



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:04 PM UTC

PDB ID : 1EM6 / pdb_00001em6
Title : HUMAN LIVER GLYCOGEN PHOSPHORYLASE A COMPLEXED WITH GLCNAC AND CP-526,423
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Deposited on : 2000-03-16
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

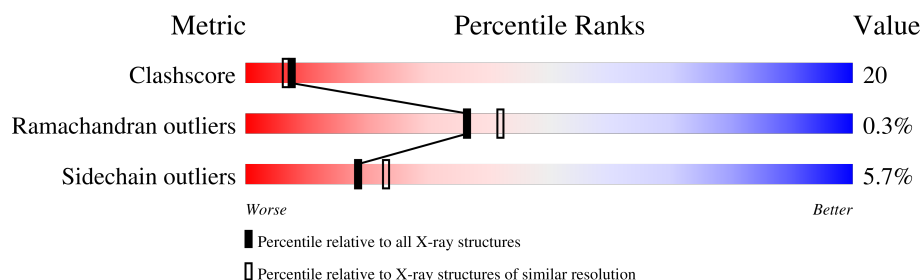
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	847	
1	B	847	

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
5	MPD	B	1902	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13599 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.

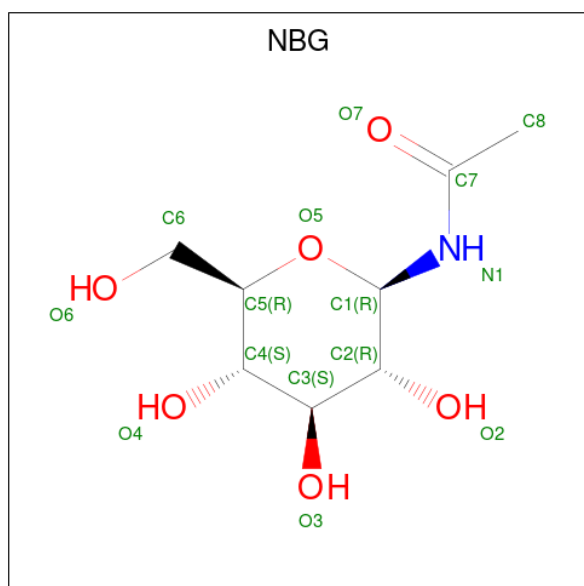
- Molecule 1 is a protein called LIVER GLYCOGEN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	787	Total	C	N	O	S	0	0	0
			6380	4097	1082	1172	29			
1	B	787	Total	C	N	O	S	0	0	0
			6380	4097	1082	1172	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	569	ARG	SER	SEE REMARK 999	UNP P06737
B	569	ARG	SER	SEE REMARK 999	UNP P06737

- Molecule 2 is N-acetyl-beta-D-glucopyranosylamine (CCD ID: NBG) (formula: $C_8H_{15}NO_6$).



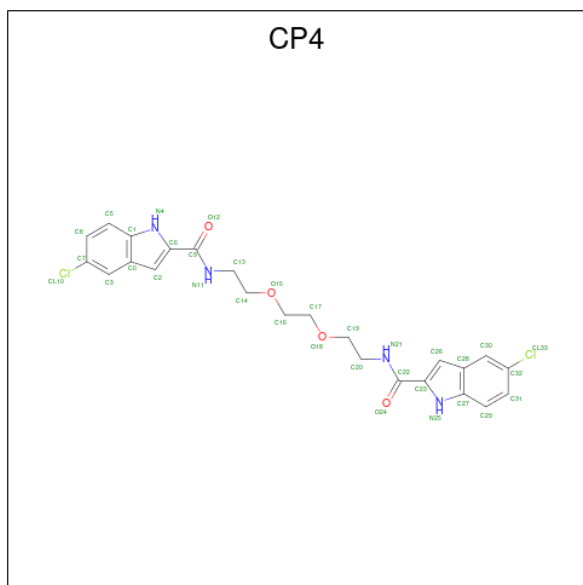
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

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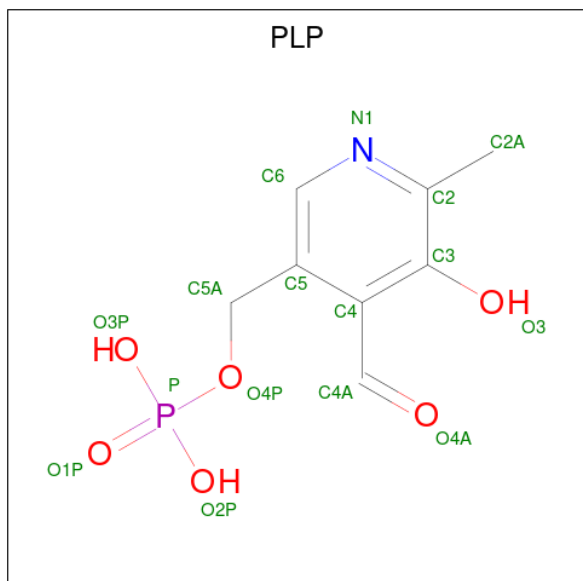
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is BIS[5-CHLORO-1H-INDOL-2-YL-CARBONYL-AMINOETHYL]-ETHYLENE GLYCOL (CCD ID: CP4) (formula: $C_{24}H_{24}Cl_2N_4O_4$).



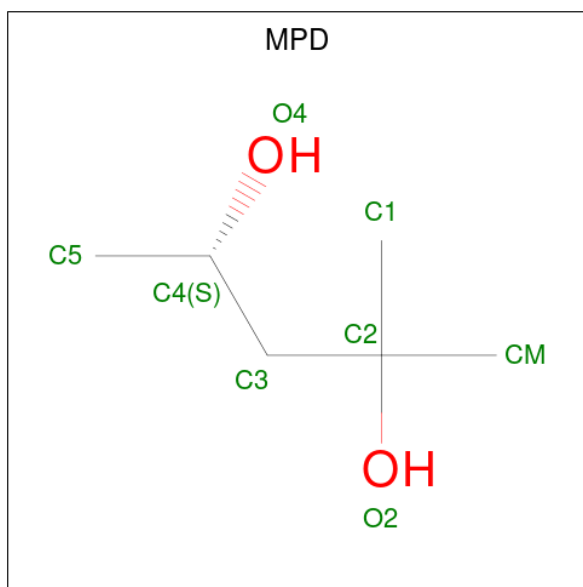
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0
			34	24	2	4	4	0

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is water.

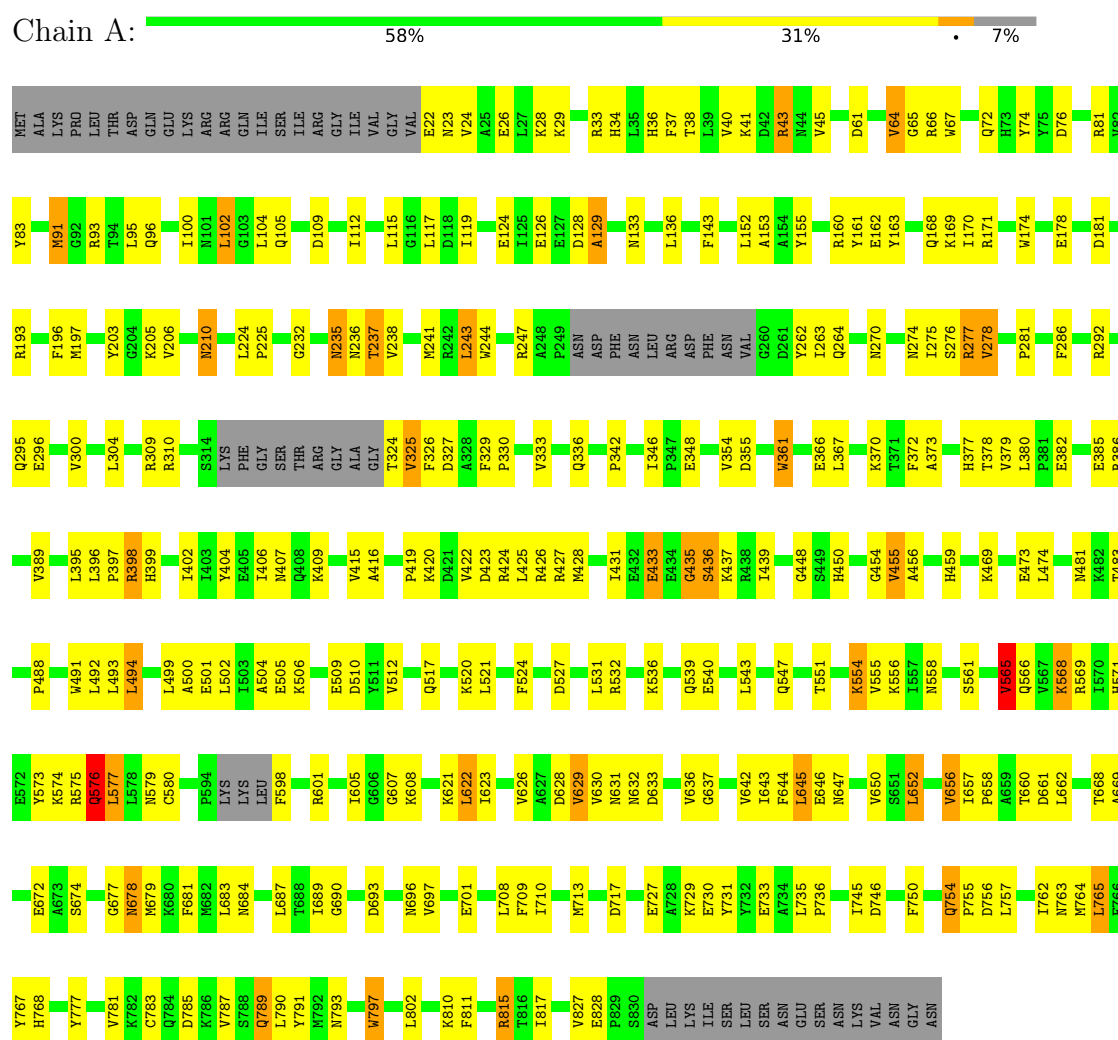
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	379	Total	O	0	0
			379	379		
6	B	358	Total	O	0	0
			358	358		

3 Residue-property plots

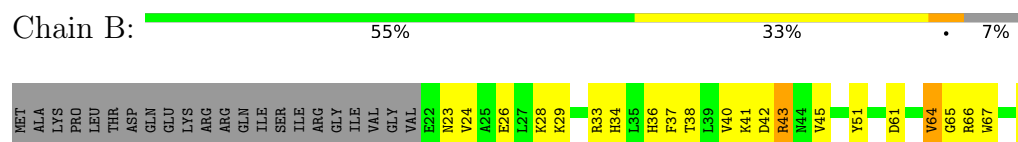
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: LIVER GLYCOGEN PHOSPHORYLASE



• Molecule 1: LIVER GLYCOGEN PHOSPHORYLASE



R81	V278	E366	I439	K544	D633	I710	W797
V82	L279	L367	G448	F545	V636	F711	T816
Y83	Y280	L387	S449	S546	G637	G712	L802
M91	L183	K370	H450	Q547	V642	M713	K810
G92	R184	T371	G454	F548	I643	D717	R815
R93	R193	F372	V455	T551	F644	A720	T816
T94	F196	A373	A456	K554	L645	K723	T817
L95	M197	H377	K457	V555	E646	W726	E827
Q96	M197	T378	I458	N558	N647	E727	E828
I100	Y203	V379	H459	S561	K649	A728	S830
M101	N210	F381	K469	V565	V650	E729	ASP
L102	T211	E382	E473	Q566	L652	E730	LEU
Q105	K214	E385	M481	V567	V656	Y731	LYS
N106	W215	R386	K482	K568	I657	Y732	LYS
D109	I216	V389	T483	R569	P658	E733	ILE
E110	L224	L395	P488	I570	A659	A734	SER
A111	P225	L396	H571	E572	T660	L735	LEU
I112	P225	L396	H571	E572	D661	P736	SER
L115	G232	P397	L492	K574	L662	I745	ASN
G116	N235	R398	L493	R575	T668	D746	GLU
L117	N236	H399	L494	Q576	A669	W750	SER
D118	N237	I402	L499	L578	G670	F750	ASN
I119	V238	I403	A500	L578	T671	Q754	LYS
E126	M241	Y404	E501	C580	E672	P755	VAL
E127	R242	E405	L502	F594	A673	D756	ASN
D128	L243	I406	E505	L594	S674	L757	GLY
A129	W244	Q408	K506	LYS	G675	F758	ASN
N133	R247	Q409	I507	LEU	T676	K759	ASN
L136	A248	H410	G508	F598	M678	I762	LYS
F143	P249	I414	E509	F598	M679	N763	VAL
M147	ASP	V415	D510	R601	F681	M764	ASN
M147	PHE	A416	V512	I605	M682	L765	GLY
L152	ASN	F329	Q517	G605	L683	F766	ASN
A153	ASN	P330	K419	G607	N684	Y767	ASN
A154	LEU	V333	K420	K608	L687	H768	
Y155	ARG	Q336	D421	M615	T688	F774	
Y155	ASP	Q336	V422	L615	F689	Y777	
R160	PHE	D339	R423	I619	G690	W781	
Y161	ASN	D339	L425	I620	D693	K782	
E162	VAL	P342	R426	K621	N696	C783	
Y163	G260	A345	R427	L622	V697	Q784	
Q168	D261	I346	M428	I623	E698	D785	
Q168	Y262	P347	I431	V626	M699	K786	
K169	Q264	E348	E432	G627	A700	W787	
I170	N270	E348	E433	D628	E701	S788	
R171	N274	V354	E434	V629	E702	Q789	
W174	L275	D355	G435	M541	L708	L790	
E178	S276	K437	K437	N632	F709	Y791	
	R277	R361	R438			N793	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	123.31Å 123.31Å 122.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.00 – 2.20	Depositor
% Data completeness (in resolution range)	92.7 (99.00-2.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13599	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

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: PLP, MPD, NBG, CP4

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	0.40	0/6522	0.91	24/8822 (0.3%)
1	B	0.40	0/6522	0.91	25/8822 (0.3%)
All	All	0.40	0/13044	0.91	49/17644 (0.3%)

There are no bond length outliers.

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	VAL	N-CA-C	7.21	117.30	110.74
1	B	575	ARG	N-CA-C	7.20	121.33	111.39
1	A	575	ARG	N-CA-C	7.19	121.31	111.39
1	B	754	GLN	CA-C-N	7.14	128.76	119.84
1	B	754	GLN	C-N-CA	7.14	128.76	119.84

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	6380	0	6361	247	2
1	B	6380	0	6361	275	1
2	A	15	0	15	1	0
2	B	15	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	34	0	24	0	0
4	A	15	0	7	0	0
4	B	15	0	6	0	0
5	B	8	0	14	0	0
6	A	379	0	0	21	0
6	B	358	0	0	33	1
All	All	13599	0	12803	518	2

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 20.

The worst 5 of 518 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:133:ASN:HD22	1:B:569:ARG:NH2	1.56	1.02
1:B:789:GLN:HE21	1:B:789:GLN:HA	1.24	1.02
1:A:133:ASN:HD22	1:A:569:ARG:NH2	1.60	1.00
1:A:789:GLN:HE21	1:A:789:GLN:HA	1.24	0.98
1:A:133:ASN:HD21	1:A:281:PRO:HA	1.29	0.97

All (2) 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:A:505:GLU:OE1	1:B:312:LYS:NZ[2_555]	2.03	0.17
1:A:210:ASN:OD1	6:B:2026:HOH:O[2_665]	2.16	0.04

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	779/847 (92%)	737 (95%)	39 (5%)	3 (0%)	30	34
1	B	779/847 (92%)	733 (94%)	44 (6%)	2 (0%)	36	42
All	All	1558/1694 (92%)	1470 (94%)	83 (5%)	5 (0%)	36	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	436	SER
1	B	436	SER
1	A	435	GLY
1	B	435	GLY
1	A	342	PRO

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	688/740 (93%)	648 (94%)	40 (6%)	18	22
1	B	688/740 (93%)	649 (94%)	39 (6%)	18	23
All	All	1376/1480 (93%)	1297 (94%)	79 (6%)	18	23

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	499	LEU
1	B	683	LEU
1	B	532	ARG
1	B	577	LEU
1	B	765	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	678	ASN

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Mol	Chain	Res	Type
1	B	789	GLN
1	A	678	ASN
1	A	579	ASN
1	B	793	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](#)

6 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	$\# Z > 2$
5	MPD	B	1902	-	7,7,7	0.74	0	9,10,10	0.71	0
2	NBG	B	1861	-	15,15,15	1.54	3 (20%)	21,21,21	1.23	2 (9%)
4	PLP	A	860	1	15,15,16	1.61	2 (13%)	21,22,23	1.28	3 (14%)
3	CP4	A	862	-	37,37,37	2.03	14 (37%)	50,50,50	2.00	12 (24%)
4	PLP	B	1860	1	15,15,16	1.99	2 (13%)	21,22,23	1.39	2 (9%)
2	NBG	A	861	-	15,15,15	1.48	3 (20%)	21,21,21	1.08	1 (4%)

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	MPD	B	1902	-	1/1/2/2	2/5/5/5	-
2	NBG	B	1861	-	-	0/6/26/26	0/1/1/1
4	PLP	A	860	1	-	1/6/6/8	0/1/1/1
3	CP4	A	862	-	-	2/21/21/21	0/4/4/4
4	PLP	B	1860	1	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1860	PLP	C4A-C4	-6.16	1.39	1.51
3	A	862	CP4	C6-N4	-4.65	1.31	1.38
4	A	860	PLP	C4A-C4	-4.41	1.42	1.51
3	A	862	CP4	C23-N25	-4.21	1.32	1.38
2	A	861	NBG	C2-C1	4.01	1.57	1.53

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	862	CP4	C3-C0-C1	5.15	122.31	119.13
3	A	862	CP4	C1-C0-C2	-5.10	102.62	106.80
3	A	862	CP4	C27-C28-C26	-4.80	102.87	106.80
3	A	862	CP4	C30-C28-C27	4.66	122.01	119.13
3	A	862	CP4	O24-C22-C23	-3.80	116.20	121.09

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1902	MPD	C4

All (5) torsion outliers are listed below:

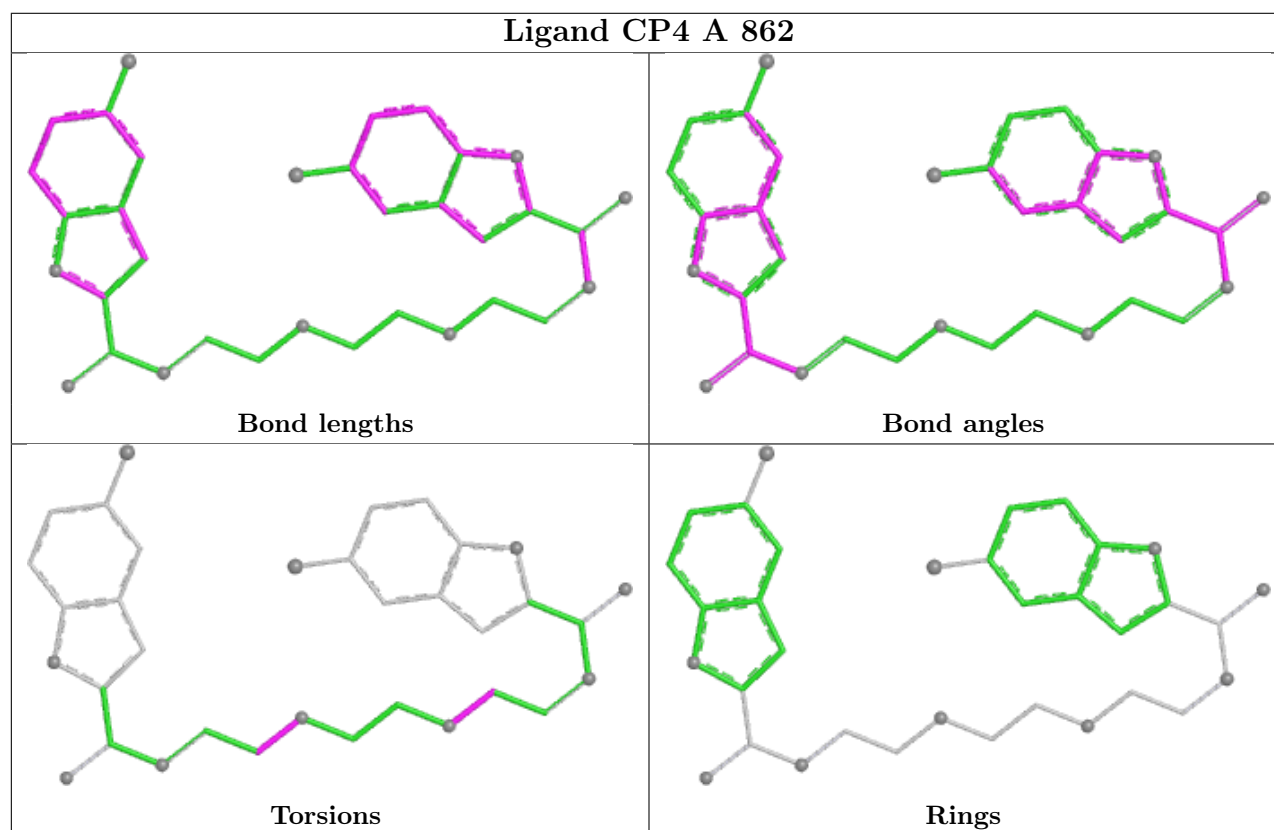
Mol	Chain	Res	Type	Atoms
5	B	1902	MPD	C2-C3-C4-O4
5	B	1902	MPD	C2-C3-C4-C5
4	A	860	PLP	C4-C5-C5A-O4P
3	A	862	CP4	C20-C19-O18-C17
3	A	862	CP4	C13-C14-O15-C16

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1861	NBG	1	0
2	A	861	NBG	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 ⓘ

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.