Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2024 – 01:27 PM EDT

PDB ID	:	4HAU
Title	:	Crystal structure of CRM1 inhibitor Ratjadone A in complex with CRM1-Ran-RanBP1
Authors	:	Sun, Q.; Chook, Y.M.
Deposited on	:	2012-09-27
Resolution	:	2.00 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

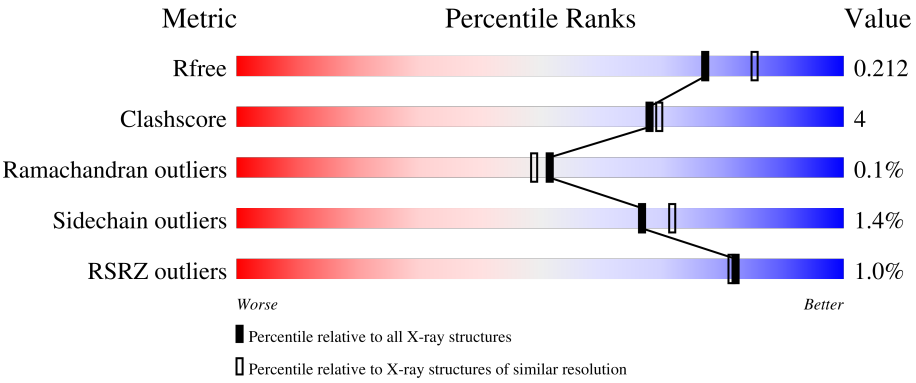
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.00 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))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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% 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	216	83% 9% 8%
2	B	140	79% 7% • 14%
3	C	1023	% 91% 7% •

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
6	EDO	C	1106	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 12576 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 GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	5	0
			1647	1061	285	295	6			

- Molecule 2 is a protein called Ran-specific GTPase-activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	3	0
			1023	647	179	193	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	98	LYS	ALA	CONFLICT	UNP P41920

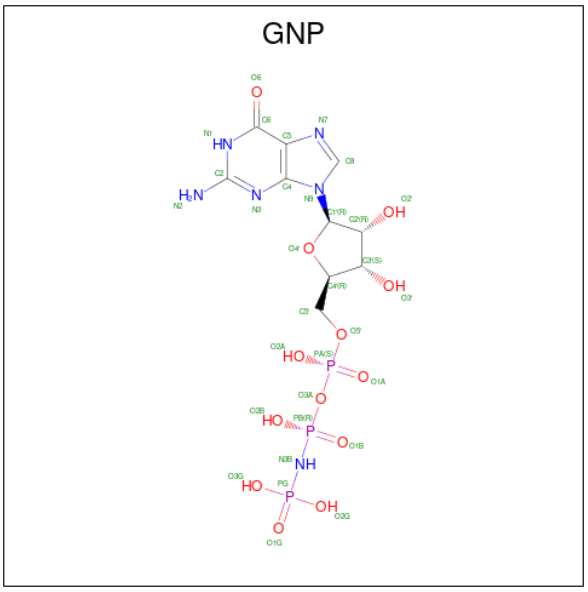
- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1014	Total	C	N	O	S	0	48	0
			8462	5447	1382	1590	43			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	EXPRESSION TAG	UNP P30822
C	0	ALA	-	EXPRESSION TAG	UNP P30822
C	205	ALA	SER	CONFLICT	UNP P30822
C	539	CYS	THR	ENGINEERED MUTATION	UNP P30822
C	1022	CYS	TYR	ENGINEERED MUTATION	UNP P30822

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

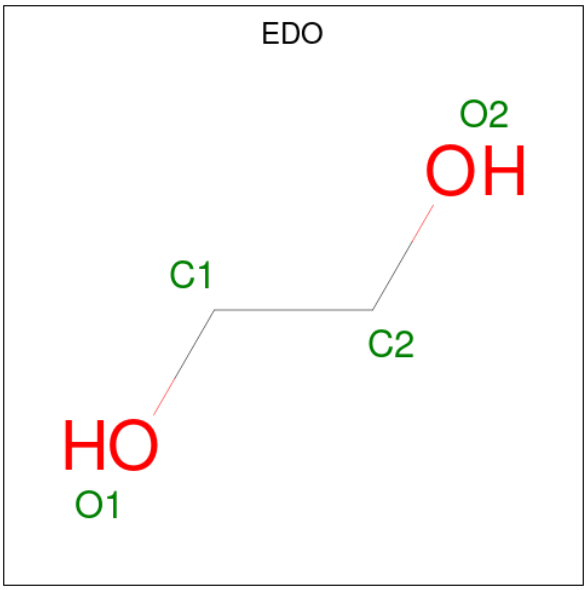


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

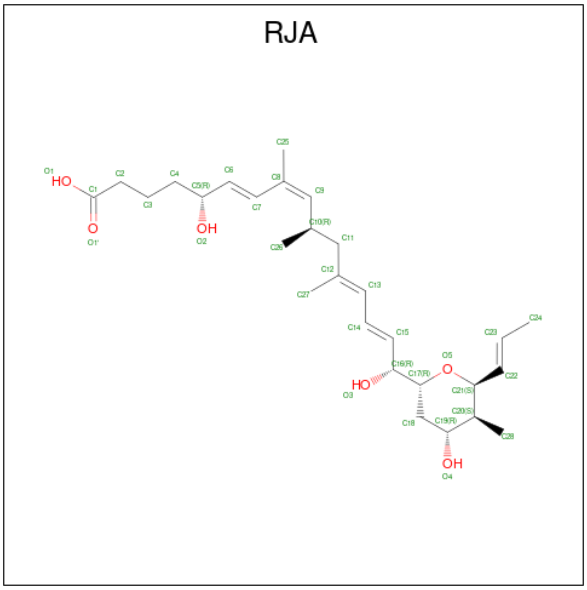
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



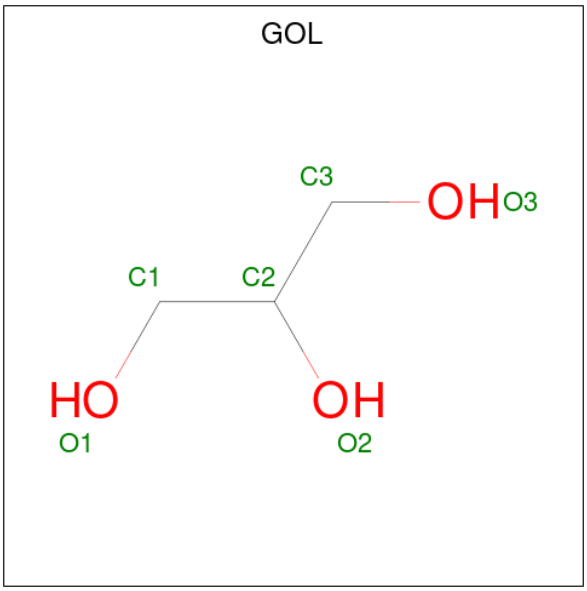
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0

- Molecule 7 is Ratjadone A, bound form (three-letter code: RJA) (formula: $C_{28}H_{44}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 34 28 6	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	3	Total Cl 3 3	0	0

- Molecule 10 is water.

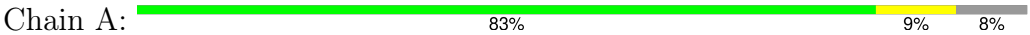
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	214	Total O 214 214	0	0
10	B	72	Total O 72 72	0	0
10	C	1054	Total O 1054 1054	0	0

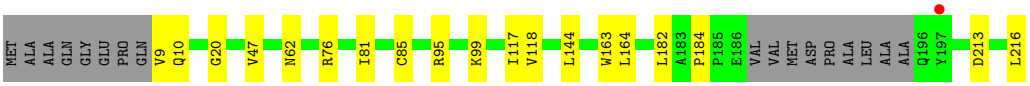
3 Residue-property plots (i)

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: GTP-binding nuclear protein Ran

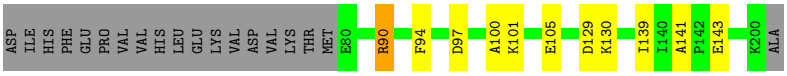
Chain A:





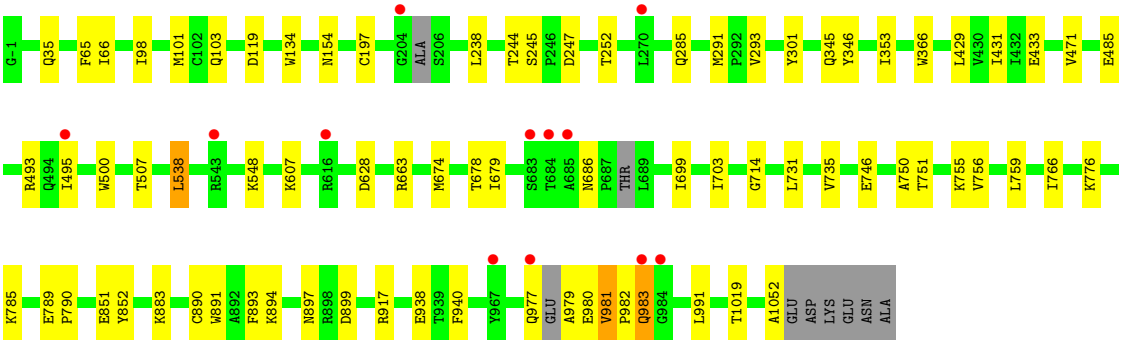
• Molecule 2: Ran-specific GTPase-activating protein 1

Chain B:



• Molecule 3: Exportin-1

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	106.18Å 106.18Å 306.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 47.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.00) 99.2 (47.09-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.148 , 0.207 0.161 , 0.212	Depositor DCC
R_{free} test set	5905 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 58.7	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	0.97	EDS
Total number of atoms	12576	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: CL, EDO, GOL, RJA, MG, GNP

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	0.56	0/1692	0.61	0/2287
2	B	0.53	0/1039	0.64	0/1383
3	C	0.55	2/8719 (0.0%)	0.58	0/11804
All	All	0.55	2/11450 (0.0%)	0.59	0/15474

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	366	TRP	CD2-CE2	5.12	1.47	1.41
3	C	134	TRP	CD2-CE2	5.01	1.47	1.41

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	1647	0	1650	21	0
2	B	1023	0	1023	9	0
3	C	8462	0	8591	55	0
4	A	32	0	13	1	0
5	A	1	0	0	0	0
6	A	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	8	0	12	6	0
7	C	34	0	41	3	0
8	C	18	0	24	1	0
9	C	3	0	0	0	0
10	A	214	0	0	5	0
10	B	72	0	0	0	0
10	C	1054	0	0	10	0
All	All	12576	0	11366	86	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 4.

All (86) 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:C:917[B]:ARG:HH11	3:C:917[B]:ARG:CG	1.75	0.99
3:C:917[B]:ARG:HG3	3:C:917[B]:ARG:NH1	1.66	0.99
3:C:917[B]:ARG:HH11	3:C:917[B]:ARG:HG3	0.84	0.99
7:C:1101:RJA:H17	7:C:1101:RJA:H28B	1.54	0.88
3:C:1019[B]:THR:HG21	6:C:1106:EDO:C2	2.11	0.80
2:B:90:ARG:CG	2:B:90:ARG:HH21	1.96	0.79
3:C:1019[B]:THR:HG21	6:C:1106:EDO:H11	1.64	0.78
3:C:1019[B]:THR:HG21	6:C:1106:EDO:C1	2.15	0.76
3:C:197[B]:CYS:SG	10:C:2208:HOH:O	2.45	0.74
3:C:66:ILE:HG23	10:C:2228:HOH:O	1.89	0.72
3:C:1019[B]:THR:HG21	6:C:1106:EDO:H21	1.71	0.71
3:C:977:GLN:O	3:C:979:ALA:N	2.25	0.69
1:A:9:VAL:HG13	1:A:10:GLN:H	1.61	0.66
1:A:9:VAL:HG12	10:A:544:HOH:O	1.97	0.65
3:C:981:VAL:HG22	3:C:982:PRO:HD2	1.80	0.64
3:C:894:LYS:NZ	3:C:938:GLU:OE1	2.31	0.64
3:C:244:THR:HG22	3:C:285:GLN:OE1	1.98	0.63
3:C:1019[B]:THR:CG2	6:C:1106:EDO:H21	2.29	0.63
3:C:495:ILE:HD12	3:C:538:LEU:HD23	1.81	0.63
3:C:293[B]:VAL:HG12	3:C:346:TYR:CE2	2.34	0.61
2:B:97:ASP:O	2:B:100:ALA:O	2.20	0.59
2:B:90:ARG:NH2	2:B:90:ARG:HG2	2.17	0.58
3:C:238:LEU:O	3:C:252:THR:HG21	2.04	0.58
1:A:99[B]:LYS:N	1:A:99[B]:LYS:HE2	2.19	0.57
3:C:674:MET:O	3:C:678:THR:HG23	2.06	0.56
3:C:899:ASP:C	10:C:2210:HOH:O	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:ARG:CG	2:B:90:ARG:NH2	2.59	0.55
3:C:103:GLN:NE2	10:C:1907:HOH:O	2.36	0.55
1:A:47:VAL:CG1	1:A:62[B]:ASN:HD21	2.21	0.54
3:C:851:GLU:HG2	3:C:852:TYR:CD1	2.42	0.54
1:A:47:VAL:HG13	1:A:62[B]:ASN:HD21	1.70	0.54
1:A:95:ARG:O	1:A:99[B]:LYS:HE2	2.08	0.54
3:C:1019[B]:THR:CG2	6:C:1106:EDO:C2	2.84	0.54
3:C:890:CYS:O	3:C:893:PHE:HB2	2.07	0.54
2:B:90:ARG:HH21	2:B:90:ARG:HG3	1.70	0.51
1:A:81:ILE:HD11	3:C:65:PHE:CG	2.45	0.51
3:C:703[B]:ILE:HD13	3:C:766:ILE:HG13	1.93	0.51
3:C:891:TRP:CE3	8:C:1104:GOL:H12	2.45	0.50
3:C:1052:ALA:HB3	10:C:2218:HOH:O	2.11	0.49
7:C:1101:RJA:H28B	7:C:1101:RJA:C17	2.36	0.49
3:C:981:VAL:HG22	3:C:982:PRO:CD	2.43	0.49
3:C:429[B]:LEU:HD11	3:C:433:GLU:OE2	2.12	0.49
1:A:99[B]:LYS:HE2	1:A:99[B]:LYS:H	1.77	0.48
3:C:735[A]:VAL:HG13	3:C:759:LEU:HB3	1.95	0.48
3:C:789[B]:GLU:HB2	3:C:790:PRO:HD3	1.94	0.48
1:A:20:GLY:H	4:A:301:GNP:HNB3	1.62	0.48
3:C:293[B]:VAL:HG12	3:C:346:TYR:CZ	2.48	0.48
3:C:699:ILE:HG21	3:C:731:LEU:HD21	1.95	0.48
3:C:979:ALA:HA	3:C:983:GLN:NE2	2.29	0.48
1:A:117:ILE:HB	1:A:144:LEU:HD22	1.96	0.48
1:A:118:VAL:HG22	1:A:163:TRP:CE3	2.50	0.47
3:C:245[A]:SER:HB2	3:C:247[A]:ASP:OD2	2.15	0.47
3:C:507[B]:THR:HG23	10:C:2246:HOH:O	2.14	0.47
1:A:76[A]:ARG:NE	10:A:568:HOH:O	2.48	0.46
3:C:98:ILE:HA	3:C:101[B]:MET:HE2	1.98	0.46
2:B:129:ASP:O	2:B:130:LYS:HB2	2.15	0.46
3:C:293[A]:VAL:HG11	3:C:345:GLN:HB3	1.98	0.46
1:A:47:VAL:HG13	1:A:62[B]:ASN:ND2	2.30	0.46
3:C:495:ILE:CD1	3:C:538:LEU:HD23	2.44	0.46
3:C:548:LYS:HD3	10:C:2216:HOH:O	2.14	0.45
2:B:141:ALA:HB1	2:B:143:GLU:OE1	2.16	0.45
3:C:119:ASP:OD2	3:C:154:ASN:ND2	2.48	0.45
1:A:76[B]:ARG:CZ	10:A:587:HOH:O	2.63	0.45
3:C:679:ILE:HD13	3:C:699:ILE:CG1	2.47	0.45
1:A:9:VAL:HG13	1:A:10:GLN:N	2.28	0.44
3:C:301:TYR:CD1	3:C:353:ILE:HD13	2.52	0.44
3:C:493[B]:ARG:HA	3:C:493[B]:ARG:HD2	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:PHE:CE2	2:B:105[A]:GLU:HG2	2.53	0.43
3:C:500:TRP:CZ3	3:C:538:LEU:HD11	2.53	0.43
1:A:99[B]:LYS:NZ	10:A:478:HOH:O	2.51	0.43
3:C:679:ILE:HD13	3:C:699:ILE:HG12	2.00	0.43
3:C:746:GLU:HB2	3:C:750:ALA:HB2	2.01	0.42
1:A:184:PRO:HG2	2:B:139:ILE:HG12	2.01	0.42
3:C:485[A]:GLU:HG3	10:C:1610:HOH:O	2.19	0.42
3:C:751:THR:HA	3:C:756:VAL:HG11	2.01	0.42
3:C:897:ASN:ND2	10:C:1696:HOH:O	2.52	0.42
7:C:1101:RJA:H14	7:C:1101:RJA:H27	1.83	0.42
1:A:85:CYS:HB2	1:A:164:LEU:HD22	2.01	0.42
1:A:213:ASP:HB2	10:A:606:HOH:O	2.20	0.42
3:C:485[B]:GLU:CG	10:C:1887:HOH:O	2.68	0.41
1:A:95:ARG:O	1:A:99[B]:LYS:CE	2.68	0.41
3:C:431[B]:ILE:HD11	3:C:471:VAL:HG11	2.02	0.41
3:C:714:GLY:HA2	3:C:776:LYS:HD2	2.03	0.41
3:C:789[A]:GLU:HB3	3:C:790:PRO:HD3	2.02	0.41
3:C:917[B]:ARG:CG	3:C:917[B]:ARG:NH1	2.47	0.40
1:A:216:LEU:HD23	1:A:216:LEU:HA	1.94	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	200/216 (93%)	194 (97%)	6 (3%)	0	100	100
2	B	121/140 (86%)	114 (94%)	7 (6%)	0	100	100
3	C	1054/1023 (103%)	1039 (99%)	14 (1%)	1 (0%)	51	49
All	All	1375/1379 (100%)	1347 (98%)	27 (2%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	686	ASN

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	179/185 (97%)	178 (99%)	1 (1%)	86 90
2	B	107/122 (88%)	105 (98%)	2 (2%)	57 61
3	C	967/932 (104%)	952 (98%)	15 (2%)	62 67
All	All	1253/1239 (101%)	1235 (99%)	18 (1%)	67 72

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	LEU
2	B	90	ARG
2	B	101	LYS
3	C	35	GLN
3	C	291	MET
3	C	538	LEU
3	C	607	LYS
3	C	628	ASP
3	C	663	ARG
3	C	755	LYS
3	C	785[A]	LYS
3	C	785[B]	LYS
3	C	883	LYS
3	C	940	PHE
3	C	980	GLU
3	C	981	VAL
3	C	983	GLN
3	C	991	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
3	C	203	GLN
3	C	434	ASN
3	C	983	GLN

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)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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	$\#\|Z\| > 2$
7	RJA	C	1101	3	33,34,34	0.58	0	37,44,44	1.84	7 (18%)
8	GOL	C	1103	-	5,5,5	0.55	0	5,5,5	0.47	0
6	EDO	A	303	-	3,3,3	0.44	0	2,2,2	0.29	0
8	GOL	C	1102	-	5,5,5	0.33	0	5,5,5	0.42	0
6	EDO	A	304	-	3,3,3	0.48	0	2,2,2	0.26	0
8	GOL	C	1104	-	5,5,5	0.28	0	5,5,5	0.40	0
6	EDO	C	1105	-	3,3,3	0.53	0	2,2,2	0.33	0
4	GNP	A	301	5	29,34,34	1.42	3 (10%)	33,54,54	2.01	7 (21%)
6	EDO	C	1106	-	3,3,3	0.60	0	2,2,2	0.01	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
7	RJA	C	1101	3	-	7/32/48/48	1/1/1/1
8	GOL	C	1103	-	-	1/4/4/4	-
6	EDO	A	303	-	-	1/1/1/1	-
8	GOL	C	1102	-	-	4/4/4/4	-
6	EDO	A	304	-	-	0/1/1/1	-
8	GOL	C	1104	-	-	2/4/4/4	-
6	EDO	C	1105	-	-	1/1/1/1	-
4	GNP	A	301	5	-	3/14/38/38	0/3/3/3
6	EDO	C	1106	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	GNP	PB-N3B	3.87	1.73	1.63
4	A	301	GNP	C5-C6	3.56	1.47	1.41
4	A	301	GNP	PG-N3B	3.29	1.71	1.63

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	1101	RJA	C17-C16-C15	-5.46	102.65	111.28
4	A	301	GNP	O1G-PG-N3B	-5.27	104.01	111.77
4	A	301	GNP	C2-N1-C6	4.70	122.49	115.96
4	A	301	GNP	C2-N3-C4	4.29	120.11	115.48
7	C	1101	RJA	C10-C9-C8	-4.00	121.29	128.13
7	C	1101	RJA	C14-C13-C12	-3.95	122.13	127.69
4	A	301	GNP	C4-C5-C6	-3.71	115.56	121.23
4	A	301	GNP	N3-C2-N1	-3.60	122.64	127.21
4	A	301	GNP	C5-C6-N1	-3.50	118.75	123.42
7	C	1101	RJA	C6-C7-C8	-3.23	119.38	126.32
7	C	1101	RJA	C13-C14-C15	-3.19	117.05	124.43
7	C	1101	RJA	C27-C12-C11	2.14	120.02	115.28
7	C	1101	RJA	O5-C17-C18	2.01	112.05	109.78
4	A	301	GNP	O2A-PA-O1A	2.00	121.77	112.44

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GNP	PG-N3B-PB-O1B
4	A	301	GNP	PA-O3A-PB-O1B
4	A	301	GNP	PA-O3A-PB-O2B
7	C	1101	RJA	O3-C16-C17-O5
7	C	1101	RJA	O3-C16-C17-C18
7	C	1101	RJA	C15-C16-C17-O5
8	C	1102	GOL	O1-C1-C2-C3
8	C	1104	GOL	C1-C2-C3-O3
8	C	1104	GOL	O2-C2-C3-O3
8	C	1102	GOL	C1-C2-C3-O3
8	C	1102	GOL	O1-C1-C2-O2
6	C	1105	EDO	O1-C1-C2-O2
7	C	1101	RJA	C4-C5-C6-C7
8	C	1102	GOL	O2-C2-C3-O3
8	C	1103	GOL	O2-C2-C3-O3
7	C	1101	RJA	C15-C16-C17-C18
7	C	1101	RJA	C1-C2-C3-C4
6	A	303	EDO	O1-C1-C2-O2
6	C	1106	EDO	O1-C1-C2-O2
7	C	1101	RJA	C25-C8-C9-C10

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1101	RJA	C17-C18-C19-C20-C21-O5

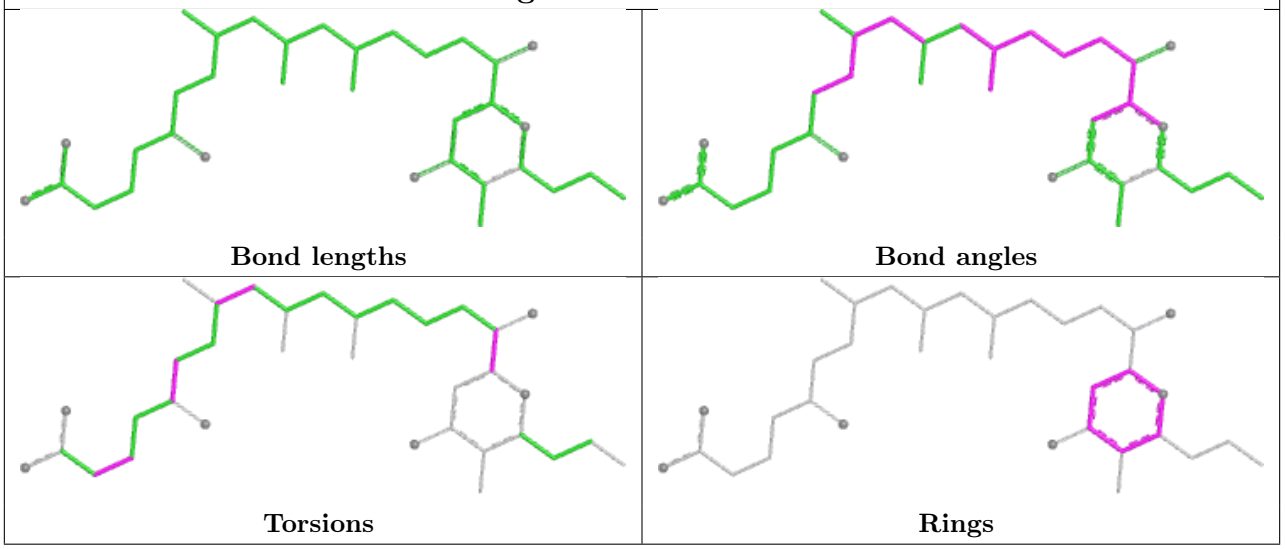
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1101	RJA	3	0
8	C	1104	GOL	1	0
4	A	301	GNP	1	0
6	C	1106	EDO	6	0

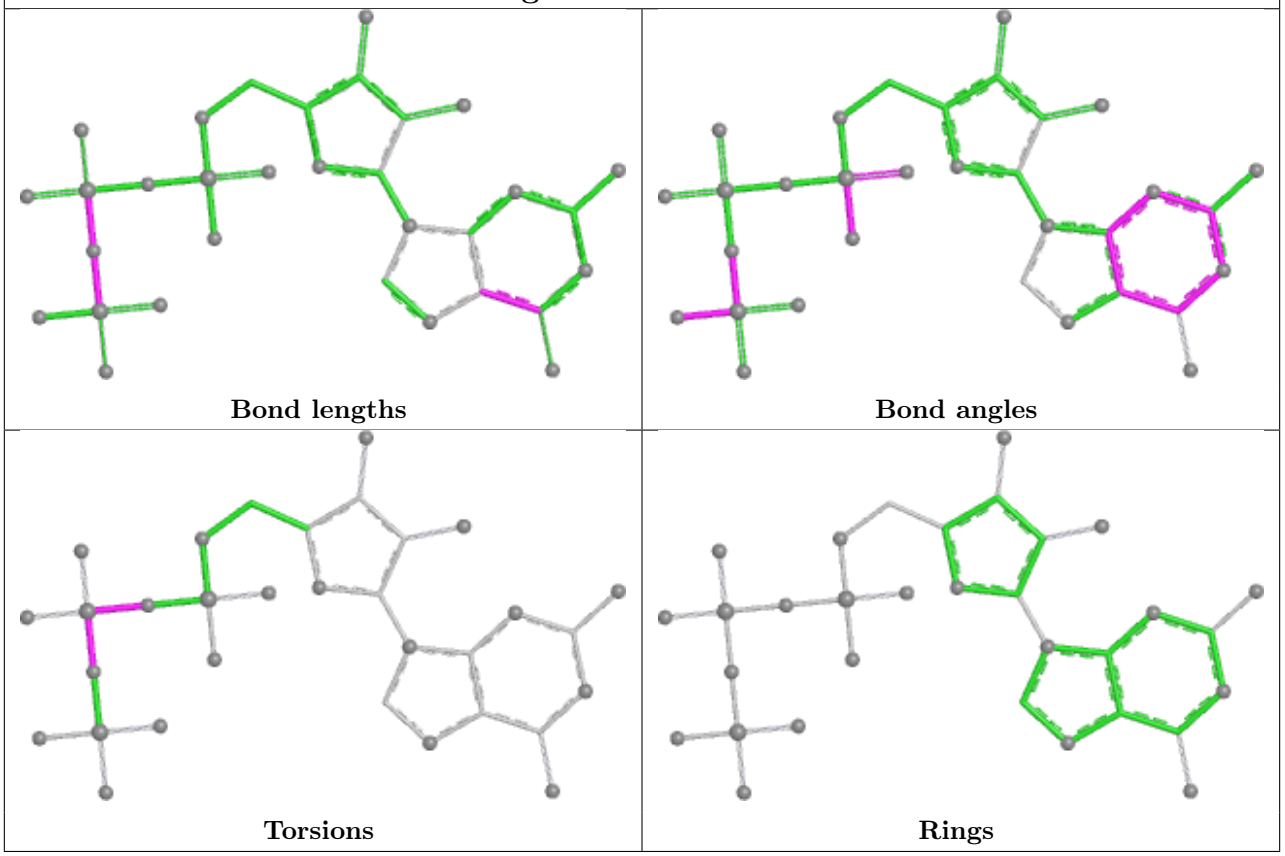
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 RJA C 1101



Ligand GNP A 301



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	199/216 (92%)	-0.43	1 (0%) 91 90	16, 25, 47, 70	0
2	B	121/140 (86%)	-0.39	0 100 100	25, 35, 57, 89	0
3	C	1014/1023 (99%)	-0.48	12 (1%) 79 78	15, 28, 52, 84	0
All	All	1334/1379 (96%)	-0.46	13 (0%) 82 81	15, 29, 53, 89	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	543	ARG	3.5
3	C	983	GLN	3.5
1	A	197	TYR	3.3
3	C	270	LEU	3.0
3	C	495	ILE	3.0
3	C	685	ALA	2.9
3	C	684	THR	2.7
3	C	204	GLY	2.4
3	C	683	SER	2.2
3	C	967	TYR	2.2
3	C	616	ARG	2.1
3	C	984	GLY	2.1
3	C	977	GLN	2.1

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 (i)

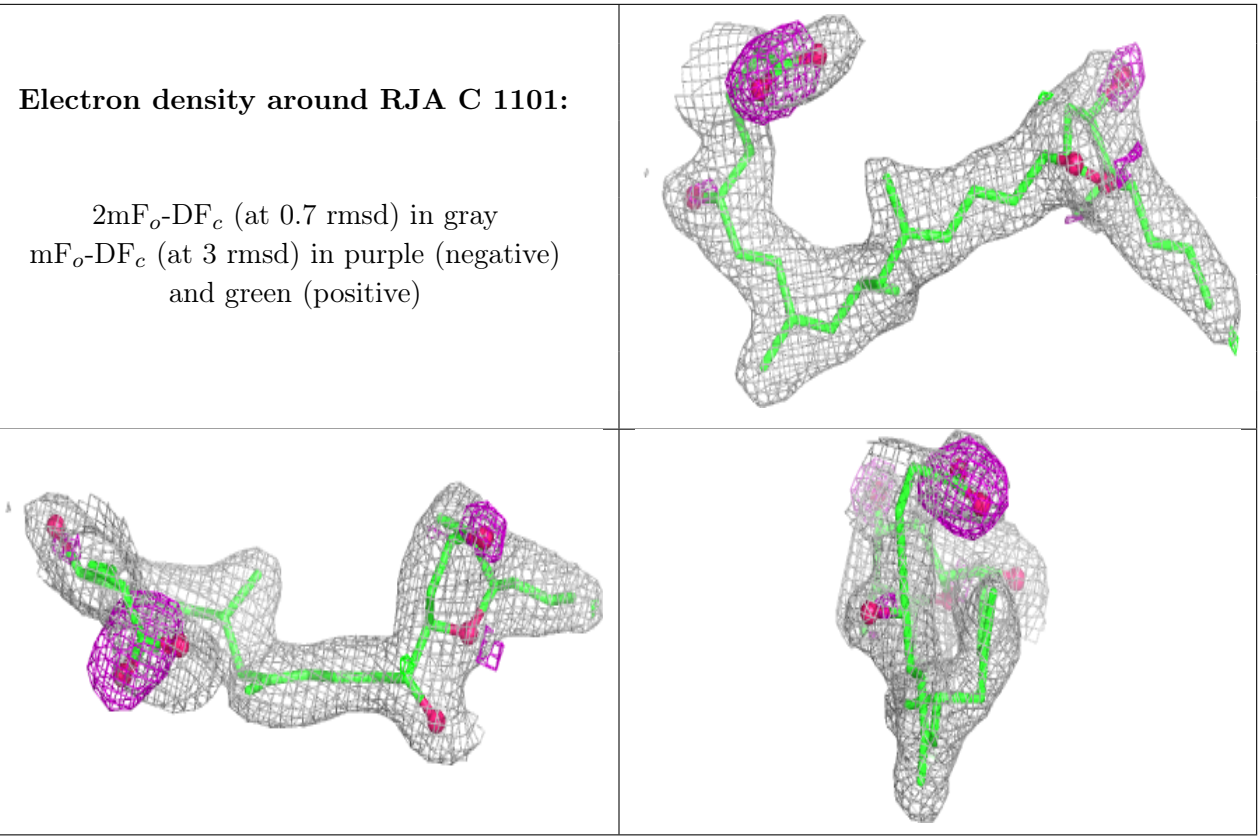
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	EDO	A	303	4/4	0.81	0.13	60,62,64,65	0
8	GOL	C	1103	6/6	0.82	0.23	41,48,52,53	0
8	GOL	C	1102	6/6	0.85	0.24	62,64,65,70	0
6	EDO	A	304	4/4	0.87	0.34	51,52,56,57	0
6	EDO	C	1106	4/4	0.88	0.17	48,50,52,53	0
9	CL	C	1107	1/1	0.89	0.10	62,62,62,62	0
7	RJA	C	1101	34/34	0.90	0.18	24,32,39,41	0
6	EDO	C	1105	4/4	0.91	0.13	40,49,49,50	0
8	GOL	C	1104	6/6	0.94	0.08	42,48,49,50	0
9	CL	C	1108	1/1	0.94	0.14	53,53,53,53	0
9	CL	C	1109	1/1	0.95	0.11	64,64,64,64	0
5	MG	A	302	1/1	0.98	0.06	22,22,22,22	0
4	GNP	A	301	32/32	0.99	0.09	18,22,24,24	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.

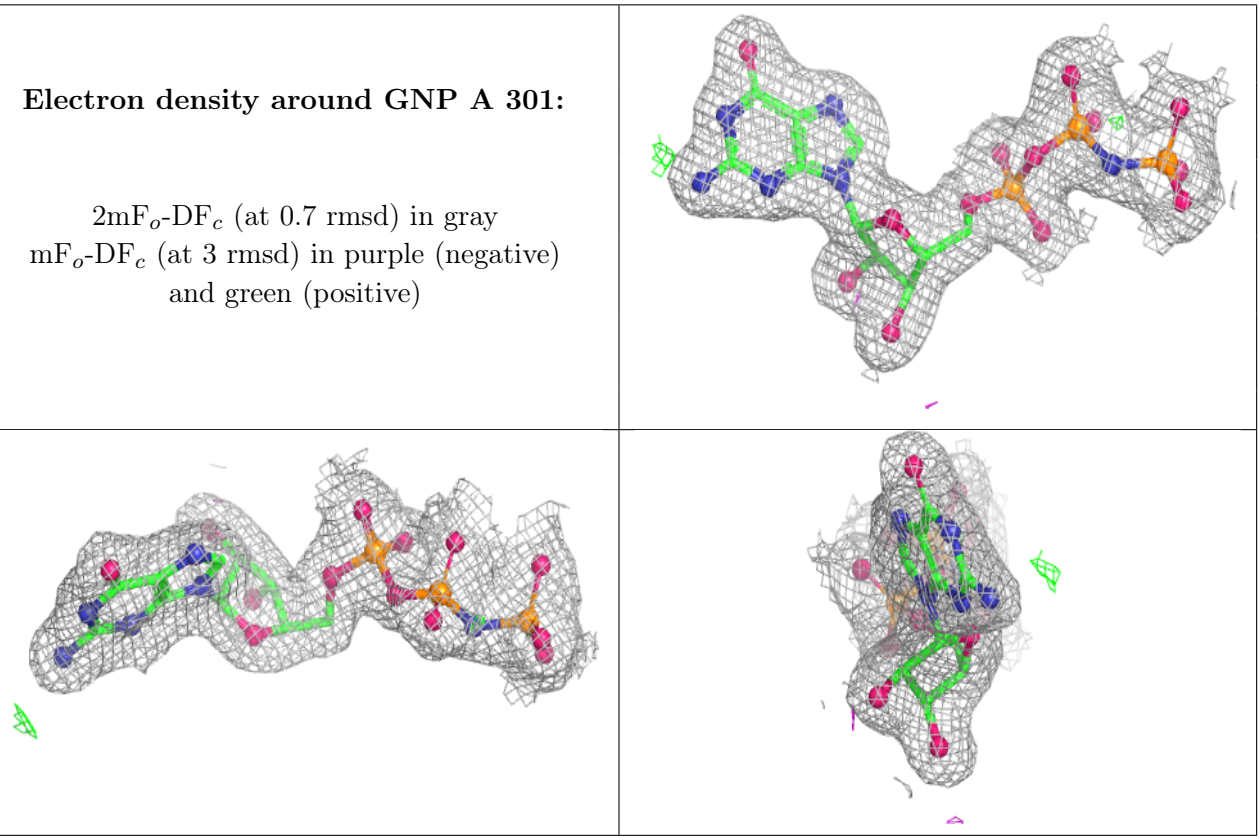
Electron density around RJA C 1101:

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



Electron density around GNP A 301:

$2mF_o$-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.