



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:54 AM UTC

PDB ID : 6XJS / pdb_00006xjs
Title : Crystal Structure of KPT-330 bound to CRM1 (E582K, 537-DLTVK-541 to GLCEQ)
Authors : Baumhardt, J.M.; Chook, Y.M.
Deposited on : 2020-06-24
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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

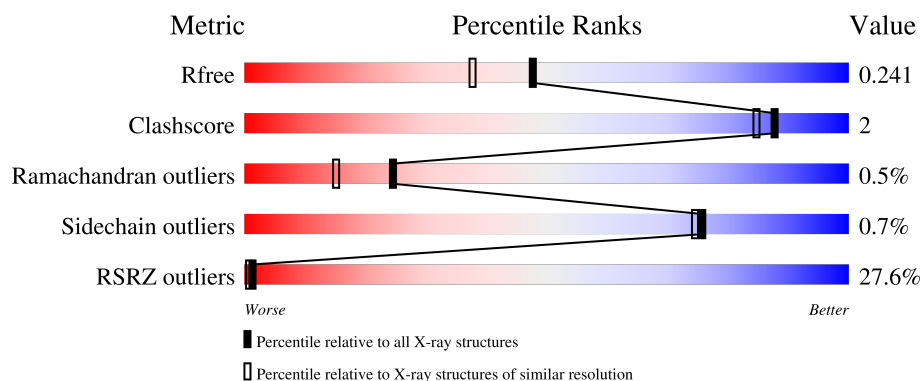
1 Overall quality at a glance

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}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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 $\leq 5\%$. 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	20% 94% . .
2	B	140	41% 84% . 12%
3	C	1024	26% 93% 5% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22807 atoms, of which 11190 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	208	Total	C	H	N	O	S	0	5	0
			3391	1093	1697	291	304	6			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	123	Total	C	H	N	O	S	0	3	0
			2060	652	1031	181	191	5			

- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	1011	Total	C	H	N	O	S	0	42	0
			16744	5337	8434	1368	1560	45			

There are 46 discrepancies between the modelled and reference sequences:

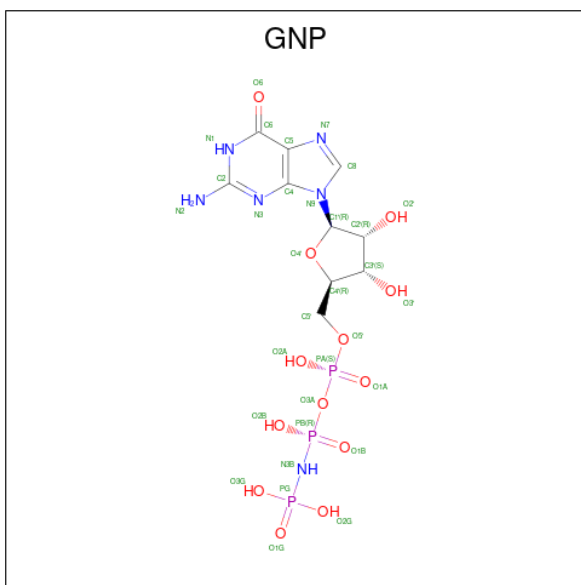
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P30822
C	-1	GLY	-	expression tag	UNP P30822
C	0	SER	-	expression tag	UNP P30822
C	?	-	VAL	deletion	UNP P30822
C	?	-	GLN	deletion	UNP P30822
C	?	-	ARG	deletion	UNP P30822
C	?	-	LEU	deletion	UNP P30822
C	?	-	PRO	deletion	UNP 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	582	LYS	GLU	engineered mutation	UNP P30822
C	1022	CYS	TYR	conflict	UNP P30822

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

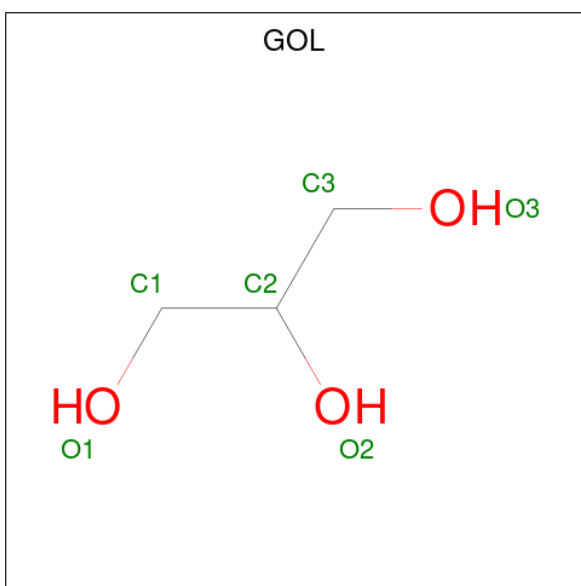


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	H	N	O	P	0	0
			44	10	12	6	13	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

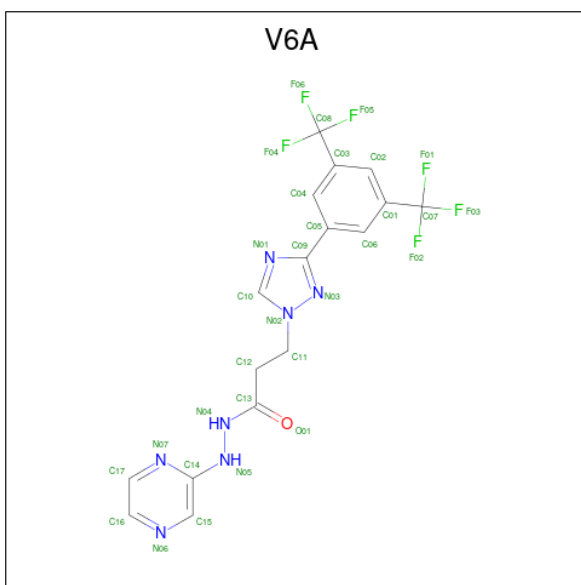
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total 14	C 3	H 8	O 3	14	0
6	C	1	Total 14	C 3	H 8	O 3	0	0

- Molecule 7 is selinexor, bound form (CCD ID: V6A) (formula: $\text{C}_{17}\text{H}_{13}\text{F}_6\text{N}_7\text{O}$) (labeled as "Ligand of Interest" by depositor).



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

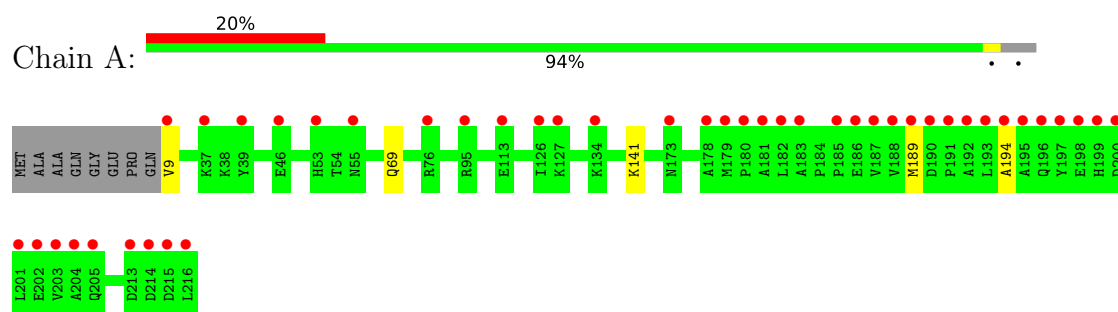
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	91	Total O 91 91	0	0
8	B	27	Total O 27 27	0	0
8	C	390	Total O 390 390	0	0

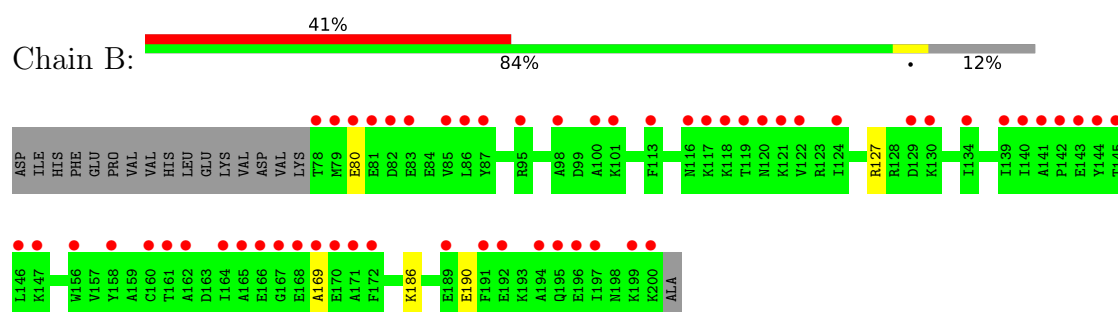
3 Residue-property plots

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.

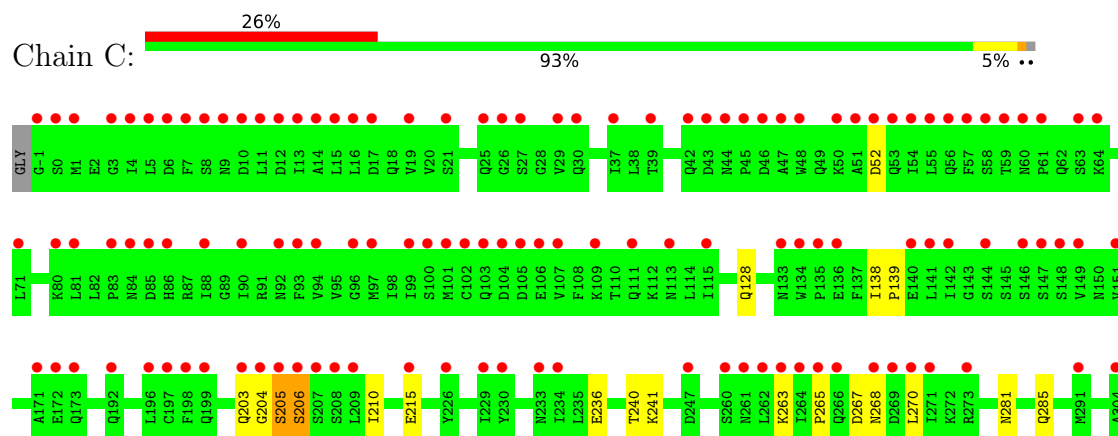
- Molecule 1: GTP-binding nuclear protein Ran

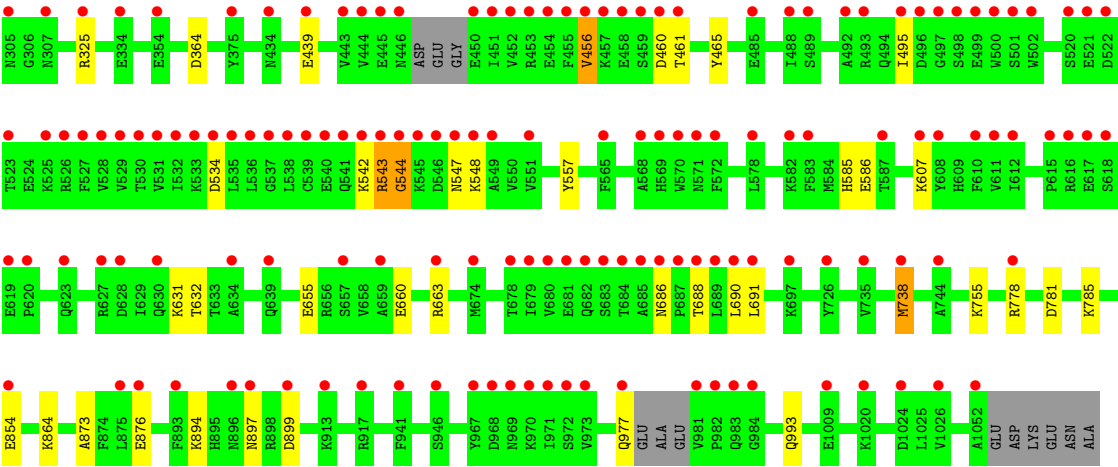


- Molecule 2: Ran-specific GTPase-activating protein 1



- Molecule 3: Exportin-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.04Å 106.04Å 305.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.20 – 1.94 38.20 – 1.94	Depositor EDS
% Data completeness (in resolution range)	67.7 (38.20-1.94) 92.5 (38.20-1.94)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.202 , 0.240 0.212 , 0.241	Depositor DCC
R_{free} test set	2000 reflections (1.67%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22807	wwPDB-VP
Average B, all atoms (Å ²)	52.0	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, GNP, MG, 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	0.13	0/1754	0.32	0/2379
2	B	0.12	0/1059	0.29	0/1413
3	C	0.15	0/8608	0.31	0/11658
All	All	0.14	0/11421	0.31	0/15450

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	203	GLN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1694	1697	1676	3	0
2	B	1029	1031	1021	2	0
3	C	8310	8434	8265	38	1
4	A	32	12	12	0	0
5	A	1	0	0	0	0
6	C	12	16	16	3	0
7	C	31	0	0	1	0
8	A	91	0	0	2	0
8	B	27	0	0	0	0
8	C	390	0	0	15	0
All	All	11617	11190	10990	44	1

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 2.

All (44) 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)
7:C:1103:V6A:N05	8:C:1201:HOH:O	1.69	1.25
3:C:977:GLN:O	8:C:1202:HOH:O	1.91	0.88
3:C:236:GLU:OE1	8:C:1203:HOH:O	1.94	0.85
3:C:778:ARG:NH2	8:C:1205:HOH:O	2.11	0.83
3:C:864:LYS:NZ	8:C:1206:HOH:O	2.19	0.75
3:C:585:HIS:NE2	6:C:1102:GOL:O3	2.22	0.72
3:C:993:GLN:NE2	8:C:1204:HOH:O	2.10	0.65
3:C:897:ASN:ND2	8:C:1214:HOH:O	2.32	0.62
1:A:141:LYS:NZ	8:A:401:HOH:O	2.32	0.60
3:C:543:ARG:HA	3:C:548:LYS:HE2	1.86	0.58
1:A:9:VAL:N	8:A:402:HOH:O	2.37	0.56
3:C:607:LYS:NZ	8:C:1210:HOH:O	2.27	0.56
3:C:543:ARG:O	3:C:544:GLY:C	2.49	0.56
2:B:80:GLU:OE1	2:B:127:ARG:NH2	2.35	0.55
3:C:204[B]:GLY:HA2	3:C:210:ILE:HD11	1.89	0.54
3:C:461:THR:HG22	8:C:1213:HOH:O	2.07	0.54
3:C:781:ASP:O	3:C:785:LYS:HE2	2.09	0.53
3:C:691:LEU:O	3:C:755:LYS:NZ	2.38	0.53
3:C:268:ASN:OD1	3:C:270:LEU:N	2.41	0.52
3:C:460:ASP:OD1	3:C:460:ASP:N	2.43	0.52
2:B:186:LYS:NZ	2:B:190:GLU:OE1	2.43	0.51
3:C:205[A]:SER:OG	3:C:206[A]:SER:N	2.44	0.51
3:C:690:LEU:HD13	3:C:738:MET:HE1	1.95	0.49
3:C:465:TYR:OH	3:C:557:TYR:OH	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:899:ASP:HB3	8:C:1527:HOH:O	2.12	0.48
3:C:655:GLU:HG2	3:C:660:GLU:HG3	1.96	0.47
3:C:128:GLN:NE2	8:C:1217:HOH:O	2.35	0.46
3:C:632:THR:N	6:C:1102:GOL:O2	2.50	0.45
3:C:688:THR:O	3:C:691:LEU:HG	2.17	0.45
3:C:267:ASP:N	3:C:267:ASP:OD1	2.51	0.44
3:C:456:VAL:HA	8:C:1390:HOH:O	2.16	0.44
1:A:189:MET:HE1	1:A:194:ALA:HA	1.99	0.43
3:C:138:ILE:HB	3:C:139:PRO:HD3	2.00	0.43
3:C:364[B]:ASP:OD1	8:C:1207:HOH:O	2.22	0.42
3:C:268:ASN:OD1	3:C:268:ASN:C	2.63	0.41
3:C:873:ALA:O	3:C:876:GLU:HG3	2.19	0.41
3:C:240:THR:OG1	3:C:241:LYS:N	2.53	0.41
3:C:542:LYS:HB3	3:C:547:ASN:CG	2.45	0.41
3:C:495:ILE:HD11	3:C:534:ASP:HB3	2.03	0.40
3:C:894:LYS:NZ	8:C:1238:HOH:O	2.53	0.40
3:C:263:LYS:HD2	3:C:325:ARG:HD2	2.03	0.40
3:C:281:ASN:O	3:C:285:GLN:HG2	2.22	0.40
3:C:632:THR:HA	6:C:1102:GOL:O2	2.21	0.40
3:C:439:GLU:HG3	8:C:1331:HOH:O	2.21	0.40

All (1) 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:660:GLU:OE2	3:C:663:ARG:NH2[7_555]	2.19	0.01

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	211/216 (98%)	206 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	124/140 (89%)	116 (94%)	7 (6%)	1 (1%)	16	7
3	C	1047/1024 (102%)	1016 (97%)	24 (2%)	7 (1%)	18	9
All	All	1382/1380 (100%)	1338 (97%)	36 (3%)	8 (1%)	24	11

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	205[A]	SER
3	C	205[B]	SER
3	C	206[A]	SER
3	C	206[B]	SER
2	B	169	ALA
3	C	544	GLY
3	C	265	PRO
3	C	686	ASN

5.3.2 Protein sidechains ⓘ

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	185/185 (100%)	183 (99%)	2 (1%)	65	60
2	B	108/121 (89%)	108 (100%)	0	100	100
3	C	960/933 (103%)	951 (99%)	9 (1%)	70	67
All	All	1253/1239 (101%)	1242 (99%)	11 (1%)	76	67

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69[A]	GLN
1	A	69[B]	GLN
3	C	52	ASP
3	C	215[A]	GLU
3	C	215[B]	GLU
3	C	456	VAL

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Mol	Chain	Res	Type
3	C	543	ARG
3	C	586	GLU
3	C	631	LYS
3	C	738	MET
3	C	854	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	154	ASN
3	C	31	GLN
3	C	49	GLN
3	C	313	GLN
3	C	418	HIS
3	C	477	HIS
3	C	642	HIS
3	C	742	GLN
3	C	925	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
6	GOL	C	1102	-	5,5,5	0.57	0	5,5,5	0.75	0
7	V6A	C	1103	3	33,33,33	2.37	11 (33%)	46,48,48	2.61	13 (28%)
6	GOL	C	1101	-	5,5,5	0.43	0	5,5,5	0.46	0
4	GNP	A	301	5	34,34,34	3.70	17 (50%)	47,54,54	1.66	9 (19%)

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
6	GOL	C	1102	-	-	2/4/4/4	-
7	V6A	C	1103	3	-	3/26/26/26	0/3/3/3
6	GOL	C	1101	-	-	4/4/4/4	-
4	GNP	A	301	5	-	7/18/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	GNP	C2-N2	8.71	1.54	1.34
4	A	301	GNP	O4'-C1'	8.51	1.61	1.42
7	C	1103	V6A	C13-N04	8.33	1.45	1.34
4	A	301	GNP	PA-O3A	7.41	1.67	1.59
4	A	301	GNP	PB-O3A	7.08	1.67	1.59
4	A	301	GNP	C2'-C1'	-7.05	1.31	1.53
4	A	301	GNP	PB-O1B	5.81	1.55	1.46
4	A	301	GNP	O4'-C4'	-5.39	1.33	1.45
7	C	1103	V6A	C09-N03	-4.41	1.27	1.33
4	A	301	GNP	PG-O1G	4.09	1.52	1.46
4	A	301	GNP	O2'-C2'	3.95	1.52	1.43
7	C	1103	V6A	C09-N01	-3.65	1.30	1.36
7	C	1103	V6A	C14-N05	3.59	1.47	1.38
7	C	1103	V6A	N02-N03	-3.49	1.31	1.35
4	A	301	GNP	C6-N1	-3.20	1.32	1.38
7	C	1103	V6A	C10-N02	-3.13	1.27	1.33
4	A	301	GNP	O3'-C3'	-2.91	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	GNP	PB-N3B	2.65	1.70	1.63
7	C	1103	V6A	O01-C13	-2.65	1.18	1.23
4	A	301	GNP	O6-C6	-2.55	1.18	1.23
4	A	301	GNP	PA-O5'	2.47	1.69	1.59
7	C	1103	V6A	C02-C03	-2.43	1.35	1.39
7	C	1103	V6A	C02-C01	-2.37	1.35	1.39
4	A	301	GNP	PG-N3B	2.35	1.69	1.63
7	C	1103	V6A	C06-C01	-2.28	1.36	1.39
4	A	301	GNP	PB-O2B	-2.06	1.51	1.56
4	A	301	GNP	C4-N9	-2.04	1.32	1.38
7	C	1103	V6A	C04-C05	-2.03	1.36	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1103	V6A	C11-N02-N03	7.86	127.51	119.56
7	C	1103	V6A	N02-C10-N01	-7.07	107.05	110.82
7	C	1103	V6A	C10-N01-C09	6.91	108.65	102.71
4	A	301	GNP	C5-C4-N3	-5.22	120.09	128.39
7	C	1103	V6A	C15-C14-N07	-4.98	119.04	121.26
7	C	1103	V6A	C12-C13-N04	4.72	120.25	114.70
4	A	301	GNP	C2-N3-C4	4.37	119.83	112.30
7	C	1103	V6A	N05-C14-N07	3.79	120.67	114.83
7	C	1103	V6A	N03-C09-N01	-3.74	107.01	114.62
7	C	1103	V6A	C05-C09-N03	3.30	128.94	123.19
7	C	1103	V6A	C10-N02-N03	-3.16	108.40	109.97
4	A	301	GNP	C2-N1-C6	-2.94	119.77	125.11
4	A	301	GNP	N9-C8-N7	-2.92	107.98	113.40
4	A	301	GNP	N9-C4-N3	2.72	131.39	125.95
4	A	301	GNP	C5-C6-N1	2.60	119.88	113.25
4	A	301	GNP	O6-C6-C5	-2.50	119.93	126.53
7	C	1103	V6A	C17-C16-N06	-2.49	118.87	121.96
7	C	1103	V6A	O01-C13-N04	-2.43	119.95	122.84
7	C	1103	V6A	F06-C08-F05	2.30	114.07	105.77
7	C	1103	V6A	F06-C08-C03	-2.18	108.22	112.90
4	A	301	GNP	C8-N7-C5	2.17	108.13	104.26
4	A	301	GNP	C1'-N9-C4	-2.11	120.25	126.49

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GNP	PG-N3B-PB-O1B
4	A	301	GNP	PG-N3B-PB-O3A
6	C	1101	GOL	C1-C2-C3-O3
7	C	1103	V6A	N02-C11-C12-C13
7	C	1103	V6A	C12-C13-N04-N05
6	C	1101	GOL	O1-C1-C2-C3
6	C	1102	GOL	O1-C1-C2-C3
6	C	1101	GOL	O1-C1-C2-O2
7	C	1103	V6A	O01-C13-N04-N05
4	A	301	GNP	O4'-C4'-C5'-O5'
4	A	301	GNP	C3'-C4'-C5'-O5'
6	C	1101	GOL	O2-C2-C3-O3
4	A	301	GNP	C5'-O5'-PA-O3A
4	A	301	GNP	C5'-O5'-PA-O1A
4	A	301	GNP	C5'-O5'-PA-O2A
6	C	1102	GOL	O1-C1-C2-O2

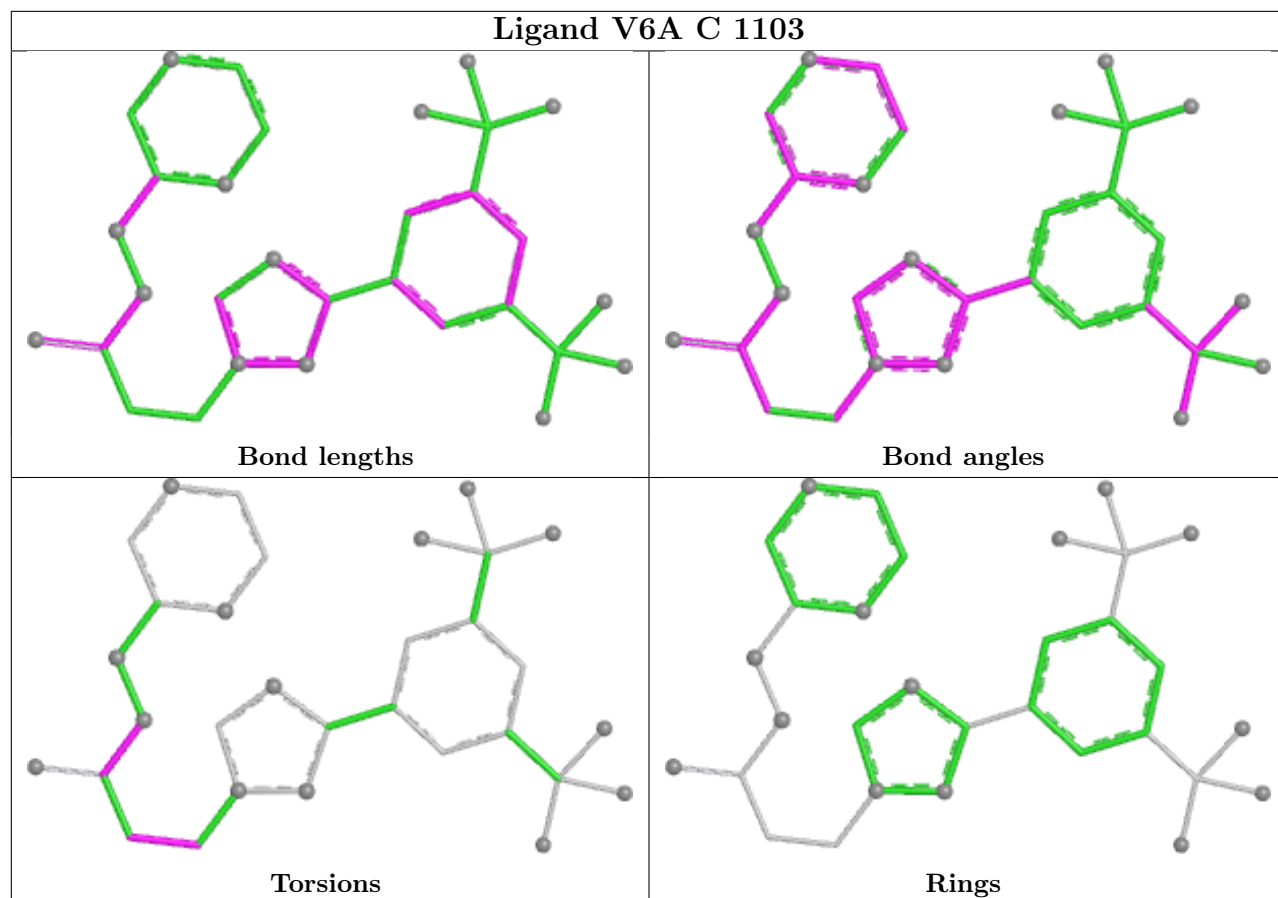
There are no ring outliers.

2 monomers are involved in 4 short contacts:

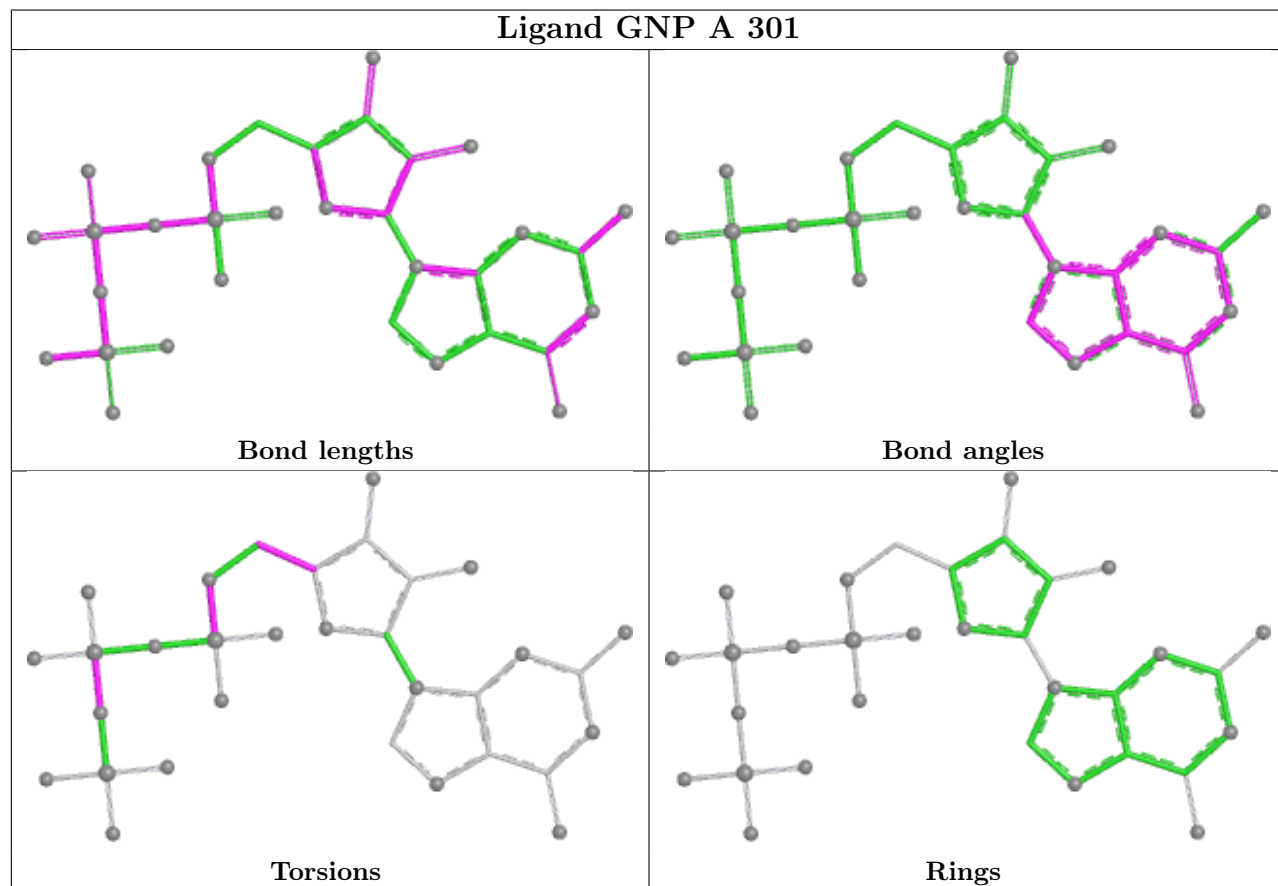
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1102	GOL	3	0
7	C	1103	V6A	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand V6A C 1103



Ligand GNP A 301



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	208/216 (96%)	1.32	44 (21%) 2 2	21, 41, 115, 173	3 (1%)
2	B	123/140 (87%)	2.04	57 (46%) 0 0	21, 63, 101, 141	2 (1%)
3	C	1011/1024 (98%)	1.39	270 (26%) 1 1	16, 45, 87, 143	25 (2%)
All	All	1342/1380 (97%)	1.44	371 (27%) 1 1	16, 47, 91, 173	30 (2%)

All (371) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	205[A]	SER	14.8
3	C	456	VAL	13.9
3	C	206[A]	SER	12.0
3	C	455	PHE	10.0
3	C	457	LYS	9.6
3	C	446	ASN	9.3
3	C	459	SER	8.7
3	C	264	ILE	8.7
3	C	93	PHE	8.5
1	A	197	TYR	8.2
3	C	460	ASP	7.9
1	A	188	VAL	7.6
3	C	204[A]	GLY	7.4
3	C	458	GLU	7.0
1	A	191	PRO	6.9
3	C	-1	GLY	6.9
3	C	57	PHE	6.8
1	A	193	LEU	6.7
3	C	691	LEU	6.7
1	A	192	ALA	6.6
1	A	187	VAL	6.6
3	C	497	GLY	6.5
1	A	194	ALA	6.4

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Mol	Chain	Res	Type	RSRZ
3	C	967	TYR	6.4
3	C	262	LEU	6.4
3	C	689	LEU	6.3
3	C	135	PRO	6.3
3	C	81	LEU	6.2
3	C	981	VAL	6.2
3	C	0	SER	6.1
2	B	78	THR	6.1
3	C	134	TRP	5.9
3	C	687	PRO	5.9
3	C	261	ASN	5.8
3	C	454	GLU	5.8
2	B	129	ASP	5.8
2	B	79	MET	5.8
3	C	270	LEU	5.8
1	A	180	PRO	5.7
3	C	502	TRP	5.7
3	C	544	GLY	5.6
1	A	179	MET	5.6
3	C	9	ASN	5.5
1	A	216	LEU	5.4
3	C	291[A]	MET	5.3
1	A	195	ALA	5.3
3	C	523	THR	5.3
1	A	9	VAL	5.3
1	A	189	MET	5.2
3	C	690	LEU	5.1
3	C	538	LEU	5.0
3	C	8	SER	5.0
3	C	679	ILE	5.0
3	C	7	PHE	4.9
3	C	451	ILE	4.9
3	C	207[A]	SER	4.9
1	A	199	HIS	4.9
3	C	682	GLN	4.9
2	B	199	LYS	4.7
2	B	200	LYS	4.7
3	C	539	CYS	4.7
3	C	147[A]	SER	4.7
3	C	685	ALA	4.6
3	C	611	VAL	4.6
1	A	198	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
3	C	684	THR	4.6
3	C	11	LEU	4.6
3	C	500	TRP	4.5
3	C	203	GLN	4.5
3	C	146	SER	4.5
3	C	532	ILE	4.4
3	C	263	LYS	4.4
3	C	85	ASP	4.3
3	C	496	ASP	4.3
3	C	627	ARG	4.2
3	C	726	TYR	4.2
1	A	190	ASP	4.2
3	C	265	PRO	4.2
3	C	982	PRO	4.2
3	C	495	ILE	4.2
3	C	520	SER	4.2
3	C	663	ARG	4.2
3	C	1052	ALA	4.2
3	C	148[A]	SER	4.1
3	C	498	SER	4.1
3	C	453	ARG	4.0
2	B	82	ASP	4.0
3	C	149	VAL	4.0
3	C	445	GLU	4.0
3	C	51	ALA	4.0
1	A	213	ASP	3.9
3	C	226	TYR	3.9
3	C	266	GLN	3.9
3	C	59	THR	3.9
2	B	197	ILE	3.9
3	C	107	VAL	3.9
3	C	492	ALA	3.8
3	C	534	ASP	3.8
3	C	55	LEU	3.8
3	C	52	ASP	3.8
1	A	183	ALA	3.8
3	C	683	SER	3.8
3	C	526	ARG	3.8
1	A	186	GLU	3.7
2	B	145	THR	3.7
3	C	172	GLU	3.7
3	C	681	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
3	C	688	THR	3.7
3	C	3	GLY	3.7
3	C	103[A]	GLN	3.7
3	C	39[A]	THR	3.7
3	C	977	GLN	3.7
3	C	230	TYR	3.6
3	C	686	ASN	3.6
3	C	452	VAL	3.6
3	C	674	MET	3.6
3	C	88	ILE	3.6
1	A	95	ARG	3.6
3	C	983	GLN	3.6
3	C	10	ASP	3.6
3	C	53	GLN	3.5
3	C	450	GLU	3.5
2	B	167	GLY	3.5
3	C	876	GLU	3.5
3	C	102[A]	CYS	3.5
3	C	899	ASP	3.5
3	C	533	LYS	3.5
3	C	680	VAL	3.5
3	C	354	GLU	3.5
1	A	182	LEU	3.5
3	C	984	GLY	3.5
3	C	12	ASP	3.5
2	B	101	LYS	3.5
2	B	169	ALA	3.5
3	C	537	GLY	3.5
3	C	86	HIS	3.4
3	C	545	LYS	3.4
1	A	76	ARG	3.4
3	C	271	ILE	3.4
3	C	612	ILE	3.4
2	B	118	LYS	3.4
3	C	109	LYS	3.4
3	C	6	ASP	3.4
3	C	56	GLN	3.4
1	A	196	GLN	3.4
3	C	444	VAL	3.4
1	A	178	ALA	3.4
3	C	536	LEU	3.4
2	B	168	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
3	C	247	ASP	3.3
3	C	229	ILE	3.3
2	B	171	ALA	3.3
3	C	522	ASP	3.3
3	C	13	ILE	3.3
3	C	29	VAL	3.3
2	B	117	LYS	3.3
3	C	529	VAL	3.3
2	B	161	THR	3.3
3	C	893	PHE	3.3
3	C	946	SER	3.2
1	A	204	ALA	3.2
2	B	98	ALA	3.2
2	B	142	PRO	3.2
2	B	80	GLU	3.2
3	C	540	GLU	3.2
1	A	127[A]	LYS	3.2
3	C	618	SER	3.2
1	A	215	ASP	3.2
2	B	143	GLU	3.2
3	C	461	THR	3.2
3	C	83	PRO	3.2
3	C	443	VAL	3.2
3	C	973	VAL	3.2
3	C	50	LYS	3.2
3	C	84	ASN	3.1
3	C	151	VAL	3.1
3	C	616	ARG	3.1
1	A	185	PRO	3.1
3	C	46	ASP	3.1
3	C	628	ASP	3.1
3	C	615	PRO	3.1
2	B	81	GLU	3.1
3	C	260	SER	3.1
2	B	196	GLU	3.1
3	C	105	ASP	3.0
3	C	582	LYS	3.0
3	C	100	SER	3.0
2	B	119	THR	3.0
1	A	214	ASP	3.0
3	C	104	ASP	3.0
3	C	192[A]	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	5	LEU	3.0
3	C	141	LEU	3.0
2	B	189	GLU	3.0
3	C	14	ALA	3.0
3	C	434	ASN	3.0
3	C	489	SER	2.9
3	C	1	MET	2.9
1	A	201	LEU	2.9
3	C	43	ASP	2.9
1	A	173	ASN	2.9
3	C	54	ILE	2.9
3	C	142	ILE	2.9
3	C	44	ASN	2.9
2	B	100	ALA	2.9
3	C	208[A]	SER	2.9
3	C	15	LEU	2.9
3	C	305	ASN	2.8
3	C	587	THR	2.8
3	C	375	TYR	2.8
3	C	548	LYS	2.8
3	C	917	ARG	2.8
3	C	570	TRP	2.8
3	C	607	LYS	2.8
3	C	619	GLU	2.8
2	B	194	ALA	2.8
3	C	96	GLY	2.8
3	C	196	LEU	2.8
3	C	1020	LYS	2.8
2	B	85	VAL	2.8
3	C	623	GLN	2.8
1	A	202	GLU	2.8
3	C	99	ILE	2.8
3	C	488	ILE	2.8
3	C	48	TRP	2.8
3	C	269	ASP	2.8
3	C	897	ASN	2.7
3	C	525	LYS	2.7
3	C	778	ARG	2.7
3	C	233	ASN	2.7
3	C	80	LYS	2.7
3	C	530	THR	2.7
3	C	678	THR	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	541	GLN	2.7
2	B	86	LEU	2.7
3	C	136	GLU	2.7
2	B	130	LYS	2.7
1	A	39	TYR	2.6
3	C	42	GLN	2.6
3	C	972	SER	2.6
3	C	92	ASN	2.6
3	C	630	GLN	2.6
3	C	617	GLU	2.6
3	C	133	ASN	2.6
3	C	198	PHE	2.6
3	C	969	ASN	2.6
3	C	521	GLU	2.6
2	B	162	ALA	2.6
3	C	970	LYS	2.6
3	C	571	ASN	2.6
3	C	896	ASN	2.6
2	B	191	PHE	2.6
3	C	111	GLN	2.6
2	B	134	ILE	2.6
3	C	37	ILE	2.6
2	B	122	VAL	2.6
2	B	116	ASN	2.6
3	C	106	GLU	2.5
3	C	854	GLU	2.5
3	C	115	ILE	2.5
3	C	549	ALA	2.5
3	C	543	ARG	2.5
2	B	158	TYR	2.5
2	B	121	LYS	2.5
1	A	53	HIS	2.5
2	B	165	ALA	2.5
3	C	47	ALA	2.5
3	C	16	LEU	2.5
3	C	547	ASN	2.5
2	B	139	ILE	2.5
3	C	27	SER	2.5
3	C	499	GLU	2.5
1	A	181	ALA	2.5
3	C	101	MET	2.5
3	C	528	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	160	CYS	2.4
1	A	55	ASN	2.4
3	C	501	SER	2.4
3	C	4	ILE	2.4
2	B	141	ALA	2.4
3	C	268	ASN	2.4
2	B	166	GLU	2.4
3	C	215[A]	GLU	2.4
3	C	639	GLN	2.4
3	C	1009	GLU	2.4
1	A	126[A]	ILE	2.4
3	C	1024	ASP	2.4
3	C	30	GLN	2.4
3	C	60	ASN	2.4
3	C	738	MET	2.4
2	B	124	ILE	2.4
2	B	140	ILE	2.4
3	C	140	GLU	2.4
3	C	334	GLU	2.4
3	C	97	MET	2.4
3	C	58	SER	2.4
1	A	200	ASP	2.3
3	C	535	LEU	2.3
3	C	583	PHE	2.3
1	A	113	GLU	2.3
3	C	659	ALA	2.3
3	C	26	GLY	2.3
3	C	19	VAL	2.3
3	C	531	VAL	2.3
3	C	197[A]	CYS	2.3
3	C	209	LEU	2.3
2	B	87	TYR	2.3
3	C	744	ALA	2.3
3	C	697	LYS	2.3
1	A	203	VAL	2.3
3	C	546	ASP	2.3
2	B	144	TYR	2.3
2	B	172	PHE	2.3
3	C	941	PHE	2.3
2	B	170	GLU	2.3
3	C	173	GLN	2.3
3	C	199	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	875	LEU	2.3
2	B	164	ILE	2.2
3	C	113[A]	ASN	2.2
3	C	542	LYS	2.2
3	C	71	LEU	2.2
3	C	527	PHE	2.2
3	C	971	ILE	2.2
1	A	37	LYS	2.2
3	C	493	ARG	2.2
3	C	94	VAL	2.2
3	C	25	GLN	2.2
3	C	45	PRO	2.2
3	C	634	ALA	2.2
3	C	572	PHE	2.2
3	C	90	ILE	2.2
2	B	120	ASN	2.2
3	C	569	HIS	2.2
3	C	913	LYS	2.2
3	C	273	ARG	2.2
3	C	735[A]	VAL	2.2
3	C	21	SER	2.2
3	C	144	SER	2.2
3	C	578	LEU	2.2
3	C	61	PRO	2.2
3	C	620	PRO	2.2
2	B	113	PHE	2.1
3	C	485	GLU	2.1
3	C	610	PHE	2.1
2	B	156	TRP	2.1
2	B	95[A]	ARG	2.1
3	C	64	LYS	2.1
3	C	304	ALA	2.1
3	C	551	VAL	2.1
2	B	147	LYS	2.1
2	B	83	GLU	2.1
2	B	195	GLN	2.1
3	C	171	ALA	2.1
3	C	234	ILE	2.1
3	C	439	GLU	2.1
3	C	568	ALA	2.1
3	C	968	ASP	2.1
1	A	46	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	134	LYS	2.0
2	B	192	GLU	2.0
3	C	63	SER	2.0
3	C	608	TYR	2.0
1	A	205	GLN	2.0
3	C	1026	VAL	2.0
2	B	146	LEU	2.0
3	C	17	ASP	2.0
3	C	657	SER	2.0
3	C	565	PHE	2.0
3	C	307	ASN	2.0
3	C	325	ARG	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

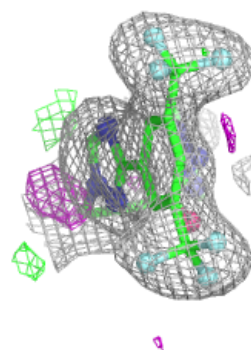
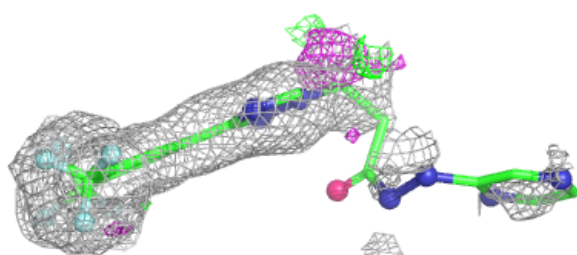
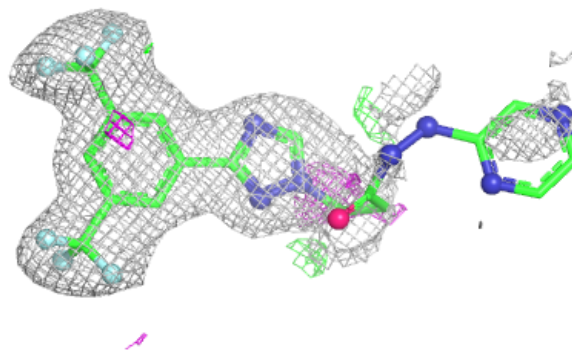
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	C	1102	6/6	0.60	0.21	48,57,66,66	0
7	V6A	C	1103	31/31	0.85	0.19	46,57,112,113	0
6	GOL	C	1101	6/6	-	-	14,17,18,19	14
4	GNP	A	301	32/32	0.87	0.13	1,2,7,8	0
5	MG	A	302	1/1	0.98	0.25	9,9,9,9	0

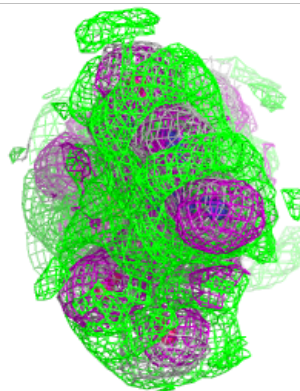
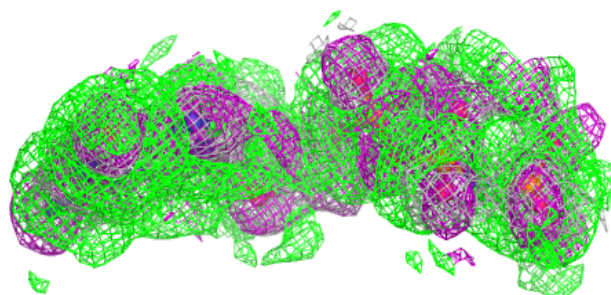
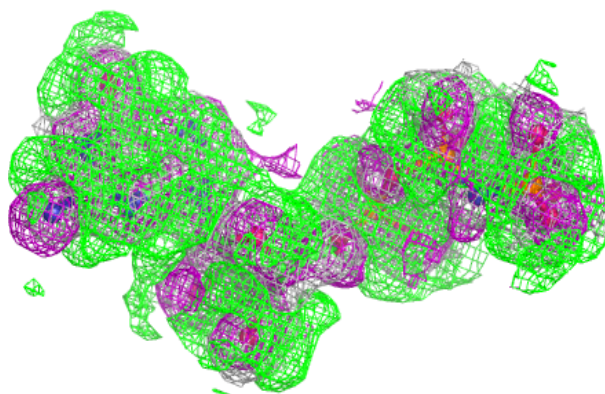
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around V6A C 1103:

$2mF_o-DF_c$ (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.