



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:06 AM UTC

PDB ID : 6XL4 / pdb_00006xl4
Title : EGFR(T790M/V948R) in complex with AZD9291 and DDC4002
Authors : Heppner, D.E.; Beyett, T.S.; Eck, M.J.
Deposited on : 2020-06-28
Resolution : 2.06 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

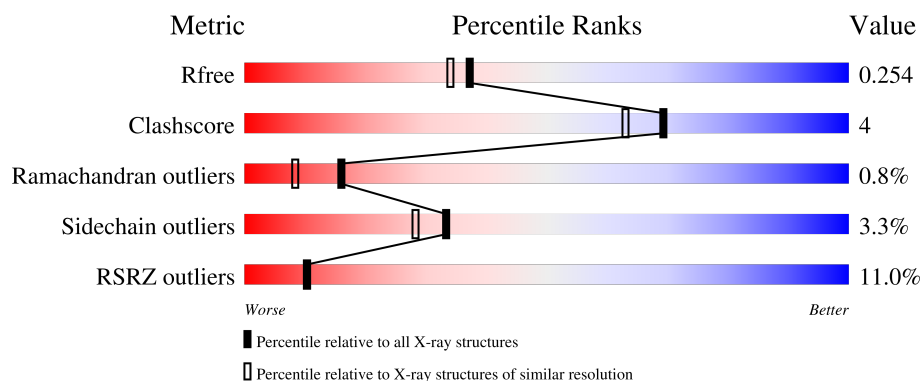
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	328	6% 80% 9% 11%
1	B	328	9% 77% 10% 11%
1	C	328	14% 80% 9% 8%
1	D	328	11% 81% 10% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9977 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.

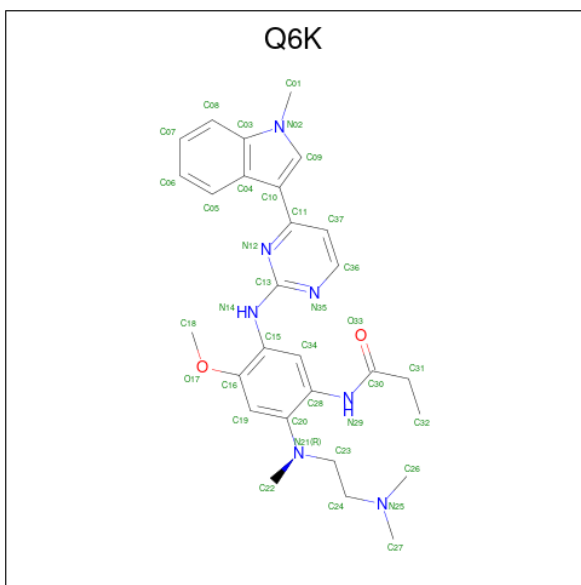
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2360	1515	402	424	19			
1	B	292	Total	C	N	O	S	0	0	0
			2347	1507	400	421	19			
1	C	302	Total	C	N	O	S	0	0	0
			2419	1551	411	438	19			
1	D	300	Total	C	N	O	S	0	0	0
			2400	1540	408	433	19			

There are 8 discrepancies between the modelled and reference sequences:

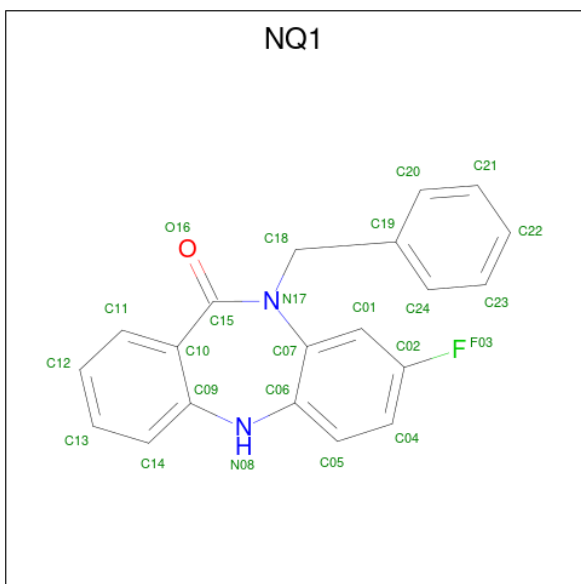
Chain	Residue	Modelled	Actual	Comment	Reference
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
B	948	ARG	VAL	engineered mutation	UNP P00533
C	790	MET	THR	engineered mutation	UNP P00533
C	948	ARG	VAL	engineered mutation	UNP P00533
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533

- Molecule 2 is {N}-[2-[2-(dimethylamino)ethyl-methyl-amino]-4-methoxy-5-[[4-(1-methylindol-3-yl)pyrimidin-2-yl]amino]phenyl]propanamide (CCD ID: Q6K) (formula: C₂₈H₃₅N₇O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			37	28	7	2		
2	B	1	Total	C	N	O	0	0
			37	28	7	2		

- Molecule 3 is 10-benzyl-8-fluoro-5,10-dihydro-11H-dibenzo[b,e][1,4]diazepin-11-one (CCD ID: NQ1) (formula: C₂₀H₁₅FN₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			24	20	1	2	1		

Continued on next page...

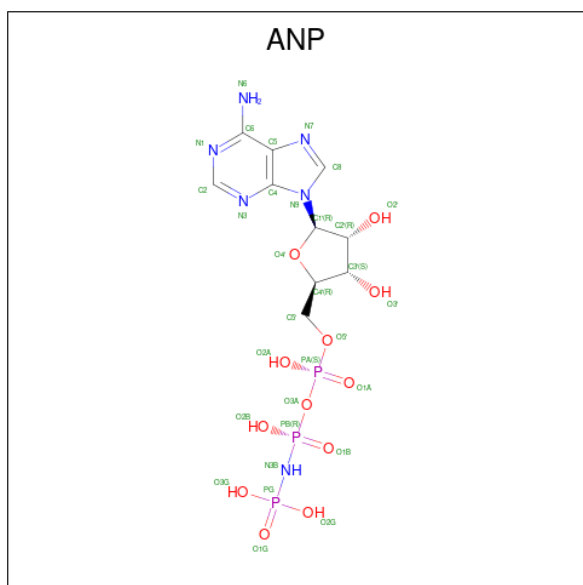
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			24	20	1	2	1		
3	D	1	Total	C	F	N	O	0	0
			24	20	1	2	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	79	Total	O	0	0
			79	79		
6	B	66	Total	O	0	0
			66	66		

Continued on next page...

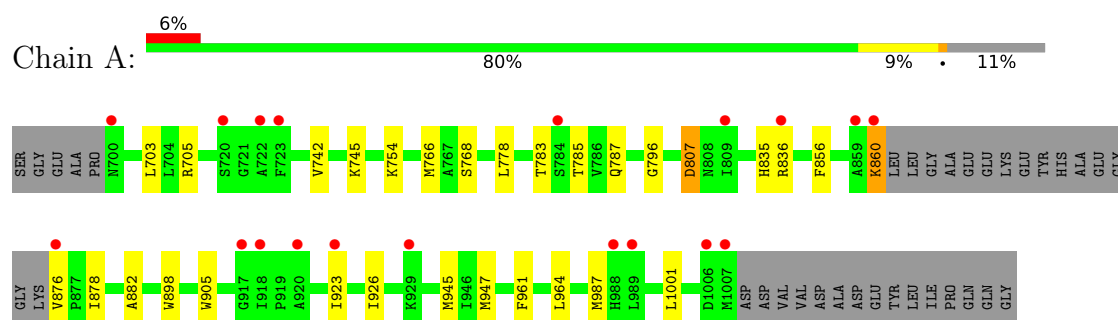
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	69	Total	O	0	0
			69	69		
6	D	59	Total	O	0	0
			59	59		

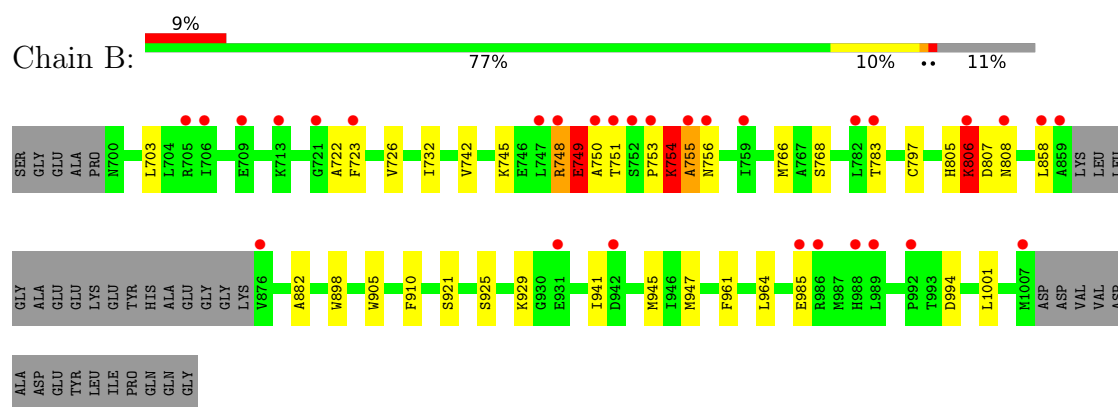
3 Residue-property plots [i](#)

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.

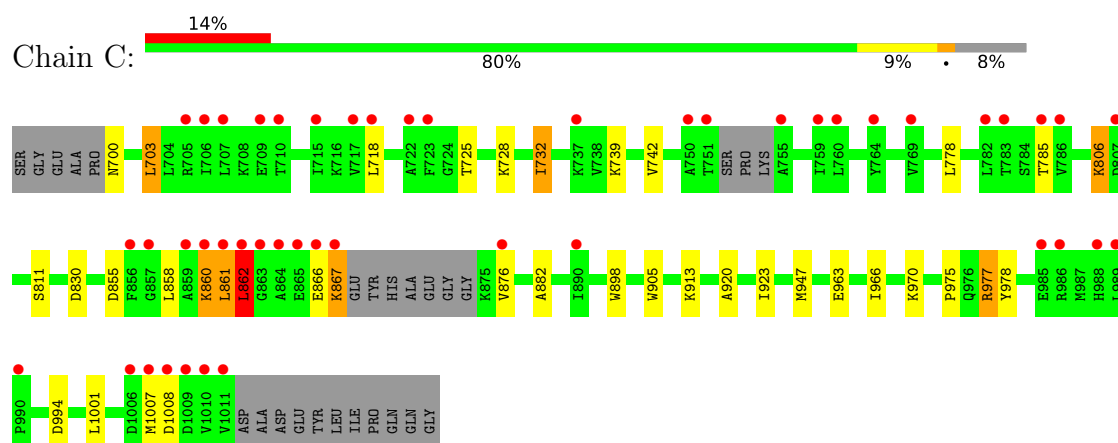
• Molecule 1: Epidermal growth factor receptor



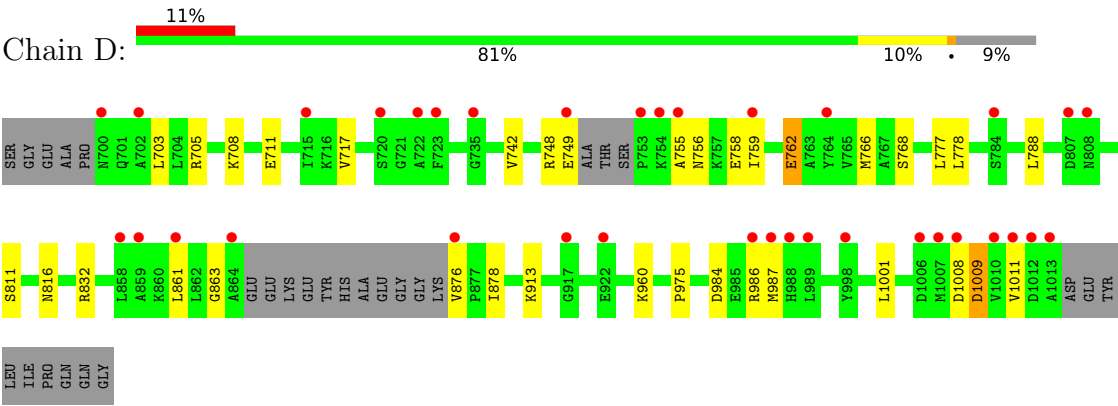
• Molecule 1: Epidermal growth factor receptor



• Molecule 1: Epidermal growth factor receptor



● Molecule 1: Epidermal growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.54Å 101.71Å 86.97Å 90.00° 102.72° 90.00°	Depositor
Resolution (Å)	84.84 – 2.06 84.84 – 2.06	Depositor EDS
% Data completeness (in resolution range)	98.9 (84.84-2.06) 89.3 (84.84-2.06)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.214 , 0.252 0.216 , 0.254	Depositor DCC
R_{free} test set	3628 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.896	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9977	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2650e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, NQ1, Q6K

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	0/2412	0.49	2/3262 (0.1%)
1	B	0.27	0/2399	0.59	6/3246 (0.2%)
1	C	0.30	0/2469	0.62	4/3338 (0.1%)
1	D	0.32	0/2451	0.50	3/3315 (0.1%)
All	All	0.29	0/9731	0.55	15/13161 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	861	LEU	N-CA-C	-12.85	97.63	113.18
1	B	806	LYS	CA-C-N	-7.91	109.69	122.26
1	B	806	LYS	C-N-CA	-7.91	109.69	122.26
1	C	866	GLU	N-CA-C	-7.86	103.58	113.02
1	B	722	ALA	N-CA-C	-7.68	104.40	114.31
1	D	1009	ASP	N-CA-C	6.46	119.49	109.60
1	C	860	LYS	CB-CA-C	6.11	120.29	110.09
1	C	860	LYS	N-CA-C	-6.08	105.52	113.17
1	B	807	ASP	CB-CA-C	5.69	119.10	109.55
1	B	805	HIS	O-C-N	5.59	129.51	121.97
1	B	754	LYS	N-CA-C	5.43	122.36	110.80
1	D	986	ARG	N-CA-C	-5.25	105.97	112.38
1	D	755	ALA	N-CA-C	5.24	114.94	108.19
1	A	807	ASP	CA-C-N	-5.10	114.56	122.67
1	A	807	ASP	C-N-CA	-5.10	114.56	122.67

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	2360	0	2398	17	0
1	B	2347	0	2382	20	0
1	C	2419	0	2445	20	0
1	D	2400	0	2425	20	0
2	A	37	0	0	1	0
2	B	37	0	0	2	0
3	A	24	0	0	1	0
3	B	24	0	0	1	0
3	D	24	0	0	1	0
4	D	1	0	0	0	0
5	D	31	0	13	0	0
6	A	79	0	0	0	0
6	B	66	0	0	1	0
6	C	69	0	0	1	0
6	D	59	0	0	2	0
All	All	9977	0	9663	68	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (68) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:753:PRO:HG2	1:B:754:LYS:HE2	1.47	0.96
1:B:754:LYS:O	1:B:755:ALA:HB3	1.86	0.75
1:B:994:ASP:OD1	1:D:705:ARG:NH1	2.22	0.73
1:A:742:VAL:HG12	1:C:1001:LEU:HD11	1.75	0.68
1:D:703:LEU:HD13	1:D:768:SER:HA	1.78	0.65
1:B:754:LYS:O	1:B:755:ALA:CB	2.46	0.64
1:B:742:VAL:HG12	1:D:1001:LEU:HD11	1.82	0.62
1:D:987:MET:HE1	6:D:1247:HOH:O	2.00	0.61
1:A:705:ARG:NH1	1:C:994:ASP:OD1	2.34	0.59
1:A:1001:LEU:HD11	1:C:742:VAL:HG12	1.85	0.58
1:A:703:LEU:HD13	1:A:768:SER:HA	1.86	0.57
1:D:759:ILE:HD13	1:D:861:LEU:HD11	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:963:GLU:OE2	1:D:913:LYS:NZ	2.21	0.56
1:B:703:LEU:HD13	1:B:768:SER:HA	1.89	0.55
1:D:777:LEU:HD11	1:D:788:LEU:HB3	1.87	0.55
1:B:1001:LEU:HD11	1:D:742:VAL:HG12	1.87	0.55
1:D:816:ASN:HD21	1:D:1011:VAL:H	1.55	0.53
1:C:867:LYS:HD2	1:C:876:VAL:HG11	1.89	0.53
1:A:783:THR:OG1	1:A:785:THR:O	2.26	0.52
1:B:905:TRP:HD1	1:B:947:MET:HE1	1.75	0.52
1:C:966:ILE:HG22	1:C:970:LYS:HE2	1.92	0.52
1:A:766:MET:HG3	3:A:1302:NQ1:C14	2.40	0.51
1:A:807:ASP:O	1:A:987:MET:HE1	2.11	0.51
1:A:1001:LEU:HD13	1:C:778:LEU:HD23	1.93	0.50
1:D:708:LYS:HB2	1:D:711:GLU:HG3	1.94	0.50
1:D:766:MET:HG3	3:D:1103:NQ1:C14	2.42	0.50
1:A:796:GLY:HA2	2:A:1301:Q6K:C34	2.43	0.49
1:D:811:SER:OG	1:D:975:PRO:HB2	2.14	0.48
1:B:726:VAL:HG21	2:B:1202:Q6K:C03	2.43	0.48
1:C:732:ILE:HD11	1:C:739:LYS:HG2	1.95	0.48
1:D:762:GLU:HG2	1:D:861:LEU:HD13	1.95	0.48
1:A:961:PHE:HA	1:A:964:LEU:HD12	1.96	0.47
1:B:749:GLU:H	1:B:749:GLU:HG3	1.49	0.47
1:B:905:TRP:HB2	1:B:947:MET:HE3	1.97	0.47
1:C:806:LYS:HB3	1:C:806:LYS:HE3	1.66	0.47
1:A:835:HIS:CD2	1:A:856:PHE:HB3	2.50	0.46
1:D:777:LEU:HD21	1:D:788:LEU:HD22	1.97	0.46
1:B:783:THR:OG1	6:B:1301:HOH:O	2.21	0.46
1:C:913:LYS:HE3	6:C:1168:HOH:O	2.14	0.46
1:D:876:VAL:N	6:D:1209:HOH:O	2.49	0.46
1:C:862:LEU:HD13	1:C:862:LEU:HA	1.73	0.45
1:D:876:VAL:HG23	1:D:878:ILE:HG12	1.98	0.45
1:A:905:TRP:HD1	1:A:947:MET:HE1	1.81	0.45
1:D:748:ARG:HH22	1:D:863:GLY:H	1.64	0.44
1:B:941:ILE:HG13	1:B:945:MET:HG2	2.00	0.44
1:B:925:SER:O	1:B:929:LYS:HG2	2.17	0.44
1:C:861:LEU:HD23	1:C:861:LEU:HA	1.81	0.44
1:B:748:ARG:HD2	1:B:748:ARG:HA	1.39	0.43
1:A:745:LYS:O	1:A:787:GLN:HA	2.18	0.43
1:A:836:ARG:HH11	1:A:860:LYS:HG2	1.83	0.43
1:B:766:MET:HG3	3:B:1201:NQ1:C14	2.48	0.43
1:A:876:VAL:HG23	1:A:878:ILE:HG12	2.01	0.43
1:D:1001:LEU:HD12	1:D:1001:LEU:HA	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.54	0.43
1:C:882:ALA:HA	1:C:898:TRP:CD2	2.54	0.43
1:C:905:TRP:HD1	1:C:947:MET:HE1	1.84	0.43
1:B:797:CYS:HB3	2:B:1202:Q6K:C31	2.49	0.42
1:B:961:PHE:HA	1:B:964:LEU:HD12	2.00	0.42
1:C:718:LEU:HD21	1:C:728:LYS:HB2	2.01	0.42
1:C:977:ARG:HD2	1:C:978:TYR:CE2	2.55	0.42
1:C:700:ASN:HB3	1:C:703:LEU:HD13	2.02	0.41
1:C:830:ASP:HB3	1:D:717:VAL:HG11	2.02	0.41
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.56	0.41
1:B:806:LYS:O	1:B:910:PHE:CD1	2.74	0.41
1:C:920:ALA:HA	1:C:923:ILE:HG12	2.03	0.40
1:D:960:LYS:HB3	1:D:960:LYS:HE3	1.88	0.40
1:A:923:ILE:HD13	1:A:926:ILE:HD11	2.03	0.40
1:C:811:SER:OG	1:C:975:PRO:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	289/328 (88%)	284 (98%)	5 (2%)	0	100	100
1	B	288/328 (88%)	275 (96%)	6 (2%)	7 (2%)	4	1
1	C	296/328 (90%)	282 (95%)	13 (4%)	1 (0%)	36	30
1	D	294/328 (90%)	279 (95%)	14 (5%)	1 (0%)	36	30
All	All	1167/1312 (89%)	1120 (96%)	38 (3%)	9 (1%)	16	8

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	754	LYS
1	B	756	ASN
1	B	806	LYS
1	C	862	LEU
1	B	755	ALA
1	D	756	ASN
1	B	749	GLU
1	B	750	ALA
1	B	808	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	261/288 (91%)	257 (98%)	4 (2%)	57	58
1	B	259/288 (90%)	249 (96%)	10 (4%)	28	23
1	C	265/288 (92%)	252 (95%)	13 (5%)	22	15
1	D	263/288 (91%)	255 (97%)	8 (3%)	36	32
All	All	1048/1152 (91%)	1013 (97%)	35 (3%)	33	28

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	754	LYS
1	A	778	LEU
1	A	860	LYS
1	A	945	MET
1	B	723	PHE
1	B	732	ILE
1	B	745	LYS
1	B	748	ARG
1	B	749	GLU
1	B	751	THR
1	B	806	LYS
1	B	858	LEU
1	B	921	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	985	GLU
1	C	703	LEU
1	C	725	THR
1	C	732	ILE
1	C	785	THR
1	C	806	LYS
1	C	855	ASP
1	C	858	LEU
1	C	860	LYS
1	C	862	LEU
1	C	867	LYS
1	C	977	ARG
1	C	1007	MET
1	C	1008	ASP
1	D	749	GLU
1	D	758	GLU
1	D	762	GLU
1	D	778	LEU
1	D	832	ARG
1	D	984	ASP
1	D	1008	ASP
1	D	1009	ASP

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	812	GLN
1	A	816	ASN
1	A	893	HIS
1	B	812	GLN
1	B	816	ASN
1	C	894	GLN
1	C	988	HIS
1	D	816	ASN
1	D	976	GLN
1	D	988	HIS

5.3.3 RNA ⓘ

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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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$
2	Q6K	B	1202	-	40,40,40	5.69	26 (65%)	56,56,56	2.27	14 (25%)
3	NQ1	D	1103	-	27,27,27	2.60	7 (25%)	37,38,38	1.51	7 (18%)
3	NQ1	B	1201	-	27,27,27	2.58	7 (25%)	37,38,38	1.49	7 (18%)
5	ANP	D	1102	4	33,33,33	0.94	4 (12%)	45,52,52	0.57	0
3	NQ1	A	1302	-	27,27,27	2.59	7 (25%)	37,38,38	1.42	5 (13%)
2	Q6K	A	1301	1	40,40,40	5.69	26 (65%)	56,56,56	2.13	14 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Q6K	B	1202	-	-	8/25/25/25	0/4/4/4
3	NQ1	D	1103	-	-	2/4/4/4	0/4/4/4
3	NQ1	B	1201	-	-	0/4/4/4	0/4/4/4
5	ANP	D	1102	4	-	3/18/38/38	0/3/3/3
3	NQ1	A	1302	-	-	2/4/4/4	0/4/4/4
2	Q6K	A	1301	1	-	6/25/25/25	0/4/4/4

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	Q6K	C05-C04	12.11	1.58	1.39
2	B	1202	Q6K	C05-C04	12.11	1.58	1.39
2	A	1301	Q6K	C28-C20	12.01	1.53	1.40
2	B	1202	Q6K	C08-C03	11.96	1.58	1.39
2	A	1301	Q6K	C08-C03	11.84	1.58	1.39
2	B	1202	Q6K	C28-C20	11.35	1.53	1.40
2	B	1202	Q6K	C13-N35	10.33	1.49	1.34
2	A	1301	Q6K	C13-N35	10.31	1.49	1.34
2	A	1301	Q6K	C34-C28	9.70	1.54	1.39
2	B	1202	Q6K	C34-C28	9.55	1.54	1.39
2	A	1301	Q6K	C34-C15	9.30	1.54	1.39
2	B	1202	Q6K	C34-C15	9.05	1.53	1.39
2	B	1202	Q6K	C19-C16	8.49	1.53	1.38
2	A	1301	Q6K	C19-C16	8.24	1.52	1.38
2	B	1202	Q6K	C19-C20	7.94	1.52	1.39
2	A	1301	Q6K	C19-C20	7.68	1.52	1.39
3	D	1103	NQ1	C15-N17	7.51	1.45	1.36
2	A	1301	Q6K	C11-N12	7.45	1.45	1.34
2	B	1202	Q6K	C11-N12	7.44	1.45	1.34
3	B	1201	NQ1	C15-N17	7.41	1.45	1.36
3	A	1302	NQ1	C15-N17	7.33	1.45	1.36
2	B	1202	Q6K	C06-C05	7.31	1.51	1.38
2	A	1301	Q6K	C06-C05	7.27	1.51	1.38
2	A	1301	Q6K	C07-C08	7.18	1.51	1.38
2	B	1202	Q6K	C07-C08	7.08	1.51	1.38
2	B	1202	Q6K	C15-C16	6.40	1.53	1.40
2	A	1301	Q6K	C15-C16	6.21	1.53	1.40
2	B	1202	Q6K	C37-C36	6.05	1.50	1.38
2	A	1301	Q6K	C37-C36	5.94	1.50	1.38
2	B	1202	Q6K	C36-N35	5.56	1.46	1.34
2	A	1301	Q6K	C36-N35	5.51	1.46	1.34
2	A	1301	Q6K	C37-C11	5.48	1.49	1.39
2	B	1202	Q6K	C37-C11	5.46	1.49	1.39
3	D	1103	NQ1	C06-N08	5.30	1.48	1.41
2	B	1202	Q6K	C13-N12	5.25	1.49	1.34
2	A	1301	Q6K	C13-N12	5.18	1.49	1.34
2	B	1202	Q6K	C07-C06	5.17	1.49	1.38
3	A	1302	NQ1	C09-N08	5.15	1.47	1.41
3	A	1302	NQ1	C06-N08	5.13	1.47	1.41
3	D	1103	NQ1	C09-N08	5.10	1.47	1.41
3	B	1201	NQ1	C09-N08	5.09	1.47	1.41
2	B	1202	Q6K	C30-N29	5.09	1.46	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	Q6K	C07-C06	5.07	1.49	1.38
3	B	1201	NQ1	C06-N08	5.02	1.47	1.41
2	B	1202	Q6K	C13-N14	4.94	1.46	1.36
2	A	1301	Q6K	C30-N29	4.81	1.45	1.35
3	B	1201	NQ1	C07-N17	4.63	1.47	1.43
3	A	1302	NQ1	C07-N17	4.61	1.47	1.43
2	A	1301	Q6K	C13-N14	4.61	1.46	1.36
2	A	1301	Q6K	C04-C10	-4.40	1.37	1.47
3	D	1103	NQ1	C07-N17	4.34	1.47	1.43
2	B	1202	Q6K	C04-C10	-4.23	1.38	1.47
3	B	1201	NQ1	C10-C15	3.72	1.55	1.50
3	D	1103	NQ1	C10-C15	3.58	1.55	1.50
3	A	1302	NQ1	C10-C15	3.48	1.55	1.50
3	D	1103	NQ1	C06-C07	-3.22	1.37	1.40
3	B	1201	NQ1	C06-C07	-3.14	1.37	1.40
3	A	1302	NQ1	C06-C07	-3.11	1.37	1.40
2	B	1202	Q6K	C15-N14	2.78	1.47	1.39
2	A	1301	Q6K	C15-N14	2.67	1.47	1.39
2	A	1301	Q6K	C20-N21	2.66	1.47	1.41
5	D	1102	ANP	PG-O1G	2.62	1.50	1.46
3	A	1302	NQ1	C10-C09	-2.60	1.37	1.41
3	B	1201	NQ1	C10-C09	-2.59	1.37	1.41
3	D	1103	NQ1	C10-C09	-2.59	1.37	1.41
2	B	1202	Q6K	C09-C10	2.55	1.39	1.37
2	B	1202	Q6K	C20-N21	2.52	1.46	1.41
5	D	1102	ANP	PG-N3B	2.49	1.69	1.63
2	A	1301	Q6K	C09-C10	2.48	1.39	1.37
5	D	1102	ANP	PB-O1B	2.39	1.49	1.46
2	A	1301	Q6K	O33-C30	-2.30	1.18	1.23
2	A	1301	Q6K	C11-C10	2.27	1.54	1.48
2	B	1202	Q6K	C11-C10	2.27	1.54	1.48
2	B	1202	Q6K	C28-N29	2.26	1.46	1.41
2	B	1202	Q6K	O33-C30	-2.16	1.19	1.23
2	A	1301	Q6K	C28-N29	2.08	1.45	1.41
5	D	1102	ANP	PB-O3A	-2.02	1.56	1.59

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1202	Q6K	N35-C13-N12	-7.72	118.95	126.42
2	A	1301	Q6K	N35-C13-N12	-7.18	119.48	126.42
2	B	1202	Q6K	C36-N35-C13	6.13	120.55	115.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	Q6K	C36-N35-C13	5.88	120.33	115.42
2	B	1202	Q6K	C11-N12-C13	5.73	121.21	116.87
2	A	1301	Q6K	C11-N12-C13	5.12	120.75	116.87
3	B	1201	NQ1	C07-N17-C15	5.09	130.05	124.75
3	A	1302	NQ1	C07-N17-C15	4.80	129.75	124.75
3	D	1103	NQ1	C07-N17-C15	4.55	129.48	124.75
2	B	1202	Q6K	C10-C09-N02	-4.54	107.65	110.95
2	A	1301	Q6K	C10-C09-N02	-4.44	107.72	110.95
2	A	1301	Q6K	C04-C10-C09	4.29	108.25	106.02
2	B	1202	Q6K	C04-C10-C09	4.10	108.15	106.02
2	A	1301	Q6K	C36-C37-C11	4.10	119.54	117.02
2	B	1202	Q6K	C31-C30-N29	3.92	124.77	114.65
2	A	1301	Q6K	O17-C16-C15	3.90	119.67	114.81
2	B	1202	Q6K	C36-C37-C11	3.78	119.34	117.02
2	B	1202	Q6K	O17-C16-C15	3.73	119.46	114.81
3	D	1103	NQ1	C18-N17-C07	-3.48	114.40	118.13
2	B	1202	Q6K	O33-C30-N29	-3.35	117.64	123.64
3	B	1201	NQ1	C18-N17-C07	-3.32	114.57	118.13
2	A	1301	Q6K	C37-C36-N35	-3.25	120.00	123.97
2	B	1202	Q6K	C37-C36-N35	-3.16	120.10	123.97
3	B	1201	NQ1	O16-C15-N17	-2.92	118.33	121.09
3	A	1302	NQ1	C18-N17-C07	-2.81	115.11	118.13
2	B	1202	Q6K	C37-C11-N12	-2.63	119.85	122.92
2	A	1301	Q6K	C37-C11-N12	-2.58	119.91	122.92
2	B	1202	Q6K	C24-C23-N21	-2.53	108.27	112.41
3	D	1103	NQ1	C19-C18-N17	2.46	117.46	113.46
3	A	1302	NQ1	O16-C15-N17	-2.45	118.77	121.09
3	D	1103	NQ1	O16-C15-N17	-2.36	118.86	121.09
2	A	1301	Q6K	C15-N14-C13	-2.27	122.29	129.22
3	D	1103	NQ1	C10-C15-N17	2.25	122.85	119.69
3	D	1103	NQ1	C04-C02-C01	-2.24	120.27	123.23
3	A	1302	NQ1	C05-C06-C07	2.24	121.75	118.94
3	D	1103	NQ1	C05-C04-C02	2.23	120.67	118.38
3	A	1302	NQ1	C10-C15-N17	2.15	122.70	119.69
2	A	1301	Q6K	C18-O17-C16	-2.14	114.38	117.51
3	B	1201	NQ1	C05-C06-C07	2.12	121.60	118.94
2	A	1301	Q6K	C19-C20-N21	-2.08	117.66	120.90
3	B	1201	NQ1	C10-C15-N17	2.08	122.61	119.69
3	B	1201	NQ1	C05-C04-C02	2.07	120.50	118.38
2	B	1202	Q6K	C18-O17-C16	-2.05	114.51	117.51
2	A	1301	Q6K	O17-C16-C19	-2.05	120.55	124.08
3	B	1201	NQ1	C04-C02-C01	-2.02	120.56	123.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1202	Q6K	O17-C16-C19	-2.02	120.60	124.08
2	A	1301	Q6K	C28-C20-N21	2.00	122.31	118.29

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	Q6K	C24-C23-N21-C22
2	B	1202	Q6K	C19-C20-N21-C23
5	D	1102	ANP	PG-N3B-PB-O1B
5	D	1102	ANP	PA-O3A-PB-O2B
2	B	1202	Q6K	O33-C30-N29-C28
2	B	1202	Q6K	C31-C30-N29-C28
2	A	1301	Q6K	C23-C24-N25-C26
2	A	1301	Q6K	N21-C23-C24-N25
2	B	1202	Q6K	C15-C16-O17-C18
2	B	1202	Q6K	C19-C16-O17-C18
2	B	1202	Q6K	C23-C24-N25-C26
2	A	1301	Q6K	C28-C20-N21-C23
2	B	1202	Q6K	C23-C24-N25-C27
2	B	1202	Q6K	C28-C20-N21-C23
3	D	1103	NQ1	N17-C18-C19-C20
2	A	1301	Q6K	C19-C20-N21-C23
3	A	1302	NQ1	N17-C18-C19-C20
2	A	1301	Q6K	C23-C24-N25-C27
3	D	1103	NQ1	N17-C18-C19-C24
5	D	1102	ANP	PA-O3A-PB-O1B
3	A	1302	NQ1	N17-C18-C19-C24

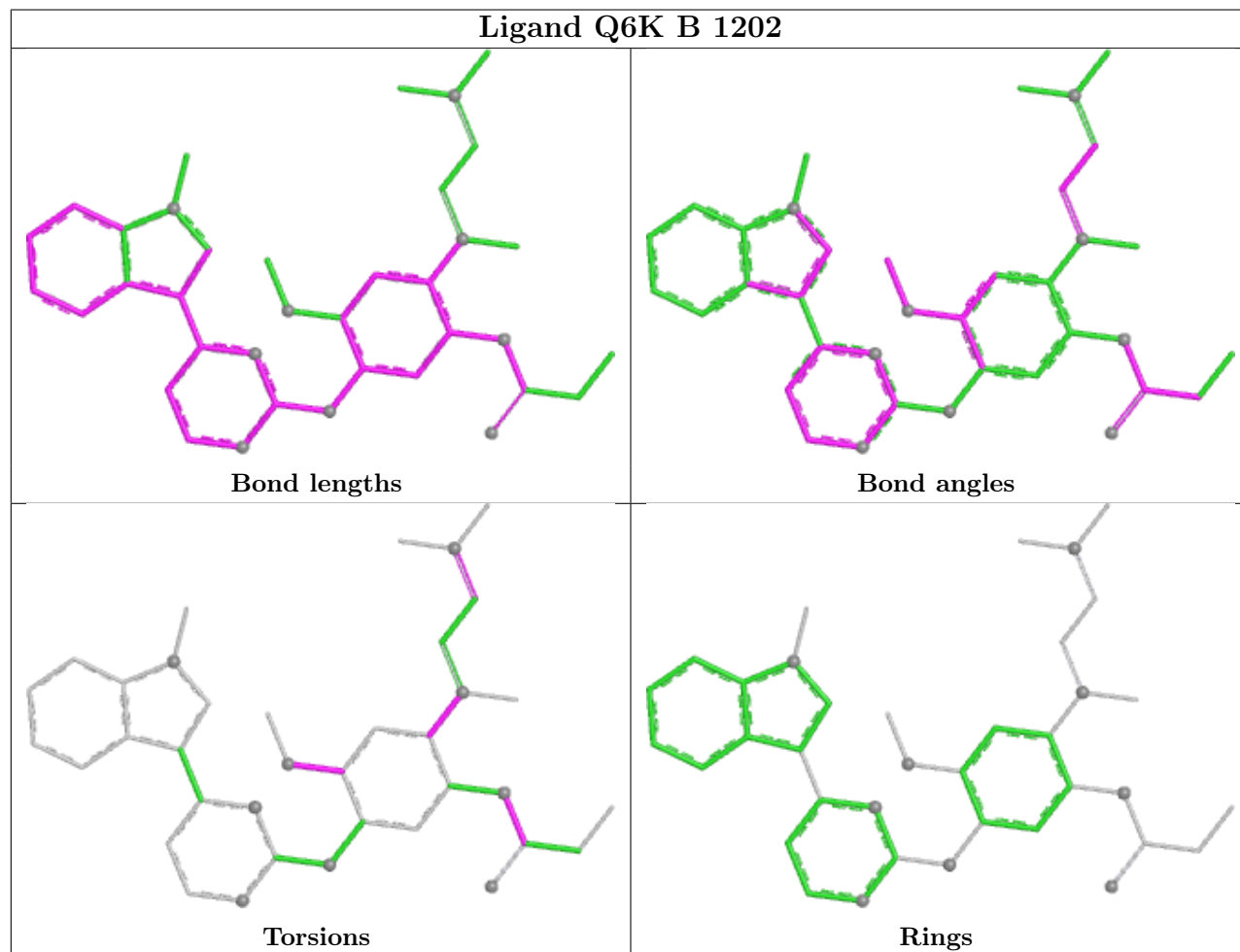
There are no ring outliers.

5 monomers are involved in 6 short contacts:

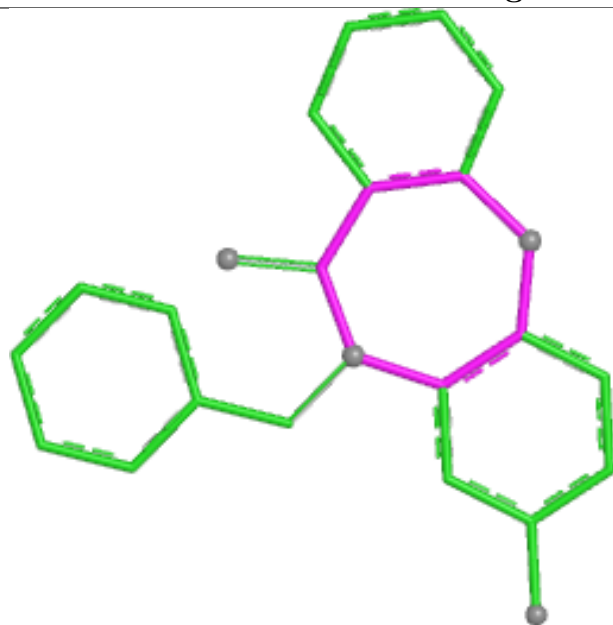
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1202	Q6K	2	0
3	D	1103	NQ1	1	0
3	B	1201	NQ1	1	0
3	A	1302	NQ1	1	0
2	A	1301	Q6K	1	0

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

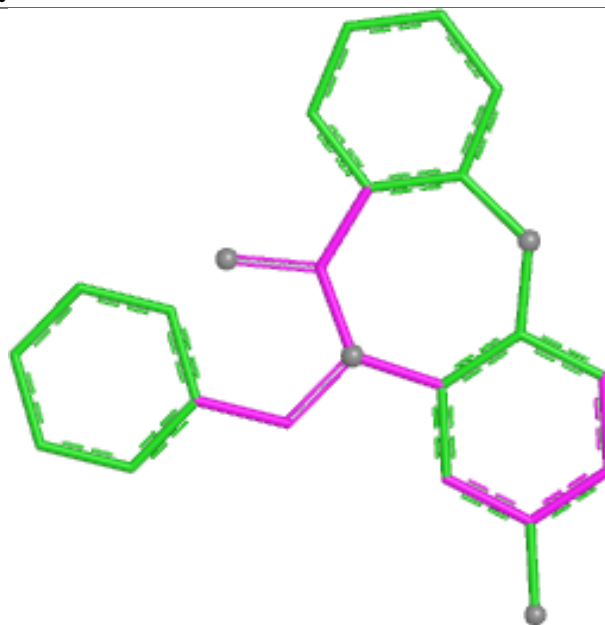
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



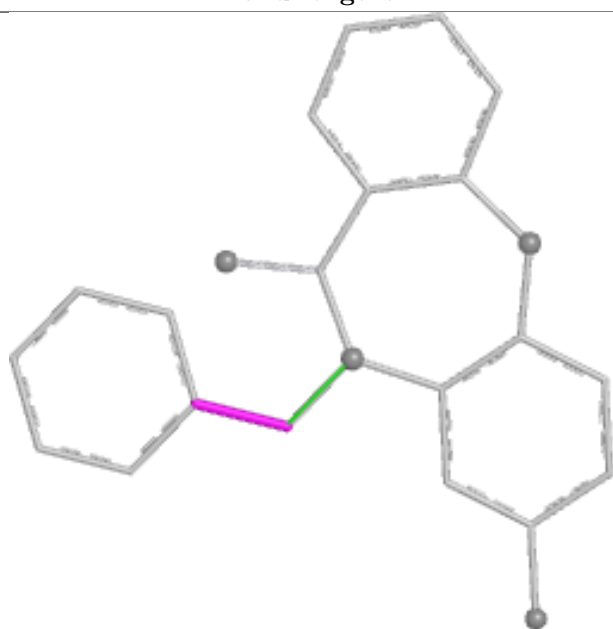
Ligand NQ1 D 1103



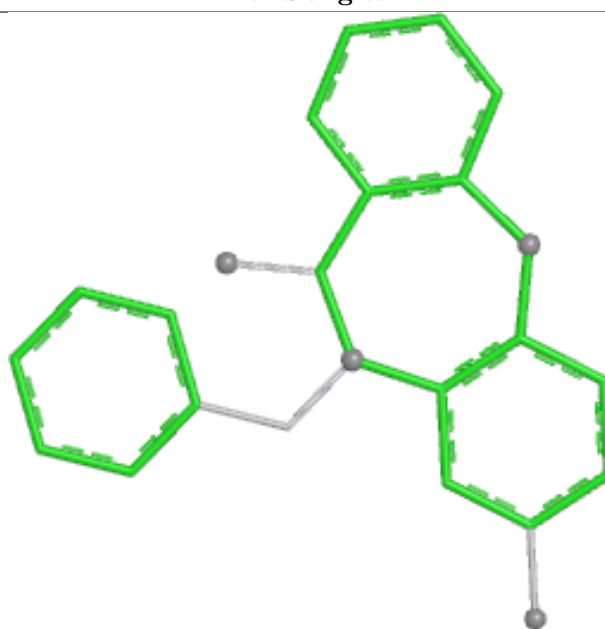
Bond lengths



Bond angles

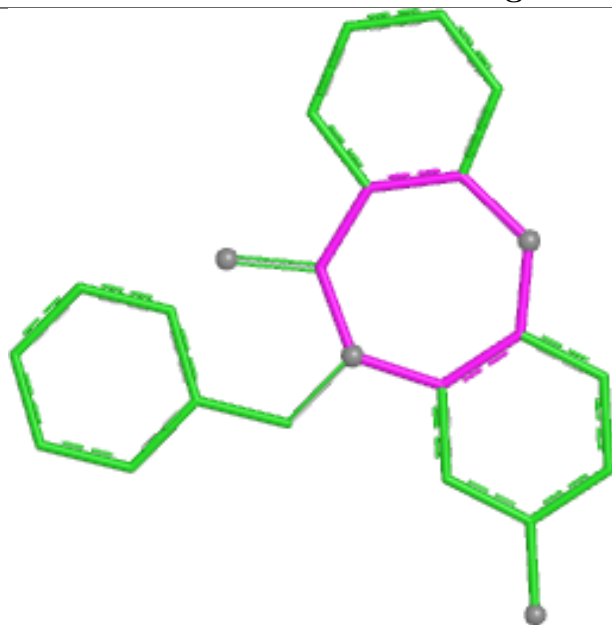


Torsions

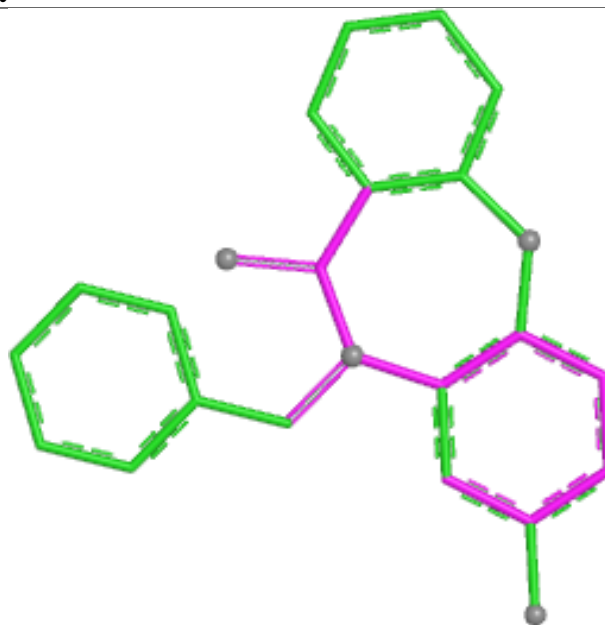


Rings

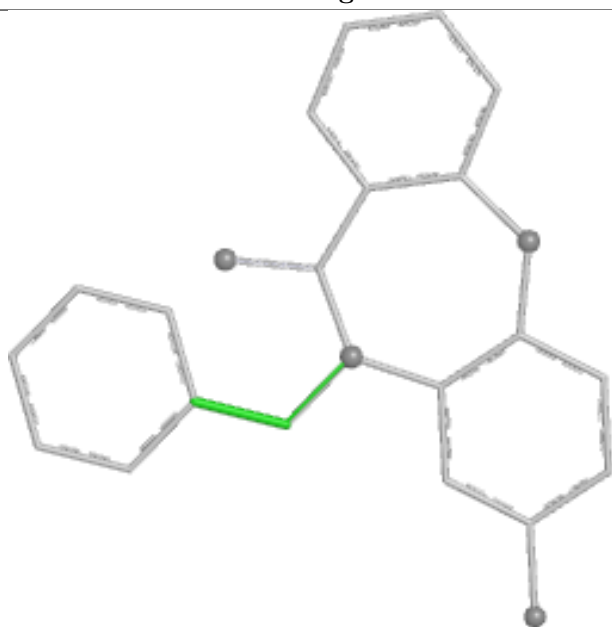
Ligand NQ1 B 1201



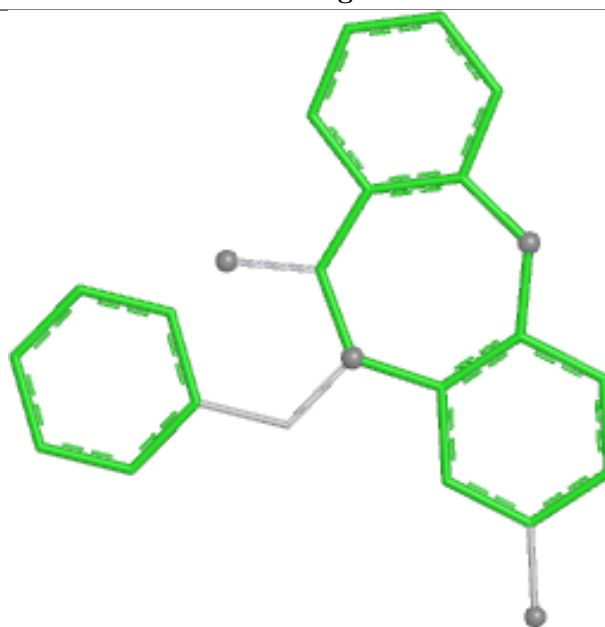
Bond lengths



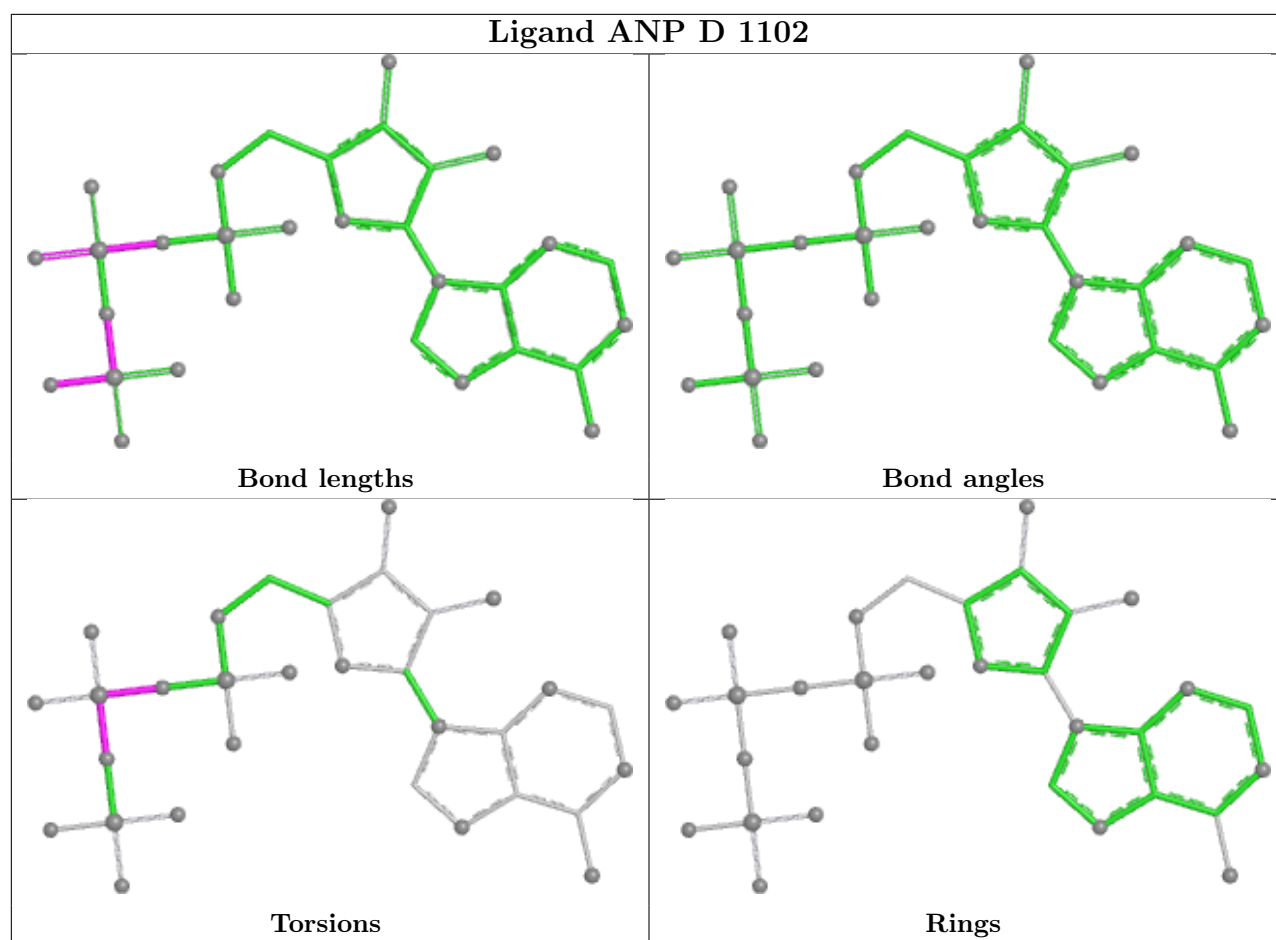
Bond angles



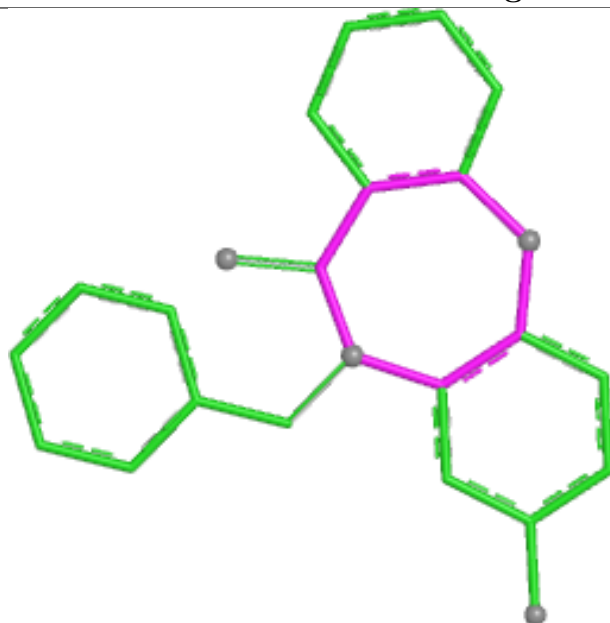
Torsions



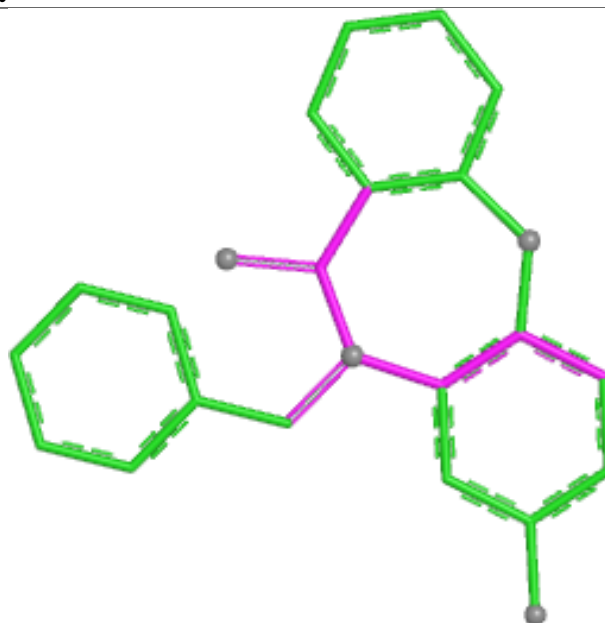
Rings



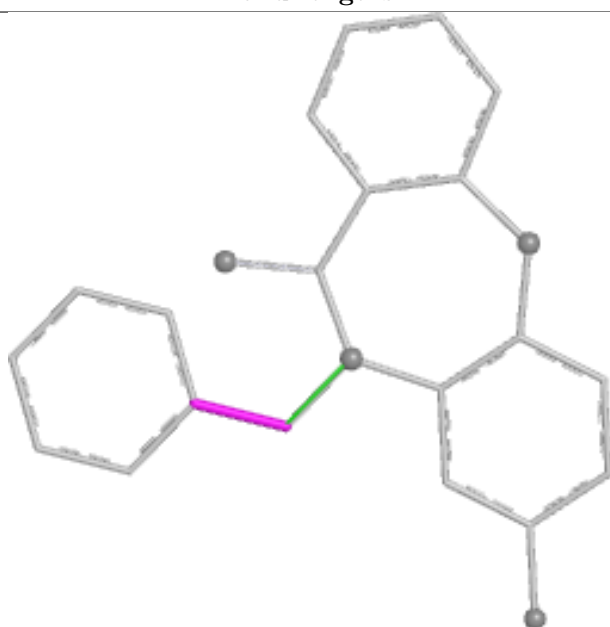
Ligand NQ1 A 1302



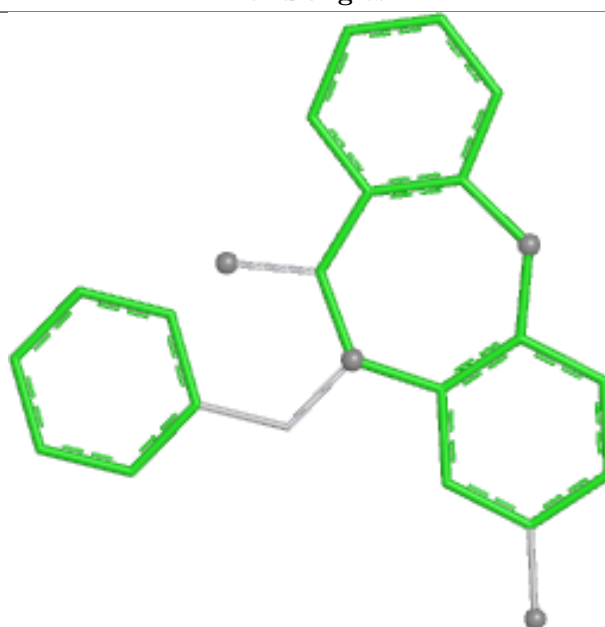
Bond lengths



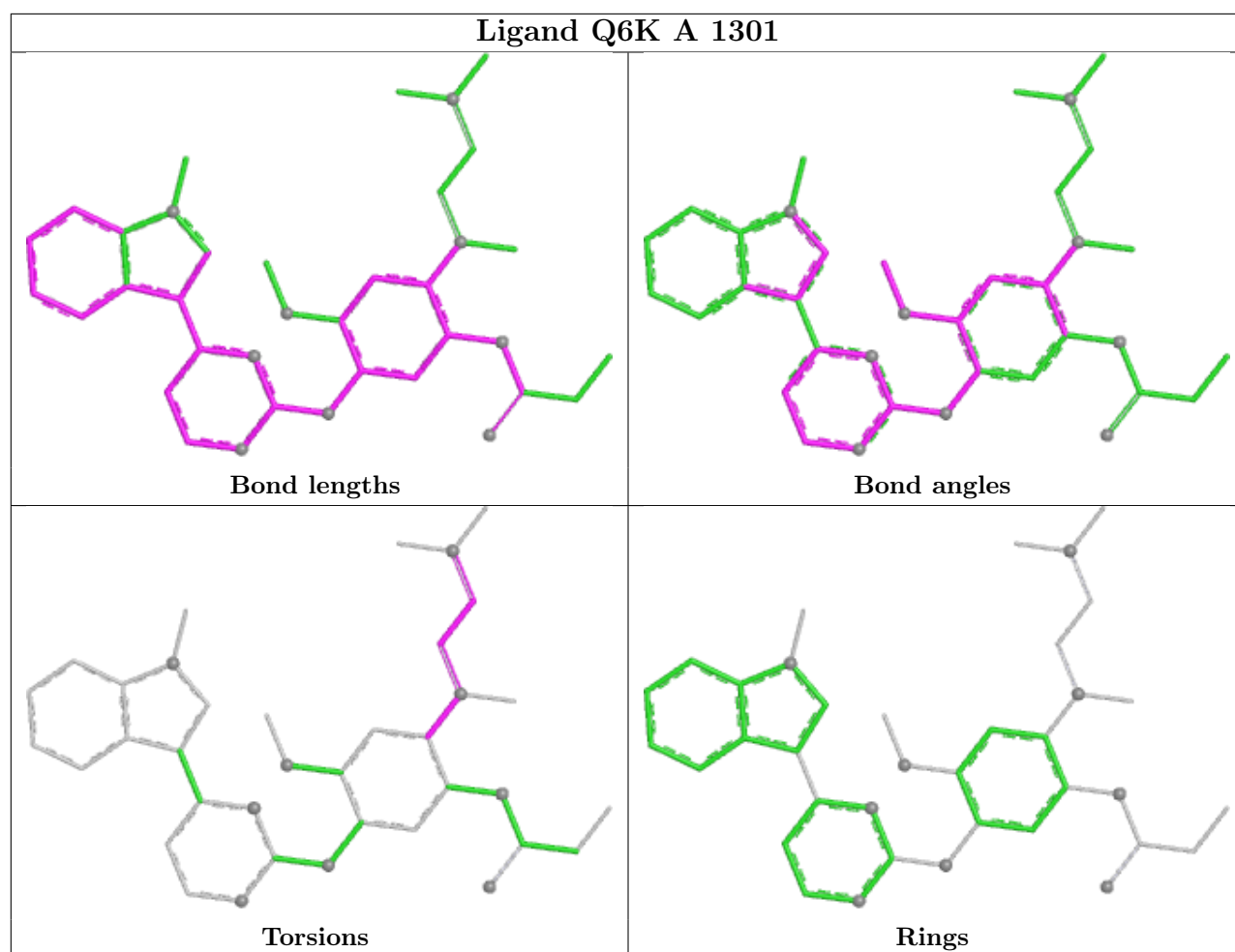
Bond angles



Torsions



Rings



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, 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	293/328 (89%)	0.60	19 (6%)	25 24	22, 35, 59, 86	0
1	B	292/328 (89%)	0.76	30 (10%)	12 12	22, 37, 67, 112	0
1	C	302/328 (92%)	0.89	47 (15%)	5 5	20, 37, 70, 106	0
1	D	300/328 (91%)	0.85	35 (11%)	9 9	23, 39, 74, 97	0
All	All	1187/1312 (90%)	0.77	131 (11%)	10 10	20, 37, 67, 112	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	859	ALA	5.4
1	B	753	PRO	5.2
1	B	723	PHE	4.8
1	C	862	LEU	4.6
1	D	1010	VAL	4.4
1	C	751	THR	4.3
1	D	1011	VAL	4.3
1	D	753	PRO	4.3
1	C	859	ALA	4.2
1	D	1013	ALA	4.2
1	C	1011	VAL	4.2
1	C	988	HIS	4.0
1	D	864	ALA	4.0
1	C	722	ALA	3.9
1	C	750	ALA	3.9
1	B	989	LEU	3.8
1	D	858	LEU	3.7
1	C	755	ALA	3.7
1	C	864	ALA	3.7
1	C	1010	VAL	3.7
1	C	867	LYS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	722	ALA	3.4
1	D	859	ALA	3.4
1	A	988	HIS	3.3
1	D	987	MET	3.3
1	C	760	LEU	3.3
1	C	1007	MET	3.3
1	C	876	VAL	3.2
1	D	989	LEU	3.2
1	B	751	THR	3.2
1	B	808	ASN	3.2
1	C	860	LYS	3.2
1	B	750	ALA	3.2
1	C	856	PHE	3.2
1	B	1007	MET	3.2
1	B	755	ALA	3.1
1	C	717	VAL	3.1
1	C	986	ARG	3.1
1	A	859	ALA	3.1
1	C	1006	ASP	3.1
1	D	755	ALA	3.1
1	C	861	LEU	3.0
1	C	786	VAL	3.0
1	A	918	ILE	3.0
1	C	989	LEU	2.9
1	A	1007	MET	2.9
1	D	876	VAL	2.9
1	C	759	ILE	2.9
1	C	807	ASP	2.9
1	A	722	ALA	2.9
1	B	747	LEU	2.9
1	B	721	GLY	2.8
1	C	865	GLU	2.8
1	C	764	TYR	2.8
1	B	756	ASN	2.7
1	A	1006	ASP	2.7
1	C	985	GLU	2.7
1	C	723	PHE	2.7
1	D	986	ARG	2.7
1	C	769	VAL	2.7
1	D	1008	ASP	2.7
1	B	709	GLU	2.7
1	C	782	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	1012	ASP	2.6
1	D	759	ILE	2.6
1	D	754	LYS	2.6
1	A	723	PHE	2.6
1	D	807	ASP	2.6
1	A	860	LYS	2.6
1	C	863	GLY	2.5
1	C	1008	ASP	2.5
1	C	707	LEU	2.5
1	A	917	GLY	2.5
1	B	876	VAL	2.5
1	D	735	GLY	2.5
1	B	931	GLU	2.5
1	A	784	SER	2.5
1	B	752	SER	2.5
1	C	785	THR	2.5
1	A	836	ARG	2.5
1	C	706	ILE	2.5
1	C	990	PRO	2.4
1	B	782	LEU	2.4
1	D	720	SER	2.4
1	D	988	HIS	2.4
1	D	702	ALA	2.4
1	D	922	GLU	2.4
1	D	700	ASN	2.4
1	B	705	ARG	2.4
1	D	1007	MET	2.4
1	C	715	ILE	2.3
1	B	985	GLU	2.3
1	D	749	GLU	2.3
1	A	809	ILE	2.3
1	C	783	THR	2.3
1	B	806	LYS	2.3
1	D	917	GLY	2.3
1	C	718	LEU	2.3
1	D	784	SER	2.2
1	D	998	TYR	2.2
1	B	988	HIS	2.2
1	A	700	ASN	2.2
1	C	1009	ASP	2.2
1	D	1006	ASP	2.2
1	B	858	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	748	ARG	2.2
1	C	710	THR	2.2
1	B	942	ASP	2.2
1	A	923	ILE	2.1
1	C	866	GLU	2.1
1	D	715	ILE	2.1
1	D	861	LEU	2.1
1	C	737	LYS	2.1
1	C	709	GLU	2.1
1	B	992	PRO	2.1
1	D	723	PHE	2.1
1	B	986	ARG	2.1
1	A	920	ALA	2.1
1	B	713	LYS	2.1
1	A	720	SER	2.1
1	D	808	ASN	2.1
1	B	783	THR	2.1
1	B	706	ILE	2.1
1	C	705	ARG	2.1
1	C	890	ILE	2.1
1	A	989	LEU	2.1
1	A	929	LYS	2.1
1	C	857	GLY	2.0
1	B	759	ILE	2.0
1	A	876	VAL	2.0
1	D	764	TYR	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](#)

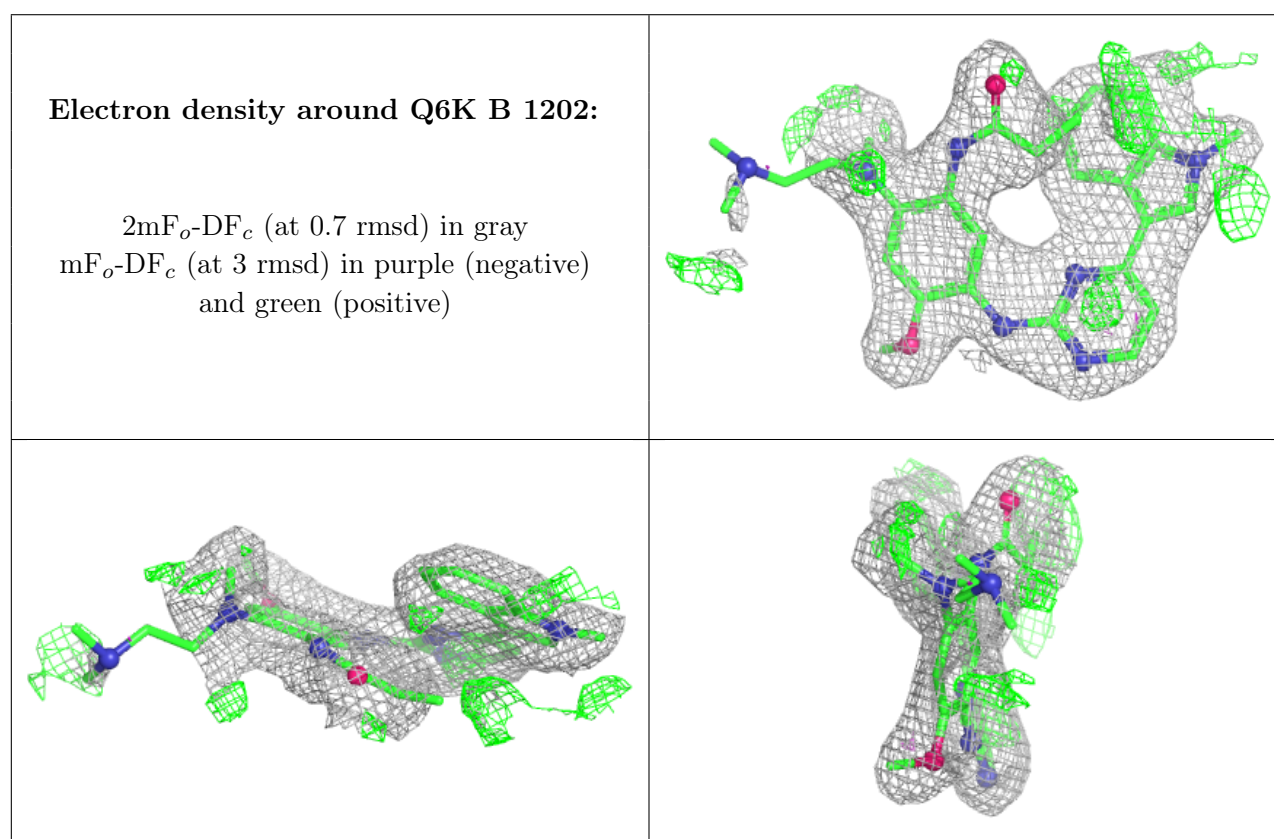
There are no oligosaccharides in this entry.

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, 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.

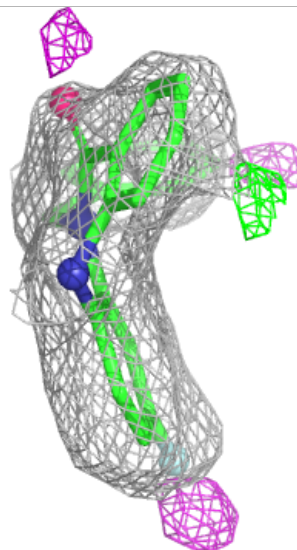
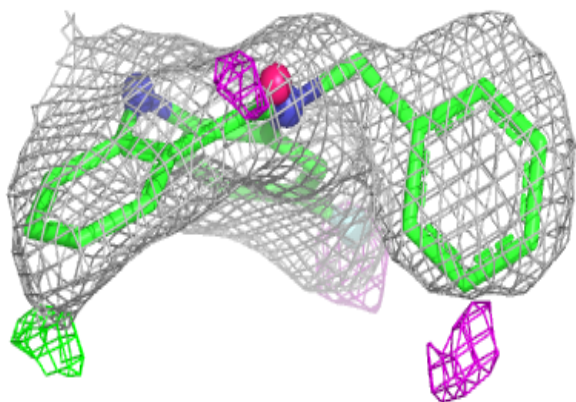
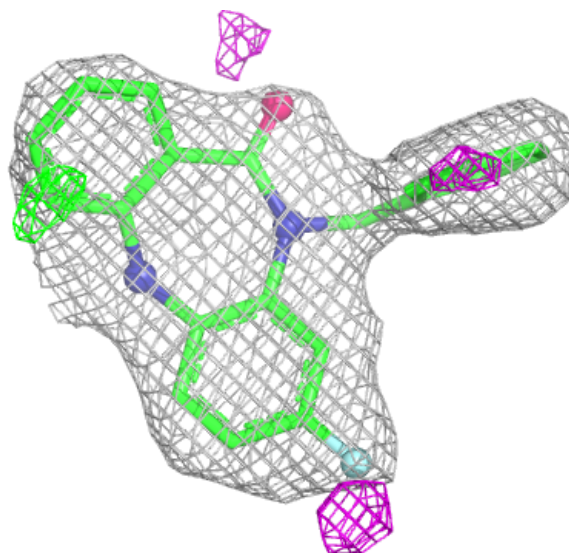
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	Q6K	B	1202	37/37	0.83	0.15	25,39,75,79	0
3	NQ1	B	1201	24/24	0.86	0.10	34,42,50,54	0
3	NQ1	D	1103	24/24	0.87	0.12	33,42,50,53	0
3	NQ1	A	1302	24/24	0.92	0.10	25,31,42,47	0
2	Q6K	A	1301	37/37	0.93	0.10	18,32,45,51	0
5	ANP	D	1102	31/31	0.94	0.07	26,37,43,47	0
4	MG	D	1101	1/1	0.98	0.05	36,36,36,36	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.



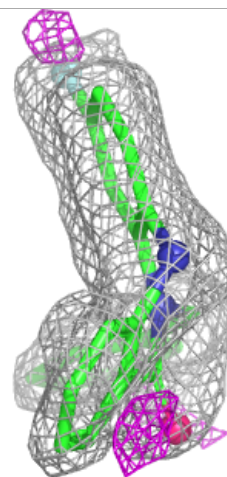
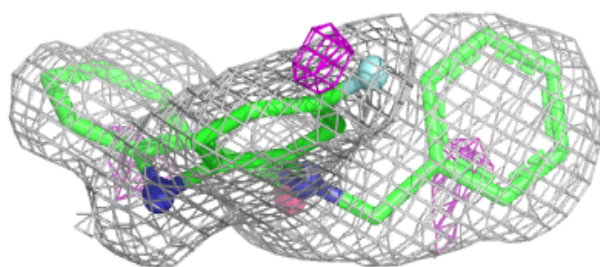
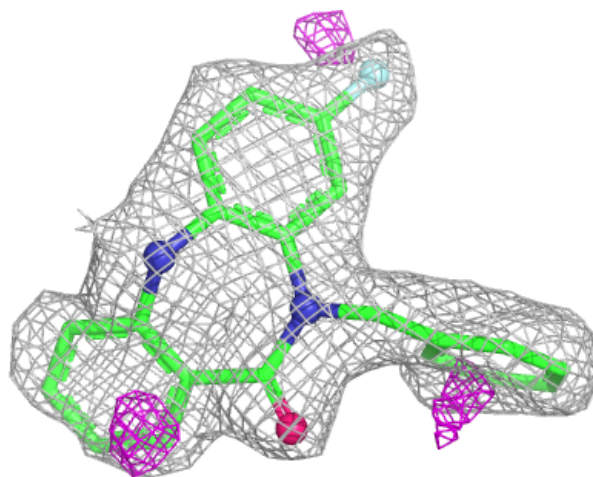
Electron density around NQ1 B 1201:

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



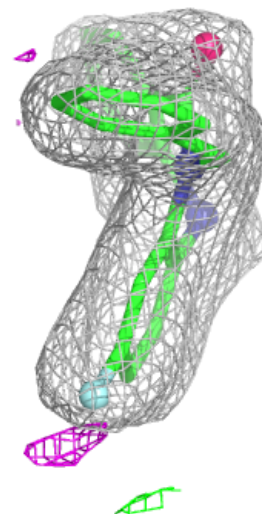
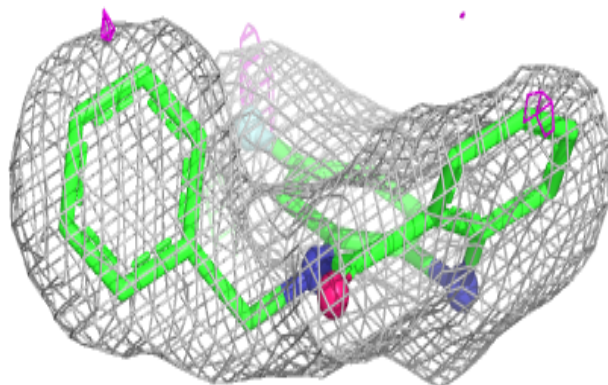
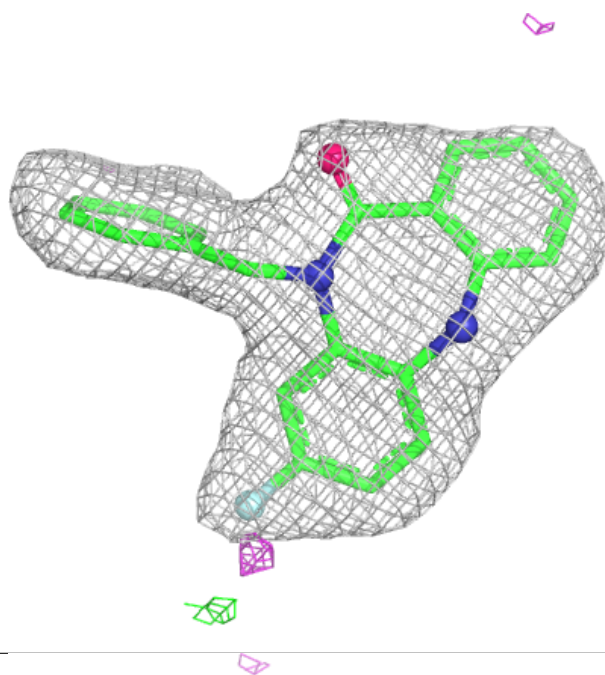
Electron density around NQ1 D 1103:

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



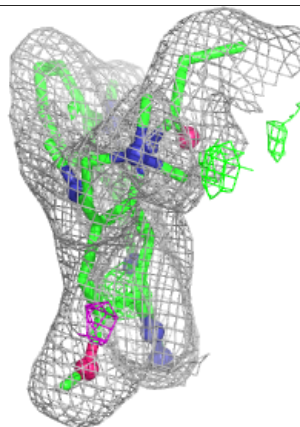
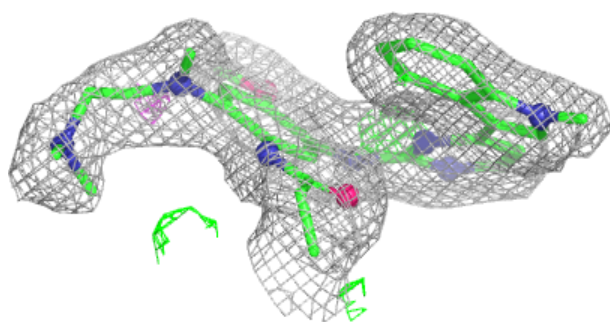
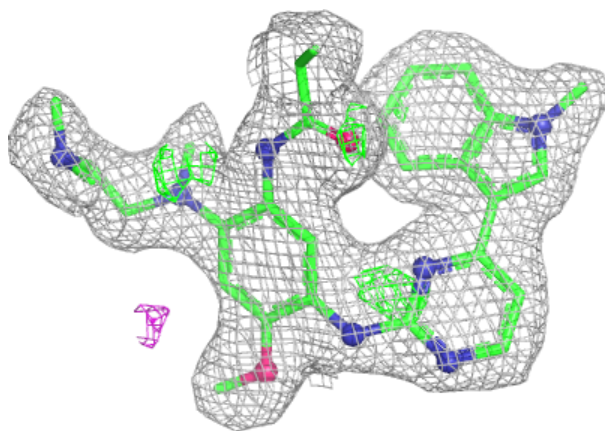
Electron density around NQ1 A 1302:

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

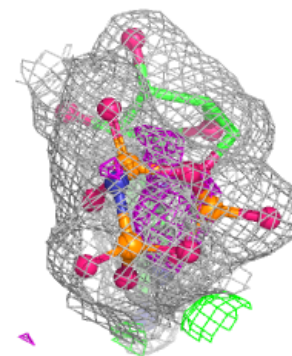
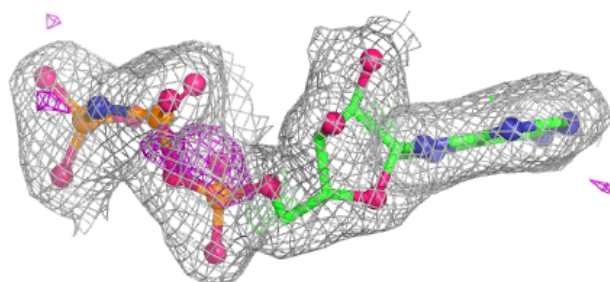
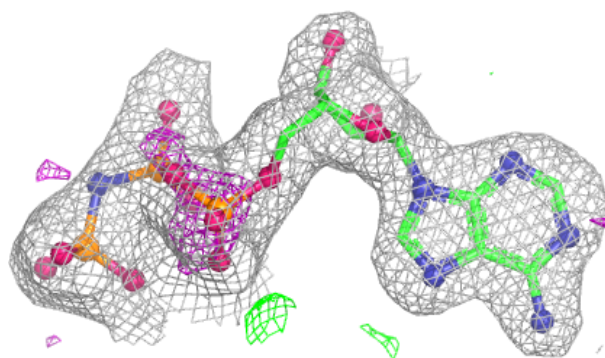


Electron density around Q6K A 1301:

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

**Electron density around ANP D 1102:**

$2mF_o-DF_c$ (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.