Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2021 – 12:42 PM EDT

PDB ID	:	7MWZ
Title	:	Structure of drosophila STING in complex with 3'2'-cGAMP
Authors	:	Slavik, K.M.; Ragucci, A.E.; Kranzusch, P.J.
Deposited on	:	2021-05-17
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 following versions of software and data (see references ⓘ) were used in the production of this report:

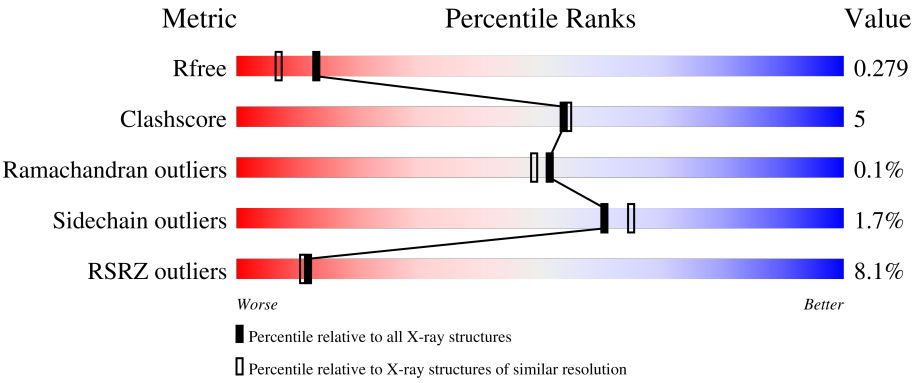
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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	356	4% 89% 10%
1	B	356	8% 82% 17%
1	C	356	10% 85% 12%
1	D	356	9% 73% 11% 15%

2 Entry composition

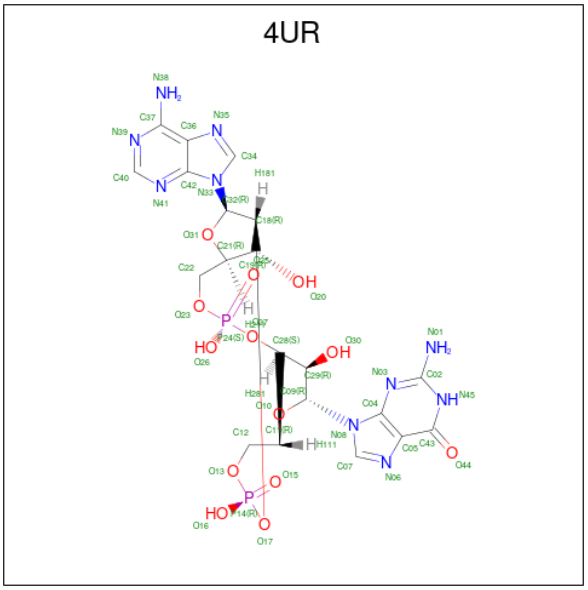
There are 3 unique types of molecules in this entry. The entry contains 11544 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 STING.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	0	0
			2834	1809	497	514	14			
1	B	352	Total	C	N	O	S	0	0	0
			2845	1818	498	515	14			
1	C	349	Total	C	N	O	S	0	0	0
			2828	1808	494	512	14			
1	D	301	Total	C	N	O	S	0	0	0
			2436	1559	423	441	13			

- Molecule 2 is 3'2'-cGAMP (three-letter code: 4UR) (formula: $C_{20}H_{24}N_{10}O_{13}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			45	20	10	13	2		
2	C	1	Total	C	N	O	P	0	0
			45	20	10	13	2		

- Molecule 3 is water.

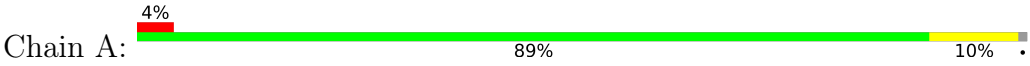
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	170	Total O 170 170	0	0
3	B	137	Total O 137 137	0	0
3	C	113	Total O 113 113	0	0
3	D	91	Total O 91 91	0	0

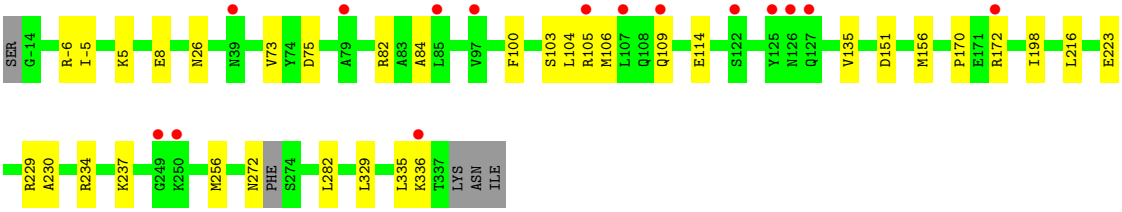
3 Residue-property plots (i)

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: STING

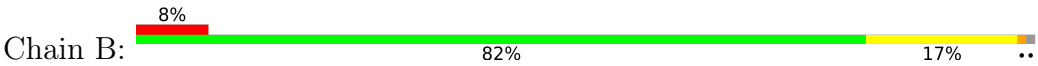
Chain A:

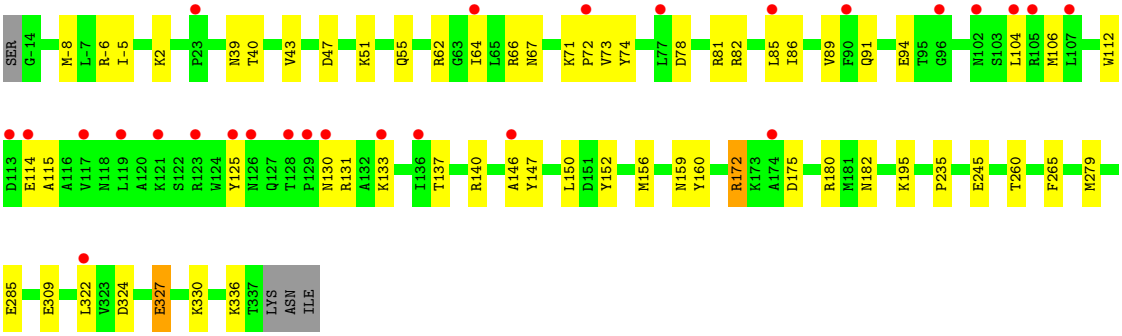




• Molecule 1: STING

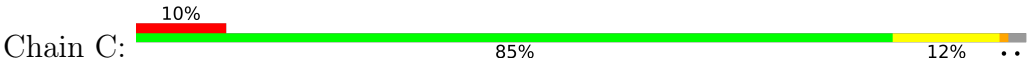
Chain B:

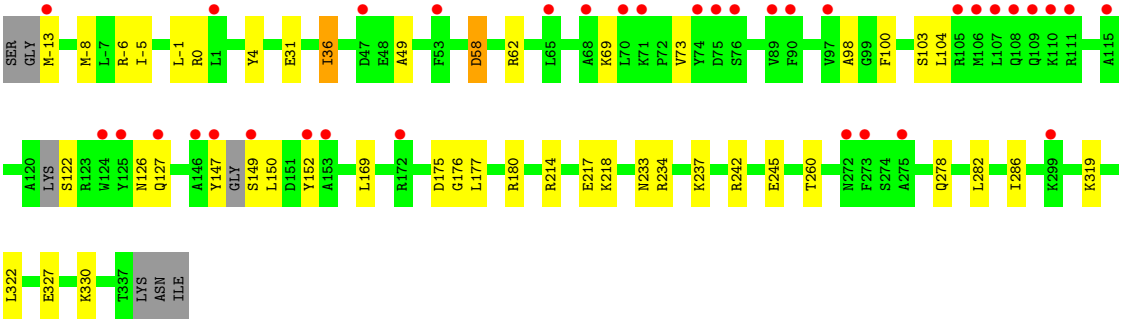




• Molecule 1: STING

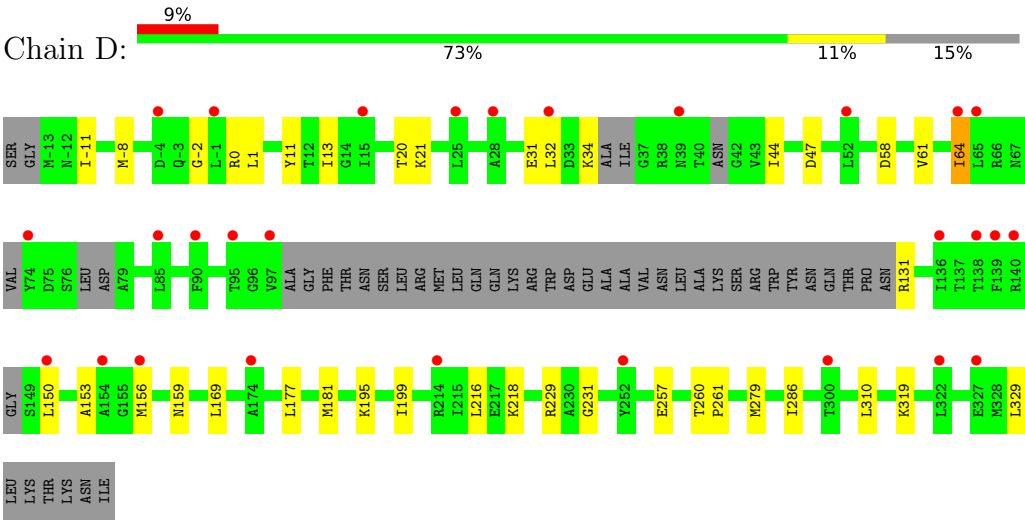
Chain C:





• Molecule 1: STING

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.92Å 95.05Å 140.14Å 90.00° 93.93° 90.00°	Depositor
Resolution (Å)	48.84 – 2.00 48.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.84-2.00) 99.6 (48.84-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.247 , 0.283 0.244 , 0.279	Depositor DCC
R_{free} test set	2006 reflections (2.24%)	wwPDB-VP
Wilson B-factor (Å^2)	43.2	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 42.5	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	0.95	EDS
Total number of atoms	11544	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.91 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6964e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: 4UR

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	0.24	0/2891	0.47	0/3897
1	B	0.24	0/2904	0.48	0/3916
1	C	0.23	0/2885	0.45	0/3889
1	D	0.24	0/2480	0.46	0/3332
All	All	0.24	0/11160	0.47	0/15034

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	2834	0	2862	25	0
1	B	2845	0	2872	42	0
1	C	2828	0	2851	32	0
1	D	2436	0	2453	28	0
2	B	45	0	24	2	0
2	C	45	0	24	3	0
3	A	170	0	0	9	0
3	B	137	0	0	10	0
3	C	113	0	0	13	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	91	0	0	7	0
All	All	11544	0	11086	117	2

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 5.

All (117) 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:B:112:TRP:O	3:B:501:HOH:O	1.81	0.98
1:C:322:LEU:O	3:C:502:HOH:O	1.98	0.82
1:C:233:ASN:OD1	3:C:501:HOH:O	1.98	0.81
1:B:85:LEU:O	3:B:502:HOH:O	1.99	0.80
1:B:245:GLU:OE2	3:B:503:HOH:O	2.02	0.78
1:A:100:PHE:HB3	1:A:103:SER:HB2	1.66	0.77
1:A:223:GLU:OE1	3:A:401:HOH:O	2.06	0.74
1:B:67:ASN:ND2	3:B:507:HOH:O	2.21	0.73
1:C:31:GLU:OE2	3:C:503:HOH:O	2.08	0.72
1:C:149:SER:N	3:C:504:HOH:O	2.22	0.72
1:B:322:LEU:HB3	3:B:518:HOH:O	1.90	0.71
1:D:13:ILE:HG21	1:D:32:LEU:HD13	1.75	0.67
1:B:260:THR:HG1	2:B:401:4UR:H301	1.33	0.67
1:A:109:GLN:NE2	3:A:412:HOH:O	2.28	0.66
1:C:127:GLN:NE2	3:C:508:HOH:O	2.29	0.65
1:A:170:PRO:O	1:A:172:ARG:NH1	2.30	0.64
1:B:245:GLU:OE1	1:B:330:LYS:NZ	2.22	0.64
1:D:257:GLU:OE1	3:D:402:HOH:O	2.15	0.64
1:A:272:ASN:O	3:A:403:HOH:O	2.14	0.64
1:C:278:GLN:HG2	1:D:-2:GLY:HA3	1.79	0.64
1:D:218:LYS:NZ	3:D:409:HOH:O	2.31	0.64
1:B:309:GLU:OE2	3:B:504:HOH:O	2.15	0.63
1:C:-13:MET:SD	3:C:504:HOH:O	2.55	0.63
1:B:73:VAL:HG21	1:B:104:LEU:HB3	1.80	0.63
1:A:26:ASN:HB2	1:D:34:LYS:HD2	1.80	0.62
1:C:260:THR:OG1	2:C:401:4UR:O30	2.03	0.62
1:A:282:LEU:HD13	1:B:-6:ARG:HH12	1.64	0.61
1:B:172:ARG:NH1	3:B:510:HOH:O	2.34	0.61
1:A:105:ARG:HG3	3:A:412:HOH:O	2.01	0.60
1:B:78:ASP:OD2	1:B:81:ARG:NH1	2.29	0.59
1:C:237:LYS:HA	3:C:520:HOH:O	2.02	0.59
2:C:401:4UR:H221	3:C:551:HOH:O	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:603:HOH:O	1:D:156:MET:SD	2.58	0.58
1:B:182:ASN:OD1	1:B:195:LYS:NZ	2.38	0.57
1:D:31:GLU:OE2	3:D:403:HOH:O	2.17	0.57
1:B:125:TYR:OH	1:B:133:LYS:NZ	2.28	0.57
1:B:-8:MET:HG3	1:B:147:TYR:CZ	2.40	0.57
1:C:217:GLU:HG3	1:C:242:ARG:HG3	1.87	0.57
1:A:73:VAL:HG11	1:A:104:LEU:HD22	1.85	0.57
1:C:214:ARG:NH1	1:C:327:GLU:OE2	2.38	0.57
1:B:106:MET:HB2	1:B:115:ALA:HB2	1.86	0.56
1:B:74:TYR:HD2	1:B:85:LEU:HD23	1.71	0.55
1:C:69:LYS:HE3	1:C:98:ALA:HB1	1.89	0.55
1:B:94:GLU:HB3	3:B:507:HOH:O	2.05	0.54
1:A:229:ARG:HB3	1:A:234:ARG:HG3	1.90	0.54
1:B:55:GLN:N	3:B:505:HOH:O	2.31	0.54
3:A:483:HOH:O	1:B:260:THR:HG21	2.07	0.54
1:B:2:LYS:HG2	1:B:43:VAL:HG22	1.90	0.54
1:B:172:ARG:HH21	1:B:175:ASP:HB3	1.73	0.53
1:D:216:LEU:HD11	1:D:329:LEU:HD12	1.89	0.53
1:A:8:GLU:OE1	3:A:404:HOH:O	2.19	0.52
1:B:62:ARG:HB3	1:B:66:ARG:HH12	1.74	0.52
1:B:51:LYS:O	3:B:505:HOH:O	2.19	0.51
1:D:169:LEU:HD22	1:D:177:LEU:HG	1.92	0.51
1:C:-5:ILE:HG12	1:D:279:MET:HE1	1.93	0.51
2:C:401:4UR:H341	2:C:401:4UR:O23	2.12	0.50
1:C:169:LEU:HD22	1:C:177:LEU:HD22	1.94	0.50
1:C:69:LYS:HB3	3:C:511:HOH:O	2.13	0.49
1:C:234:ARG:HH21	1:D:260:THR:HG21	1.78	0.48
1:A:216:LEU:HD11	1:A:329:LEU:HD12	1.95	0.48
1:A:-5:ILE:HD13	1:B:279:MET:HE1	1.95	0.47
1:A:156:MET:HE1	1:B:156:MET:HG3	1.97	0.47
1:B:64:ILE:HD11	1:B:89:VAL:HG21	1.96	0.47
1:B:112:TRP:HB3	1:B:140:ARG:HA	1.95	0.47
1:A:-6:ARG:NH2	1:B:285:GLU:OE1	2.48	0.47
1:B:156:MET:HE1	1:B:265:PHE:HB2	1.97	0.47
1:C:100:PHE:HB3	1:C:103:SER:HB2	1.96	0.47
1:D:11:TYR:N	3:D:412:HOH:O	2.48	0.47
1:B:175:ASP:OD2	1:B:180:ARG:NH2	2.48	0.47
3:C:551:HOH:O	1:D:159:ASN:HB3	2.14	0.47
1:D:58:ASP:HA	1:D:61:VAL:HB	1.96	0.46
1:C:218:LYS:HE2	3:D:433:HOH:O	2.14	0.46
1:A:198:ILE:HB	1:A:256:MET:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ASP:OD1	1:C:176:GLY:N	2.48	0.46
1:A:230:ALA:HB3	1:B:260:THR:HG22	1.97	0.46
1:D:20:THR:OG1	1:D:21:LYS:N	2.49	0.46
1:C:152:TYR:HB2	1:D:150:LEU:O	2.16	0.46
1:D:153:ALA:HB2	1:D:286:ILE:HG23	1.97	0.45
1:A:237:LYS:HD3	1:B:235:PRO:HD3	1.97	0.45
1:D:131:ARG:N	3:D:419:HOH:O	2.48	0.45
1:C:0:ARG:HD2	1:C:4:TYR:CD1	2.52	0.45
1:A:336:LYS:HG2	1:A:336:LYS:O	2.17	0.45
1:D:199:ILE:HB	1:D:310:LEU:HD23	2.00	0.44
1:C:147:TYR:O	1:C:149:SER:N	2.51	0.44
1:D:181:MET:HE2	1:D:195:LYS:HD3	2.00	0.44
1:A:5:LYS:NZ	3:A:419:HOH:O	2.34	0.44
1:B:71:LYS:HG3	1:B:72:PRO:HD3	1.99	0.44
1:A:106:MET:SD	1:A:114:GLU:HB3	2.58	0.44
1:C:237:LYS:NZ	3:C:526:HOH:O	2.49	0.43
1:C:-1:LEU:HD11	1:C:49:ALA:HB1	2.00	0.43
1:C:245:GLU:OE1	1:C:330:LYS:NZ	2.52	0.43
1:B:-5:ILE:HD11	1:B:150:LEU:HD12	1.99	0.43
1:D:-11:ILE:HA	1:D:-8:MET:HG2	2.00	0.43
1:D:0:ARG:HA	1:D:0:ARG:HD2	1.75	0.43
1:A:5:LYS:NZ	3:A:434:HOH:O	2.52	0.42
1:B:91:GLN:HB2	1:B:131:ARG:CZ	2.48	0.42
1:C:-8:MET:HG3	1:C:147:TYR:CZ	2.55	0.42
1:B:62:ARG:HB3	1:B:66:ARG:NH1	2.34	0.42
1:B:159:ASN:ND2	2:B:401:4UR:H121	2.34	0.42
1:D:145:ASP:OD1	3:D:404:HOH:O	2.22	0.42
1:A:84:ALA:HB1	1:A:135:VAL:HG13	2.02	0.42
1:C:218:LYS:NZ	1:D:231:GLY:O	2.52	0.42
1:B:137:THR:HB	1:B:146:ALA:HB2	2.02	0.42
1:C:122:SER:O	1:C:126:ASN:ND2	2.50	0.41
1:D:32:LEU:HD11	1:D:44:ILE:HG21	2.02	0.41
1:D:1:LEU:HB3	1:D:44:ILE:O	2.21	0.41
1:C:73:VAL:HG11	1:C:104:LEU:HD22	2.03	0.41
1:C:282:LEU:O	1:C:286:ILE:HG12	2.20	0.41
1:A:5:LYS:NZ	3:A:435:HOH:O	2.52	0.41
1:C:-6:ARG:NH2	3:C:532:HOH:O	2.53	0.41
1:D:260:THR:OG1	1:D:261:PRO:HD3	2.20	0.41
1:B:82:ARG:O	1:B:86:ILE:HG13	2.21	0.41
1:B:324:ASP:HB3	1:B:327:GLU:HB2	2.02	0.41
1:C:58:ASP:HB3	1:C:62:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:VAL:HA	1:D:64:ILE:HD11	2.03	0.40
1:B:152:TYR:O	1:B:156:MET:HG3	2.21	0.40
1:A:75:ASP:HA	1:A:82:ARG:HH21	1.87	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:529:HOH:O	3:C:589:HOH:O[2_446]	2.08	0.12
3:C:508:HOH:O	3:C:509:HOH:O[2_446]	2.12	0.08

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	347/356 (98%)	339 (98%)	8 (2%)	0	100	100
1	B	350/356 (98%)	342 (98%)	8 (2%)	0	100	100
1	C	343/356 (96%)	330 (96%)	12 (4%)	1 (0%)	41	37
1	D	287/356 (81%)	277 (96%)	10 (4%)	0	100	100
All	All	1327/1424 (93%)	1288 (97%)	38 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	36	ILE

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	300/305 (98%)	298 (99%)	2 (1%)	84	88
1	B	301/305 (99%)	292 (97%)	9 (3%)	41	41
1	C	300/305 (98%)	295 (98%)	5 (2%)	60	65
1	D	259/305 (85%)	255 (98%)	4 (2%)	65	69
All	All	1160/1220 (95%)	1140 (98%)	20 (2%)	60	65

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	ASP
1	A	335	LEU
1	B	39	ASN
1	B	40	THR
1	B	47	ASP
1	B	114	GLU
1	B	130	ASN
1	B	160	TYR
1	B	172	ARG
1	B	327	GLU
1	B	336	LYS
1	C	36	ILE
1	C	58	ASP
1	C	150	LEU
1	C	180	ARG
1	C	319	LYS
1	D	47	ASP
1	D	64	ILE
1	D	229	ARG
1	D	319	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	159	ASN

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)

2 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	4UR	C	401	-	43,51,51	3.19	20 (46%)	52,80,80	3.14	17 (32%)
2	4UR	B	401	-	43,51,51	3.17	20 (46%)	52,80,80	3.07	16 (30%)

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	4UR	C	401	-	-	9/22/62/62	0/6/7/7
2	4UR	B	401	-	-	8/22/62/62	0/6/7/7

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	4UR	C04-N03	9.63	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	4UR	C04-N03	9.52	1.50	1.35
2	B	401	4UR	C43-C05	7.73	1.54	1.41
2	C	401	4UR	C43-C05	7.59	1.54	1.41
2	C	401	4UR	C02-N01	7.06	1.48	1.33
2	B	401	4UR	C02-N01	7.05	1.48	1.33
2	C	401	4UR	C02-N45	6.14	1.46	1.35
2	C	401	4UR	C43-N45	6.07	1.43	1.33
2	B	401	4UR	C02-N45	6.04	1.46	1.35
2	B	401	4UR	C43-N45	6.00	1.43	1.33
2	C	401	4UR	P14-O17	5.31	1.74	1.60
2	B	401	4UR	P14-O17	5.18	1.74	1.60
2	C	401	4UR	P24-O27	4.43	1.72	1.60
2	B	401	4UR	P24-O27	4.36	1.71	1.60
2	B	401	4UR	O31-C32	3.97	1.46	1.41
2	C	401	4UR	O31-C32	3.89	1.46	1.41
2	C	401	4UR	P14-O13	3.32	1.72	1.59
2	B	401	4UR	P14-O13	3.26	1.72	1.59
2	B	401	4UR	C37-N38	3.18	1.45	1.34
2	C	401	4UR	C37-N38	3.15	1.45	1.34
2	C	401	4UR	C29-C28	-2.83	1.46	1.52
2	B	401	4UR	C29-C28	-2.72	1.46	1.52
2	B	401	4UR	C40-N41	2.66	1.36	1.32
2	C	401	4UR	O10-C09	2.59	1.44	1.41
2	C	401	4UR	C40-N41	2.54	1.36	1.32
2	B	401	4UR	C19-C18	-2.52	1.47	1.52
2	C	401	4UR	C19-C18	-2.52	1.47	1.52
2	B	401	4UR	O10-C09	2.43	1.44	1.41
2	C	401	4UR	O31-C21	-2.41	1.39	1.45
2	C	401	4UR	C36-C42	-2.40	1.34	1.40
2	B	401	4UR	O31-C21	-2.38	1.39	1.45
2	C	401	4UR	P24-O23	2.35	1.68	1.59
2	C	401	4UR	C02-N03	2.34	1.45	1.34
2	B	401	4UR	P24-O23	2.33	1.68	1.59
2	B	401	4UR	C02-N03	2.30	1.45	1.34
2	B	401	4UR	C36-C42	-2.24	1.35	1.40
2	B	401	4UR	C28-C11	-2.14	1.47	1.52
2	C	401	4UR	C28-C11	-2.13	1.47	1.52
2	B	401	4UR	O44-C43	-2.03	1.19	1.24
2	C	401	4UR	O44-C43	-2.02	1.19	1.24

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	4UR	C09-N08-C04	11.86	147.47	126.64
2	B	401	4UR	C09-N08-C04	11.58	146.98	126.64
2	C	401	4UR	C36-C37-N38	10.67	136.57	120.35
2	B	401	4UR	C36-C37-N38	10.66	136.55	120.35
2	C	401	4UR	N38-C37-N39	-7.40	103.21	118.57
2	B	401	4UR	N38-C37-N39	-7.37	103.28	118.57
2	C	401	4UR	N41-C40-N39	-5.74	119.71	128.68
2	C	401	4UR	C32-N33-C42	-5.66	116.70	126.64
2	B	401	4UR	N03-C02-N45	-5.50	119.89	127.22
2	B	401	4UR	N41-C40-N39	-5.48	120.11	128.68
2	C	401	4UR	N03-C02-N45	-5.43	119.98	127.22
2	B	401	4UR	C32-N33-C42	-4.37	118.95	126.64
2	B	401	4UR	C02-N03-C04	4.11	120.05	115.36
2	C	401	4UR	C02-N03-C04	4.03	119.96	115.36
2	C	401	4UR	O26-P24-O27	3.37	120.09	106.78
2	B	401	4UR	O26-P24-O27	3.16	119.25	106.78
2	B	401	4UR	P14-O17-C18	-2.92	108.76	119.41
2	C	401	4UR	O16-P14-O17	2.70	117.45	106.78
2	B	401	4UR	O16-P14-O17	2.66	117.29	106.78
2	C	401	4UR	P14-O17-C18	-2.63	109.84	119.41
2	B	401	4UR	C05-C43-N45	-2.59	119.89	123.43
2	C	401	4UR	C05-C43-N45	-2.55	119.94	123.43
2	C	401	4UR	C28-C29-C09	2.55	105.53	99.89
2	B	401	4UR	C28-C29-C09	2.53	105.50	99.89
2	B	401	4UR	C43-N45-C02	2.49	119.88	115.93
2	C	401	4UR	C43-N45-C02	2.38	119.72	115.93
2	B	401	4UR	O16-P14-O13	2.15	117.74	107.75
2	C	401	4UR	P14-O13-C12	-2.15	109.07	121.68
2	C	401	4UR	C18-C19-C21	2.07	106.48	101.99
2	C	401	4UR	O16-P14-O13	2.06	117.33	107.75
2	B	401	4UR	N01-C02-N45	2.03	120.41	117.25
2	C	401	4UR	N01-C02-N45	2.03	120.40	117.25
2	B	401	4UR	P14-O13-C12	-2.01	109.90	121.68

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	4UR	C18-O17-P14-O13
2	B	401	4UR	C22-O23-P24-O25
2	B	401	4UR	C22-O23-P24-O26
2	C	401	4UR	C12-O13-P14-O15
2	C	401	4UR	C12-O13-P14-O16

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Mol	Chain	Res	Type	Atoms
2	C	401	4UR	C18-O17-P14-O13
2	B	401	4UR	C29-C28-O27-P24
2	C	401	4UR	C29-C28-O27-P24
2	B	401	4UR	C22-O23-P24-O27
2	C	401	4UR	C12-O13-P14-O17
2	B	401	4UR	C11-C28-O27-P24
2	C	401	4UR	C11-C28-O27-P24
2	B	401	4UR	C12-O13-P14-O17
2	C	401	4UR	C18-O17-P14-O15
2	C	401	4UR	C22-O23-P24-O26
2	C	401	4UR	C18-O17-P14-O16
2	B	401	4UR	C12-O13-P14-O15

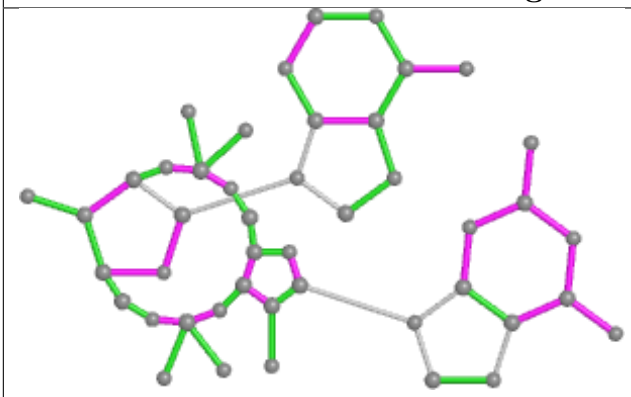
There are no ring outliers.

2 monomers are involved in 5 short contacts:

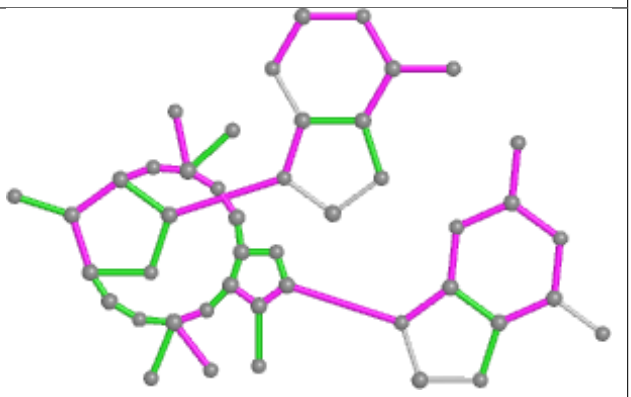
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	4UR	3	0
2	B	401	4UR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

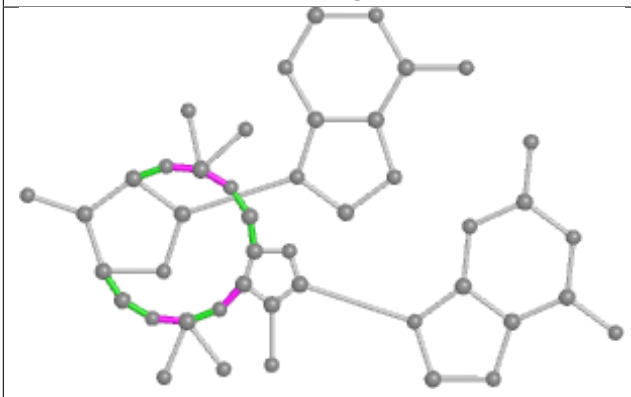
Ligand 4UR C 401



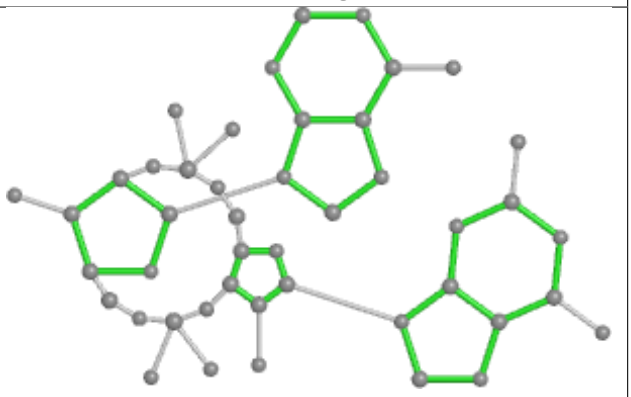
Bond lengths



Bond angles

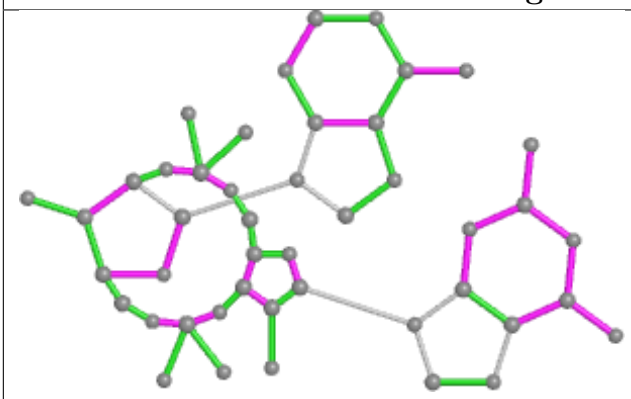


Torsions

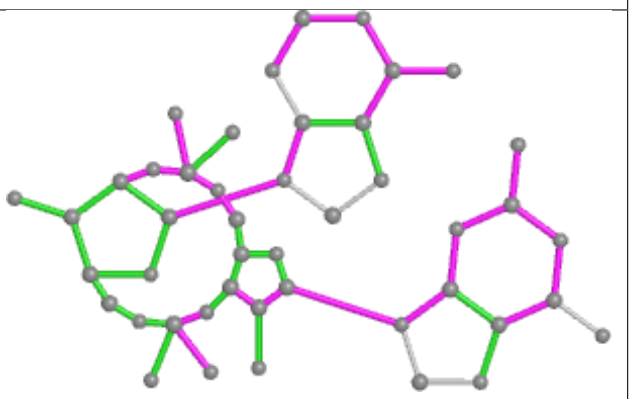


Rings

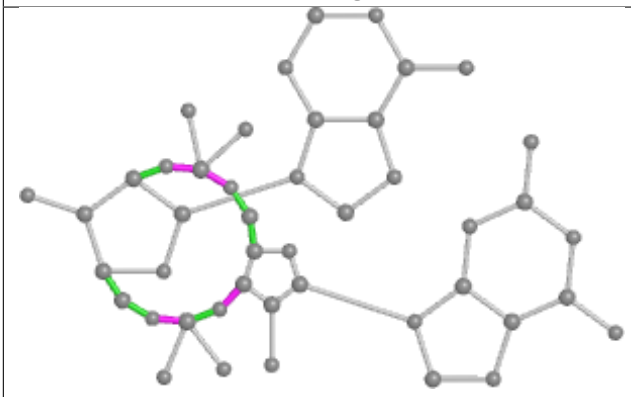
Ligand 4UR B 401



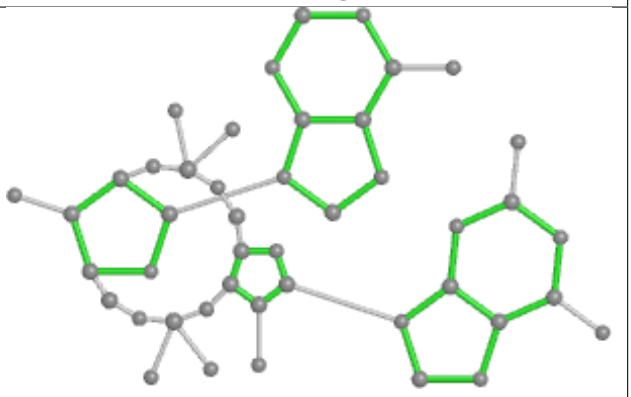
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	351/356 (98%)	0.28	15 (4%)	35	34	27, 50, 85, 106	0
1	B	352/356 (98%)	0.53	27 (7%)	13	12	28, 56, 103, 118	0
1	C	349/356 (98%)	0.59	35 (10%)	7	6	38, 63, 102, 119	0
1	D	301/356 (84%)	0.74	32 (10%)	6	5	46, 71, 100, 119	0
All	All	1353/1424 (95%)	0.53	109 (8%)	12	11	27, 60, 99, 119	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	117	VAL	8.3
1	A	109	GLN	5.4
1	D	136	ILE	5.3
1	B	64	ILE	4.9
1	D	322	LEU	4.4
1	C	125	TYR	4.2
1	D	64	ILE	4.1
1	D	327	GLU	4.0
1	A	105	ARG	3.8
1	C	65	LEU	3.8
1	B	130	ASN	3.8
1	B	126	ASN	3.7
1	D	300	THR	3.7
1	B	85	LEU	3.7
1	D	331	SER	3.7
1	C	299	LYS	3.7
1	A	336	LYS	3.6
1	B	72	PRO	3.6
1	D	150	LEU	3.6
1	D	85	LEU	3.5
1	B	136	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	109	GLN	3.4
1	D	39	ASN	3.4
1	B	121	LYS	3.3
1	D	139	PHE	3.3
1	C	76	SER	3.3
1	A	172	ARG	3.3
1	D	32	LEU	3.3
1	B	107	LEU	3.0
1	D	28	ALA	3.0
1	B	125	TYR	3.0
1	B	113	ASP	3.0
1	D	214	ARG	2.9
1	C	89	VAL	2.8
1	B	128	THR	2.8
1	C	111	ARG	2.8
1	D	138	THR	2.8
1	A	107	LEU	2.8
1	C	106	MET	2.7
1	B	104	LEU	2.7
1	A	79	ALA	2.7
1	B	123	ARG	2.7
1	D	65	LEU	2.7
1	C	110	LYS	2.7
1	C	127	GLN	2.7
1	B	23	PRO	2.7
1	D	252	TYR	2.7
1	C	68	ALA	2.7
1	C	147	TYR	2.6
1	C	70	LEU	2.6
1	A	249	GLY	2.6
1	C	53	PHE	2.6
1	C	107	LEU	2.6
1	D	25	LEU	2.6
1	D	145	ASP	2.5
1	D	97	VAL	2.5
1	B	77	LEU	2.5
1	C	74	TYR	2.5
1	C	152	TYR	2.5
1	D	74	TYR	2.5
1	A	39	ASN	2.5
1	D	154	ALA	2.4
1	A	127	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	1	LEU	2.4
1	A	125	TYR	2.4
1	C	272	ASN	2.4
1	D	140	ARG	2.4
1	B	102	ASN	2.4
1	A	126	ASN	2.4
1	D	95	THR	2.4
1	C	124	TRP	2.3
1	B	90	PHE	2.3
1	C	97	VAL	2.3
1	C	75	ASP	2.3
1	C	115	ALA	2.3
1	D	-1	LEU	2.3
1	B	133	LYS	2.3
1	C	108	GLN	2.3
1	B	119	LEU	2.3
1	C	146	ALA	2.3
1	B	174	ALA	2.2
1	D	332	HIS	2.2
1	A	97	VAL	2.2
1	C	172	ARG	2.2
1	C	71	LYS	2.2
1	D	15	ILE	2.2
1	A	122	SER	2.2
1	B	129	PRO	2.2
1	D	52	LEU	2.2
1	A	85	LEU	2.1
1	C	90	PHE	2.1
1	C	47	ASP	2.1
1	C	105	ARG	2.1
1	D	174	ALA	2.1
1	D	144	TRP	2.1
1	C	153	ALA	2.1
1	C	275	ALA	2.1
1	B	114	GLU	2.1
1	C	149	SER	2.1
1	C	-13	MET	2.1
1	D	90	PHE	2.1
1	D	-4	ASP	2.1
1	C	273	PHE	2.1
1	B	322	LEU	2.0
1	D	156	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	146	ALA	2.0
1	B	96	GLY	2.0
1	B	105	ARG	2.0
1	A	250	LYS	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)

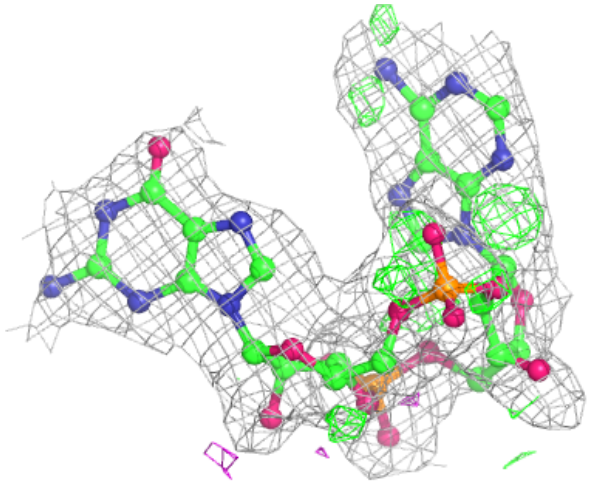
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

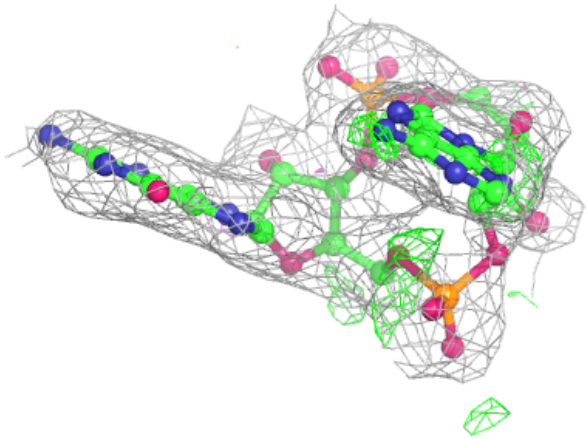
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	4UR	C	401	45/45	0.87	0.17	42,52,62,65	0
2	4UR	B	401	45/45	0.90	0.15	28,35,42,44	0

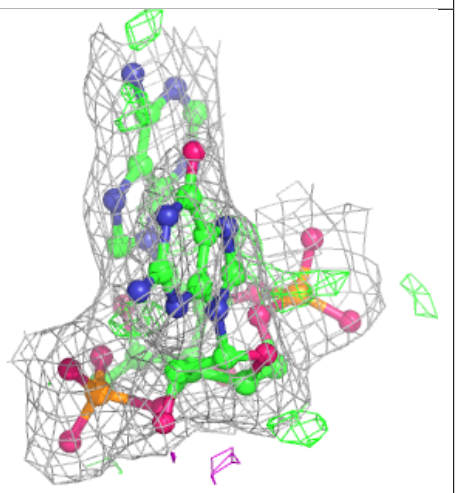
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4UR C 401:

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

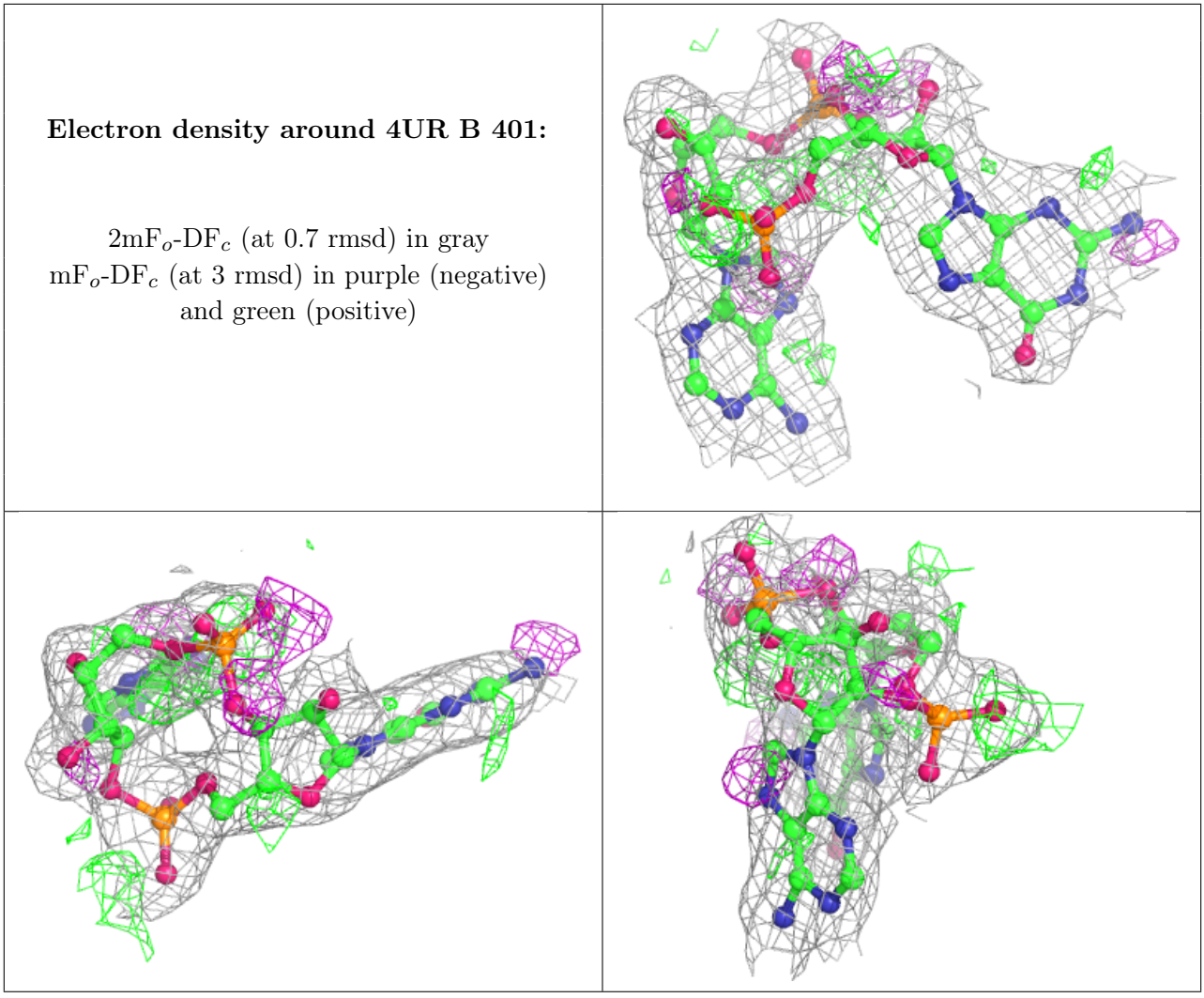






Electron density around 4UR B 401:

$2mF_o$-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.