wwPDB X-ray Structure Validation Summary Report (i)

Jan 8, 2023 – 12:49 PM EST

PDB ID	:	1RUH
Title	:	RHINOVIRUS 14 MUTANT N1219S COMPLEXED WITH ANTIVIRAL COMPOUND WIN 52084
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Deposited on	:	1995-06-09
Resolution	:	3.00 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:

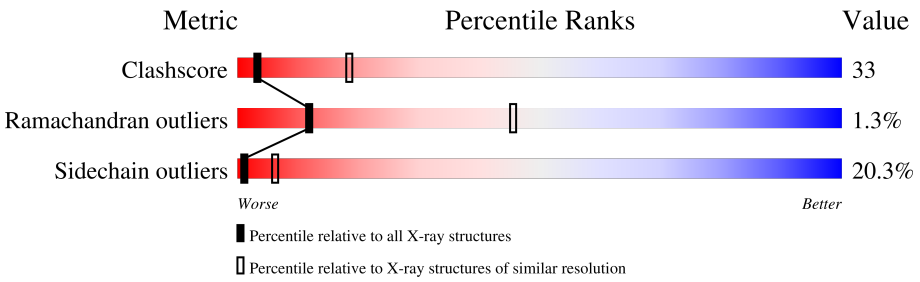
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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	1	289	33% 39% 16% 6% 6%
2	2	262	43% 36% 13% 5% •
3	3	236	42% 36% 17% 6%
4	4	68	18% 16% 16% 9% 41%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6292 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 RHINOVIRUS 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	273	2168	1372	374	414	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	219	SER	ASN	engineered mutation	UNP P03303

- Molecule 2 is a protein called RHINOVIRUS 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	255	1952	1238	330	372	12	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	170	LEU	ILE	conflict	UNP P03303

- Molecule 3 is a protein called RHINOVIRUS 14.

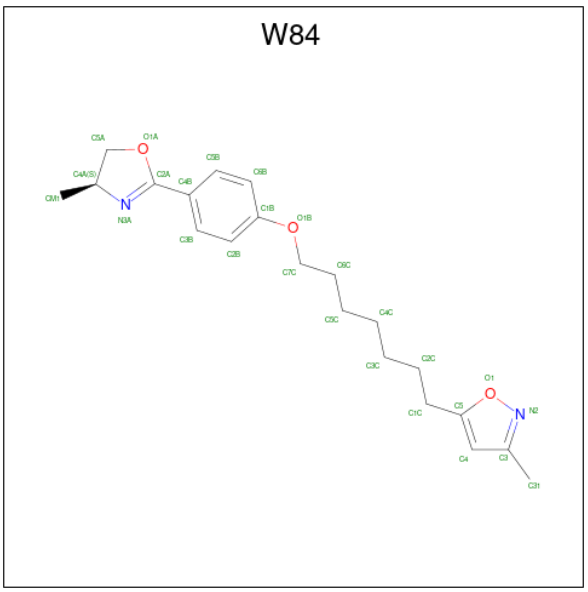
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	236	1849	1184	305	353	7	0	0	0

- Molecule 4 is a protein called RHINOVIRUS 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	4	40	297	186	47	62	2	0	0	0

- Molecule 5 is 5-(7-(5-HYDRO-4-METHYL-2-OXAZOLYL)PHENOXY)HEPTYL)-3-MET

HYL ISOXAZOLE (three-letter code: W84) (formula: $C_{21}H_{28}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	1	1	26	21	2	3	0	0

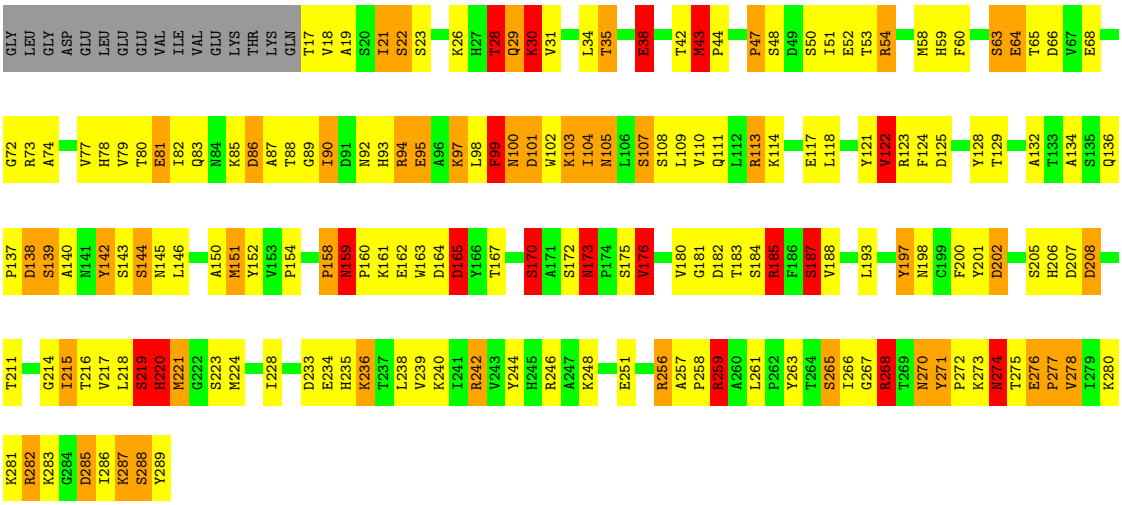
3 Residue-property plots (i)

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.

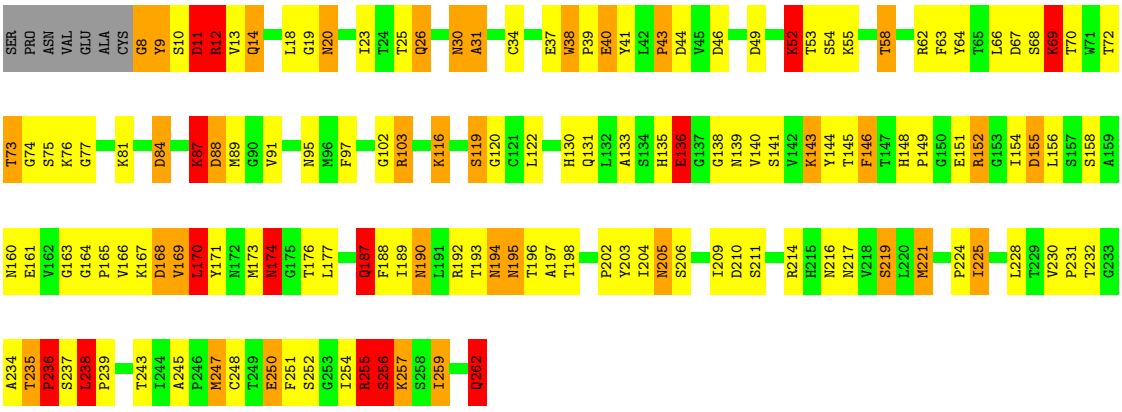
• Molecule 1: RHINOVIRUS 14

Chain 1: 33% 39% 16% 6% 6%



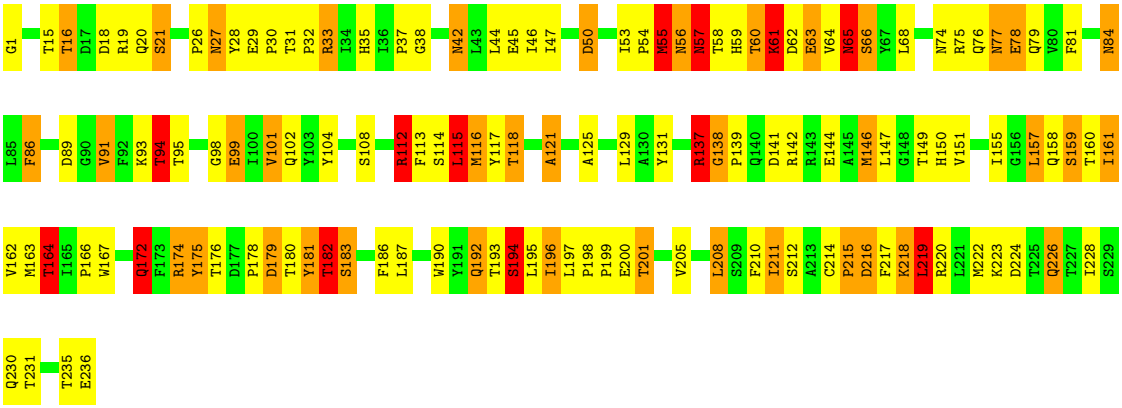
• Molecule 2: RHINOVIRUS 14

Chain 2: 43% 36% 13% 5%



• Molecule 3: RHINOVIRUS 14

Chain 3: 42% 36% 17% 6%



- Molecule 4: RHINOVIRUS 14

Chain 4: 18% 16% 16% 9% 41%

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 3	Depositor
Cell constants a, b, c, α, β, γ	445.10Å 445.10Å 445.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6292	wwPDB-VP
Average B, all atoms (Å^2)	1.0	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: W84

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	1	1.95	40/2226 (1.8%)	2.35	120/3028 (4.0%)
2	2	1.85	32/2001 (1.6%)	2.17	79/2735 (2.9%)
3	3	1.76	21/1898 (1.1%)	2.16	75/2597 (2.9%)
4	4	2.30	13/302 (4.3%)	2.46	21/406 (5.2%)
All	All	1.88	106/6427 (1.6%)	2.24	295/8766 (3.4%)

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	1	0	4
2	2	0	2
All	All	0	6

The worst 5 of 106 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	220	HIS	C-N	-25.12	0.76	1.34
1	1	219	SER	C-N	-18.77	0.90	1.34
1	1	170	SER	CB-OG	-14.30	1.23	1.42
1	1	150	ALA	C-N	14.03	1.66	1.34
1	1	285	ASP	CA-CB	11.82	1.79	1.53

The worst 5 of 295 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	246	ARG	NE-CZ-NH1	22.50	131.55	120.30
1	1	256	ARG	NE-CZ-NH2	20.44	130.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	123	ARG	NE-CZ-NH1	19.20	129.90	120.30
2	2	255	ARG	NE-CZ-NH2	-18.68	110.96	120.30
1	1	285	ASP	CB-CG-OD1	-17.64	102.43	118.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	219	SER	Mainchain
1	1	220	HIS	Mainchain
1	1	259	ARG	Sidechain
1	1	268	ARG	Sidechain
2	2	12	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	1	2168	0	2103	175	0
2	2	1952	0	1926	126	0
3	3	1849	0	1831	149	0
4	4	297	0	294	36	0
5	1	26	0	27	7	0
All	All	6292	0	6181	411	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 33.

The worst 5 of 411 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)
3:3:57:ASN:CB	3:3:57:ASN:CA	1.75	1.58
4:4:33:LYS:CE	4:4:33:LYS:NZ	1.67	1.55
2:2:52:LYS:NZ	2:2:52:LYS:CE	1.68	1.54
1:1:285:ASP:CB	1:1:285:ASP:CA	1.80	1.54
1:1:220:HIS:C	1:1:221:MET:CA	1.94	1.33

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	1	271/289 (94%)	251 (93%)	16 (6%)	4 (2%)	10 42
2	2	253/262 (97%)	233 (92%)	18 (7%)	2 (1%)	19 57
3	3	234/236 (99%)	216 (92%)	15 (6%)	3 (1%)	12 45
4	4	38/68 (56%)	34 (90%)	3 (8%)	1 (3%)	5 27
All	All	796/855 (93%)	734 (92%)	52 (6%)	10 (1%)	12 45

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	3	57	ASN
3	3	77	ASN
1	1	99	PHE
1	1	139	SER
1	1	165	ASP

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	1	239/253 (94%)	191 (80%)	48 (20%)	1 6
2	2	223/229 (97%)	179 (80%)	44 (20%)	1 7
3	3	209/209 (100%)	171 (82%)	38 (18%)	1 9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	4	33/57 (58%)	20 (61%)	13 (39%)	0	0
All	All	704/748 (94%)	561 (80%)	143 (20%)	1	6

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	182	THR
3	3	201	THR
4	4	29	ILE
2	2	11	ASP
1	1	287	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
2	2	195	ASN
3	3	226	GLN
2	2	217	ASN
3	3	102	GLN
2	2	216	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)

1 ligand is 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	$\#\|Z\| > 2$
5	W84	1	290	-	25,28,28	3.05	6 (24%)	31,36,36	2.83	8 (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
5	W84	1	290	-	-	5/14/24/24	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	290	W84	C2A-N3A	10.92	1.43	1.27
5	1	290	W84	C4A-N3A	-7.32	1.35	1.48
5	1	290	W84	O1A-C2A	-4.18	1.29	1.36
5	1	290	W84	C4-C5	-3.90	1.34	1.39
5	1	290	W84	O1A-C5A	-3.77	1.38	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	1	290	W84	CM1-C4A-N3A	7.78	133.42	111.63
5	1	290	W84	O1A-C2A-N3A	-7.71	110.16	118.17
5	1	290	W84	O1A-C2A-C4B	6.22	124.09	115.85
5	1	290	W84	O1A-C5A-C4A	5.38	111.47	104.94
5	1	290	W84	C4A-N3A-C2A	4.90	113.05	106.44

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1	290	W84	C3C-C4C-C5C-C6C
5	1	290	W84	C1C-C2C-C3C-C4C
5	1	290	W84	C2C-C1C-C5-C4

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Mol	Chain	Res	Type	Atoms
5	1	290	W84	C5-C1C-C2C-C3C
5	1	290	W84	C6C-C7C-O1B-C1B

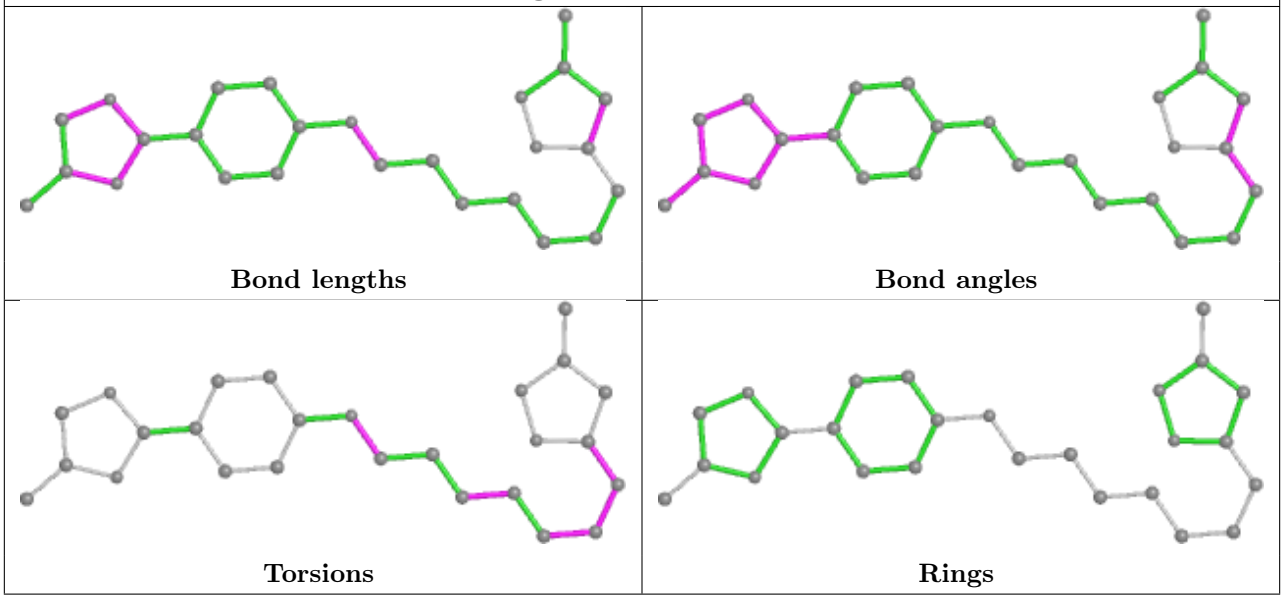
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	290	W84	7	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 W84 1 290



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	150:ALA	C	151:MET	N	1.66
1	1	219:SER	C	220:HIS	N	0.90
1	1	220:HIS	C	221:MET	N	0.76

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.