Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2023 – 09:46 AM EDT

PDB ID	:	7L5E
Title	:	Crystal Structure of KPT-330 bound to CRM1 (537-DLTVK-541 to GLCEQ)
Authors	:	Baumhardt, J.M.; Chook, Y.M.
Deposited on	:	2020-12-21
Resolution	:	1.94 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

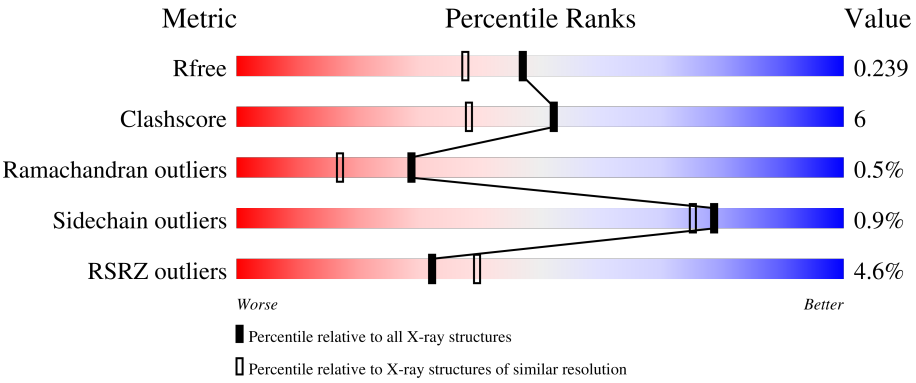
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	4% 86% 8% 6%
2	B	140	3% 79% 8% 13%
3	C	1024	5% 85% 12% ••

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11658 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
			Total	C	N	O	S			
1	A	202	1657	1068	287	296	6	0	4	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	122	1005	637	178	186	4	0	2	0

- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	1009	8296	5319	1373	1558	46	0	32	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P30822
C	-1	GLY	-	expression tag	UNP P30822
C	0	SER	-	expression tag	UNP P30822
C	?	-	VAL	deletion	UNP P30822
C	?	-	GLN	deletion	UNP P30822
C	?	-	ARG	deletion	UNP P30822
C	?	-	LEU	deletion	UNP P30822
C	?	-	PRO	deletion	UNP P30822
C	?	-	ALA	deletion	UNP P30822
C	?	-	THR	deletion	UNP P30822
C	?	-	GLU	deletion	UNP P30822
C	?	-	MET	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	PRO	deletion	UNP P30822

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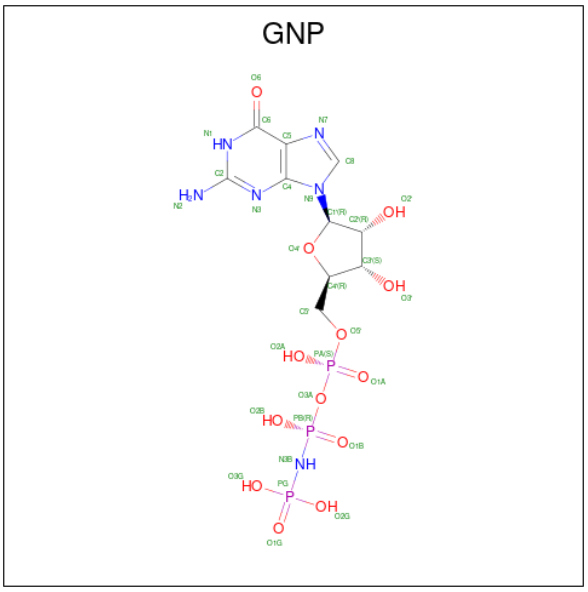
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LEU	deletion	UNP P30822
C	?	-	ILE	deletion	UNP P30822
C	?	-	GLN	deletion	UNP P30822
C	?	-	LEU	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	VAL	deletion	UNP P30822
C	?	-	GLY	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	GLN	deletion	UNP P30822
C	?	-	ALA	deletion	UNP P30822
C	?	-	ILE	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	THR	deletion	UNP P30822
C	?	-	GLY	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	GLY	deletion	UNP P30822
C	?	-	ALA	deletion	UNP P30822
C	?	-	LEU	deletion	UNP P30822
C	?	-	ASN	deletion	UNP P30822
C	?	-	PRO	deletion	UNP P30822
C	?	-	GLU	deletion	UNP P30822
C	?	-	TYR	deletion	UNP P30822
C	?	-	MET	deletion	UNP P30822
C	?	-	LYS	deletion	UNP P30822
C	?	-	ARG	deletion	UNP P30822
C	?	-	PHE	deletion	UNP P30822
C	537	GLY	ASP	engineered mutation	UNP P30822
C	539	CYS	THR	engineered mutation	UNP P30822
C	540	GLU	VAL	engineered mutation	UNP P30822
C	541	GLN	LYS	engineered mutation	UNP P30822
C	1022	CYS	TYR	conflict	UNP P30822

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

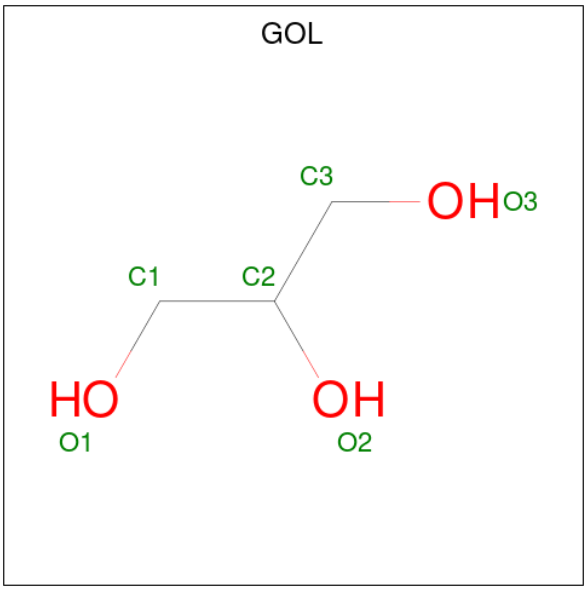


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

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

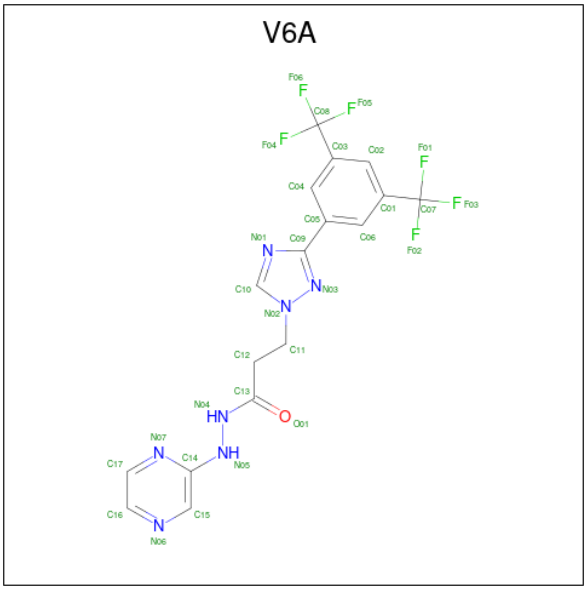
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is selinexor, bound form (three-letter code: V6A) (formula: $C_{17}H_{13}F_6N_7O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C F N O 31 17 6 7 1	0	0

- Molecule 8 is water.

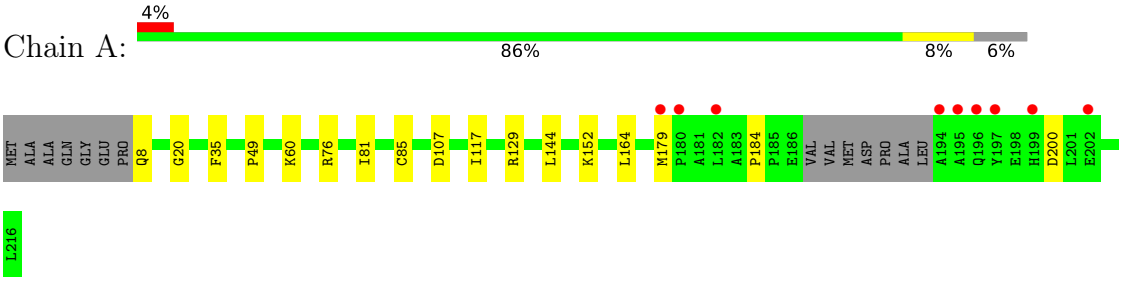
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	118	Total O 118 118	0	0
8	B	34	Total O 34 34	0	0
8	C	478	Total O 478 478	0	0

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.

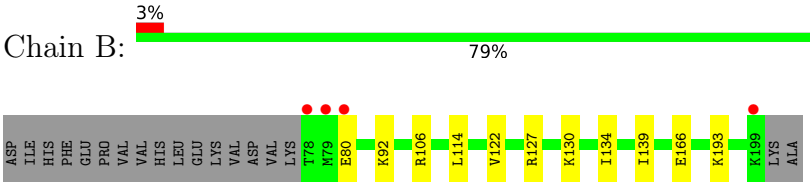
• Molecule 1: GTP-binding nuclear protein Ran

Chain A:



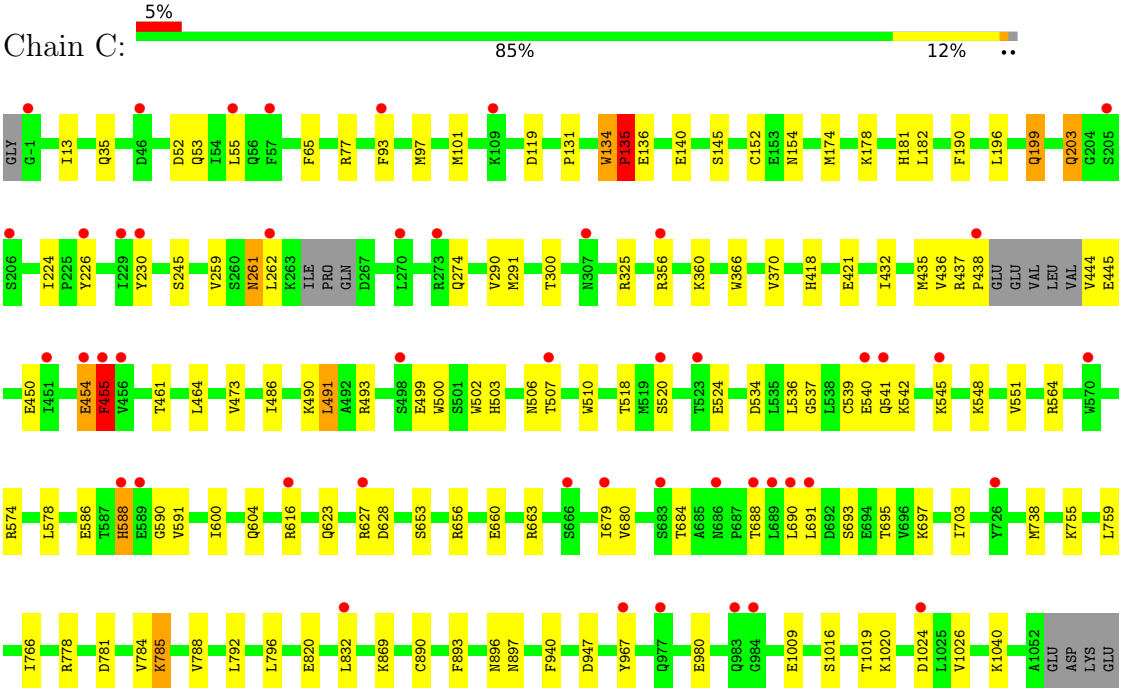
• Molecule 2: Ran-specific GTPase-activating protein 1

Chain B:



• Molecule 3: Exportin-1

Chain C:



ASN
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.43Å 105.43Å 305.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.80 – 1.94 45.80 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.80-1.94) 99.8 (45.80-1.94)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.226 , 0.245 0.223 , 0.239	Depositor DCC
R_{free} test set	2000 reflections (1.58%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.5	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	11658	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: GNP, MG, GOL, V6A

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	0.28	0/1697	0.50	0/2299
2	B	0.26	0/1023	0.53	1/1369 (0.1%)
3	C	0.34	1/8460 (0.0%)	0.48	6/11459 (0.1%)
All	All	0.32	1/11180 (0.0%)	0.49	7/15127 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	135	PRO	N-CD	15.45	1.69	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	455	PHE	N-CA-C	8.21	133.18	111.00
3	C	135	PRO	CA-N-CD	-7.82	100.56	111.50
2	B	130	LYS	CB-CA-C	-6.82	96.76	110.40
3	C	135	PRO	N-CA-CB	6.71	111.35	103.30
3	C	491	LEU	CB-CG-CD1	-5.42	101.78	111.00
3	C	134	TRP	N-CA-C	-5.24	96.85	111.00
3	C	454	GLU	N-CA-C	5.05	124.64	111.00

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	1657	0	1650	14	0
2	B	1005	0	990	8	0
3	C	8296	0	8319	102	1
4	A	32	0	12	1	0
5	A	1	0	0	0	0
6	A	6	0	8	1	0
7	C	31	0	0	4	0
8	A	118	0	0	3	0
8	B	34	0	0	2	0
8	C	478	0	0	13	2
All	All	11658	0	10979	122	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 6.

All (122) 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:135:PRO:CD	3:C:135:PRO:N	1.69	1.45
3:C:491:LEU:HD11	3:C:534:ASP:HB3	1.56	0.87
3:C:356[B]:ARG:HH21	3:C:461:THR:HG22	1.42	0.85
3:C:679:ILE:HD11	3:C:695:THR:HG23	1.62	0.82
3:C:134:TRP:C	3:C:135:PRO:CD	2.53	0.77
3:C:503:HIS:O	3:C:503:HIS:CG	2.39	0.75
3:C:660:GLU:OE2	8:C:1201:HOH:O	2.04	0.74
3:C:438:PRO:O	3:C:445:GLU:N	2.22	0.71
3:C:520:SER:OG	8:C:1202:HOH:O	2.08	0.70
3:C:540:GLU:HG2	3:C:541:GLN:HE21	1.57	0.67
3:C:262:LEU:O	3:C:325[B]:ARG:NH2	2.26	0.67
3:C:503:HIS:O	3:C:503:HIS:ND1	2.28	0.66
3:C:539:CYS:HB2	7:C:1101:V6A:C11	2.24	0.66
3:C:1020:LYS:NZ	8:C:1214:HOH:O	2.31	0.64
3:C:653:SER:O	3:C:656:ARG:NH1	2.29	0.63
3:C:539:CYS:SG	7:C:1101:V6A:C11	2.88	0.62
3:C:1016[B]:SER:HB3	3:C:1020:LYS:HZ1	1.65	0.61
3:C:493:ARG:HE	3:C:499:GLU:CD	2.05	0.59
3:C:261[A]:ASN:OD1	8:C:1203:HOH:O	2.17	0.59
3:C:181:HIS:ND1	8:C:1215:HOH:O	2.32	0.58
3:C:588:HIS:HB3	3:C:591:VAL:HB	1.86	0.58
3:C:680:VAL:O	3:C:684:THR:HB	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ASP:OD2	6:A:303:GOL:O1	2.23	0.57
2:B:106:ARG:NH2	2:B:166:GLU:HG3	2.19	0.57
3:C:437:ARG:HG2	3:C:510:TRP:CH2	2.40	0.57
2:B:80:GLU:OE1	2:B:127:ARG:NH2	2.35	0.56
3:C:503:HIS:HA	3:C:506:ASN:HB2	1.88	0.56
3:C:486:ILE:O	3:C:490:LYS:HG2	2.06	0.56
3:C:896:ASN:ND2	3:C:947:ASP:O	2.29	0.56
2:B:166:GLU:OE1	8:B:301:HOH:O	2.17	0.56
3:C:199:GLN:O	3:C:203:GLN:HB3	2.06	0.56
3:C:97:MET:O	3:C:101:MET:HG3	2.06	0.55
3:C:502:TRP:O	3:C:503:HIS:HB3	2.06	0.55
3:C:590:GLY:N	8:C:1213:HOH:O	2.30	0.55
1:A:117:ILE:HB	1:A:144:LEU:HD22	1.89	0.55
3:C:356[B]:ARG:NH2	3:C:461:THR:HG22	2.17	0.54
3:C:691:LEU:HD11	3:C:738[B]:MET:SD	2.48	0.54
3:C:536:LEU:HA	3:C:539:CYS:SG	2.48	0.53
3:C:325[B]:ARG:NH1	8:C:1223:HOH:O	2.38	0.53
3:C:432:ILE:O	3:C:507[B]:THR:HG22	2.09	0.53
1:A:200:ASP:OD2	8:A:401:HOH:O	2.19	0.53
3:C:623:GLN:O	3:C:627:ARG:HG3	2.09	0.53
3:C:586:GLU:HB3	3:C:588:HIS:HB2	1.90	0.52
3:C:55:LEU:HB2	3:C:93:PHE:HZ	1.74	0.52
3:C:540:GLU:OE1	3:C:541:GLN:NE2	2.43	0.52
3:C:540:GLU:CG	3:C:541:GLN:HE21	2.21	0.52
3:C:545:LYS:O	3:C:588:HIS:HE1	1.93	0.52
3:C:781:ASP:O	3:C:785:LYS:HE2	2.10	0.51
3:C:491:LEU:HD11	3:C:534:ASP:CB	2.36	0.51
3:C:473:VAL:HG13	3:C:518:THR:HG22	1.92	0.50
3:C:897:ASN:ND2	8:C:1238:HOH:O	2.43	0.50
3:C:174:MET:CE	3:C:182:LEU:HD12	2.41	0.50
3:C:226:TYR:HB3	8:C:1253:HOH:O	2.11	0.50
7:C:1101:V6A:N07	7:C:1101:V6A:C13	2.73	0.50
1:A:179:MET:HE3	2:B:134:ILE:H	1.75	0.50
3:C:52:ASP:HA	3:C:93:PHE:CZ	2.47	0.50
3:C:755:LYS:HZ2	3:C:759:LEU:HD11	1.77	0.49
3:C:436:VAL:HG22	3:C:437:ARG:H	1.78	0.49
3:C:119:ASP:OD2	3:C:154:ASN:ND2	2.45	0.48
3:C:174:MET:HE3	3:C:182:LEU:HD12	1.96	0.48
3:C:600:ILE:O	3:C:604:GLN:HG3	2.13	0.48
1:A:85:CYS:HB2	1:A:164:LEU:HD22	1.95	0.48
3:C:77:ARG:NH1	3:C:1040:LYS:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1009:GLU:OE1	8:C:1204:HOH:O	2.20	0.47
3:C:784:VAL:HG12	3:C:785:LYS:HD3	1.97	0.47
3:C:688:THR:O	3:C:691:LEU:N	2.41	0.47
3:C:967:TYR:CZ	3:C:1019:THR:HG21	2.50	0.47
2:B:92:LYS:NZ	8:B:304:HOH:O	2.38	0.47
3:C:13:ILE:HD11	3:C:53:GLN:HG2	1.96	0.47
1:A:76:ARG:HG2	1:A:76:ARG:HH21	1.80	0.46
2:B:193:LYS:HB3	2:B:193:LYS:HE3	1.78	0.46
3:C:418:HIS:HA	3:C:421:GLU:HG3	1.97	0.46
3:C:820:GLU:OE2	3:C:869:LYS:NZ	2.32	0.46
3:C:190:PHE:CZ	3:C:224:ILE:HG21	2.50	0.46
3:C:890:CYS:O	3:C:893:PHE:HB2	2.16	0.46
3:C:245:SER:HB2	8:C:1274:HOH:O	2.15	0.45
3:C:693:SER:O	3:C:697:LYS:HG2	2.16	0.45
3:C:688:THR:HA	3:C:691:LEU:CD1	2.47	0.45
3:C:491:LEU:C	3:C:491:LEU:HD13	2.38	0.45
3:C:500:TRP:CZ2	3:C:542:LYS:HD2	2.51	0.45
3:C:539:CYS:CB	7:C:1101:V6A:C11	2.92	0.45
3:C:356[B]:ARG:HD3	3:C:464:LEU:HD22	1.99	0.44
3:C:145:SER:O	3:C:152:CYS:HB2	2.17	0.44
3:C:506:ASN:HB3	3:C:510:TRP:CZ2	2.52	0.44
3:C:537:GLY:O	3:C:541:GLN:NE2	2.49	0.44
1:A:49:PRO:HB3	1:A:60:LYS:HE2	1.99	0.44
3:C:131:PRO:HA	3:C:134:TRP:O	2.18	0.44
1:A:20:GLY:H	4:A:301:GNP:HNB3	1.65	0.44
3:C:539:CYS:HB3	3:C:551:VAL:HG11	1.98	0.44
3:C:55:LEU:HD12	3:C:93:PHE:CZ	2.52	0.44
3:C:259:VAL:C	3:C:261[B]:ASN:H	2.22	0.43
3:C:574:ARG:O	3:C:578:LEU:HD23	2.18	0.43
3:C:196:LEU:HA	3:C:199:GLN:HG2	2.00	0.43
3:C:366:TRP:O	3:C:370:VAL:HG22	2.18	0.43
3:C:437:ARG:HG3	8:C:1491:HOH:O	2.19	0.43
1:A:8:GLN:HA	8:A:466:HOH:O	2.19	0.42
1:A:81:ILE:HD11	3:C:65:PHE:CG	2.54	0.42
3:C:548:LYS:O	3:C:548:LYS:HD2	2.19	0.42
1:A:76:ARG:HG2	1:A:76:ARG:NH2	2.35	0.42
3:C:755:LYS:HD3	3:C:755:LYS:HA	1.80	0.42
1:A:129:ARG:NH2	8:A:408:HOH:O	2.40	0.42
3:C:491:LEU:CD1	3:C:534:ASP:HB3	2.39	0.42
3:C:688:THR:HA	3:C:691:LEU:HD12	2.01	0.41
1:A:184:PRO:HG2	2:B:139:ILE:HG12	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:300:THR:HG21	8:C:1641:HOH:O	2.19	0.41
3:C:174:MET:HE3	3:C:178:LYS:HG2	2.01	0.41
3:C:788:VAL:O	3:C:792:LEU:HG	2.21	0.41
3:C:536:LEU:HA	3:C:536:LEU:HD23	1.84	0.41
3:C:796:LEU:HD12	3:C:832:LEU:HG	2.03	0.41
3:C:136:GLU:HG3	3:C:140:GLU:OE2	2.21	0.41
3:C:230:TYR:O	3:C:274:GLN:NE2	2.54	0.41
3:C:356[B]:ARG:HD2	3:C:360:LYS:HE3	2.02	0.41
3:C:690:LEU:HD12	3:C:690:LEU:HA	1.89	0.41
3:C:454:GLU:O	3:C:455:PHE:CB	2.69	0.41
1:A:35:PHE:CZ	1:A:152:LYS:HD2	2.56	0.41
3:C:290:VAL:HG12	3:C:291:MET:CE	2.51	0.41
3:C:1024:ASP:OD1	3:C:1026:VAL:HG22	2.21	0.41
3:C:524:GLU:CD	3:C:564:ARG:HH21	2.25	0.40
3:C:703[B]:ILE:HD13	3:C:766:ILE:HG13	2.03	0.40
3:C:755:LYS:NZ	3:C:759:LEU:HD11	2.36	0.40
3:C:796:LEU:CD1	3:C:832:LEU:HG	2.52	0.40
2:B:114:LEU:O	2:B:122:VAL:HA	2.22	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:663:ARG:NH2	8:C:1201:HOH:O[7_465]	2.10	0.10
8:C:1236:HOH:O	8:C:1616:HOH:O[3_554]	2.16	0.04

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	202/216 (94%)	197 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	122/140 (87%)	117 (96%)	5 (4%)	0	100	100
3	C	1037/1024 (101%)	1007 (97%)	24 (2%)	6 (1%)	25	13
All	All	1361/1380 (99%)	1321 (97%)	34 (2%)	6 (0%)	29	24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	455	PHE
3	C	980	GLU
3	C	135	PRO
3	C	450	GLU
3	C	588	HIS
3	C	444	VAL

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	178/185 (96%)	178 (100%)	0	100	100
2	B	102/121 (84%)	102 (100%)	0	100	100
3	C	932/933 (100%)	920 (99%)	12 (1%)	69	62
All	All	1212/1239 (98%)	1200 (99%)	12 (1%)	78	71

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	35	GLN
3	C	199	GLN
3	C	203	GLN
3	C	261[A]	ASN
3	C	261[B]	ASN
3	C	435[A]	MET
3	C	435[B]	MET
3	C	616	ARG

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Mol	Chain	Res	Type
3	C	628	ASP
3	C	778	ARG
3	C	785	LYS
3	C	940	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	203	GLN
3	C	307	ASN
3	C	541	GLN
3	C	588	HIS
3	C	727	ASN
3	C	801	ASN
3	C	1010	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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	V6A	C	1101	-	32,33,33	2.98	11 (34%)	42,48,48	2.53	14 (33%)
6	GOL	A	303	-	5,5,5	0.38	0	5,5,5	0.27	0
4	GNP	A	301	5	29,34,34	5.09	16 (55%)	33,54,54	1.80	8 (24%)

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	V6A	C	1101	-	-	5/26/26/26	0/3/3/3
6	GOL	A	303	-	-	2/4/4/4	-
4	GNP	A	301	5	-	6/14/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	GNP	C2'-C1'	-14.91	1.31	1.53
4	A	301	GNP	O4'-C1'	14.88	1.61	1.41
4	A	301	GNP	C2-N2	10.46	1.54	1.33
7	C	1101	V6A	C13-N04	9.54	1.47	1.34
7	C	1101	V6A	C10-N02	-8.21	1.25	1.33
4	A	301	GNP	PB-O3A	6.92	1.67	1.59
7	C	1101	V6A	C14-N05	5.93	1.48	1.38
4	A	301	GNP	PB-O1B	5.53	1.54	1.46
4	A	301	GNP	O4'-C4'	-5.40	1.32	1.45
4	A	301	GNP	O2'-C2'	4.22	1.52	1.43
7	C	1101	V6A	C09-N01	-4.16	1.29	1.35
4	A	301	GNP	PG-O1G	3.94	1.52	1.46
7	C	1101	V6A	C10-N01	-3.48	1.29	1.35
7	C	1101	V6A	C09-N03	-3.43	1.26	1.34
4	A	301	GNP	O3'-C3'	-3.08	1.35	1.43
7	C	1101	V6A	C11-N02	-3.05	1.42	1.47
4	A	301	GNP	C5-C4	-2.76	1.33	1.40
4	A	301	GNP	PB-N3B	2.67	1.70	1.63
7	C	1101	V6A	O01-C13	-2.45	1.18	1.23
4	A	301	GNP	PA-O5'	2.39	1.69	1.59
4	A	301	GNP	O6-C6	-2.34	1.18	1.24
4	A	301	GNP	C5-C6	-2.33	1.37	1.41
4	A	301	GNP	PG-N3B	2.27	1.69	1.63
7	C	1101	V6A	C02-C01	-2.23	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	GNP	PB-O2B	-2.04	1.51	1.56
7	C	1101	V6A	C06-C05	-2.02	1.36	1.39
7	C	1101	V6A	C02-C03	-2.01	1.36	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	1101	V6A	C15-C14-N07	-8.38	117.41	121.27
7	C	1101	V6A	N03-C09-N01	-8.23	107.89	114.72
4	A	301	GNP	N3-C2-N1	-5.32	120.12	127.22
7	C	1101	V6A	C14-N05-N04	-4.14	110.22	119.04
7	C	1101	V6A	N01-C10-N02	-4.04	106.44	112.21
4	A	301	GNP	C2-N3-C4	3.96	119.88	115.36
7	C	1101	V6A	F05-C08-C03	-3.39	105.49	112.93
7	C	1101	V6A	C17-C16-N06	-3.38	117.73	121.95
4	A	301	GNP	C1'-N9-C4	-3.02	121.34	126.64
7	C	1101	V6A	O01-C13-C12	-2.86	116.79	122.02
7	C	1101	V6A	F04-C08-C03	-2.85	106.67	112.93
4	A	301	GNP	PB-O3A-PA	-2.80	122.77	132.62
4	A	301	GNP	N2-C2-N3	2.79	122.33	117.79
7	C	1101	V6A	C17-N07-C14	2.70	121.06	117.22
7	C	1101	V6A	F06-C08-C03	2.62	118.67	112.93
4	A	301	GNP	C2-N1-C6	2.61	120.08	115.93
4	A	301	GNP	C5-C6-N1	-2.58	119.90	123.43
7	C	1101	V6A	F02-C07-C01	-2.54	107.34	112.93
7	C	1101	V6A	C11-C12-C13	-2.49	107.31	111.89
7	C	1101	V6A	C16-N06-C15	2.29	120.81	116.85
4	A	301	GNP	C3'-C2'-C1'	2.21	104.30	100.98
7	C	1101	V6A	C13-N04-N05	2.10	122.67	120.05

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GNP	PG-N3B-PB-O1B
4	A	301	GNP	C5'-O5'-PA-O3A
6	A	303	GOL	O1-C1-C2-C3
7	C	1101	V6A	C12-C11-N02-N03
7	C	1101	V6A	C13-N04-N05-C14
6	A	303	GOL	O1-C1-C2-O2
7	C	1101	V6A	C12-C11-N02-C10
4	A	301	GNP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	A	301	GNP	C3'-C4'-C5'-O5'
4	A	301	GNP	C5'-O5'-PA-O1A
4	A	301	GNP	C5'-O5'-PA-O2A
7	C	1101	V6A	C11-C12-C13-O01
7	C	1101	V6A	C11-C12-C13-N04

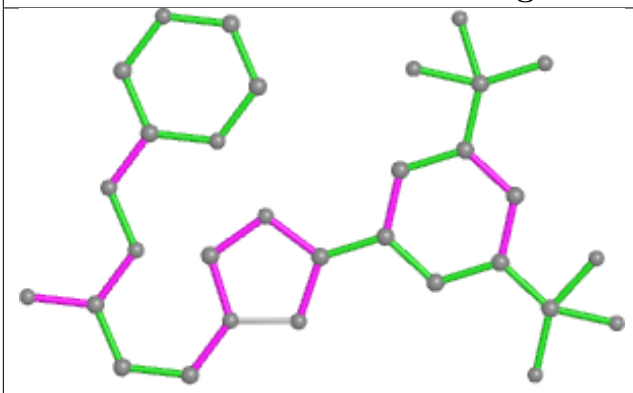
There are no ring outliers.

3 monomers are involved in 6 short contacts:

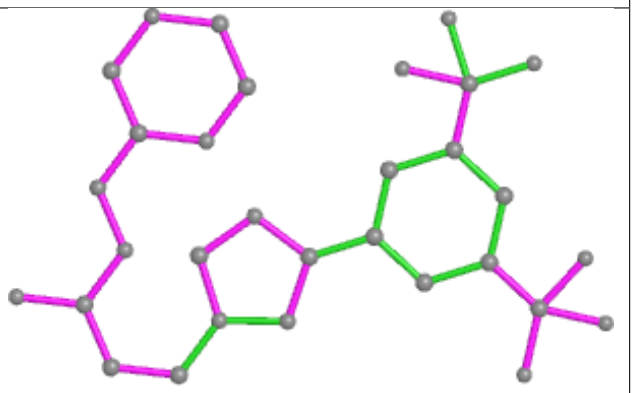
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1101	V6A	4	0
6	A	303	GOL	1	0
4	A	301	GNP	1	0

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.

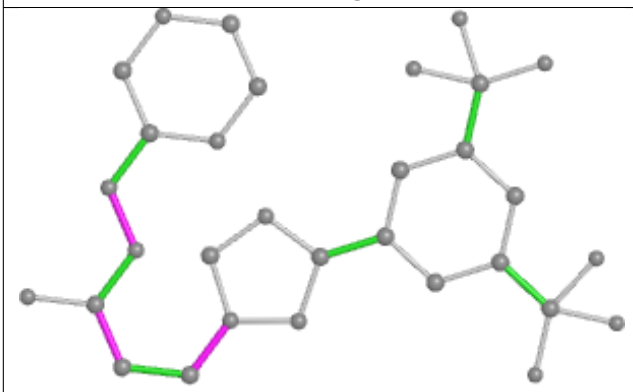
Ligand V6A C 1101



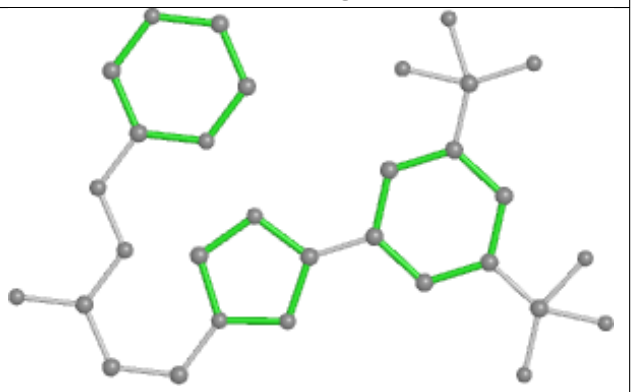
Bond lengths



Bond angles

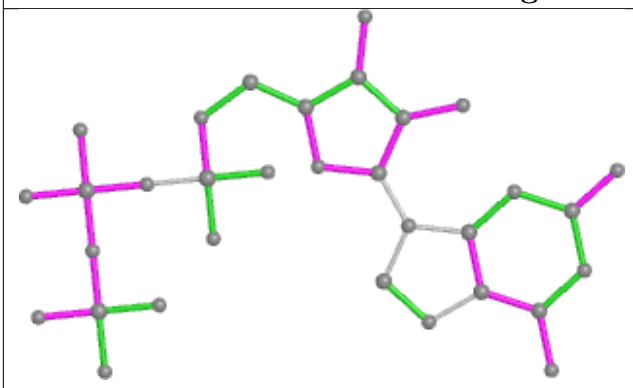


Torsions

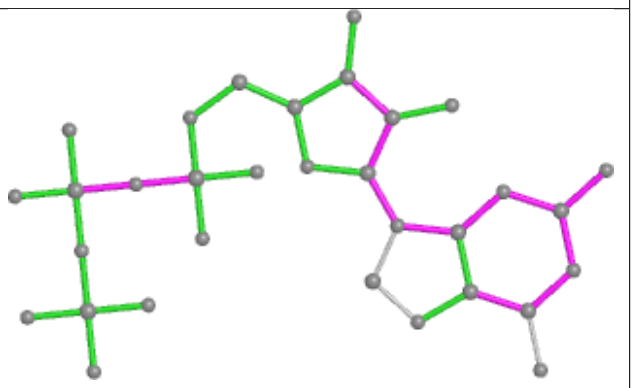


Rings

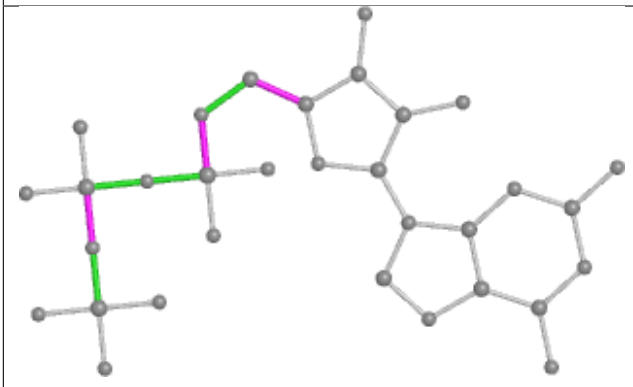
Ligand GNP A 301



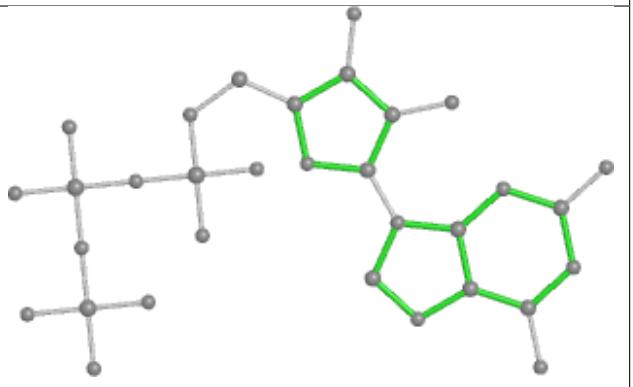
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	261[A]:ASN	C	262:LEU	N	3.32

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	202/216 (93%)	0.29	9 (4%)	33	40	20, 33, 68, 117	0
2	B	122/140 (87%)	0.21	4 (3%)	46	54	35, 49, 75, 111	0
3	C	1009/1024 (98%)	0.24	48 (4%)	30	38	19, 37, 73, 139	0
All	All	1333/1380 (96%)	0.25	61 (4%)	32	39	19, 38, 74, 139	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	689	LEU	8.6
1	A	179	MET	7.1
3	C	205	SER	5.2
3	C	55	LEU	5.2
3	C	226	TYR	5.1
2	B	79	MET	5.0
3	C	588	HIS	5.0
3	C	688	THR	4.5
1	A	194	ALA	4.4
3	C	690	LEU	4.3
2	B	78	THR	4.3
3	C	262	LEU	4.2
3	C	498	SER	4.1
3	C	451	ILE	4.0
3	C	983	GLN	4.0
3	C	679	ILE	3.9
3	C	540	GLU	3.8
1	A	195	ALA	3.7
3	C	270	LEU	3.7
1	A	196	GLN	3.7
3	C	93	PHE	3.5
3	C	726	TYR	3.4
3	C	541	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	197	TYR	3.4
3	C	984	GLY	3.3
1	A	180	PRO	3.2
3	C	967	TYR	3.2
3	C	438	PRO	3.1
3	C	686	ASN	3.0
3	C	455	PHE	3.0
3	C	977	GLN	3.0
3	C	683	SER	2.8
3	C	589	GLU	2.8
3	C	356[A]	ARG	2.6
3	C	520	SER	2.6
3	C	206	SER	2.6
3	C	616	ARG	2.5
3	C	545	LYS	2.5
1	A	199	HIS	2.5
2	B	199	LYS	2.5
1	A	182	LEU	2.4
3	C	229	ILE	2.4
3	C	109	LYS	2.3
3	C	507[A]	THR	2.3
3	C	-1	GLY	2.3
3	C	691	LEU	2.3
3	C	57	PHE	2.3
3	C	230	TYR	2.2
3	C	456	VAL	2.2
3	C	273	ARG	2.2
3	C	666[A]	SER	2.1
3	C	307	ASN	2.1
1	A	202	GLU	2.1
3	C	570	TRP	2.1
3	C	627	ARG	2.1
3	C	1024	ASP	2.1
2	B	80	GLU	2.1
3	C	523	THR	2.0
3	C	454	GLU	2.0
3	C	46	ASP	2.0
3	C	832	LEU	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)

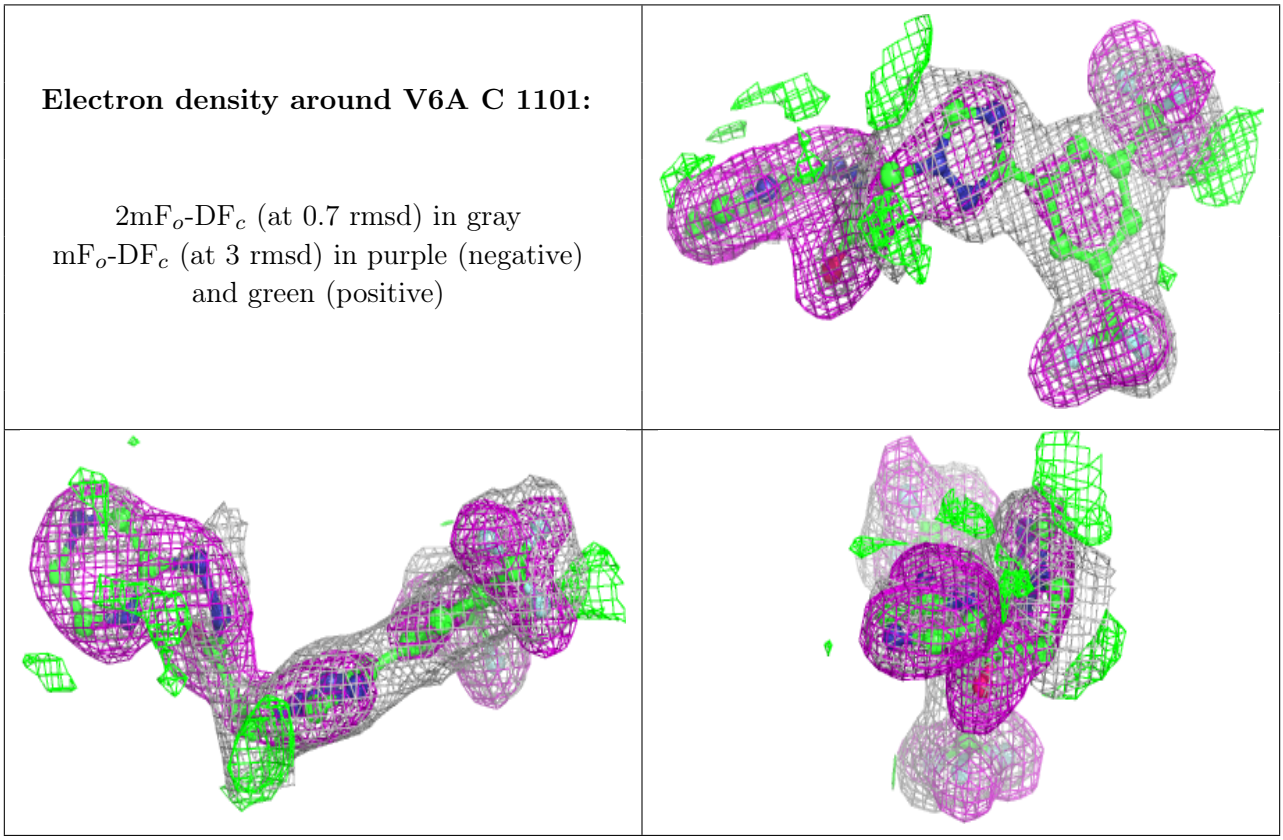
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
7	V6A	C	1101	31/31	0.75	0.36	19,19,19,19	0
6	GOL	A	303	6/6	0.77	0.28	51,66,70,72	0
4	GNP	A	301	32/32	0.92	0.14	17,24,31,33	0
5	MG	A	302	1/1	0.93	0.12	18,18,18,18	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.

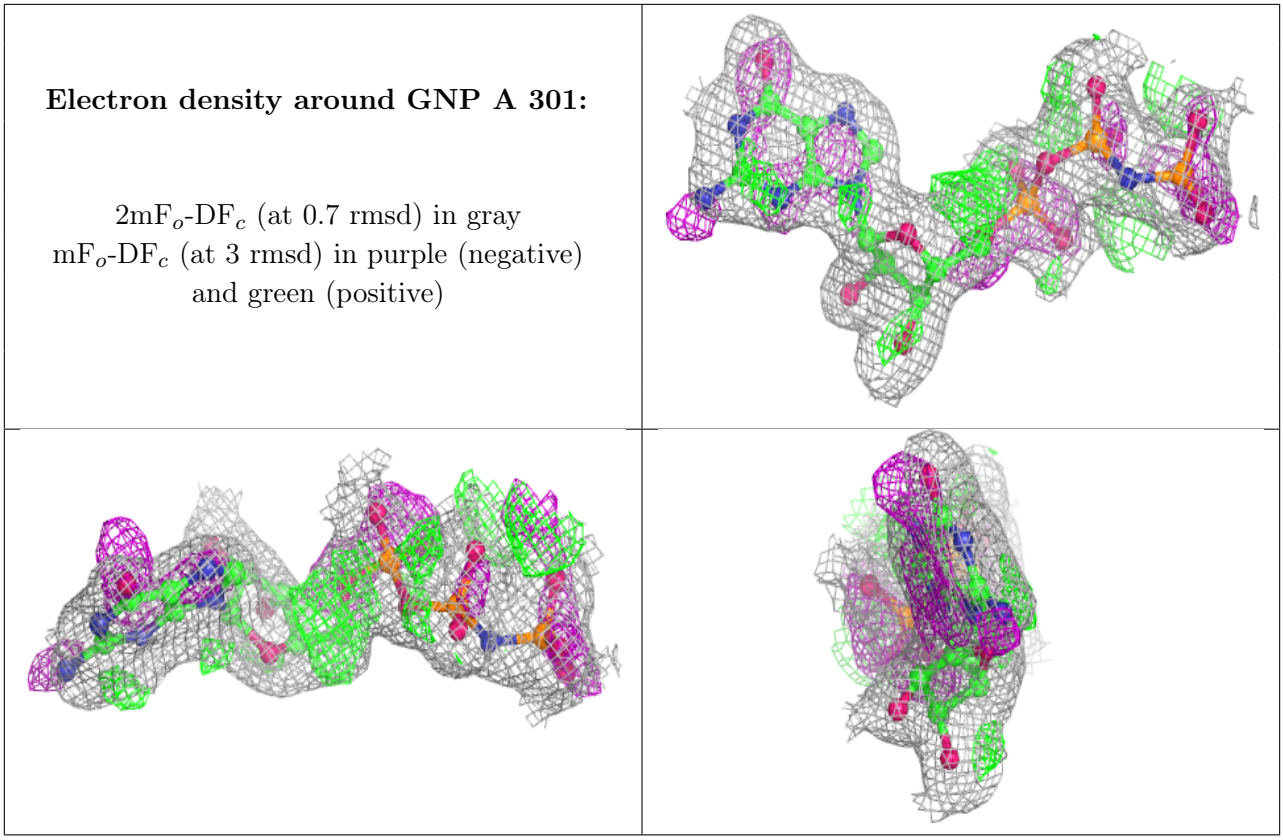
Electron density around V6A C 1101:

$2mF_o$-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.