



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:08 PM UTC

PDB ID : 9AXM / pdb_00009axm
Title : Crystal structure of ARAF/MEK1 complex with NST-628 and a RAF dimer
Authors : Quade, B.; Huang, X.
Deposited on : 2024-03-06
Resolution : 2.42 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

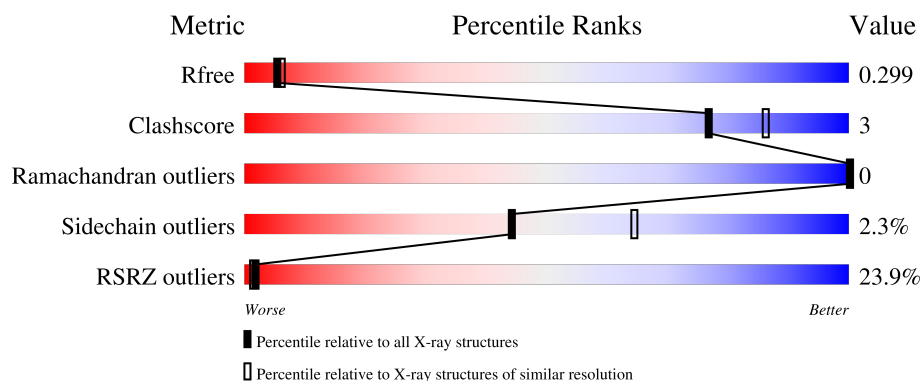
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	310	9% 90% 9%
1	C	310	59% 89% 5% 6%
2	B	280	6% 81% 9% 9%
2	D	280	13% 84% 6% 9%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8435 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	305	Total	C	N	O	S	0	1	0
			2333	1486	398	433	16			
1	C	291	Total	C	N	O	S	0	0	0
			1879	1169	334	365	11			

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	265	SER	-	linker	UNP Q02750
A	266	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 A-Raf.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	254	Total	C	N	O	S	0	0	0
			1983	1272	347	350	14			

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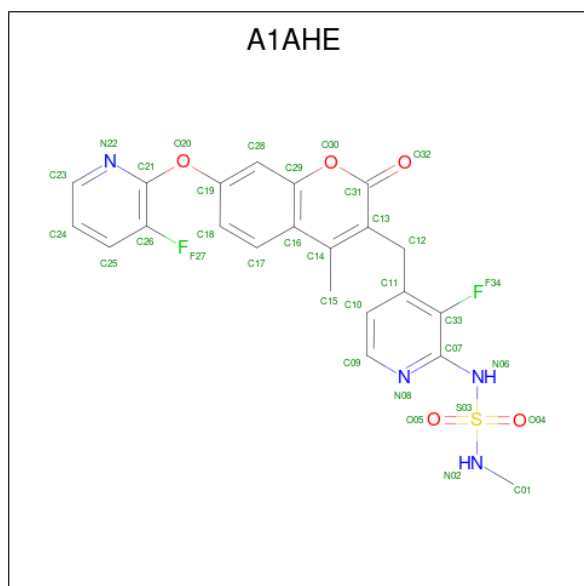
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	256	Total	C	N	O	S	0	0	0
			1969	1266	336	354	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	297	GLY	-	expression tag	UNP P10398
B	301	ASP	TYR	engineered mutation	UNP P10398
B	302	ASP	TYR	engineered mutation	UNP P10398
D	297	GLY	-	expression tag	UNP P10398
D	301	ASP	TYR	engineered mutation	UNP P10398
D	302	ASP	TYR	engineered mutation	UNP P10398

- 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 (CCD ID: A1AHE) (formula: C₂₂H₁₈F₂N₄O₅S) (labeled as "Ligand of Interest" by depositor).

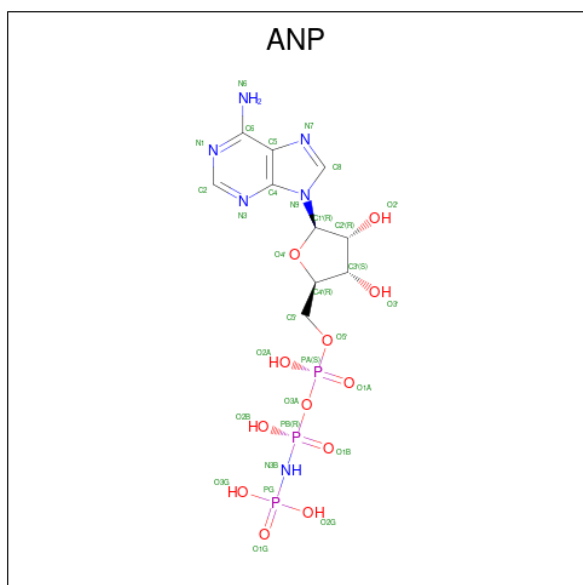


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			34	22	2	4	5	1		
3	C	1	Total	C	F	N	O	S	0	0
			34	22	2	4	5	1		

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

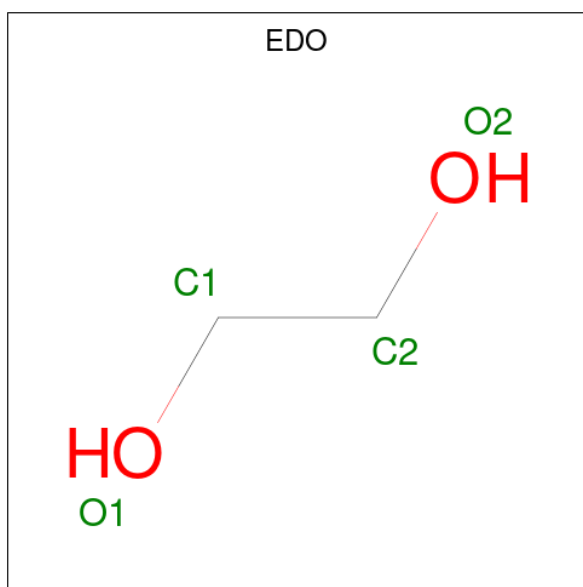
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



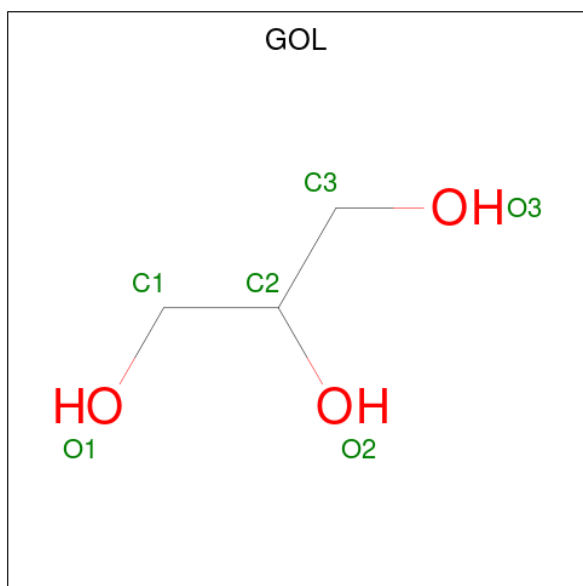
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 31 10 6 12 3	0	0
5	B	1	Total C N O P 31 10 6 12 3	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

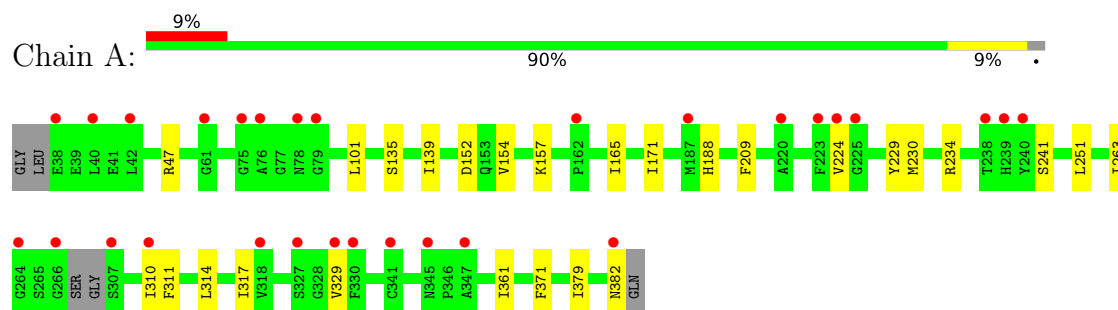
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	23	Total 23	O 23	0	0
8	B	40	Total 40	O 40	0	0
8	C	21	Total 21	O 21	0	0
8	D	33	Total 33	O 33	0	0

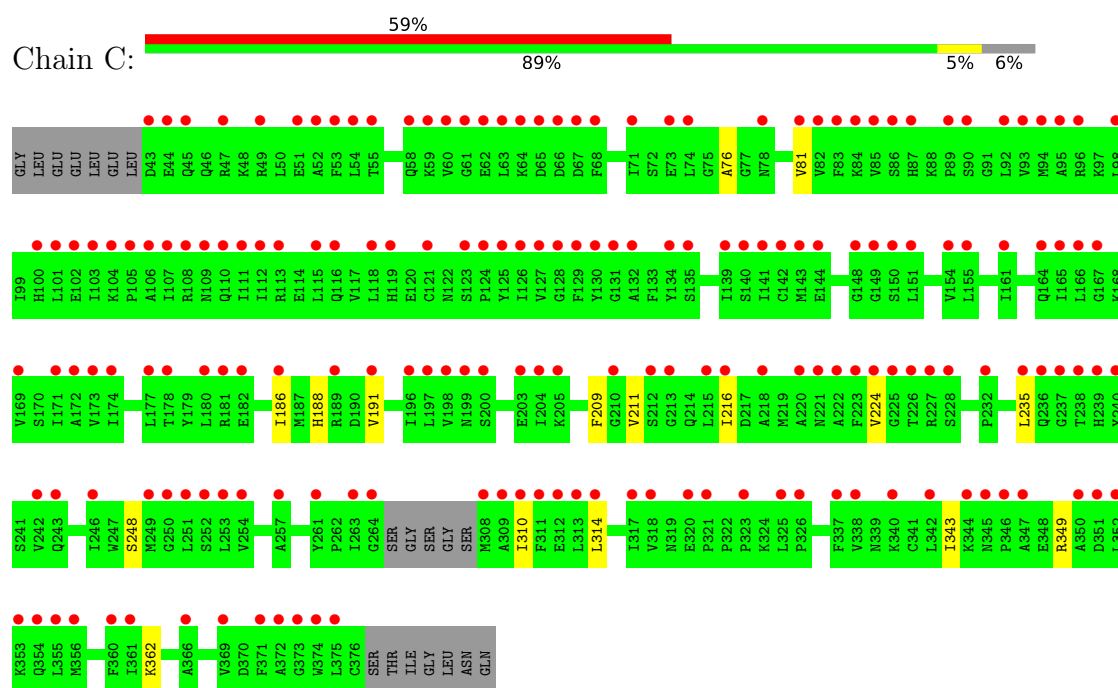
3 Residue-property plots [i](#)

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.

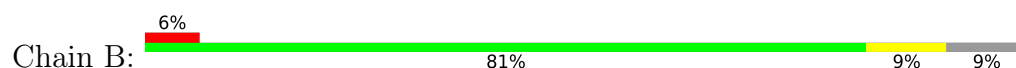
- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 1

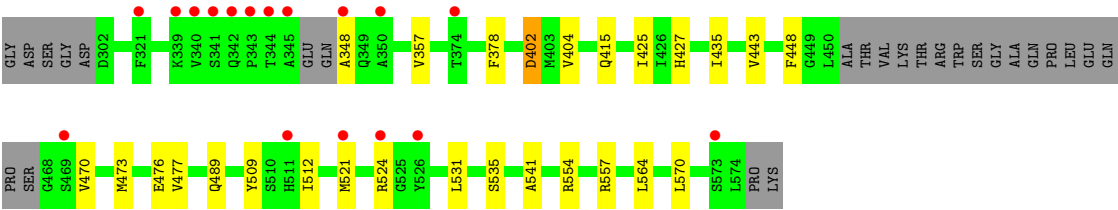


- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 1

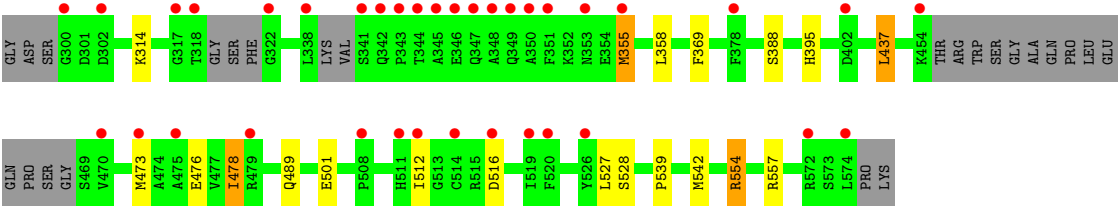
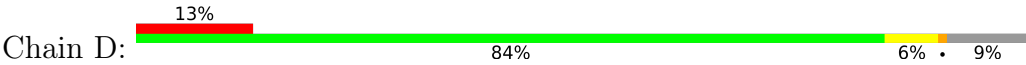


- Molecule 2: Serine/threonine-protein kinase A-Raf





● Molecule 2: Serine/threonine-protein kinase A-Raf



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	80.21Å 173.43Å 187.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.46 – 2.42 47.46 – 2.42	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.46-2.42) 100.0 (47.46-2.42)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, REFMAC 5	Depositor
R, R_{free}	0.260 , 0.301 0.260 , 0.299	Depositor DCC
R_{free} test set	2546 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8435	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, A1AHE, GOL, EDO

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	0.08	0/2376	0.25	0/3209
1	C	0.06	0/1908	0.26	0/2607
2	B	0.09	0/2029	0.25	0/2750
2	D	0.08	0/2012	0.24	0/2731
All	All	0.08	0/8325	0.25	0/11297

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2333	0	2301	15	0
1	C	1879	0	1488	9	0
2	B	1983	0	1934	14	0
2	D	1969	0	1915	12	0
3	A	34	0	0	0	0
3	C	34	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	31	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	31	0	13	0	0
6	B	4	0	6	0	0
7	C	6	0	8	0	0
7	D	12	0	16	0	0
8	A	23	0	0	0	0
8	B	40	0	0	0	0
8	C	21	0	0	0	0
8	D	33	0	0	0	0
All	All	8435	0	7694	46	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 3.

All (46) 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:A:263:ILE:HD13	1:A:317:ILE:HG12	1.72	0.70
1:A:230:MET:HE1	1:A:234:ARG:HB3	1.78	0.65
1:A:157:LYS:HZ1	1:A:382:ASN:HB2	1.67	0.59
2:D:476:GLU:OE2	2:D:557:ARG:NH2	2.37	0.58
2:B:357:VAL:HG13	2:B:425:ILE:HD12	1.88	0.56
2:D:476:GLU:HG3	2:D:554:ARG:HH11	1.70	0.56
1:C:343:ILE:O	1:C:349:ARG:NH1	2.42	0.53
1:C:235:LEU:HD21	1:C:314:LEU:HD22	1.92	0.52
2:B:473:MET:HE3	2:B:477:VAL:HG12	1.92	0.52
1:A:224:VAL:HG13	2:B:470:VAL:HG12	1.92	0.51
2:D:473:MET:HE2	2:D:478:ILE:HG13	1.93	0.51
1:A:229:TYR:HA	1:A:251:LEU:HD23	1.94	0.50
2:B:509:TYR:HB3	2:B:512:ILE:HD12	1.96	0.48
2:D:314:LYS:HD3	2:D:314:LYS:HA	1.75	0.48
1:A:311:PHE:HZ	2:B:524:ARG:HG2	1.79	0.47
2:B:348:ALA:HA	2:B:378:PHE:CZ	2.50	0.47
2:D:512:ILE:HD13	2:D:527:LEU:HD21	1.97	0.47
2:B:402:ASP:HB2	2:B:404:VAL:HG12	1.97	0.46
1:A:101:LEU:HD12	1:A:139:ILE:HD12	1.97	0.46
2:D:437:LEU:HD23	2:D:437:LEU:HA	1.77	0.46
1:A:165:ILE:HD12	1:A:371:PHE:HD1	1.81	0.46
2:D:539:PRO:HG2	2:D:542:MET:HB2	1.99	0.45
1:A:310:ILE:O	1:A:314:LEU:HG	2.15	0.45
1:A:311:PHE:CZ	2:B:524:ARG:HG2	2.52	0.45
2:B:476:GLU:OE2	2:B:557:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:HIS:CD2	1:A:209:PHE:HB3	2.52	0.44
1:C:188:HIS:HA	1:C:209:PHE:HB2	1.97	0.44
2:B:489:GLN:HG2	2:B:554:ARG:O	2.17	0.44
1:C:235:LEU:HD21	2:D:516:ASP:HB3	1.99	0.44
1:A:171:ILE:HG12	1:A:361:ILE:HG23	2.00	0.43
2:B:415:GLN:NE2	2:B:564:LEU:HD21	2.33	0.43
1:A:230:MET:HB3	1:A:230:MET:HE3	1.52	0.43
1:C:362:LYS:HB3	1:C:362:LYS:HE2	1.61	0.43
2:B:427:HIS:CD2	2:B:448:PHE:HB3	2.54	0.43
1:A:230:MET:CE	1:A:234:ARG:HB3	2.48	0.43
1:C:310:ILE:O	1:C:314:LEU:HG	2.17	0.42
2:D:395:HIS:NE2	2:D:501:GLU:OE1	2.46	0.42
1:C:76:ALA:HA	1:C:81:VAL:HA	2.02	0.42
1:C:191:VAL:O	1:C:248:SER:HB3	2.19	0.42
2:B:435:ILE:HG23	2:B:443:VAL:HG13	2.00	0.41
2:D:355:MET:HE3	2:D:355:MET:HB3	1.67	0.41
1:A:154:VAL:HG13	1:A:379:ILE:HG21	2.01	0.41
2:B:541:ALA:HB3	2:B:570:LEU:HD13	2.01	0.41
2:D:358:LEU:HB3	2:D:369:PHE:HB2	2.02	0.41
2:D:489:GLN:HG2	2:D:554:ARG:O	2.20	0.41
1:C:216:ILE:HA	3:C:401:A1AHE:F34	2.10	0.41

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	302/310 (97%)	293 (97%)	9 (3%)	0	100	100
1	C	287/310 (93%)	275 (96%)	12 (4%)	0	100	100
2	B	248/280 (89%)	238 (96%)	10 (4%)	0	100	100
2	D	248/280 (89%)	236 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1085/1180 (92%)	1042 (96%)	43 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	248/265 (94%)	243 (98%)	5 (2%)	48	68
1	C	137/265 (52%)	134 (98%)	3 (2%)	45	66
2	B	208/243 (86%)	204 (98%)	4 (2%)	50	70
2	D	206/243 (85%)	200 (97%)	6 (3%)	37	57
All	All	799/1016 (79%)	781 (98%)	18 (2%)	44	64

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	135	SER
1	A	152	ASP
1	A	241	SER
1	A	329	VAL
2	B	402	ASP
2	B	521	MET
2	B	531	LEU
2	B	535	SER
1	C	186	ILE
1	C	211	VAL
1	C	224	VAL
2	D	355	MET
2	D	388	SER
2	D	437	LEU
2	D	478	ILE
2	D	528	SER

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Mol	Chain	Res	Type
2	D	554	ARG

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

Mol	Chain	Res	Type
1	A	236	GLN
1	A	239	HIS
2	B	330	HIS
2	B	433	ASN
2	B	438	HIS
2	D	311	GLN
2	D	405	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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	ANP	A	403	4	33,33,33	0.90	4 (12%)	45,52,52	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	D	602	-	5,5,5	0.95	0	5,5,5	1.04	0
6	EDO	B	603	-	3,3,3	0.42	0	2,2,2	0.39	0
3	A1AHE	A	401	-	36,37,37	1.48	4 (11%)	47,54,54	1.86	9 (19%)
5	ANP	B	602	4	33,33,33	0.92	4 (12%)	45,52,52	0.63	0
7	GOL	D	601	-	5,5,5	0.93	0	5,5,5	1.09	0
3	A1AHE	C	401	-	36,37,37	1.40	4 (11%)	47,54,54	1.76	8 (17%)
7	GOL	C	402	-	5,5,5	0.93	0	5,5,5	1.09	0

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	ANP	A	403	4	-	4/18/38/38	0/3/3/3
7	GOL	D	602	-	-	0/4/4/4	-
6	EDO	B	603	-	-	1/1/1/1	-
3	A1AHE	A	401	-	-	0/15/16/16	0/4/4/4
5	ANP	B	602	4	-	2/18/38/38	0/3/3/3
7	GOL	D	601	-	-	1/4/4/4	-
3	A1AHE	C	401	-	-	2/15/16/16	0/4/4/4
7	GOL	C	402	-	-	2/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	A1AHE	S03-N02	5.02	1.67	1.61
3	C	401	A1AHE	S03-N02	4.87	1.67	1.61
3	A	401	A1AHE	C26-C21	2.73	1.42	1.38
3	C	401	A1AHE	C26-C21	2.69	1.42	1.38
5	B	602	ANP	PG-O1G	2.51	1.50	1.46
3	A	401	A1AHE	C07-C33	2.49	1.43	1.40
5	B	602	ANP	PG-N3B	2.48	1.69	1.63
5	A	403	ANP	PG-N3B	2.42	1.69	1.63
5	B	602	ANP	PB-O1B	2.42	1.49	1.46
5	A	403	ANP	PG-O1G	2.34	1.49	1.46
3	A	401	A1AHE	C28-C29	2.28	1.42	1.38
5	A	403	ANP	PB-O1B	2.27	1.49	1.46
3	C	401	A1AHE	C28-C29	2.22	1.42	1.38
5	A	403	ANP	PB-O3A	-2.21	1.56	1.59
3	C	401	A1AHE	F34-C33	-2.18	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	602	ANP	PB-O3A	-2.16	1.56	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	A1AHE	C31-C13-C14	-6.31	115.96	120.35
3	C	401	A1AHE	C31-C13-C14	-5.80	116.31	120.35
3	A	401	A1AHE	C11-C12-C13	4.06	120.78	114.05
3	C	401	A1AHE	C11-C12-C13	3.75	120.26	114.05
3	A	401	A1AHE	O30-C31-O32	-3.72	111.32	116.22
3	A	401	A1AHE	O30-C31-C13	3.66	122.41	117.86
3	C	401	A1AHE	O30-C31-O32	-3.63	111.44	116.22
3	C	401	A1AHE	O30-C31-C13	3.47	122.18	117.86
3	A	401	A1AHE	O20-C21-C26	3.45	122.00	117.57
3	C	401	A1AHE	O20-C21-C26	3.39	121.92	117.57
3	A	401	A1AHE	C17-C16-C29	-2.78	114.56	118.21
3	C	401	A1AHE	C17-C16-C29	-2.63	114.76	118.21
3	A	401	A1AHE	C10-C11-C33	-2.41	114.68	116.46
3	C	401	A1AHE	C10-C11-C33	-2.39	114.70	116.46
3	A	401	A1AHE	C15-C14-C16	-2.24	115.94	118.49
3	A	401	A1AHE	C17-C16-C14	2.09	125.94	122.75
3	C	401	A1AHE	C29-O30-C31	-2.01	120.34	122.26

There are no chirality outliers.

All (12) torsion outliers are listed below:

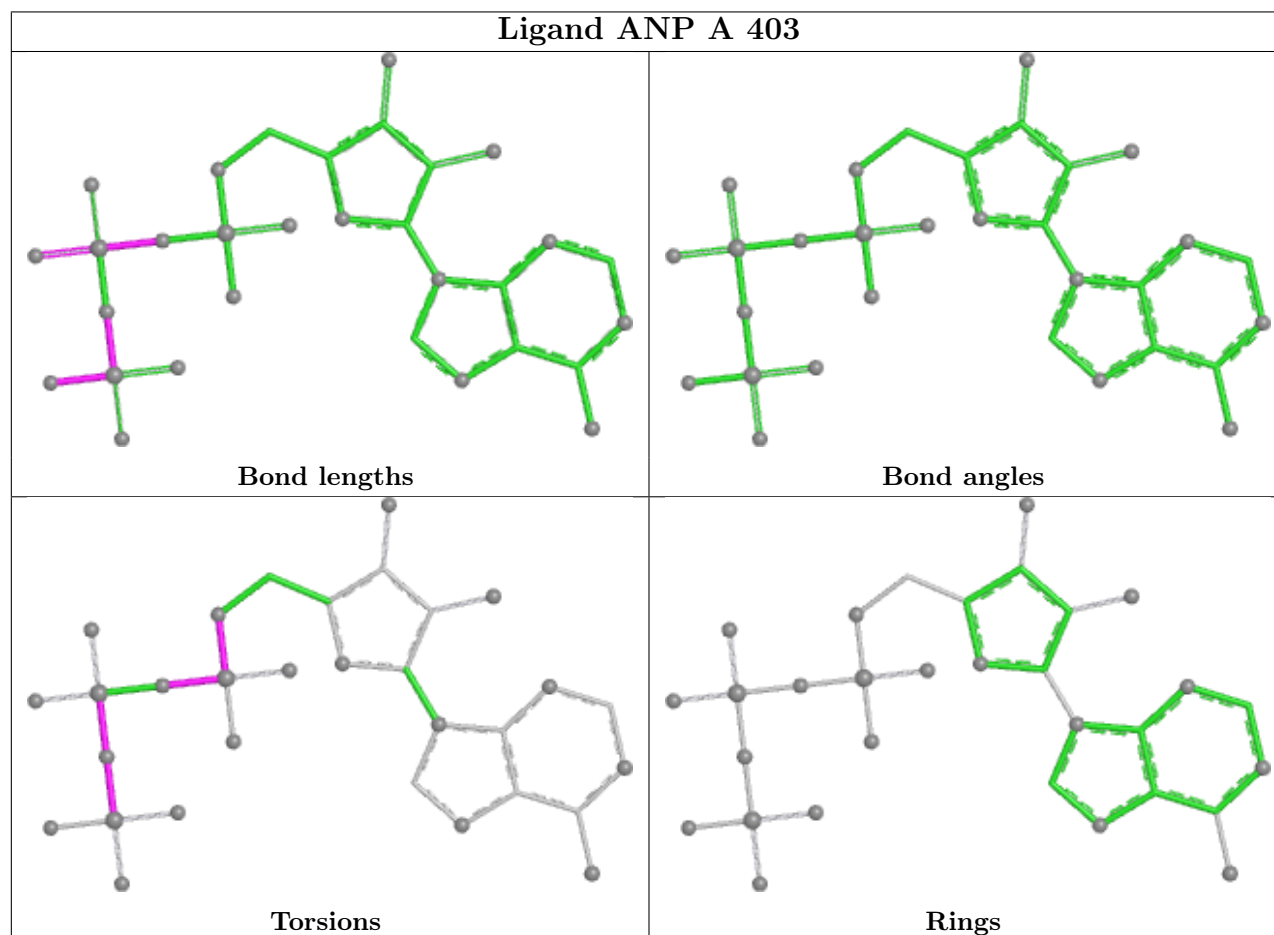
Mol	Chain	Res	Type	Atoms
5	A	403	ANP	PB-N3B-PG-O1G
5	A	403	ANP	PG-N3B-PB-O1B
5	A	403	ANP	C5'-O5'-PA-O1A
5	B	602	ANP	PA-O3A-PB-O2B
7	C	402	GOL	C1-C2-C3-O3
7	C	402	GOL	O2-C2-C3-O3
3	C	401	A1AHE	C01-N02-S03-O04
3	C	401	A1AHE	C01-N02-S03-O05
5	A	403	ANP	PB-O3A-PA-O2A
7	D	601	GOL	O1-C1-C2-O2
6	B	603	EDO	O1-C1-C2-O2
5	B	602	ANP	PA-O3A-PB-O1B

There are no ring outliers.

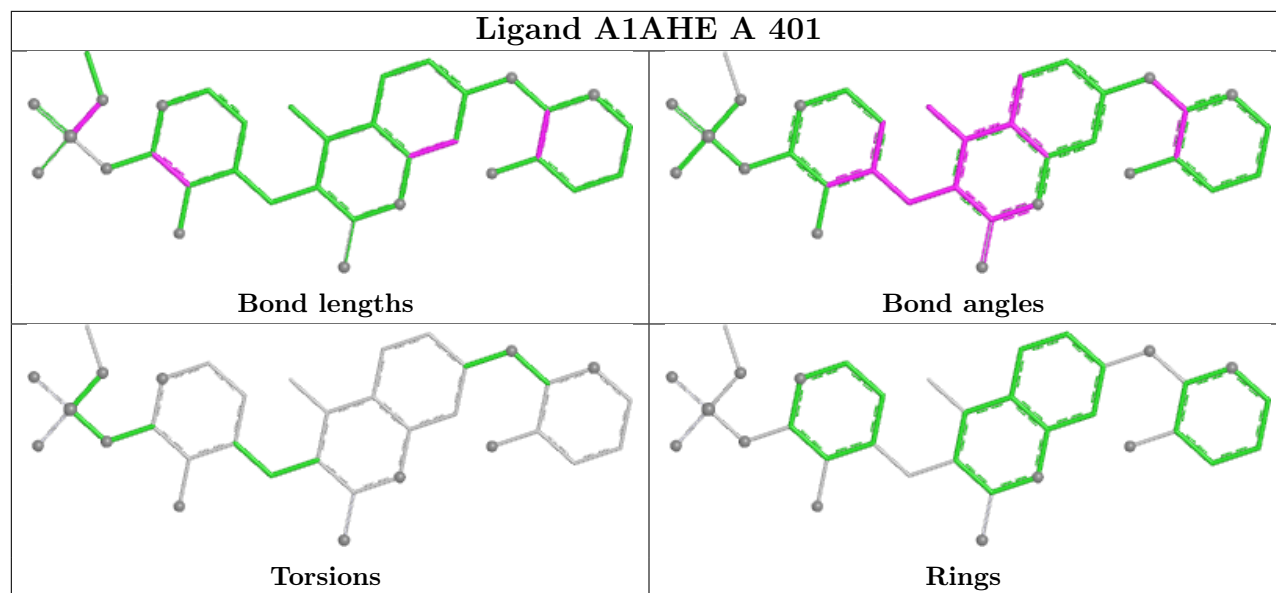
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	A1AHE	1	0

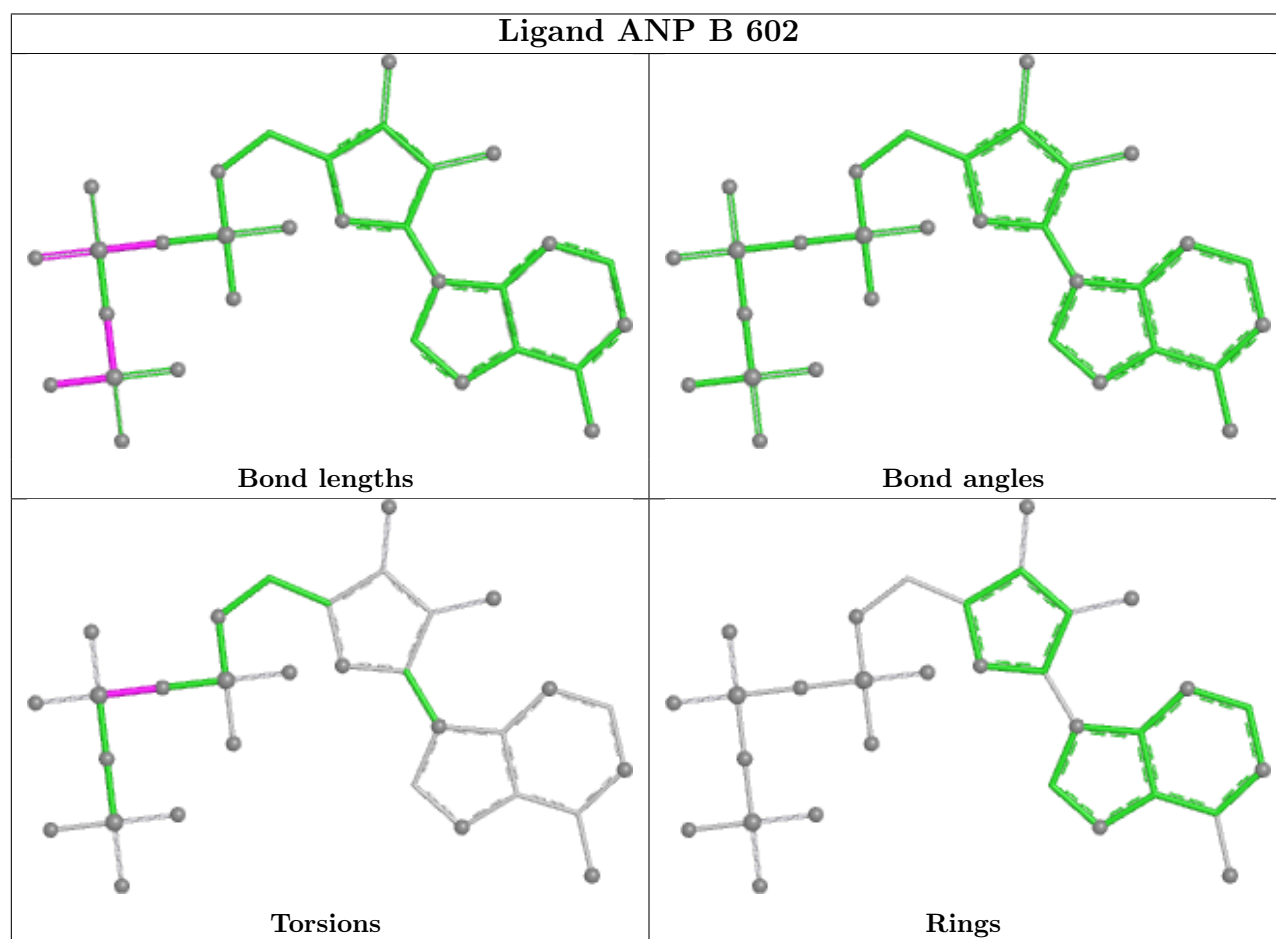
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

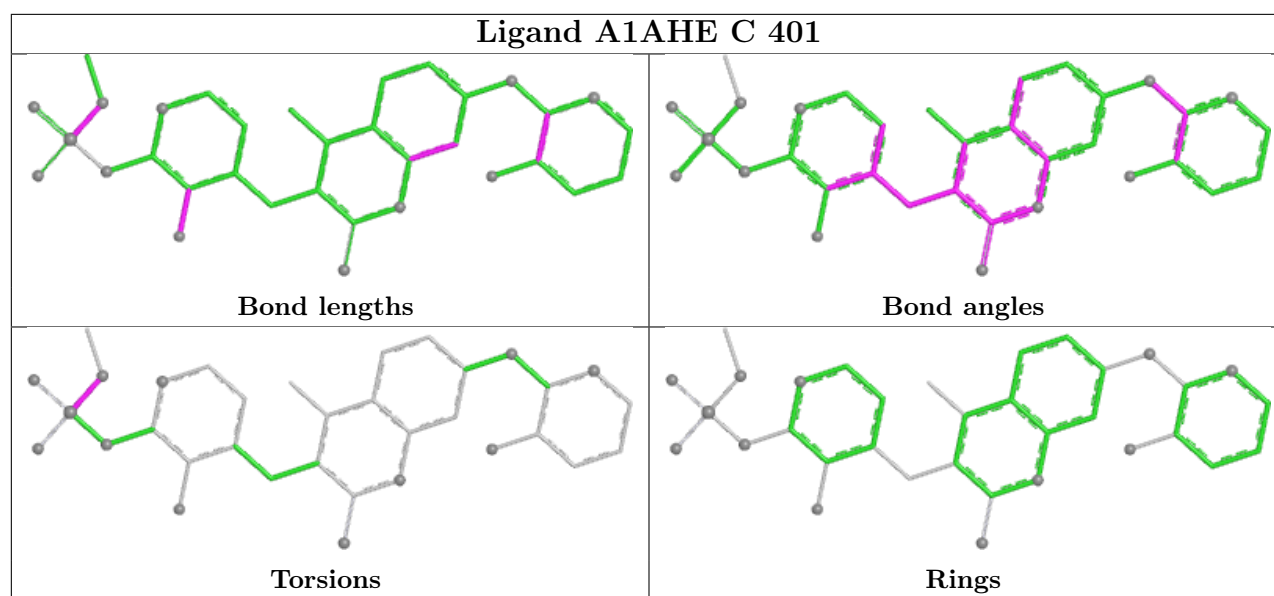


Ligand A1AHE A 401



Ligand ANP B 602





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	305/310 (98%)	0.86	29 (9%) 14 10	23, 58, 87, 116	1 (0%)
1	C	291/310 (93%)	2.52	182 (62%) 0 0	80, 109, 156, 185	0
2	B	254/280 (90%)	0.71	17 (6%) 24 20	34, 53, 91, 154	0
2	D	256/280 (91%)	0.84	36 (14%) 6 5	31, 53, 95, 172	0
All	All	1106/1180 (93%)	1.26	264 (23%) 2 1	23, 62, 135, 185	1 (0%)

All (264) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	199	ASN	6.2
1	C	60	VAL	6.0
1	C	78	ASN	5.7
1	A	240	TYR	5.7
1	C	212	SER	5.5
1	C	87	HIS	5.3
1	C	121	CYS	5.2
2	D	346	GLU	5.2
1	C	191	VAL	5.1
1	C	198	VAL	5.0
2	B	345	ALA	5.0
1	C	144	GLU	5.0
1	C	213	GLY	4.9
1	C	116	GLN	4.9
1	C	186	ILE	4.8
1	C	355	LEU	4.8
1	C	105	PRO	4.8
1	C	239	HIS	4.8
1	C	164	GLN	4.6
1	C	65	ASP	4.6
1	C	128	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
2	D	574	LEU	4.5
1	C	131	GLY	4.4
1	C	171	ILE	4.4
1	C	95	ALA	4.3
1	C	89	PRO	4.3
1	C	222	ALA	4.3
1	C	177	LEU	4.3
1	C	106	ALA	4.2
1	C	238	THR	4.1
1	C	143	MET	4.1
1	C	54	LEU	4.1
2	D	322	GLY	4.0
1	C	196	ILE	4.0
1	A	266	GLY	4.0
2	B	526	TYR	4.0
1	C	62	GLU	4.0
1	C	51	GLU	4.0
2	D	351	PHE	4.0
2	D	300	GLY	4.0
1	C	197	LEU	4.0
1	C	204	ILE	3.9
2	B	344	THR	3.9
2	D	345	ALA	3.9
1	C	109	ASN	3.9
1	C	253	LEU	3.9
1	C	178	THR	3.9
2	D	378	PHE	3.8
1	C	47	ARG	3.8
2	B	321	PHE	3.8
1	C	108	ARG	3.8
1	C	225	GLY	3.8
2	D	343	PRO	3.8
1	C	371	PHE	3.8
1	C	141	ILE	3.7
1	C	182	GLU	3.7
1	C	43	ASP	3.7
1	C	86	SER	3.7
1	C	58	GLN	3.7
1	C	67	ASP	3.7
1	C	94	MET	3.7
1	C	249	MET	3.7
1	C	63	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	127	VAL	3.6
1	C	101	LEU	3.6
1	C	352	LEU	3.6
1	C	119	HIS	3.5
1	C	338	VAL	3.5
1	C	115	LEU	3.5
1	C	366	ALA	3.5
2	D	318	THR	3.5
2	D	344	THR	3.5
1	C	374	TRP	3.5
2	B	348	ALA	3.5
1	C	45	GLN	3.4
1	C	55	THR	3.4
1	C	203	GLU	3.4
2	D	342	GLN	3.4
1	C	52	ALA	3.4
1	C	216	ILE	3.4
1	C	66	ASP	3.4
1	C	169	VAL	3.4
1	C	49	ARG	3.4
1	C	142	CYS	3.3
1	C	44	GLU	3.3
1	C	139	ILE	3.3
1	C	165	ILE	3.3
1	C	310	ILE	3.3
1	C	104	LYS	3.3
1	A	239	HIS	3.3
1	A	238	THR	3.3
1	C	174	ILE	3.3
1	C	372	ALA	3.3
1	C	132	ALA	3.2
1	C	118	LEU	3.2
2	D	348	ALA	3.2
2	D	520	PHE	3.2
1	A	78	ASN	3.2
1	C	321	PRO	3.2
1	A	75	GLY	3.1
1	C	61	GLY	3.1
1	C	226	THR	3.1
1	C	347	ALA	3.1
1	A	307	SER	3.1
2	B	343	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	130	TYR	3.1
1	C	309	ALA	3.1
1	C	375	LEU	3.1
1	C	113	ARG	3.1
1	C	112	ILE	3.1
1	C	254	VAL	3.1
2	B	341	SER	3.0
1	A	310	ILE	3.0
1	C	148	GLY	3.0
1	C	345	ASN	3.0
1	C	350	ALA	3.0
1	C	74	LEU	3.0
1	C	223	PHE	3.0
1	C	82	VAL	2.9
1	C	172	ALA	2.9
1	C	342	LEU	2.9
1	C	236	GLN	2.9
2	D	514	CYS	2.9
1	C	103	ILE	2.9
1	C	111	ILE	2.9
1	C	361	ILE	2.9
1	C	173	VAL	2.9
1	C	220	ALA	2.9
1	C	252	SER	2.9
1	C	189	ARG	2.9
1	C	124	PRO	2.9
1	C	83	PHE	2.9
1	C	161	ILE	2.9
1	A	327	SER	2.8
1	A	345	ASN	2.8
2	D	353	ASN	2.8
1	C	125	TYR	2.8
1	C	240	TYR	2.8
2	B	573	SER	2.8
1	C	85	VAL	2.8
1	C	151	LEU	2.8
1	C	64	LYS	2.8
1	C	134	TYR	2.8
1	C	264	GLY	2.8
1	C	140	SER	2.8
1	A	224	VAL	2.8
1	C	154	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	215	LEU	2.8
1	C	314	LEU	2.8
1	C	228	SER	2.8
1	C	155	LEU	2.8
1	C	102	GLU	2.8
1	C	68	PHE	2.8
1	C	369	VAL	2.7
2	D	470	VAL	2.7
1	C	326	PRO	2.7
1	C	235	LEU	2.7
1	C	53	PHE	2.7
1	A	318	VAL	2.7
2	D	350	ALA	2.7
2	D	347	GLN	2.7
2	B	511	HIS	2.7
1	C	353	LYS	2.6
1	C	81	VAL	2.6
1	C	93	VAL	2.6
1	C	224	VAL	2.6
2	D	302	ASP	2.6
1	C	100	HIS	2.6
1	A	225	GLY	2.6
2	D	475	ALA	2.6
1	C	180	LEU	2.6
1	A	220	ALA	2.6
1	C	135	SER	2.6
1	A	264	GLY	2.5
1	A	38	GLU	2.5
1	C	360	PHE	2.5
2	D	338	LEU	2.5
2	D	355	MET	2.5
1	C	167	GLY	2.5
1	C	129	PHE	2.5
1	C	166	LEU	2.5
1	C	90	SER	2.5
1	C	96	ARG	2.5
1	C	261	TYR	2.5
1	A	79	GLY	2.5
1	C	59	LYS	2.5
2	B	340	VAL	2.5
2	D	511	HIS	2.5
1	A	329	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	346	PRO	2.4
1	C	373	GLY	2.4
2	D	317	GLY	2.4
2	B	339	LYS	2.4
2	D	512	ILE	2.4
1	C	325	LEU	2.4
1	C	107	ILE	2.4
1	C	92	LEU	2.4
1	A	382	ASN	2.4
1	C	205	LYS	2.4
1	C	312	GLU	2.4
1	C	317	ILE	2.4
2	B	521	MET	2.4
1	C	313	LEU	2.4
2	D	516	ASP	2.4
1	C	84	LYS	2.4
1	C	344	LYS	2.4
2	D	454	LYS	2.4
1	C	246	ILE	2.3
2	D	402	ASP	2.3
1	C	200	SER	2.3
1	C	149	GLY	2.3
1	C	227	ARG	2.3
2	B	524	ARG	2.3
2	D	473	MET	2.3
1	A	341	CYS	2.3
1	C	243	GLN	2.3
1	C	73	GLU	2.3
1	A	223	PHE	2.3
1	C	337	PHE	2.3
1	C	318	VAL	2.3
1	A	187	MET	2.2
1	C	71	ILE	2.2
1	C	251	LEU	2.2
1	C	308	MET	2.2
1	C	218	ALA	2.2
1	A	40	LEU	2.2
1	C	98	LEU	2.2
1	C	356	MET	2.2
1	C	126	ILE	2.2
1	A	347	ALA	2.2
1	C	257	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	526	TYR	2.2
1	A	61	GLY	2.2
1	C	237	GLY	2.2
2	D	519	ILE	2.2
1	C	323	PRO	2.2
2	D	508	PRO	2.2
1	C	340	LYS	2.2
1	C	221	ASN	2.2
2	B	350	ALA	2.2
1	C	210	GLY	2.2
1	C	351	ASP	2.2
1	C	250	GLY	2.1
1	C	311	PHE	2.1
1	A	76	ALA	2.1
1	C	263	ILE	2.1
2	D	572	ARG	2.1
1	C	123	SER	2.1
2	D	341	SER	2.1
1	C	110	GLN	2.1
1	C	354	GLN	2.1
2	B	342	GLN	2.1
2	D	479	ARG	2.1
1	C	150	SER	2.1
2	D	349	GLN	2.1
1	C	320	GLU	2.1
1	C	232	PRO	2.1
1	A	330	PHE	2.0
1	C	242	VAL	2.0
1	A	42	LEU	2.0
2	B	374	THR	2.0
1	C	181	ARG	2.0
1	A	162	PRO	2.0
2	B	469	SER	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 ⓘ

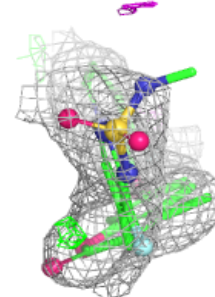
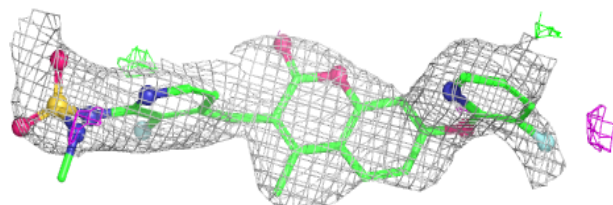
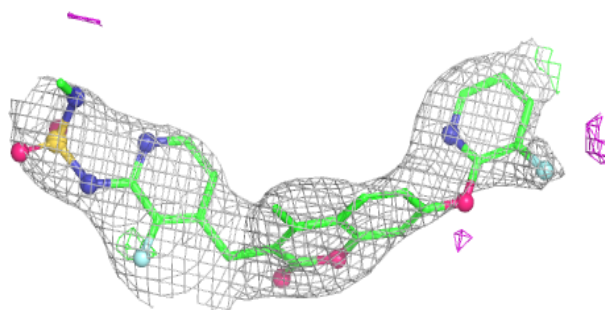
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	B	603	4/4	0.58	0.23	71,72,79,87	0
3	A1AHE	C	401	34/34	0.68	0.17	94,104,112,113	0
7	GOL	D	602	6/6	0.72	0.24	53,58,64,71	0
7	GOL	C	402	6/6	0.73	0.16	68,79,84,91	0
7	GOL	D	601	6/6	0.82	0.14	56,56,68,69	0
5	ANP	B	602	31/31	0.92	0.09	34,53,63,75	0
5	ANP	A	403	31/31	0.93	0.09	40,52,71,78	0
3	A1AHE	A	401	34/34	0.95	0.09	39,51,60,61	0
4	MG	B	601	1/1	0.98	0.14	53,53,53,53	0
4	MG	A	402	1/1	1.00	0.03	50,50,50,50	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.

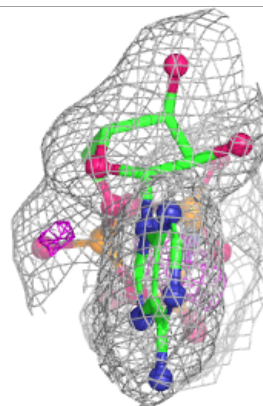
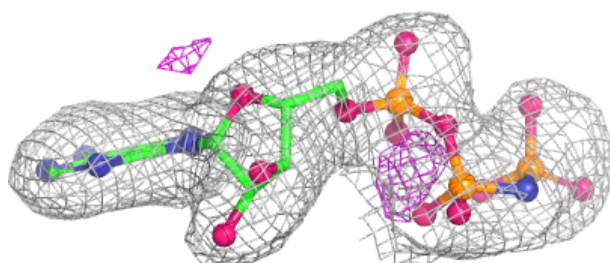
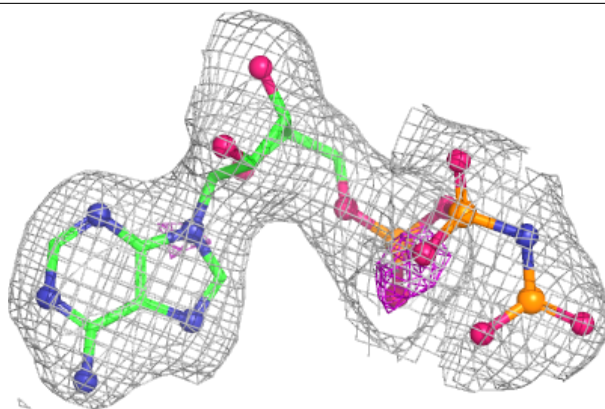
Electron density around A1AHE C 401:

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

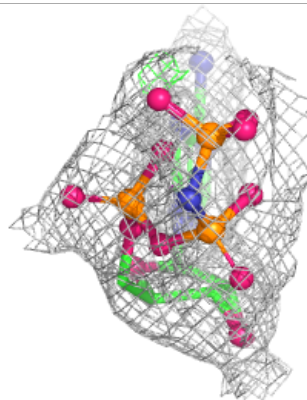
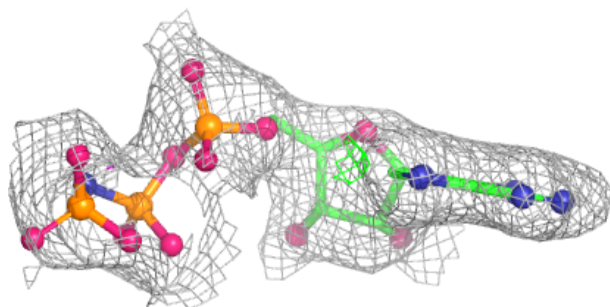
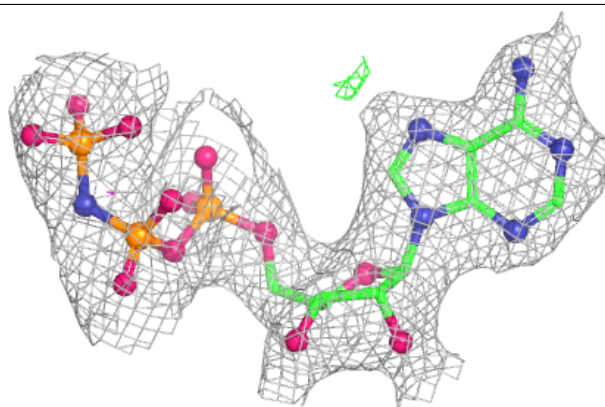


Electron density around ANP B 602:

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

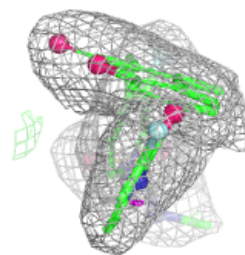
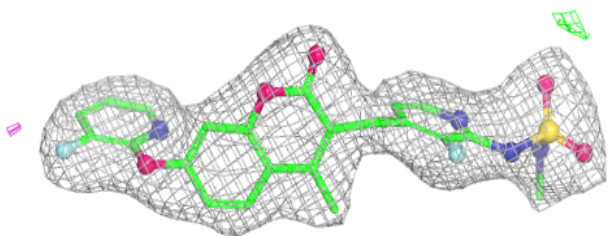
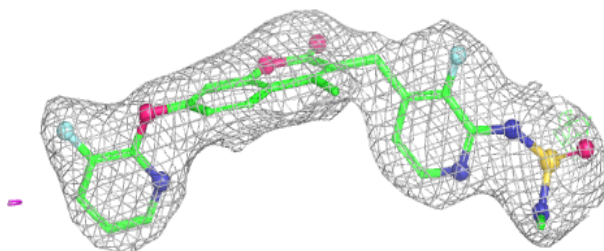
**Electron density around ANP A 403:**

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.