Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2022 – 05:26 pm BST

PDB ID	:	7QMP
Title	:	Endothiapepsin in complex with compound TL00150 at room-temperature (temperature ramping down structure 17)
Authors	:	Huang, C.Y.; Aumonier, S.; Wang, M.
Deposited on	:	2021-12-20
Resolution	:	1.79 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 (i)) were used in the production of this report:

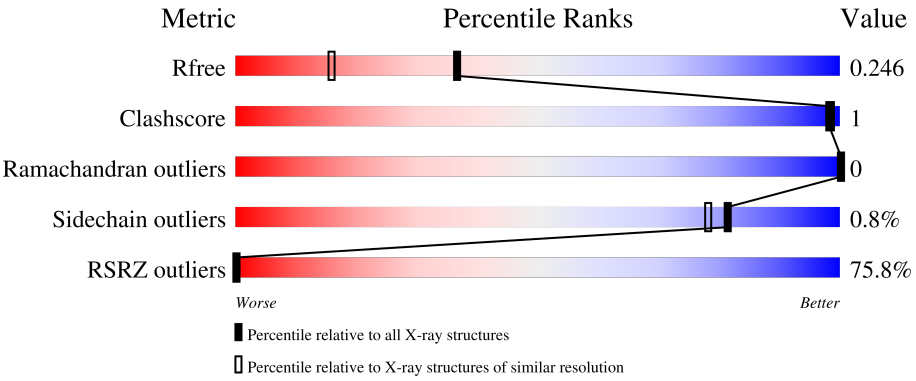
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 1.79 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))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	A	419	60% 77% · 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	U1H	A	2601	-	-	-	X

2 Entry composition

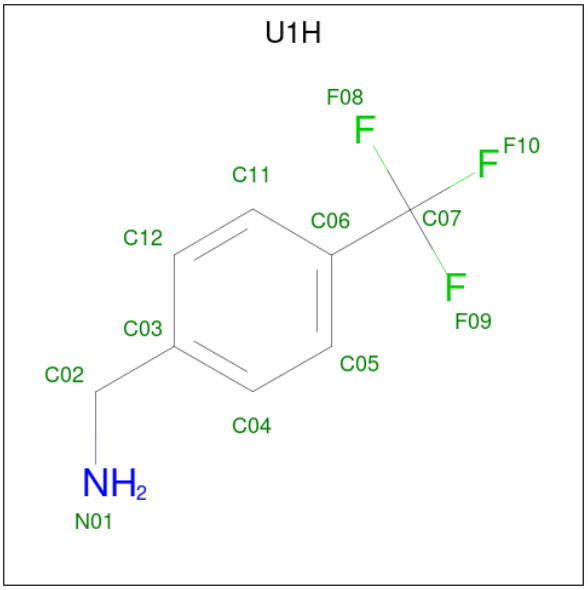
There are 5 unique types of molecules in this entry. The entry contains 2613 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Endothiapepsin.

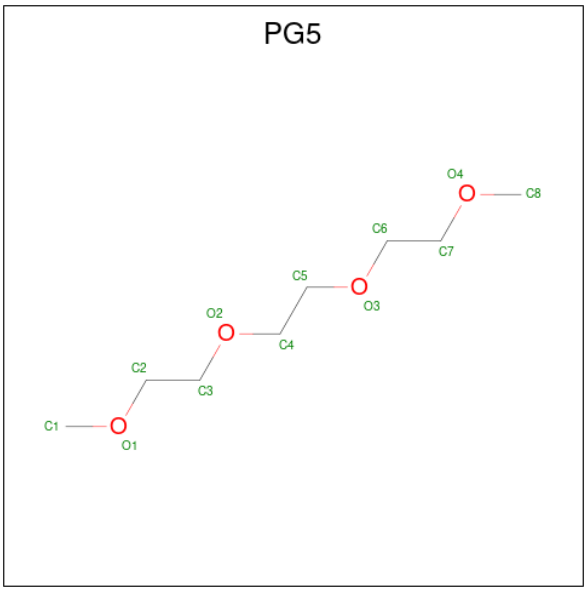
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2379	1509	361	507	2			

- Molecule 2 is [4-(trifluoromethyl)phenyl]methanamine (three-letter code: U1H) (formula: $C_8H_8F_3N$) (labeled as "Ligand of Interest" by depositor).



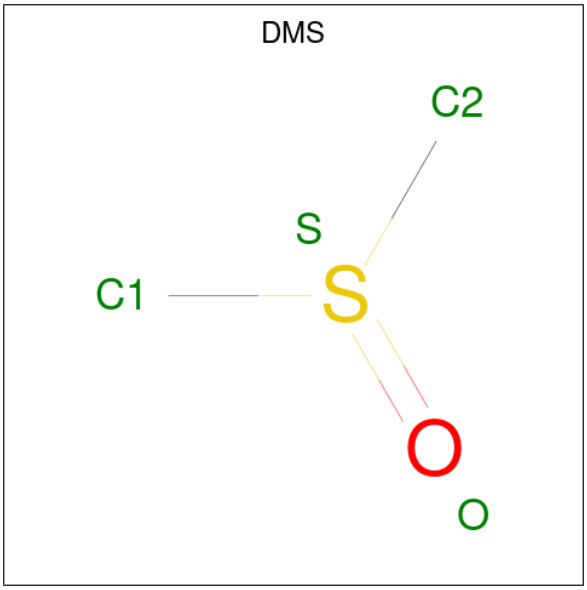
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	N	0	0
			12	8	3	1		
2	A	1	Total	C	F	N	0	0
			12	8	3	1		

- Molecule 3 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY]-ETHANE (three-letter code: PG5) (formula: $C_8H_{18}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 8 4	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 4 2 1 1	0	0
4	A	1	Total C O S 4 2 1 1	0	0
4	A	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is water.

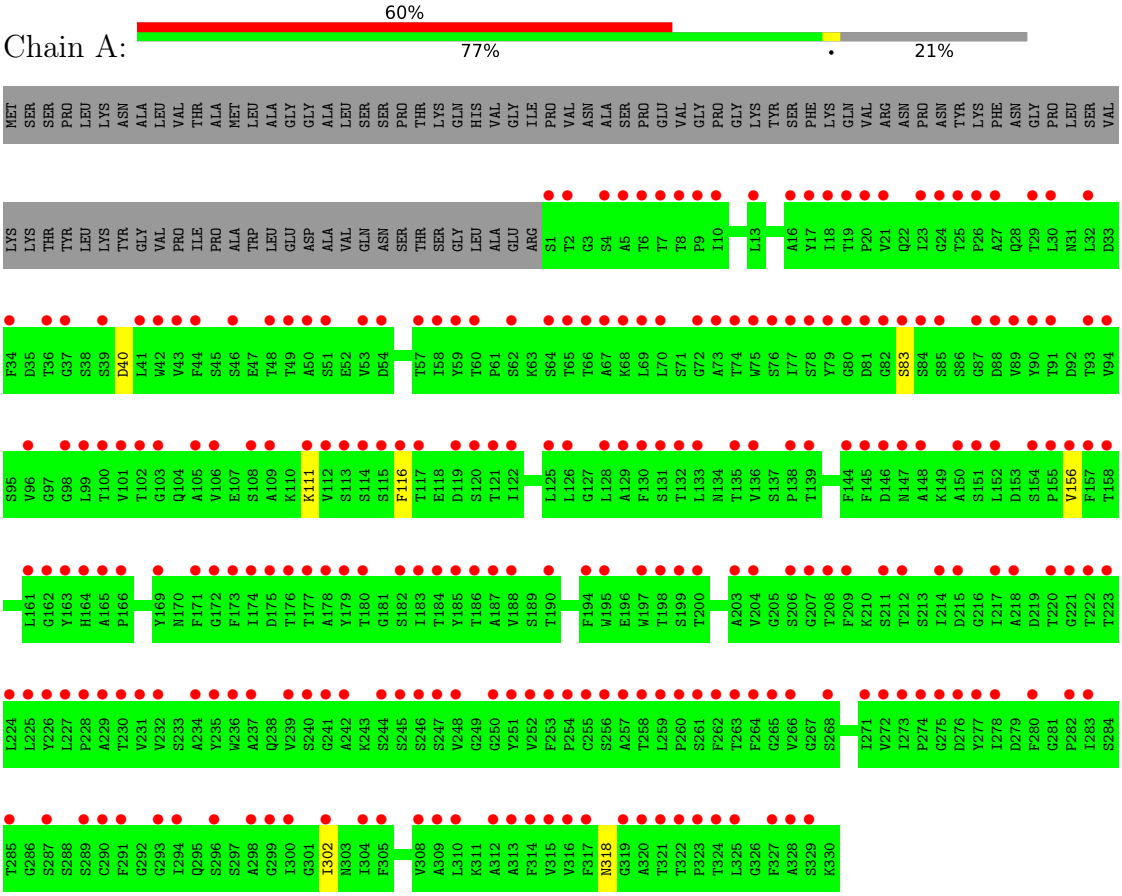
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	186	Total	O	0	0
			186	186		

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 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: Endothiapepsin

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	45.79Å 74.00Å 53.50Å 90.00° 109.70° 90.00°	Depositor
Resolution (Å)	37.00 – 1.79 43.11 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.00-1.79) 99.6 (43.11-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.207 , 0.246 0.206 , 0.246	Depositor DCC
R_{free} test set	1572 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2613	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: DMS, PG5, U1H

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	0.31	0/2435	0.54	0/3335

There are no bond length outliers.

There are no bond angle outliers.

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	2379	0	2245	3	0
2	A	24	0	0	0	0
3	A	12	0	18	0	0
4	A	12	0	18	0	0
5	A	186	0	0	1	0
All	All	2613	0	2281	3	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 1.

All (3) 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:A:156:VAL:HG12	1:A:318:ASN:HA	1.95	0.48
1:A:83:SER:HB3	1:A:116:PHE:CE2	2.55	0.42
1:A:302:ILE:HG13	5:A:2757:HOH:O	2.20	0.41

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	328/419 (78%)	324 (99%)	4 (1%)	0	100 100

There are no Ramachandran outliers to report.

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	258/336 (77%)	256 (99%)	2 (1%)	81 78

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	111	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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)

6 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	U1H	A	2601	-	12,12,12	0.73	0	17,17,17	1.17	0
3	PG5	A	2602	-	11,11,11	0.49	0	10,10,10	0.26	0
2	U1H	A	2606	-	12,12,12	0.78	0	17,17,17	1.05	0
4	DMS	A	2603	-	3,3,3	0.73	0	3,3,3	0.18	0
4	DMS	A	2605	-	3,3,3	0.72	0	3,3,3	0.32	0
4	DMS	A	2604	-	3,3,3	0.73	0	3,3,3	0.12	0

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	U1H	A	2601	-	-	0/8/8/8	0/1/1/1
2	U1H	A	2606	-	-	0/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PG5	A	2602	-	-	6/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

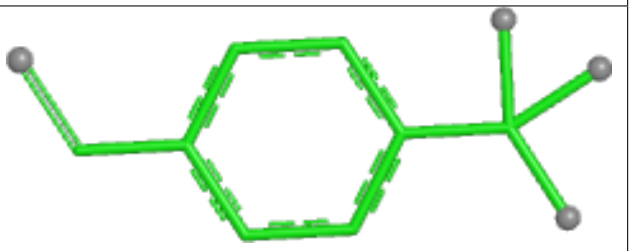
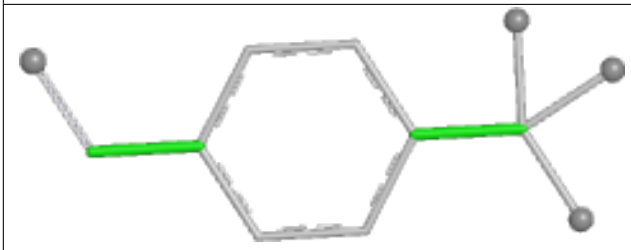
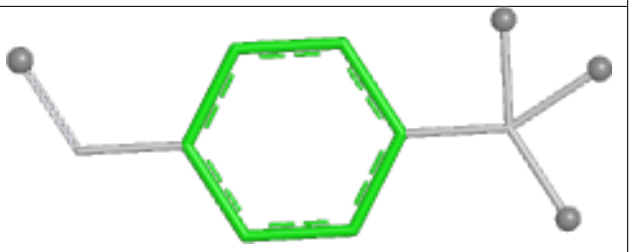
All (6) torsion outliers are listed below:

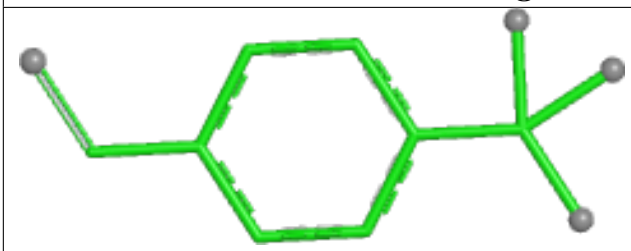
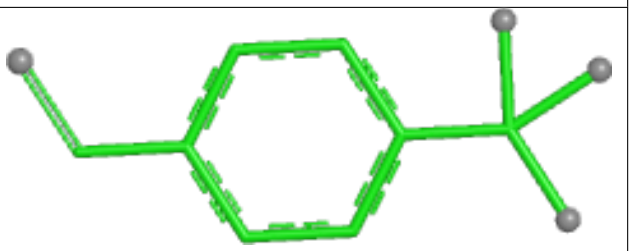
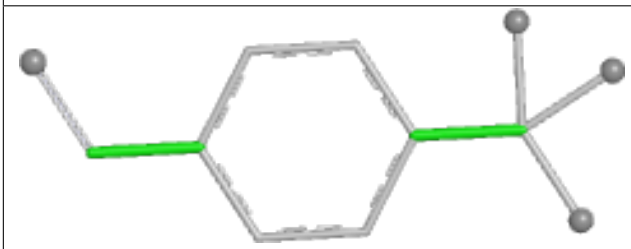
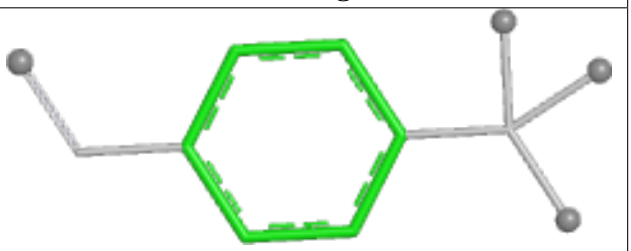
Mol	Chain	Res	Type	Atoms
3	A	2602	PG5	O1-C2-C3-O2
3	A	2602	PG5	C6-C7-O4-C8
3	A	2602	PG5	C2-C3-O2-C4
3	A	2602	PG5	C3-C2-O1-C1
3	A	2602	PG5	O2-C4-C5-O3
3	A	2602	PG5	O3-C6-C7-O4

There are no ring outliers.

No monomer is involved in short contacts.

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 U1H A 2601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand U1H A 2606	
 Bond lengths	 Bond angles
 Torsions	 Rings

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

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, 95^{th} 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	A	330/419 (78%)	2.91	250 (75%)	0	0	22, 30, 44, 56	0

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	GLY	8.0
1	A	79	TYR	6.5
1	A	156	VAL	6.5
1	A	80	GLY	6.1
1	A	58	ILE	6.0
1	A	252	VAL	6.0
1	A	258	THR	5.8
1	A	190	THR	5.8
1	A	273	ILE	5.7
1	A	246	SER	5.5
1	A	122	ILE	5.4
1	A	283	ILE	5.4
1	A	248	VAL	5.4
1	A	300	ILE	5.3
1	A	150	ALA	5.2
1	A	188	VAL	5.1
1	A	27	ALA	5.1
1	A	294	ILE	5.0
1	A	231	VAL	5.0
1	A	313	ALA	4.9
1	A	144	PHE	4.9
1	A	321	THR	4.8
1	A	280	PHE	4.7
1	A	187	ALA	4.7
1	A	316	VAL	4.7
1	A	312	ALA	4.7
1	A	51	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	234	ALA	4.6
1	A	152	LEU	4.5
1	A	113	SER	4.5
1	A	299	GLY	4.4
1	A	83	SER	4.4
1	A	74	THR	4.4
1	A	266	VAL	4.4
1	A	10	ILE	4.4
1	A	204	VAL	4.4
1	A	44	PHE	4.4
1	A	114	SER	4.4
1	A	315	VAL	4.4
1	A	163	TYR	4.3
1	A	302	ILE	4.3
1	A	69	LEU	4.3
1	A	186	THR	4.3
1	A	327	PHE	4.3
1	A	230	THR	4.3
1	A	54	ASP	4.2
1	A	121	THR	4.2
1	A	136	VAL	4.2
1	A	148	ALA	4.2
1	A	178	ALA	4.2
1	A	259	LEU	4.2
1	A	42	TRP	4.1
1	A	43	VAL	4.1
1	A	128	LEU	4.1
1	A	75	TRP	4.1
1	A	240	SER	4.1
1	A	90	TYR	4.0
1	A	217	ILE	4.0
1	A	36	THR	4.0
1	A	236	TRP	3.9
1	A	139	THR	3.9
1	A	195	TRP	3.9
1	A	261	SER	3.9
1	A	117	THR	3.9
1	A	251	TYR	3.9
1	A	287	SER	3.9
1	A	272	VAL	3.9
1	A	177	THR	3.9
1	A	239	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	7	THR	3.9
1	A	227	LEU	3.8
1	A	255	CYS	3.8
1	A	26	PRO	3.8
1	A	155	PRO	3.8
1	A	67	ALA	3.8
1	A	57	THR	3.8
1	A	21	VAL	3.7
1	A	41	LEU	3.7
1	A	101	VAL	3.7
1	A	285	THR	3.7
1	A	271	ILE	3.7
1	A	304	ILE	3.7
1	A	49	THR	3.7
1	A	65	THR	3.7
1	A	161	LEU	3.6
1	A	89	VAL	3.6
1	A	232	VAL	3.6
1	A	165	ALA	3.6
1	A	194	PHE	3.6
1	A	209	PHE	3.6
1	A	278	ILE	3.6
1	A	158	THR	3.6
1	A	200	THR	3.5
1	A	73	ALA	3.5
1	A	5	ALA	3.5
1	A	129	ALA	3.5
1	A	198	THR	3.5
1	A	197	TRP	3.5
1	A	93	THR	3.5
1	A	46	SER	3.5
1	A	2	THR	3.4
1	A	247	SER	3.4
1	A	225	LEU	3.4
1	A	84	SER	3.4
1	A	13	LEU	3.4
1	A	96	VAL	3.4
1	A	106	VAL	3.4
1	A	109	ALA	3.4
1	A	23	ILE	3.4
1	A	214	ILE	3.4
1	A	81	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	173	PHE	3.4
1	A	18	ILE	3.3
1	A	17	TYR	3.3
1	A	68	LYS	3.3
1	A	182	SER	3.3
1	A	146	ASP	3.3
1	A	264	PHE	3.3
1	A	53	VAL	3.3
1	A	166	PRO	3.3
1	A	320	ALA	3.3
1	A	305	PHE	3.3
1	A	224	LEU	3.3
1	A	151	SER	3.2
1	A	112	VAL	3.2
1	A	325	LEU	3.2
1	A	229	ALA	3.2
1	A	64	SER	3.2
1	A	329	SER	3.2
1	A	108	SER	3.2
1	A	309	ALA	3.2
1	A	119	ASP	3.2
1	A	78	SER	3.2
1	A	212	THR	3.2
1	A	183	ILE	3.1
1	A	208	THR	3.1
1	A	223	THR	3.1
1	A	277	TYR	3.1
1	A	145	PHE	3.1
1	A	237	ALA	3.1
1	A	133	LEU	3.1
1	A	48	THR	3.0
1	A	226	TYR	3.0
1	A	274	PRO	3.0
1	A	125	LEU	3.0
1	A	29	THR	3.0
1	A	66	THR	3.0
1	A	34	PHE	3.0
1	A	59	TYR	3.0
1	A	6	THR	3.0
1	A	222	THR	3.0
1	A	310	LEU	3.0
1	A	105	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	268	SER	3.0
1	A	111	LYS	3.0
1	A	88	ASP	2.9
1	A	138	PRO	2.9
1	A	235	TYR	2.9
1	A	253	PHE	2.9
1	A	176	THR	2.9
1	A	179	TYR	2.9
1	A	324	THR	2.9
1	A	103	GLY	2.9
1	A	135	THR	2.9
1	A	203	ALA	2.9
1	A	1	SER	2.8
1	A	19	THR	2.8
1	A	256	SER	2.8
1	A	70	LEU	2.8
1	A	291	PHE	2.8
1	A	323	PRO	2.8
1	A	91	THR	2.8
1	A	76	SER	2.7
1	A	157	PHE	2.7
1	A	244	SER	2.7
1	A	169	TYR	2.7
1	A	317	PHE	2.7
1	A	77	ILE	2.7
1	A	16	ALA	2.7
1	A	132	THR	2.7
1	A	25	THR	2.6
1	A	126	LEU	2.6
1	A	130	PHE	2.6
1	A	164	HIS	2.6
1	A	293	GLY	2.6
1	A	87	GLY	2.5
1	A	322	THR	2.5
1	A	314	PHE	2.5
1	A	174	ILE	2.5
1	A	206	SER	2.5
1	A	32	LEU	2.5
1	A	99	LEU	2.5
1	A	20	PRO	2.5
1	A	180	THR	2.5
1	A	185	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	207	GLY	2.5
1	A	147	ASN	2.5
1	A	102	THR	2.5
1	A	220	THR	2.5
1	A	276	ASP	2.4
1	A	115	SER	2.4
1	A	131	SER	2.4
1	A	94	VAL	2.4
1	A	254	PRO	2.4
1	A	241	GLY	2.4
1	A	37	GLY	2.4
1	A	175	ASP	2.4
1	A	308	VAL	2.4
1	A	85	SER	2.4
1	A	215	ASP	2.4
1	A	275	GLY	2.4
1	A	242	ALA	2.3
1	A	298	ALA	2.3
1	A	265	GLY	2.3
1	A	263	THR	2.3
1	A	282	PRO	2.3
1	A	262	PHE	2.3
1	A	245	SER	2.2
1	A	24	GLY	2.2
1	A	98	GLY	2.2
1	A	290	CYS	2.2
1	A	39	SER	2.2
1	A	154	SER	2.2
1	A	199	SER	2.2
1	A	184	THR	2.2
1	A	218	ALA	2.2
1	A	62	SER	2.2
1	A	120	SER	2.2
1	A	100	THR	2.2
1	A	319	GLY	2.2
1	A	116	PHE	2.2
1	A	4	SER	2.2
1	A	211	SER	2.2
1	A	9	PRO	2.2
1	A	250	GLY	2.2
1	A	72	GLY	2.1
1	A	8	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	50	ALA	2.1
1	A	257	ALA	2.1
1	A	289	SER	2.1
1	A	60	THR	2.1
1	A	296	SER	2.1
1	A	162	GLY	2.1
1	A	221	GLY	2.1
1	A	328	ALA	2.1
1	A	228	PRO	2.0
1	A	260	PRO	2.0
1	A	171	PHE	2.0
1	A	30	LEU	2.0
1	A	172	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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, 95^{th} 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.

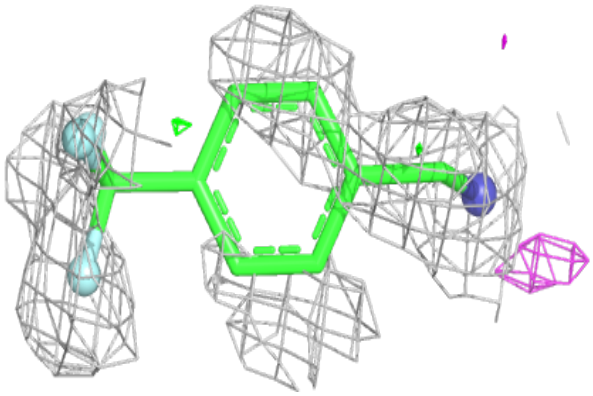
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	U1H	A	2601	12/12	0.05	0.43	23,41,51,52	12
2	U1H	A	2606	12/12	0.40	0.33	31,41,49,49	12
4	DMS	A	2604	4/4	0.54	0.40	44,51,55,60	4
3	PG5	A	2602	12/12	0.71	0.24	36,39,49,50	12
4	DMS	A	2605	4/4	0.73	0.22	40,47,49,56	4
4	DMS	A	2603	4/4	0.76	0.28	25,34,41,47	4

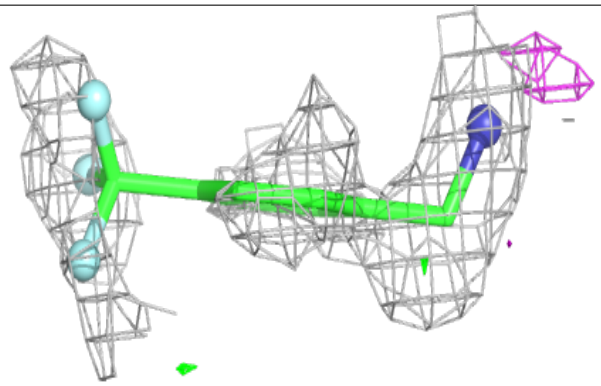
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

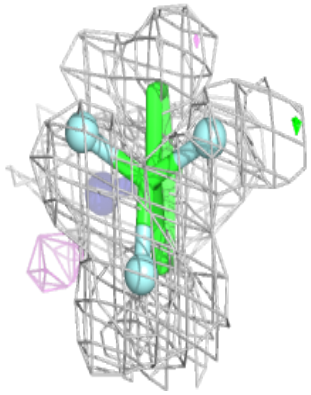
orientation to approximate a three-dimensional view.

Electron density around U1H A 2601:

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

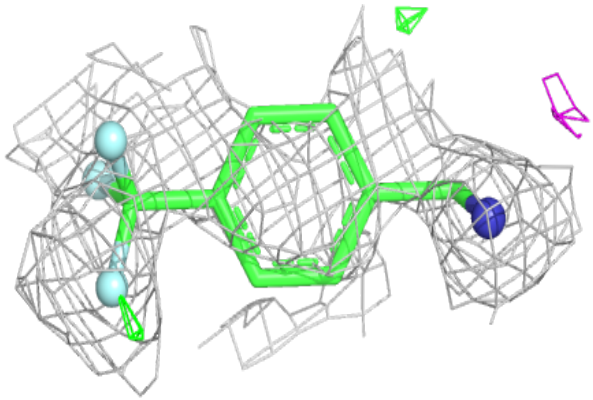


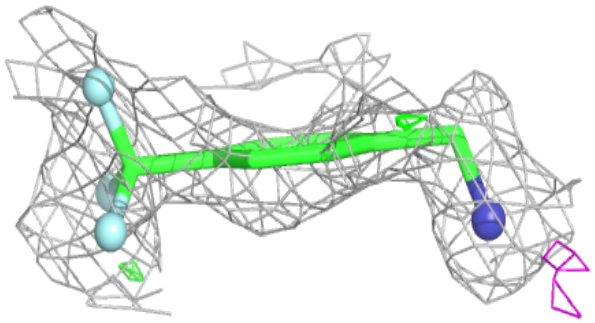


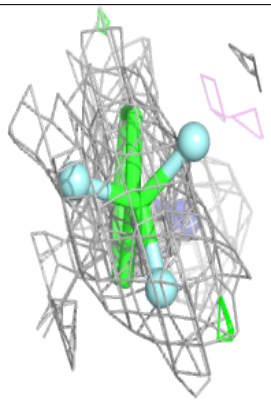


Electron density around U1H A 2606:

$2mF_o$-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 (i)

There are no such residues in this entry.