Full wwPDB X-ray Structure Validation Report (i)

Jul 26, 2023 – 03:44 AM EDT

PDB ID	:	1A0Q
Title	:	29G11 COMPLEXED WITH PHENYL [1-(1-N-SUCCINYLAMINO)PENTYL] PHOSPHONATE
Authors	:	Buchbinder, J.L.; Stephenson, R.C.; Scanlan, T.S.; Fletterick, R.J.
Deposited on	:	1997-12-05
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

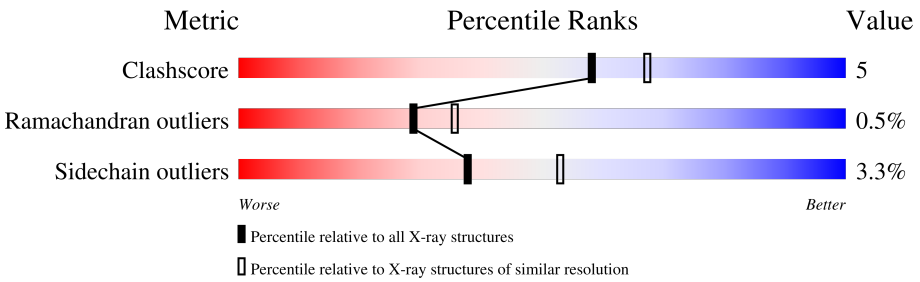
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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	L	212	81% 15% •
2	H	217	80% 12% • 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3301 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 29G11 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	211	1643	1032	278	328	5	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	4	LEU	MET	conflict	GB 12002896
L	22	THR	ALA	conflict	GB 12002896
L	26	SER	ASN	conflict	GB 12002896
L	30	LYS	ASN	conflict	GB 12002896
L	34	GLY	ALA	conflict	GB 12002896
L	43	GLN	GLY	conflict	GB 12002896
L	55	LEU	GLN	conflict	GB 12002896
L	63	ARG	SER	conflict	GB 12002896
L	92	TYR	ASP	conflict	GB 12002896
L	141	SER	PRO	conflict	GB 12002896
L	187	GLU	GLY	conflict	GB 12002896

- Molecule 2 is a protein called 29G11 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	205	1540	977	249	308	6	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	8	ASP	GLY	conflict	GB 3399661
H	9	ALA	PRO	conflict	GB 3399661
H	20	ILE	MET	conflict	GB 3399661
H	31	ASP	SER	conflict	GB 3399661
H	32	HIS	TYR	conflict	GB 3399661

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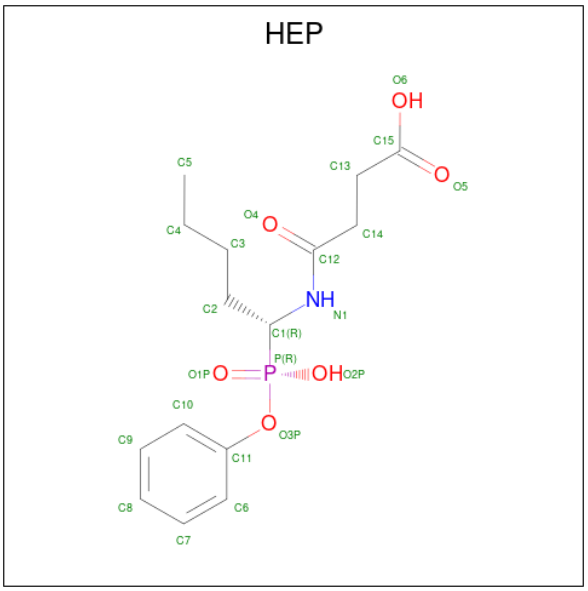
Chain	Residue	Modelled	Actual	Comment	Reference
H	34	ILE	MET	conflict	GB 3399661
H	42	GLU	GLY	conflict	GB 3399661
H	52	SER	ASN	conflict	GB 3399661
H	53	GLY	TYR	conflict	GB 3399661
H	55	GLY	ASP	conflict	GB 3399661
H	56	ASP	GLY	conflict	GB 3399661
H	57	ILE	THR	conflict	GB 3399661
H	71	ALA	SER	conflict	GB 3399661
H	81	GLN	GLU	conflict	GB 3399661
H	82A	ASN	SER	conflict	GB 3399661
H	91	LEU	TYR	conflict	GB 3399661
H	93	LYS	VAL	conflict	GB 3399661
H	?	-	GLY	deletion	GB 3399661
H	97	TYR	ARG	conflict	GB 3399661
H	98	GLY	PRO	conflict	GB 3399661
H	99	ARG	TYR	conflict	GB 3399661
H	100	SER	TYR	conflict	GB 3399661
H	100A	ASN	ALA	conflict	GB 3399661
H	100B	VAL	MET	conflict	GB 3399661
H	108	THR	SER	conflict	GB 3399661
H	109	LEU	VAL	conflict	GB 3399661

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	L	1	1	1	0	0
			Total	Zn		
3	H	2	2	2	0	0

- Molecule 4 is PHENYL[1-(N-SUCCINYLAMINO)PENTYL]PHOSPHONATE (three-letter code: HEP) (formula: $C_{15}H_{22}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	H	1	23	15	1	6	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	L	45	45	45	0	0
			Total	O		
5	H	47	47	47	0	0

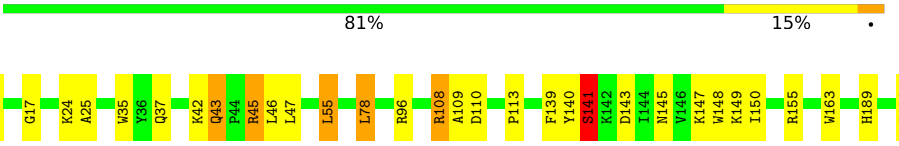
3 Residue-property plots (i)

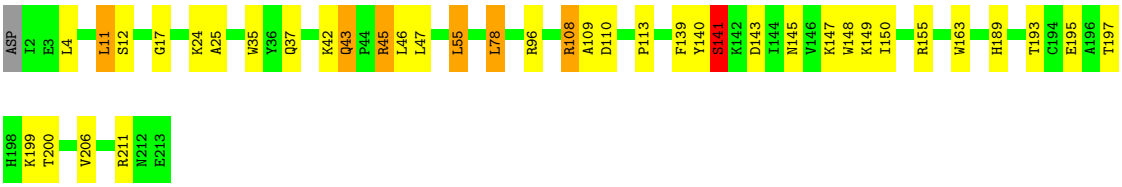
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: 29G11 FAB (LIGHT CHAIN)

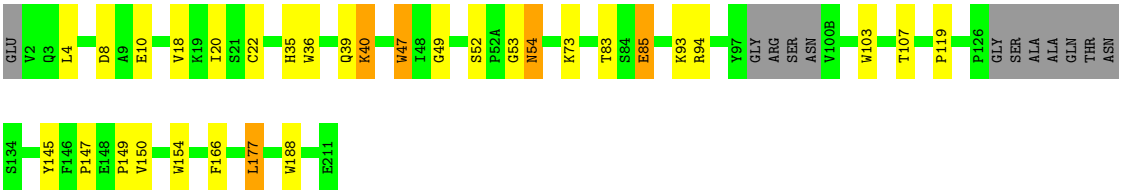
Chain L:





- Molecule 2: 29G11 FAB (HEAVY CHAIN)

Chain H:



4 Data and refinement statistics (i)

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	36.78Å 82.61Å 132.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30	Depositor
% Data completeness (in resolution range)	93.0 (50.00-2.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.203 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3301	wwPDB-VP
Average B, all atoms ($Å^2$)	25.0	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: ZN, HEP

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	L	0.67	0/1681	1.36	19/2277 (0.8%)
2	H	0.68	0/1577	1.35	14/2150 (0.7%)
All	All	0.67	0/3258	1.36	33/4427 (0.7%)

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	L	0	1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	163	TRP	CD1-CG-CD2	8.17	112.84	106.30
1	L	140	TYR	CA-C-N	-8.10	99.39	117.20
2	H	47	TRP	CD1-CG-CD2	8.06	112.75	106.30
2	H	188	TRP	CD1-CG-CD2	8.03	112.72	106.30
2	H	103	TRP	CD1-CG-CD2	7.87	112.59	106.30
1	L	35	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	L	163	TRP	CE2-CD2-CG	-7.76	101.09	107.30
2	H	154	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	L	35	TRP	CE2-CD2-CG	-7.67	101.16	107.30
2	H	188	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	L	148	TRP	CD1-CG-CD2	7.48	112.29	106.30
1	L	108	ARG	NE-CZ-NH2	-7.27	116.67	120.30
2	H	47	TRP	CE2-CD2-CG	-7.18	101.55	107.30
2	H	36	TRP	CD1-CG-CD2	7.16	112.02	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	148	TRP	CE2-CD2-CG	-7.14	101.59	107.30
2	H	36	TRP	CE2-CD2-CG	-7.08	101.64	107.30
2	H	154	TRP	CE2-CD2-CG	-7.02	101.69	107.30
2	H	103	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	L	141	SER	N-CA-C	-6.97	92.17	111.00
1	L	140	TYR	O-C-N	6.36	132.88	122.70
1	L	108	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	L	45	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	L	163	TRP	CG-CD2-CE3	5.88	139.19	133.90
2	H	177	LEU	CA-CB-CG	5.87	128.79	115.30
1	L	45	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	L	163	TRP	CB-CG-CD1	-5.81	119.45	127.00
1	L	35	TRP	CG-CD2-CE3	5.58	138.93	133.90
1	L	11	LEU	CA-CB-CG	5.56	128.08	115.30
1	L	148	TRP	CG-CD2-CE3	5.30	138.67	133.90
2	H	39	GLN	CA-C-N	-5.18	105.81	117.20
2	H	47	TRP	CG-CD1-NE1	-5.16	104.94	110.10
2	H	40	LYS	CA-C-N	5.14	131.51	117.10
1	L	35	TRP	CB-CG-CD1	-5.12	120.34	127.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	43	GLN	Peptide

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	L	1643	0	1590	18	0
2	H	1540	0	1503	12	0
3	H	2	0	0	0	0
3	L	1	0	0	0	0
4	H	23	0	20	1	0
5	H	47	0	0	0	0
5	L	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3301	0	3113	30	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 5.

All (30) 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:L:149:LYS:HB2	1:L:193:THR:HB	1.77	0.66
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.49	0.59
1:L:43:GLN:HG3	1:L:45:ARG:HB2	1.85	0.58
2:H:4:LEU:HG	2:H:22:CYS:SG	2.48	0.53
1:L:145:ASN:HB3	1:L:197:THR:HB	1.92	0.51
1:L:147:LYS:HB3	1:L:195:GLU:HB3	1.91	0.50
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.93	0.50
1:L:17:GLY:O	1:L:78:LEU:HD22	2.13	0.48
1:L:195:GLU:HG3	1:L:206:VAL:HG22	1.96	0.48
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.48	0.47
1:L:189:HIS:O	1:L:211:ARG:HD3	2.15	0.47
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.95	0.47
1:L:46:LEU:HG	1:L:55:LEU:HD13	1.95	0.47
2:H:20:ILE:HD12	2:H:107:THR:HG21	1.97	0.47
1:L:110:ASP:OD2	1:L:199:LYS:HE2	2.14	0.46
2:H:53:GLY:HA2	2:H:73:LYS:HE2	1.98	0.46
2:H:83:THR:OG1	2:H:85:GLU:HG2	2.15	0.45
1:L:4:LEU:HD23	1:L:25:ALA:HA	1.97	0.45
2:H:93:LYS:HG2	2:H:94:ARG:N	2.32	0.44
1:L:11:LEU:HD12	1:L:12:SER:H	1.82	0.44
2:H:166:PHE:O	2:H:177:LEU:HB2	2.18	0.43
1:L:11:LEU:HD12	1:L:12:SER:N	2.33	0.43
2:H:10:GLU:HG2	2:H:18:VAL:HG21	2.01	0.42
1:L:150:ILE:HD12	1:L:155:ARG:HG3	2.01	0.41
2:H:52:SER:HB3	2:H:54:ASN:HB2	2.01	0.41
1:L:42:LYS:HB3	1:L:43:GLN:H	1.68	0.41
1:L:110:ASP:HB3	1:L:200:THR:HG22	2.02	0.41
2:H:35:HIS:CD2	4:H:214:HEP:H10	2.56	0.41
1:L:108:ARG:HG2	1:L:109:ALA:N	2.36	0.41
1:L:113:PRO:HB3	1:L:139:PHE:HB3	2.04	0.40

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	L	209/212 (99%)	202 (97%)	6 (3%)	1 (0%)	29	35
2	H	199/217 (92%)	192 (96%)	6 (3%)	1 (0%)	29	35
All	All	408/429 (95%)	394 (97%)	12 (3%)	2 (0%)	29	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	141	SER
2	H	40	LYS

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	L	185/189 (98%)	179 (97%)	6 (3%)	39	54
2	H	175/187 (94%)	169 (97%)	6 (3%)	37	51
All	All	360/376 (96%)	348 (97%)	12 (3%)	38	53

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	24	LYS
1	L	55	LEU
1	L	78	LEU
1	L	96	ARG

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Mol	Chain	Res	Type
1	L	141	SER
1	L	143	ASP
2	H	8	ASP
2	H	54	ASN
2	H	85	GLU
2	H	147	PRO
2	H	149	PRO
2	H	150	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	37	GLN
1	L	138	ASN
1	L	198	HIS
2	H	5	GLN
2	H	32	HIS
2	H	35	HIS
2	H	82(A)	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	HEP	H	214	-	23,23,23	2.67	4 (17%)	23,30,30	1.33	4 (17%)

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	HEP	H	214	-	-	3/24/24/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	214	HEP	P-C1	-11.24	1.74	1.84
4	H	214	HEP	P-O2P	-3.53	1.48	1.56
4	H	214	HEP	P-O3P	3.52	1.62	1.58
4	H	214	HEP	O6-C15	-2.11	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	214	HEP	O2P-P-O1P	3.34	119.73	111.58
4	H	214	HEP	O1P-P-C1	-3.18	109.80	114.20
4	H	214	HEP	C13-C14-C12	2.28	116.56	112.56
4	H	214	HEP	O3P-P-O1P	-2.21	110.20	114.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	214	HEP	C14-C13-C15-O5
4	H	214	HEP	C14-C13-C15-O6
4	H	214	HEP	N1-C1-P-O1P

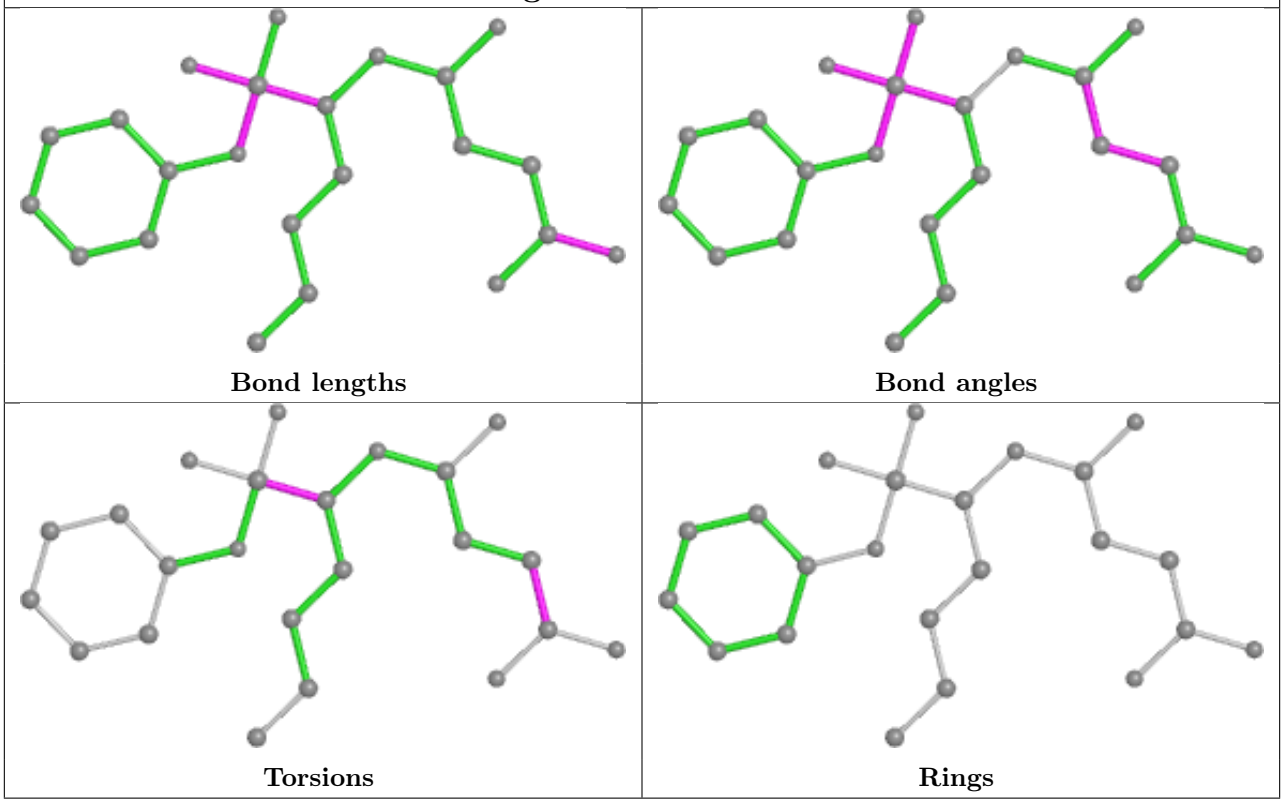
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	214	HEP	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 HEP H 214



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.