wwPDB X-ray Structure Validation Summary Report (i)

Jul 31, 2023 – 07:16 AM EDT

PDB ID	:	1XKB
Title	:	FACTOR XA COMPLEXED WITH A SYNTHETIC INHIBITOR FX-2212 A,(2S)-(3'-AMIDINO-3-BIPHENYLYL)-5-(4-PYRIDYLAMINO)PENTANOIC ACID
Authors	:	Kamata, K.; Kim, S.H.
Deposited on	:	1998-03-19
Resolution	:	2.40 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

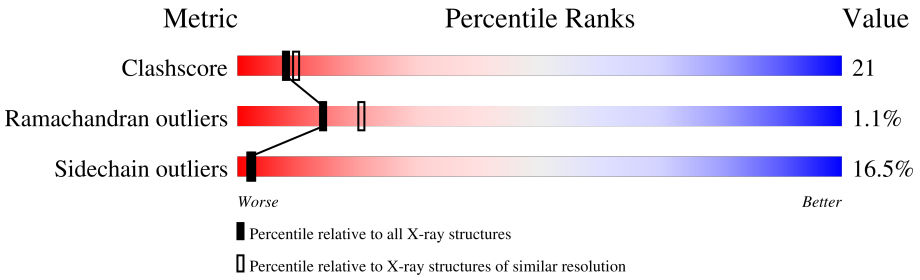
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	95	48% 40% 7% .
1	B	95	39% 46% 9% 5%
2	C	235	61% 33% 5% .
2	D	235	55% 37% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5433 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 BLOOD COAGULATION FACTOR XA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	91	Total	C	N	O	S	0	0	0
			682	408	116	145	13			
1	B	90	Total	C	N	O	S	0	0	0
			676	405	117	141	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	BHD	ASP	modified residue	UNP P00742
B	63	BHD	ASP	modified residue	UNP P00742

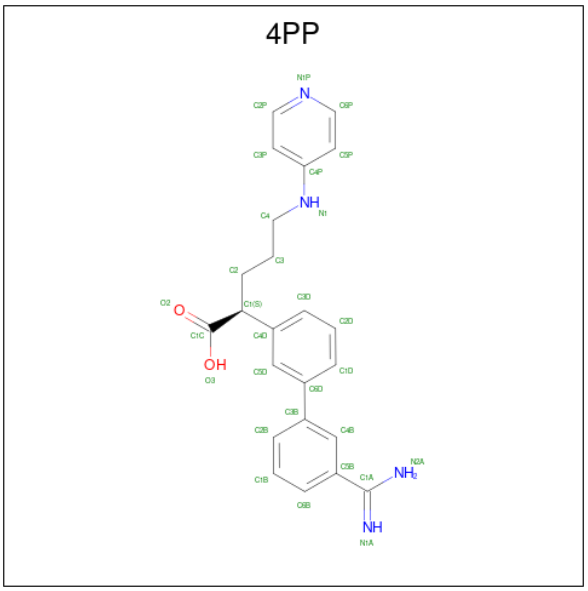
- Molecule 2 is a protein called BLOOD COAGULATION FACTOR XA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	235	Total	C	N	O	S	0	0	0
			1863	1172	327	350	14			
2	D	234	Total	C	N	O	S	0	0	0
			1852	1166	323	349	14			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is (2S)-(3'-AMIDINO-3-BIPHENYL)-5-(4-PYRIDYLAMINO)PENTANOIC ACID (three-letter code: 4PP) (formula: $C_{23}H_{24}N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O 29 23 4 2	0	0
4	D	1	Total C N O 29 23 4 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	27	Total O 27 27	0	0
5	C	123	Total O 123 123	0	0
5	B	25	Total O 25 25	0	0
5	D	124	Total O 124 124	0	0

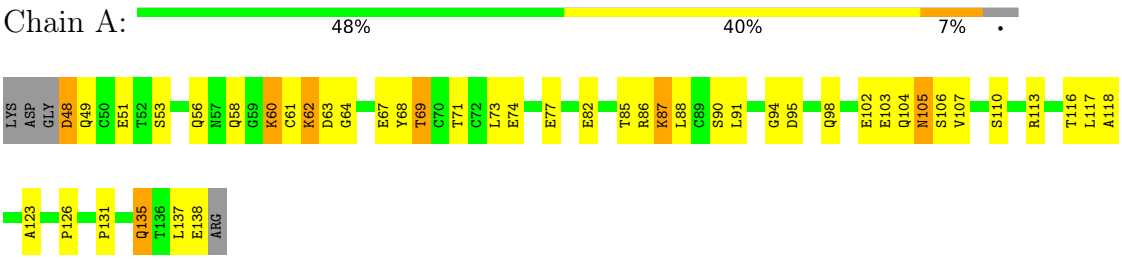
3 Residue-property plots (i)

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 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.

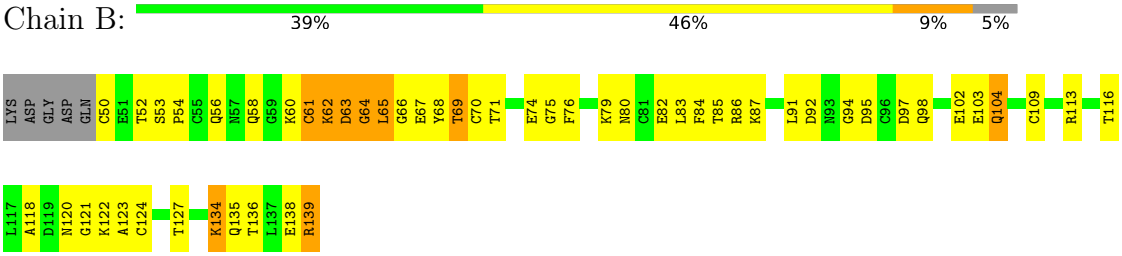
• Molecule 1: BLOOD COAGULATION FACTOR XA

Chain A:



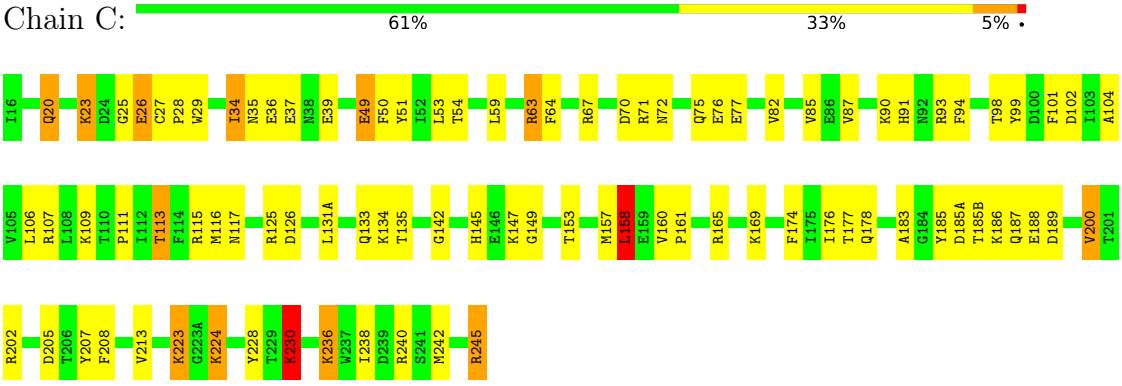
• Molecule 1: BLOOD COAGULATION FACTOR XA

Chain B:



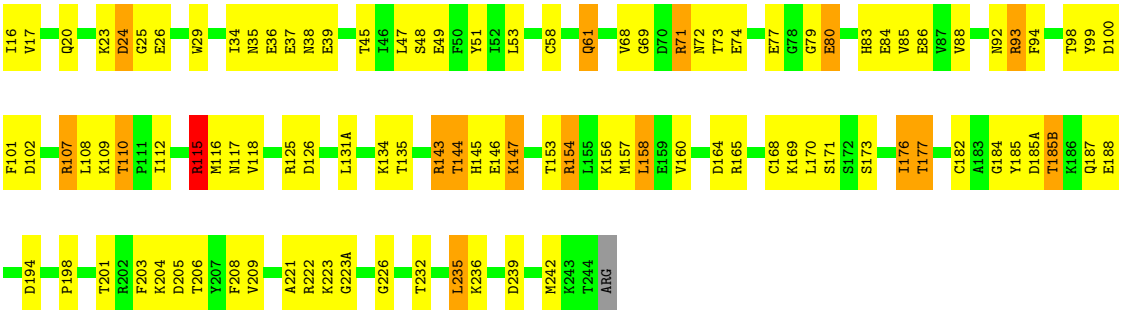
• Molecule 2: BLOOD COAGULATION FACTOR XA

Chain C:



• Molecule 2: BLOOD COAGULATION FACTOR XA

Chain D:


I16 V17 Q20 K23 D24 G25 E26 W29 I34 N35 E36 E37 N38 E39 T45 I46 L47 S48 E49 F50 Y51 I52 L53 C58 Q61 V68 G69 D70 R71 N72 T73 E74 E77 G78 G79 E80 H83 E84 V85 E86 V87 V88 N92 R93 F94 T98 Y99 D100
F101 D102 R107 L108 K109 T110 P111 I112 R115 M116 N117 V118 R125 D126 L131A K134 T135 R143 T144 H145 E146 K147 T153 R154 L155 K156 M157 L158 E159 V160 D164 R165 C168 K169 L170 S171 S172 S173 I176 T177 C182 A183 G184 Y185 D185A T185B K186 Q187 E188
D194 P198 T201 R202 F203 K204 D205 T206 Y207 F208 V209 A221 R222 K223 G223A G226 T232 L235 K236 D239 M242 K243 T244 ARG

4 Data and refinement statistics (i)

Xtriage (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	58.27Å 105.22Å 63.24Å 90.00° 103.40° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40	Depositor
% Data completeness (in resolution range)	86.3 (8.00-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.206 , 0.294	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5433	wwPDB-VP
Average B, all atoms (Å^2)	24.0	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: CA, 4PP, BHD

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	0.37	0/682	0.61	0/916
1	B	0.39	0/676	0.62	1/907 (0.1%)
2	C	0.38	0/1901	0.65	1/2560 (0.0%)
2	D	0.40	0/1890	0.66	1/2546 (0.0%)
All	All	0.39	0/5149	0.64	3/6929 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	158	LEU	CA-CB-CG	6.31	129.81	115.30
1	B	64	GLY	N-CA-C	-5.65	98.98	113.10
2	D	115	ARG	NE-CZ-NH2	-5.62	117.49	120.30

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	682	0	614	32	0
1	B	676	0	614	44	0
2	C	1863	0	1821	82	0
2	D	1852	0	1808	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	C	29	0	22	1	0
4	D	29	0	22	1	0
5	A	27	0	0	0	0
5	B	25	0	0	0	0
5	C	123	0	0	6	0
5	D	124	0	0	7	0
All	All	5433	0	4901	215	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 21.

The worst 5 of 215 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)
2:D:232:THR:HA	2:D:235:LEU:HD22	1.54	0.89
1:A:62:LYS:HG3	1:A:69:THR:HG22	1.54	0.89
1:B:138:GLU:HG3	1:B:139:ARG:CZ	2.05	0.87
1:A:48:ASP:HA	1:A:51:GLU:HB2	1.61	0.83
1:B:138:GLU:HG2	2:D:116:MET:SD	2.21	0.79

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	88/95 (93%)	79 (90%)	9 (10%)	0	100 100
1	B	87/95 (92%)	71 (82%)	13 (15%)	3 (3%)	3 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	233/235 (99%)	217 (93%)	13 (6%)	3 (1%)	12 17
2	D	232/235 (99%)	216 (93%)	15 (6%)	1 (0%)	34 48
All	All	640/660 (97%)	583 (91%)	50 (8%)	7 (1%)	14 20

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	GLY
1	B	64	GLY
2	D	125	ARG
2	C	142	GLY
2	C	187	GLN

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	77/80 (96%)	58 (75%)	19 (25%)	0 0
1	B	76/80 (95%)	61 (80%)	15 (20%)	1 1
2	C	200/200 (100%)	177 (88%)	23 (12%)	5 7
2	D	199/200 (100%)	165 (83%)	34 (17%)	2 2
All	All	552/560 (99%)	461 (84%)	91 (16%)	2 2

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	20	GLN
2	D	110	THR
2	D	24	ASP
2	D	77	GLU
2	D	147	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	57	ASN
1	B	104	GLN
2	D	178	GLN
2	D	75	GLN
1	A	135	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	BHD	A	63	3,1	6,8,9	1.08	0	8,10,12	0.88	0
1	BHD	B	63	1	6,8,9	1.00	0	8,10,12	1.65	2 (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
1	BHD	A	63	3,1	-	4/9/10/12	-
1	BHD	B	63	1	-	5/9/10/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	63	BHD	OB-CB-CA	3.09	113.80	107.28
1	B	63	BHD	OD2-CG-CB	2.45	119.89	113.27

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	63	BHD	OB-CB-CG-OD1
1	A	63	BHD	OB-CB-CG-OD2
1	B	63	BHD	CA-CB-CG-OD1
1	B	63	BHD	CA-CB-CG-OD2
1	A	63	BHD	CA-CB-CG-OD1

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	63	BHD	2	0
1	B	63	BHD	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
4	4PP	C	998	-	30,31,31	2.07	10 (33%)	32,41,41	1.31	4 (12%)
4	4PP	D	999	-	30,31,31	2.17	15 (50%)	32,41,41	1.21	2 (6%)

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
4	4PP	C	998	-	-	2/19/23/23	0/3/3/3
4	4PP	D	999	-	-	6/19/23/23	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	998	4PP	C4P-N1	4.08	1.50	1.38
4	D	999	4PP	C4P-N1	4.04	1.50	1.38
4	C	998	4PP	C5B-C1A	3.89	1.54	1.47
4	D	999	4PP	C5B-C1A	3.66	1.54	1.47
4	D	999	4PP	C5D-C4D	3.46	1.44	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	998	4PP	C4-N1-C4P	-4.69	112.58	122.94
4	D	999	4PP	C4-N1-C4P	-4.23	113.58	122.94
4	C	998	4PP	O3-C1C-O2	-2.26	118.96	124.09
4	C	998	4PP	C5P-C6P-N1P	-2.22	119.75	123.62
4	C	998	4PP	C3P-C2P-N1P	-2.22	119.75	123.62

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	998	4PP	C1C-C1-C2-C3
4	C	998	4PP	C4D-C1-C2-C3
4	D	999	4PP	C2-C1-C1C-O2
4	D	999	4PP	C2-C1-C1C-O3
4	D	999	4PP	C2-C3-C4-N1

There are no ring outliers.

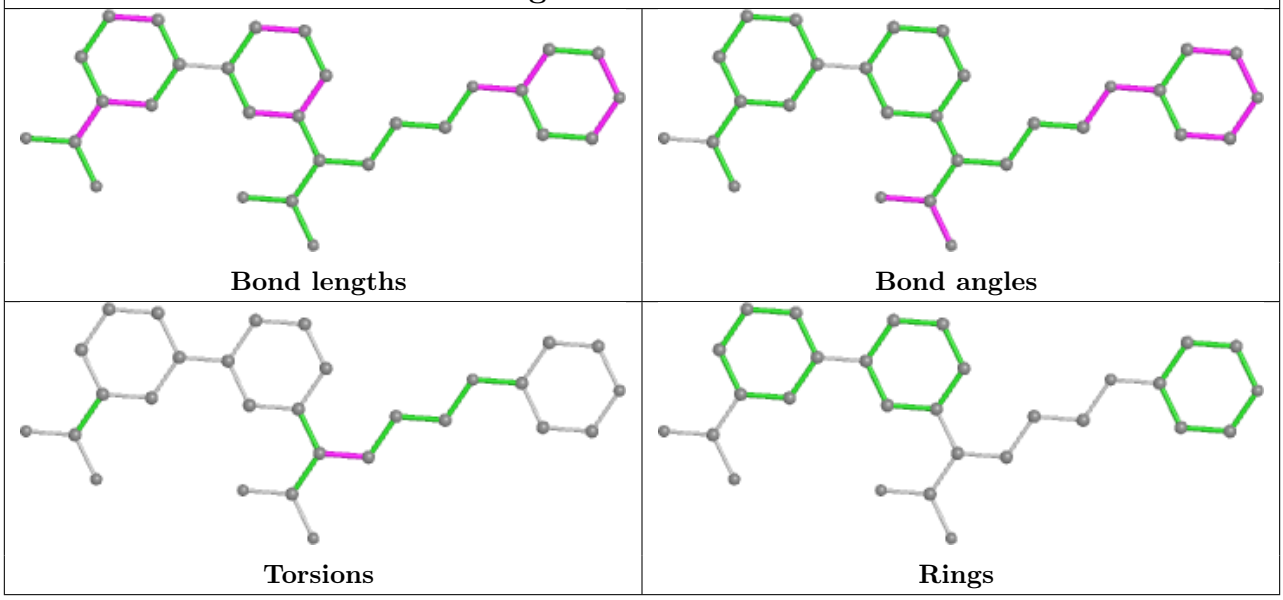
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	998	4PP	1	0
4	D	999	4PP	1	0

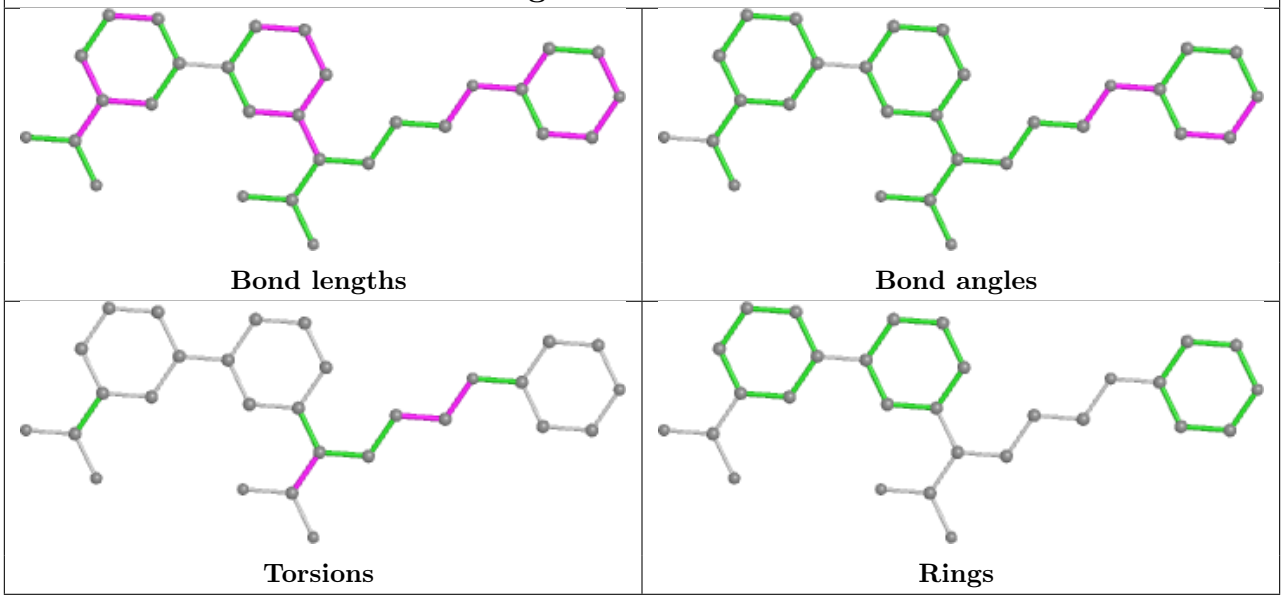
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 4PP C 998



Ligand 4PP D 999



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.