Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 02:00 am BST

PDB ID	:	4CSW
Title	:	Rhodothermus marinus YCFD-like ribosomal protein L16 Arginyl hydroxylase
Authors	:	McDonough, M.A.; Sekirnik, R.; Schofield, C.J.
Deposited on	:	2014-03-11
Resolution	:	2.82 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 following versions of software and data (see references (i)) were used in the production of this report:

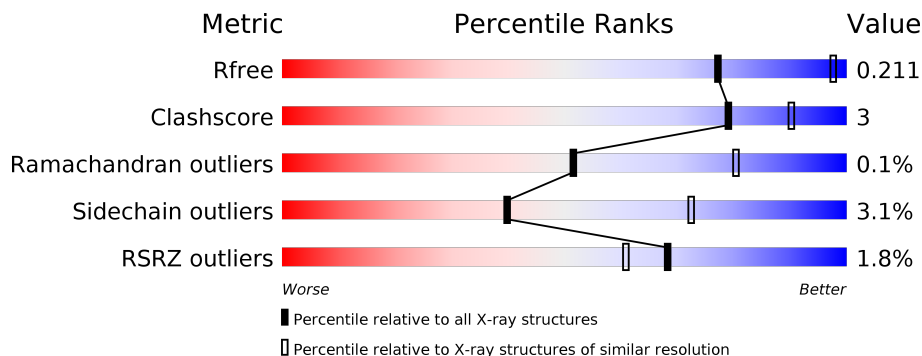|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.82 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		0.211
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		3.1%
RSRZ outliers		1.8%

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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 on 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	406	88% 7% •
1	B	406	85% 11% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6264 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 CUPIN 4 FAMILY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total 3050	C 1966	N 537	O 540	S 7	0	1	0
1	B	388	Total 3015	C 1949	N 525	O 534	S 7	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	HIS	-	expression tag	UNP D0MK34
A	-12	HIS	-	expression tag	UNP D0MK34
A	-11	HIS	-	expression tag	UNP D0MK34
A	-10	HIS	-	expression tag	UNP D0MK34
A	-9	SER	-	expression tag	UNP D0MK34
A	-8	SER	-	expression tag	UNP D0MK34
A	-7	GLY	-	expression tag	UNP D0MK34
A	-6	LEU	-	expression tag	UNP D0MK34
A	-5	VAL	-	expression tag	UNP D0MK34
A	-4	PRO	-	expression tag	UNP D0MK34
A	-3	ARG	-	expression tag	UNP D0MK34
A	-2	GLY	-	expression tag	UNP D0MK34
A	-1	SER	-	expression tag	UNP D0MK34
A	0	HIS	-	expression tag	UNP D0MK34
B	-13	HIS	-	expression tag	UNP D0MK34
B	-12	HIS	-	expression tag	UNP D0MK34
B	-11	HIS	-	expression tag	UNP D0MK34
B	-10	HIS	-	expression tag	UNP D0MK34
B	-9	SER	-	expression tag	UNP D0MK34
B	-8	SER	-	expression tag	UNP D0MK34
B	-7	GLY	-	expression tag	UNP D0MK34
B	-6	LEU	-	expression tag	UNP D0MK34
B	-5	VAL	-	expression tag	UNP D0MK34
B	-4	PRO	-	expression tag	UNP D0MK34
B	-3	ARG	-	expression tag	UNP D0MK34

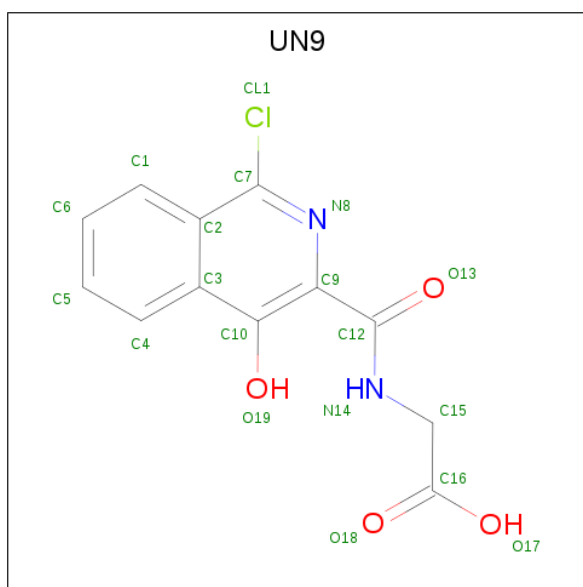*Continued on next page...*

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP D0MK34
B	-1	SER	-	expression tag	UNP D0MK34
B	0	HIS	-	expression tag	UNP D0MK34

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).
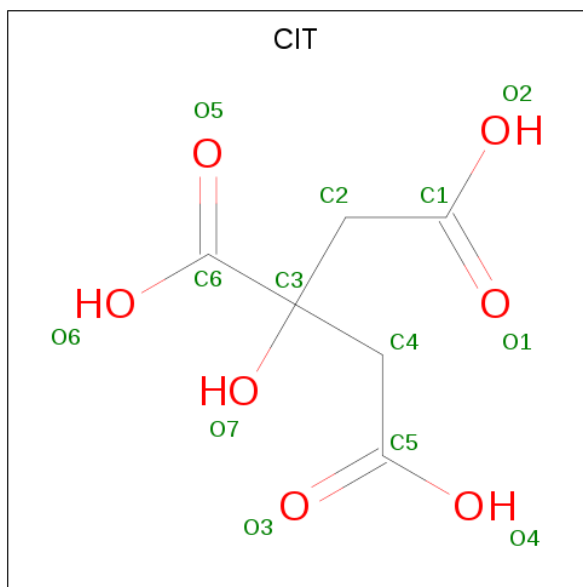
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 13	C 6	O 7	0	0

- Molecule 3 is N-[(1-CHLORO-4-HYDROXYISOQUINOLIN-3-YL)CARBONYL]GLYCINE (three-letter code: UN9) (formula: $C_{12}H_9ClN_2O_4$).

UN9

CL1
Cl

C1
C6
C7
N8
C2
C5
C3
C9　O13
O
C4
C10　C12
OH　HN
O19　N14　C15

C16
O
O18　OH
O17

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			19	12	1	2	4		
3	A	1	Total	C	Cl	N	O	0	0
			19	12	1	2	4		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3
OH O3

C1　C2

HO　OH
O1　O2

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

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Mn 1	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	84	Total 84	O 84	0	0
6	B	57	Total 57	O 57	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: CUPIN 4 FAMILY PROTEIN
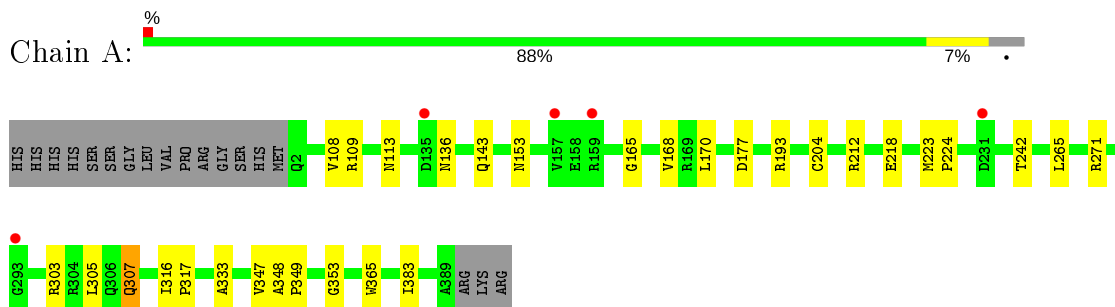
- Molecule 1: CUPIN 4 FAMILY PROTEIN
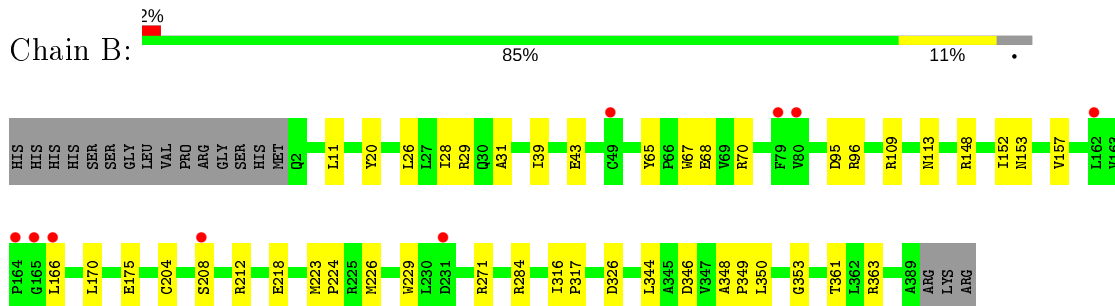
4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	158.30Å 87.69Å 90.61Å 90.00° 113.10° 90.00°	Depositor
Resolution (Å)	30.21 – 2.82	Depositor
	30.21 – 2.82	EDS
% Data completeness	96.8 (30.21-2.82)	Depositor
(in resolution range)	97.5 (30.21-2.82)	EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.18 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.168 , 0.210	Depositor
	0.169 , 0.211	DCC
R_{free} test set	2000 reflections (7.27%)	wwPDB-VP
Wilson B-factor (Å^2)	64.2	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.7	EDS
L-test for twinning[2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6264	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: GOL, MN, CIT, UN9

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	0.22	0/3141	0.41	0/4300
1	B	0.22	0/3102	0.41	0/4251
All	All	0.22	0/6243	0.41	0/8551

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	3050	0	3021	16	0
1	B	3015	0	2970	17	0
2	A	13	0	5	0	0
3	A	38	0	16	0	0
4	A	6	0	8	1	0
5	B	1	0	0	0	0
6	A	84	0	0	4	0
6	B	57	0	0	1	0
All	All	6264	0	6020	34	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 3.

All (34) 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:212:ARG:NH2	1:A:218:GLU:OE2	2.15	0.78
1:A:136:ASN:OD1	1:A:193:ARG:NH1	2.21	0.74
1:A:109:ARG:NH2	1:A:353:GLY:O	2.28	0.66
1:A:271:ARG:NH1	6:A:2041:HOH:O	2.31	0.61
1:B:109:ARG:NH1	1:B:113:ASN:OD1	2.33	0.61
1:A:271:ARG:NH2	6:A:2061:HOH:O	2.36	0.57
1:A:333:ALA:HB1	1:A:383:ILE:HG12	1.89	0.55
1:B:109:ARG:NH2	1:B:353:GLY:O	2.44	0.51
1:A:265:LEU:O	6:A:2062:HOH:O	2.19	0.50
1:B:153:ASN:ND2	1:B:175:GLU:O	2.41	0.50
1:B:284:ARG:NH1	6:B:2029:HOH:O	2.45	0.49
1:B:350:LEU:HD11	1:B:361:THR:CG2	2.43	0.49
1:B:95:ASP:OD2	1:B:96:ARG:NH1	2.46	0.48
4:A:1393:GOL:O1	6:A:2084:HOH:O	2.20	0.47
1:B:229:TRP:O	1:B:271:ARG:NH1	2.43	0.47
1:A:109:ARG:NH1	1:A:113:ASN:OD1	2.48	0.47
1:B:67:TRP:HB2	1:B:166:LEU:HD22	1.97	0.47
1:B:212:ARG:NH2	1:B:218:GLU:OE2	2.49	0.47
1:A:348:ALA:HB3	1:A:349:PRO:HD3	1.96	0.46
1:B:20:TYR:CZ	1:B:26:LEU:HD12	2.50	0.46
1:A:143:GLN:NE2	1:A:204:CYS:SG	2.87	0.46
1:A:108:VAL:HG12	1:A:108:VAL:O	2.16	0.45
1:A:347:VAL:HG12	1:A:365:TRP:CD2	2.51	0.45
1:A:153:ASN:ND2	1:A:177:ASP:OD2	2.49	0.45
1:A:303:ARG:NH2	1:A:307:GLN:OE1	2.51	0.44
1:B:39:ILE:HG12	1:B:43:GLU:HB2	2.00	0.43
1:A:223:MET:N	1:A:224:PRO:CD	2.81	0.42
1:B:28:ILE:CG2	1:B:31:ALA:HB2	2.49	0.42
1:B:68:GLU:OE1	1:B:70:ARG:NH1	2.53	0.42
1:B:223:MET:N	1:B:224:PRO:CD	2.84	0.41
1:B:316:ILE:N	1:B:317:PRO:CD	2.84	0.41
1:B:26:LEU:CD2	1:B:28:ILE:HG13	2.52	0.40
1:A:316:ILE:N	1:A:317:PRO:CD	2.84	0.40
1:B:348:ALA:N	1:B:349:PRO:HD2	2.36	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	A	387/406 (95%)	376 (97%)	10 (3%)	1 (0%)	41	70
1	B	386/406 (95%)	374 (97%)	12 (3%)	0	100	100
All	All	773/812 (95%)	750 (97%)	22 (3%)	1 (0%)	51	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	GLY

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	310/337 (92%)	305 (98%)	5 (2%)	62	87
1	B	302/337 (90%)	288 (95%)	14 (5%)	27	58
All	All	612/674 (91%)	593 (97%)	19 (3%)	40	72

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	VAL
1	A	170	LEU
1	A	242	THR
1	A	305	LEU
1	A	307	GLN

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Mol	Chain	Res	Type
1	B	11	LEU
1	B	29	ARG
1	B	65	TYR
1	B	148	ARG
1	B	152	ILE
1	B	157	VAL
1	B	170	LEU
1	B	204	CYS
1	B	208	SER
1	B	226	MET
1	B	326	ASP
1	B	344	LEU
1	B	346	ASP
1	B	363	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS
1	B	154	HIS
1	B	324	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

Full wwPDB X-ray Structure Validation Report

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	$\#|Z| > 2$
3	UN9	A	1391	-	17,20,20	1.85	5 (29%)	21,28,28	2.97	7 (33%)
2	CIT	A	1390	-	3,12,12	1.16	0	3,17,17	1.49	1 (33%)
4	GOL	A	1393	-	5,5,5	0.40	0	5,5,5	0.28	0
3	UN9	A	1392	-	17,20,20	1.90	6 (35%)	21,28,28	2.95	6 (28%)

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
3	UN9	A	1391	-	-	0/7/9/9	0/2/2/2
2	CIT	A	1390	-	-	0/6/16/16	-
4	GOL	A	1393	-	-	2/4/4/4	-
3	UN9	A	1392	-	-	3/7/9/9	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1391	UN9	C12-N14	3.91	1.42	1.33
3	A	1392	UN9	C12-N14	3.82	1.42	1.33
3	A	1392	UN9	O19-C10	2.76	1.44	1.35
3	A	1391	UN9	O19-C10	2.75	1.44	1.35
3	A	1392	UN9	O13-C12	-2.66	1.17	1.23
3	A	1391	UN9	O13-C12	-2.62	1.18	1.23
3	A	1392	UN9	C3-C2	-2.58	1.38	1.43
3	A	1391	UN9	C3-C2	-2.53	1.38	1.43
3	A	1392	UN9	C7-N8	2.39	1.37	1.30
3	A	1392	UN9	C10-C3	-2.26	1.38	1.43
3	A	1391	UN9	C7-N8	2.12	1.36	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1391	UN9	C12-C9-N8	-10.63	106.07	115.99
3	A	1392	UN9	C12-C9-N8	-9.43	107.19	115.99
3	A	1392	UN9	C9-C12-N14	6.37	121.88	115.67
3	A	1391	UN9	C1-C2-C7	-4.22	116.97	123.67
3	A	1391	UN9	O19-C10-C3	3.89	124.89	116.64
3	A	1391	UN9	CL1-C7-N8	3.32	120.15	114.39
3	A	1392	UN9	C1-C2-C7	-3.30	118.43	123.67
3	A	1392	UN9	CL1-C7-N8	3.29	120.11	114.39
3	A	1392	UN9	O19-C10-C3	3.06	123.13	116.64
3	A	1391	UN9	C9-C10-C3	-2.57	117.84	120.54
3	A	1392	UN9	C9-C10-C3	-2.50	117.91	120.54
2	A	1390	CIT	C3-C4-C5	-2.48	111.02	114.98
3	A	1391	UN9	C1-C2-C3	2.44	121.48	118.45
3	A	1391	UN9	C10-C9-N8	2.15	124.65	121.42

There are no chirality outliers.
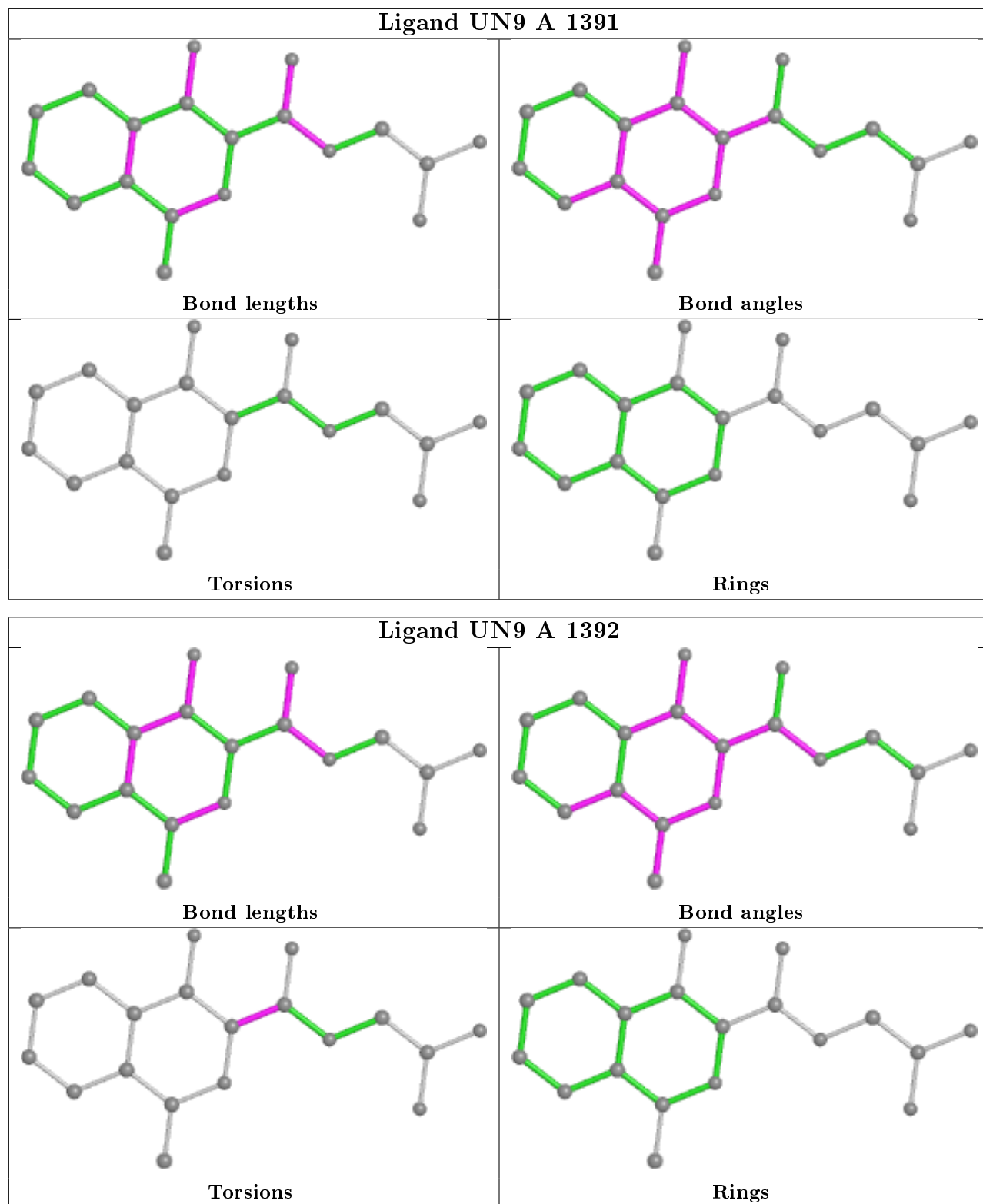
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1392	UN9	O13-C12-C9-C10
4	A	1393	GOL	O2-C2-C3-O3
3	A	1392	UN9	N14-C12-C9-C10
3	A	1392	UN9	N14-C12-C9-N8
4	A	1393	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1393	GOL	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 UN9 A 1391

Bond lengths

Bond angles

Torsions

Rings

Ligand UN9 A 1392

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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	388/406 (95%)	-0.34	5 (1%)	77	72	43, 72, 116, 179	0
1	B	388/406 (95%)	-0.28	9 (2%)	60	50	42, 79, 126, 178	0
All	All	776/812 (95%)	-0.31	14 (1%)	68	61	42, 75, 123, 179	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	79	PHE	3.8
1	A	159	ARG	3.4
1	A	293	GLY	3.4
1	B	49	CYS	3.0
1	B	80	VAL	2.7
1	B	208	SER	2.6
1	B	165	GLY	2.5
1	B	162	LEU	2.5
1	B	166	LEU	2.4
1	A	231	ASP	2.3
1	A	157	VAL	2.3
1	B	231	ASP	2.3
1	A	135[A]	ASP	2.2
1	B	164	PRO	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.
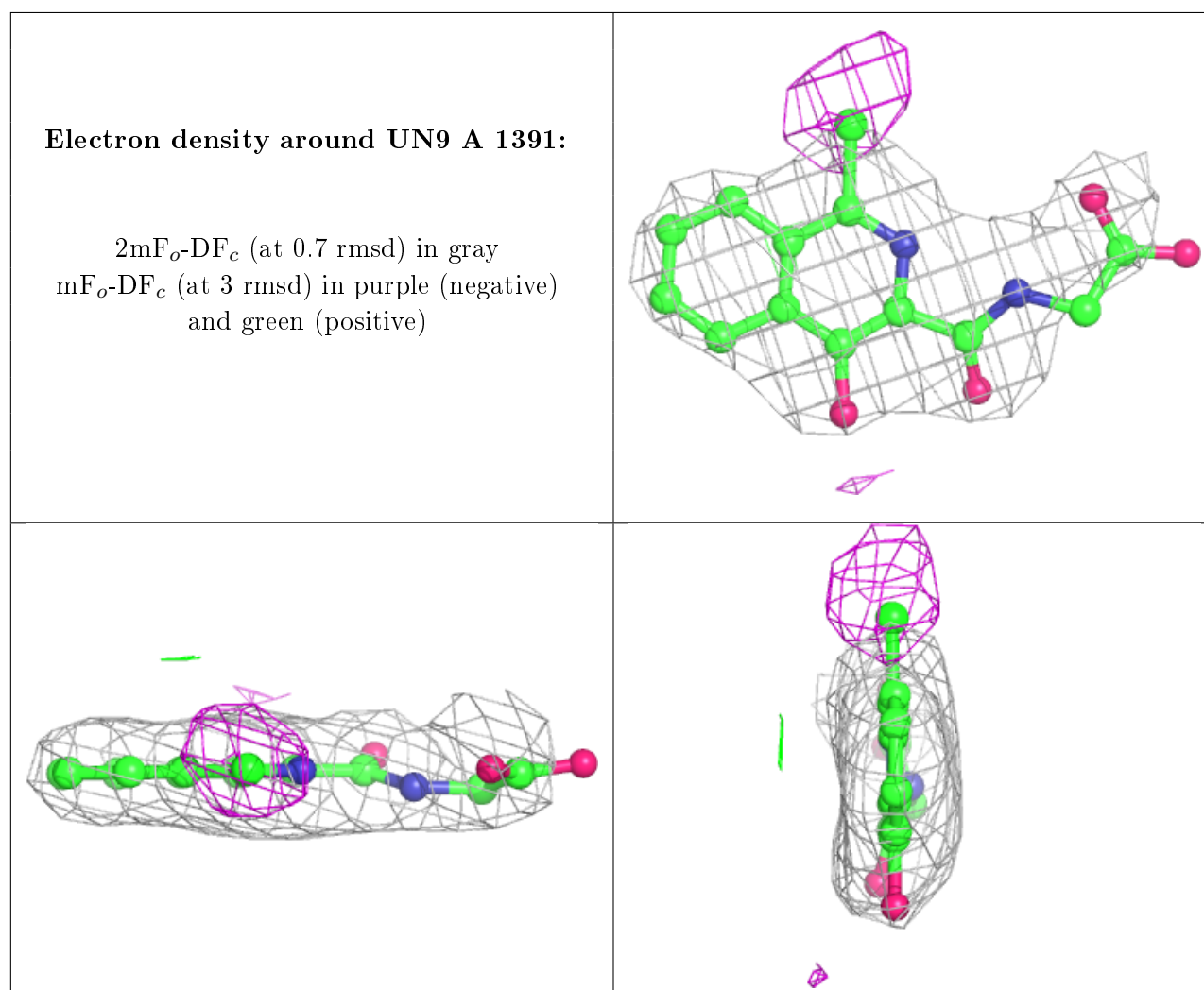
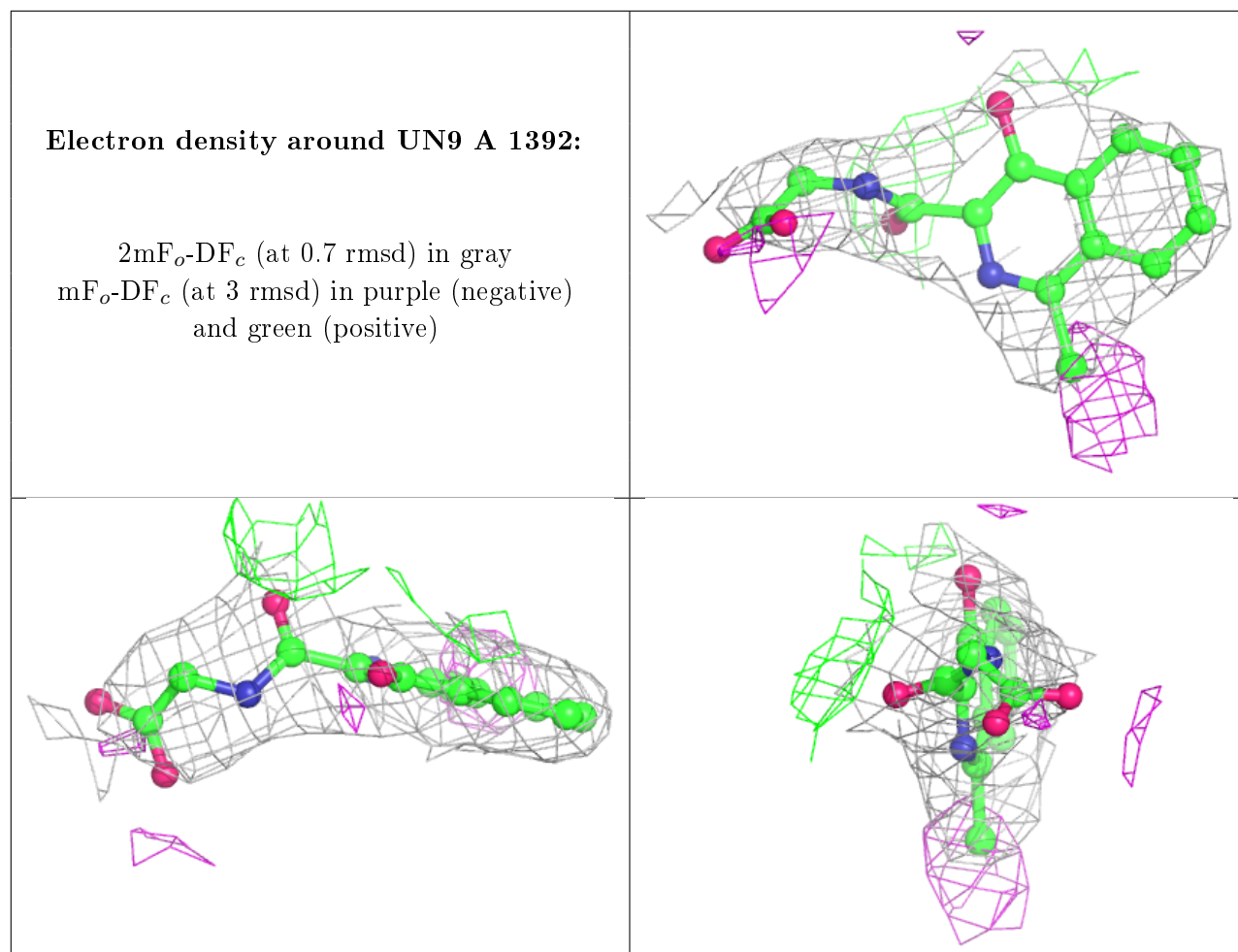## 6.3 Carbohydrates (i)

There are no carbohydrates 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($Å^2$)	Q<0.9
2	CIT	A	1390	13/13	0.74	0.21	83,98,105,114	0
4	GOL	A	1393	6/6	0.79	0.24	77,83,89,92	0
3	UN9	A	1391	19/19	0.89	0.18	65,80,115,126	0
3	UN9	A	1392	19/19	0.91	0.18	65,86,111,112	0
5	MN	B	1390	1/1	0.97	0.08	112,112,112,112	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 UN9 A 1391:

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

Electron density around UN9 A 1392:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.