



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:31 AM UTC

PDB ID : 1ABB / pdb_00001abb
Title : CONTROL OF PHOSPHORYLASE B CONFORMATION BY A MODIFIED COFACTOR: CRYSTALLOGRAPHIC STUDIES ON R-STATE GLYCOGEN PHOSPHORYLASE RECONSTITUTED WITH PYRIDOXAL 5'-DIPHOSPHATE
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Deposited on : 1992-04-09
Resolution : 2.80 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

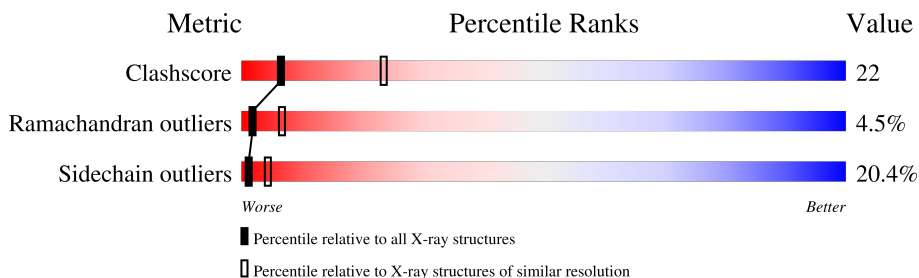
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	828	 34% 39% 20% 6%
1	B	828	 29% 39% 26% 6%
1	C	828	 31% 42% 21% 5%
1	D	828	 27% 38% 25% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26960 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	6693	4264	1185	1214	30	0	0	1
1	B	824	6693	4264	1185	1214	30	0	0	1
1	C	824	6693	4264	1185	1214	30	0	0	1
1	D	824	6693	4264	1185	1214	30	0	0	1

There are 4 discrepancies between the modelled and reference sequences:

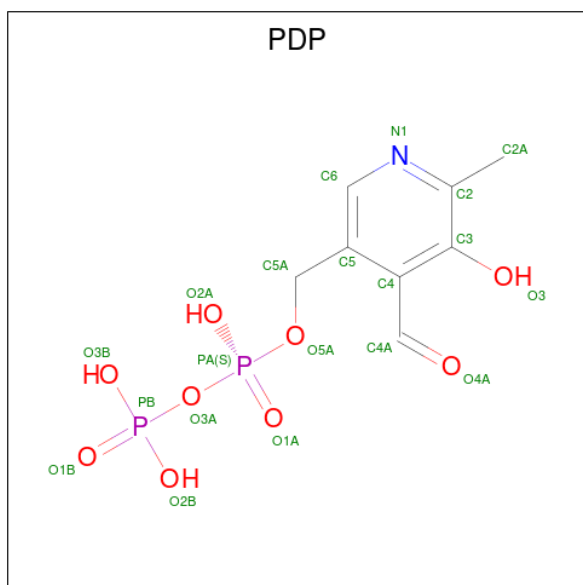
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489
B	380	ILE	LEU	conflict	UNP P00489
C	380	ILE	LEU	conflict	UNP P00489
D	380	ILE	LEU	conflict	UNP P00489

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



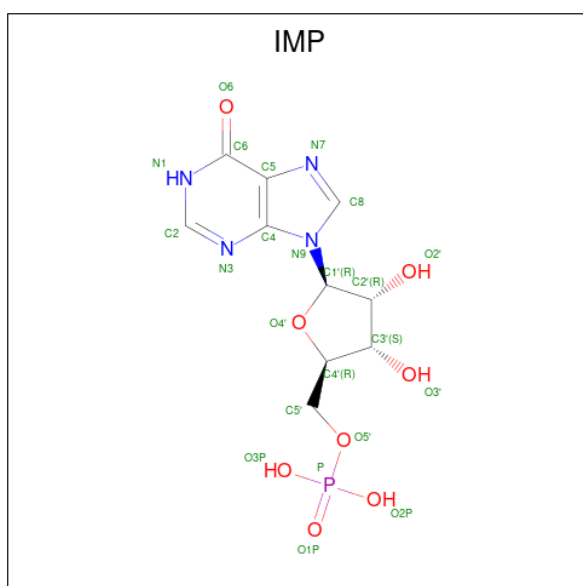
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PYRIDOXAL-5'-DIPHOSPHATE (CCD ID: PDP) (formula: $C_8H_{11}NO_9P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			19	8	1	8	2		
3	B	1	Total	C	N	O	P	0	0
			19	8	1	8	2		
3	C	1	Total	C	N	O	P	0	0
			19	8	1	8	2		
3	D	1	Total	C	N	O	P	0	0
			19	8	1	8	2		

- Molecule 4 is INOSINIC ACID (CCD ID: IMP) (formula: C₁₀H₁₃N₄O₈P).



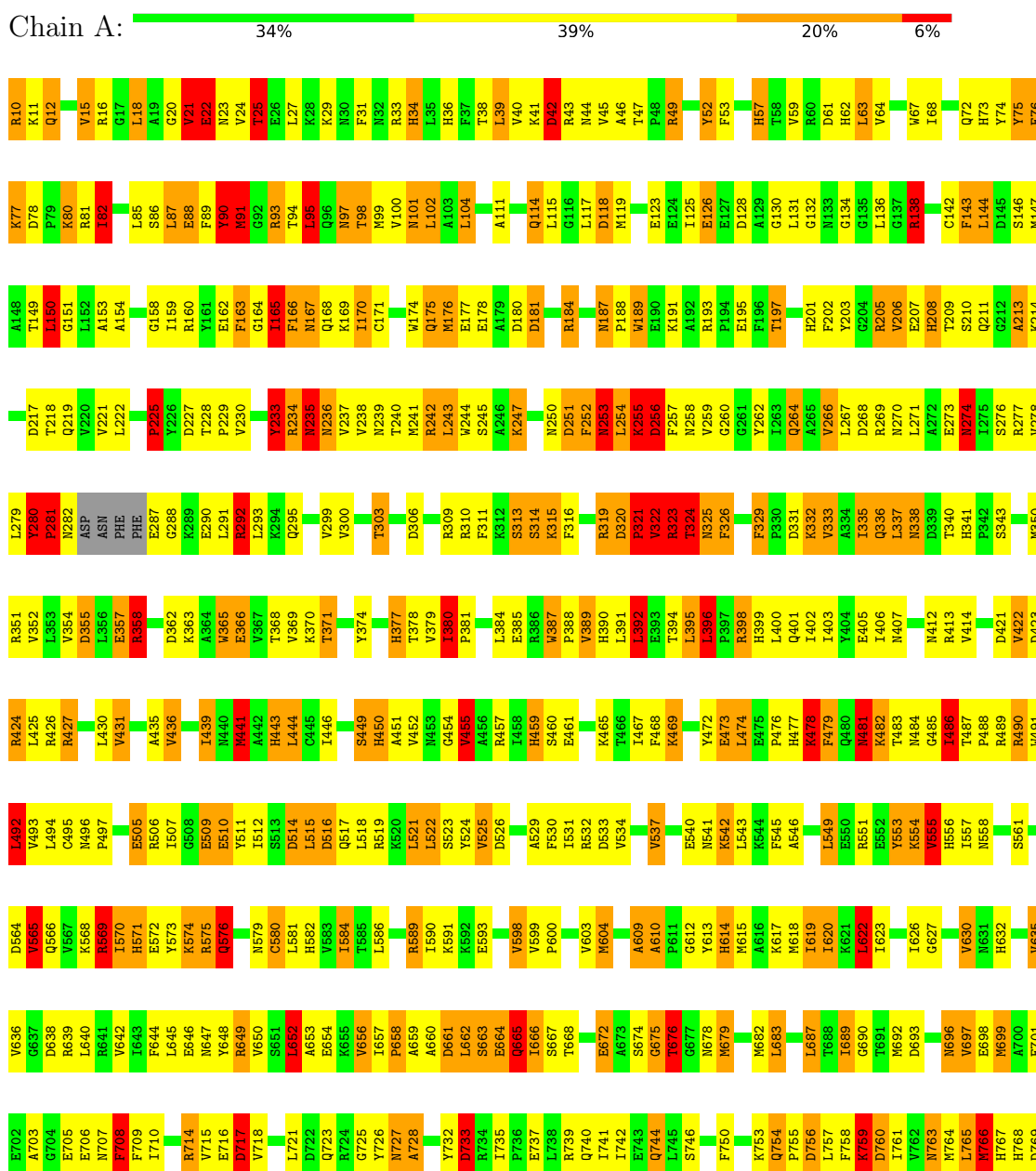
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
4	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

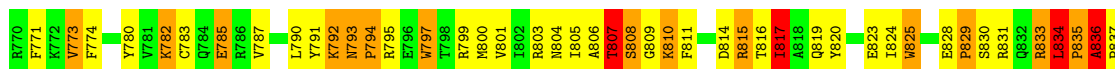
3 Residue-property plots

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.

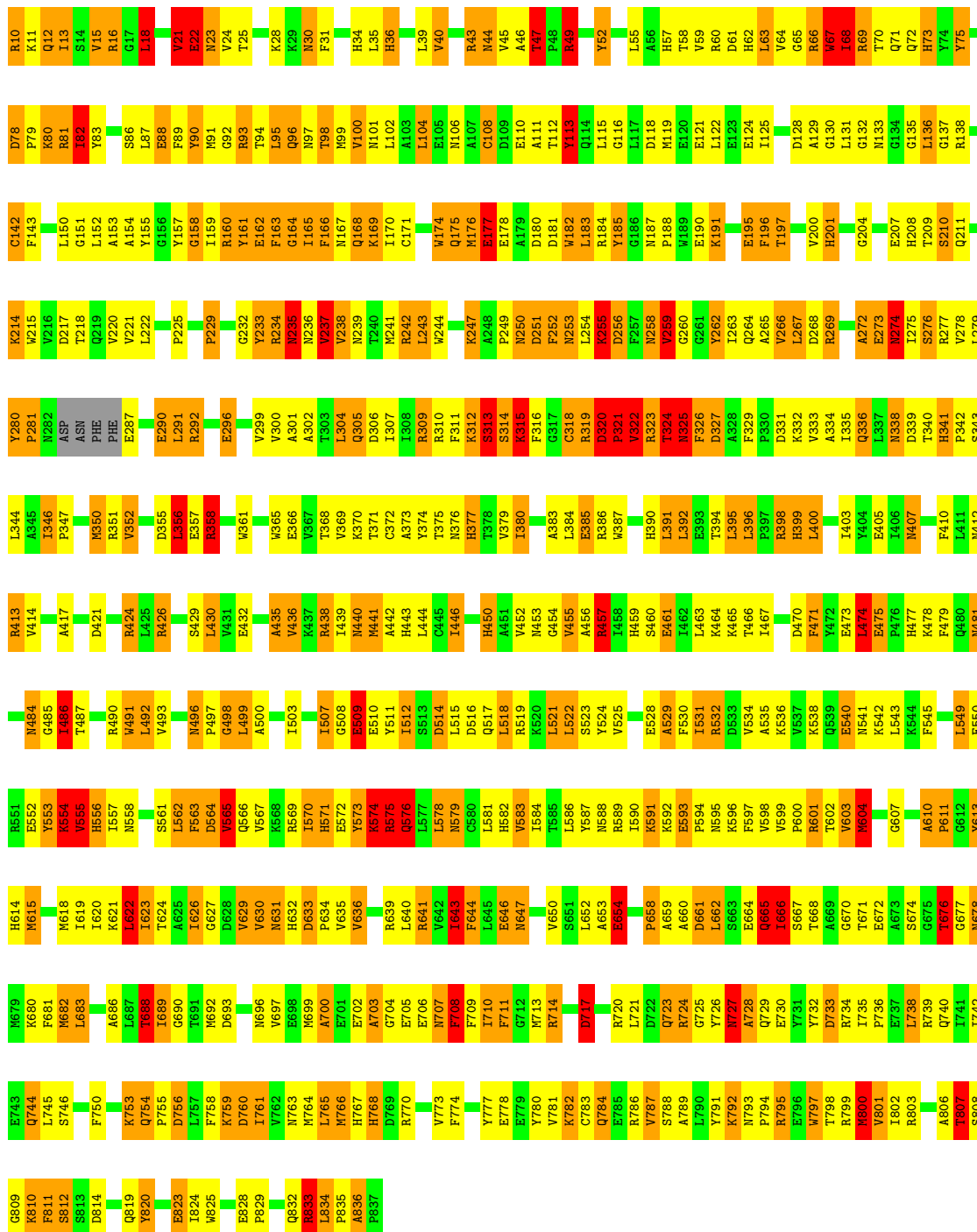
Note EDS was not executed.

- Molecule 1: GLYCOGEN PHOSPHORYLASE B





• Molecule 1: GLYCOGEN PHOSPHORYLASE B



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S808	8809	R810	F811	S812	S813	D814	R815	T816	I817	A818	O819	Y820	A821	R822	M825	G826	V827	E828	S830	R831	D832	R833	L834	F835	A836	F837	L144	D145	S146	M147	T148	A149	L150	G151	L152	A153	A154	Y155	G156	L157	F158	I159	Y160	M161	G162	R163	G164	I165	F166	M167	N168	Q169	M101	L102	A103	L104	G108	D109	E110	A111	Y112	Y113	A114	L115	G116	L117	D118	M119	L122	E123	E124	E126	G130	L131	G132	L136	G137	R138	A141	C142	F143
L200	Q401	I402	I403	Y404	E405	P406	Q408	A410	A411	A416	F418	P419	V422	D423	R427	M428	S429	L430	E357	R358	L359	D360	W361	K362	K363	A364	W365	E366	W367	T368	T371	C372	R309	R310	F311	K312	S313	S314	K315	F316	L304	O805	I307	M241	R242	L243	W244	S245	A246	K247	A248	P249	M250	D251	F252	Y253	L254	K191	E126	R192	R193	P194	E195	F196	T197	L198	P199	Q264	A265	V266	L267	D268									
R269	M270	E273	M274	T275	S276	R277	V278	L279	Y280	P281	M282	ASP	ASN	PHE	M224	M225	Y226	D227	T228	P229	L291	R292	L293	P231	K294	Q295	E296	V299	L304	O805	I307	M241	R242	L243	W244	S245	A246	K247	A248	P249	M250	D251	F252	Y253	L254	K191	E126	R192	R193	P194	E195	F196	T197	L198	P199	Q264	A265	V266	L267	D268																					
O386	L337	D338	N339	T340	H341	P342	S343	T346	P347	E348	L349	M350	R351	L353	V354	D355	L356	E357	R358	L359	D360	W361	K362	K363	A364	W365	E366	W367	T368	T371	C372	R309	R310	F311	K312	S313	S314	K315	F316	L304	O805	I307	M241	R242	L243	W244	S245	A246	K247	A248	P249	M250	D251	F252	Y253	L254	K191	E126	R192	R193	P194	E195	F196	T197	L198	P199	Q264	A265	V266	L267	D268										
L400	Q401	I402	I403	Y404	E405	P406	Q408	A410	A411	A416	F418	P419	V422	D423	R427	M428	S429	L430	E357	R358	L359	D360	W361	K362	K363	A364	W365	E366	W367	T368	T371	C372	R309	R310	F311	K312	S313	S314	K315	F316	L304	O805	I307	M241	R242	L243	W244	S245	A246	K247	A248	P249	M250	D251	F252	Y253	L254	K191	E126	R192	R193	P194	E195	F196	T197	L198	P199	Q264	A265	V266	L267	D268									
M484	Q485	T486	T487	P488	R489	A490	W491	L492	V493	F494	C495	M496	P497	G498	L499	I502	I503	A504	E505	R506	I507	G508	E509	E510	Y511	I512	S513	D514	L515	D516	Q517	L518	R519	H520	K521	L522	S523	Y524	V525	R526	D527	E528	A529	F530	I531	R532	L533	K534	L535	F536	Y537	V538	E539	K540	L541	M542	K543	P544	L545	M546	L547	L474	E475	P476	H477	K478	P479	Q480	K542	L543											
L549	E550	R551	E552	Y553	K554	R555	H556	I557	N558	P559	M560	S561	L562	F563	D564	V565	O566	R567	R568	E569	I570	H571	E572	Y573	R574	R575	L576	L577	R578	R579	C580	L581	H582	V583	I584	T585	L586	Y587	N588	R589	I590	K591	E592	E593	P594	N595	K596	F597	V598	Y599	P600	R601	T602	K538	O539	M604	N541	K542	L543																						
A609	A610	P611	G612	Y613	H614	M615	A616	K617	L618	I619	L620	K621	L622	I623	I626	G627	D628	V629	V630	M631	H632	D633	V636	G637	L640	R641	V642	L643	F644	L645	E646	M647	Y648	R649	V650	S651	L652	A653	S654	K655	V656	I657	P658	A659	A662	A663	L662	S663	E664	Q665	L666	S667	T671	S674	O675																										
T676	G677	N678	M679	K680	F681	M682	L683	N684	G685	A686	L687	T688	G689	T691	D692	D693	G694	A695	M696	E697	E698	M699	E702	A703	G704	E705	E706	N707	F708	F709	I710	F711	G712	M713	R714	Y715	E716	D717	Y718	L721	Y726	N727	A728	R729	E730	Y731	Y732	D733	R734	I735	F736	E737	L738	R739	Q740																										
I741	I742	E743	Q744	L745	S746	S747	F750	S751	P755	D756	L757	F758	K759	D760	I761	W762	N763	R764	M765	L766	H767	H768	D769	R770	F771	K772	W773	F774	E779	Y780	Y781	K782	C783	Q784	E785	R786	Y787	S788	A789	L790	Y791	K792	N793	P794	R795	E796	W797	T798	R799	M800	Y801	R802	R803	M804	T807																										
S808	G809	R810	F811	S812	S813	D814	R815	T816	I817	A818	O819	Y820	A821	R822	M825	G826	V827	E828	S830	R831	D832	R833	L834	F835	A836	F837	L144	D145	S146	M147	T148	A149	L150	G151	L152	A153	A154	Y155	G156	L157	F158	I159	Y160	M161	G162	R163	G164	I165	F166	M167	N168	Q169	M101	L102	A103	L104	G108	D109	E110	A111	Y112	Y113	A114	L115	G116	L117	D118	M119	L122	E123	E124	E126	G130	L131	G132	L136	G137	R138	A141	C142	F143

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 188.10Å 88.10Å 90.00° 109.29° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	26960	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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: PDP, IMP, 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	1.38	52/6843 (0.8%)	2.47	463/9258 (5.0%)
1	B	1.48	59/6843 (0.9%)	2.44	483/9258 (5.2%)
1	C	1.34	49/6843 (0.7%)	2.41	424/9258 (4.6%)
1	D	1.41	55/6843 (0.8%)	2.47	487/9258 (5.3%)
All	All	1.40	215/27372 (0.8%)	2.45	1857/37032 (5.0%)

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	10
1	C	0	4
1	D	0	7
All	All	0	27

The worst 5 of 215 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	68	ILE	N-CA	-37.23	0.99	1.46
1	B	80	LYS	CA-CB	-14.12	1.30	1.53
1	B	68	ILE	CB-CG1	13.90	1.81	1.53
1	A	657	ILE	CA-CB	11.59	1.59	1.54
1	B	69	ARG	CB-CG	10.60	1.84	1.52

The worst 5 of 1857 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	HIS	CA-CB-CG	25.28	139.08	113.80
1	A	16	ARG	N-CA-C	17.30	131.87	111.11
1	C	455	VAL	N-CA-CB	-16.68	90.47	112.16
1	A	61	ASP	CA-CB-CG	16.39	128.99	112.60
1	B	68	ILE	CB-CG1-CD1	16.11	147.63	113.80

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	ARG	Sidechain
1	A	280	TYR	Peptide
1	A	320	ASP	Peptide
1	A	52	TYR	Sidechain
1	A	90	TYR	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	6693	0	6653	247	3
1	B	6693	0	6653	300	3
1	C	6693	0	6653	284	0
1	D	6693	0	6653	356	6
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
3	A	19	0	7	2	0
3	B	19	0	7	2	0
3	C	19	0	6	1	0
3	D	19	0	6	1	0
4	A	23	0	11	2	0
4	B	23	0	11	4	0
4	C	23	0	11	1	0
4	D	23	0	11	1	0
All	All	26960	0	26682	1167	6

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 22.

The worst 5 of 1167 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:68:ILE:CB	1:B:68:ILE:CG1	1.81	1.57
1:B:69:ARG:CG	1:B:69:ARG:CB	1.84	1.54
1:B:73:HIS:CD2	1:B:834:LEU:HD21	1.61	1.30
1:B:69:ARG:CG	1:B:69:ARG:CA	2.33	1.06
1:B:73:HIS:CD2	1:B:834:LEU:CD2	2.32	1.01

The worst 5 of 6 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:510:GLU:N	1:D:323:ARG:NH2[2_646]	1.85	0.35
1:B:595:ASN:O	1:D:22:GLU:O[2_746]	1.87	0.33
1:A:25:THR:OG1	1:D:822:ARG:O[2_646]	1.98	0.22
1:B:595:ASN:OD1	1:D:21:VAL:N[2_746]	2.04	0.16
1:B:595:ASN:OD1	1:D:20:GLY:C[2_746]	2.10	0.10

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	820/828 (99%)	676 (82%)	104 (13%)	40 (5%)	1	6
1	B	820/828 (99%)	699 (85%)	83 (10%)	38 (5%)	2	6
1	C	820/828 (99%)	680 (83%)	107 (13%)	33 (4%)	2	8
1	D	820/828 (99%)	665 (81%)	117 (14%)	38 (5%)	2	6
All	All	3280/3312 (99%)	2720 (83%)	411 (12%)	149 (4%)	2	7

5 of 149 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	ARG
1	A	151	GLY
1	A	233	TYR
1	A	236	ASN
1	A	321	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	712/717 (99%)	569 (80%)	143 (20%)	1	4
1	B	712/717 (99%)	574 (81%)	138 (19%)	1	5
1	C	712/717 (99%)	575 (81%)	137 (19%)	1	5
1	D	712/717 (99%)	549 (77%)	163 (23%)	1	3
All	All	2848/2868 (99%)	2267 (80%)	581 (20%)	1	4

5 of 581 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	266	VAL
1	D	800	MET
1	D	315	LYS
1	D	262	TYR
1	D	540	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	167	ASN
1	D	665	GLN
1	D	235	ASN
1	D	453	ASN
1	B	377	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](#)

12 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	PDP	B	932	1	18,19,20	2.02	4 (22%)	26,29,30	1.41	5 (19%)
2	SO4	C	900	-	4,4,4	0.22	0	6,6,6	0.52	0
4	IMP	D	920	-	25,25,25	1.35	3 (12%)	37,38,38	1.51	5 (13%)
3	PDP	A	931	1	18,19,20	2.15	2 (11%)	26,29,30	1.32	4 (15%)
2	SO4	D	900	-	4,4,4	0.11	0	6,6,6	0.40	0
4	IMP	B	920	-	25,25,25	1.60	4 (16%)	37,38,38	1.83	7 (18%)
2	SO4	B	900	-	4,4,4	0.35	0	6,6,6	0.53	0
3	PDP	D	934	1	18,19,20	2.77	4 (22%)	26,29,30	1.17	3 (11%)
4	IMP	A	920	-	25,25,25	1.68	5 (20%)	37,38,38	1.75	7 (18%)
3	PDP	C	933	1	18,19,20	1.35	3 (16%)	26,29,30	1.16	3 (11%)
4	IMP	C	920	-	25,25,25	1.55	6 (24%)	37,38,38	1.81	9 (24%)
2	SO4	A	900	-	4,4,4	0.34	0	6,6,6	0.42	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	PDP	B	932	1	-	4/12/12/14	0/1/1/1
4	IMP	D	920	-	-	1/10/26/26	0/3/3/3
3	PDP	A	931	1	-	5/12/12/14	0/1/1/1
4	IMP	B	920	-	-	1/10/26/26	0/3/3/3
4	IMP	A	920	-	-	0/10/26/26	0/3/3/3
3	PDP	D	934	1	-	5/12/12/14	0/1/1/1
3	PDP	C	933	1	-	5/12/12/14	0/1/1/1
4	IMP	C	920	-	-	0/10/26/26	0/3/3/3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	934	PDP	PA-O3A	9.31	1.69	1.59
3	A	931	PDP	PA-O3A	7.41	1.67	1.59
3	D	934	PDP	C3-C2	-5.04	1.35	1.41
3	B	932	PDP	C3-C2	-4.66	1.36	1.41
4	A	920	IMP	O6-C6	4.49	1.32	1.23

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	920	IMP	C2-N1-C6	-5.24	117.91	125.09
4	B	920	IMP	C5-C6-N1	5.02	118.00	110.78
4	D	920	IMP	C5-C6-N1	4.78	117.66	110.78
4	A	920	IMP	C5-C6-N1	4.70	117.54	110.78
4	B	920	IMP	C2-N1-C6	-4.61	118.77	125.09

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

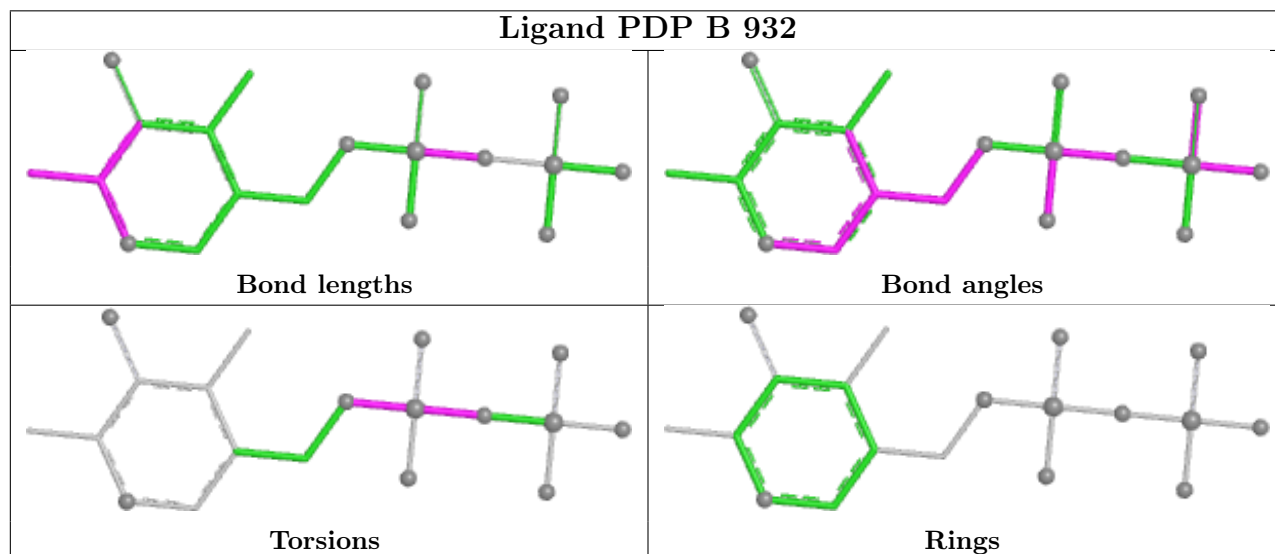
Mol	Chain	Res	Type	Atoms
3	A	931	PDP	C5A-O5A-PA-O1A
3	A	931	PDP	C5A-O5A-PA-O3A
3	A	931	PDP	C5A-O5A-PA-O2A
3	B	932	PDP	C5A-O5A-PA-O3A
3	C	933	PDP	C5A-O5A-PA-O2A

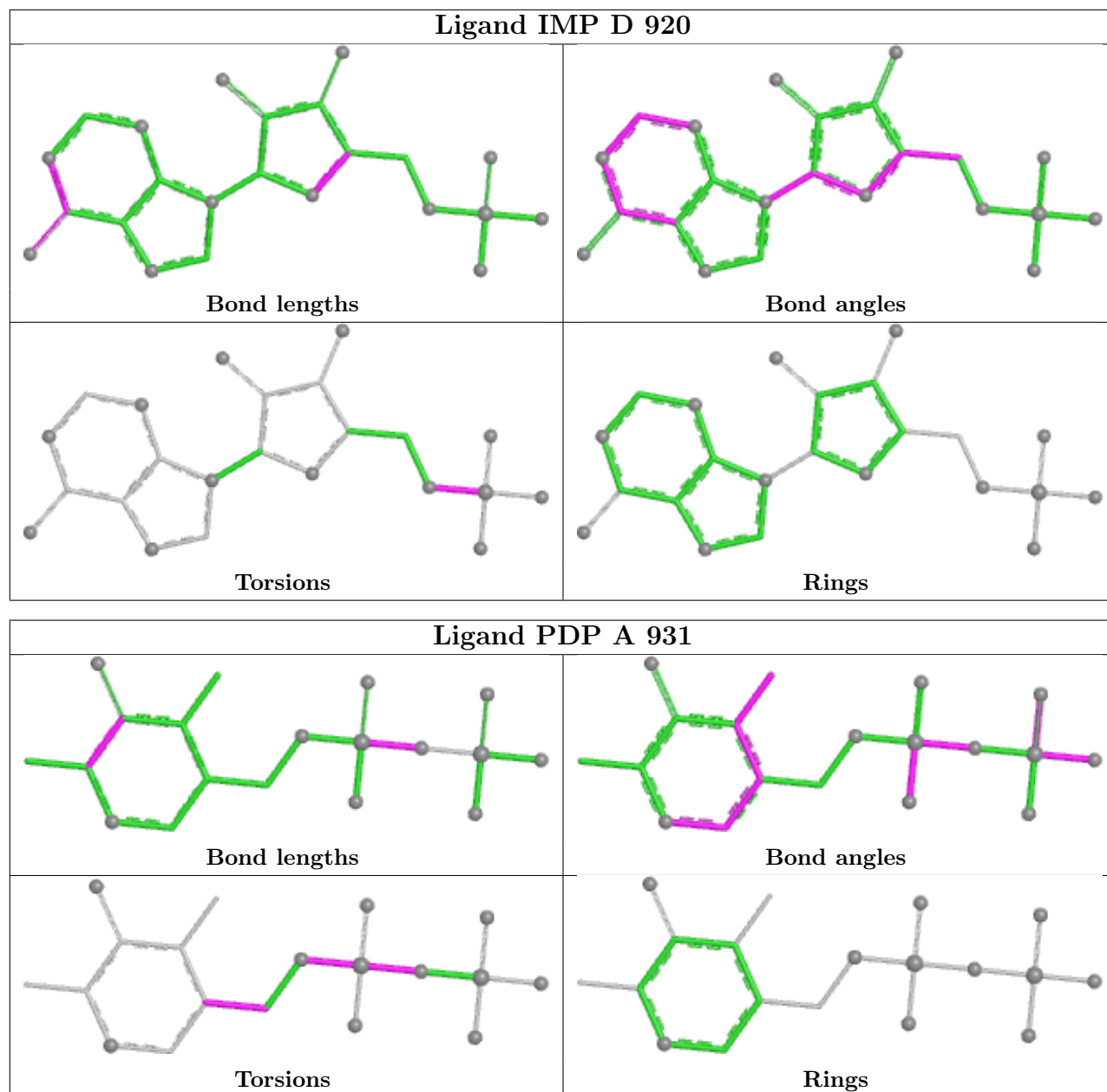
There are no ring outliers.

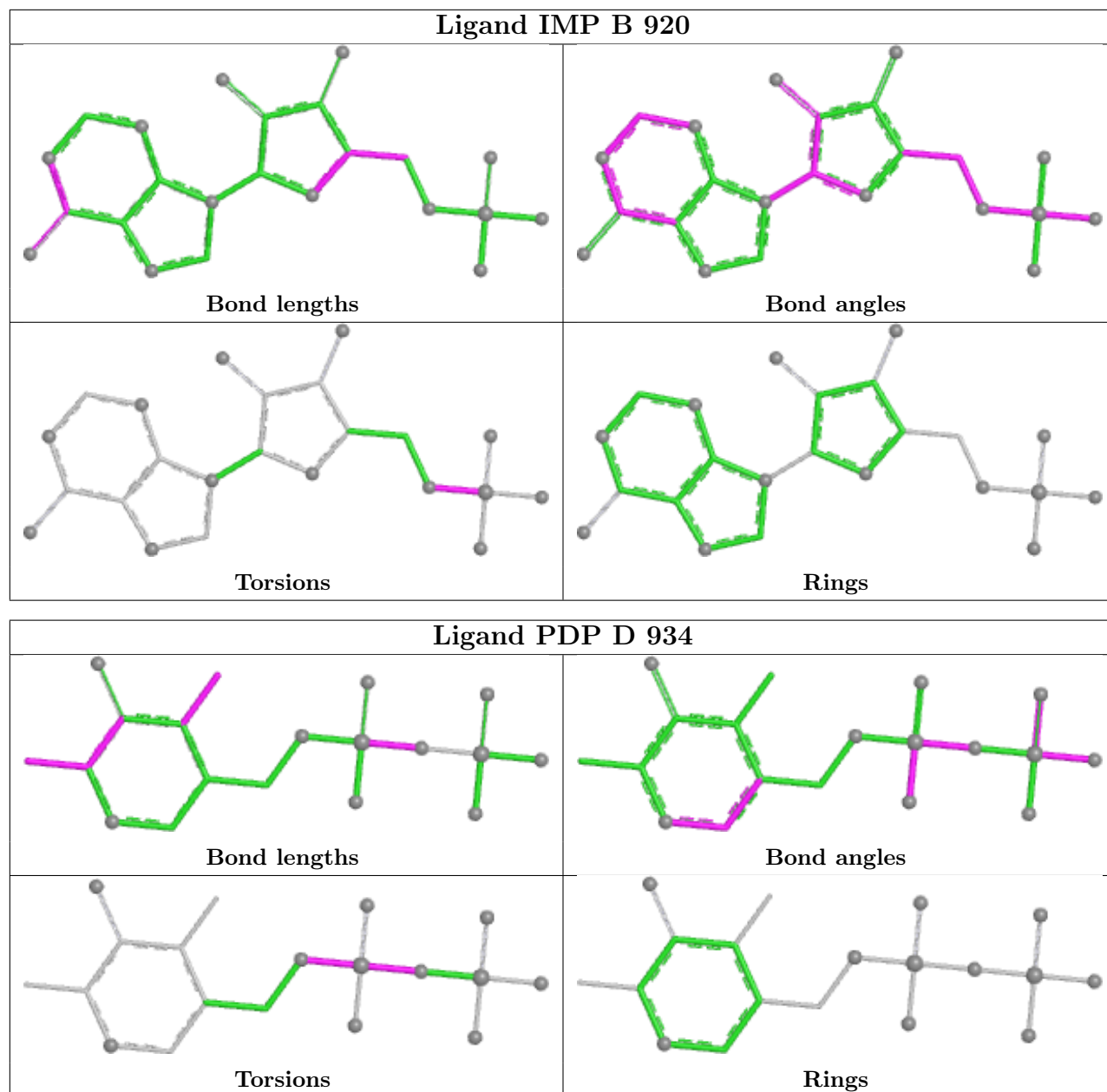
9 monomers are involved in 15 short contacts:

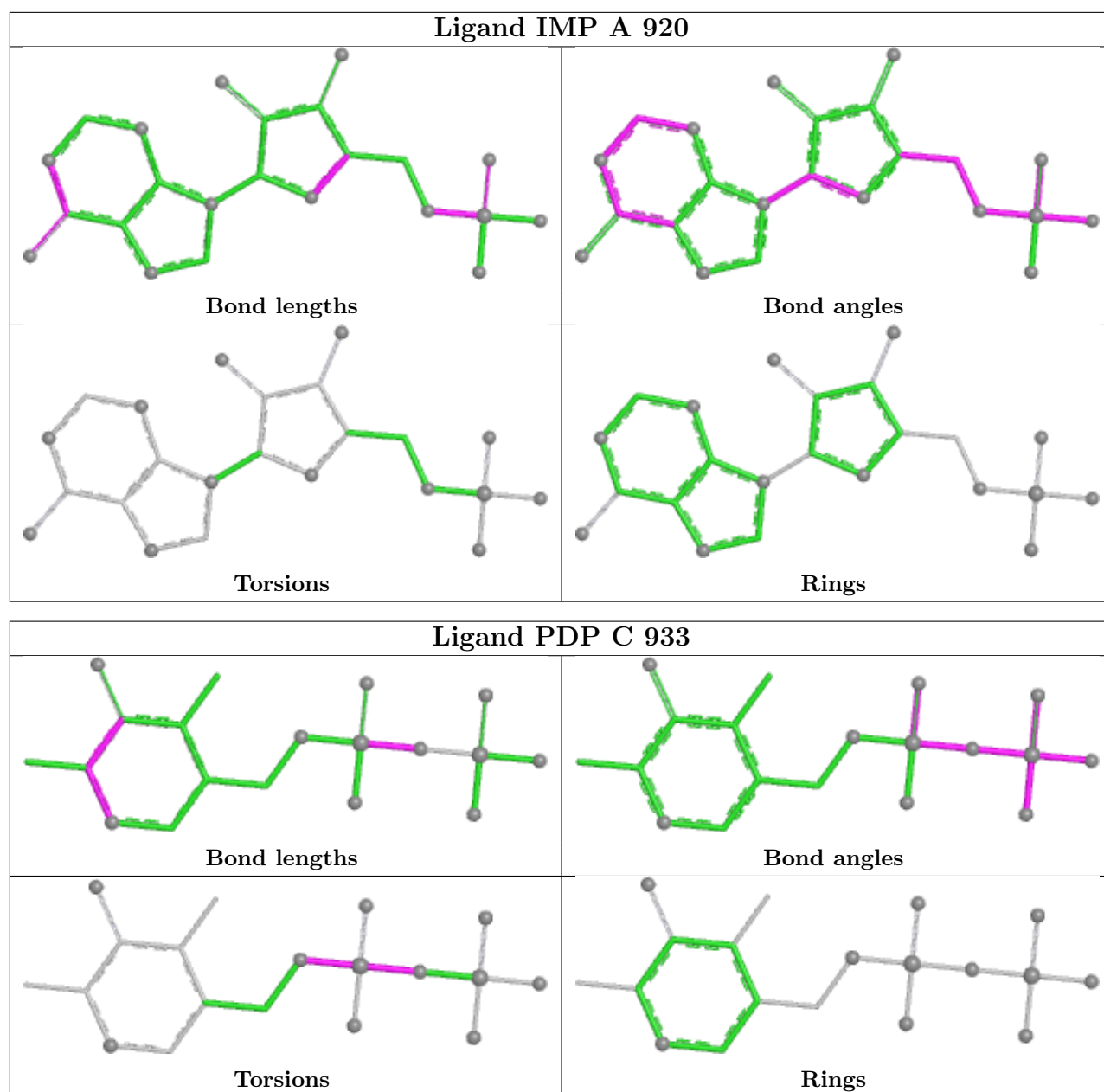
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	932	PDP	2	0
4	D	920	IMP	1	0
3	A	931	PDP	2	0
2	D	900	SO4	1	0
4	B	920	IMP	4	0
3	D	934	PDP	1	0
4	A	920	IMP	2	0
3	C	933	PDP	1	0
4	C	920	IMP	1	0

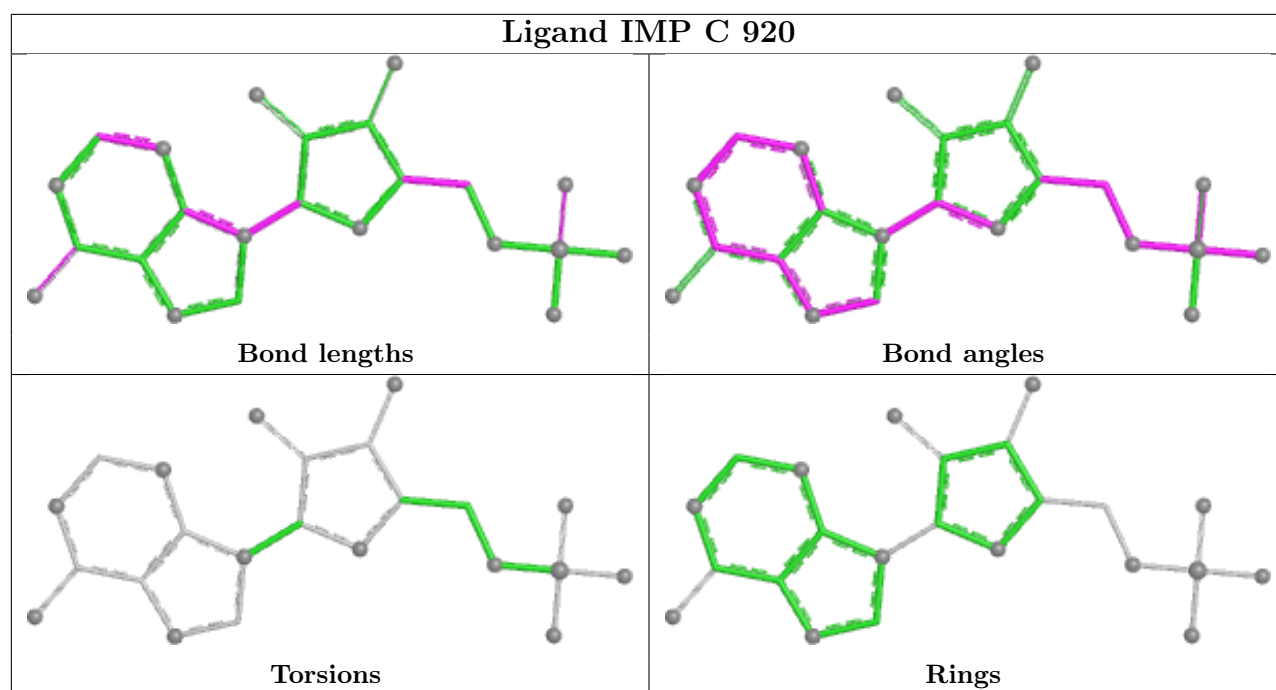
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.