Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2026 – 06:17 PM EST

PDB ID	:	36KQ / pdb_000036kq
Title	:	Tri-complex of Compound 23, KRas G12D, and CypA
Authors	:	Tomlinson, A.C.A.; Yano, J.K.
Deposited on	:	2026-06-16
Resolution	:	1.25 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:

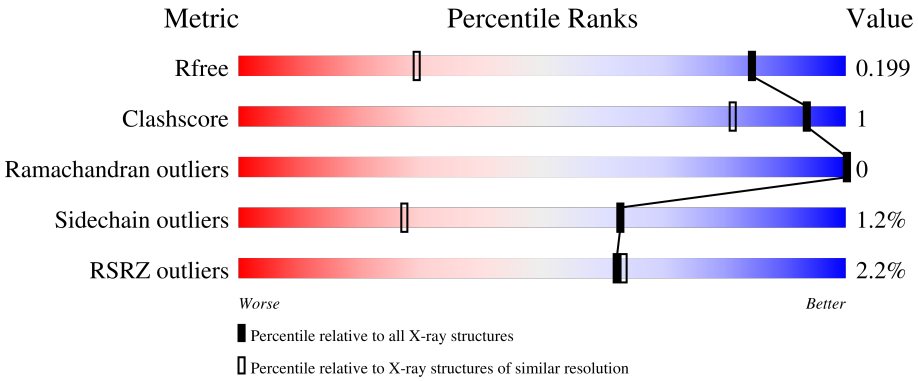
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.25 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	1693 (1.28-1.24)
Clashscore	190562	1730 (1.28-1.24)
Ramachandran outliers	187476	1695 (1.28-1.24)
Sidechain outliers	187428	1694 (1.28-1.24)
RSRZ outliers	180081	1693 (1.28-1.24)

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	170	6% 96%
1	B	170	2% 92% 8%
2	C	166	% 95%
2	D	166	97%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6351 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 Isoform 2B of GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	0	0
			1359	850	233	269	7			
1	B	170	Total	C	N	O	S	0	0	0
			1360	850	233	270	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P01116
A	12	ASP	GLY	engineered mutation	UNP P01116
B	0	SER	-	expression tag	UNP P01116
B	12	ASP	GLY	engineered mutation	UNP P01116

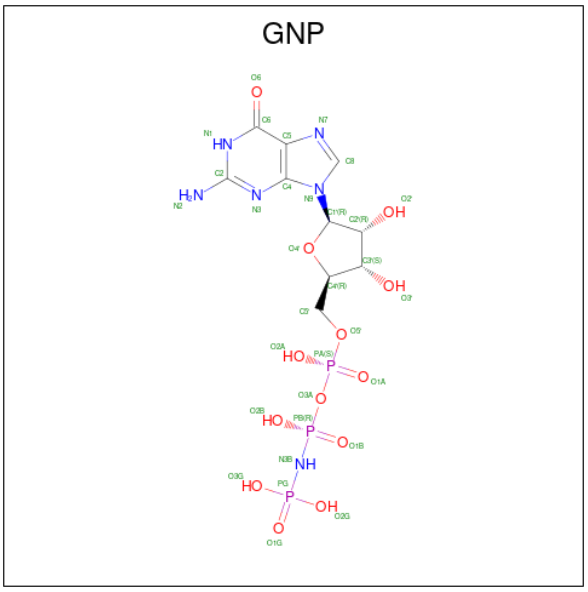
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	163	Total	C	N	O	S	0	1	0
			1259	798	220	233	8			
2	D	165	Total	C	N	O	S	0	1	0
			1268	805	219	235	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP P62937
D	0	SER	-	expression tag	UNP P62937

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

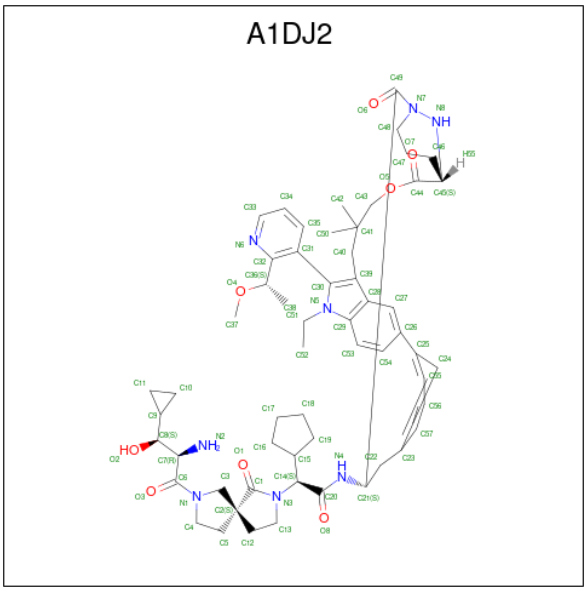


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is (2S)-2-{(5S)-7-[(2R,3S)-2-amino-3-cyclopropyl-3-hydroxypropanoyl]-1-oxo-2,7-diazaspiro[4.4]nonan-2-yl}-2-cyclopentyl-N-[(1P,8S,10R,14S,21M)-22-ethyl-21-{2-[(1S)-1-methoxyethyl]pyridin-3-yl}-18,18-dimethyl-9,15-dioxo-16-oxa-10,22,28-triazapentacyclo[18.5.2.1 2,6 .1 10,14 .0 23,27]nonacosa-1(25),2(29),3,5,20,23,26-heptaen-8-yl]acetamide (non-preferred name) (CCD ID: A1DJ2) (formula: $C_{57}H_{74}N_8O_8$) (labeled as "Ligand of Interest" by depositor).

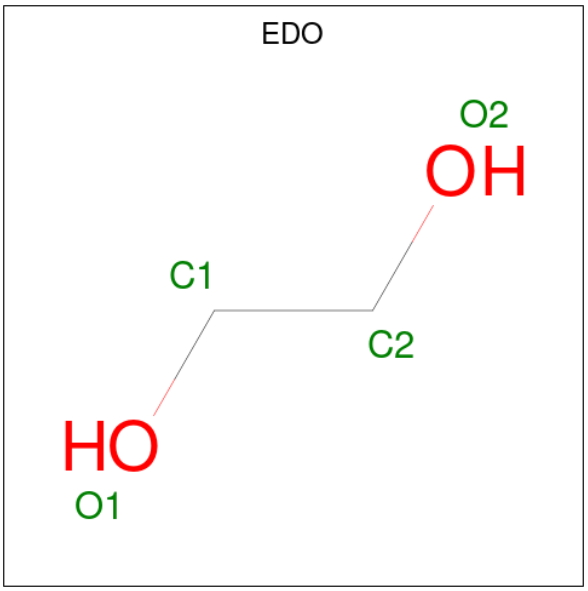


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	73	57	8	8	0	0
5	B	1	Total	C	N	O	0	0
			73	57	8	8		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
6	A	1	1	1	0	0
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 4 2 2	0	0

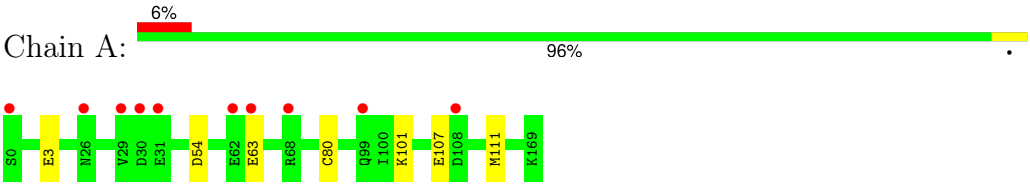
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	215	Total O 215 215	0	0
8	B	235	Total O 235 235	0	0
8	C	217	Total O 217 217	0	0
8	D	220	Total O 220 220	0	0

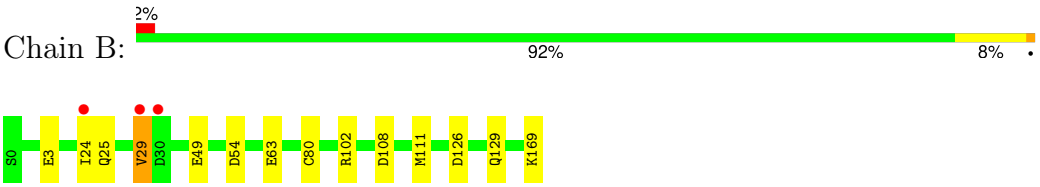
3 Residue-property plots (i)

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.

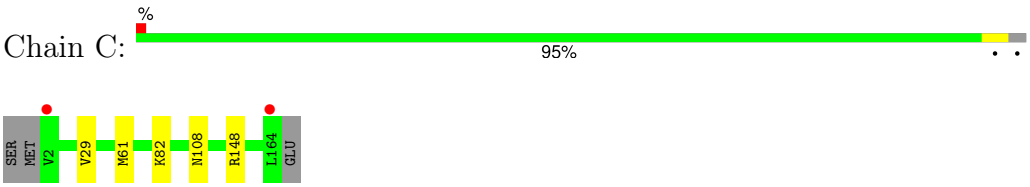
• Molecule 1: Isoform 2B of GTPase KRas



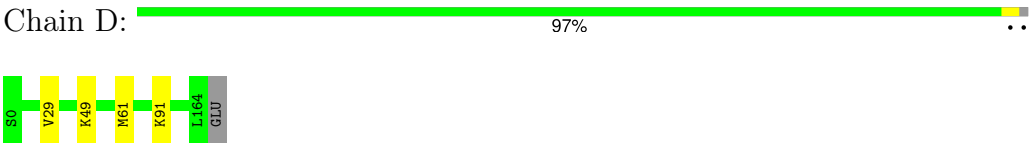
• Molecule 1: Isoform 2B of GTPase KRas



• Molecule 2: Peptidyl-prolyl cis-trans isomerase A



• Molecule 2: Peptidyl-prolyl cis-trans isomerase A



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.15Å 101.79Å 65.96Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	31.05 – 1.25 31.05 – 1.25	Depositor EDS
% Data completeness (in resolution range)	98.3 (31.05-1.25) 98.3 (31.05-1.25)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 1.25Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.179 , 0.199 0.178 , 0.199	Depositor DCC
R_{free} test set	8558 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	14.4	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 32.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.067 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6351	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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: EDO, A1DJ2, GNP, CL, MG

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	0/1380	0.48	0/1860
1	B	0.24	0/1381	0.49	0/1860
2	C	0.22	0/1287	0.49	0/1725
2	D	0.22	0/1299	0.51	0/1740
All	All	0.23	0/5347	0.49	0/7185

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	1359	0	1338	3	0
1	B	1360	0	1338	8	0
2	C	1259	0	1231	2	0
2	D	1268	0	1249	2	0
3	A	32	0	13	0	0
3	B	32	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	73	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	73	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	B	4	0	6	0	0
8	A	215	0	0	0	3
8	B	235	0	0	3	4
8	C	217	0	0	1	4
8	D	220	0	0	2	1
All	All	6351	0	5188	15	6

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 1.

All (15) 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)
2:C:148[B]:ARG:NH1	8:C:201:HOH:O	2.15	0.79
1:B:126:ASP:HB2	1:B:129:GLN:HG3	1.79	0.64
1:A:101:LYS:HE3	1:A:107:GLU:HA	1.80	0.64
1:B:80:CYS:SG	1:B:111:MET:HE3	2.47	0.54
1:A:80:CYS:SG	1:A:111:MET:HE3	2.49	0.53
1:B:3:GLU:OE2	1:B:54:ASP:OD2	2.26	0.53
1:B:49:GLU:OE1	8:B:301:HOH:O	2.18	0.53
2:D:49:LYS:NZ	8:D:202:HOH:O	2.34	0.53
1:B:108:ASP:OD2	1:B:169:LYS:NZ	2.45	0.49
1:B:29:VAL:O	8:B:302:HOH:O	2.20	0.49
2:D:91:LYS:HD2	8:D:375:HOH:O	2.14	0.47
1:A:3:GLU:OE2	1:A:54:ASP:OD2	2.33	0.47
1:B:24:ILE:HG22	1:B:25:GLN:HG3	1.97	0.47
1:B:102:ARG:NH1	8:B:304:HOH:O	2.25	0.47
2:C:82:LYS:HA	2:C:108:ASN:O	2.20	0.41

All (6) 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)
8:A:418:HOH:O	8:C:201:HOH:O[2_447]	2.01	0.19
8:A:438:HOH:O	8:B:472:HOH:O[2_447]	2.02	0.18
8:B:401:HOH:O	8:C:342:HOH:O[2_446]	2.04	0.16
8:B:472:HOH:O	8:C:358:HOH:O[1_655]	2.04	0.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:411:HOH:O	8:D:306:HOH:O[1_455]	2.14	0.06
8:B:461:HOH:O	8:C:380:HOH:O[2_446]	2.15	0.05

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	168/170 (99%)	164 (98%)	4 (2%)	0	100	100
1	B	168/170 (99%)	164 (98%)	4 (2%)	0	100	100
2	C	162/166 (98%)	156 (96%)	6 (4%)	0	100	100
2	D	164/166 (99%)	157 (96%)	7 (4%)	0	100	100
All	All	662/672 (98%)	641 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	151/151 (100%)	150 (99%)	1 (1%)	76	47
1	B	151/151 (100%)	149 (99%)	2 (1%)	61	24
2	C	132/134 (98%)	130 (98%)	2 (2%)	57	20
2	D	134/134 (100%)	132 (98%)	2 (2%)	57	20
All	All	568/570 (100%)	561 (99%)	7 (1%)	63	27

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	B	29	VAL
1	B	63	GLU
2	C	29	VAL
2	C	61	MET
2	D	29	VAL
2	D	61	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	99	GLN
1	B	26	ASN
1	B	95	HIS
1	B	129	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
5	A1DJ2	B	204	1	80,82,82	1.36	7 (8%)	90,123,123	1.37	7 (7%)
3	GNP	B	201	4	34,34,34	1.88	6 (17%)	47,54,54	1.11	4 (8%)
5	A1DJ2	A	203	1	80,82,82	1.42	6 (7%)	90,123,123	1.64	11 (12%)
7	EDO	B	203	-	3,3,3	0.23	0	2,2,2	0.37	0
3	GNP	A	201	4	34,34,34	1.82	5 (14%)	47,54,54	1.08	3 (6%)

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
5	A1DJ2	B	204	1	-	8/75/121/121	0/8/10/10
3	GNP	B	201	4	-	4/18/38/38	0/3/3/3
5	A1DJ2	A	203	1	-	8/75/121/121	0/8/10/10
7	EDO	B	203	-	-	0/1/1/1	-
3	GNP	A	201	4	-	4/18/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	203	A1DJ2	N8-N7	-7.04	1.35	1.43
5	B	204	A1DJ2	N8-N7	-7.04	1.35	1.43
5	A	203	A1DJ2	C30-C39	6.62	1.48	1.37
5	B	204	A1DJ2	C30-C39	6.12	1.47	1.37
3	B	201	GNP	PB-O3A	5.79	1.66	1.59
3	A	201	GNP	PB-O3A	5.69	1.66	1.59
3	B	201	GNP	PG-N3B	5.62	1.78	1.63
3	A	201	GNP	PG-N3B	5.43	1.77	1.63
3	A	201	GNP	PG-O1G	3.97	1.52	1.46
3	B	201	GNP	PG-O1G	3.93	1.52	1.46
5	A	203	A1DJ2	O5-C44	3.89	1.41	1.33
5	B	204	A1DJ2	O5-C44	3.57	1.40	1.33
3	B	201	GNP	PB-O1B	3.06	1.50	1.46
3	A	201	GNP	PB-O1B	2.74	1.50	1.46
3	B	201	GNP	PB-O2B	-2.63	1.49	1.56
3	A	201	GNP	PB-O2B	-2.51	1.50	1.56
5	A	203	A1DJ2	C29-N5	-2.50	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	203	A1DJ2	C30-N5	-2.40	1.35	1.39
5	B	204	A1DJ2	C31-C32	-2.31	1.39	1.41
3	B	201	GNP	PA-O3A	2.25	1.61	1.59
5	A	203	A1DJ2	C28-C39	-2.16	1.40	1.44
5	B	204	A1DJ2	C28-C39	-2.15	1.40	1.44
5	B	204	A1DJ2	C29-N5	-2.07	1.35	1.39
5	B	204	A1DJ2	C30-N5	-2.06	1.36	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	203	A1DJ2	C11-C9-C8	-8.81	109.24	119.87
5	A	203	A1DJ2	C10-C9-C8	-6.48	112.05	119.87
5	B	204	A1DJ2	C11-C9-C8	-5.37	113.39	119.87
5	B	204	A1DJ2	C10-C9-C8	-4.96	113.89	119.87
3	B	201	GNP	O1G-PG-N3B	-4.43	105.24	111.77
5	A	203	A1DJ2	C28-C39-C30	-4.18	103.67	107.12
3	A	201	GNP	O1G-PG-N3B	-4.11	105.72	111.77
5	B	204	A1DJ2	C13-N3-C1	3.91	115.96	113.47
3	B	201	GNP	O2B-PB-O1B	3.87	118.16	109.87
3	A	201	GNP	O2B-PB-O1B	3.81	118.04	109.87
5	B	204	A1DJ2	C5-C2-C1	-3.42	107.77	112.13
5	B	204	A1DJ2	C28-C39-C30	-3.08	104.57	107.12
5	A	203	A1DJ2	C31-C30-C39	-2.91	125.31	128.34
5	A	203	A1DJ2	C12-C13-N3	-2.77	100.24	103.19
5	B	204	A1DJ2	C12-C13-N3	-2.71	100.31	103.19
5	A	203	A1DJ2	C13-N3-C1	2.70	115.19	113.47
5	A	203	A1DJ2	C33-N6-C32	2.37	121.63	116.92
3	B	201	GNP	O3A-PB-N3B	-2.36	100.05	106.59
3	B	201	GNP	O2G-PG-O3G	2.32	113.83	107.59
5	A	203	A1DJ2	O5-C44-O7	-2.24	120.05	124.14
5	A	203	A1DJ2	C29-N5-C30	2.23	110.16	108.37
5	B	204	A1DJ2	C33-N6-C32	2.18	121.26	116.92
3	A	201	GNP	O3A-PB-N3B	-2.14	100.65	106.59
5	A	203	A1DJ2	C52-C51-N5	-2.11	104.16	111.57
5	A	203	A1DJ2	C29-C28-C39	2.10	109.28	107.38

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	GNP	PB-N3B-PG-O1G

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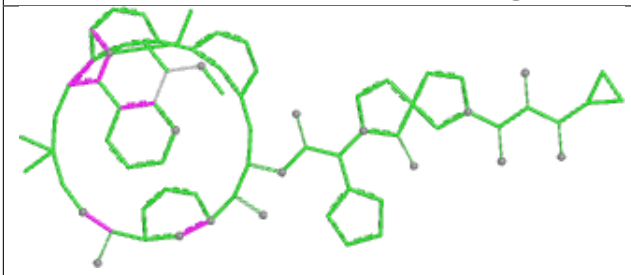
Mol	Chain	Res	Type	Atoms
3	A	201	GNP	PG-N3B-PB-O1B
3	A	201	GNP	PA-O3A-PB-O2B
3	B	201	GNP	PB-N3B-PG-O1G
3	B	201	GNP	PG-N3B-PB-O1B
3	B	201	GNP	PA-O3A-PB-O2B
5	A	203	A1DJ2	C31-C32-C36-C38
5	A	203	A1DJ2	N1-C6-C7-N2
5	A	203	A1DJ2	O3-C6-C7-N2
5	B	204	A1DJ2	C31-C32-C36-C38
5	B	204	A1DJ2	N1-C6-C7-N2
5	B	204	A1DJ2	O3-C6-C7-N2
5	A	203	A1DJ2	N4-C21-C22-C23
5	B	204	A1DJ2	N4-C21-C22-C23
5	A	203	A1DJ2	C31-C32-C36-O4
5	B	204	A1DJ2	C31-C32-C36-O4
5	A	203	A1DJ2	C32-C36-O4-C37
5	B	204	A1DJ2	C49-C21-C22-C23
5	A	203	A1DJ2	C49-C21-C22-C23
5	B	204	A1DJ2	C32-C36-O4-C37
5	A	203	A1DJ2	C15-C14-N3-C13
5	B	204	A1DJ2	C15-C14-N3-C13
3	A	201	GNP	PA-O3A-PB-O1B
3	B	201	GNP	PA-O3A-PB-O1B

There are no ring outliers.

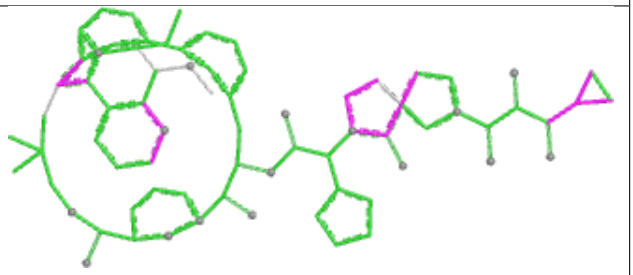
No monomer is involved in short contacts.

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.

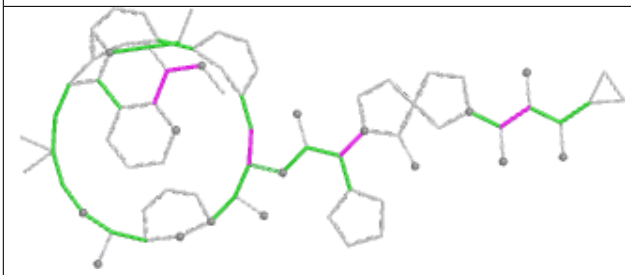
Ligand A1DJ2 B 204



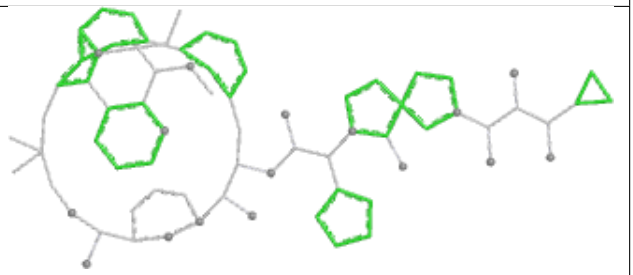
Bond lengths



Bond angles

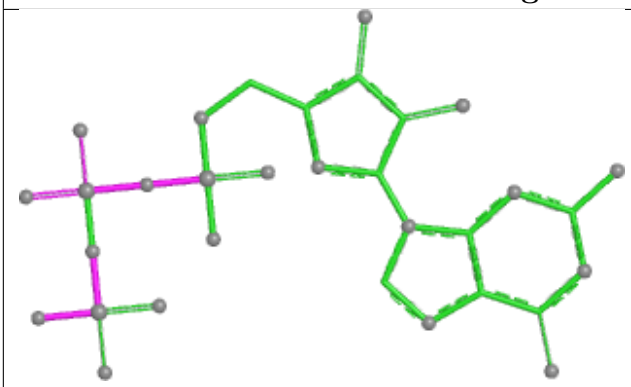


Torsions

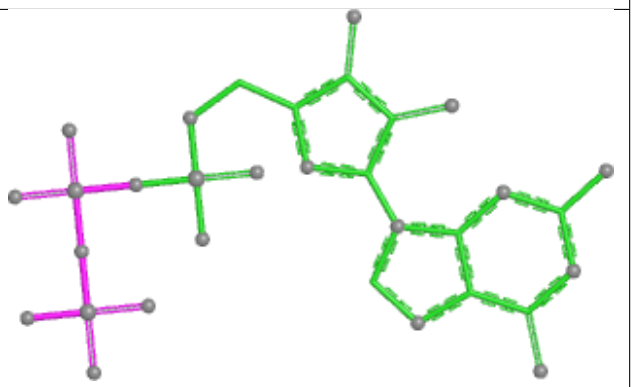


Rings

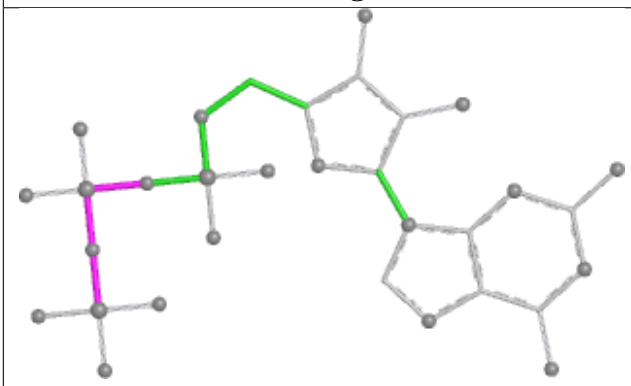
Ligand GNP B 201



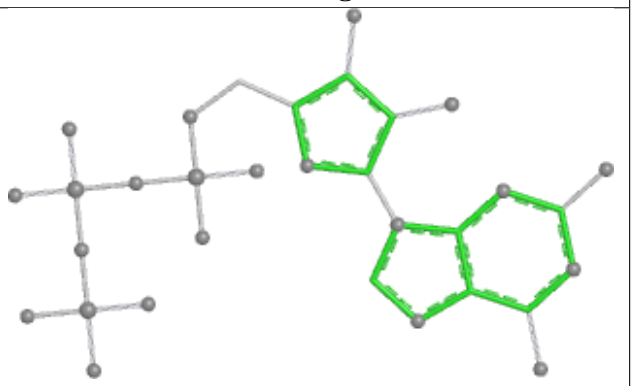
Bond lengths



Bond angles

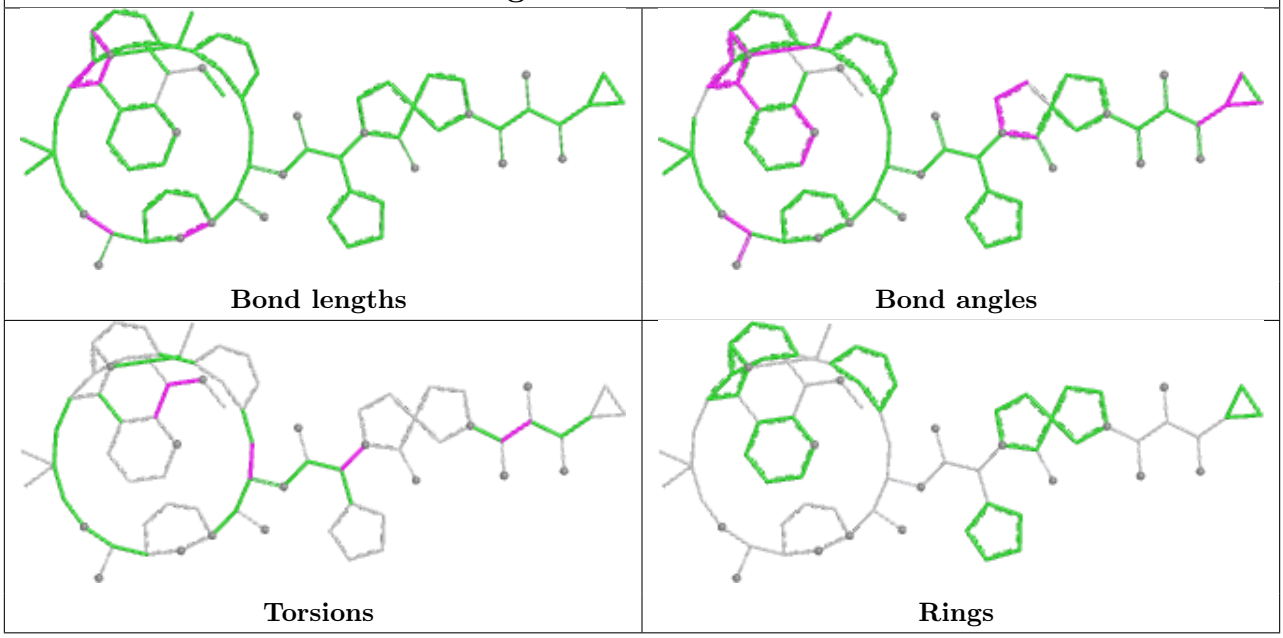


Torsions

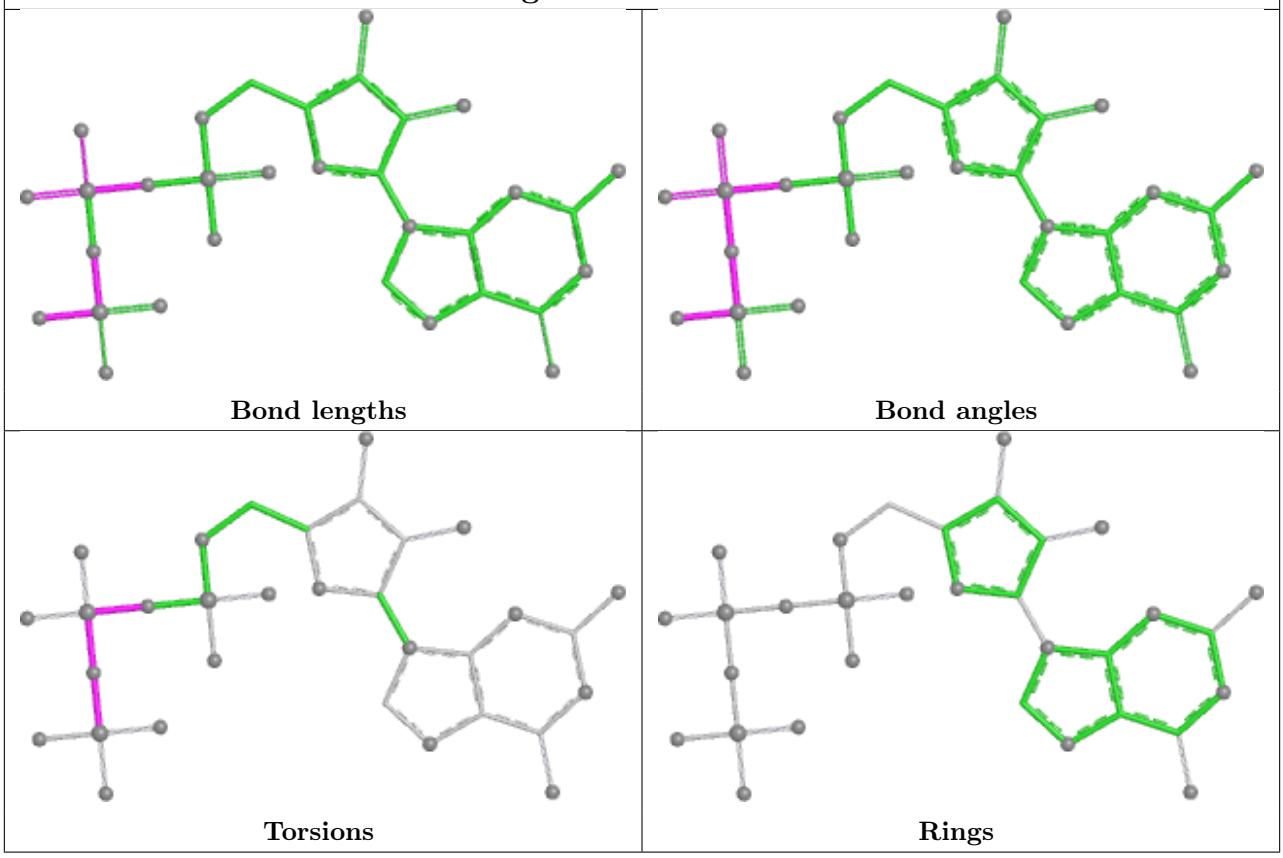


Rings

Ligand A1DJ2 A 203



Ligand GNP A 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	170/170 (100%)	0.58	10 (5%) 28 29	11, 18, 29, 38	0
1	B	170/170 (100%)	0.41	3 (1%) 67 68	11, 17, 28, 35	0
2	C	163/166 (98%)	0.06	2 (1%) 76 77	8, 16, 23, 37	1 (0%)
2	D	165/166 (99%)	-0.01	0 100 100	10, 15, 22, 26	1 (0%)
All	All	668/672 (99%)	0.26	15 (2%) 62 63	8, 16, 27, 38	2 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	VAL	7.7
1	A	29	VAL	6.8
2	C	2	VAL	6.1
1	A	63	GLU	2.8
1	B	24	ILE	2.6
1	A	68	ARG	2.4
1	A	62	GLU	2.4
1	A	0	SER	2.4
1	A	31	GLU	2.4
1	B	30	ASP	2.4
1	A	108	ASP	2.2
1	A	30	ASP	2.2
1	A	26	ASN	2.1
2	C	164	LEU	2.0
1	A	99	GLN	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 (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

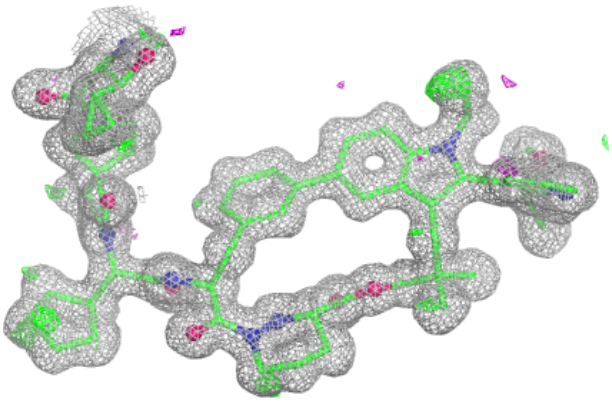
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

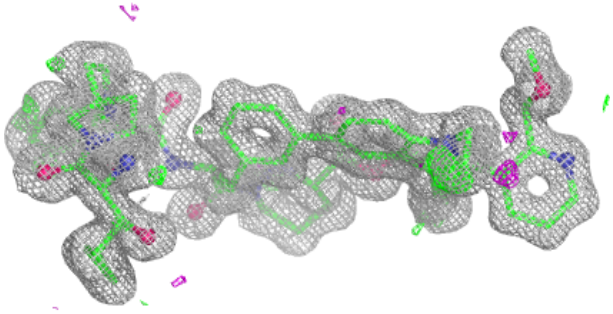
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	B	203	4/4	0.90	0.10	20,22,24,25	0
5	A1DJ2	A	203	73/73	0.96	0.06	9,11,19,21	0
5	A1DJ2	B	204	73/73	0.97	0.06	9,10,17,19	0
3	GNP	A	201	32/32	0.99	0.04	11,14,18,20	0
3	GNP	B	201	32/32	0.99	0.04	10,13,17,18	0
6	CL	A	204	1/1	0.99	0.08	16,16,16,16	0
4	MG	A	202	1/1	0.99	0.02	12,12,12,12	0
6	CL	B	205	1/1	1.00	0.09	17,17,17,17	0
4	MG	B	202	1/1	1.00	0.02	11,11,11,11	0

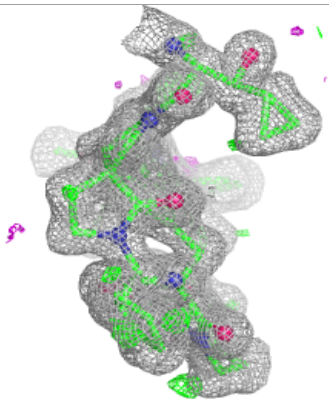
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1DJ2 A 203:

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

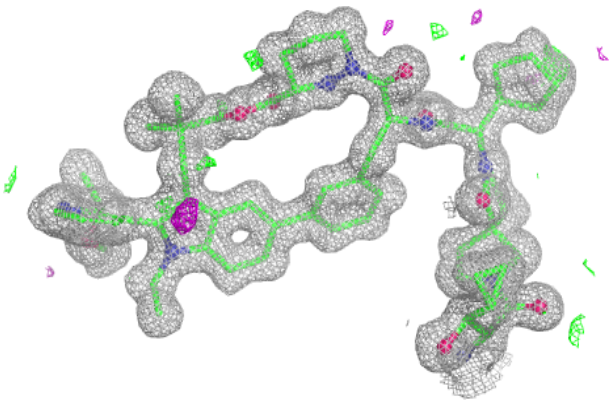


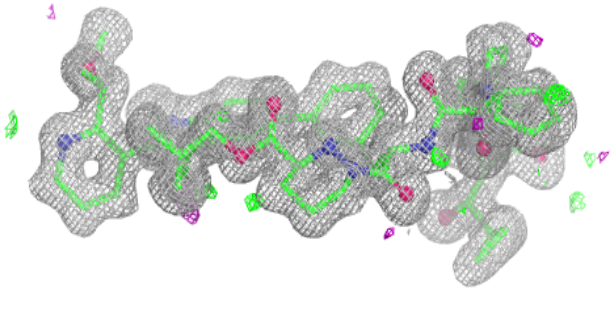


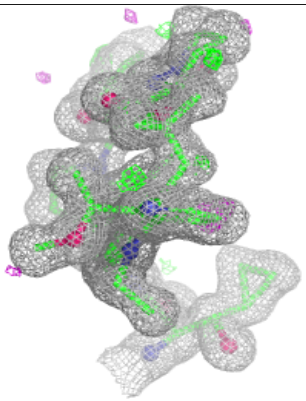


Electron density around A1DJ2 B 204:

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

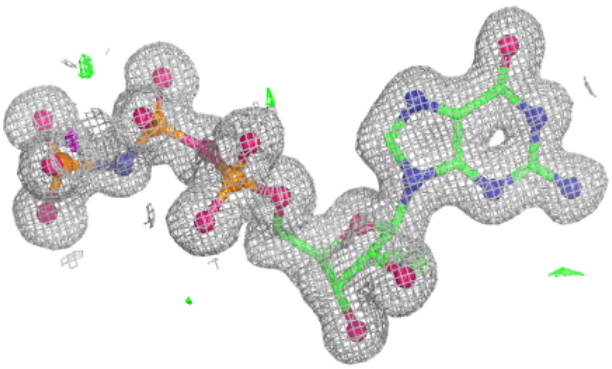


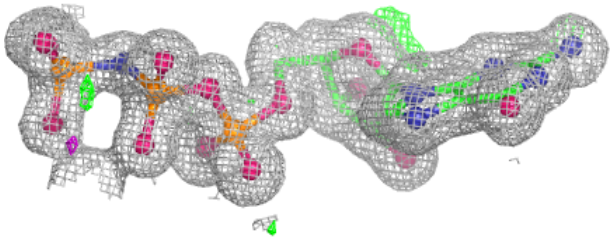


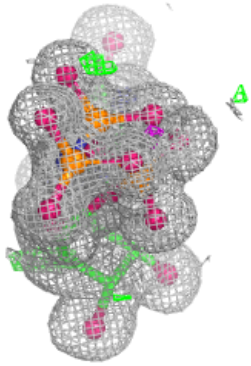


Electron density around GNP A 201:

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

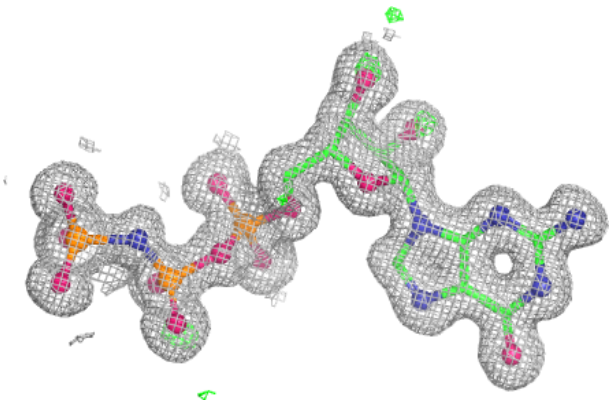


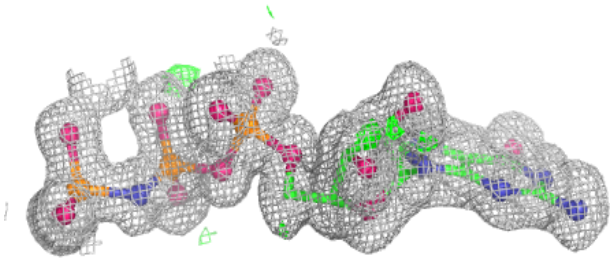


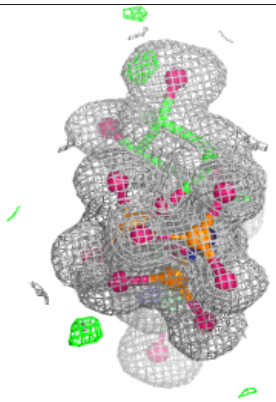


Electron density around GNP B 201:

$2mF_o$-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.