



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:03 PM UTC

PDB ID : 6B2F / pdb_00006b2f
Title : Phosphotriesterase variant S5 + TS analogue
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Deposited on : 2017-09-20
Resolution : 1.77 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

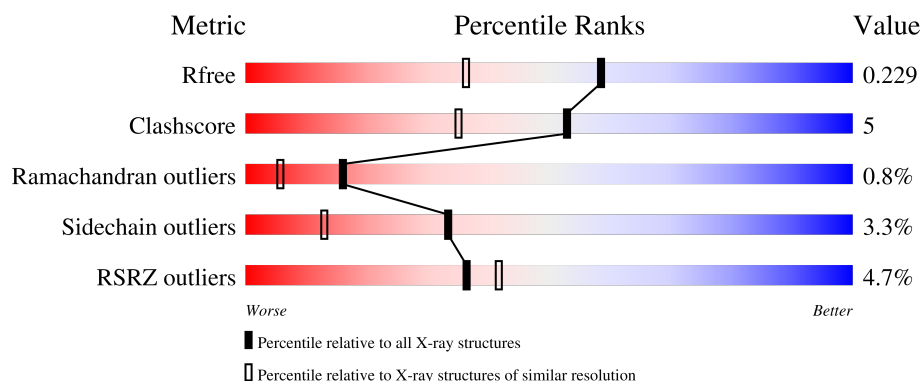
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	333	 4% 83% 11% .. 5%
1	G	333	 5% 84% 12% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5427 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 Phosphotriesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	12	0
			2530	1591	467	466	6			
1	G	326	Total	C	N	O	S	0	5	0
			2530	1592	460	472	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	216	LEU	PHE	conflict	UNP A0A060GYS1
A	233	ALA	ASP	conflict	UNP A0A060GYS1
A	254	SER	HIS	conflict	UNP A0A060GYS1
A	271	HIS	LEU	conflict	UNP A0A060GYS1
A	293	THR	MET	conflict	UNP A0A060GYS1
A	306	ILE	PHE	conflict	UNP A0A060GYS1
A	320	GLY	VAL	conflict	UNP A0A060GYS1
G	216	LEU	PHE	conflict	UNP A0A060GYS1
G	233	ALA	ASP	conflict	UNP A0A060GYS1
G	254	SER	HIS	conflict	UNP A0A060GYS1
G	271	HIS	LEU	conflict	UNP A0A060GYS1
G	293	THR	MET	conflict	UNP A0A060GYS1
G	306	ILE	PHE	conflict	UNP A0A060GYS1
G	320	GLY	VAL	conflict	UNP A0A060GYS1

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

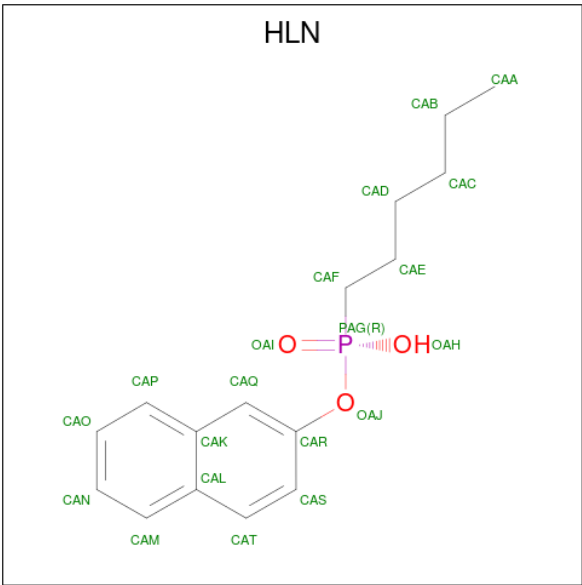
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	G	2	Total	Zn	0	0
			2	2		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is hexyl(naphthalen-2-yloxy)phosphinic acid (CCD ID: HLN) (formula: $C_{16}H_{21}O_3P$) (labeled as "Ligand of Interest" by depositor).

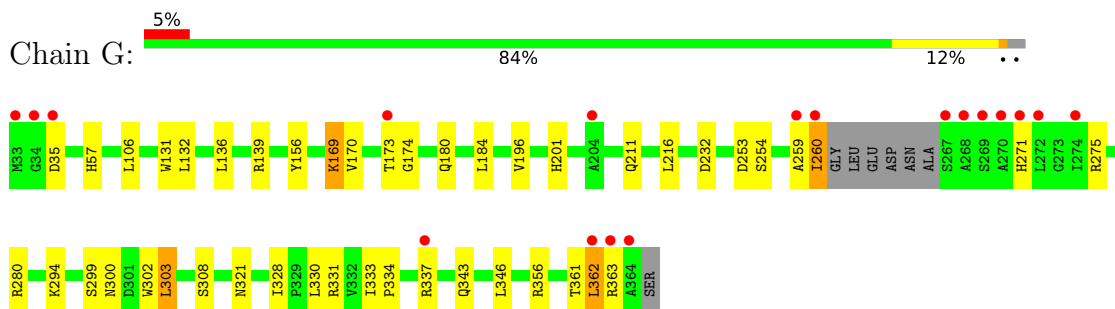


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			20	16	3	1		
4	G	1	Total	C	O	P	0	0
			20	16	3	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	131	Total	O	0	0
			131	131		
5	G	144	Total	O	0	0
			144	144		

- Molecule 1: Phosphotriesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.66Å 85.02Å 87.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.56 – 1.77 30.56 – 1.77	Depositor EDS
% Data completeness (in resolution range)	97.8 (30.56-1.77) 97.8 (30.56-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 1.77Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.196 , 0.230 0.196 , 0.229	Depositor DCC
R_{free} test set	3058 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.027 for -h,l,k 0.029 for -l,-k,-h 0.025 for k,h,-l 0.013 for k,l,h 0.013 for l,h,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5427	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: ZN, MPD, HLN, KCX

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	0.32	0/2560	0.60	4/3469 (0.1%)
1	G	0.31	0/2561	0.56	0/3474
All	All	0.31	0/5121	0.58	4/6943 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	THR	CA-C-N	8.24	136.53	121.70
1	A	361	THR	C-N-CA	8.24	136.53	121.70
1	A	362	LEU	CA-C-N	6.73	133.82	121.70
1	A	362	LEU	C-N-CA	6.73	133.82	121.70

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	2530	0	2565	26	0
1	G	2530	0	2558	23	1
2	A	2	0	0	0	0
2	G	2	0	0	0	0
3	A	32	0	56	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	16	0	28	2	0
4	A	20	0	20	0	0
4	G	20	0	20	0	0
5	A	131	0	0	3	0
5	G	144	0	0	2	0
All	All	5427	0	5247	52	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 5.

All (52) 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:314:MET:SD	5:A:2521:HOH:O	2.33	0.85
1:A:207[A]:ARG:NH1	1:A:236:ASP:OD2	2.16	0.78
1:A:118[A]:ARG:NH1	5:A:2504:HOH:O	2.29	0.66
1:A:288:ILE:HG12	1:A:293:THR:HG22	1.79	0.64
3:A:2407:MPD:O4	3:A:2407:MPD:O2	2.17	0.61
1:A:225:ARG:HD2	1:A:361:THR:O	2.01	0.60
1:A:88:ARG:NH1	1:A:119:ALA:O	2.36	0.59
1:G:131:TRP:CG	1:G:132:LEU:H	2.21	0.57
1:A:131:TRP:CG	1:A:132:LEU:H	2.23	0.57
1:A:288:ILE:HA	1:A:293:THR:HG22	1.90	0.54
3:A:2407:MPD:HM1	3:A:2407:MPD:H53	1.92	0.51
3:A:2406:MPD:O4	3:A:2406:MPD:O2	2.27	0.50
1:G:361:THR:O	1:G:362:LEU:HB2	2.10	0.50
1:A:136[B]:LEU:HD23	1:G:308:SER:HB3	1.94	0.49
1:A:206:GLN:O	1:A:207[B]:ARG:HG2	2.12	0.49
1:G:259:ALA:O	1:G:260:ILE:HB	2.11	0.49
1:G:169:KCX:OQ2	1:G:201:HIS:HB2	2.12	0.49
1:A:258:SER:OG	1:A:280:ARG:NE	2.46	0.49
3:G:2405:MPD:O2	3:G:2405:MPD:O4	2.23	0.48
1:G:136:LEU:HD13	1:G:139:ARG:NH2	2.29	0.48
1:A:59:CYS:HB3	5:A:2600:HOH:O	2.13	0.48
1:A:344:GLU:CD	1:A:344:GLU:H	2.22	0.48
1:A:144:GLU:O	1:A:148[A]:GLN:HG2	2.13	0.47
1:G:57:HIS:O	1:G:303:LEU:HA	2.13	0.47
1:G:156:TYR:HB2	3:G:2405:MPD:O4	2.13	0.47
1:G:253:ASP:HB3	5:G:2622:HOH:O	2.13	0.47
1:A:293:THR:HA	1:A:296:ILE:HD12	1.96	0.46
1:A:148[B]:GLN:HE22	3:A:2405:MPD:H13	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ARG:HH22	3:A:2407:MPD:H11	1.81	0.46
1:G:337[A]:ARG:NH2	1:G:343:GLN:OE1	2.47	0.46
1:G:173:THR:HG23	1:G:180:GLN:HE22	1.81	0.46
1:A:51:PHE:C	1:A:51:PHE:HD1	2.24	0.45
1:A:51:PHE:C	1:A:51:PHE:CD1	2.94	0.45
1:G:170:VAL:HG21	1:G:184:LEU:HD23	1.98	0.45
1:G:232:ASP:OD2	1:G:280:ARG:NH1	2.47	0.45
1:G:174:GLY:O	1:G:211[A]:GLN:NE2	2.50	0.45
1:G:106:LEU:HD12	5:G:2519:HOH:O	2.16	0.45
1:G:333:ILE:HG23	1:G:346:LEU:HD13	1.99	0.45
1:A:135:PRO:O	1:A:139[A]:ARG:HG3	2.17	0.44
1:G:302:TRP:CH2	1:G:321:ASN:HB3	2.53	0.43
1:G:330:LEU:C	1:G:331:ARG:HD2	2.43	0.43
1:A:333:ILE:HB	1:A:334:PRO:HD3	2.01	0.43
1:G:333:ILE:HB	1:G:334:PRO:HD3	2.00	0.43
1:A:136[A]:LEU:HG	1:A:139[A]:ARG:NH2	2.34	0.43
1:A:57:HIS:O	1:A:303:LEU:HA	2.19	0.42
1:G:294:LYS:O	1:G:356[B]:ARG:NH2	2.52	0.42
1:G:300:ASN:OD1	1:G:328:ILE:HG12	2.19	0.42
1:A:361:THR:HA	1:A:362:LEU:CB	2.49	0.42
1:G:131:TRP:CG	1:G:132:LEU:N	2.88	0.42
1:A:57:HIS:HB2	1:A:303:LEU:HB3	2.03	0.41
1:A:302:TRP:CH2	1:A:321:ASN:HB3	2.56	0.41
1:G:356[B]:ARG:HB3	1:G:356[B]:ARG:NH1	2.36	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:G:271:HIS:O	1:G:280:ARG:NH2[2_555]	2.06	0.14

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	325/333 (98%)	313 (96%)	10 (3%)	2 (1%)	21	9
1	G	327/333 (98%)	313 (96%)	11 (3%)	3 (1%)	14	4
All	All	652/666 (98%)	626 (96%)	21 (3%)	5 (1%)	16	6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	275	ARG
1	G	362	LEU
1	A	362	LEU
1	A	363	ARG
1	G	363	ARG

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	264/264 (100%)	253 (96%)	11 (4%)	26	7
1	G	264/264 (100%)	257 (97%)	7 (3%)	39	19
All	All	528/528 (100%)	510 (97%)	18 (3%)	33	12

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

Mol	Chain	Res	Type
1	A	35	ASP
1	A	46	ILE
1	A	51	PHE
1	A	202	THR
1	A	207[A]	ARG
1	A	207[B]	ARG
1	A	274	ILE
1	A	276	SER
1	A	299	SER

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Mol	Chain	Res	Type
1	A	303	LEU
1	A	361	THR
1	G	35	ASP
1	G	196	VAL
1	G	216	LEU
1	G	254	SER
1	G	260	ILE
1	G	299	SER
1	G	303	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	295	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
1	KCX	G	169	1,2	10,11,12	1.23	2 (20%)	6,12,14	1.63	2 (33%)
1	KCX	A	169	1,2	10,11,12	1.27	1 (10%)	6,12,14	1.12	1 (16%)

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
1	KCX	G	169	1,2	-	1/9/10/12	-
1	KCX	A	169	1,2	-	2/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	KCX	CE-NZ	2.93	1.52	1.46
1	G	169	KCX	OQ1-CX	2.71	1.26	1.21
1	G	169	KCX	CE-NZ	2.14	1.51	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	169	KCX	OQ1-CX-NZ	-3.32	119.87	124.92
1	A	169	KCX	OQ1-CX-NZ	-2.60	120.98	124.92
1	G	169	KCX	CE-NZ-CX	-2.06	118.49	121.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	169	KCX	C-CA-CB-CG
1	A	169	KCX	O-C-CA-CB
1	G	169	KCX	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	169	KCX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	MPD	A	2403	-	7,7,7	0.70	0	9,10,10	0.36	0
3	MPD	A	2405	-	7,7,7	0.72	0	9,10,10	0.39	0
3	MPD	A	2406	-	7,7,7	0.69	0	9,10,10	0.54	0
3	MPD	G	2403	-	7,7,7	0.78	0	9,10,10	0.40	0
3	MPD	G	2405	-	7,7,7	0.74	0	9,10,10	0.29	0
4	HLN	G	2404	2	21,21,21	2.18	3 (14%)	25,28,28	1.02	1 (4%)
3	MPD	A	2407	-	7,7,7	0.68	0	9,10,10	0.58	0
4	HLN	A	2404	2	21,21,21	2.08	2 (9%)	25,28,28	1.33	2 (8%)

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
3	MPD	A	2403	-	-	3/5/5/5	-
3	MPD	A	2405	-	-	0/5/5/5	-
3	MPD	A	2406	-	-	4/5/5/5	-
3	MPD	G	2403	-	-	3/5/5/5	-
3	MPD	G	2405	-	-	3/5/5/5	-
4	HLN	G	2404	2	-	9/12/12/12	0/2/2/2
3	MPD	A	2407	-	-	4/5/5/5	-
4	HLN	A	2404	2	-	4/12/12/12	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2404	HLN	PAG-OAJ	7.81	1.66	1.58
4	A	2404	HLN	PAG-OAJ	7.28	1.66	1.58
4	A	2404	HLN	PAG-CAF	4.88	1.87	1.80
4	G	2404	HLN	PAG-CAF	4.55	1.86	1.80
4	G	2404	HLN	PAG-OAH	-2.36	1.50	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2404	HLN	OAJ-PAG-OAI	-4.64	102.79	113.52
4	G	2404	HLN	CAD-CAE-CAF	-3.00	106.32	112.61
4	A	2404	HLN	OAH-PAG-CAF	2.77	112.07	105.54

There are no chirality outliers.

All (30) torsion outliers are listed below:

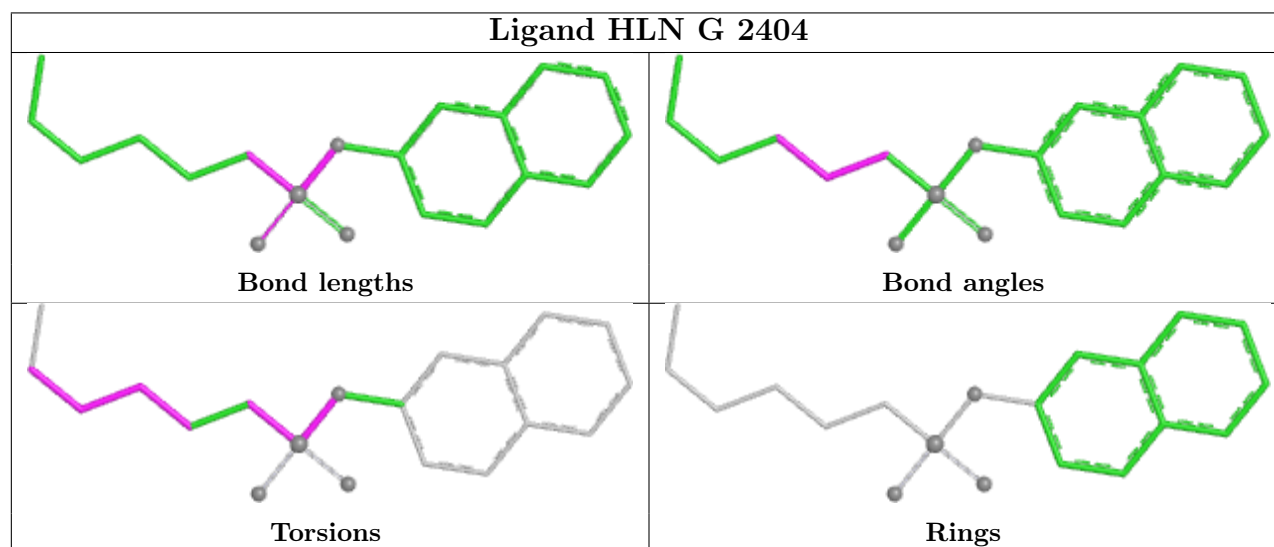
Mol	Chain	Res	Type	Atoms
3	A	2406	MPD	C2-C3-C4-C5
3	A	2407	MPD	C2-C3-C4-C5
4	A	2404	HLN	CAR-OAJ-PAG-CAF
4	G	2404	HLN	CAE-CAF-PAG-OAH
4	G	2404	HLN	CAE-CAF-PAG-OAI
4	G	2404	HLN	CAE-CAF-PAG-OAJ
4	G	2404	HLN	CAR-OAJ-PAG-OAH
4	G	2404	HLN	CAR-OAJ-PAG-OAI
4	A	2404	HLN	CAR-OAJ-PAG-OAI
4	G	2404	HLN	CAB-CAC-CAD-CAE
4	A	2404	HLN	CAD-CAE-CAF-PAG
4	A	2404	HLN	CAA-CAB-CAC-CAD
4	G	2404	HLN	CAA-CAB-CAC-CAD
4	G	2404	HLN	CAC-CAD-CAE-CAF
3	A	2406	MPD	C1-C2-C3-C4
3	A	2403	MPD	O2-C2-C3-C4
3	A	2407	MPD	O2-C2-C3-C4
3	G	2403	MPD	O2-C2-C3-C4
3	G	2405	MPD	O2-C2-C3-C4
3	A	2406	MPD	C2-C3-C4-O4
3	A	2403	MPD	C1-C2-C3-C4
3	A	2403	MPD	CM-C2-C3-C4
3	A	2406	MPD	CM-C2-C3-C4
3	A	2407	MPD	C1-C2-C3-C4
3	A	2407	MPD	CM-C2-C3-C4
3	G	2403	MPD	C1-C2-C3-C4
3	G	2403	MPD	CM-C2-C3-C4
3	G	2405	MPD	C1-C2-C3-C4
3	G	2405	MPD	CM-C2-C3-C4
4	G	2404	HLN	CAR-OAJ-PAG-CAF

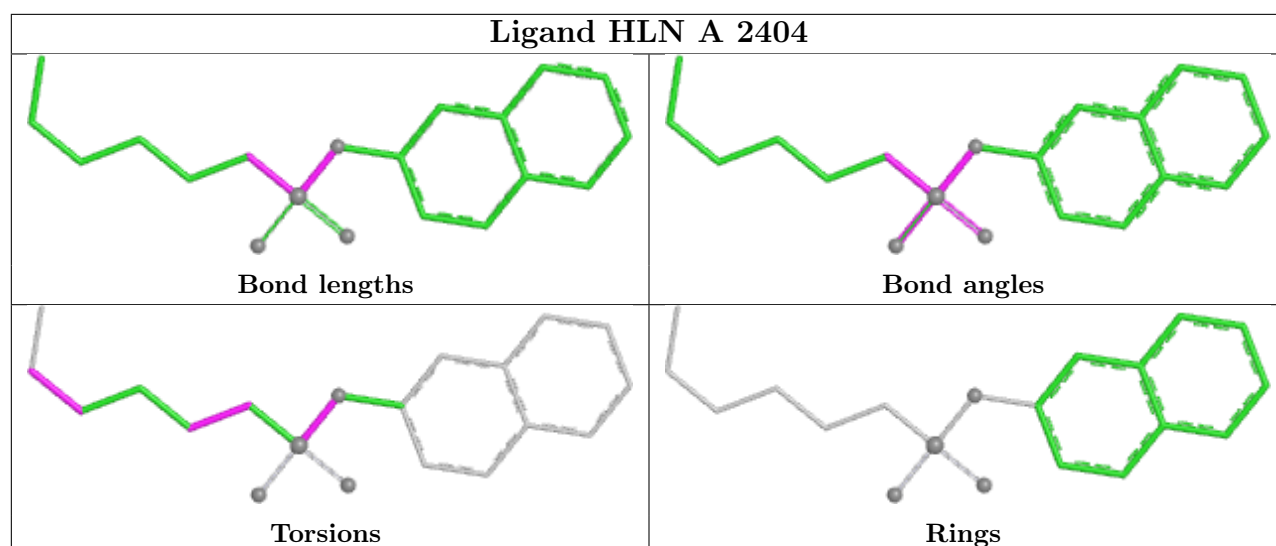
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2405	MPD	1	0
3	A	2406	MPD	1	0
3	G	2405	MPD	2	0
3	A	2407	MPD	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.





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	317/333 (95%)	-0.00	12 (3%)	44 50	9, 21, 41, 67	12 (3%)
1	G	325/333 (97%)	0.18	18 (5%)	30 36	9, 25, 50, 82	5 (1%)
All	All	642/666 (96%)	0.09	30 (4%)	36 42	9, 23, 46, 82	17 (2%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	270	ALA	8.8
1	A	274	ILE	7.5
1	G	274	ILE	6.5
1	G	268	ALA	5.6
1	G	33	MET	5.4
1	G	260	ILE	5.1
1	G	259	ALA	5.1
1	G	269	SER	5.0
1	G	364	ALA	4.9
1	G	362	LEU	4.3
1	G	267	SER	3.9
1	A	34	GLY	3.9
1	A	260	ILE	3.9
1	A	364	ALA	3.8
1	A	259	ALA	3.8
1	A	362	LEU	3.6
1	G	272	LEU	3.5
1	G	271	HIS	3.5
1	A	363	ARG	3.3
1	G	363	ARG	3.2
1	G	34	GLY	3.1
1	A	275	ARG	2.9
1	G	337[A]	ARG	2.7
1	A	174	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	361	THR	2.6
1	G	204	ALA	2.5
1	A	35	ASP	2.4
1	G	35	ASP	2.4
1	G	173	THR	2.3
1	A	202	THR	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KCX	G	169	12/13	0.93	0.07	15,18,25,28	0
1	KCX	A	169	12/13	0.96	0.06	13,15,20,21	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MPD	G	2403	8/8	0.52	0.24	39,40,43,44	0
3	MPD	A	2407	8/8	0.63	0.18	35,40,40,42	0
3	MPD	A	2405	8/8	0.68	0.18	41,44,45,46	0
3	MPD	A	2406	8/8	0.73	0.16	42,44,46,47	0
3	MPD	G	2405	8/8	0.76	0.16	47,50,51,52	0
3	MPD	A	2403	8/8	0.79	0.15	39,41,44,45	0
4	HLN	G	2404	20/20	0.87	0.16	24,47,62,62	0
4	HLN	A	2404	20/20	0.91	0.17	22,52,74,74	0
2	ZN	A	2401	1/1	1.00	0.01	16,16,16,16	0
2	ZN	A	2402	1/1	1.00	0.01	19,19,19,19	1

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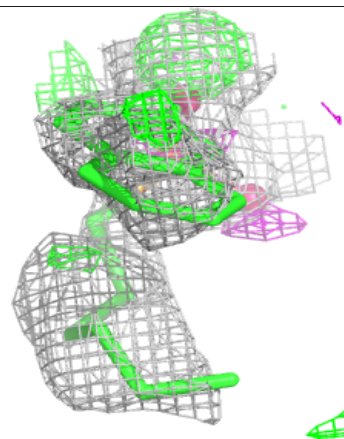
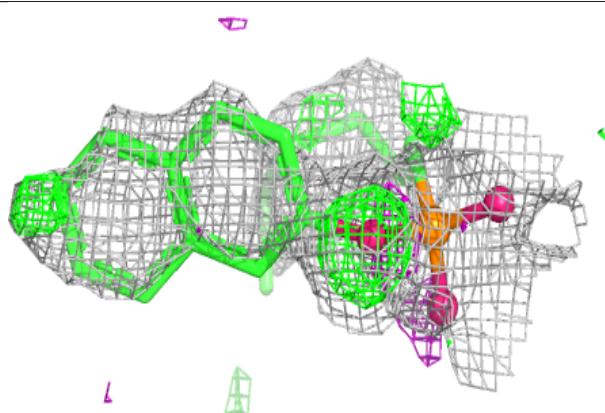
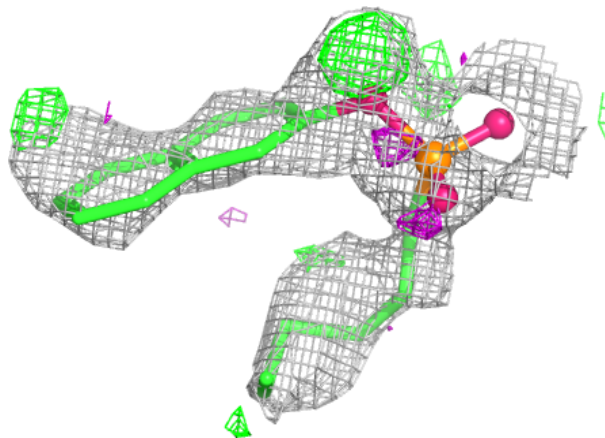
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	G	2401	1/1	1.00	0.01	16,16,16,16	1
2	ZN	G	2402	1/1	1.00	0.01	23,23,23,23	1

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.

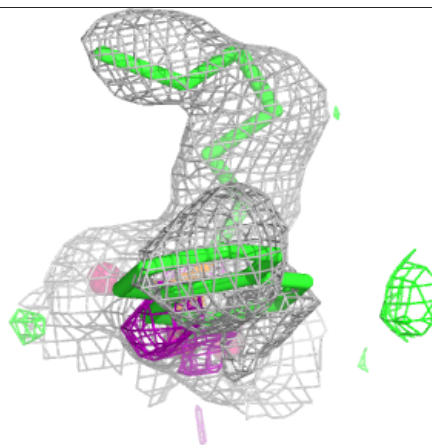
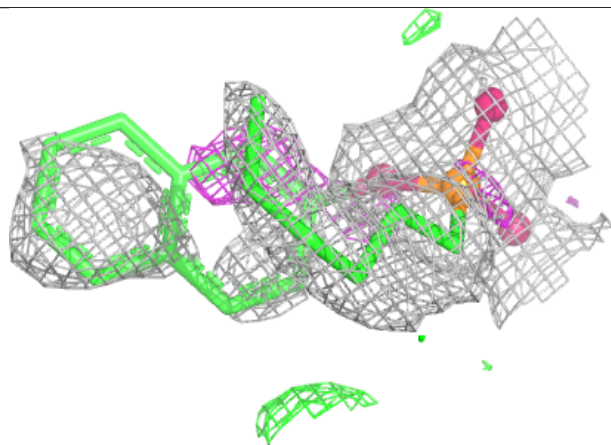
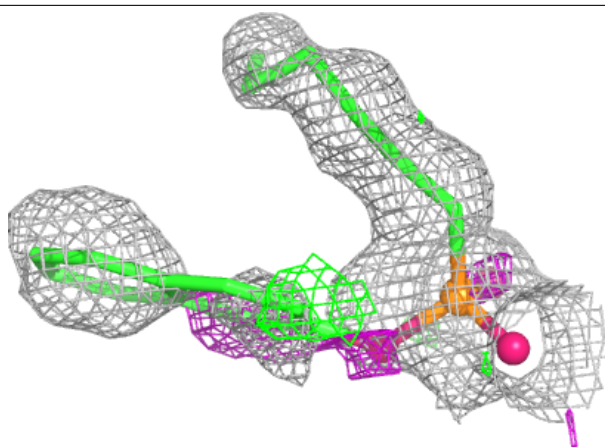
Electron density around HLN G 2404:

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 HLN A 2404:

$2mF_o - DF_c$ (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.