



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:34 AM UTC

PDB ID : 7GPB / pdb_00007gpb
Title : STRUCTURAL MECHANISM FOR GLYCOGEN PHOSPHORYLASE
CONTROL BY PHOSPHORYLATION AND AMP
Authors : Barford, D.; Hu, S.-H.; Johnson, L.N.
Deposited on : 1990-11-13
Resolution : 2.90 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)
Xtrriage (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

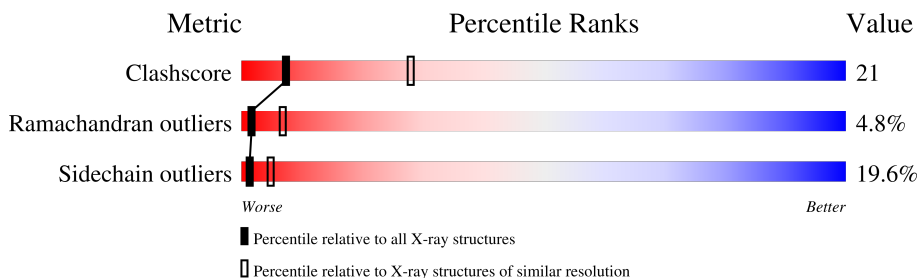
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	842	32% 41% 20% 5% •
1	B	842	34% 41% 18% 5% •
1	C	842	36% 40% 18% ••
1	D	842	29% 39% 24% 6% •

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
2	SO4	A	901	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26955 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 GLYCOGEN PHOSPHORYLASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	824	6692	4264	1185	1213	30	0	0	1
1	B	824	6692	4264	1185	1213	30	0	0	1
1	C	824	6692	4264	1185	1213	30	0	0	1
1	D	824	6692	4264	1185	1213	30	0	0	1

There are 4 discrepancies between the modelled and reference sequences:

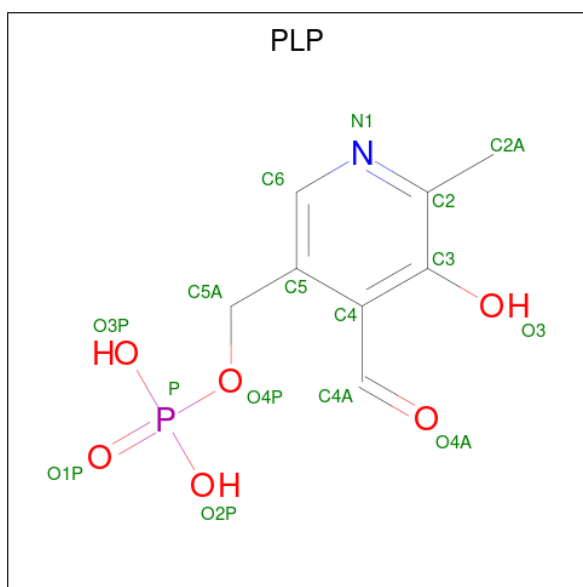
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489
B	380	ILE	LEU	conflict	UNP P00489
C	380	ILE	LEU	conflict	UNP P00489
D	380	ILE	LEU	conflict	UNP P00489

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



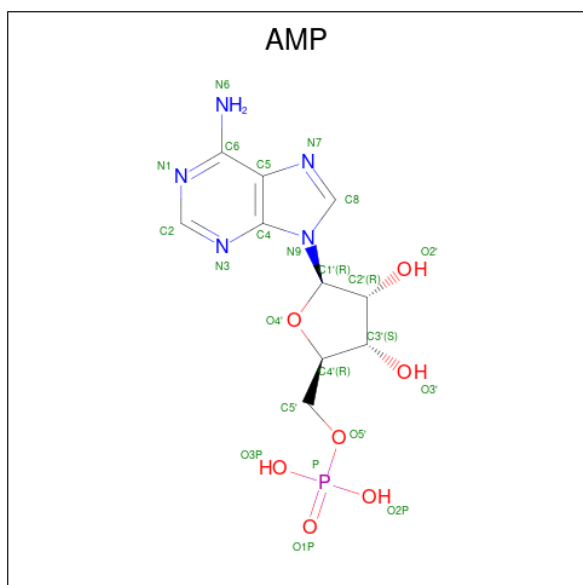
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



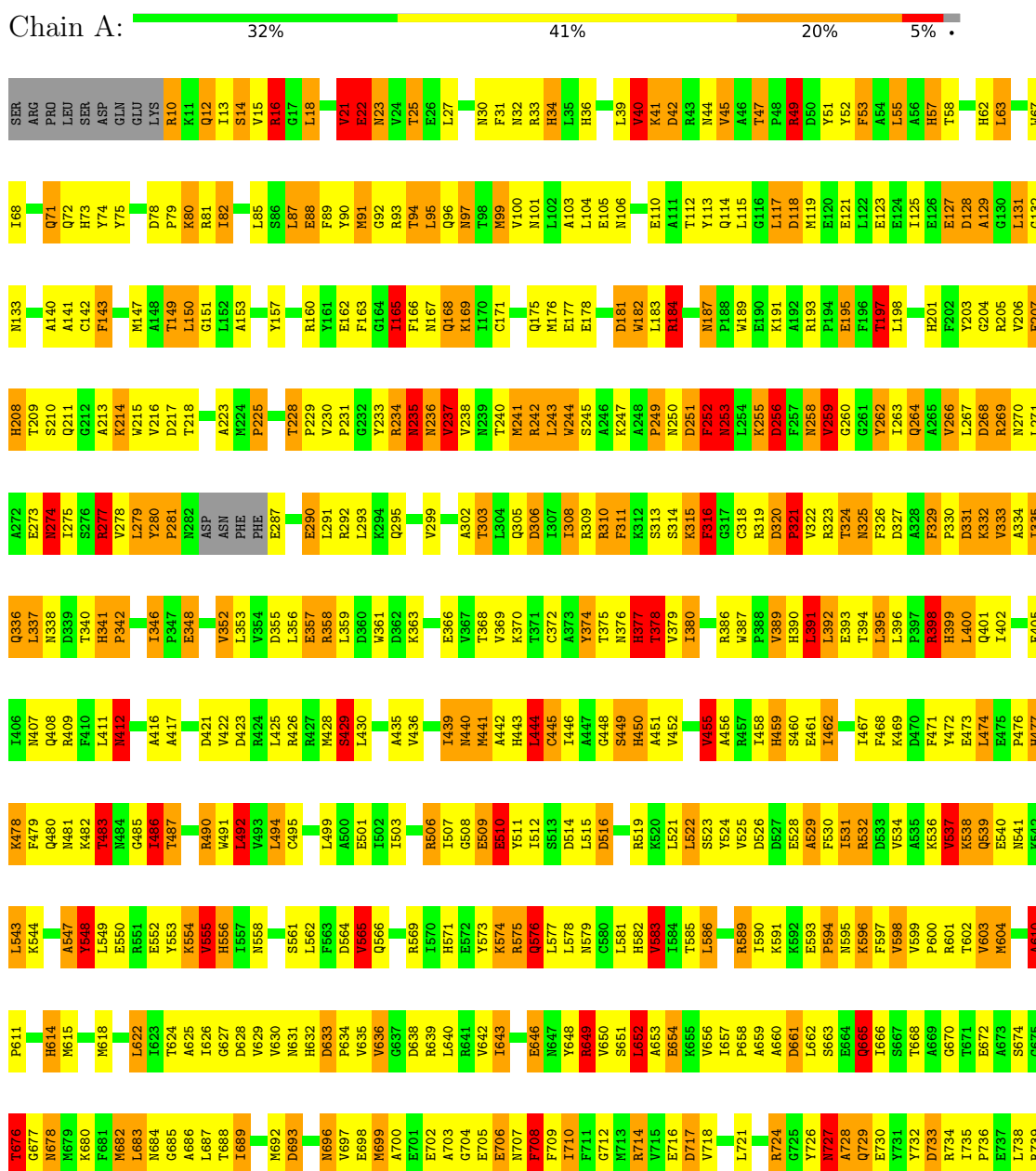
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	B	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	C	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	D	1	Total 23	C 10	N 5	O 7	P 1	0	0

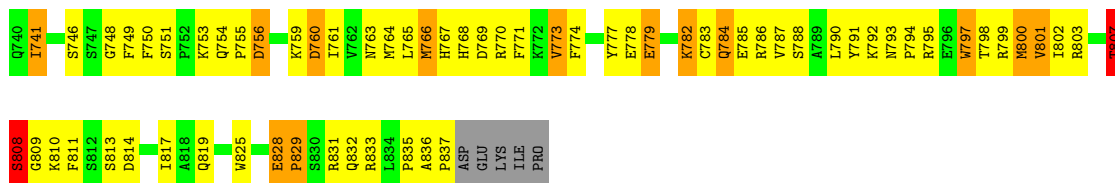
3 Residue-property plots [i](#)

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 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.

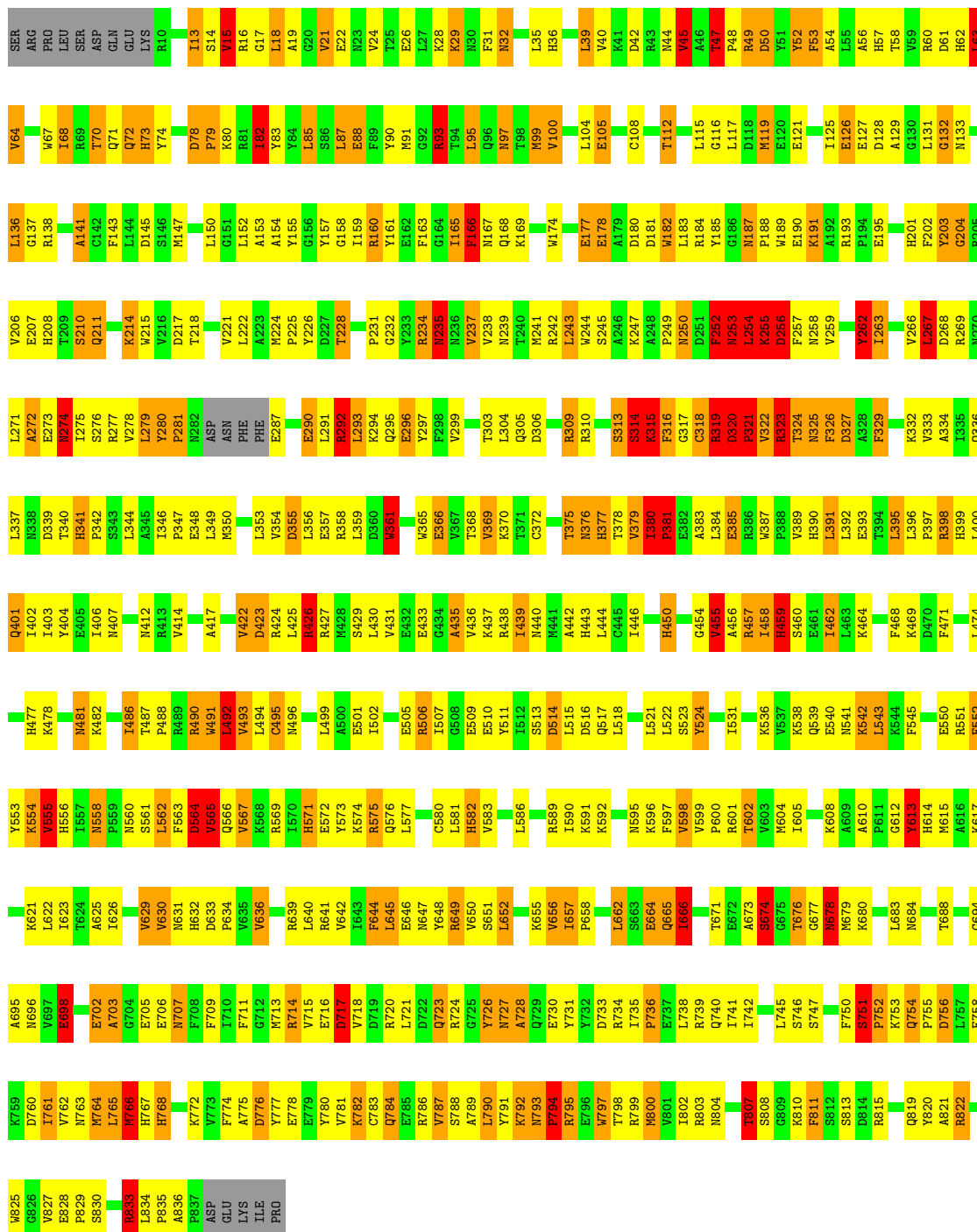
- Molecule 1: GLYCOGEN PHOSPHORYLASE B



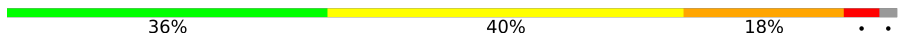


• Molecule 1: GLYCOGEN PHOSPHORYLASE B

Chain B: 34% 41% 18% 5%

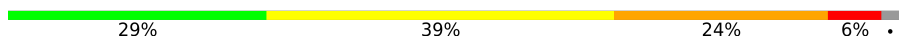


• Molecule 1: GLYCOGEN PHOSPHORYLASE B

Chain C: 

SER	ARG	PRO	LEU	SER	ASP	GLN	GLU	LYS	R10	R11	K11	Q12	I13	S14	V15	R16	G17	L18	G18	A19	G20	V21	T25	E26	L27	F31	N32	R33	H34	L35	H36	F37	L38	V40	K41	D42	R43	M44	V45	A46	T47	P48	R49	Y52	L55	A56	H57	T58	V59	R60	D61	H62	L63	V64	R66			
I67	I68	R69	R70	LEU	Q71	H72	H73	Y74	Y75	E76	K77	K80	R81	I82	Y83	Y84	L85	E88	F89	M90	M91	G92	R93	L94	R95	Q96	M99	V100	H101	L102	A103	L104	M119	E120	E121	I125	E126	D127	D128	A129	G130	G132	L136	C142	F143	V144	L144	M147	A148	T149	L150	G151						
L152	A153	A154	Y155	G156	R160	Y161	F162	F163	F164	K165	I166	M167	K168	Q169	W174	Q175	M176	E177	E178	D181	W182	F183	L183	R184	M187	E190	H191	A192	R193	P194	E195	F196	T197	L198	P199	H201	G204	R205	V206	E207	H208	T209	S210	Q211	W215	V216	A217	P218	Q219	M224	K289	L289	E290					
Y226	D227	T228	P229	V230	P231	G232	Y233	R234	N235	N236	V237	V238	M239	T240	M241	R242	L243	W244	K247	N250	D251	F252	M253	L254	K255	R256	F257	N258	V259	Y262	I263	Q264	A265	V266	L267	D268	R269	E273	N274	I275	S276	R277	V278	Y280	P281	N282	ASP	ASN	PHE	PHE	E287	G288	E290					
L291	R292	L293	K294	Q295	F298	V299	V300	A301	A302	T303	L304	Q305	D306	I307	I308	R309	R310	F311	R312	S313	S314	K315	F316	C317	C318	R319	D320	P321	V322	R323	T324	N325	D326	D327	A328	F329	P330	D331	K332	G336	L337	M338	D339	H341	P342	S343	I346	P347	E348	L349	M350	R351	V352	D355				
L356	E357	R358	L359	W361	D362	K363	A364	W365	E366	T367	T368	V369	K370	T371	Y374	T375	N376	H377	T378	V379	I380	P381	E382	A383	L384	E385	P388	V389	H390	L391	L392	E393	T394	L395	L396	P397	R398	H399	L400	Q401	Y404	M407	H409	F410	N412	D421	L349	V422	D423	R426	W491	L492						
M428	S429	L430	V431	E432	W433	A436	K437	R438	I439	H443	L444	C445	I446	A447	G448	S449	H450	A451	V452	M453	G454	V455	A456	A457	I458	H459	S460	L463	K464	K465	T466	I467	F468	F471	Y472	E473	L474	E475	P476	H477	K478	P479	Q480	M481	K482	T483	N484	G485	V486	T487	R490	W491	L492					
V493	L494	C495	H496	P497	G498	L499	I502	A503	A504	E505	R506	E509	E510	C445	S513	D514	Q517	L518	R519	V520	L521	L522	S523	Y524	V525	M526	D527	E528	A529	F530	L531	R532	T533	V534	A535	K536	V537	K538	V603	M604	L605	M641	K642	L543	A609	A610	P611	H614	M615	M692	D693	M618	T619	V553	A654	R621	L622	H556
F559	M560	S561	L562	F563	D564	V565	Q566	V567	K568	R569	I570	H571	E572	Y573	K574	R575	Q576	M579	H582	V583	L586	Y587	M588	R589	T590	K591	K592	E593	P594	F597	V598	V599	P600	R601	T602	V603	M604	L605	G606	K608	A609	A610	P611	H614	M615	M692	D693	M618	T619	V553	A654	R621	L622	H556				
T624	A625	I626	V630	M631	H632	D633	D638	R639	L645	E646	N647	Y648	R649	V650	S651	L652	A653	E654	K655	V656	P658	D661	L662	S663	W664	I665	T671	S674	G675	T676	G677	M678	M679	K680	L683	T688	L689	G690	T691	M692	D693	M618	T619	V553	A654	R621	L622	H556										
M699	A700	E701	E702	A703	G704	E705	W706	N707	F708	F709	I710	F711	R714	V715	E716	R720	L721	D722	Y726	L727	A728	Q729	E730	D733	R734	L735	F736	E737	L738	R739	Q740	I741	L742	E743	Q744	L745	G746	S747	G748	S751	F752	K753	Q754	P755	F758	K759	D760	L761	E762	N763	R764	L765	M766					
H767	H768	D769	R770	F771	K772	V773	F774	E778	E779	Y780	V781	K782	C783	Q784	E785	R786	V787	K792	N793	F794	R795	T798	R799	M800	W801	R802	R803	N804	L805	A806	T807	S808	Q809	K810	F811	S812	S813	D814	I817	A818	Q819	Y820	A821	R822	Q754	P755	F758	K759	D760	L761	E762	N763	R764	L765	M766			
L834	F835	A836	F837	ASP	GLU	LYS	ILE	PRO	R10	K11	Q12	I13	S14	V15	R16	G17	L18	A19	G20	V21	E22	N23	V24	T25	E26	L27	M800	W801	R802	R803	N804	L805	A806	T807	S808	Q809	K810	F811	S812	S813	D814	I817	A818	Q819	Y820	A821	R822	Q754	P755	F758	K759	D760	L761	E762	N763	R764	L765	M766

• Molecule 1: GLYCOGEN PHOSPHORYLASE B

Chain D: 

SER	ARG	PRO	LEU	SER	ASP	GLN	GLU	LYS	R10	K11	Q12	I13	S14	V15	R16	G17	L18	A19	G20	V21	E22	N23	V24	T25	E26	L27	K28	R29	N30	R33	R34	L35	H36	F37	T38	L39	V40	K41	D42	R43	Y44	V45	A46	P48	R49	D50	Y51	Y52	H57	R60	D61	H62	L63	V64
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M793	F794	E795	F796	M797	F798	R799	M800	R801	R802	R803	R804	R805	A806	R807	S808	R809	R810	F811	S812	S813	D814	R815	R816	A817	A818	Q819	Y820	A821	R822	E823	T824	M825	G826	V827	P828	S829	G830	G831	G832	G833	G834	G835	G836	G837	G838	G839	G840	G841	G842	G843	G844	G845	G846	G847	G848	G849	G850	G851	G852	G853	G854	G855	G856	G857	G858	G859	G860	G861	G862	G863	G864	G865	G866	G867	G868	G869	G870	G871	G872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	G1000
L131	G132	M133	L136	G137	R138	F143	L144	D145	S146	M147	A148	T149	L150	K80	G151	L152	A153	A154	Y155	G156	R160	Y161	E162	F163	G164	R93	T94	F165	F166	M167	Q168	K169	L170	M99	C171	G172	G173	L101	L102	A103	Q175	M176	E177	E178	A179	D180	D181	Y113	Q114	L115	R184	M119	P188	W189	E190	E123	E124	I125	E126	E127	D128	A129	G130																																																																																																																																																
H201	R205	V206	E207	H208	T209	S210	Q211	K214	D215	S146	M147	A148	T218	Q219	K219	V220	M224	P225	Y226	D227	T228	P229	V230	P231	G232	G233	R234	N235	N236	V237	V238	M239	T240	M241	R242	L243	W244	S245	K247	A248	P249	M250	D251	F252	N253	L254	K255	D256	F257	N258	V259	R193	Y262	I263	Q264	P198	A199	V266																																																																																																																																																					
L267	D268	R269	N270	E273	M274	L275	N388	R277	T340	H341	P342	S343	L344	A345	L411	N481	P347	E348	L349	M350	R351	V352	L356	E357	R358	K289	E290	L291	R292	L293	K294	Q295	D360	E296	W361	Y297	F298	V299	V300	A301	A302	T303	L304	Q305	D306	I307	R309	K312	S313	S314	K315	F316	N253	G317	C318	R319	D320	P321	V322	R323	T324	N325	F326	F329																																																																																																																																															
P330	D331	K332	V333	A334	I335	O336	L337	D339	T340	H341	P342	S343	L344	A345	L411	N481	P347	E348	L349	M350	R351	V352	L356	E357	R358	K289	E290	L291	R292	L293	K294	Q295	D360	E296	W361	Y297	F298	V299	V300	A301	A302	T303	L304	Q305	D306	I307	R309	K312	S313	S314	K315	F316	N253	G317	C318	R319	D320	P321	V322	R323	T324	N325	F326	F329																																																																																																																																															
E393	T394	L395	L396	P397	R398	H399	L400	Q401	L402	N407	Q408	R409	F410	L411	A345	L411	N481	P347	E348	L349	M350	R351	V352	L356	E357	R358	K289	E290	L291	R292	L293	K294	Q295	D360	E296	W361	Y297	F298	V299	V300	A301	A302	T303	L304	Q305	D306	I307	R309	K312	S313	S314	K315	F316	N253	G317	C318	R319	D320	P321	V322	R323	T324	N325	F326	F329																																																																																																																																														
L463	K464	K465	T466	R467	V468	K469	D470	L474	E475	H476	P477	K478	Q480	N481	P482	T483	M484	G485	E550	T486	R551	E552	Y553	R489	A490	W491	L492	V493	N568	L494	C495	M496	P497	G498	L499	A500	V367	R437	R438	I439	N440	H443	L444	C445	I446	S449	H450	V379	A451	V452	M453	G454	V455	L521	S523	R457	I458	K459	S460	E461	E528																																																																																																																																																		
A529	F530	I531	R532	D533	V534	A535	D470	L474	E475	H476	P477	K478	Q480	N481	P482	T483	M484	G485	E550	T486	R551	E552	Y553	R489	A490	W491	L492	V493	N568	L494	C495	M496	P497	G498	L499	A500	V367	R437	R438	I439	N440	H443	L444	C445	I446	S449	H450	V379	A451	V452	M453	G454	V455	L521	S523	R457	I458	K459	S460	E461	E528																																																																																																																																																		
F590	K591	K592	E593	P594	M595	K596	F597	V598	P599	R600	T601	V602	V603	G606	L543	F545	A546	A547	Y548	L549	H614	M615	A616	K617	M618	L619	L622	N631	H632	D633	P634	V635	A700	G637	L640	R641	V642	L643	F644	L645	E646	V647	Y648	G649	C590	L581	H582	S651	V583	I584	M587	K588	V656	R655	L657	R589																																																																																																																																																							
R658	A659	G660	D661	L662	S663	E664	Q665	I666	A669	A673	S674	G675	T676	G677	N678	M679	K680	F681	N682	L683	N684	L687	P688	L689	G690	T691	K759	D760	I761	V762	A695	N696	V697	E698	N699	A700	E701	E702	G704	E705	E706	M707	F708	F709	I710	F711	G712	M713	R714	V715	W716	D717	W718	L721																																																																																																																																																									
R724	G725	Y726	N727	A728	Y732	D733	R734	I735	L738	R739	G740	I741	Q744	G748	F749	F750	S751	P752	K753	Q754	P755	D756	L757	F758	K759	D760	I761	V762	M763	M764	L765	M766	H767	R768	D769	V773	F774	A775	D776	Y777	E778	E779	K782	C783	Q784	R785	R786	W787	S788	A789	L790	Y791	K792																																																																																																																																																										

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.00Å 190.00Å 88.20Å 90.00° 109.35° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.171 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	26955	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: AMP, PLP, SO4

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	1.29	43/6842 (0.6%)	2.34	408/9258 (4.4%)
1	B	1.28	44/6842 (0.6%)	2.25	324/9258 (3.5%)
1	C	1.28	45/6842 (0.7%)	2.27	349/9258 (3.8%)
1	D	1.26	38/6842 (0.6%)	2.31	360/9258 (3.9%)
All	All	1.28	170/27368 (0.6%)	2.29	1441/37032 (3.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
1	C	0	5
1	D	0	8
All	All	0	25

The worst 5 of 170 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	100	VAL	CA-CB	11.80	1.70	1.54
1	C	657	ILE	CA-CB	9.83	1.59	1.54
1	A	829	PRO	CA-CB	-8.38	1.41	1.53
1	D	626	ILE	CA-CB	8.34	1.64	1.54
1	C	630	VAL	CA-CB	8.31	1.64	1.54

The worst 5 of 1441 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	67	TRP	CG-CD2-CE3	-36.55	97.35	133.90
1	D	67	TRP	NE1-CE2-CZ2	-24.67	93.09	130.10
1	B	477	HIS	CA-CB-CG	13.92	127.72	113.80
1	A	181	ASP	CA-CB-CG	13.84	126.44	112.60
1	C	575	ARG	N-CA-C	13.75	130.00	113.23

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain
1	A	277	ARG	Sidechain
1	A	280	TYR	Peptide
1	A	47	THR	Peptide
1	A	49	ARG	Sidechain

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	6692	0	6653	261	1
1	B	6692	0	6653	249	0
1	C	6692	0	6653	263	0
1	D	6692	0	6653	347	1
2	A	10	0	0	2	0
2	B	10	0	0	1	0
2	C	10	0	0	1	0
2	D	5	0	0	0	0
3	A	15	0	6	1	0
3	B	15	0	7	1	0
3	C	15	0	7	1	0
3	D	15	0	7	2	0
4	A	23	0	12	3	0
4	B	23	0	12	1	0
4	C	23	0	12	1	0
4	D	23	0	12	2	0
All	All	26955	0	26687	1101	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 21.

The worst 5 of 1101 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:D:85:LEU:HD21	1:D:303:THR:HG21	1.43	1.00
1:D:251:ASP:HB3	1:D:255:LYS:HB3	1.46	0.98
1:D:707:ASN:HA	1:D:800:MET:SD	2.04	0.97
1:A:45:VAL:HG21	4:B:920:AMP:H3'	1.44	0.97
1:D:91:MET:HE1	1:D:144:LEU:HD12	1.48	0.94

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:A:509:GLU:N	1:D:321:PRO:O[2_646]	2.18	0.02

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	820/842 (97%)	669 (82%)	116 (14%)	35 (4%)	2	8
1	B	820/842 (97%)	687 (84%)	92 (11%)	41 (5%)	1	6
1	C	820/842 (97%)	708 (86%)	82 (10%)	30 (4%)	2	11
1	D	820/842 (97%)	669 (82%)	100 (12%)	51 (6%)	1	3
All	All	3280/3368 (97%)	2733 (83%)	390 (12%)	157 (5%)	2	7

5 of 157 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	321	PRO
1	A	358	ARG
1	A	553	TYR
1	A	674	SER

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	712/731 (97%)	563 (79%)	149 (21%)	1	4
1	B	712/731 (97%)	571 (80%)	141 (20%)	1	5
1	C	712/731 (97%)	583 (82%)	129 (18%)	2	6
1	D	712/731 (97%)	574 (81%)	138 (19%)	1	5
All	All	2848/2924 (97%)	2291 (80%)	557 (20%)	1	5

5 of 557 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	281	PRO
1	D	337	LEU
1	D	274	ASN
1	D	575	ARG
1	B	313	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	274	ASN
1	D	744	GLN
1	D	376	ASN
1	D	576	GLN
1	B	412	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](#)

15 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
3	PLP	A	999	1	15,15,16	1.87	5 (33%)	21,22,23	1.07	2 (9%)
3	PLP	D	999	1	15,15,16	1.12	1 (6%)	21,22,23	1.87	2 (9%)
3	PLP	B	999	1	15,15,16	1.60	1 (6%)	21,22,23	1.09	1 (4%)
3	PLP	C	999	1	15,15,16	1.14	1 (6%)	21,22,23	0.98	1 (4%)
2	SO4	B	900	-	4,4,4	0.46	0	6,6,6	0.44	0
2	SO4	A	901	-	4,4,4	0.34	0	6,6,6	0.33	0
4	AMP	C	920	-	25,25,25	0.75	0	37,38,38	0.73	0
2	SO4	D	900	-	4,4,4	0.24	0	6,6,6	0.32	0
2	SO4	A	900	-	4,4,4	0.24	0	6,6,6	0.37	0
4	AMP	D	920	-	25,25,25	0.75	0	37,38,38	0.67	0
4	AMP	A	920	-	25,25,25	0.74	0	37,38,38	0.78	0
4	AMP	B	920	-	25,25,25	0.73	0	37,38,38	0.72	0
2	SO4	C	901	-	4,4,4	0.32	0	6,6,6	0.41	0
2	SO4	C	900	-	4,4,4	0.36	0	6,6,6	0.34	0
2	SO4	B	901	-	4,4,4	0.41	0	6,6,6	0.26	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
3	PLP	A	999	1	-	0/6/6/8	0/1/1/1
3	PLP	D	999	1	-	0/6/6/8	0/1/1/1
3	PLP	B	999	1	-	0/6/6/8	0/1/1/1
3	PLP	C	999	1	-	0/6/6/8	0/1/1/1
4	AMP	D	920	-	-	3/10/26/26	0/3/3/3
4	AMP	A	920	-	-	3/10/26/26	0/3/3/3
4	AMP	B	920	-	-	2/10/26/26	0/3/3/3
4	AMP	C	920	-	-	3/10/26/26	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	999	PLP	C3-C2	-3.98	1.36	1.41
3	A	999	PLP	C3-C2	-3.92	1.36	1.41
3	A	999	PLP	P-O2P	-2.57	1.45	1.54
3	C	999	PLP	C3-C2	-2.55	1.38	1.41
3	A	999	PLP	C5-C4	-2.41	1.37	1.40

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	999	PLP	O4P-C5A-C5	7.49	123.39	109.36
3	C	999	PLP	C6-C5-C4	2.34	120.01	118.10
3	A	999	PLP	C5-C6-N1	-2.28	120.12	123.83
3	D	999	PLP	C5-C6-N1	-2.26	120.16	123.83
3	B	999	PLP	O4P-C5A-C5	2.22	113.52	109.36

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

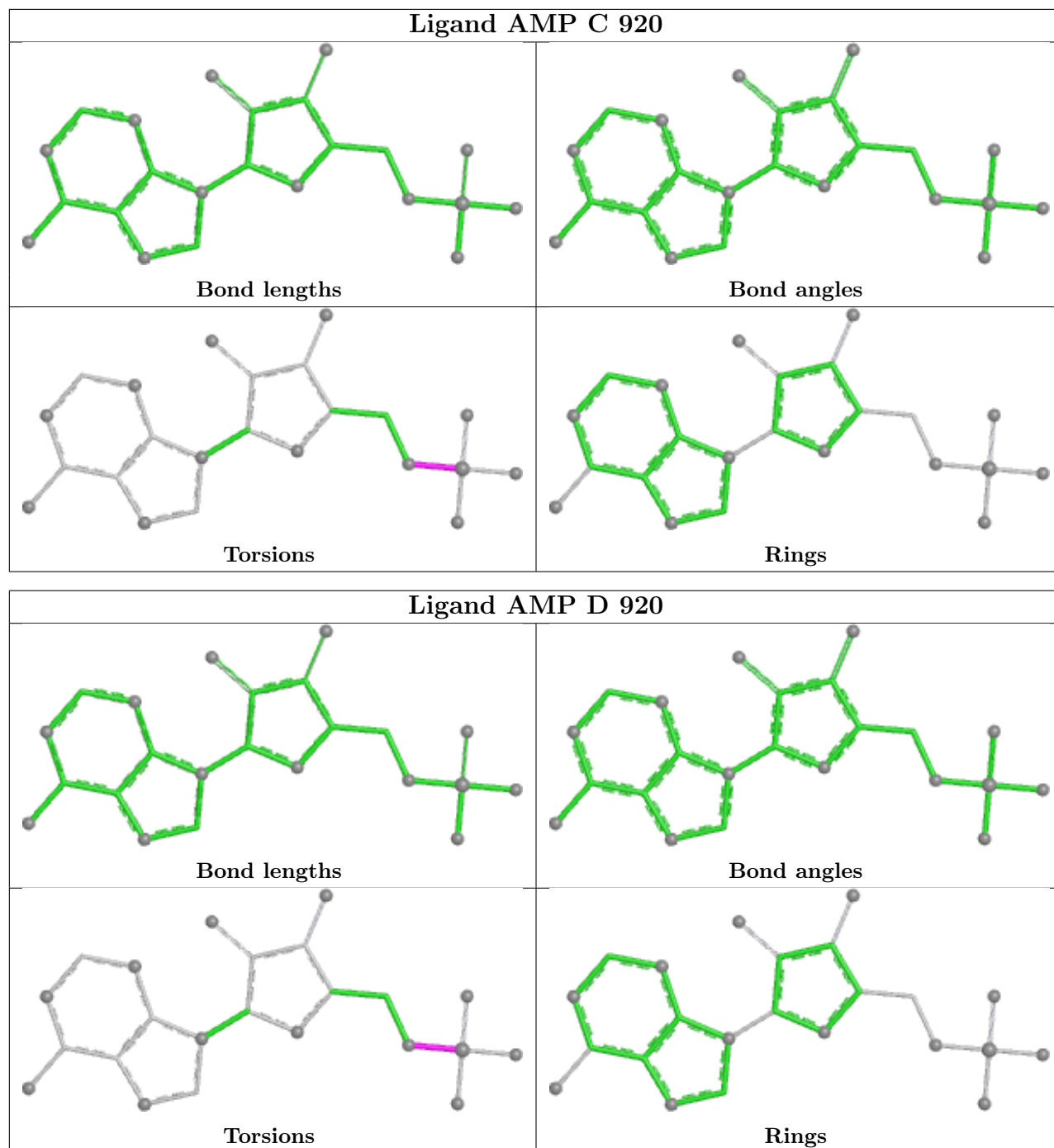
Mol	Chain	Res	Type	Atoms
4	A	920	AMP	C5'-O5'-P-O2P
4	A	920	AMP	C5'-O5'-P-O3P
4	B	920	AMP	C5'-O5'-P-O2P
4	B	920	AMP	C5'-O5'-P-O3P
4	C	920	AMP	C5'-O5'-P-O2P

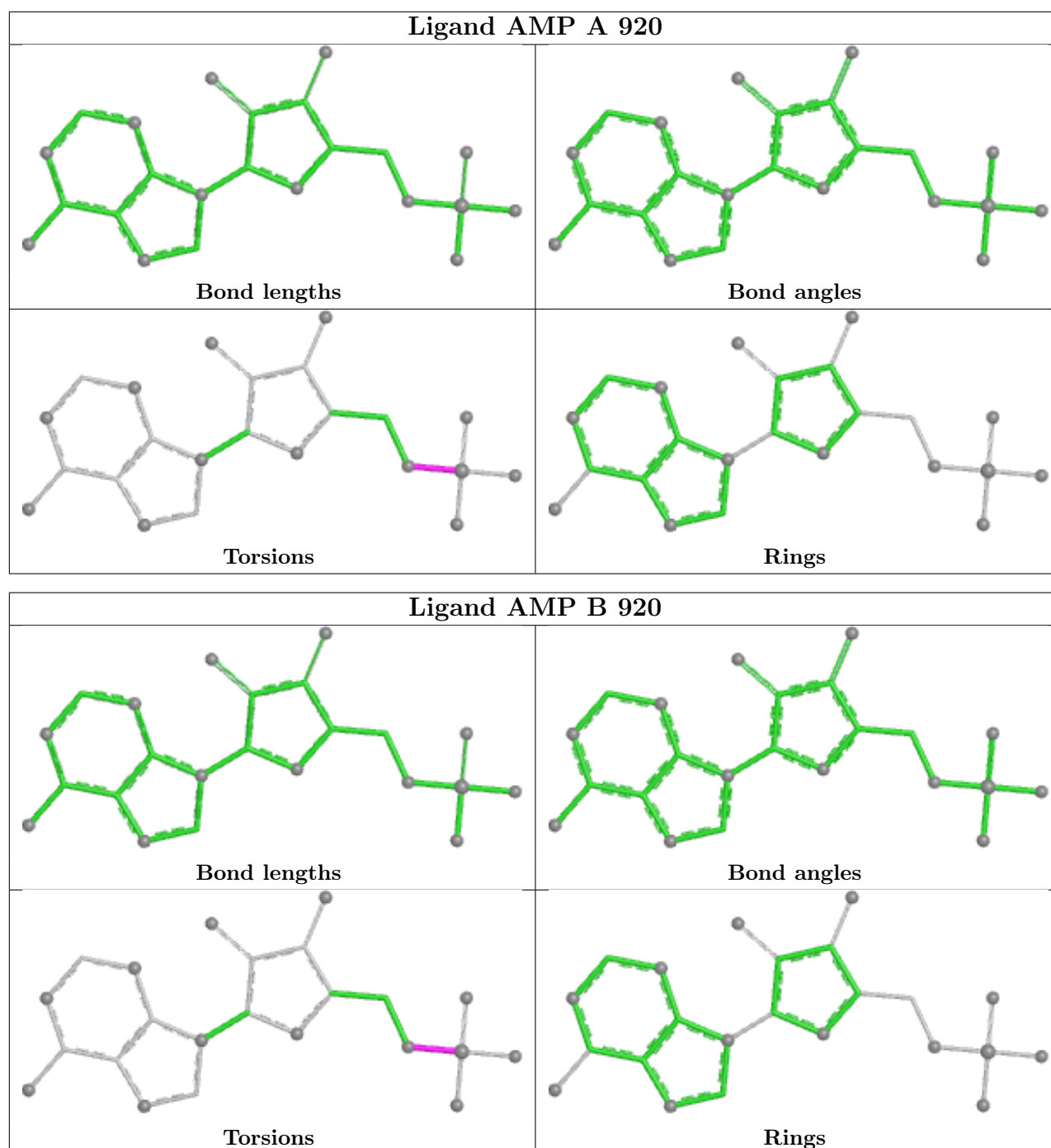
There are no ring outliers.

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	PLP	1	0
3	D	999	PLP	2	0
3	B	999	PLP	1	0
3	C	999	PLP	1	0
2	A	901	SO4	2	0
4	C	920	AMP	1	0
4	D	920	AMP	2	0
4	A	920	AMP	3	0
4	B	920	AMP	1	0
2	C	901	SO4	1	0
2	B	901	SO4	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 [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

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.