wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2020 – 10:15 PM BST

PDB ID	:	1EM6
Title	:	HUMAN LIVER GLYCOGEN PHOSPHORYLASE A COMPLEXED WITH GLCNAC AND CP-526,423
Authors	:	Rath, V.L.; Ammirati, M.; Danley, D.E.; Ekstrom, J.L.; Hynes, T.R.; Olson, T.V.; Hoover, D.J.
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

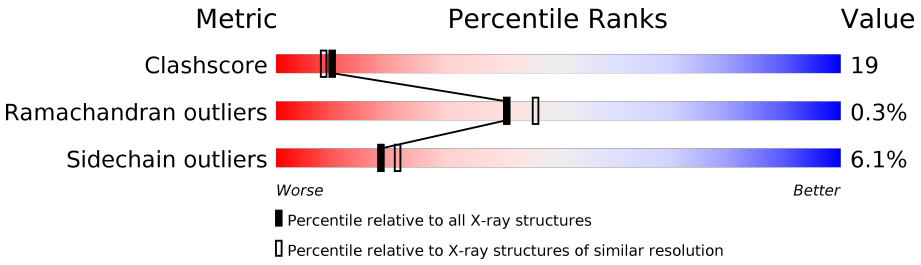
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 on 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	847	61% 29% • 7%
1	B	847	58% 32% • 7%

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

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.

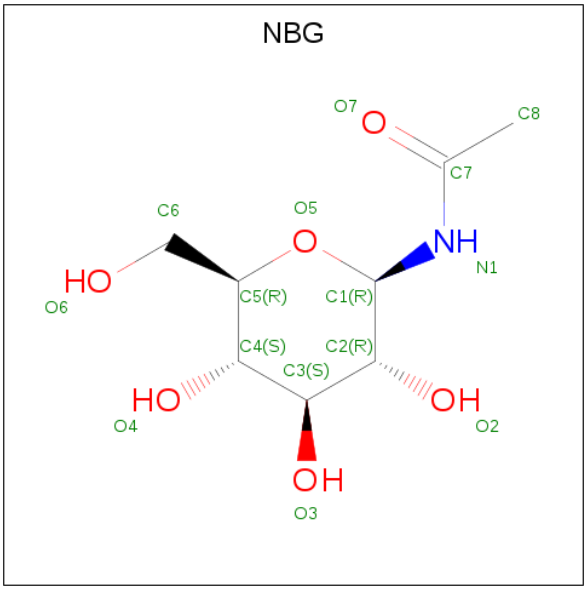
- Molecule 1 is a protein called LIVER GLYCOGEN PHOSPHORYLASE.

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 (three-letter code: 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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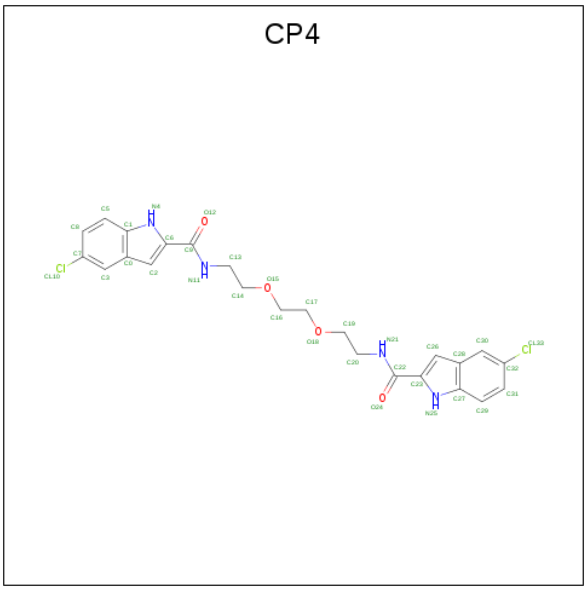
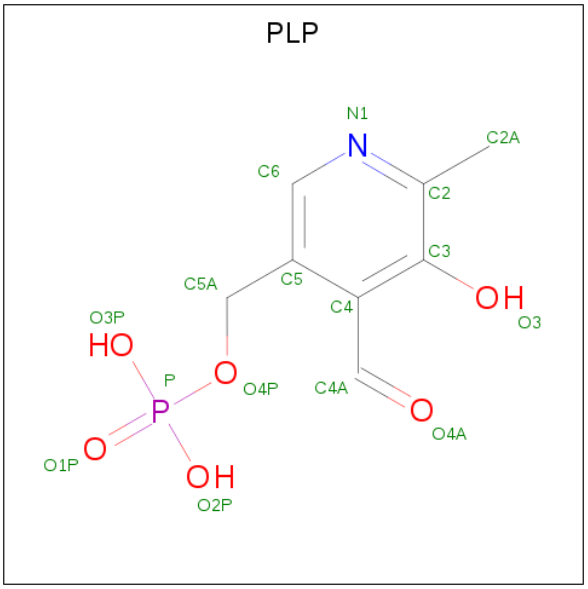
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is BIS[5-CHLORO-1H-INDOL-2-YL-CARBONYL-AMINOETHYL]-ETHYLEN E GLYCOL (three-letter code: CP4) (formula: $C_{24}H_{24}Cl_2N_4O_4$).



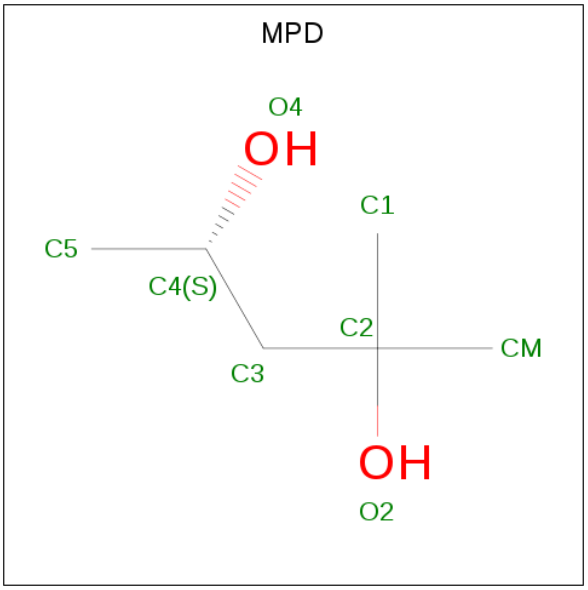
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			34	24	2	4	4		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: 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 (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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		

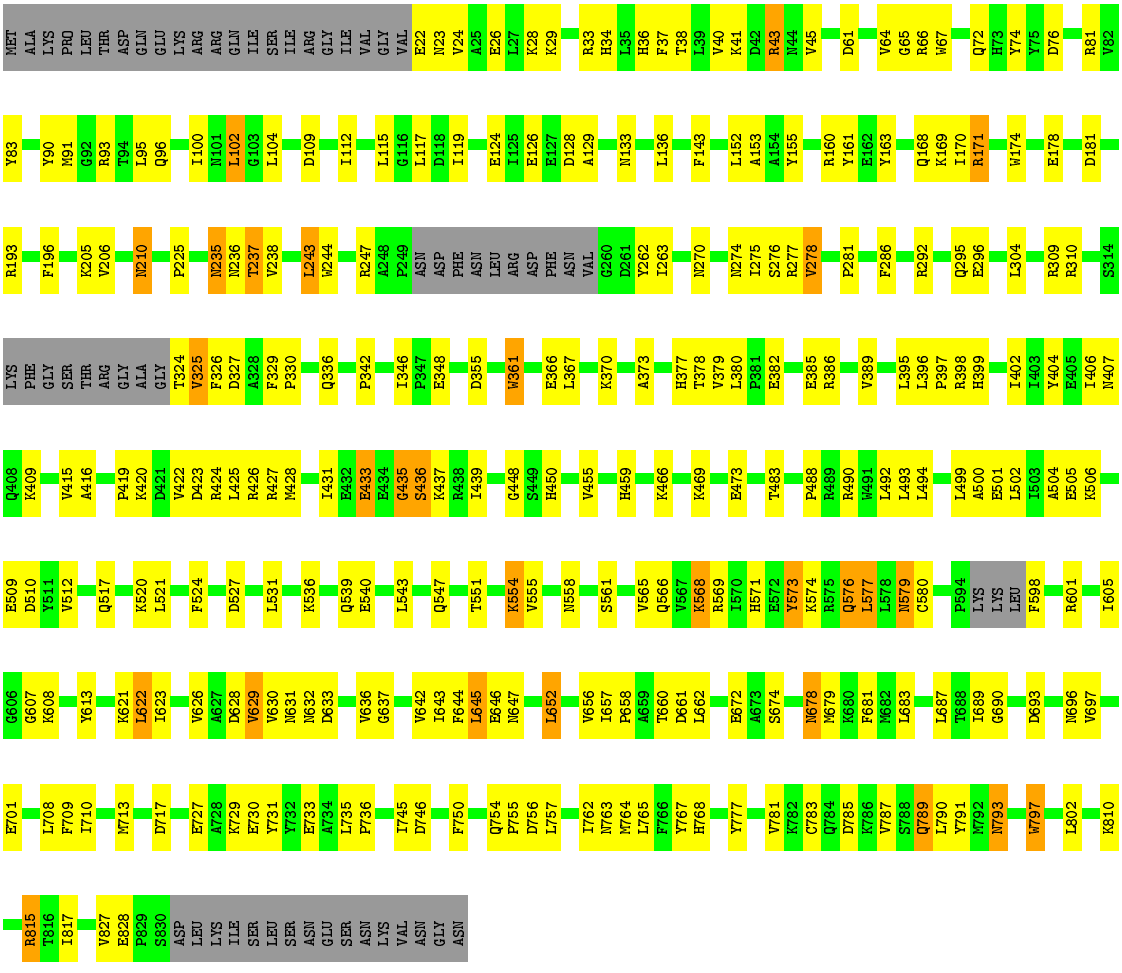
3 Residue-property plots (i)

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

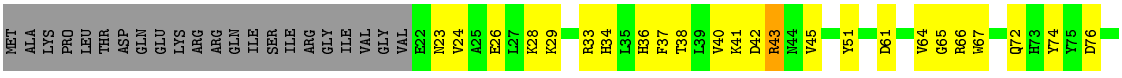
- Molecule 1: LIVER GLYCOGEN PHOSPHORYLASE

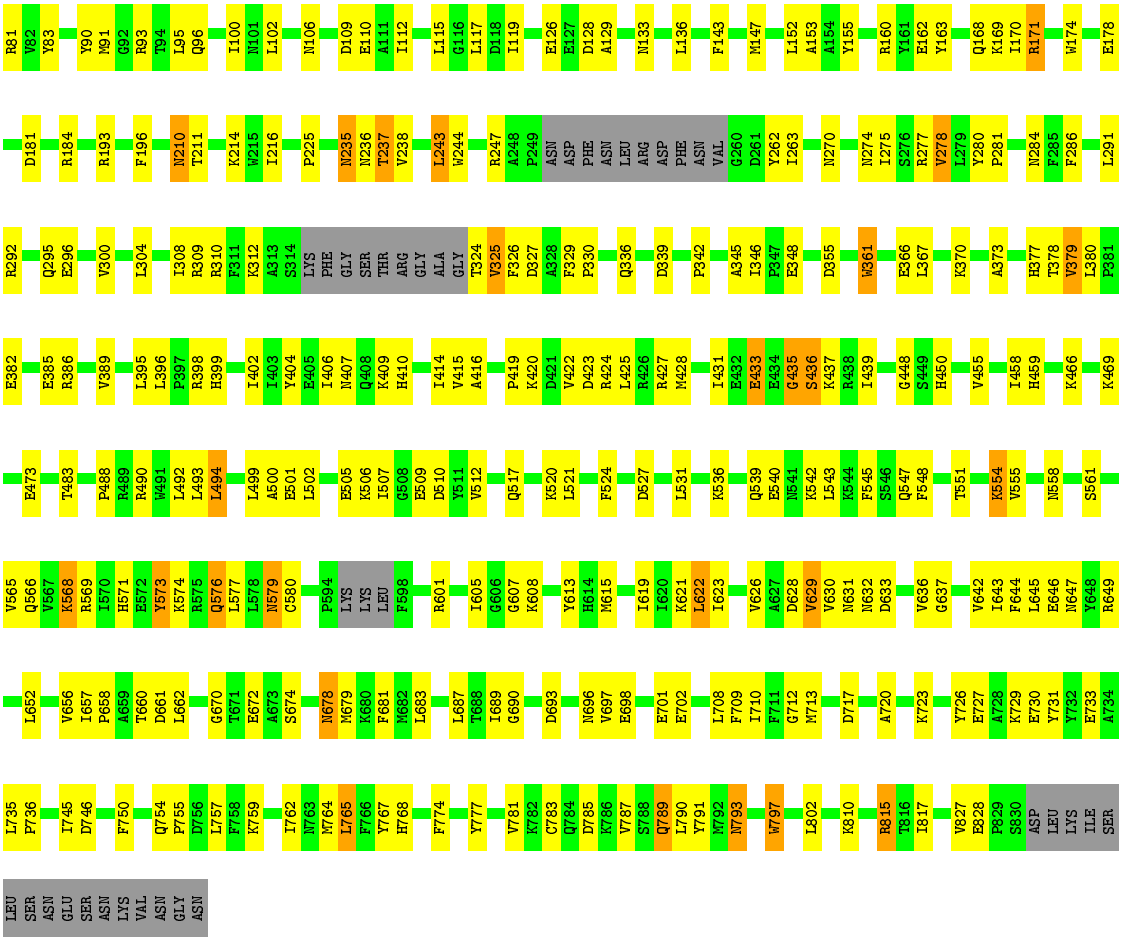
Chain A:



- Molecule 1: LIVER GLYCOGEN PHOSPHORYLASE

Chain B:




R81 V82 Y83 Y90 M91 G92 R93 T94 L95 Q96 I100 N101 L102 N106 D109 E110 A111 I112 L115 G116 L117 D118 I119 E126 E127 D128 A129 N133 L136 F143 M147 L152 A153 A154 Y155 R160 Y161 E162 Y163 Q168 K169 I170 R171 W174 E178
D181 R184 R193 F196 N210 T211 K214 W215 I216 P225 N235 N236 T237 V238 L243 W244 R247 A248 P249 ASN ASP PHE ASN LEU ARG ASP PHE ASN VAL G260 D261 Y262 I263 N270 N274 I275 S276 R277 V278 L279 Y280 P281 N284 F285 F286 L291
R292 Q295 E296 V300 L304 I308 R309 R310 F311 K312 A313 S314 LYS PHE GLY SER THR ARG GLY ALA GLY T324 V325 F326 D327 A328 F329 P330 Q336 D339 P342 A345 I346 P347 E348 D355 W361 E366 L367 K370 A373 H377 T378 V379 L380 P381
E382 E385 R386 V389 L395 L396 P397 R398 H399 I402 I403 Y404 E405 I406 N407 Q408 K409 H410 I414 V415 A416 P419 K420 D421 V422 D423 R424 L425 R426 R427 M428 I431 E432 E433 E434 G435 S436 K437 R438 I439 G448 S449 H450 V455 I458 H459 K466 K469
E473 T483 P488 R489 R490 W491 L492 L493 L494 L499 A500 E501 L502 E505 K506 I507 G508 E509 D510 Y511 V512 Q517 K520 L521 F524 D527 L531 K536 Q539 E540 N541 K542 L543 K544 F545 S546 Q547 F548 T551 K554 V555 N558 S561
V565 Q566 V567 K568 R569 I570 H571 E572 Y573 K574 R575 Q576 L577 L578 N579 C580 P594 LYS LYS LEU F598 R601 I605 G606 G607 K608 Y613 H614 M615 I619 I620 K621 L622 I623 V626 A627 D628 V629 V630 N631 N632 D633 V636 G637 V642 I643 F644 L645 E646 N647 Y648 R649
L652 V656 I657 P658 A659 T660 D661 L662 G670 T671 E672 A673 S674 N678 M679 K680 F681 M682 L683 L687 T688 I689 G690 D693 N696 V697 E698 E701 E702 L708 F709 I710 F711 G712 M713 D717 A720 K723 Y726 E727 A728 K729 E730 Y731 Y732 E733 A734
L735 P736 I745 D746 F750 Q754 P755 D756 L757 F758 K759 I762 N763 M764 L765 F766 Y767 H768 F774 Y777 V781 K782 C783 Q784 D785 K786 V787 S788 Q789 L790 Y791 M792 N793 W797 L802 K810 R815 T816 I817 V827 E828 P829 S830 ASP LEU LYS ILE SER
LEU SER ASN GLU SER ASN LYS VAL ASN GLY ASN

4 Data and refinement statistics (i)

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CP4, MPD, NBG, PLP

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	0.35	0/6522	0.60	0/8822
1	B	0.35	0/6522	0.60	0/8822
All	All	0.35	0/13044	0.60	0/17644

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

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	236	2
1	B	6380	0	6361	258	1
2	A	15	0	15	1	0
2	B	15	0	15	1	0
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	32	1
All	All	13599	0	12803	490	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 19.

The worst 5 of 490 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:HA	1:B:789:GLN:HE21	1.24	1.02
1:A:133:ASN:HD22	1:A:569:ARG:NH2	1.60	1.00
1:A:789:GLN:HA	1:A:789:GLN:HE21	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%)	34	37
1	B	779/847 (92%)	733 (94%)	44 (6%)	2 (0%)	41	46
All	All	1558/1694 (92%)	1470 (94%)	83 (5%)	5 (0%)	41	46

All (5) Ramachandran outliers are listed below:

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

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

5.3.2 Protein sidechains (i)

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%)	647 (94%)	41 (6%)	19	22
1	B	688/740 (93%)	645 (94%)	43 (6%)	18	20
All	All	1376/1480 (93%)	1292 (94%)	84 (6%)	18	21

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	789	GLN
1	B	210	ASN
1	B	730	GLU
1	A	797	TRP
1	B	90	TYR

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

Mol	Chain	Res	Type
1	A	793	ASN
1	B	106	ASN
1	B	754	GLN
1	A	822	GLN
1	B	34	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 monosaccharides 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	$\#\|Z\| > 2$
2	NBG	B	1861	-	15,15,15	1.61	3 (20%)	21,21,21	1.24	2 (9%)
4	PLP	B	1860	1	15,15,16	1.92	2 (13%)	20,22,23	1.40	2 (10%)
2	NBG	A	861	-	15,15,15	1.53	3 (20%)	21,21,21	1.09	1 (4%)
4	PLP	A	860	1	15,15,16	1.55	1 (6%)	20,22,23	1.29	4 (20%)
5	MPD	B	1902	-	7,7,7	0.71	0	9,10,10	0.66	0
3	CP4	A	862	-	33,37,37	1.84	10 (30%)	40,50,50	1.90	10 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NBG	B	1861	-	-	0/6/26/26	0/1/1/1
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
4	PLP	A	860	1	-	1/6/6/8	0/1/1/1
5	MPD	B	1902	-	1/1/2/2	1/5/5/5	-
3	CP4	A	862	-	-	2/15/21/21	0/4/4/4

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1860	PLP	C4A-C4	-5.93	1.39	1.51
4	A	860	PLP	C4A-C4	-4.24	1.42	1.51
2	A	861	NBG	C2-C1	4.13	1.57	1.52
3	A	862	CP4	C5-C8	3.58	1.44	1.36
2	B	1861	NBG	C1-N1	3.56	1.47	1.43

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	862	CP4	C23-C22-N21	4.43	121.79	115.59
3	A	862	CP4	C2-C0-C1	-4.19	102.62	106.27
3	A	862	CP4	C6-C9-N11	3.92	121.07	115.59
3	A	862	CP4	C26-C28-C27	-3.90	102.87	106.27
3	A	862	CP4	C6-N4-C1	3.72	112.20	104.45

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1902	MPD	C4

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1902	MPD	C2-C3-C4-O4
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.

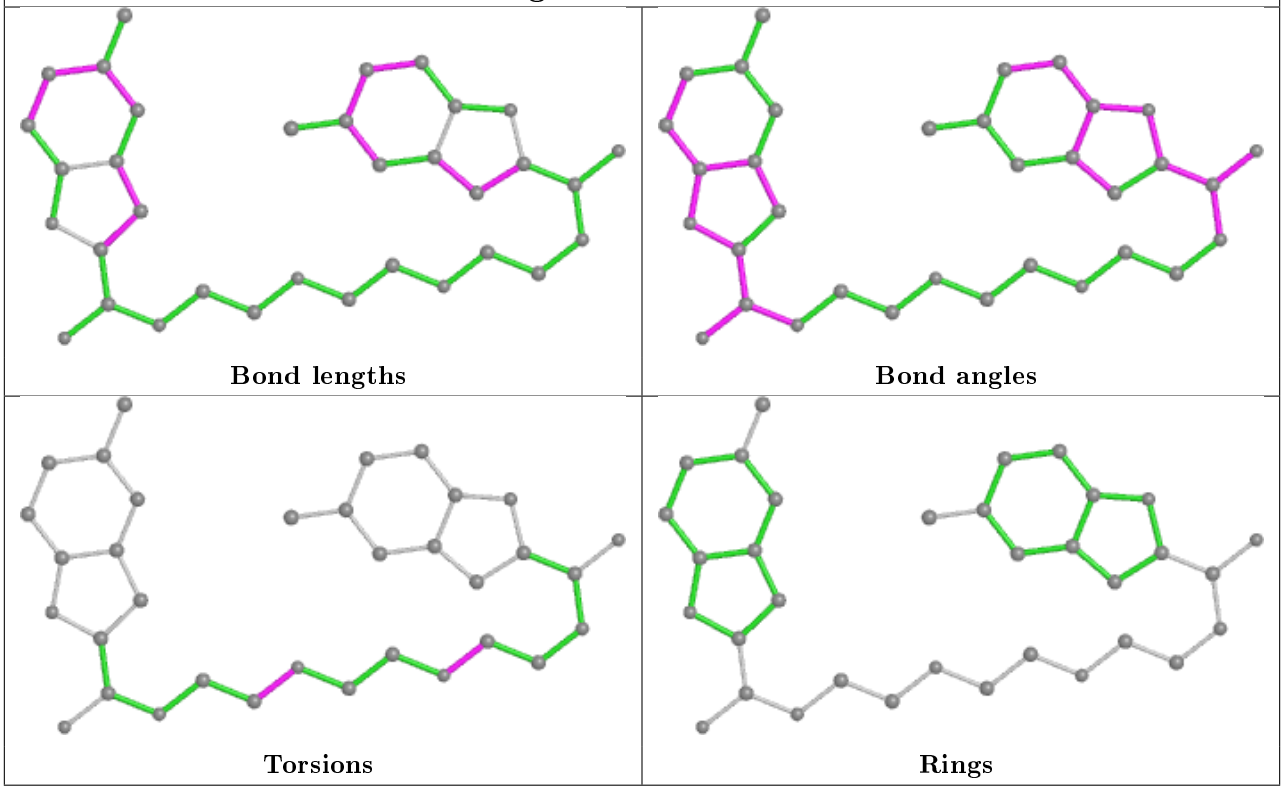
2 monomers are involved in 2 short contacts:

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 then 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 CP4 A 862



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.