	10	24	4		
3	A	1	Total	C	H	N	0	0
			38	10	24	4		

- Molecule 4 is L-ornithine (CCD ID: ORN) (formula: $C_5H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			20	5	11	2	2		

- Molecule 5 is 1,4-DIAMINOBTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



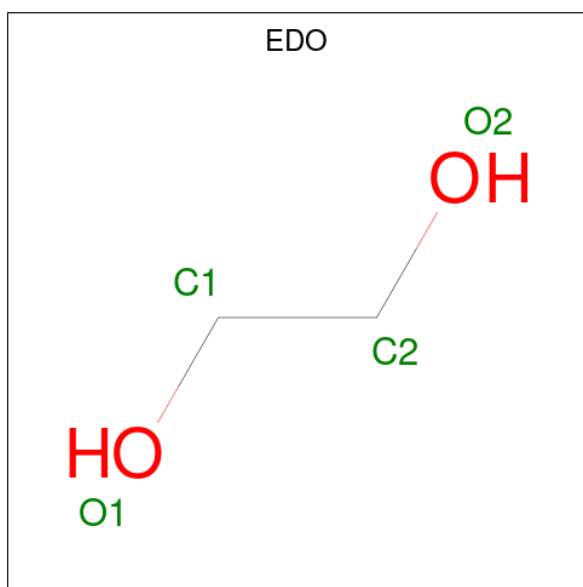
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	N		
			18	4	12	2	0	0
5	A	1	Total	C	H	N		
			18	4	12	2	0	0
5	A	1	Total	C	H	N		
			18	4	12	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	N	0	0
			18	4	12	2		
5	B	1	Total	C	H	N	0	0
			18	4	12	2		
5	B	1	Total	C	H	N	0	0
			18	4	12	2		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



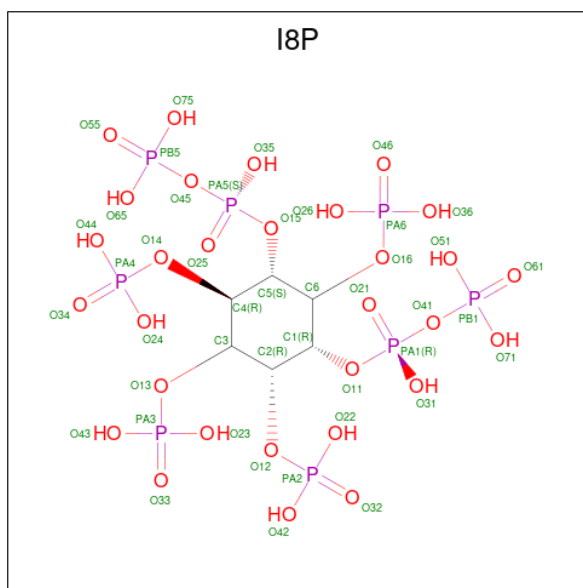
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		

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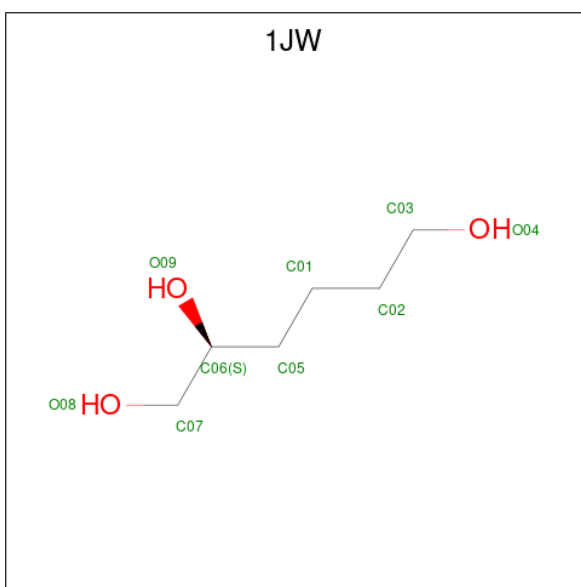
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 7 is (1R,3S,4R,5S,6R)-2,4,5,6-tetrakis(phosphonoxy)cyclohexane-1,3-diyl bis[trihydrogen (diphosphate)] (CCD ID: I8P) (formula: $C_6H_{20}O_{30}P_8$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	O	P	0	0
			50	6	6	30	8		
7	B	1	Total	C	H	O	P	0	0
			50	6	6	30	8		

- Molecule 8 is (2S)-hexane-1,2,6-triol (CCD ID: 1JW) (formula: $C_6H_{14}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	H	O	0	0
			23	6	14	3		
8	B	1	Total	C	H	O	0	0
			23	6	14	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	27	Total	O	0	0
			27	27		
9	B	24	Total	O	0	0
			24	24		

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	114.59Å 114.59Å 172.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.68 – 2.36 49.68 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.68-2.36) 99.9 (49.68-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.37Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, R_{free}	0.228 , 0.275 0.228 , 0.275	Depositor DCC
R_{free} test set	2707 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	69.2	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16377	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: I8P, ORN, PUT, EDO, SPM, ZN, 1JW

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	0.13	0/4025	0.27	0/5421
1	B	0.13	0/3973	0.29	0/5349
All	All	0.13	0/7998	0.28	0/10770

There are no bond length outliers.

There are no bond angle outliers.

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	3935	4027	4027	58	0
1	B	3884	3978	3977	81	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	48	52	3	0
4	A	9	11	11	1	0
5	A	24	48	48	1	0
5	B	12	24	24	0	0
6	A	36	54	54	1	0
6	B	24	36	36	1	0
7	A	44	6	6	1	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	44	6	6	3	0
8	B	18	28	0	0	0
9	A	27	0	0	2	0
9	B	24	0	0	0	0
All	All	8111	8266	8241	140	1

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 9.

All (140) 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:A:973:ILE:CD1	1:A:1028:LEU:HD11	1.72	1.18
1:A:973:ILE:HD11	1:A:1028:LEU:HD11	1.29	1.12
1:A:973:ILE:CD1	1:A:1028:LEU:CD1	2.57	0.83
1:A:956:ASP:O	1:A:960:LEU:HD12	1.78	0.82
1:B:575:GLU:OE2	1:B:575:GLU:HA	1.80	0.81
1:A:973:ILE:HD13	1:A:1028:LEU:HD11	1.61	0.80
1:B:830:MET:HE1	1:B:935:ALA:CB	2.13	0.78
1:B:826:LEU:HG	1:B:830:MET:HE2	1.65	0.78
1:A:973:ILE:HD13	1:A:1028:LEU:HD21	1.65	0.76
1:A:738:LEU:HD21	1:A:746:PRO:HB3	1.66	0.76
1:B:725:LYS:O	1:B:729:ASP:OD2	2.07	0.72
1:B:579:ILE:HD12	1:B:584:ASP:HB3	1.74	0.70
1:B:972:ASP:OD2	1:B:987:TYR:OH	2.09	0.69
1:B:687:ARG:HG3	1:B:687:ARG:HH11	1.56	0.69
3:A:1203:SPM:N14	9:A:1301:HOH:O	2.27	0.68
1:B:715:LYS:HA	1:B:719:ASP:OD1	1.94	0.67
1:B:581:ASN:OD1	1:B:584:ASP:N	2.25	0.66
1:B:613:LEU:HD22	1:B:624:ILE:HD11	1.79	0.65
1:B:625:GLN:OE1	7:B:1210:I8P:O35	2.15	0.65
1:A:632:LYS:N	1:A:632:LYS:HD3	2.13	0.64
1:A:817:LYS:O	1:A:817:LYS:NZ	2.22	0.63
1:A:750:ALA:O	1:A:945:LYS:NZ	2.32	0.62
1:B:589:LEU:C	1:B:589:LEU:HD13	2.25	0.62
1:B:783:LYS:NZ	1:B:788:MET:HE1	2.15	0.62
1:A:659:GLU:OE2	1:A:1065:TYR:OH	2.14	0.62
1:B:816:GLU:HA	1:B:816:GLU:OE1	1.99	0.61
1:A:807:LYS:NZ	1:A:825:GLU:OE1	2.32	0.60
1:B:570:LEU:O	1:B:573:HIS:HD2	1.85	0.60
1:A:956:ASP:C	1:A:960:LEU:HD12	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:788:MET:O	1:B:843:ASN:ND2	2.34	0.59
1:B:673:LYS:CD	1:B:673:LYS:H	2.16	0.58
1:A:973:ILE:HD13	1:A:1028:LEU:CD2	2.34	0.58
1:B:1059:GLN:OE1	1:B:1059:GLN:HA	2.03	0.57
1:B:804:ARG:NH2	1:B:833:ASP:OD1	2.37	0.57
1:A:749:PHE:CE1	1:A:945:LYS:HD2	2.39	0.57
1:A:749:PHE:HE1	1:A:945:LYS:HD2	1.68	0.57
1:B:593:ARG:NH2	1:B:614:GLU:OE1	2.38	0.57
1:A:973:ILE:HD13	1:A:1028:LEU:CD1	2.33	0.56
1:B:783:LYS:HE3	1:B:788:MET:HE1	1.87	0.56
1:A:605:LYS:NZ	7:A:1215:I8P:O25	2.27	0.56
1:B:835:LEU:HD21	1:B:1066:ILE:HG12	1.88	0.55
1:B:1093:ARG:HD3	1:B:1094:VAL:HG23	1.89	0.55
1:A:1028:LEU:HD12	1:A:1028:LEU:N	2.21	0.54
1:B:570:LEU:O	1:B:573:HIS:CD2	2.59	0.54
1:B:581:ASN:OD1	1:B:583:ASN:N	2.40	0.54
1:A:666:GLN:O	1:A:670:LEU:HD23	2.09	0.53
1:B:783:LYS:CE	1:B:788:MET:HE1	2.39	0.53
1:B:673:LYS:HD2	1:B:673:LYS:N	2.24	0.53
1:B:687:ARG:HG3	1:B:687:ARG:NH1	2.19	0.53
1:B:627:LYS:HE2	7:B:1210:I8P:O75	2.08	0.52
1:A:1031:SER:N	1:A:1039:SER:O	2.37	0.51
1:B:627:LYS:CE	7:B:1210:I8P:O75	2.58	0.51
1:B:973:ILE:HD11	1:B:1026:PHE:HB3	1.92	0.51
1:A:749:PHE:CE1	1:A:945:LYS:CD	2.93	0.51
1:B:673:LYS:CD	1:B:673:LYS:N	2.74	0.51
1:A:973:ILE:HD11	1:A:1028:LEU:CD1	2.19	0.50
1:B:1009:ARG:HD2	1:B:1076:LYS:HD3	1.91	0.50
1:A:556:LYS:O	1:A:822:LYS:NZ	2.43	0.50
1:B:788:MET:HA	1:B:788:MET:HE2	1.92	0.50
1:B:1009:ARG:HD2	1:B:1076:LYS:CD	2.42	0.50
1:A:680:LYS:HD3	1:A:682:PHE:CZ	2.47	0.50
1:A:977:LYS:HD2	1:A:1080:MET:CE	2.42	0.49
1:A:715:LYS:HG2	1:A:719:ASP:OD2	2.12	0.49
1:B:816:GLU:OE1	1:B:816:GLU:CA	2.60	0.49
1:A:1084:GLN:OE1	1:A:1088:ARG:NH1	2.46	0.49
1:A:804[A]:ARG:NH1	9:A:1304:HOH:O	2.46	0.49
1:B:589:LEU:HD11	1:B:593:ARG:NE	2.28	0.49
1:A:780:PHE:CD1	1:A:785:VAL:HG21	2.48	0.48
1:A:973:ILE:CD1	1:A:1028:LEU:CG	2.91	0.48
1:A:819:ASP:OD1	1:A:820:PRO:HD2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:771:TYR:CZ	1:B:775:ILE:HD11	2.49	0.48
1:B:554:LYS:HZ1	1:B:644:LYS:HD3	1.78	0.48
1:A:1080:MET:SD	1:A:1084:GLN:NE2	2.87	0.48
1:B:952:ALA:O	1:B:956:ASP:OD2	2.32	0.48
1:A:540:LYS:HD3	1:A:1030:GLU:OE1	2.14	0.47
1:A:926:MET:N	1:A:926:MET:HE2	2.28	0.47
1:B:757:GLU:HG2	1:B:760:LEU:HD23	1.95	0.47
1:A:580[A]:ARG:NH2	6:A:1208:EDO:O2	2.46	0.47
1:B:641:PHE:C	1:B:641:PHE:CD1	2.92	0.47
1:B:788:MET:SD	1:B:843:ASN:HB3	2.54	0.47
1:B:999:ASN:O	1:B:1003:GLU:HG2	2.15	0.47
1:A:725:LYS:O	1:A:729:ASP:OD2	2.33	0.47
1:B:554:LYS:NZ	1:B:644:LYS:HD3	2.30	0.47
1:A:1043:ARG:NH1	1:A:1075:THR:O	2.48	0.46
1:B:581:ASN:OD1	1:B:583:ASN:HB2	2.16	0.46
1:B:578:VAL:HG22	1:B:625:GLN:HG2	1.96	0.46
1:B:993:HIS:O	1:B:997:LEU:HB2	2.15	0.46
1:B:554:LYS:O	1:B:555:GLN:HG2	2.16	0.46
1:B:744:GLU:OE1	1:B:745:ALA:N	2.47	0.46
1:B:783:LYS:HE3	1:B:788:MET:CE	2.46	0.46
1:B:725:LYS:HG3	1:B:729:ASP:OD2	2.15	0.46
1:B:589:LEU:HD11	1:B:593:ARG:HE	1.81	0.46
1:A:537:TRP:CZ2	1:A:1041:SER:HB3	2.51	0.45
1:B:584:ASP:O	1:B:588:VAL:HG23	2.17	0.45
1:B:737:PRO:HA	1:B:740:ARG:HD3	1.98	0.45
1:A:651:HIS:ND1	1:B:1062:ASP:OD2	2.43	0.45
1:A:1003:GLU:HA	1:A:1003:GLU:OE1	2.16	0.45
1:B:788:MET:HG3	1:B:840:PHE:CE1	2.52	0.45
1:B:596:LEU:C	1:B:596:LEU:HD13	2.42	0.44
1:B:973:ILE:HG22	1:B:1080:MET:HE3	1.98	0.44
1:B:788:MET:HG3	1:B:840:PHE:HE1	1.82	0.44
1:A:540:LYS:NZ	1:A:977:LYS:O	2.50	0.44
1:A:616:LYS:NZ	1:A:803:GLU:OE1	2.40	0.44
1:A:924:ARG:O	1:A:926:MET:CE	2.66	0.43
1:A:972:ASP:OD2	1:A:987:TYR:OH	2.27	0.43
1:B:684:SER:HB3	1:B:689:VAL:HG11	1.99	0.43
1:A:759:TYR:CE1	1:A:760:LEU:HD23	2.53	0.43
1:B:778:ASN:O	1:B:782:LYS:HG2	2.18	0.43
1:A:713:ILE:HD11	5:A:1212:PUT:C1	2.48	0.43
1:B:579:ILE:CG2	1:B:585:LEU:HD23	2.49	0.43
1:B:1046:MET:C	1:B:1046:MET:SD	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:762:ILE:HG21	1:B:818:VAL:HG21	2.00	0.43
1:B:613:LEU:CD2	1:B:624:ILE:HD11	2.46	0.42
1:B:673:LYS:H	1:B:673:LYS:HD2	1.81	0.42
1:B:830:MET:HE1	1:B:935:ALA:HB3	1.95	0.42
1:B:958:GLY:HA2	1:B:996:THR:HB	2.01	0.42
1:B:976:MET:HE3	1:B:985:VAL:HG23	2.01	0.42
1:B:792:TRP:CE3	6:B:1206:EDO:H21	2.55	0.42
1:B:556:LYS:HB3	1:B:644:LYS:HG2	2.00	0.42
1:A:560:SER:HB3	1:A:638:LYS:HD2	2.01	0.42
1:A:945:LYS:HE3	3:A:1203:SPM:N1	2.34	0.42
1:A:1042:ILE:CD1	1:A:1080:MET:HG2	2.50	0.42
1:B:776:MET:HE3	1:B:802:LYS:HG3	2.01	0.42
1:A:959:LEU:O	1:A:963:LEU:HB2	2.19	0.41
1:A:1042:ILE:HD11	1:A:1080:MET:HG2	2.02	0.41
3:A:1202:SPM:N10	4:A:1204:ORN:O	2.53	0.41
1:A:627:LYS:HD3	1:A:642:ILE:CD1	2.51	0.41
1:A:838[A]:ARG:NH1	1:A:842:GLU:OE2	2.52	0.41
1:B:973:ILE:HD11	1:B:1026:PHE:CB	2.50	0.41
1:B:559:HIS:HB3	1:B:605:LYS:HD3	2.02	0.41
1:A:965:LEU:O	1:A:969:ILE:HG13	2.21	0.41
1:B:540:LYS:O	1:B:982:PRO:HA	2.20	0.41
1:B:548:ALA:HB2	1:B:689:VAL:HG22	2.03	0.41
1:B:788:MET:SD	1:B:843:ASN:CB	3.09	0.41
1:B:797:ASP:HB2	1:B:798:PRO:HD2	2.03	0.41
1:B:1086:LYS:O	1:B:1090:LYS:HG2	2.21	0.41
1:A:773:LYS:HB3	1:A:773:LYS:HE2	1.77	0.41
1:A:679:ILE:HD13	1:A:984:CYS:HB3	2.02	0.40
1:B:749:PHE:CE2	1:B:945:LYS:HG3	2.56	0.40
1:A:995:TYR:CE2	1:A:1018:LEU:HD12	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:GLY:N	7:A:1215:I8P:O75[4_545]	1.30	0.90

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	481/507 (95%)	469 (98%)	12 (2%)	0	100	100
1	B	474/507 (94%)	465 (98%)	9 (2%)	0	100	100
All	All	955/1014 (94%)	934 (98%)	21 (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	436/456 (96%)	436 (100%)	0	100	100
1	B	429/456 (94%)	429 (100%)	0	100	100
All	All	865/912 (95%)	865 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	573	HIS
1	A	640	GLN
1	A	678	ASN
1	A	778	ASN
1	A	1077	HIS
1	B	573	HIS

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Mol	Chain	Res	Type
1	B	786	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](#)

Of 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 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	$\# Z > 2$
5	PUT	A	1212	-	5,5,5	0.76	0	4,4,4	0.22	0
6	EDO	A	1207	-	3,3,3	0.25	0	2,2,2	0.32	0
3	SPM	A	1203	-	13,13,13	0.34	0	12,12,12	0.97	0
6	EDO	A	1217	-	3,3,3	0.24	0	2,2,2	0.34	0
6	EDO	B	1207	-	3,3,3	0.26	0	2,2,2	0.35	0
3	SPM	A	1202	-	13,13,13	0.37	0	12,12,12	0.50	0
5	PUT	B	1208	-	5,5,5	0.76	0	4,4,4	0.23	0
6	EDO	B	1206	-	3,3,3	0.27	0	2,2,2	0.28	0
6	EDO	A	1214	-	3,3,3	0.25	0	2,2,2	0.36	0
6	EDO	A	1210	-	3,3,3	0.24	0	2,2,2	0.34	0
6	EDO	A	1211	-	3,3,3	0.25	0	2,2,2	0.36	0
6	EDO	B	1205	-	3,3,3	0.26	0	2,2,2	0.35	0
5	PUT	B	1203	-	5,5,5	0.76	0	4,4,4	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	B	1211	-	3,3,3	0.25	0	2,2,2	0.37	0
5	PUT	A	1218	-	5,5,5	0.75	0	4,4,4	0.21	0
8	1JW	B	1204	-	8,8,8	0.54	0	7,8,8	1.04	0
8	1JW	B	1202	-	8,8,8	0.90	0	7,8,8	0.71	0
7	I8P	A	1215	-	42,44,44	1.68	6 (14%)	68,74,74	0.87	3 (4%)
6	EDO	A	1208	-	3,3,3	0.25	0	2,2,2	0.32	0
6	EDO	B	1209	-	3,3,3	0.25	0	2,2,2	0.32	0
4	ORN	A	1204	-	7,8,8	1.06	0	6,9,9	0.40	0
5	PUT	A	1206	-	5,5,5	0.75	0	4,4,4	0.22	0
6	EDO	A	1213	-	3,3,3	0.25	0	2,2,2	0.32	0
6	EDO	B	1212	-	3,3,3	0.25	0	2,2,2	0.36	0
7	I8P	B	1210	-	42,44,44	1.61	6 (14%)	68,74,74	0.87	2 (2%)
6	EDO	A	1209	-	3,3,3	0.25	0	2,2,2	0.34	0
5	PUT	A	1205	-	5,5,5	0.75	0	4,4,4	0.23	0
6	EDO	A	1216	-	3,3,3	0.26	0	2,2,2	0.35	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
5	PUT	A	1212	-	-	2/3/3/3	-
6	EDO	A	1207	-	-	1/1/1/1	-
3	SPM	A	1203	-	-	2/11/11/11	-
6	EDO	A	1217	-	-	0/1/1/1	-
6	EDO	B	1207	-	-	1/1/1/1	-
3	SPM	A	1202	-	-	4/11/11/11	-
5	PUT	B	1208	-	-	1/3/3/3	-
6	EDO	B	1206	-	-	0/1/1/1	-
6	EDO	A	1214	-	-	0/1/1/1	-
6	EDO	A	1210	-	-	1/1/1/1	-
6	EDO	A	1211	-	-	0/1/1/1	-
6	EDO	B	1205	-	-	0/1/1/1	-
5	PUT	B	1203	-	-	1/3/3/3	-
6	EDO	B	1211	-	-	0/1/1/1	-
5	PUT	A	1218	-	-	1/3/3/3	-
8	1JW	B	1204	-	-	2/7/7/7	-
8	1JW	B	1202	-	-	4/7/7/7	-
7	I8P	A	1215	-	-	10/42/66/66	0/1/1/1
6	EDO	A	1208	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	1209	-	-	1/1/1/1	-
4	ORN	A	1204	-	-	2/8/8/8	-
5	PUT	A	1206	-	-	1/3/3/3	-
6	EDO	A	1213	-	-	1/1/1/1	-
6	EDO	B	1212	-	-	0/1/1/1	-
7	I8P	B	1210	-	-	5/42/66/66	0/1/1/1
6	EDO	A	1209	-	-	0/1/1/1	-
5	PUT	A	1205	-	-	1/3/3/3	-
6	EDO	A	1216	-	-	0/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1210	I8P	PA1-O41	5.08	1.65	1.59
7	A	1215	I8P	PA5-O45	5.06	1.65	1.59
7	A	1215	I8P	PA1-O41	4.90	1.64	1.59
7	B	1210	I8P	PA5-O45	3.91	1.63	1.59
7	A	1215	I8P	PA3-O13	3.39	1.65	1.59
7	A	1215	I8P	PA4-O14	3.39	1.65	1.59
7	B	1210	I8P	PA4-O14	3.36	1.65	1.59
7	B	1210	I8P	PA3-O13	3.33	1.65	1.59
7	A	1215	I8P	PA2-O12	3.18	1.65	1.59
7	B	1210	I8P	PA6-O16	3.12	1.65	1.59
7	B	1210	I8P	PA2-O12	3.04	1.64	1.59
7	A	1215	I8P	PA6-O16	2.96	1.64	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1210	I8P	PA4-O14-C4	-2.39	117.04	123.43
7	B	1210	I8P	C3-C2-C1	2.26	115.38	110.43
7	A	1215	I8P	PA6-O16-C6	-2.19	117.59	123.43
7	A	1215	I8P	PA3-O13-C3	-2.13	117.74	123.43
7	A	1215	I8P	O35-PA5-O45	2.05	112.81	107.27

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1215	I8P	C5-O15-PA5-O45
7	A	1215	I8P	PA1-O41-PB1-O71

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Mol	Chain	Res	Type	Atoms
7	B	1210	I8P	C5-O15-PA5-O45
8	B	1202	1JW	C01-C05-C06-C07
8	B	1204	1JW	C05-C06-C07-O08
3	A	1202	SPM	C6-C7-C8-C9
5	A	1218	PUT	C1-C2-C3-C4
8	B	1202	1JW	C01-C05-C06-O09
3	A	1202	SPM	C7-C8-C9-N10
8	B	1204	1JW	O09-C06-C07-O08
4	A	1204	ORN	CA-CB-CG-CD
3	A	1203	SPM	C2-C3-C4-N5
7	A	1215	I8P	C4-O14-PA4-O34
5	A	1205	PUT	C1-C2-C3-C4
7	A	1215	I8P	PB1-O41-PA1-O21
5	B	1208	PUT	C1-C2-C3-C4
5	A	1206	PUT	C1-C2-C3-C4
3	A	1203	SPM	N1-C2-C3-C4
7	B	1210	I8P	PB5-O45-PA5-O35
6	A	1208	EDO	O1-C1-C2-O2
5	A	1212	PUT	N1-C1-C2-C3
5	B	1203	PUT	N1-C1-C2-C3
6	A	1207	EDO	O1-C1-C2-O2
6	B	1207	EDO	O1-C1-C2-O2
3	A	1202	SPM	C8-C9-N10-C11
8	B	1202	1JW	O09-C06-C07-O08
7	A	1215	I8P	C3-O13-PA3-O33
3	A	1202	SPM	C3-C4-N5-C6
6	A	1213	EDO	O1-C1-C2-O2
6	B	1209	EDO	O1-C1-C2-O2
6	A	1210	EDO	O1-C1-C2-O2
7	A	1215	I8P	C1-O11-PA1-O21
7	A	1215	I8P	C5-O15-PA5-O25
7	A	1215	I8P	C5-O15-PA5-O35
7	B	1210	I8P	C5-O15-PA5-O35
7	B	1210	I8P	PB5-O45-PA5-O25
5	A	1212	PUT	C2-C3-C4-N2
7	A	1215	I8P	C4-O14-PA4-O44
7	B	1210	I8P	C4-O14-PA4-O44
8	B	1202	1JW	C02-C01-C05-C06
7	A	1215	I8P	C6-O16-PA6-O46
4	A	1204	ORN	OXT-C-CA-N

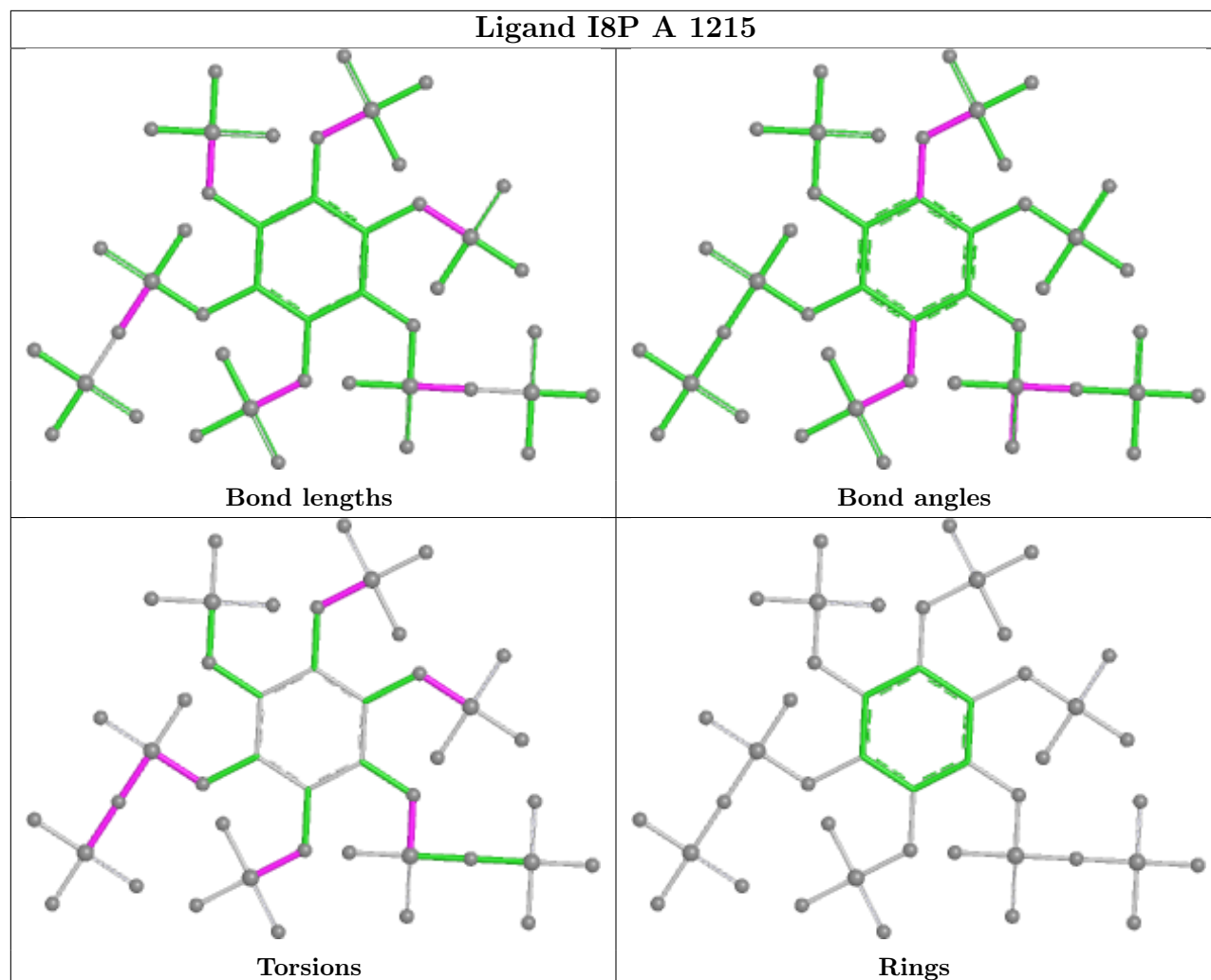
There are no ring outliers.

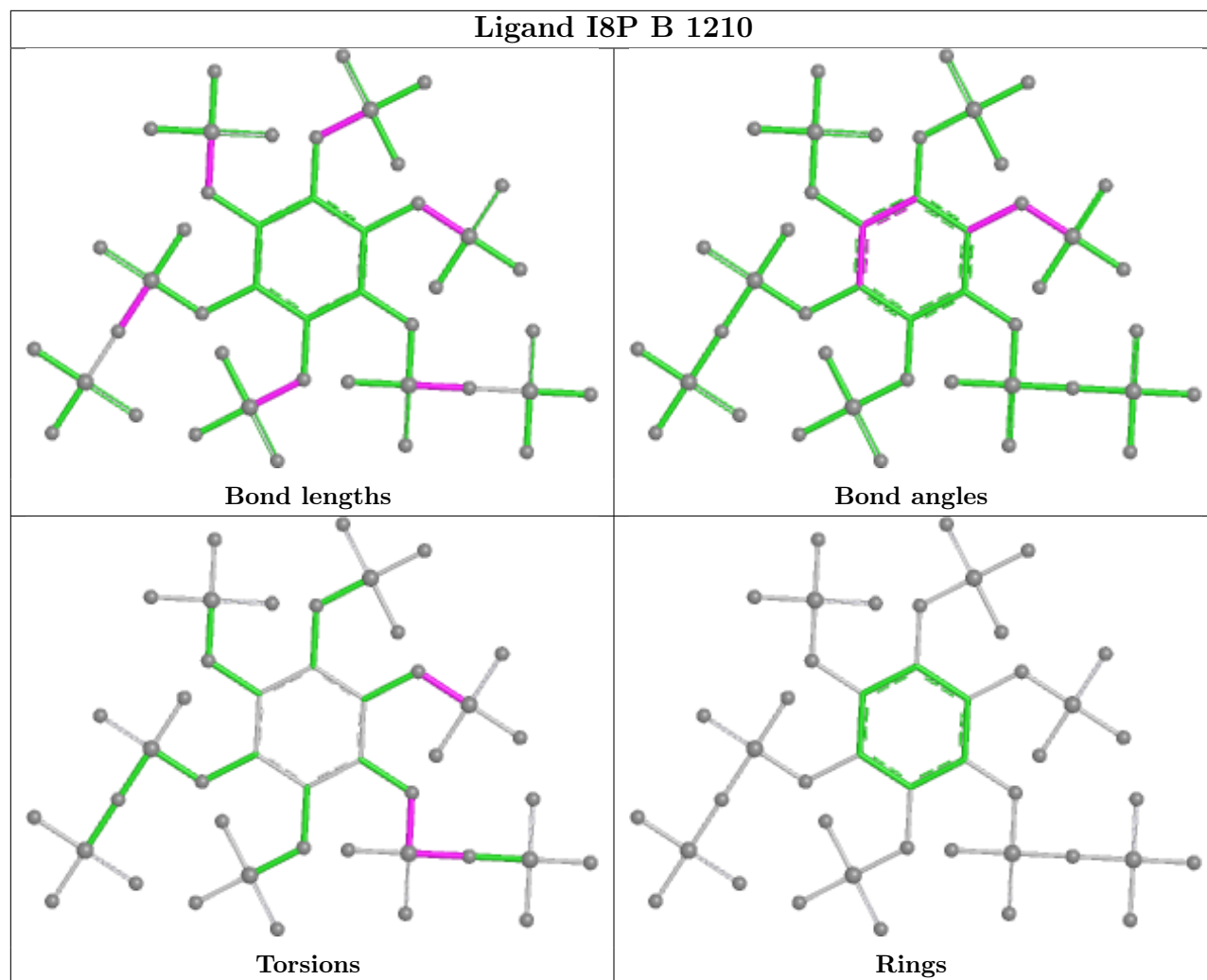
8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1212	PUT	1	0
3	A	1203	SPM	2	0
3	A	1202	SPM	1	0
6	B	1206	EDO	1	0
7	A	1215	I8P	1	1
6	A	1208	EDO	1	0
4	A	1204	ORN	1	0
7	B	1210	I8P	3	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 I8P A 1215





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	482/507 (95%)	0.60	32 (6%) 24 27	41, 88, 152, 214	3 (0%)
1	B	477/507 (94%)	0.69	35 (7%) 21 24	40, 87, 159, 194	3 (0%)
All	All	959/1014 (94%)	0.65	67 (6%) 22 25	40, 88, 157, 214	6 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1028	LEU	5.4
1	B	566	PHE	4.9
1	A	848	GLY	4.0
1	A	537	TRP	4.0
1	B	848	GLY	3.9
1	B	1094	VAL	3.8
1	A	1042	ILE	3.7
1	B	706	LEU	3.6
1	A	723	ALA	3.6
1	A	1034	ALA	3.6
1	A	785	VAL	3.3
1	A	924	ARG	3.1
1	B	587	ILE	3.0
1	A	925	PHE	3.0
1	B	577	VAL	3.0
1	B	707	GLY	2.9
1	B	626	LEU	2.9
1	A	538	VAL	2.9
1	B	624	ILE	2.9
1	A	749	PHE	2.8
1	B	600	ALA	2.8
1	B	642	ILE	2.7
1	A	1091	PHE	2.6
1	B	628	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	932	TYR	2.6
1	B	723	ALA	2.5
1	A	973	ILE	2.5
1	B	567	ILE	2.5
1	A	632	LYS	2.5
1	B	572	GLY	2.5
1	B	625	GLN	2.5
1	B	604	ALA	2.5
1	B	788	MET	2.4
1	B	561	PHE	2.4
1	A	746	PRO	2.4
1	B	820	PRO	2.4
1	A	724	ALA	2.4
1	A	1035	SER	2.4
1	B	594	ILE	2.4
1	A	727	LEU	2.4
1	A	755	MET	2.3
1	B	641	PHE	2.3
1	B	569	LEU	2.3
1	B	596	LEU	2.3
1	A	949	ILE	2.3
1	B	565	ILE	2.3
1	B	785	VAL	2.3
1	B	840	PHE	2.3
1	B	1085	GLN	2.3
1	A	820	PRO	2.3
1	B	578	VAL	2.3
1	A	1033	ASP	2.2
1	A	932	TYR	2.2
1	A	1093	ARG	2.2
1	B	926	MET	2.2
1	A	835	LEU	2.2
1	A	539	PHE	2.2
1	A	543	ALA	2.2
1	A	1083	VAL	2.1
1	A	742	GLY	2.1
1	A	743	LYS	2.1
1	B	1058	VAL	2.1
1	A	1036	GLY	2.1
1	B	557	PHE	2.1
1	B	1093	ARG	2.1
1	B	786	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	823	ILE	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
4	ORN	A	1204	9/9	0.57	0.14	111,139,148,150	0
7	I8P	B	1210	44/44	0.63	0.12	102,125,189,224	0
5	PUT	B	1203	6/6	0.65	0.17	90,114,120,120	0
8	1JW	B	1204	9/9	0.70	0.20	74,100,121,125	0
3	SPM	A	1203	14/14	0.74	0.19	86,113,127,134	0
6	EDO	A	1208	4/4	0.77	0.17	104,125,132,132	0
5	PUT	A	1218	6/6	0.78	0.21	97,119,142,142	0
6	EDO	A	1216	4/4	0.81	0.24	67,87,103,105	0
5	PUT	A	1212	6/6	0.82	0.16	84,110,128,128	0
6	EDO	A	1213	4/4	0.83	0.17	75,90,105,105	0
6	EDO	A	1209	4/4	0.83	0.17	74,90,102,104	0
6	EDO	B	1209	4/4	0.84	0.17	80,96,106,108	0
3	SPM	A	1202	14/14	0.84	0.16	94,118,135,139	0
6	EDO	B	1206	4/4	0.84	0.14	90,108,119,124	0
6	EDO	A	1210	4/4	0.85	0.14	68,86,91,104	0
7	I8P	A	1215	44/44	0.85	0.10	66,89,122,170	0
8	1JW	B	1202	9/9	0.87	0.13	86,104,119,123	0
6	EDO	A	1217	4/4	0.87	0.15	72,87,91,100	0
6	EDO	A	1211	4/4	0.88	0.17	69,84,97,97	0
6	EDO	B	1205	4/4	0.88	0.23	80,97,107,107	0
6	EDO	B	1207	4/4	0.89	0.15	73,88,99,103	0
6	EDO	A	1207	4/4	0.89	0.17	71,90,108,108	0

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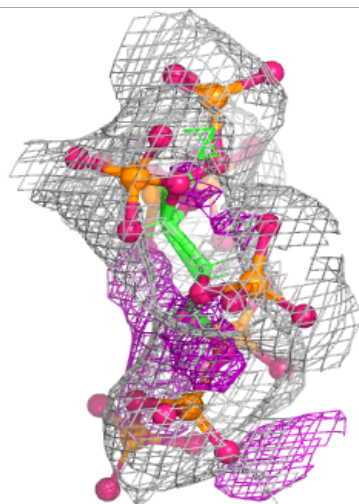
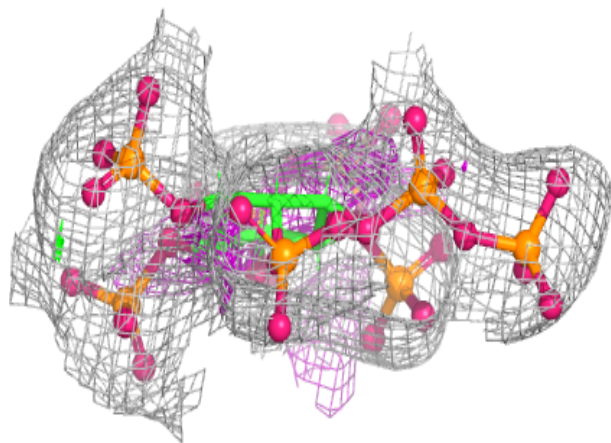
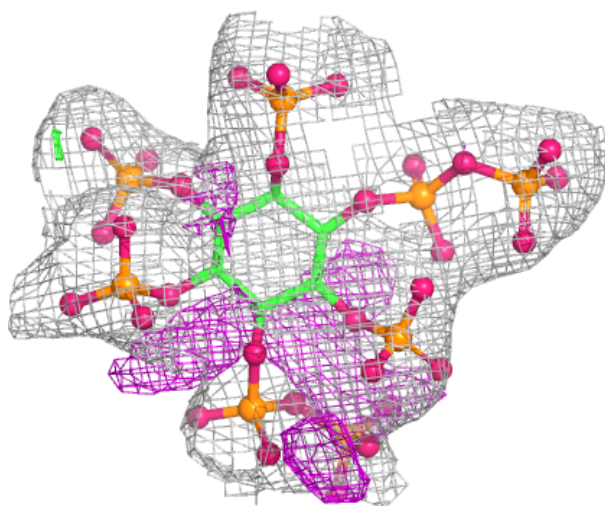
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PUT	A	1206	6/6	0.90	0.19	79,97,106,106	0
6	EDO	B	1212	4/4	0.90	0.15	80,96,104,112	0
6	EDO	B	1211	4/4	0.91	0.19	104,125,128,128	0
5	PUT	B	1208	6/6	0.92	0.12	69,84,102,102	0
6	EDO	A	1214	4/4	0.92	0.21	71,86,87,103	0
5	PUT	A	1205	6/6	0.93	0.14	76,94,111,111	0
2	ZN	B	1201	1/1	0.98	0.04	58,58,58,58	0
2	ZN	A	1201	1/1	0.99	0.08	61,61,61,61	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.

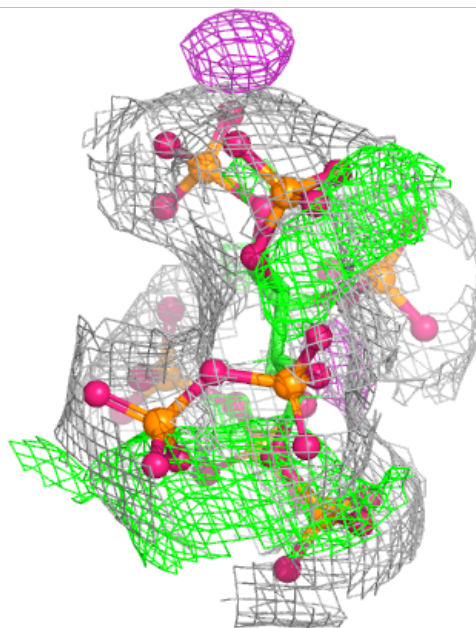
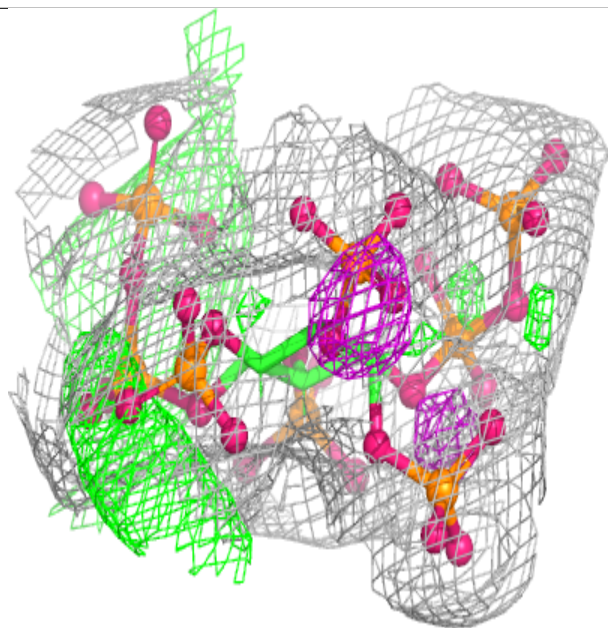
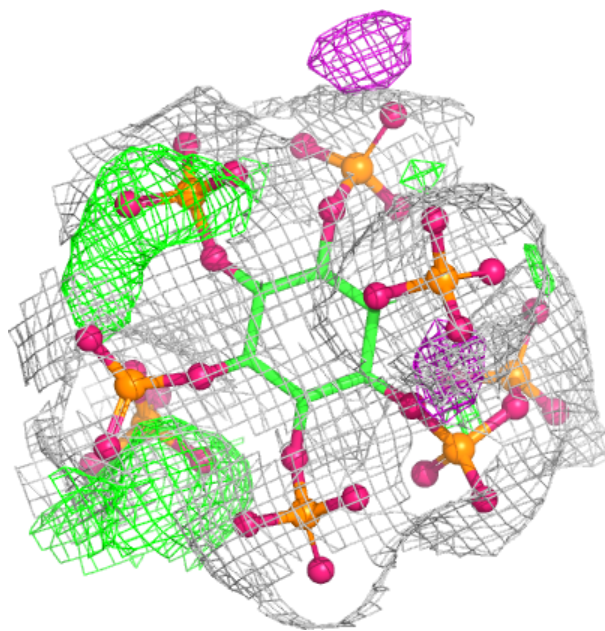
Electron density around I8P B 1210:

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



Electron density around I8P A 1215:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.