



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:15 PM BST

PDB ID : 5N9R
Title : Crystal structure of USP7 in complex with a potent, selective and reversible small-molecule inhibitor
Authors : Harrison, T.; Gavory, G.; O'Dowd, C.; Helm, M.; Flasz, I.; Arkoudis, E.; Dossang, A.; Hughes, C.; Cassidy, E.; McClelland, K.; Odrzywol, E.; Page, N.; Barker, O.; Miel, H.
Deposited on : 2017-02-27
Resolution : 2.23 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 ⓘ symbol.

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 : 2.13.1
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) : 2.13.1

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6388 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 Ubiquitin carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	356	2939	1855	506	560	18	0	6	0
1	B	347	2824	1784	480	542	18	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

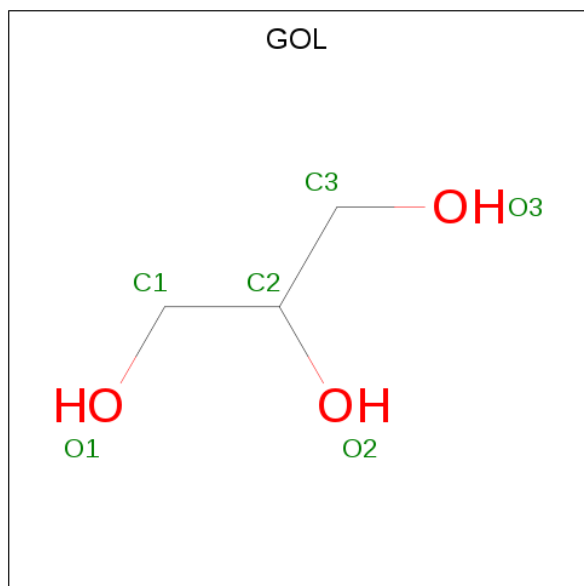
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	MET	-	initiating methionine	UNP Q93009
A	561	HIS	-	expression tag	UNP Q93009
A	562	HIS	-	expression tag	UNP Q93009
B	206	MET	-	initiating methionine	UNP Q93009
B	561	HIS	-	expression tag	UNP Q93009
B	562	HIS	-	expression tag	UNP Q93009

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



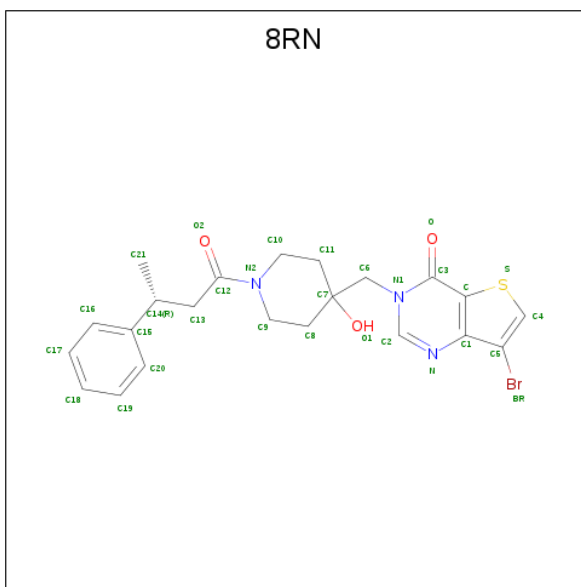
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



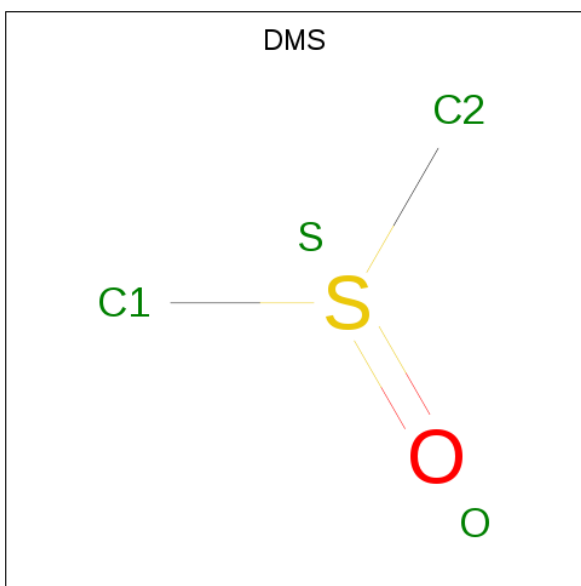
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 7-bromanyl-3-[[4-oxidanyl-1-[(3 {R})-3-phenylbutanoyl]piperidin-4-yl]methyl]thieno[3,2-d]pyrimidin-4-one (three-letter code: 8RN) (formula: C₂₂H₂₄BrN₃O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	Br	C	N	O			S
4	A	1	30	1	22	3	3	1	0	0
4	B	1	30	1	22	3	3	1	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

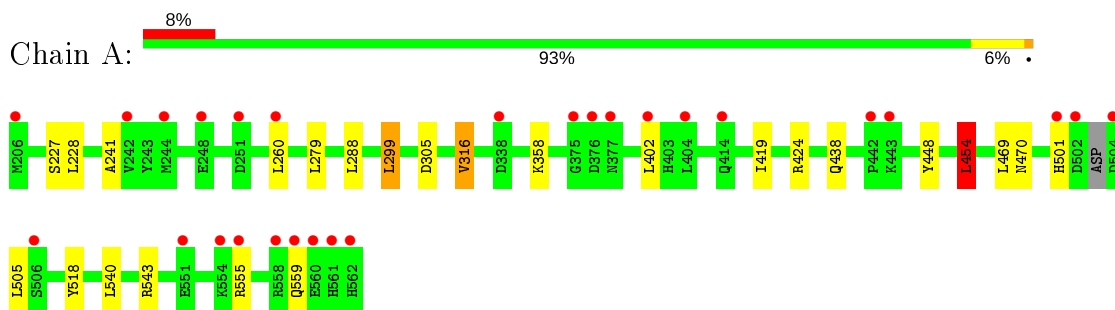
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	295	Total 295	O 295	0	0
6	B	233	Total 233	O 233	0	0

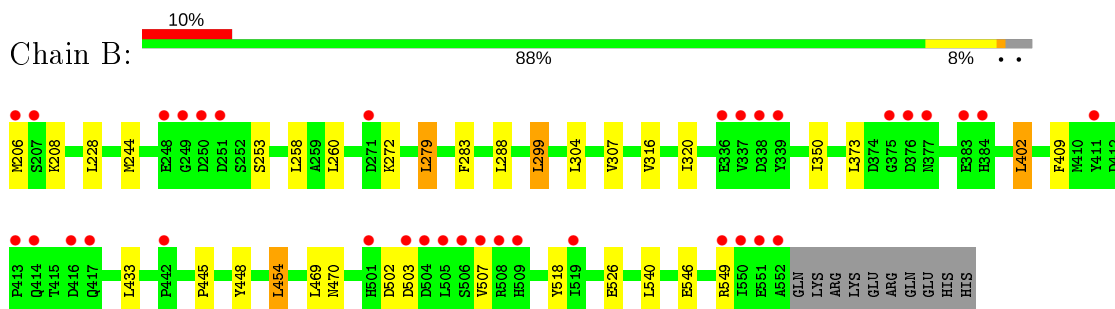
3 Residue-property plots [i](#)

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 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: Ubiquitin carboxyl-terminal hydrolase 7



- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.94Å 66.94Å 81.09Å 90.00° 105.09° 90.00°	Depositor
Resolution (Å)	20.00 – 2.23 19.71 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.23) 99.4 (19.71-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.59 (at 2.23Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.148 , 0.212 0.161 , 0.219	Depositor DCC
R_{free} test set	1848 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtrriage
Anisotropy	0.066	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6388	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: GOL, 8RN, DMS, SO4

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	0.46	0/3018	0.69	1/4064 (0.0%)
1	B	0.46	0/2890	0.70	1/3898 (0.0%)
All	All	0.46	0/5908	0.69	2/7962 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	LEU	CA-CB-CG	5.93	128.94	115.30
1	B	454	LEU	CA-CB-CG	5.63	128.25	115.30

There are no chirality outliers.

There are no planarity outliers.

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	A	2939	0	2885	6	0
1	B	2824	0	2761	7	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
3	A	6	0	8	0	0
3	B	12	0	16	0	0
4	A	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	30	0	0	0	0
5	B	4	0	6	0	0
6	A	295	0	0	1	0
6	B	233	0	0	1	0
All	All	6388	0	5676	13	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 (13) 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:305[B]:ASP:OD2	6:A:1101:HOH:O	1.88	0.90
1:B:307:VAL:HG23	1:B:320:ILE:CD1	2.31	0.60
1:A:419:ILE:O	1:A:419:ILE:HD12	2.03	0.59
1:B:307:VAL:HG23	1:B:320:ILE:HD11	1.86	0.57
1:A:227:SER:HB3	1:A:454:LEU:HD13	1.87	0.55
1:B:228:LEU:HD23	1:B:299:LEU:HD13	1.89	0.55
1:A:228:LEU:HD23	1:A:299:LEU:HD13	1.95	0.48
1:B:448:TYR:HB3	1:B:518:TYR:HB3	1.95	0.48
1:A:448:TYR:HB3	1:A:518:TYR:HB3	1.95	0.47
1:A:241:ALA:HA	1:A:316:VAL:HG21	2.00	0.44
1:B:350:ILE:HD12	1:B:402:LEU:HD21	2.01	0.42
1:B:304:LEU:HD12	6:B:1297:HOH:O	2.18	0.42
1:B:279:LEU:HD22	1:B:283:PHE:HE1	1.86	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	358/357 (100%)	350 (98%)	8 (2%)	0	100	100
1	B	347/357 (97%)	333 (96%)	14 (4%)	0	100	100
All	All	705/714 (99%)	683 (97%)	22 (3%)	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	329/324 (102%)	311 (94%)	18 (6%)	21	20
1	B	316/324 (98%)	290 (92%)	26 (8%)	11	8
All	All	645/648 (100%)	601 (93%)	44 (7%)	15	13

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	LEU
1	A	279	LEU
1	A	288	LEU
1	A	299	LEU
1	A	316	VAL
1	A	358	LYS
1	A	402	LEU
1	A	424	ARG
1	A	438	GLN
1	A	454	LEU
1	A	469	LEU
1	A	470	ASN
1	A	501	HIS
1	A	505	LEU
1	A	540	LEU
1	A	543	ARG
1	A	555	ARG
1	A	559	GLN

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Mol	Chain	Res	Type
1	B	206	MET
1	B	208	LYS
1	B	244	MET
1	B	253	SER
1	B	258	LEU
1	B	260	LEU
1	B	272	LYS
1	B	279	LEU
1	B	288	LEU
1	B	299	LEU
1	B	316	VAL
1	B	373	LEU
1	B	402	LEU
1	B	409	PHE
1	B	433	LEU
1	B	445	PRO
1	B	454	LEU
1	B	469	LEU
1	B	470	ASN
1	B	502	ASP
1	B	503	ASP
1	B	507	VAL
1	B	526	GLU
1	B	540	LEU
1	B	546	GLU
1	B	549	ARG

Some 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

9 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
5	DMS	B	1003	-	3,3,3	0.55	0	3,3,3	0.49	0
4	8RN	A	1003	-	30,33,33	2.16	4 (13%)	29,48,48	1.59	5 (17%)
3	GOL	A	1002	-	5,5,5	0.47	0	5,5,5	0.41	0
3	GOL	B	1005	-	5,5,5	0.31	0	5,5,5	0.16	0
2	SO4	B	1002	-	4,4,4	0.33	0	6,6,6	0.14	0
3	GOL	B	1004	-	5,5,5	0.36	0	5,5,5	0.36	0
2	SO4	A	1001	-	4,4,4	0.33	0	6,6,6	0.35	0
4	8RN	B	1006	-	30,33,33	2.19	4 (13%)	29,48,48	1.72	4 (13%)
2	SO4	B	1001	-	4,4,4	0.32	0	6,6,6	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	1004	-	-	2/4/4/4	-
3	GOL	A	1002	-	-	2/4/4/4	-
4	8RN	A	1003	-	-	4/17/29/29	0/4/4/4
4	8RN	B	1006	-	-	4/17/29/29	0/4/4/4
3	GOL	B	1005	-	-	1/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	8RN	C1-N	7.60	1.46	1.37
4	B	1006	8RN	C1-N	7.36	1.46	1.37
4	B	1006	8RN	C4-S	-6.91	1.62	1.70
4	A	1003	8RN	C4-S	-6.39	1.62	1.70
4	B	1006	8RN	C8-C7	3.76	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	8RN	C8-C7	3.58	1.56	1.52
4	B	1006	8RN	C12-N2	2.07	1.39	1.35
4	A	1003	8RN	C11-C7	2.02	1.54	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1006	8RN	C4-S-C	6.26	98.72	91.24
4	A	1003	8RN	C4-S-C	5.72	98.08	91.24
4	B	1006	8RN	C-C1-N	-3.60	120.72	124.96
4	A	1003	8RN	C-C1-N	-3.35	121.01	124.96
4	B	1006	8RN	O2-C12-C13	-3.29	116.26	122.20
4	A	1003	8RN	C13-C12-N2	2.96	124.24	118.52
4	B	1006	8RN	C13-C12-N2	2.88	124.08	118.52
4	A	1003	8RN	O2-C12-N2	-2.32	117.52	122.05
4	A	1003	8RN	O2-C12-C13	-2.24	118.16	122.20

There are no chirality outliers.

All (13) torsion outliers are listed below:

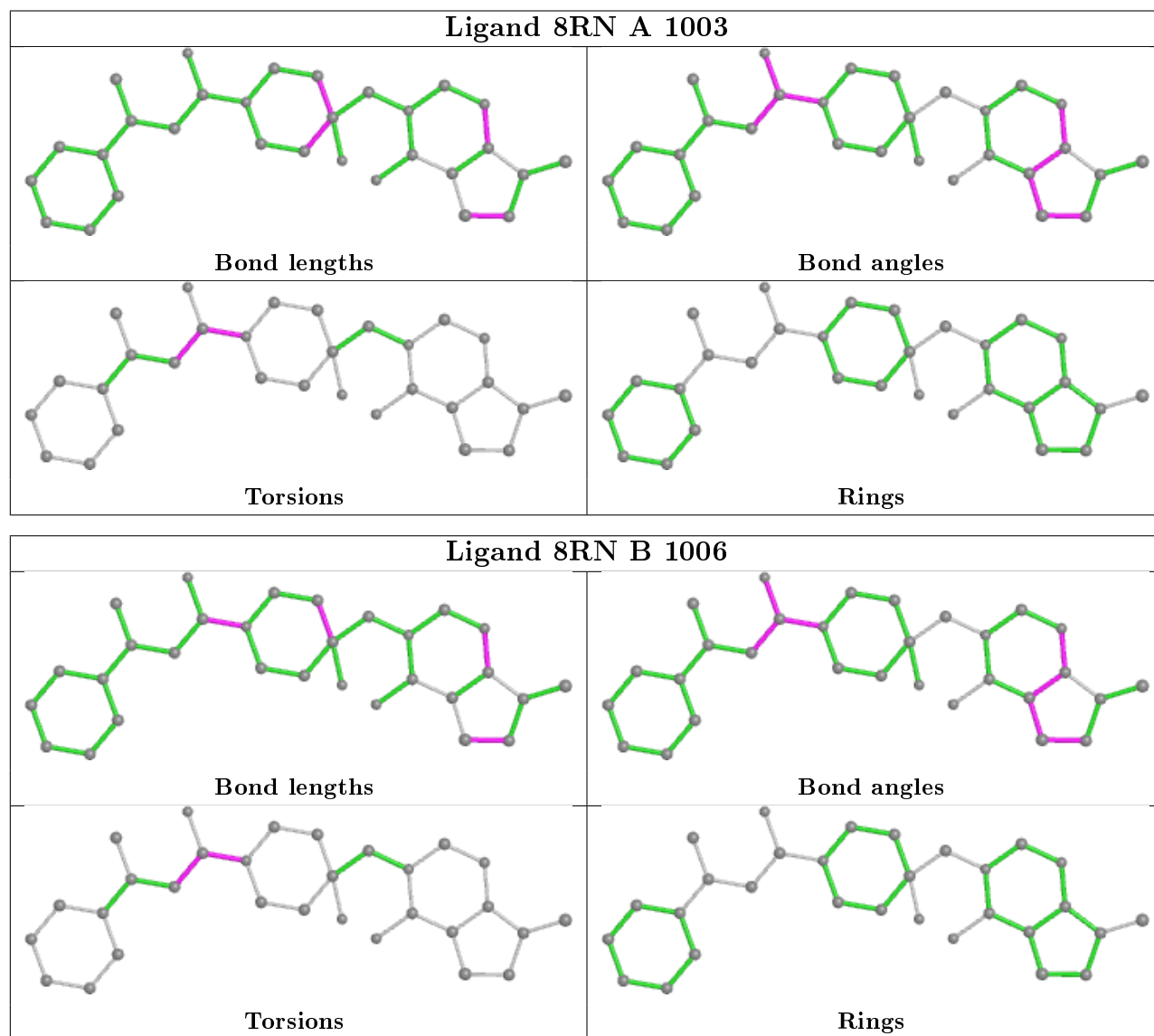
Mol	Chain	Res	Type	Atoms
3	A	1002	GOL	O1-C1-C2-C3
4	A	1003	8RN	C13-C12-N2-C9
3	B	1004	GOL	C1-C2-C3-O3
3	B	1004	GOL	O2-C2-C3-O3
3	A	1002	GOL	O1-C1-C2-O2
4	B	1006	8RN	C13-C12-N2-C9
4	A	1003	8RN	O2-C12-N2-C9
4	B	1006	8RN	O2-C12-N2-C9
4	A	1003	8RN	O2-C12-C13-C14
4	B	1006	8RN	O2-C12-C13-C14
4	A	1003	8RN	N2-C12-C13-C14
4	B	1006	8RN	N2-C12-C13-C14
3	B	1005	GOL	O1-C1-C2-C3

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 than 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.



5.7 Other polymers [i](#)

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	A	356/357 (99%)	0.14	27 (7%) 13 13	39, 58, 97, 143	0
1	B	347/357 (97%)	0.36	35 (10%) 7 6	39, 58, 117, 162	0
All	All	703/714 (98%)	0.25	62 (8%) 10 9	39, 58, 110, 162	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	505	LEU	11.8
1	B	552	ALA	9.0
1	B	206	MET	7.6
1	B	207	SER	7.4
1	B	507	VAL	6.9
1	B	506	SER	6.3
1	B	504	ASP	6.0
1	B	501	HIS	5.6
1	B	414	GLN	5.5
1	A	561	HIS	5.4
1	B	376	ASP	5.1
1	A	376	ASP	5.1
1	A	558	ARG	4.9
1	A	555	ARG	4.7
1	A	206	MET	4.4
1	A	502	ASP	4.1
1	A	559	GLN	4.0
1	B	551	GLU	3.9
1	B	503	ASP	3.7
1	B	375	GLY	3.5
1	B	508	ARG	3.5
1	A	442	PRO	3.4
1	A	562	HIS	3.4
1	B	250	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	375	GLY	3.3
1	B	549	ARG	3.3
1	B	337	VAL	3.2
1	B	251	ASP	3.1
1	A	377	ASN	3.1
1	B	338	ASP	3.0
1	A	443	LYS	3.0
1	A	560	GLU	2.9
1	B	384	HIS	2.9
1	A	251	ASP	2.9
1	B	271	ASP	2.8
1	A	402	LEU	2.8
1	B	416	ASP	2.7
1	A	551	GLU	2.7
1	B	248	GLU	2.7
1	A	504	ASP	2.7
1	A	414	GLN	2.7
1	A	554	LYS	2.6
1	A	501	HIS	2.6
1	A	242	VAL	2.6
1	A	338	ASP	2.6
1	B	336	GLU	2.6
1	B	413	PRO	2.5
1	B	442	PRO	2.5
1	B	509	HIS	2.5
1	A	404	LEU	2.5
1	B	339	TYR	2.4
1	A	248	GLU	2.4
1	A	506	SER	2.4
1	B	550	ILE	2.3
1	B	377	ASN	2.3
1	A	260	LEU	2.3
1	B	249	GLY	2.3
1	A	244	MET	2.2
1	B	417	GLN	2.2
1	B	411	TYR	2.2
1	B	383	GLU	2.2
1	B	519	ILE	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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

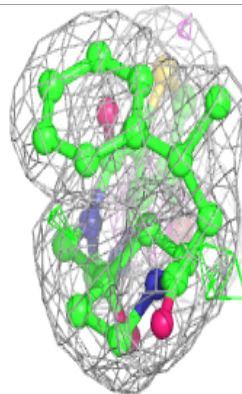
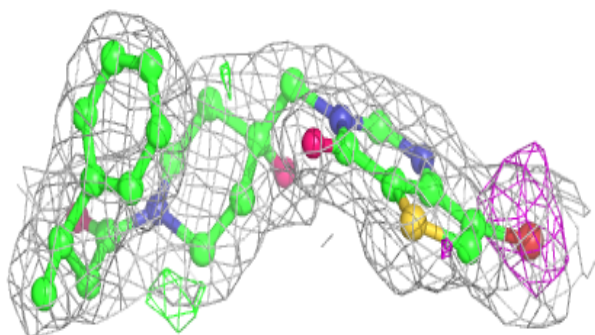
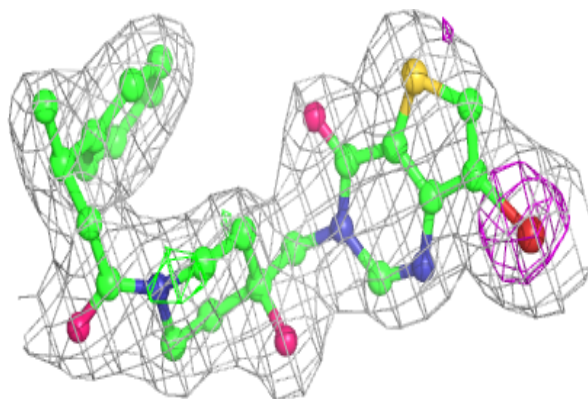
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	B	1005	6/6	0.85	0.20	68,72,77,78	0
3	GOL	B	1004	6/6	0.86	0.30	68,81,87,95	0
3	GOL	A	1002	6/6	0.90	0.19	69,75,79,79	0
5	DMS	B	1003	4/4	0.93	0.23	66,78,82,85	4
4	8RN	A	1003	30/30	0.94	0.16	38,42,48,70	0
2	SO4	A	1001	5/5	0.94	0.12	60,66,87,96	0
4	8RN	B	1006	30/30	0.94	0.16	41,45,51,71	0
2	SO4	B	1002	5/5	0.97	0.27	87,91,98,99	0
2	SO4	B	1001	5/5	0.98	0.07	72,77,82,94	0

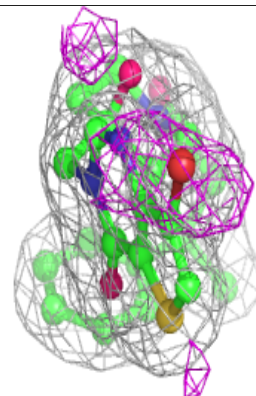
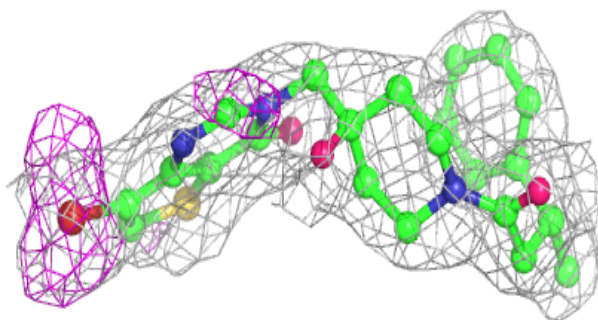
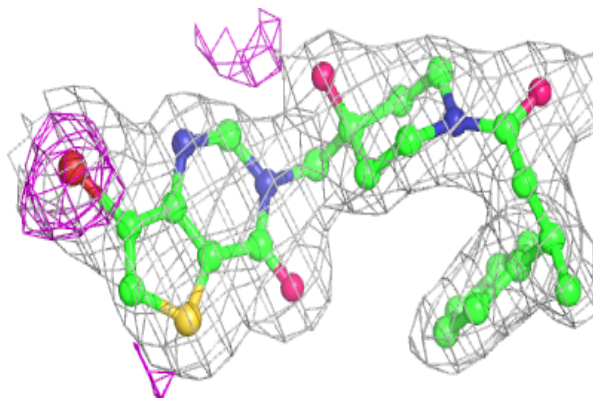
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8RN A 1003:

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

**Electron density around 8RN B 1006:**

$2mF_o-DF_c$ (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.