Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 03:18 AM EDT

PDB ID	:	6WS5
Title	:	Rational drug design of phenazopyridine derivatives as novel inhibitors of Rev1-CT
Authors	:	McPherson, K.S.; Korzhnev, D.M.
Deposited on	:	2020-04-30
Resolution	:	2.47 Å(reported)

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

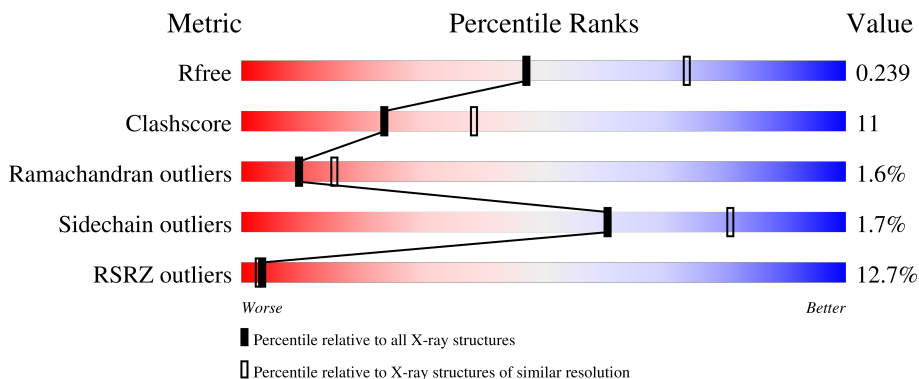|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.47 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	Percentile Ranks	Value
Rfree		0.239
Clashscore		11
Ramachandran outliers		1.6%
Sidechain outliers		1.7%
RSRZ outliers		12.7%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	HHH	95	3% 77% 22% •
2	CCC	227	15% 63% 23% • 12%
3	ZZZ	52	6% 27% 12% • 60%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 5191 atoms, of which 2626 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 DNA repair protein REV1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	HHH	95	Total	C	H	N	O	S	35	0	0
			1553	494	783	120	151	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
HHH	1157	GLY	-	expression tag	UNP Q9UBZ9

- Molecule 2 is a protein called Mitotic spindle assembly checkpoint protein MAD2B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	CCC	199	Total	C	H	N	O	S	80	0	0
			3274	1041	1660	272	291	10			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-13	MET	-	expression tag	UNP Q9UI95
CCC	-12	GLY	-	expression tag	UNP Q9UI95
CCC	-11	SER	-	expression tag	UNP Q9UI95
CCC	-10	SER	-	expression tag	UNP Q9UI95
CCC	-9	HIS	-	expression tag	UNP Q9UI95
CCC	-8	HIS	-	expression tag	UNP Q9UI95
CCC	-7	HIS	-	expression tag	UNP Q9UI95
CCC	-6	HIS	-	expression tag	UNP Q9UI95
CCC	-5	HIS	-	expression tag	UNP Q9UI95
CCC	-4	HIS	-	expression tag	UNP Q9UI95
CCC	-3	SER	-	expression tag	UNP Q9UI95
CCC	-2	GLN	-	expression tag	UNP Q9UI95
CCC	-1	ASP	-	expression tag	UNP Q9UI95
CCC	0	PRO	-	expression tag	UNP Q9UI95
CCC	1	ASN	-	expression tag	UNP Q9UI95

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	2	SER	-	expression tag	UNP Q9UI95
CCC	124	ALA	ARG	engineered mutation	UNP Q9UI95

- Molecule 3 is a protein called DNA polymerase zeta catalytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	ZZZ	21	Total 336	C 101	H 174	N 29	O 30	S 2	6	0	0

- Molecule 4 is 3-[(Z)-(2,3-difluorophenyl)diazenyl]pyridine-2,6-diamine (three-letter code: U8M) (formula: $C_{11}H_9F_2N_5$) (labeled as "Ligand of Interest" by depositor).

U8M
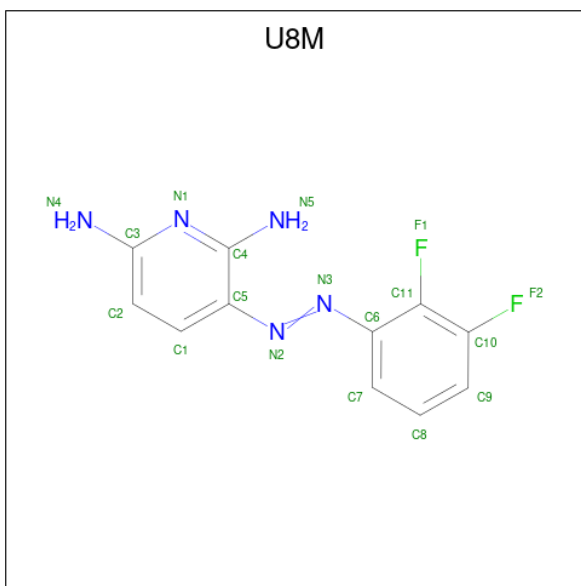
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	HHH	1	Total 27	C 11	F 2	H 9	N 5	4	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	HHH	1	Total 1	O 1	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.
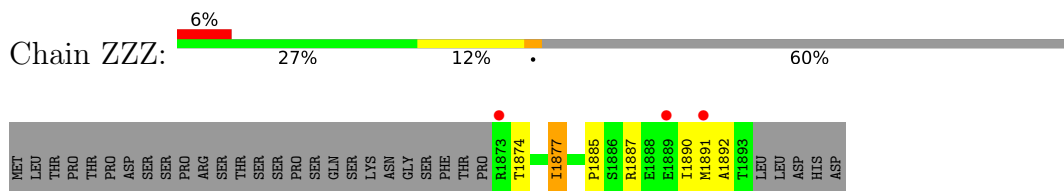
• Molecule 1: DNA repair protein REV1

Chain HHH:
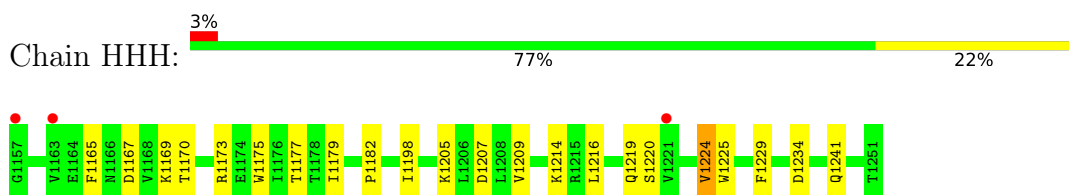
• Molecule 2: Mitotic spindle assembly checkpoint protein MAD2B

Chain CCC:
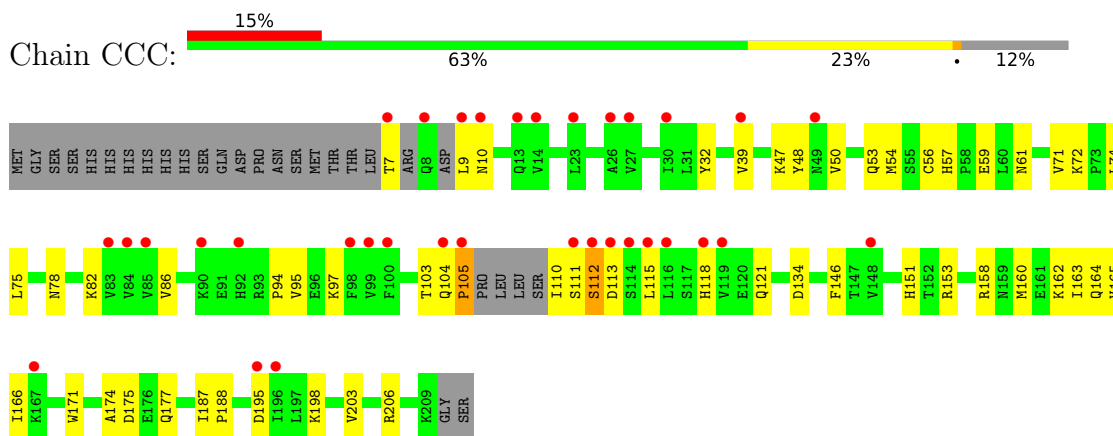
• Molecule 3: DNA polymerase zeta catalytic subunit

Chain ZZZ:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	50.02Å 73.02Å 85.55Å	Depositor
a, b, c, α, β, γ	90.00° 90.00° 90.00°	
Resolution (Å)	29.51 – 2.47	Depositor
	29.49 – 2.47	EDS
% Data completeness	99.5 (29.51-2.47)	Depositor
(in resolution range)	99.6 (29.49-2.47)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.201 , 0.237	Depositor
	0.208 , 0.239	DCC
R_{free} test set	620 reflections (5.31%)	wwPDB-VP
Wilson B-factor (Å^2)	63.5	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 55.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5191	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: U8M

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	HHH	0.94	0/780	0.97	0/1056
2	CCC	0.90	0/1648	1.04	1/2238 (0.0%)
3	ZZZ	1.07	1/164 (0.6%)	1.14	1/221 (0.5%)
All	All	0.92	1/2592 (0.0%)	1.02	2/3515 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	ZZZ	1877	ILE	C-O	5.30	1.33	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	153	ARG	NE-CZ-NH2	-5.26	117.67	120.30
3	ZZZ	1887	ARG	NE-CZ-NH1	5.00	122.80	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	HHH	770	783	780	15	0
2	CCC	1614	1660	1648	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	ZZZ	162	174	173	5	0
4	HHH	18	9	0	2	0
5	HHH	1	0	0	0	0
All	All	2565	2626	2601	58	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 11.

All (58) 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:CCC:32:TYR:CZ	2:CCC:53:GLN:NE2	2.54	0.76
2:CCC:163:ILE:CD1	2:CCC:171:TRP:HB2	2.17	0.74
2:CCC:78:ASN:HD21	2:CCC:104:GLN:CB	2.07	0.68
1:HHH:1214:LYS:HG3	1:HHH:1229:PHE:CZ	2.33	0.64
2:CCC:163:ILE:CD1	2:CCC:171:TRP:CB	2.77	0.63
2:CCC:78:ASN:HD21	2:CCC:104:GLN:HB2	1.63	0.62
2:CCC:32:TYR:CE1	2:CCC:39:VAL:HG23	2.35	0.62
2:CCC:163:ILE:HD13	2:CCC:171:TRP:CB	2.31	0.61
2:CCC:7:THR:O	2:CCC:113:ASP:O	2.19	0.60
2:CCC:59:GLU:HG2	3:ZZZ:1885:PRO:HG3	1.84	0.59
2:CCC:56:CYS:HA	2:CCC:61:ASN:HD21	1.67	0.59
2:CCC:95:VAL:HA	2:CCC:206:ARG:HD3	1.85	0.58
2:CCC:115:LEU:O	2:CCC:118:HIS:HB3	2.02	0.58
1:HHH:1205:LYS:O	1:HHH:1209:VAL:HG23	2.04	0.57
2:CCC:32:TYR:CE1	2:CCC:53:GLN:NE2	2.73	0.56
1:HHH:1182:PRO:HD2	1:HHH:1224:VAL:HG11	1.88	0.55
2:CCC:163:ILE:HD13	2:CCC:171:TRP:CG	2.42	0.55
4:HHH:1601:U8M:C1	4:HHH:1601:U8M:C11	2.86	0.54
1:HHH:1165:PHE:HE2	1:HHH:1209:VAL:HG22	1.71	0.53
3:ZZZ:1874:THR:HG21	3:ZZZ:1877:ILE:HD12	1.92	0.51
1:HHH:1182:PRO:HB3	1:HHH:1225:TRP:CH2	2.46	0.50
2:CCC:9:LEU:HG	2:CCC:10:ASN:N	2.27	0.50
1:HHH:1241:GLN:O	1:HHH:1241:GLN:HG3	2.13	0.49
2:CCC:47:LYS:HE3	2:CCC:54:MET:HE2	1.93	0.49
2:CCC:165:VAL:HG13	2:CCC:166:ILE:N	2.27	0.49
3:ZZZ:1874:THR:CG2	3:ZZZ:1877:ILE:HD12	2.42	0.48
2:CCC:74:LEU:HD11	2:CCC:163:ILE:HG23	1.96	0.48
1:HHH:1165:PHE:CE1	1:HHH:1169:LYS:HD2	2.48	0.47
2:CCC:160:MET:O	2:CCC:164:GLN:HG2	2.14	0.47
2:CCC:158:ARG:O	2:CCC:162:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:103:THR:HB	2:CCC:198:LYS:HB2	1.96	0.46
2:CCC:71:VAL:O	2:CCC:72:LYS:C	2.53	0.46
2:CCC:105:PRO:O	2:CCC:195:ASP:O	2.33	0.46
1:HHH:1207:ASP:HB2	2:CCC:188:PRO:HG2	1.97	0.46
1:HHH:1182:PRO:HD2	1:HHH:1224:VAL:CG1	2.46	0.46
4:HHH:1601:U8M:C1	4:HHH:1601:U8M:C6	2.89	0.45
2:CCC:75:LEU:O	2:CCC:78:ASN:N	2.35	0.45
1:HHH:1216:LEU:O	1:HHH:1219:GLN:HG2	2.17	0.45
2:CCC:57:HIS:NE2	3:ZZZ:1890:ILE:HD13	2.33	0.44
2:CCC:118:HIS:O	2:CCC:121:GLN:HB2	2.17	0.44
2:CCC:174:ALA:HB3	3:ZZZ:1877:ILE:HG22	2.00	0.44
1:HHH:1167:ASP:O	1:HHH:1170:THR:HB	2.18	0.43
1:HHH:1173:ARG:O	1:HHH:1177:THR:OG1	2.27	0.43
1:HHH:1165:PHE:CZ	1:HHH:1169:LYS:HD2	2.53	0.43
2:CCC:121:GLN:HA	2:CCC:121:GLN:OE1	2.19	0.43
2:CCC:32:TYR:CE2	2:CCC:53:GLN:NE2	2.86	0.42
2:CCC:86:VAL:O	2:CCC:146:PHE:HA	2.20	0.42
2:CCC:110:ILE:HD13	2:CCC:110:ILE:N	2.35	0.41
2:CCC:97:LYS:O	2:CCC:203:VAL:HA	2.21	0.41
2:CCC:104:GLN:N	2:CCC:105:PRO:CD	2.84	0.41
2:CCC:48:TYR:O	2:CCC:50:VAL:HG23	2.20	0.41
2:CCC:112:SER:O	2:CCC:115:LEU:HB3	2.21	0.41
2:CCC:187:ILE:HD12	2:CCC:187:ILE:N	2.35	0.41
1:HHH:1175:TRP:HD1	1:HHH:1179:ILE:HD12	1.85	0.41
2:CCC:175:ASP:HB3	2:CCC:177:GLN:HG2	2.03	0.41
2:CCC:82:LYS:HG2	2:CCC:151:HIS:HB2	2.03	0.40
2:CCC:94:PRO:O	2:CCC:206:ARG:HD2	2.20	0.40
1:HHH:1175:TRP:CD1	1:HHH:1179:ILE:HD12	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	HHH	93/95 (98%)	81 (87%)	11 (12%)	1 (1%)	14	23
2	CCC	195/227 (86%)	178 (91%)	15 (8%)	2 (1%)	15	26
3	ZZZ	19/52 (36%)	15 (79%)	2 (10%)	2 (10%)	0	0
All	All	307/374 (82%)	274 (89%)	28 (9%)	5 (2%)	9	15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	ZZZ	1892	ALA
3	ZZZ	1891	MET
2	CCC	111	SER
2	CCC	112	SER
1	HHH	1224	VAL

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	HHH	89/89 (100%)	86 (97%)	3 (3%)	37	61
2	CCC	187/213 (88%)	185 (99%)	2 (1%)	73	88
3	ZZZ	19/49 (39%)	19 (100%)	0	100	100
All	All	295/351 (84%)	290 (98%)	5 (2%)	60	81

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	HHH	1198	ILE
1	HHH	1220	SER
1	HHH	1234	ASP
2	CCC	105	PRO
2	CCC	134	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\#|Z| > 2$
4	U8M	HHH	1601	-	17,19,19	0.63	0	21,26,26	1.23	2 (9%)

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	U8M	HHH	1601	-	-	5/5/5/5	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	HHH	1601	U8M	C1-C5-C4	2.85	118.83	116.87
4	HHH	1601	U8M	N5-C4-N1	2.85	121.07	117.03

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	HHH	1601	U8M	C4-C5-N2-N3
4	HHH	1601	U8M	C5-N2-N3-C6
4	HHH	1601	U8M	C7-C6-N3-N2
4	HHH	1601	U8M	C1-C5-N2-N3
4	HHH	1601	U8M	C11-C6-N3-N2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	HHH	1601	U8M	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 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 U8M HHH 1601

Bond lengths

Bond angles

Torsions

Rings
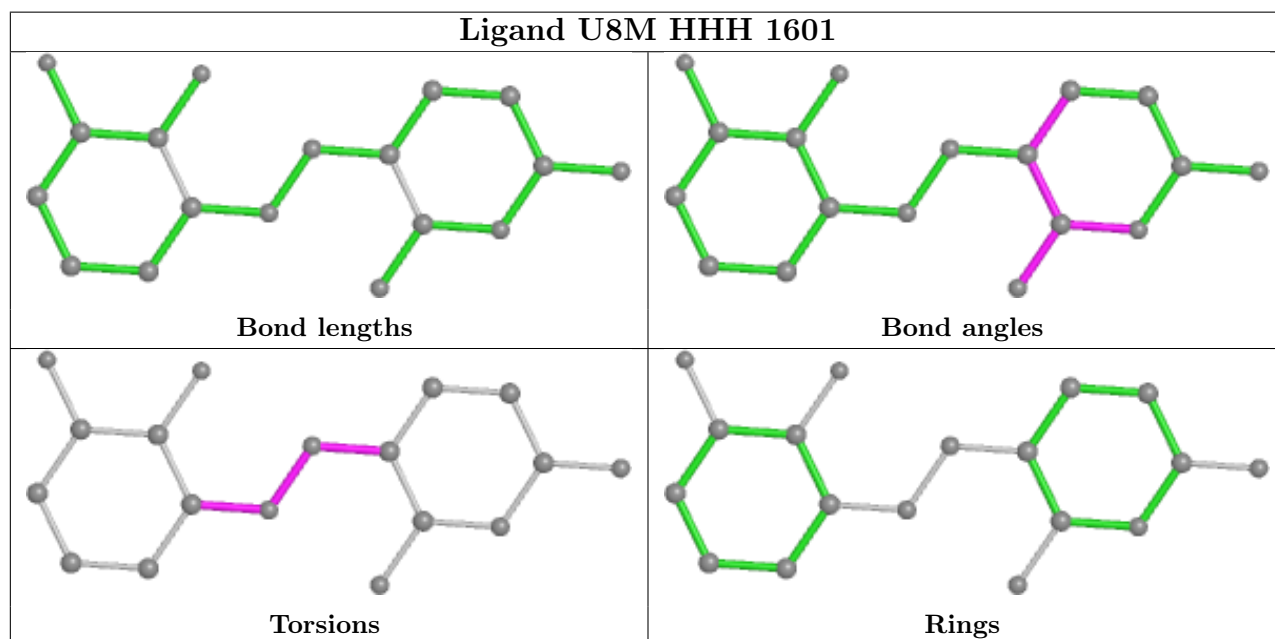
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	HHH	95/95 (100%)	-0.07	3 (3%)	47	50	45, 70, 105, 124	0
2	CCC	199/227 (87%)	0.71	34 (17%)	1	1	41, 69, 137, 205	0
3	ZZZ	21/52 (40%)	0.21	3 (14%)	2	2	45, 64, 125, 134	0
All	All	315/374 (84%)	0.45	40 (12%)	3	3	41, 70, 130, 205	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	CCC	8	GLN	7.1
2	CCC	7	THR	6.6
2	CCC	9	LEU	5.4
2	CCC	116	LEU	4.7
2	CCC	111	SER	4.7
2	CCC	105	PRO	4.4
2	CCC	115	LEU	4.3
2	CCC	10	ASN	4.3
2	CCC	100	PHE	3.9
2	CCC	104	GLN	3.5
2	CCC	27	VAL	3.4
2	CCC	85	VAL	3.4
1	HHH	1221	VAL	3.4
2	CCC	196	ILE	3.4
1	HHH	1157	GLY	3.3
2	CCC	112	SER	3.3
2	CCC	119	VAL	3.3
2	CCC	113	ASP	3.2
2	CCC	83	VAL	3.1
2	CCC	84	VAL	3.1
2	CCC	118	HIS	2.9
2	CCC	167	LYS	2.8
1	HHH	1163	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	CCC	14	VAL	2.7
2	CCC	23	LEU	2.7
2	CCC	114	SER	2.7
2	CCC	26	ALA	2.7
2	CCC	99	VAL	2.7
2	CCC	98	PHE	2.7
3	ZZZ	1889	GLU	2.6
2	CCC	195	ASP	2.5
2	CCC	30	ILE	2.4
2	CCC	49	ASN	2.4
2	CCC	13	GLN	2.4
2	CCC	148	VAL	2.2
3	ZZZ	1873	ARG	2.2
2	CCC	92	HIS	2.1
2	CCC	39	VAL	2.1
3	ZZZ	1891	MET	2.0
2	CCC	90	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

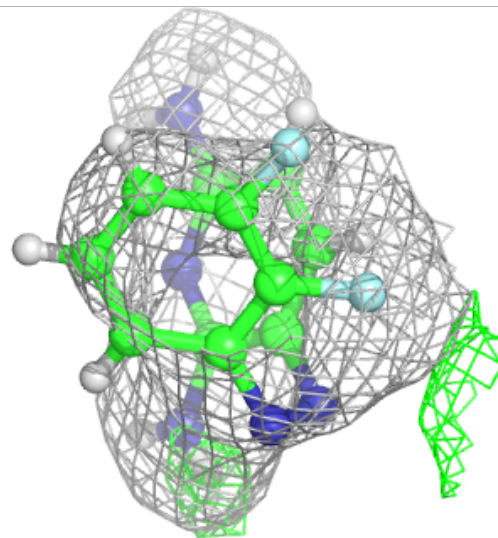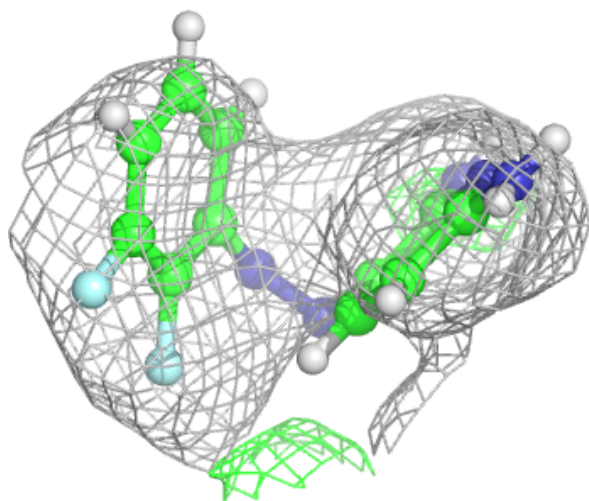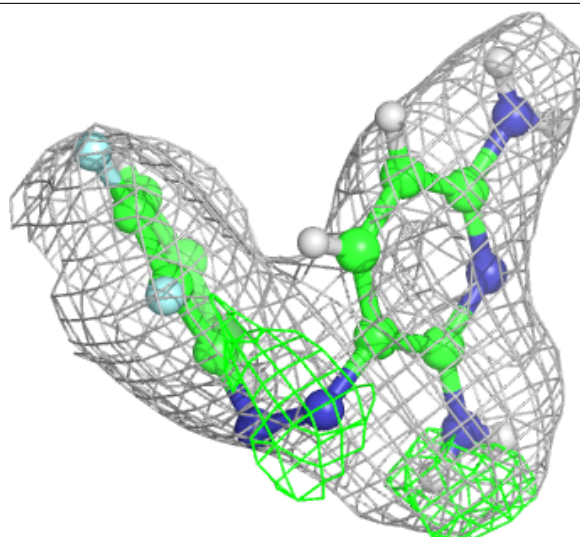There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\mathring{A}^2$)	Q<0.9
4	U8M	HHH	1601	18/18	0.70	0.17	65,119,143,146	4

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around U8M HHH 1601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.