



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:07 PM UTC

PDB ID : 4G61 / pdb_00004g61
Title : Crystal structure of IMPase/NADP phosphatase complexed with Mg²⁺ and phosphate
Authors : Bhattacharyya, S.; Dutta, D.; Ghosh, A.K.; Das, A.K.
Deposited on : 2012-07-18
Resolution : 2.30 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

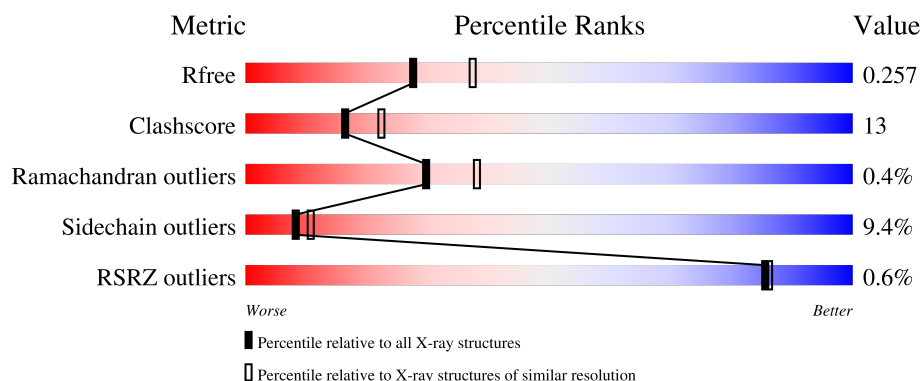
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	271	 74% 21% . .
1	B	271	 % 76% 17% . . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	308	-	-	X	-
6	DTO	B	307[A]	-	X	X	-
6	DTO	B	307[B]	-	-	X	-
7	P33	B	309	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4548 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 Inositol monophosphatase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	2	0
			2118	1363	350	392	13			
1	B	261	Total	C	N	O	S	0	1	0
			2086	1346	345	381	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q6G709
A	-4	HIS	-	expression tag	UNP Q6G709
A	-3	HIS	-	expression tag	UNP Q6G709
A	-2	HIS	-	expression tag	UNP Q6G709
A	-1	HIS	-	expression tag	UNP Q6G709
A	0	HIS	-	expression tag	UNP Q6G709
B	-5	HIS	-	expression tag	UNP Q6G709
B	-4	HIS	-	expression tag	UNP Q6G709
B	-3	HIS	-	expression tag	UNP Q6G709
B	-2	HIS	-	expression tag	UNP Q6G709
B	-1	HIS	-	expression tag	UNP Q6G709
B	0	HIS	-	expression tag	UNP Q6G709

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mg	0	0
			3	3		
2	B	3	Total	Mg	0	0
			3	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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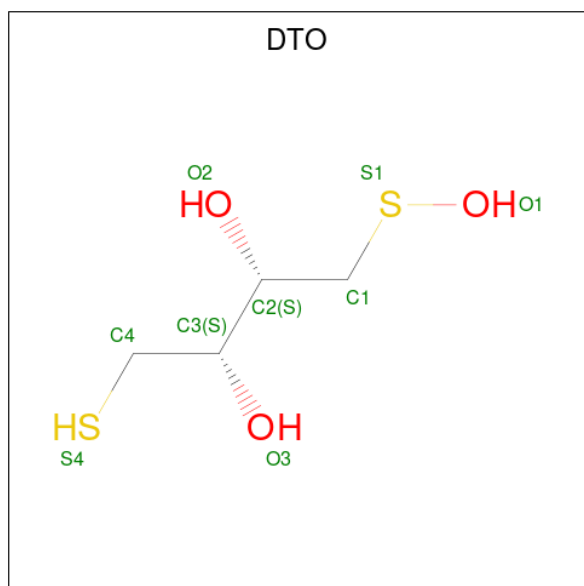
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

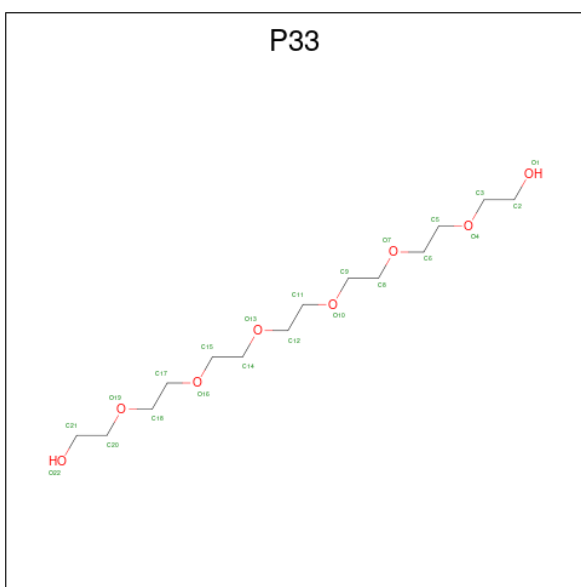
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is 1-HYDROXYSULFANYL-4-MERCAPTO-BUTANE-2,3-DIOL (CCD ID: DTO) (formula: C₄H₁₀O₃S₂).



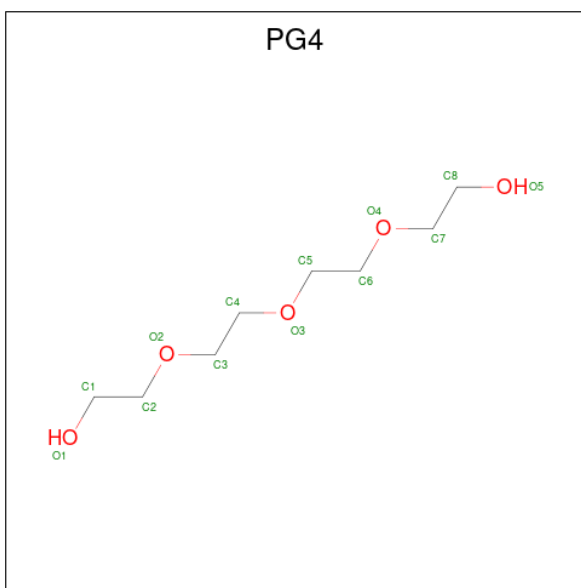
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	S	0	1
			16	8	4	4		

- Molecule 7 is 3,6,9,12,15,18-HEXA-OXAICOSANE-1,20-DIOL (CCD ID: P33) (formula: C₁₄H₃₀O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			22	14	8		

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			13	8	5		

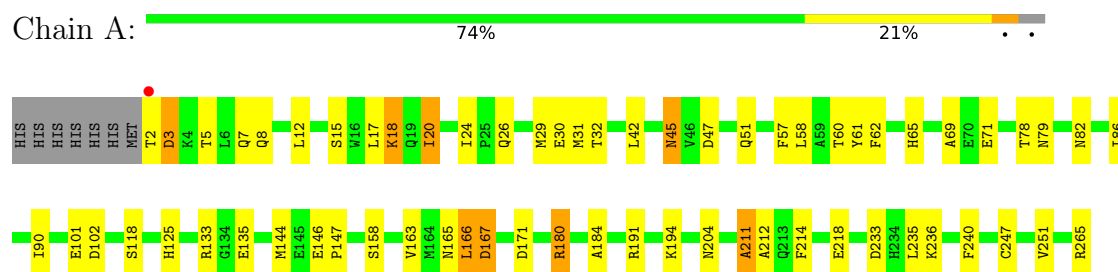
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	148	Total 148	O 148	0	0
9	B	103	Total 103	O 103	0	0

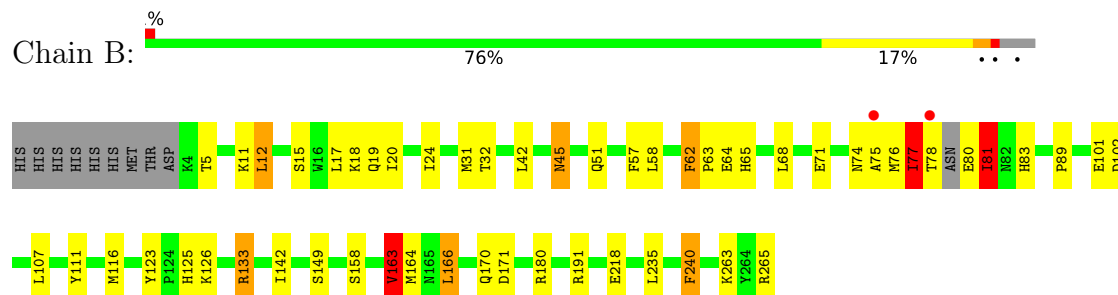
3 Residue-property plots

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: Inositol monophosphatase family protein



- Molecule 1: Inositol monophosphatase family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	60.71Å 63.05Å 141.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.67 – 2.30 19.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.67-2.30) 98.2 (19.67-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 2.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.176 , 0.255 0.176 , 0.257	Depositor DCC
R_{free} test set	1235 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4548	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% 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: PO4, P33, CL, DTO, GOL, PG4, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.09	3/2170 (0.1%)	1.10	6/2935 (0.2%)
1	B	1.11	4/2131 (0.2%)	1.13	9/2881 (0.3%)
All	All	1.10	7/4301 (0.2%)	1.12	15/5816 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	20	ILE	CA-CB	6.05	1.62	1.54
1	B	24	ILE	CA-C	5.64	1.57	1.52
1	B	76	MET	N-CA	5.52	1.52	1.46
1	A	147	PRO	CA-C	5.47	1.55	1.52
1	B	123	TYR	N-CA	-5.30	1.42	1.46
1	A	214	PHE	N-CA	5.25	1.52	1.46
1	A	163	VAL	CA-CB	5.19	1.60	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ILE	N-CA-C	7.87	125.71	109.34
1	A	180	ARG	NE-CZ-NH2	-6.38	113.45	119.20
1	A	146	GLU	CA-C-N	6.16	124.09	119.66
1	A	146	GLU	C-N-CA	6.16	124.09	119.66
1	B	81	ILE	N-CA-C	6.15	116.99	109.30
1	B	62	PHE	CA-C-N	-5.72	113.77	120.12
1	B	62	PHE	C-N-CA	-5.72	113.77	120.12
1	A	211	ALA	N-CA-C	5.66	118.17	111.33
1	B	180	ARG	NE-CZ-NH2	-5.60	114.16	119.20
1	B	76	MET	N-CA-C	5.53	116.67	108.60
1	B	180	ARG	CG-CD-NE	-5.43	100.06	112.00
1	B	133	ARG	NE-CZ-NH2	-5.37	114.37	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	LYS	CA-C-N	-5.22	115.14	120.10
1	A	236	LYS	C-N-CA	-5.22	115.14	120.10
1	B	163	VAL	N-CA-CB	-5.16	105.61	112.26

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	2118	0	2099	60	0
1	B	2086	0	2061	47	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
4	A	12	0	16	4	0
4	B	12	0	16	6	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	16	0	18	19	0
7	B	22	0	30	14	0
8	B	13	0	18	4	0
9	A	148	0	0	7	0
9	B	103	0	0	3	0
All	All	4548	0	4258	111	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 13.

All (111) 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:64:GLU:HB2	7:B:309:P33:H92	1.42	0.98
1:A:171:ASP:OD1	4:A:307:GOL:H11	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:PHE:O	1:A:61:TYR:HD2	1.46	0.97
1:B:63:PRO:HD2	7:B:309:P33:H111	1.48	0.96
1:A:191:ARG:NH2	6:B:307[B]:DTO:H42	1.82	0.92
1:A:125:HIS:CE1	6:B:307[A]:DTO:H11	2.08	0.88
1:A:184:ALA:HA	4:A:305:GOL:H12	1.62	0.81
1:A:60:THR:HB	1:A:61:TYR:CD2	2.17	0.80
1:A:31:MET:HA	1:A:45:ASN:HD21	1.48	0.79
1:A:51:GLN:HE22	1:A:71:GLU:H	1.29	0.79
1:B:171:ASP:OD1	4:B:308:GOL:C3	2.31	0.78
1:A:57:PHE:O	1:A:61:TYR:CD2	2.36	0.75
1:A:60:THR:HB	1:A:61:TYR:CE2	2.20	0.75
1:A:60:THR:HA	9:A:428:HOH:O	1.85	0.75
1:B:133:ARG:NH2	1:B:218:GLU:OE2	2.21	0.74
1:A:167:ASP:OD1	4:A:307:GOL:H32	1.88	0.73
1:B:51:GLN:HE22	1:B:71:GLU:H	1.34	0.73
1:A:5:THR:H	1:A:8:GLN:HE21	1.37	0.71
1:A:102:ASP:OD1	6:B:307[A]:DTO:S1	2.50	0.69
1:A:194:LYS:HB3	8:B:310:PG4:H52	1.75	0.69
1:A:165[A]:ASN:ND2	1:A:167:ASP:HB2	2.08	0.69
1:A:191:ARG:HH22	6:B:307[B]:DTO:H42	1.58	0.68
1:B:125:HIS:CE1	6:B:307[B]:DTO:S1	2.90	0.65
1:B:101:GLU:OE2	6:B:307[A]:DTO:O3	2.15	0.64
1:B:68:LEU:HD12	1:B:74:ASN:HB3	1.80	0.64
1:B:45:ASN:H	1:B:45:ASN:HD22	1.46	0.64
1:A:133:ARG:NH2	1:A:218:GLU:OE2	2.28	0.64
1:B:81:ILE:HD12	1:B:81:ILE:H	1.63	0.62
1:B:77:ILE:HD12	1:B:80:GLU:HA	1.81	0.62
1:B:77:ILE:O	1:B:81:ILE:HD11	2.00	0.62
3:B:301:PO4:P	9:B:406:HOH:O	2.58	0.62
1:B:64:GLU:HB2	7:B:309:P33:C9	2.24	0.61
1:A:101:GLU:OE2	6:B:307[B]:DTO:H12	2.01	0.60
1:A:7[A]:GLN:OE1	1:A:135:GLU:OE2	2.19	0.60
1:B:62:PHE:HB3	1:B:65:HIS:CD2	2.37	0.59
1:B:171:ASP:OD1	4:B:308:GOL:C2	2.49	0.59
1:A:2:THR:O	1:A:3:ASP:HB2	2.03	0.58
1:A:32:THR:H	1:A:45:ASN:ND2	2.00	0.58
1:B:163:VAL:HG13	9:B:431:HOH:O	2.02	0.58
1:B:191:ARG:NH2	6:B:307[A]:DTO:S4	2.76	0.58
1:B:64:GLU:HG2	7:B:309:P33:H152	1.85	0.58
1:A:118:SER:HB3	1:A:212:ALA:HB1	1.87	0.56
1:A:60:THR:CA	9:A:428:HOH:O	2.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:MET:HA	8:B:310:PG4:H22	1.86	0.56
1:A:171:ASP:CG	4:A:307:GOL:H11	2.31	0.56
1:A:20:ILE:HG23	1:A:24:ILE:CD1	2.35	0.55
1:A:82:ASN:HB2	9:A:546:HOH:O	2.07	0.54
1:A:233:ASP:HB3	9:A:504:HOH:O	2.06	0.54
1:B:51:GLN:HE21	1:B:89:PRO:HG3	1.72	0.54
1:A:20:ILE:CG2	1:A:24:ILE:HD11	2.37	0.54
1:B:191:ARG:NH2	6:B:307[A]:DTO:S1	2.80	0.54
1:A:18:LYS:HE2	9:A:416:HOH:O	2.07	0.53
1:B:45:ASN:HD22	1:B:45:ASN:N	2.05	0.53
1:B:78:THR:C	1:B:80:GLU:CB	2.81	0.53
1:B:171:ASP:OD1	4:B:308:GOL:H31	2.07	0.53
1:A:165[A]:ASN:ND2	1:A:167:ASP:H	2.06	0.53
1:A:125:HIS:CE1	6:B:307[B]:DTO:O2	2.62	0.53
1:A:20:ILE:HG23	1:A:24:ILE:HD11	1.90	0.53
1:A:101:GLU:OE2	6:B:307[A]:DTO:S1	2.67	0.52
1:B:64:GLU:OE2	7:B:309:P33:H181	2.09	0.52
1:B:63:PRO:HB2	7:B:309:P33:H182	1.92	0.52
1:A:20:ILE:CG2	1:A:24:ILE:CD1	2.89	0.51
1:A:31:MET:HA	1:A:45:ASN:ND2	2.23	0.51
1:A:45:ASN:HD22	1:A:45:ASN:H	1.57	0.51
1:A:165[B]:ASN:HD22	1:A:167:ASP:H	1.58	0.51
1:A:5:THR:H	1:A:8:GLN:NE2	2.07	0.51
1:B:111:TYR:HB3	1:B:116:MET:HE3	1.95	0.49
3:A:303:PO4:P	9:A:403:HOH:O	2.71	0.49
1:A:204:ASN:ND2	9:A:525:HOH:O	2.33	0.49
1:A:62:PHE:HB3	1:A:65:HIS:CG	2.48	0.49
1:A:165[A]:ASN:HD22	1:A:167:ASP:H	1.61	0.48
1:A:51:GLN:NE2	1:A:69:ALA:HB1	2.28	0.48
7:B:309:P33:H22A	7:B:309:P33:H52	1.66	0.47
1:B:240:PHE:CD2	1:B:240:PHE:C	2.92	0.47
1:A:60:THR:CB	1:A:61:TYR:CE2	2.96	0.47
1:A:125:HIS:NE2	6:B:307[A]:DTO:H11	2.30	0.46
1:A:165[A]:ASN:HD21	1:A:167:ASP:HB2	1.79	0.46
1:B:164:MET:HE3	9:B:472:HOH:O	2.15	0.46
1:B:83:HIS:CE1	7:B:309:P33:H51	2.51	0.46
1:A:118:SER:HB3	1:A:212:ALA:CB	2.45	0.46
1:B:64:GLU:CB	7:B:309:P33:H92	2.30	0.46
1:B:65:HIS:HE2	7:B:309:P33:C5	2.29	0.45
1:A:194:LYS:HG2	8:B:310:PG4:H31	1.99	0.45
1:B:171:ASP:OD1	4:B:308:GOL:O3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165[A]:ASN:HD22	1:A:167:ASP:N	2.16	0.44
1:B:171:ASP:CG	4:B:308:GOL:H31	2.42	0.44
1:A:191:ARG:HH21	6:B:307[B]:DTO:H42	1.72	0.44
1:A:61:TYR:CD2	1:A:61:TYR:N	2.85	0.43
1:A:47:ASP:OD2	1:A:90:ILE:HB	2.19	0.43
1:B:63:PRO:HG2	7:B:309:P33:H122	2.00	0.43
1:B:45:ASN:N	1:B:45:ASN:ND2	2.67	0.42
1:B:31:MET:HA	1:B:45:ASN:HD21	1.84	0.42
8:B:310:PG4:H72	8:B:310:PG4:H51	1.47	0.42
1:A:26:GLN:O	1:A:30:GLU:HG2	2.20	0.42
1:A:191:ARG:HH22	6:B:307[B]:DTO:C4	2.27	0.42
1:B:65:HIS:HE2	7:B:309:P33:H51	1.85	0.42
1:A:166:LEU:HD12	1:A:166:LEU:HA	1.88	0.41
1:B:166:LEU:HD12	1:B:166:LEU:HA	1.95	0.41
1:A:191:ARG:HH22	6:B:307[A]:DTO:C4	2.33	0.41
1:A:86:ILE:HG21	1:A:211:ALA:HB2	2.02	0.41
1:B:171:ASP:OD2	4:B:308:GOL:H31	2.21	0.41
1:B:12:LEU:HB3	1:B:57:PHE:HZ	1.84	0.41
1:A:247:CYS:O	1:A:251:VAL:HG23	2.21	0.41
1:B:102:ASP:OD1	6:B:307[A]:DTO:C4	2.69	0.41
1:B:63:PRO:HD2	7:B:309:P33:C11	2.34	0.40
1:B:64:GLU:HG2	7:B:309:P33:H121	2.03	0.40
1:B:101:GLU:OE2	6:B:307[B]:DTO:O3	2.39	0.40
1:A:191:ARG:HH22	6:B:307[A]:DTO:H42	1.86	0.40
1:B:62:PHE:HB3	1:B:65:HIS:CG	2.57	0.40
1:B:191:ARG:NH2	6:B:307[B]:DTO:S4	2.94	0.40
1:B:32:THR:H	1:B:45:ASN:ND2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	264/271 (97%)	258 (98%)	5 (2%)	1 (0%)	30	38
1	B	258/271 (95%)	253 (98%)	4 (2%)	1 (0%)	30	38
All	All	522/542 (96%)	511 (98%)	9 (2%)	2 (0%)	30	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	75	ALA
1	A	3	ASP

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	228/238 (96%)	210 (92%)	18 (8%)	11	15
1	B	221/238 (93%)	197 (89%)	24 (11%)	6	7
All	All	449/476 (94%)	407 (91%)	42 (9%)	8	11

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	15	SER
1	A	17	LEU
1	A	18	LYS
1	A	20	ILE
1	A	29	MET
1	A	42	LEU
1	A	45	ASN
1	A	58	LEU
1	A	78	THR
1	A	79	ASN
1	A	158	SER
1	A	166	LEU
1	A	167	ASP

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Mol	Chain	Res	Type
1	A	180	ARG
1	A	235	LEU
1	A	240	PHE
1	A	265	ARG
1	B	5	THR
1	B	11	LYS
1	B	12	LEU
1	B	15	SER
1	B	17	LEU
1	B	18	LYS
1	B	19	GLN
1	B	42	LEU
1	B	45	ASN
1	B	58	LEU
1	B	77	ILE
1	B	81	ILE
1	B	107	LEU
1	B	126	LYS
1	B	142	ILE
1	B	149	SER
1	B	158	SER
1	B	163	VAL
1	B	166	LEU
1	B	170	GLN
1	B	235	LEU
1	B	240	PHE
1	B	263	LYS
1	B	265	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	45	ASN
1	A	49	GLN
1	A	51	GLN
1	A	66	GLN
1	A	79	ASN
1	A	82	ASN
1	A	125	HIS
1	A	162	GLN
1	A	248	HIS

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Mol	Chain	Res	Type
1	B	45	ASN
1	B	51	GLN
1	B	53	GLN
1	B	82	ASN
1	B	125	HIS
1	B	162	GLN
1	B	170	GLN
1	B	248	HIS

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 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	$\# Z > 2$
3	PO4	B	301	2	4,4,4	1.26	0	6,6,6	1.25	2 (33%)
7	P33	B	309	-	21,21,21	0.83	0	20,20,20	0.63	0
3	PO4	A	303	2	4,4,4	1.55	0	6,6,6	1.13	0
8	PG4	B	310	-	12,12,12	1.01	0	11,11,11	0.62	0
4	GOL	A	305	-	5,5,5	0.48	0	5,5,5	1.22	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	305	-	5,5,5	0.24	0	5,5,5	0.80	0
6	DTO	B	307[B]	-	7,7,8	0.60	0	4,8,9	1.08	1 (25%)
4	GOL	B	308	-	5,5,5	0.28	0	5,5,5	0.81	0
4	GOL	A	307	-	5,5,5	0.60	0	5,5,5	0.76	0
6	DTO	B	307[A]	-	7,7,8	0.54	0	4,8,9	2.06	2 (50%)

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
7	P33	B	309	-	-	11/19/19/19	-
8	PG4	B	310	-	-	7/10/10/10	-
4	GOL	A	305	-	-	2/4/4/4	-
4	GOL	B	305	-	-	0/4/4/4	-
6	DTO	B	307[B]	-	-	8/8/8/9	-
4	GOL	B	308	-	-	4/4/4/4	-
4	GOL	A	307	-	-	4/4/4/4	-
6	DTO	B	307[A]	-	-	8/8/8/9	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	307[A]	DTO	O2-C2-C3	2.76	115.37	109.57
6	B	307[A]	DTO	C2-C1-S1	-2.63	107.10	114.43
4	A	305	GOL	O3-C3-C2	-2.49	99.15	110.38
3	B	301	PO4	O4-P-O1	-2.12	103.46	110.95
3	B	301	PO4	O4-P-O2	2.11	114.48	107.91
6	B	307[B]	DTO	C3-C4-S4	-2.02	108.79	114.43

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	307	GOL	O1-C1-C2-O2
4	B	308	GOL	C1-C2-C3-O3
6	B	307[A]	DTO	S1-C1-C2-O2

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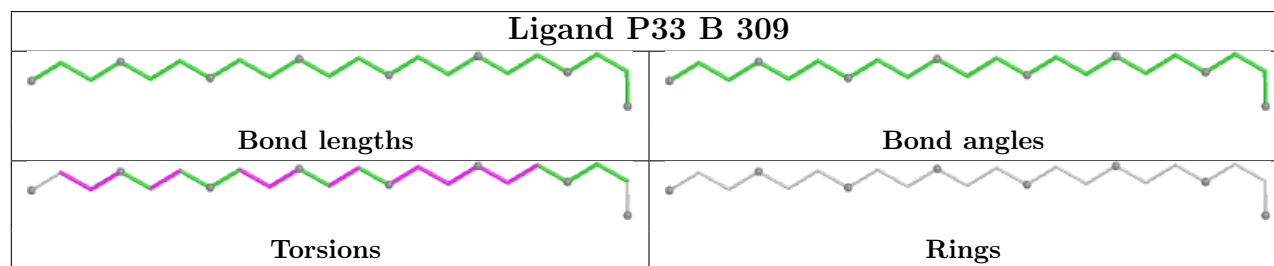
Mol	Chain	Res	Type	Atoms
6	B	307[A]	DTO	S1-C1-C2-C3
6	B	307[A]	DTO	C1-C2-C3-O3
6	B	307[A]	DTO	C1-C2-C3-C4
6	B	307[A]	DTO	O2-C2-C3-O3
6	B	307[A]	DTO	O2-C2-C3-C4
6	B	307[A]	DTO	C2-C3-C4-S4
6	B	307[A]	DTO	O3-C3-C4-S4
6	B	307[B]	DTO	S1-C1-C2-O2
6	B	307[B]	DTO	S1-C1-C2-C3
6	B	307[B]	DTO	C1-C2-C3-O3
6	B	307[B]	DTO	C1-C2-C3-C4
6	B	307[B]	DTO	O2-C2-C3-C4
6	B	307[B]	DTO	C2-C3-C4-S4
6	B	307[B]	DTO	O3-C3-C4-S4
8	B	310	PG4	C5-C6-O4-C7
7	B	309	P33	C2-C3-O4-C5
7	B	309	P33	C18-C17-O16-C15
7	B	309	P33	O13-C14-C15-O16
7	B	309	P33	O4-C5-C6-O7
8	B	310	PG4	O3-C5-C6-O4
7	B	309	P33	O7-C8-C9-O10
7	B	309	P33	O16-C17-C18-O19
8	B	310	PG4	O2-C3-C4-O3
4	A	305	GOL	O1-C1-C2-C3
4	A	307	GOL	O1-C1-C2-C3
4	A	307	GOL	C1-C2-C3-O3
4	B	308	GOL	O1-C1-C2-C3
8	B	310	PG4	O4-C7-C8-O5
4	B	308	GOL	O2-C2-C3-O3
7	B	309	P33	C15-C14-O13-C12
7	B	309	P33	O10-C11-C12-O13
6	B	307[B]	DTO	O2-C2-C3-O3
7	B	309	P33	O1-C2-C3-O4
4	A	305	GOL	O1-C1-C2-O2
8	B	310	PG4	C3-C4-O3-C5
7	B	309	P33	C14-C15-O16-C17
7	B	309	P33	C8-C9-O10-C11
8	B	310	PG4	C4-C3-O2-C2
8	B	310	PG4	C8-C7-O4-C6
4	B	308	GOL	O1-C1-C2-O2
4	A	307	GOL	O2-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	PO4	1	0
7	B	309	P33	14	0
3	A	303	PO4	1	0
8	B	310	PG4	4	0
4	A	305	GOL	1	0
6	B	307[B]	DTO	9	0
4	B	308	GOL	6	0
4	A	307	GOL	3	0
6	B	307[A]	DTO	10	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	264/271 (97%)	-0.61	1 (0%) 88 89	7, 19, 35, 51	2 (0%)
1	B	261/271 (96%)	-0.55	2 (0%) 82 83	9, 21, 39, 65	1 (0%)
All	All	525/542 (96%)	-0.58	3 (0%) 85 86	7, 20, 37, 65	3 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	78	THR	3.1
1	A	2	THR	2.6
1	B	75	ALA	2.4

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
7	P33	B	309	22/22	0.62	0.22	70,76,78,78	0
8	PG4	B	310	13/13	0.68	0.21	45,58,63,63	0

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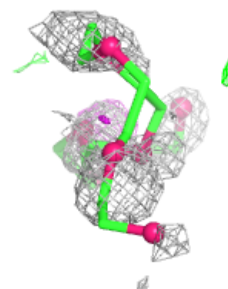
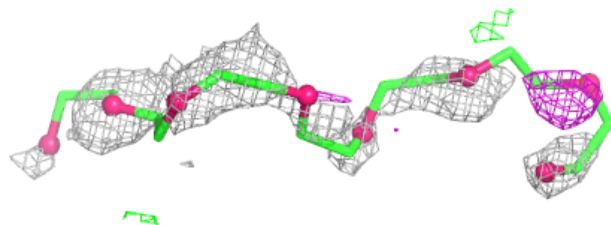
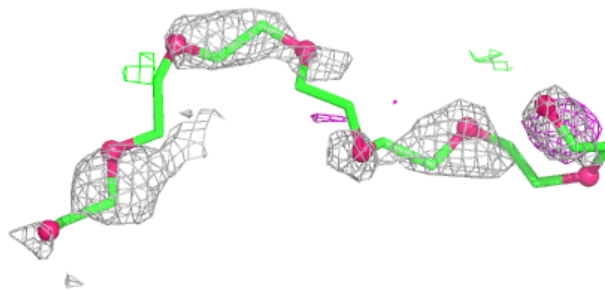
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	307	6/6	0.84	0.12	40,43,44,44	0
4	GOL	B	308	6/6	0.85	0.09	29,31,33,33	0
6	DTO	B	307[A]	8/9	0.86	0.12	19,22,27,34	8
6	DTO	B	307[B]	8/9	0.86	0.12	41,45,45,48	8
4	GOL	B	305	6/6	0.89	0.12	28,38,38,39	0
4	GOL	A	305	6/6	0.89	0.12	33,35,37,40	0
5	CL	A	306	1/1	0.98	0.04	22,22,22,22	0
2	MG	A	301	1/1	0.98	0.06	22,22,22,22	0
2	MG	A	304	1/1	0.98	0.03	16,16,16,16	0
3	PO4	A	303	5/5	0.98	0.05	14,15,19,20	0
3	PO4	B	301	5/5	0.98	0.04	20,22,24,25	0
5	CL	B	306	1/1	0.99	0.03	22,22,22,22	0
2	MG	B	304	1/1	0.99	0.06	22,22,22,22	0
2	MG	A	302	1/1	0.99	0.02	15,15,15,15	0
2	MG	B	302	1/1	0.99	0.02	24,24,24,24	0
2	MG	B	303	1/1	0.99	0.02	19,19,19,19	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 P33 B 309:

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.