



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:45 PM UTC

PDB ID : 1RWQ / pdb_00001rwq
Title : Human Dipeptidyl peptidase IV in complex with 5-aminomethyl-6-(2,4-dichloro-phenyl)-2-(3,5-dimethoxy-phenyl)-pyrimidin-4-ylamine
Authors : Hennig, M.; Thoma, R.; Stihle, M.
Deposited on : 2003-12-17
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

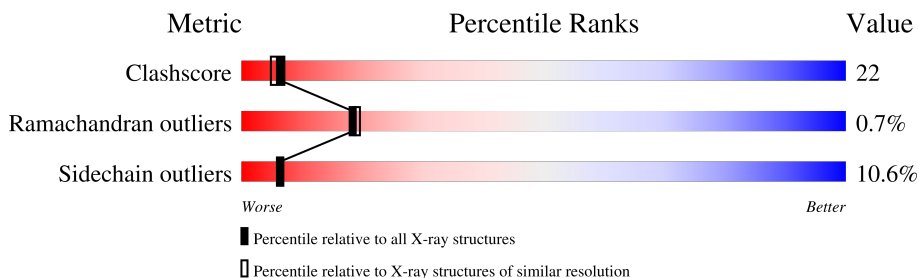
1 Overall quality at a glance

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	728	53% 37% 9%
1	B	728	55% 36% 8%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12190 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 Dipeptidyl peptidase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



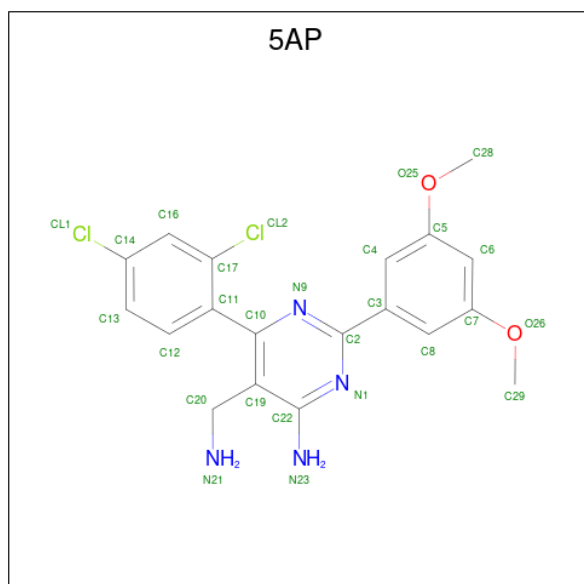
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 5-(AMINOMETHYL)-6-(2,4-DICHLOROPHENYL)-2-(3,5-DIMETHOXYPHENYL)PYRIMIDIN-4-AMINE (CCD ID: 5AP) (formula: C₁₉H₁₈Cl₂N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0
			27	19	2	4	2	0
3	B	1	Total	C	Cl	N	O	0
			27	19	2	4	2	0

- Molecule 4 is water.

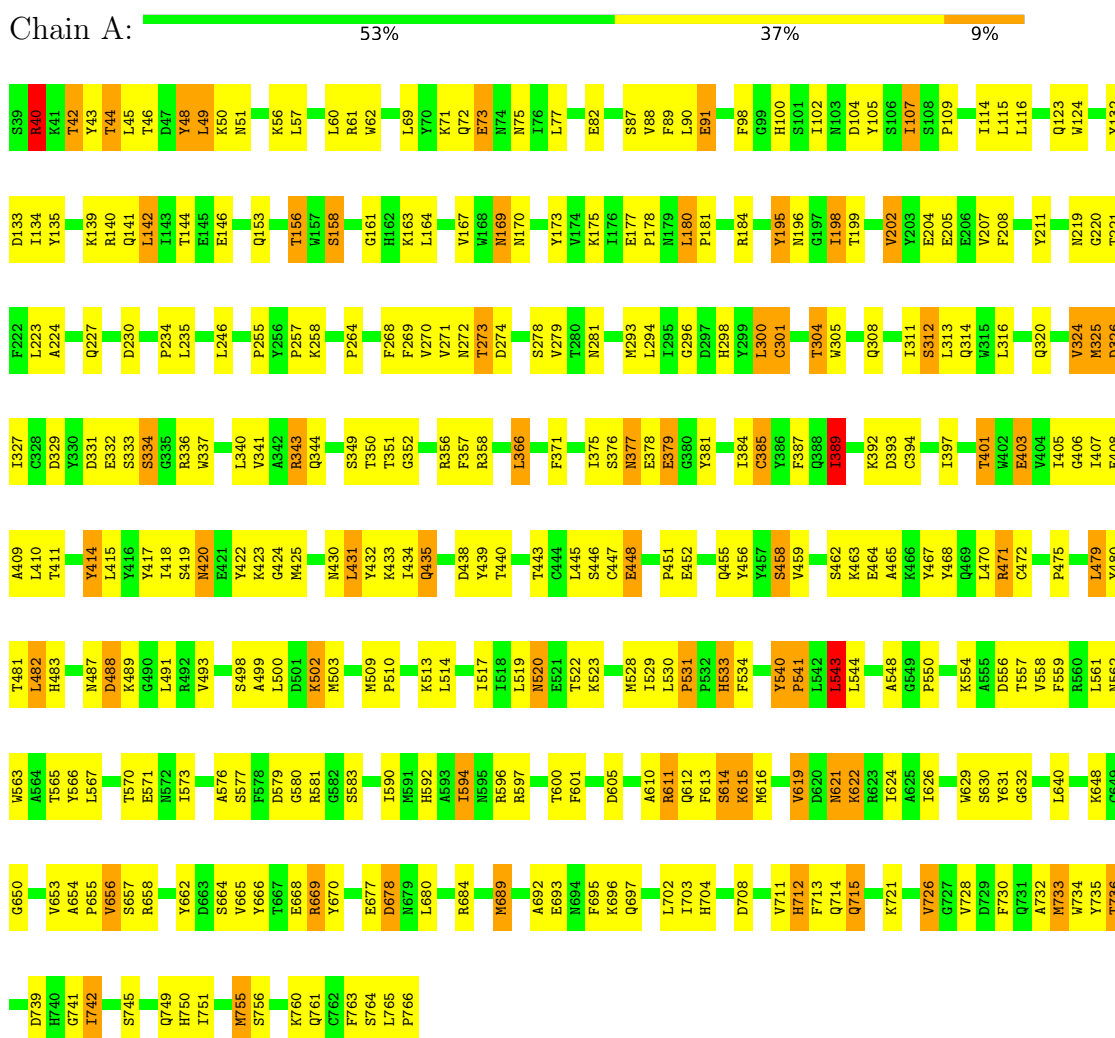
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		
4	B	51	Total	O	0	0
			51	51		

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: Dipeptidyl peptidase IV



• Molecule 1: Dipeptidyl peptidase IV



I719	S637	V558	K466	E379	L294	D200	T114	S39
V726	M638	V639	Y467	H383	I295	W201	L115	R40
Q731	L640	N562	Q469	Y386	H298	V202	E117	K41
A732	G643	V563	L470	F387	Y299	E206	Y120	Y43
H733	S644	A564	R471	F387	L300	V207	K122	T44
W734	G645	T565	C472	Q388	V303	F208	Y120	L45
Y735	V646	Y566		I389			K122	T46
T736	L567	L567					Q123	
D737	R648	L567	P478	K392	A306	Y211	W124	L49
	C649	S569	L479	D393	T307	L214	R125	K50
G741	G650	T570	Y480	C394	Q308	W215	H126	N51
I742	I651		L482		E309	W216	S127	T52
H750	A652	I574	H483	I397	R310	S217	S127	Y53
I751	V653	V575	S484	T398	I311	P218	R54	
Y752	A654	A576	S485		S312	N219	Y132	
T753		G580	V486	W402	L313	G220	D136	L60
H757	S657	R581		E403	Q314	T221	L137	
F758	R658	V493	R492	W404	I319	F222	N138	T63
I759	Y660	L494	L494	I405	L320	L223	K139	S64
		Y585	L410		N321	A224	R140	D65
			L500		Y322	Q227	Q141	H66
				Y414			L142	E67
	D663	I590	V507	L415	M325	T236	T144	T68
	S664	N591	Q508	Y416	D326	E237	E145	L69
	Y666	H592	M509		I327		E146	Y70
		A593	P510			S242	N150	Q72
R669		I594	S511	W420	Y330	D243		E73
Y670		N595	S611	E421	D331	E244		H74
M671		R596	K512	Y422	E332	S245	V155	N75
		S597	K513	K423	S333	L246	T156	
		L598	L514			Q247	W157	
T675		G599		G428		Y248	S158	V78
P676		T600	I517	R429	W337		P159	
E677		F601	I518	N430	N338			E82
D678		E602	L519	L431	C339	R253	V160	
N679		V603	M520	Y432	L340		G161	N85
L680		E604	E521	K433	R341	Y256	H162	S86
D681		D605	T522	I434	A342	P257	K163	S87
H682		Q606	K523	Q435	R343	N263	V88	
Y683		I607		L436		Y270	N179	F89
R684			Y526		E347	V271	L180	L90
		F613	Q527	K441	M348	P264	P181	E91
		S614	E528	V442	S349	T265	K175	N92
		K615	I529	T143	T350	K267	I176	S93
		M616		C444	T351		E177	T94
			P532	L445		V270	P178	F95
		V619	H533	S446	V354	V271	L180	D96
		D620	F534			N272		
		N621	D635	E452	P362	T273		N103
					H363		T188	D104
		T624	L542	Y456	F364	S277	G189	S105
N710		A625	L543		T365	S278	K190	Y106
H712		L636	L544	V459	K374	V279	E191	I107
F713			D545	S460	I374	T280	D192	S108
Q714		S630	V546	F461	S462		I193	P109
Q715				S462	S376		I194	D110
S716		G633	G549	K463	S376	Q286	Y195	G111
A717				E464	N377		N196	Q112
F718		T636	S552	A465	F379	W203		S113

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.68Å 69.14Å 422.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20	Depositor
% Data completeness (in resolution range)	84.3 (15.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.239 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12190	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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: NAG, 5AP

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	1.24	17/6135 (0.3%)	1.42	51/8344 (0.6%)
1	B	1.29	19/6135 (0.3%)	1.47	66/8344 (0.8%)
All	All	1.27	36/12270 (0.3%)	1.45	117/16688 (0.7%)

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	719	ILE	CA-CB	-10.09	1.42	1.54
1	B	630	SER	CA-C	-8.26	1.46	1.53
1	A	733	MET	SD-CE	7.58	1.98	1.79
1	A	207	VAL	C-O	-7.16	1.15	1.24
1	A	678	ASP	CA-C	7.08	1.55	1.52

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	ILE	N-CA-C	11.97	122.83	110.62
1	A	301	CYS	N-CA-C	8.66	123.97	113.41
1	A	590	ILE	N-CA-C	-8.61	104.41	111.81
1	A	133	ASP	N-CA-C	-8.34	96.33	109.50
1	B	389	ILE	N-CA-C	8.12	119.88	110.62

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	5963	0	5681	258	0
1	B	5963	0	5683	253	0
2	A	56	0	52	2	0
2	B	56	0	52	9	0
3	A	27	0	18	5	0
3	B	27	0	18	0	0
4	A	47	0	0	5	0
4	B	51	0	0	0	0
All	All	12190	0	11504	510	0

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 510 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:150:ASN:HD21	2:B:793:NAG:C1	1.45	1.28
1:B:600:THR:CG2	1:B:601:PHE:H	1.59	1.15
1:B:267:LYS:HD2	1:B:286:GLN:HE22	1.06	1.12
1:B:92:ASN:HD22	2:B:797:NAG:C1	1.65	1.08
1:B:600:THR:HG22	1:B:601:PHE:H	1.23	1.02

There are no symmetry-related clashes.

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	726/728 (100%)	665 (92%)	54 (7%)	7 (1%)	12	11
1	B	726/728 (100%)	665 (92%)	58 (8%)	3 (0%)	30	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1452/1456 (100%)	1330 (92%)	112 (8%)	10 (1%)	18	19

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	488	ASP
1	B	111	GLY
1	B	242	SER
1	A	615	LYS

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	653/653 (100%)	585 (90%)	68 (10%)	7	7
1	B	653/653 (100%)	582 (89%)	71 (11%)	6	6
All	All	1306/1306 (100%)	1167 (89%)	139 (11%)	6	6

5 of 139 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	500	LEU
1	B	521	GLU
1	B	626	ILE
1	A	482	LEU
1	A	479	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	377	ASN
1	B	562	ASN
1	B	383	HIS

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Mol	Chain	Res	Type
1	B	435	GLN
1	B	621	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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	NAG	A	794	1	14,14,15	1.00	1 (7%)	17,19,21	2.15	6 (35%)
2	NAG	B	796	1	14,14,15	0.90	1 (7%)	17,19,21	1.40	3 (17%)
2	NAG	B	793	1	14,14,15	0.67	0	17,19,21	1.27	2 (11%)
2	NAG	A	793	1	14,14,15	0.70	1 (7%)	17,19,21	2.29	6 (35%)
3	5AP	A	900	-	29,29,29	2.05	6 (20%)	37,41,41	2.29	13 (35%)
2	NAG	A	795	1	14,14,15	0.72	0	17,19,21	2.29	4 (23%)
3	5AP	B	1900	-	29,29,29	1.64	6 (20%)	37,41,41	1.89	11 (29%)
2	NAG	B	794	1	14,14,15	0.71	0	17,19,21	1.39	2 (11%)
2	NAG	A	796	1	14,14,15	0.74	0	17,19,21	1.97	5 (29%)
2	NAG	B	797	1	14,14,15	0.62	0	17,19,21	1.83	4 (23%)

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	NAG	A	794	1	-	0/6/23/26	0/1/1/1
2	NAG	B	796	1	-	1/6/23/26	0/1/1/1
2	NAG	B	793	1	-	5/6/23/26	0/1/1/1
2	NAG	A	793	1	-	5/6/23/26	0/1/1/1
3	5AP	A	900	-	-	2/12/14/14	0/3/3/3
2	NAG	A	795	1	-	5/6/23/26	0/1/1/1
3	5AP	B	1900	-	-	4/12/14/14	0/3/3/3
2	NAG	B	794	1	-	4/6/23/26	0/1/1/1
2	NAG	A	796	1	-	0/6/23/26	0/1/1/1
2	NAG	B	797	1	-	2/6/23/26	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	5AP	C11-C10	-7.98	1.41	1.49
3	B	1900	5AP	C10-N9	-3.88	1.28	1.34
3	B	1900	5AP	C19-C22	3.70	1.47	1.41
3	A	900	5AP	C10-C19	3.38	1.47	1.41
3	B	1900	5AP	C12-C11	-3.13	1.35	1.40

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	793	NAG	C4-C3-C2	-5.88	102.40	111.02
3	A	900	5AP	C22-N1-C2	5.68	124.22	117.36
3	A	900	5AP	C16-C17-C11	5.11	125.94	121.97
2	A	795	NAG	C4-C3-C2	-5.01	103.67	111.02
2	A	796	NAG	C2-N2-C7	-4.97	116.23	122.90

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	793	NAG	C3-C2-N2-C7
2	A	793	NAG	C8-C7-N2-C2
2	A	793	NAG	O7-C7-N2-C2

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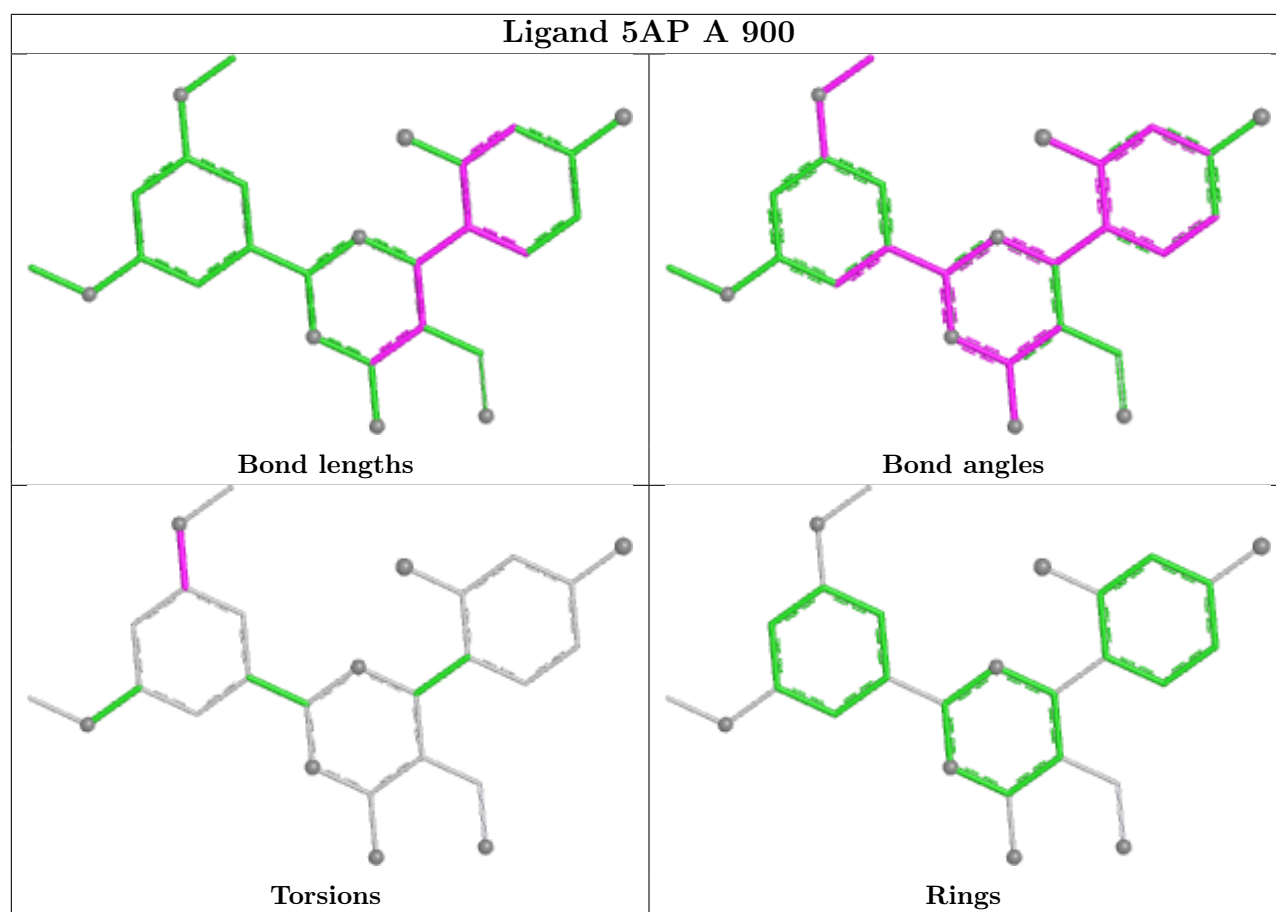
Mol	Chain	Res	Type	Atoms
2	B	793	NAG	C1-C2-N2-C7
2	B	793	NAG	C8-C7-N2-C2

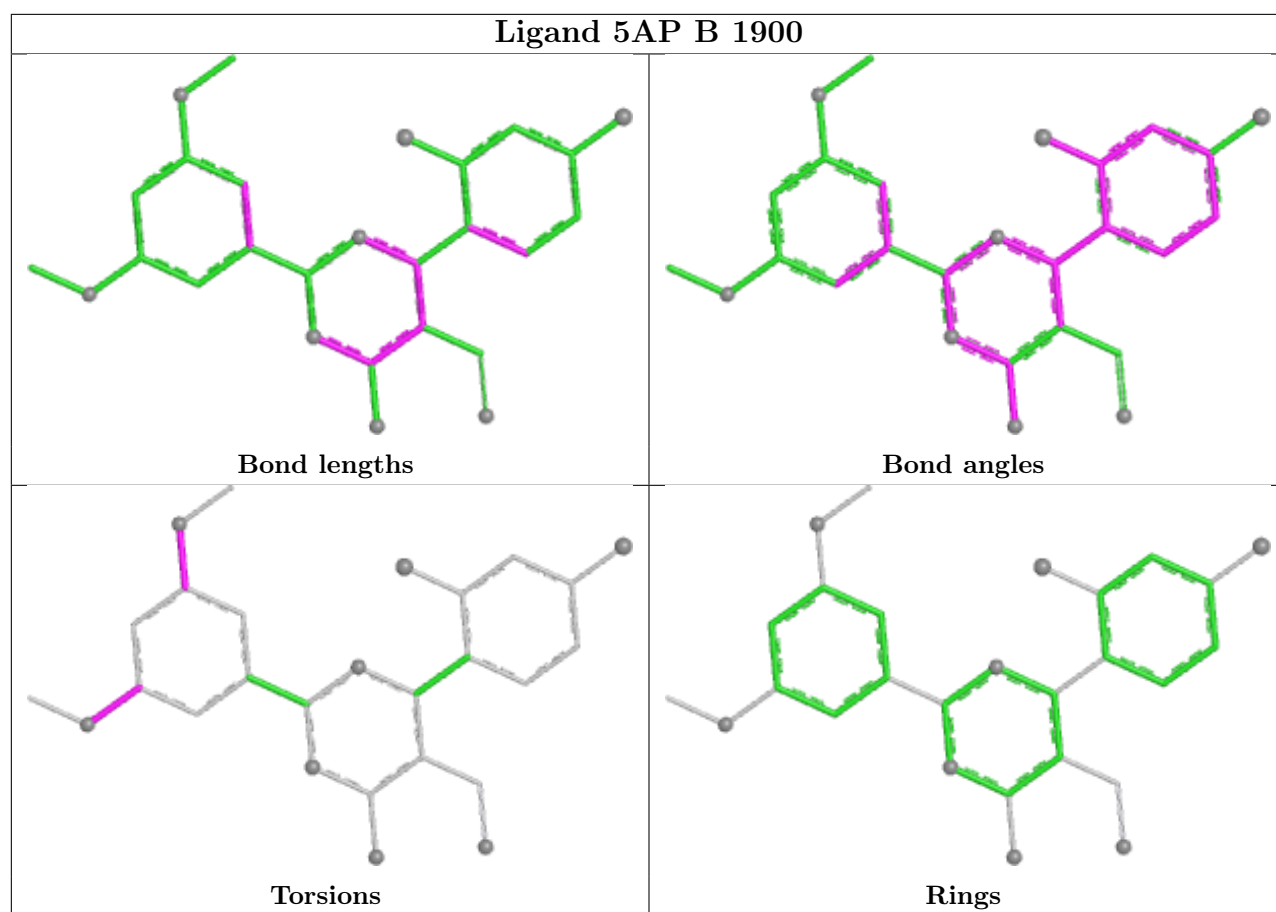
There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	793	NAG	5	0
2	A	793	NAG	1	0
3	A	900	5AP	5	0
2	A	795	NAG	1	0
2	B	794	NAG	2	0
2	B	797	NAG	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.