Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2024 – 12:07 PM EDT

PDB ID	:	9AXX
Title	:	Crystal structure of BRAF/MEK1 complex with NST-628 and an active RAF dimer
Authors	:	Quade, B.; Huang, X.
Deposited on	:	2024-03-06
Resolution	:	2.07 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:

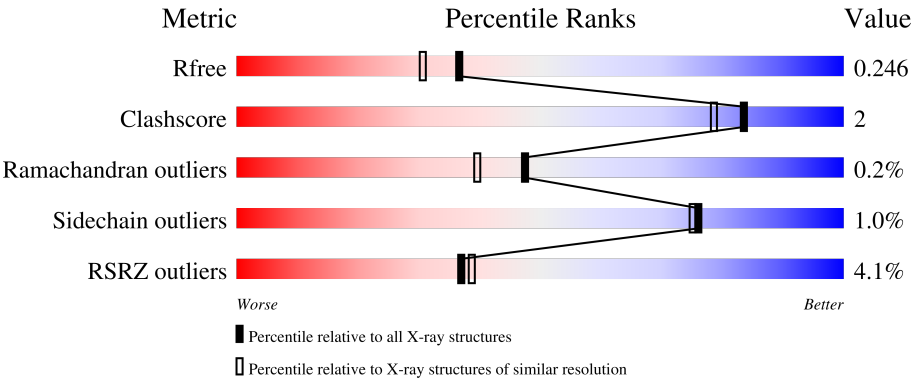
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (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 <=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	310	2% 93% · ·
1	C	310	11% 89% 7% ·
2	B	280	2% 83% 9% · 7%
2	D	280	91% 6% ·

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9276 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 Dual specificity mitogen-activated protein kinase kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	1	0
			2314	1475	392	431	16			
1	C	299	Total	C	N	O	S	0	0	0
			2252	1436	382	419	15			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	GLY	-	expression tag	UNP Q02750
A	218	ALA	SER	engineered mutation	UNP Q02750
A	222	ALA	SER	engineered mutation	UNP Q02750
A	264	GLY	-	linker	UNP Q02750
A	303	SER	-	linker	UNP Q02750
A	304	GLY	-	linker	UNP Q02750
A	305	SER	-	linker	UNP Q02750
A	306	GLY	-	linker	UNP Q02750
A	307	SER	-	linker	UNP Q02750
C	36	GLY	-	expression tag	UNP Q02750
C	218	ALA	SER	engineered mutation	UNP Q02750
C	222	ALA	SER	engineered mutation	UNP Q02750
C	264	GLY	-	linker	UNP Q02750
C	303	SER	-	linker	UNP Q02750
C	304	GLY	-	linker	UNP Q02750
C	305	SER	-	linker	UNP Q02750
C	306	GLY	-	linker	UNP Q02750
C	307	SER	-	linker	UNP Q02750

- Molecule 2 is a protein called Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	261	Total	C	N	O	S	0	1	0
			2040	1315	348	364	13			

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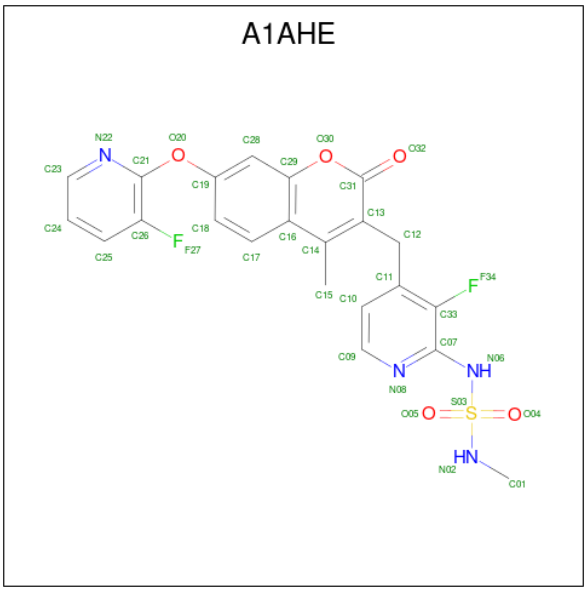
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	272	Total	C	N	O	S	0	0	0
			2141	1372	369	387	13			

There are 2 discrepancies between the modelled and reference sequences:

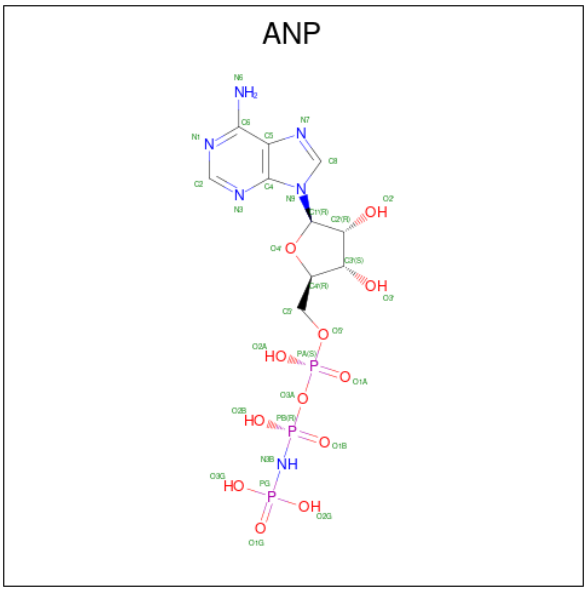
Chain	Residue	Modelled	Actual	Comment	Reference
B	444	GLY	-	expression tag	UNP P15056
D	444	GLY	-	expression tag	UNP P15056

- Molecule 3 is N-[3-fluoro-4-({7-[(3-fluoropyridin-2-yl)oxy]-4-methyl-2-oxo-2H-1-benzopyran-3-yl}methyl)pyridin-2-yl]-N'-methylsulfuric diamide (three-letter code: A1AHE) (formula: $C_{22}H_{18}F_2N_4O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			34	22	2	4	5	1		
3	C	1	Total	C	F	N	O	S	0	0
			34	22	2	4	5	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

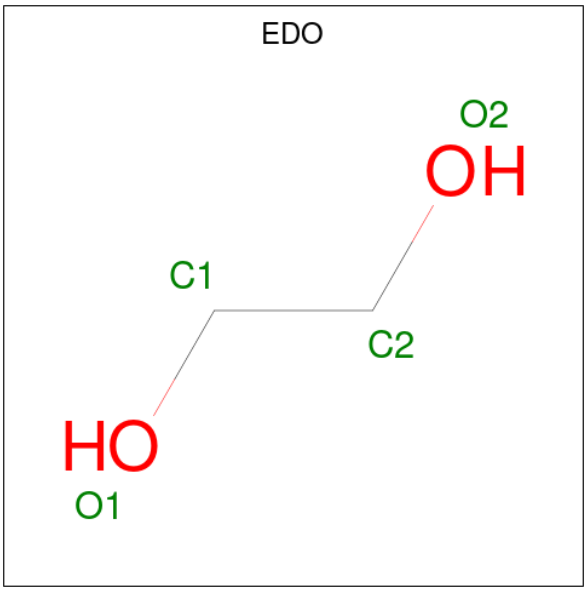


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

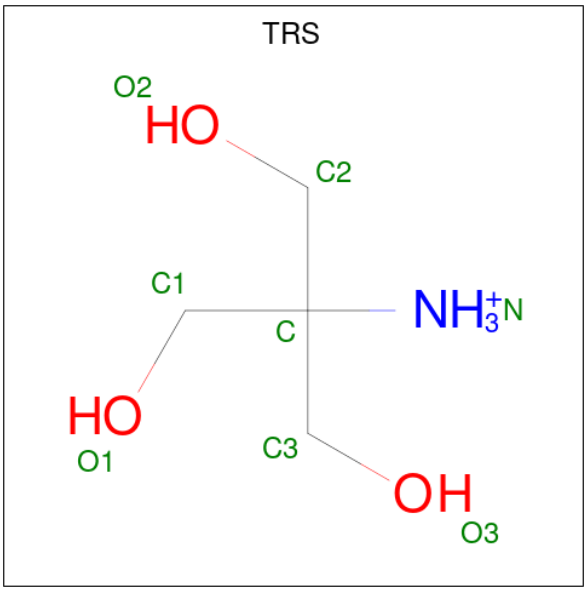
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O 8 4 1 3	0	0

- Molecule 8 is water.

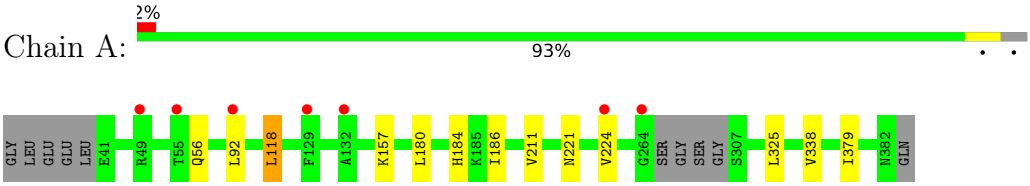
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	92	Total O 92 92	0	0
8	B	76	Total O 76 76	0	0
8	C	36	Total O 36 36	0	0
8	D	110	Total O 110 110	0	0

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.

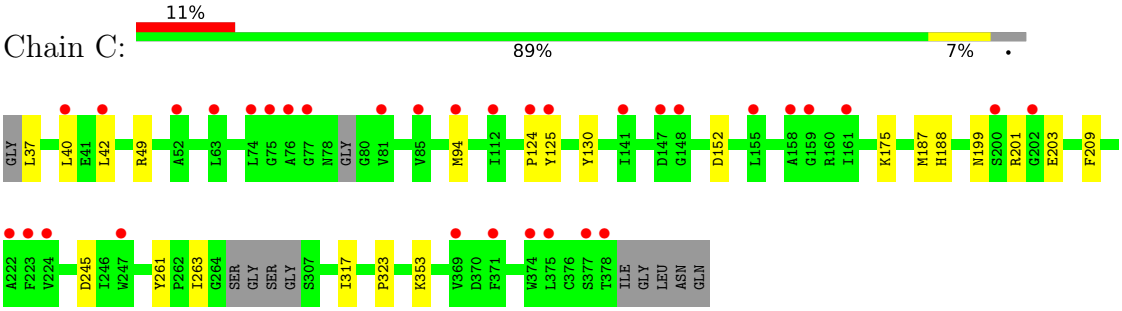
• Molecule 1: Dual specificity mitogen-activated protein kinase kinase 1

Chain A:



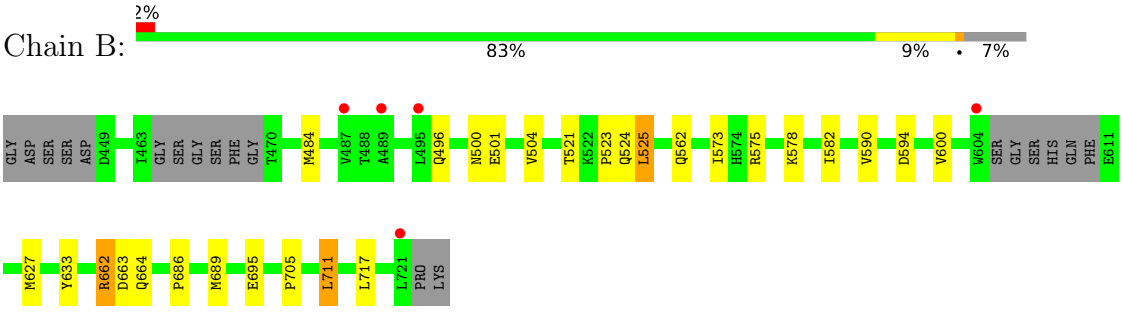
• Molecule 1: Dual specificity mitogen-activated protein kinase kinase 1

Chain C:



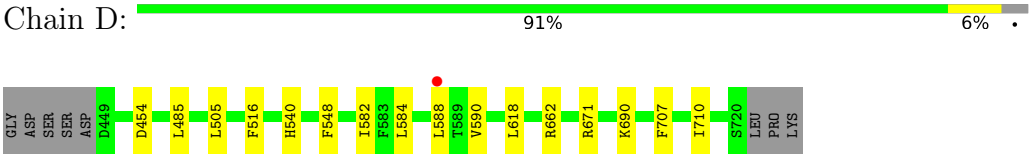
• Molecule 2: Serine/threonine-protein kinase B-raf

Chain B:



• Molecule 2: Serine/threonine-protein kinase B-raf

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.21Å 82.41Å 121.55Å 90.00° 105.65° 90.00°	Depositor
Resolution (Å)	41.20 – 2.07 58.52 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.1 (41.20-2.07) 99.2 (58.52-2.07)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, REFMAC 5	Depositor
R, R_{free}	0.213 , 0.248 0.212 , 0.246	Depositor DCC
R_{free} test set	4080 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9276	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: TRS, ANP, MG, EDO, A1AHE

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	0.26	0/2357	0.47	0/3181
1	C	0.25	0/2293	0.46	0/3103
2	B	0.26	0/2085	0.48	0/2828
2	D	0.27	0/2190	0.49	0/2965
All	All	0.26	0/8925	0.48	0/12077

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	2314	0	2295	7	0
1	C	2252	0	2181	12	0
2	B	2040	0	2003	15	0
2	D	2141	0	2128	10	0
3	A	34	0	0	0	0
3	C	34	0	0	0	0
4	A	31	0	13	0	0
4	B	31	0	13	1	0
4	C	31	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	4	0	6	0	0
6	B	16	0	24	1	0
6	C	4	0	6	2	0
6	D	20	0	30	1	0
7	B	8	0	12	0	0
8	A	92	0	0	0	0
8	B	76	0	0	2	0
8	C	36	0	0	0	0
8	D	110	0	0	0	0
All	All	9276	0	8724	43	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 2.

All (43) 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:C:199:ASN:HD21	1:C:203:GLU:HB2	1.56	0.69
2:B:695:GLU:HG2	2:B:705:PRO:HD3	1.75	0.68
1:A:224:VAL:HA	2:D:662:ARG:HD2	1.76	0.67
1:C:49:ARG:HH12	1:C:201:ARG:HB3	1.61	0.65
1:A:118:LEU:HD13	1:A:211:VAL:HG21	1.84	0.59
2:D:485:LEU:HB2	6:D:804:EDO:H22	1.84	0.59
2:B:686:PRO:HG2	2:B:717:LEU:HD21	1.87	0.54
2:B:689:MET:HB2	2:B:717:LEU:HD11	1.89	0.54
4:B:801:ANP:O2B	4:B:801:ANP:O2G	2.25	0.54
1:A:56:GLN:HB3	1:A:92:LEU:HD21	1.90	0.54
2:D:505:LEU:HB3	2:D:516:PHE:HB2	1.90	0.53
2:B:664:GLN:NE2	8:B:903:HOH:O	2.41	0.53
1:C:317:ILE:HA	6:C:404:EDO:H11	1.90	0.53
2:B:582:ILE:HG23	2:B:590:VAL:HG13	1.92	0.52
2:B:575:ARG:HG2	2:B:633:TYR:CD1	2.46	0.51
2:B:573:ILE:HG22	2:B:575:ARG:HG3	1.93	0.50
1:C:42:LEU:HD21	1:C:124:PRO:HD3	1.94	0.49
1:C:199:ASN:ND2	1:C:203:GLU:HB2	2.26	0.49
2:B:484:MET:HE2	2:B:524:GLN:HB2	1.95	0.48
1:C:261:TYR:CE2	1:C:263:ILE:HB	2.48	0.48
1:C:188:HIS:CD2	1:C:209:PHE:HB3	2.50	0.47
1:A:184:HIS:HB2	1:A:186:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:562:GLN:HA	2:B:711:LEU:HD21	1.96	0.47
2:B:578:LYS:NZ	8:B:907:HOH:O	2.47	0.47
2:D:548:PHE:CE1	2:D:588:LEU:HD21	2.51	0.46
1:C:323:PRO:HD3	6:C:404:EDO:H21	1.98	0.45
2:B:521:THR:HA	2:B:525:LEU:HD12	1.99	0.45
1:A:221:ASN:ND2	2:D:618:LEU:HD11	2.32	0.44
2:B:496:GLN:NE2	2:B:500:ASN:OD1	2.50	0.44
2:B:501:GLU:OE2	6:B:804:EDO:O2	2.35	0.44
2:D:582:ILE:HG23	2:D:590:VAL:HG13	2.00	0.43
1:C:125:TYR:CE2	1:C:175:LYS:HD3	2.53	0.43
2:D:707:PHE:HA	2:D:710:ILE:HB	2.00	0.43
2:D:454:ASP:N	2:D:454:ASP:OD1	2.50	0.43
1:C:94:MET:HG2	1:C:130:TYR:CE2	2.54	0.42
1:A:157:LYS:HD2	1:A:379:ILE:HA	2.01	0.42
1:C:37:LEU:HD12	1:C:40:LEU:HD12	2.02	0.41
2:D:540:HIS:CD2	2:D:584:LEU:HD12	2.56	0.41
2:D:690:LYS:HB3	2:D:690:LYS:HE2	1.87	0.41
2:B:662:ARG:HG2	2:B:663:ASP:N	2.35	0.41
1:C:187:MET:HB2	1:C:245:ASP:OD2	2.21	0.41
1:A:325:LEU:HG	1:A:338:VAL:HG21	2.02	0.41
2:B:504:VAL:HG22	2:B:600:VAL:HG23	2.03	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	297/310 (96%)	292 (98%)	5 (2%)	0	100 100
1	C	293/310 (94%)	284 (97%)	9 (3%)	0	100 100
2	B	256/280 (91%)	250 (98%)	4 (2%)	2 (1%)	19 9
2	D	270/280 (96%)	263 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1116/1180 (95%)	1089 (98%)	25 (2%)	2 (0%)	47 39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	523	PRO
2	B	594	ASP

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	249/265 (94%)	247 (99%)	2 (1%)	81 81
1	C	233/265 (88%)	231 (99%)	2 (1%)	78 78
2	B	214/246 (87%)	210 (98%)	4 (2%)	57 53
2	D	231/246 (94%)	230 (100%)	1 (0%)	91 91
All	All	927/1022 (91%)	918 (99%)	9 (1%)	76 75

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	LEU
1	A	180	LEU
2	B	525	LEU
2	B	627	MET
2	B	662	ARG
2	B	711	LEU
1	C	152	ASP
1	C	353	LYS
2	D	671	ARG

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

Mol	Chain	Res	Type
2	B	612	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	EDO	D	801	-	3,3,3	0.48	0	2,2,2	0.31	0
6	EDO	D	802	-	3,3,3	0.44	0	2,2,2	0.38	0
6	EDO	B	803	-	3,3,3	0.48	0	2,2,2	0.30	0
6	EDO	D	803	-	3,3,3	0.44	0	2,2,2	0.39	0
6	EDO	A	404	-	3,3,3	0.51	0	2,2,2	0.26	0
6	EDO	B	805	-	3,3,3	0.45	0	2,2,2	0.34	0
6	EDO	C	404	-	3,3,3	0.44	0	2,2,2	0.23	0
7	TRS	B	802	-	7,7,7	0.34	0	9,9,9	0.40	0
3	A1AHE	A	401	-	36,37,37	1.30	3 (8%)	50,54,54	1.48	10 (20%)
3	A1AHE	C	401	-	36,37,37	1.21	3 (8%)	50,54,54	1.50	8 (16%)
4	ANP	C	402	5	29,33,33	1.09	3 (10%)	31,52,52	1.06	2 (6%)
6	EDO	B	804	-	3,3,3	0.45	0	2,2,2	0.44	0
6	EDO	D	804	-	3,3,3	0.46	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	D	805	-	3,3,3	0.45	0	2,2,2	0.34	0
4	ANP	B	801	-	29,33,33	1.07	4 (13%)	31,52,52	1.08	3 (9%)
6	EDO	B	806	-	3,3,3	0.52	0	2,2,2	0.21	0
4	ANP	A	402	5	29,33,33	1.11	4 (13%)	31,52,52	1.11	3 (9%)

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	EDO	D	801	-	-	0/1/1/1	-
6	EDO	D	802	-	-	0/1/1/1	-
6	EDO	B	803	-	-	0/1/1/1	-
6	EDO	D	803	-	-	0/1/1/1	-
6	EDO	A	404	-	-	0/1/1/1	-
6	EDO	B	805	-	-	0/1/1/1	-
6	EDO	C	404	-	-	1/1/1/1	-
7	TRS	B	802	-	-	3/9/9/9	-
3	A1AHE	A	401	-	-	2/14/16/16	0/4/4/4
3	A1AHE	C	401	-	-	2/14/16/16	0/4/4/4
4	ANP	C	402	5	-	2/14/38/38	0/3/3/3
6	EDO	B	804	-	-	0/1/1/1	-
6	EDO	D	804	-	-	1/1/1/1	-
6	EDO	D	805	-	-	0/1/1/1	-
4	ANP	B	801	-	-	7/14/38/38	0/3/3/3
6	EDO	B	806	-	-	0/1/1/1	-
4	ANP	A	402	5	-	2/14/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	A1AHE	S03-N02	4.61	1.66	1.61
3	C	401	A1AHE	S03-N02	3.08	1.65	1.61
3	C	401	A1AHE	C26-C21	3.07	1.42	1.38
4	A	402	ANP	PG-N3B	2.80	1.70	1.63
3	A	401	A1AHE	C01-N02	2.61	1.49	1.46
4	A	402	ANP	PG-O1G	2.54	1.50	1.46
4	C	402	ANP	PG-N3B	2.53	1.70	1.63
4	B	801	ANP	PG-O1G	2.50	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402	ANP	PG-O1G	2.49	1.50	1.46
4	B	801	ANP	PG-N3B	2.49	1.69	1.63
4	C	402	ANP	PB-O1B	2.45	1.50	1.46
4	B	801	ANP	PB-O1B	2.44	1.50	1.46
4	A	402	ANP	PB-N3B	2.25	1.69	1.63
4	A	402	ANP	PB-O1B	2.23	1.49	1.46
3	A	401	A1AHE	F34-C33	-2.13	1.31	1.35
3	C	401	A1AHE	C21-N22	2.02	1.36	1.32
4	B	801	ANP	PB-N3B	2.00	1.68	1.63

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	A1AHE	O30-C31-C13	4.15	122.33	118.01
3	A	401	A1AHE	C11-C12-C13	3.74	120.56	114.12
3	A	401	A1AHE	O30-C31-C13	3.62	121.78	118.01
3	C	401	A1AHE	O30-C31-O32	-3.48	111.61	116.22
3	A	401	A1AHE	O30-C31-O32	-3.29	111.87	116.22
3	C	401	A1AHE	C11-C12-C13	3.26	119.72	114.12
4	C	402	ANP	PB-O3A-PA	-2.98	122.13	132.62
4	A	402	ANP	O1B-PB-N3B	-2.83	107.61	111.77
3	C	401	A1AHE	C33-C07-N06	2.78	124.00	120.30
3	A	401	A1AHE	C33-C07-N06	2.73	123.94	120.30
3	A	401	A1AHE	C33-C07-N08	2.69	120.62	119.33
3	C	401	A1AHE	C33-C07-N08	2.69	120.62	119.33
3	A	401	A1AHE	C29-O30-C31	-2.63	119.68	122.23
4	B	801	ANP	PB-O3A-PA	-2.61	123.42	132.62
3	C	401	A1AHE	C17-C16-C29	-2.54	114.88	118.21
3	A	401	A1AHE	C15-C14-C16	-2.30	116.00	118.57
4	B	801	ANP	O1B-PB-N3B	-2.28	108.41	111.77
4	B	801	ANP	C5-C6-N6	2.28	123.81	120.35
3	A	401	A1AHE	C10-C11-C33	-2.24	114.81	116.43
4	C	402	ANP	C5-C6-N6	2.24	123.75	120.35
4	A	402	ANP	PB-O3A-PA	-2.24	124.74	132.62
4	A	402	ANP	C5-C6-N6	2.22	123.73	120.35
3	A	401	A1AHE	C17-C16-C29	-2.17	115.37	118.21
3	C	401	A1AHE	N06-S03-N02	-2.16	103.55	109.84
3	C	401	A1AHE	C29-O30-C31	-2.15	120.14	122.23
3	A	401	A1AHE	N06-S03-N02	-2.01	103.99	109.84

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	ANP	PB-N3B-PG-O1G
4	B	801	ANP	PB-N3B-PG-O1G
4	B	801	ANP	PG-N3B-PB-O1B
4	B	801	ANP	PA-O3A-PB-O1B
4	B	801	ANP	C5'-O5'-PA-O1A
4	C	402	ANP	PB-N3B-PG-O1G
7	B	802	TRS	N-C-C2-O2
4	B	801	ANP	C3'-C4'-C5'-O5'
4	B	801	ANP	O4'-C4'-C5'-O5'
6	C	404	EDO	O1-C1-C2-O2
6	D	804	EDO	O1-C1-C2-O2
4	A	402	ANP	PB-O3A-PA-O5'
7	B	802	TRS	C3-C-C2-O2
4	B	801	ANP	PG-N3B-PB-O3A
7	B	802	TRS	C2-C-C3-O3
3	A	401	A1AHE	C01-N02-S03-O05
3	C	401	A1AHE	C01-N02-S03-O05
3	A	401	A1AHE	N08-C07-N06-S03
4	C	402	ANP	C3'-C4'-C5'-O5'
3	C	401	A1AHE	C11-C12-C13-C14

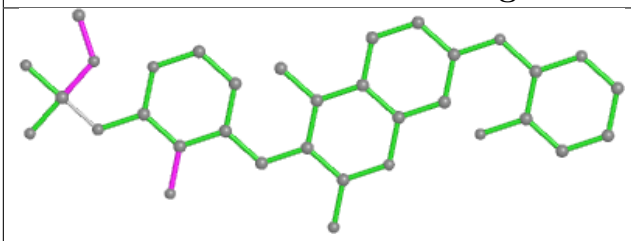
There are no ring outliers.

4 monomers are involved in 5 short contacts:

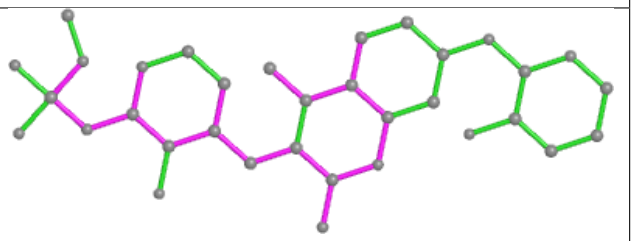
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	404	EDO	2	0
6	B	804	EDO	1	0
6	D	804	EDO	1	0
4	B	801	ANP	1	0

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

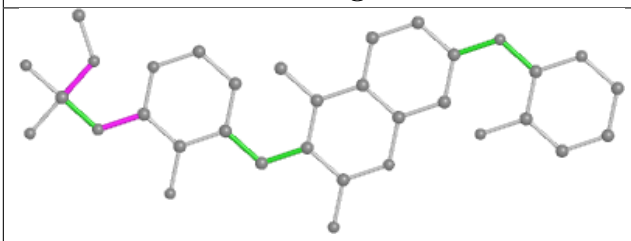
Ligand A1AHE A 401



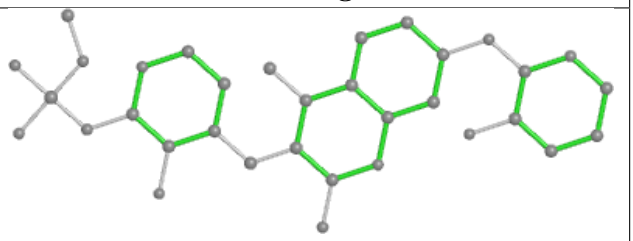
Bond lengths



Bond angles

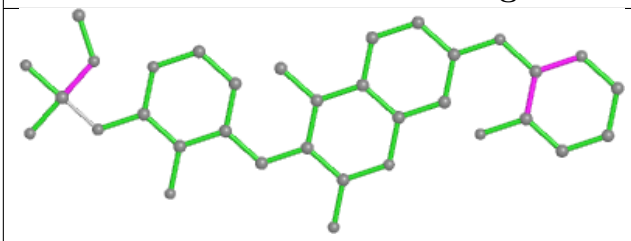


Torsions

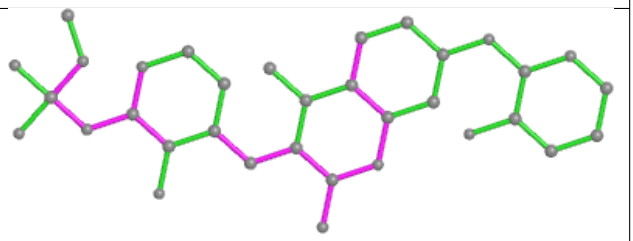


Rings

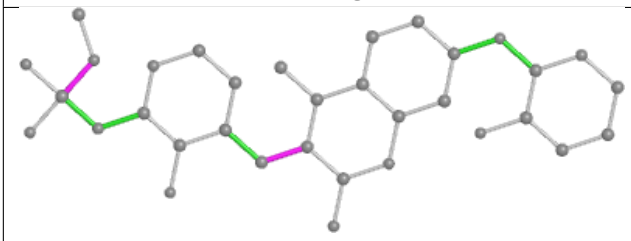
Ligand A1AHE C 401



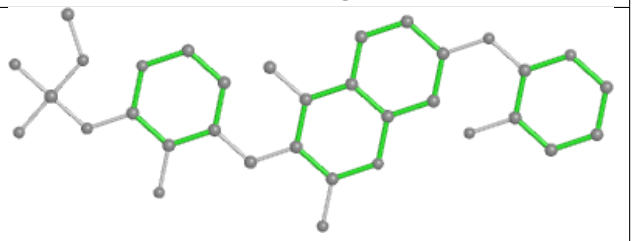
Bond lengths



Bond angles

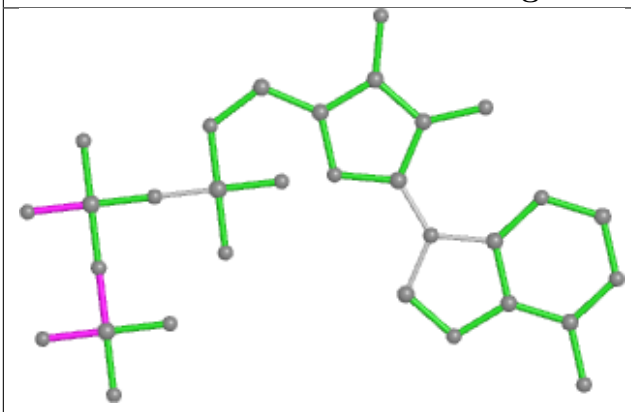


Torsions

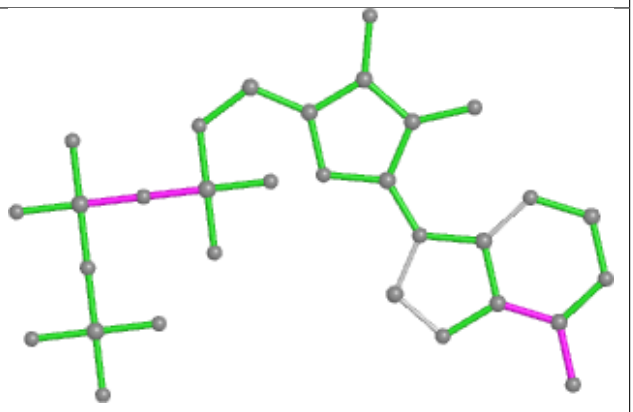


Rings

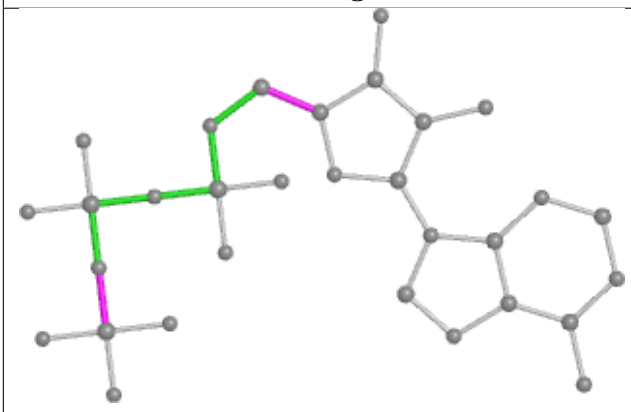
Ligand ANP C 402



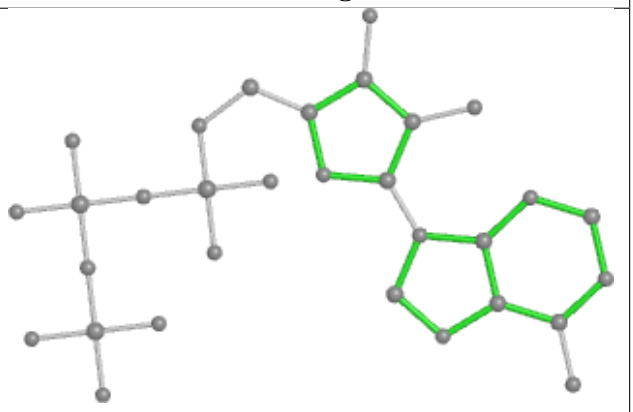
Bond lengths



Bond angles

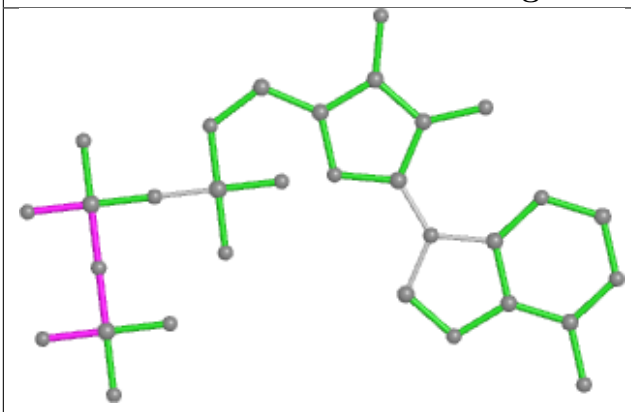


Torsions

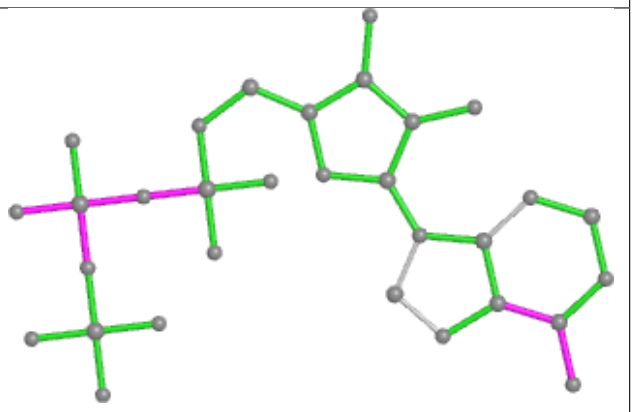


Rings

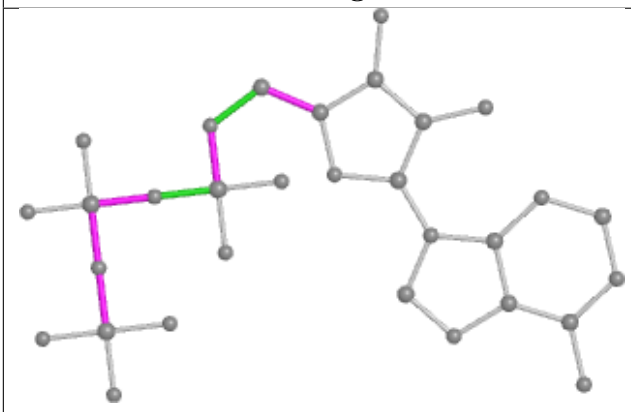
Ligand ANP B 801



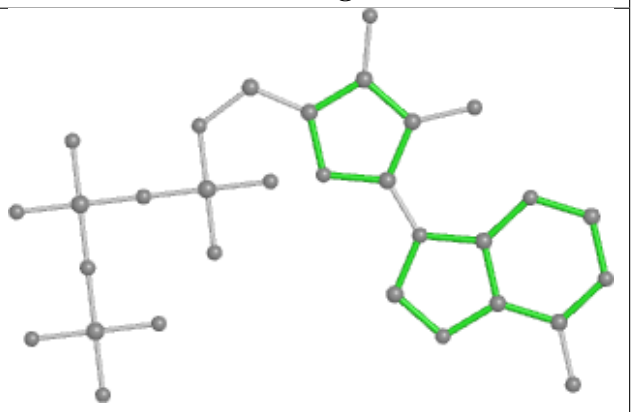
Bond lengths



Bond angles

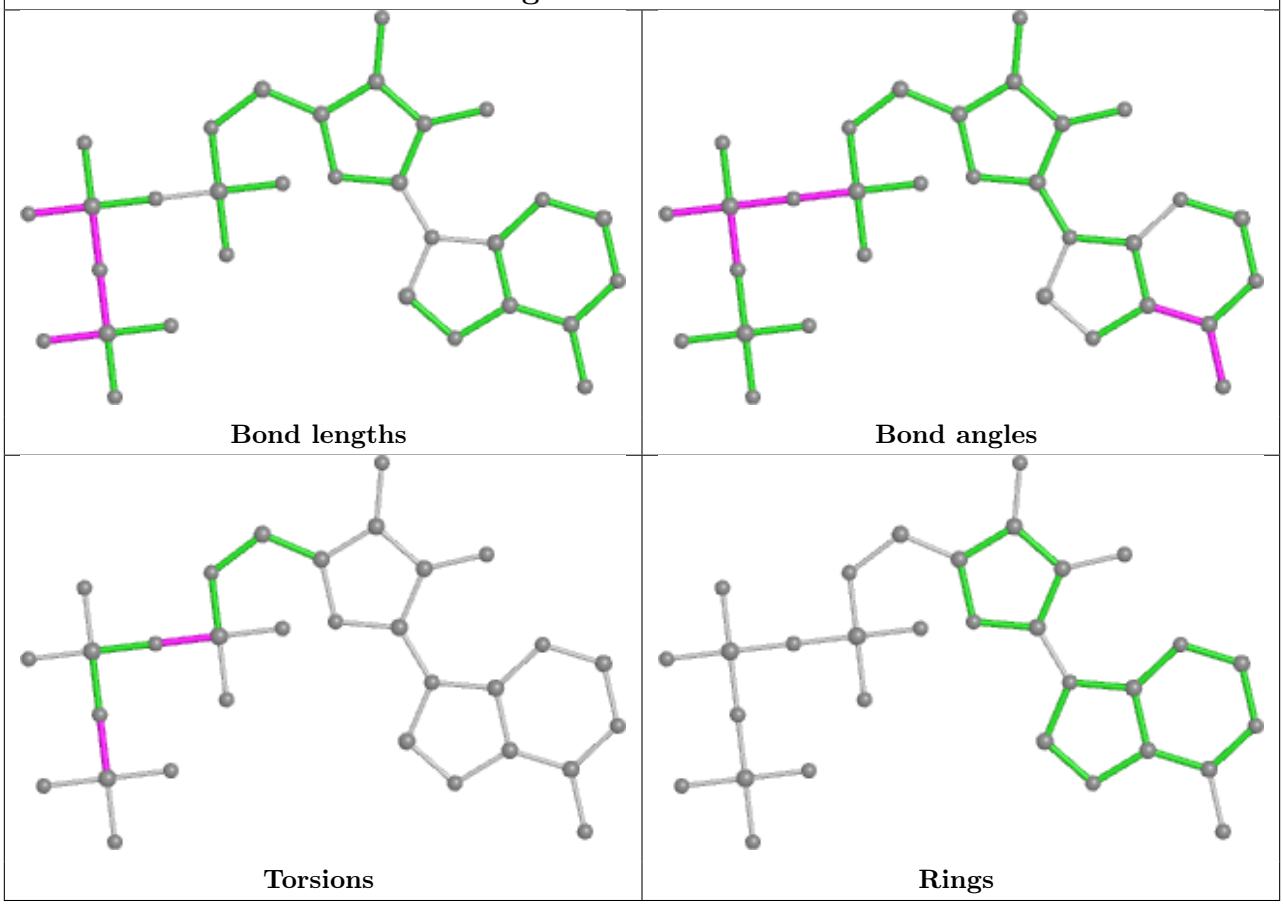


Torsions



Rings

Ligand ANP A 402



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	300/310 (96%)	0.35	7 (2%) 60 63	33, 53, 96, 125	0
1	C	299/310 (96%)	0.71	33 (11%) 5 5	46, 80, 112, 127	0
2	B	261/280 (93%)	0.15	5 (1%) 66 68	29, 50, 88, 114	0
2	D	272/280 (97%)	0.06	1 (0%) 92 93	29, 46, 70, 107	0
All	All	1132/1180 (95%)	0.33	46 (4%) 37 39	29, 56, 103, 127	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	223	PHE	6.4
2	D	588	LEU	5.9
1	C	40	LEU	5.5
1	C	375	LEU	5.0
1	A	92	LEU	4.6
1	C	374	TRP	4.5
1	C	52	ALA	4.1
1	C	371	PHE	4.0
1	C	200	SER	3.9
1	C	76	ALA	3.8
1	C	112	ILE	3.7
1	C	378	THR	3.5
1	C	161	ILE	3.5
1	C	158	ALA	3.5
1	C	155	LEU	3.4
1	C	42	LEU	3.3
1	C	224	VAL	3.0
1	C	125	TYR	2.9
1	C	94	MET	2.9
1	C	77	GLY	2.8
1	C	369	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	222	ALA	2.7
1	C	202	GLY	2.7
2	B	721	LEU	2.7
1	C	377	SER	2.6
1	C	81	VAL	2.5
2	B	489	ALA	2.5
1	A	55	THR	2.5
1	C	74	LEU	2.5
2	B	495	LEU	2.4
1	C	147	ASP	2.4
1	C	75	GLY	2.4
1	A	132	ALA	2.4
2	B	604	TRP	2.4
1	C	63	LEU	2.3
1	C	148	GLY	2.3
1	A	49	ARG	2.3
1	C	159	GLY	2.2
1	C	85	VAL	2.1
2	B	487	VAL	2.1
1	C	124	PRO	2.1
1	A	129	PHE	2.1
1	C	247	TRP	2.0
1	A	224	VAL	2.0
1	A	264	GLY	2.0
1	C	141	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

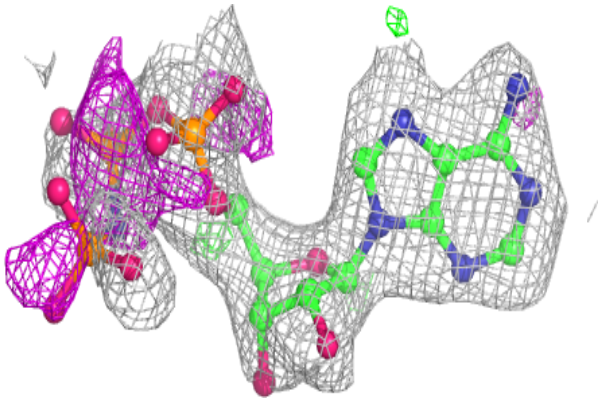
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

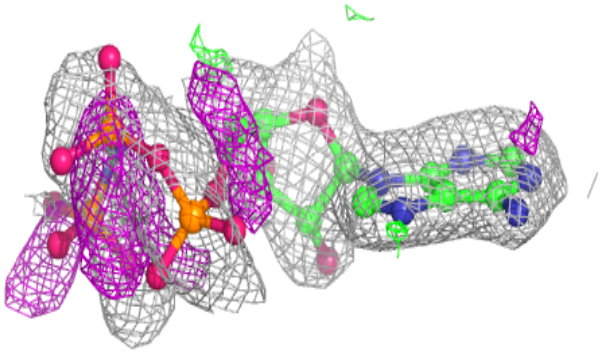
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	B	806	4/4	0.71	0.19	46,47,49,52	0
5	MG	C	403	1/1	0.72	0.07	65,65,65,65	0
4	ANP	B	801	31/31	0.79	0.29	49,84,134,141	0
6	EDO	A	404	4/4	0.81	0.19	42,49,54,55	0
7	TRS	B	802	8/8	0.81	0.20	52,61,67,72	0
6	EDO	D	804	4/4	0.82	0.20	48,53,56,61	0
6	EDO	D	805	4/4	0.83	0.29	53,56,58,58	0
6	EDO	B	805	4/4	0.84	0.17	80,80,81,85	0
6	EDO	B	803	4/4	0.88	0.27	57,59,62,70	0
5	MG	A	403	1/1	0.88	0.13	42,42,42,42	0
6	EDO	D	803	4/4	0.89	0.30	62,63,64,65	0
6	EDO	C	404	4/4	0.89	0.31	56,59,59,61	0
4	ANP	C	402	31/31	0.90	0.18	69,81,87,91	0
6	EDO	D	802	4/4	0.92	0.14	42,43,48,52	0
6	EDO	D	801	4/4	0.93	0.11	34,39,40,42	0
3	A1AHE	C	401	34/34	0.94	0.18	39,47,65,68	0
3	A1AHE	A	401	34/34	0.95	0.14	36,45,52,54	0
6	EDO	B	804	4/4	0.96	0.13	44,47,47,52	0
4	ANP	A	402	31/31	0.96	0.13	37,47,52,59	0

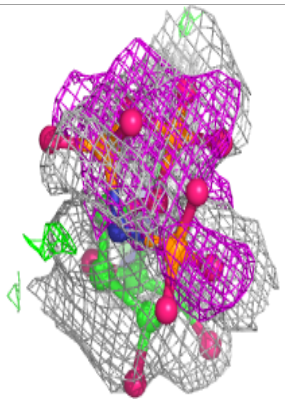
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP B 801:

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

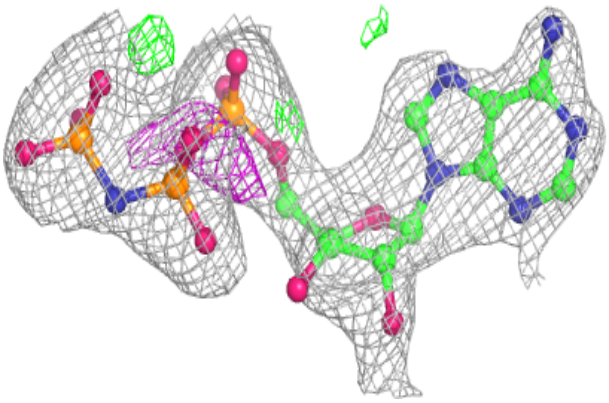


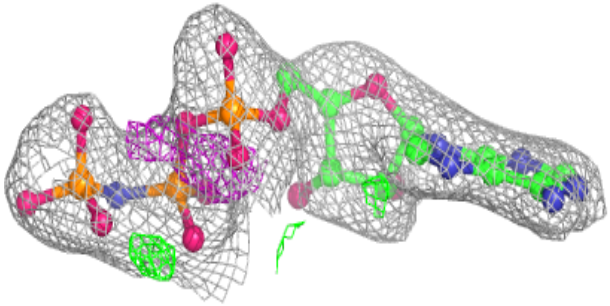


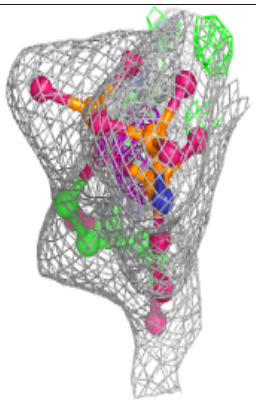


Electron density around ANP C 402:

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

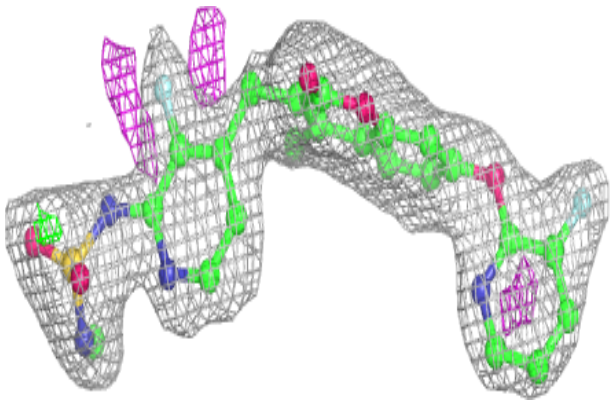


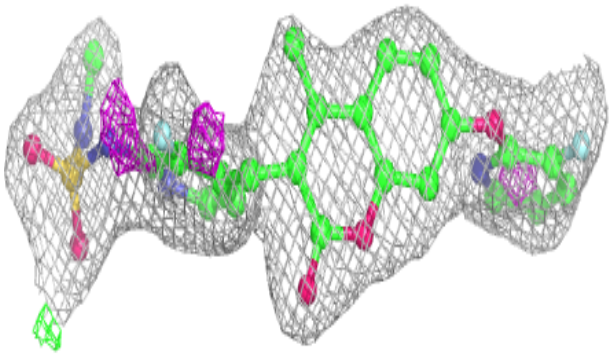


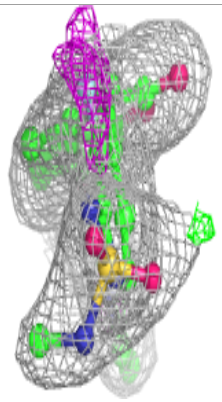


Electron density around A1AHE C 401:

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

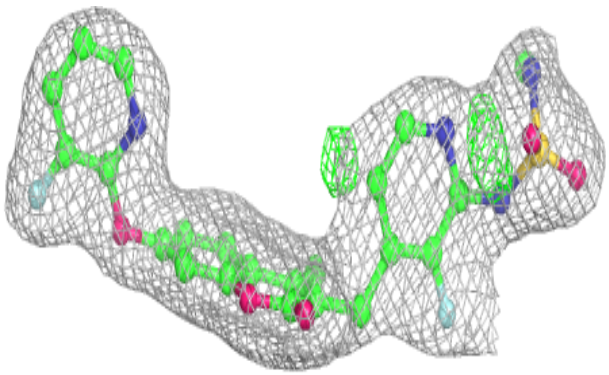


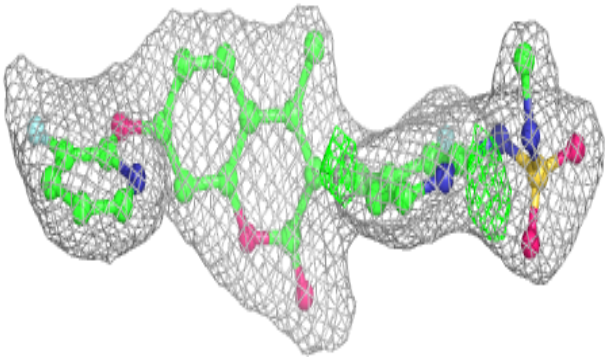


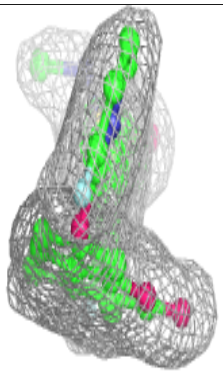


Electron density around A1AHE A 401:

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

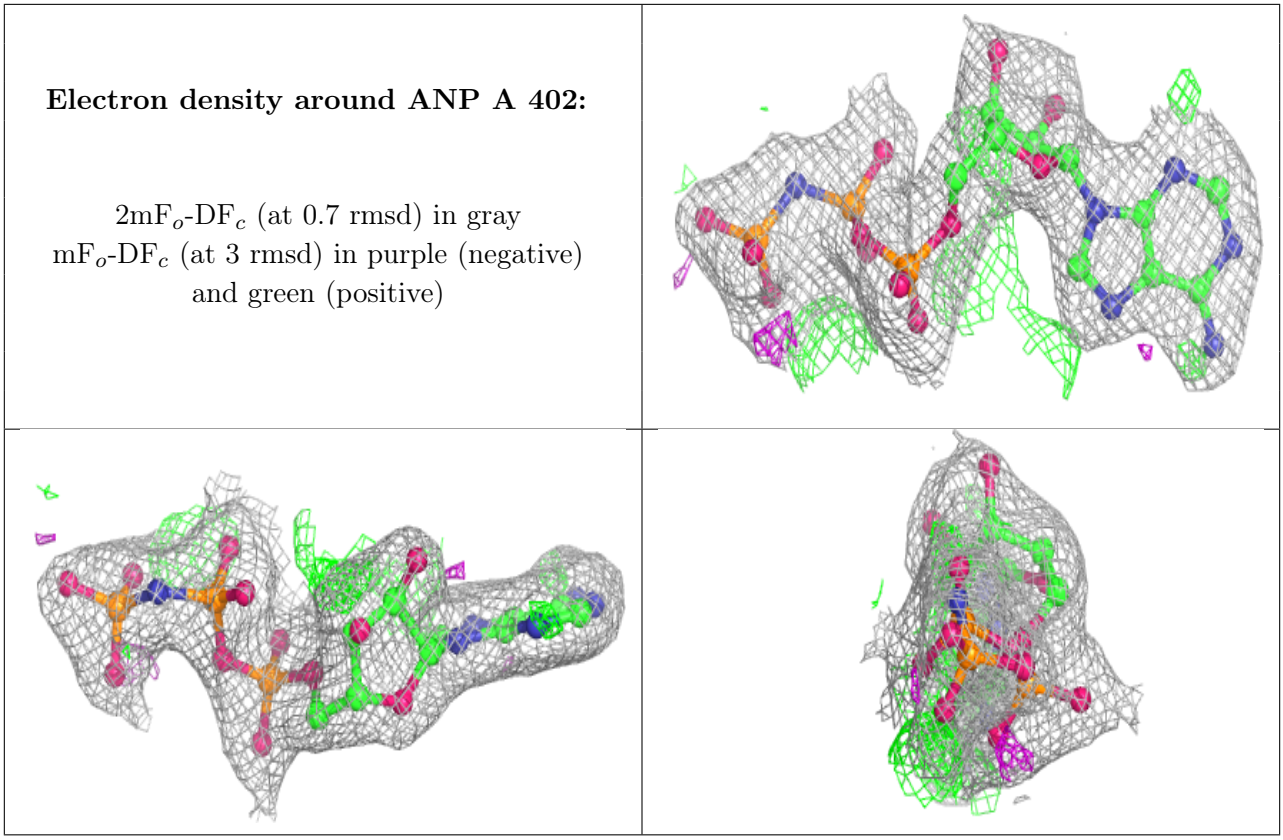






Electron density around ANP A 402:

$2mF_o$-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.