



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:01 PM UTC

PDB ID : 9AXX / pdb_00009axx
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	:	4-5-2 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

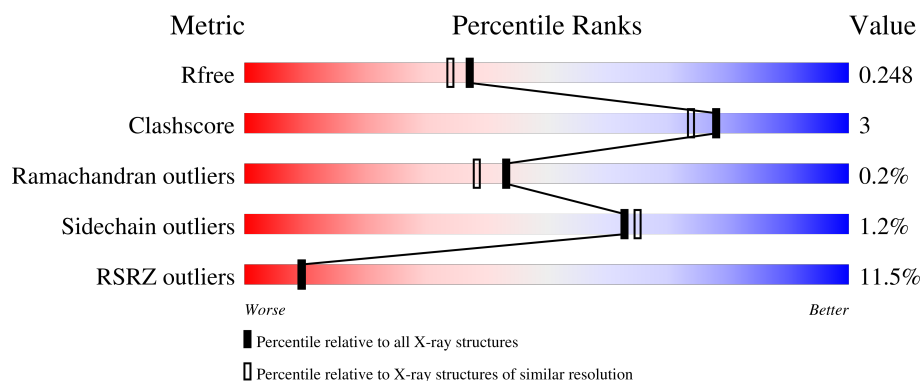
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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}	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	310	11% 92% 5% .
1	C	310	20% 87% 9% .
2	B	280	10% 82% 10% 7%
2	D	280	2% 92% 5% .

2 Entry composition

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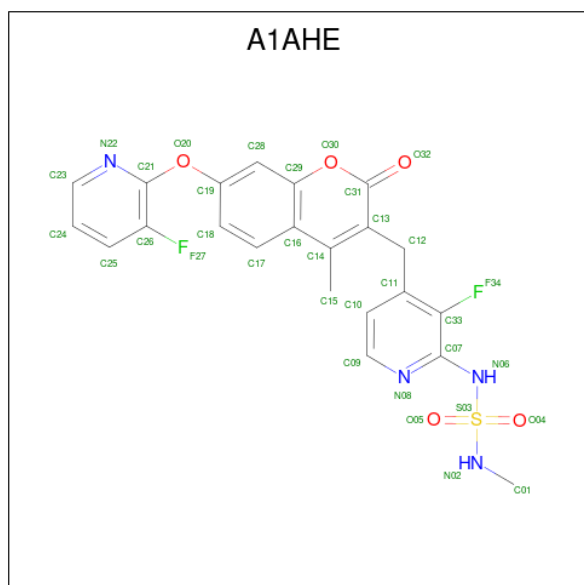
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	272	Total	C	N	O	S	0	0	0
			2141	1372	369	387	13			

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



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

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

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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

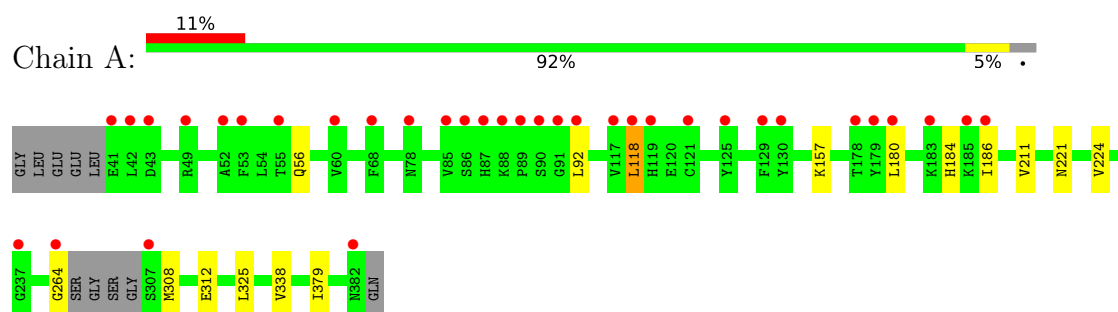
- Molecule 8 is water.

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

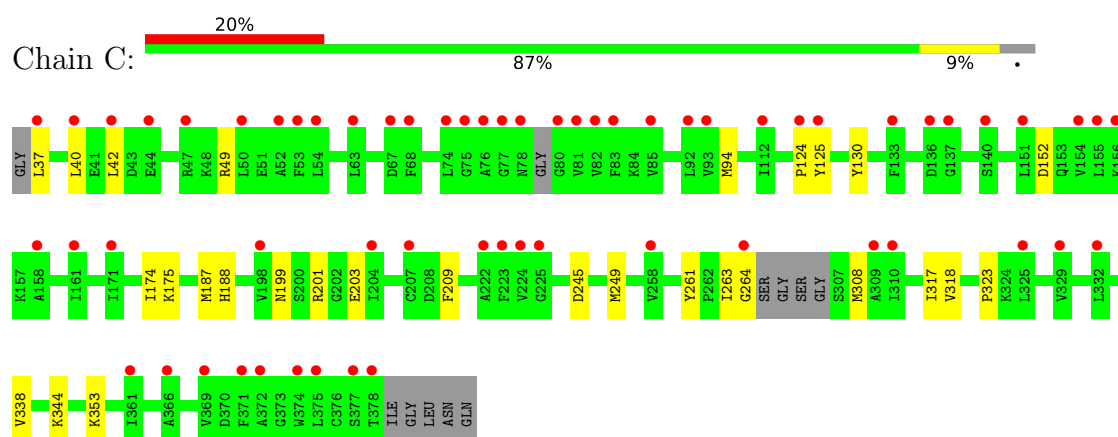
3 Residue-property plots [i](#)

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.

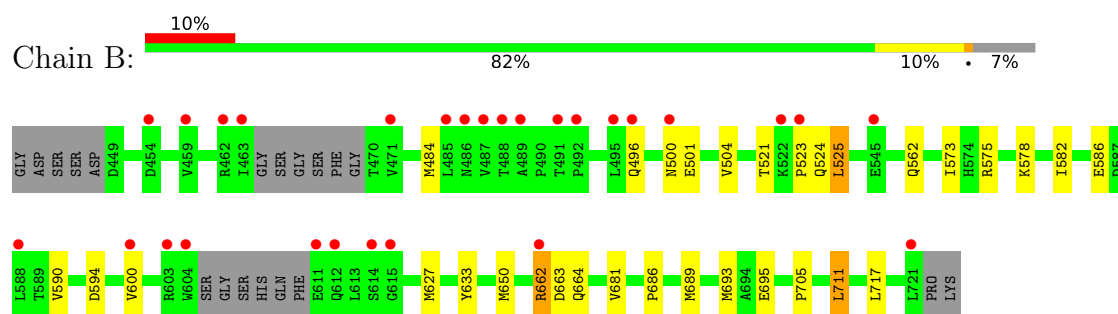
- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 1



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



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



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



4 Data and refinement statistics

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 41.20 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.1 (41.20-2.07) 99.2 (41.20-2.07)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, REFMAC 5	Depositor
R, R_{free}	0.213 , 0.248 0.213 , 0.248	Depositor DCC
R_{free} test set	4080 reflections (4.88%)	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)	0.31 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	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.*

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, EDO, A1AHE, TRS, ANP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/2357	0.31	0/3181
1	C	0.12	0/2293	0.30	0/3103
2	B	0.13	0/2085	0.32	0/2828
2	D	0.14	0/2190	0.33	0/2965
All	All	0.13	0/8925	0.31	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 [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	2314	0	2295	9	0
1	C	2252	0	2181	15	0
2	B	2040	0	2003	17	0
2	D	2141	0	2128	9	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	49	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 (49) 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:264:GLY:HA3	1:A:308:MET:HE1	1.64	0.78
1:C:264:GLY:HA3	1:C:308:MET:HE1	1.72	0.71
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
1:C:174:ILE:HD11	1:C:249:MET:HE1	1.91	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
1:C:261:TYR:CE2	1:C:263:ILE:HB	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:650:MET:HE3	2:B:689:MET:HG2	1.94	0.47
2:B:681:VAL:HG21	2:B:693:MET:HE1	1.95	0.47
1:C:188:HIS:CD2	1:C:209:PHE:HB3	2.50	0.47
2:B:484:MET:HE2	2:B:524:GLN:HB2	1.95	0.47
1:A:184:HIS:HB2	1:A:186:ILE:HG12	1.97	0.47
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
1:C:318:VAL:O	1:C:344:LYS:NZ	2.40	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
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
1:A:308:MET:HG2	1:A:312:GLU:CD	2.47	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%)	16	8
2	D	270/280 (96%)	263 (97%)	7 (3%)	0	100	100
All	All	1116/1180 (95%)	1089 (98%)	25 (2%)	2 (0%)	43	38

All (2) Ramachandran outliers are listed below:

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

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	249/265 (94%)	247 (99%)	2 (1%)	73	77
1	C	233/265 (88%)	230 (99%)	3 (1%)	61	62
2	B	214/246 (87%)	209 (98%)	5 (2%)	44	41
2	D	231/246 (94%)	230 (100%)	1 (0%)	84	87
All	All	927/1022 (91%)	916 (99%)	11 (1%)	63	65

All (11) 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	586	GLU
2	B	627	MET
2	B	662	ARG
2	B	711	LEU
1	C	152	ASP
1	C	338	VAL

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Mol	Chain	Res	Type
1	C	353	LYS
2	D	671	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	116	GLN
1	A	119	HIS
2	B	664	GLN
1	C	46	GLN
1	C	116	GLN
2	D	539	HIS
2	D	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 oligosaccharides 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	B	804	-	3,3,3	0.42	0	2,2,2	0.48	0
6	EDO	C	404	-	3,3,3	0.42	0	2,2,2	0.28	0
6	EDO	D	802	-	3,3,3	0.42	0	2,2,2	0.42	0
6	EDO	B	806	-	3,3,3	0.49	0	2,2,2	0.26	0
6	EDO	D	805	-	3,3,3	0.42	0	2,2,2	0.38	0
3	A1AHE	A	401	-	36,37,37	1.27	3 (8%)	47,54,54	1.61	9 (19%)
6	EDO	D	803	-	3,3,3	0.41	0	2,2,2	0.43	0
4	ANP	A	402	5	33,33,33	0.97	4 (12%)	45,52,52	0.75	1 (2%)
4	ANP	B	801	-	33,33,33	0.92	4 (12%)	45,52,52	0.68	1 (2%)
3	A1AHE	C	401	-	36,37,37	1.17	4 (11%)	47,54,54	1.64	7 (14%)
4	ANP	C	402	5	33,33,33	0.94	3 (9%)	45,52,52	0.63	0
6	EDO	A	404	-	3,3,3	0.48	0	2,2,2	0.30	0
6	EDO	B	803	-	3,3,3	0.45	0	2,2,2	0.35	0
6	EDO	D	801	-	3,3,3	0.45	0	2,2,2	0.36	0
6	EDO	B	805	-	3,3,3	0.42	0	2,2,2	0.39	0
7	TRS	B	802	-	7,7,7	0.35	0	9,9,9	0.42	0
6	EDO	D	804	-	3,3,3	0.43	0	2,2,2	0.44	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
6	EDO	B	804	-	-	0/1/1/1	-
6	EDO	C	404	-	-	1/1/1/1	-
6	EDO	D	802	-	-	0/1/1/1	-
6	EDO	B	806	-	-	0/1/1/1	-
6	EDO	D	805	-	-	0/1/1/1	-
3	A1AHE	A	401	-	-	3/15/16/16	0/4/4/4
6	EDO	D	803	-	-	0/1/1/1	-
4	ANP	A	402	5	-	2/18/38/38	0/3/3/3
4	ANP	B	801	-	-	7/18/38/38	0/3/3/3
3	A1AHE	C	401	-	-	2/15/16/16	0/4/4/4
4	ANP	C	402	5	-	2/18/38/38	0/3/3/3
6	EDO	A	404	-	-	0/1/1/1	-
6	EDO	B	803	-	-	0/1/1/1	-
6	EDO	D	801	-	-	0/1/1/1	-
6	EDO	B	805	-	-	0/1/1/1	-
7	TRS	B	802	-	-	8/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	D	804	-	-	1/1/1/1	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	A1AHE	S03-N02	4.72	1.66	1.61
3	C	401	A1AHE	S03-N02	3.17	1.65	1.61
4	A	402	ANP	PG-N3B	2.80	1.70	1.63
3	C	401	A1AHE	C26-C21	2.73	1.42	1.38
4	A	402	ANP	PG-O1G	2.64	1.50	1.46
4	B	801	ANP	PG-O1G	2.60	1.50	1.46
4	C	402	ANP	PG-O1G	2.59	1.50	1.46
4	C	402	ANP	PB-O1B	2.54	1.50	1.46
4	B	801	ANP	PB-O1B	2.53	1.50	1.46
4	C	402	ANP	PG-N3B	2.53	1.70	1.63
4	B	801	ANP	PG-N3B	2.49	1.69	1.63
4	A	402	ANP	PB-O1B	2.32	1.49	1.46
4	A	402	ANP	PB-N3B	2.25	1.69	1.63
3	A	401	A1AHE	F34-C33	-2.25	1.31	1.34
3	A	401	A1AHE	C01-N02	2.10	1.49	1.46
3	C	401	A1AHE	C28-C29	2.10	1.42	1.38
4	B	801	ANP	PB-N3B	2.00	1.68	1.63
3	C	401	A1AHE	C07-N08	2.00	1.38	1.35

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	A1AHE	C31-C13-C14	-5.39	116.60	120.35
3	A	401	A1AHE	C31-C13-C14	-5.08	116.81	120.35
3	A	401	A1AHE	C11-C12-C13	3.93	120.56	114.05
3	C	401	A1AHE	O30-C31-C13	3.59	122.33	117.86
3	C	401	A1AHE	O30-C31-O32	-3.50	111.61	116.22
3	C	401	A1AHE	C11-C12-C13	3.42	119.73	114.05
3	A	401	A1AHE	O30-C31-O32	-3.31	111.86	116.22
3	A	401	A1AHE	O30-C31-C13	3.15	121.78	117.86
4	A	402	ANP	O1B-PB-N3B	-2.83	107.61	111.77
3	C	401	A1AHE	O20-C21-C26	2.77	121.14	117.57
3	A	401	A1AHE	C29-O30-C31	-2.71	119.68	122.26
3	C	401	A1AHE	C17-C16-C29	-2.54	114.87	118.21
3	A	401	A1AHE	O20-C21-C26	2.50	120.79	117.57
4	B	801	ANP	O1B-PB-N3B	-2.28	108.41	111.77
3	A	401	A1AHE	C10-C11-C33	-2.24	114.81	116.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	A1AHE	C29-O30-C31	-2.22	120.14	122.26
3	A	401	A1AHE	C15-C14-C16	-2.18	116.00	118.49
3	A	401	A1AHE	C17-C16-C29	-2.17	115.37	118.21

There are no chirality outliers.

All (26) 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	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
7	B	802	TRS	C3-C-C2-O2
4	A	402	ANP	PB-O3A-PA-O5'
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
4	C	402	ANP	C3'-C4'-C5'-O5'
7	B	802	TRS	C3-C-C1-O1
7	B	802	TRS	C1-C-C2-O2
7	B	802	TRS	C1-C-C3-O3
4	B	801	ANP	PA-O3A-PB-O1B
3	A	401	A1AHE	C10-C11-C12-C13
3	C	401	A1AHE	C10-C11-C12-C13
3	A	401	A1AHE	C07-N06-S03-O04
7	B	802	TRS	N-C-C1-O1
7	B	802	TRS	N-C-C3-O3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

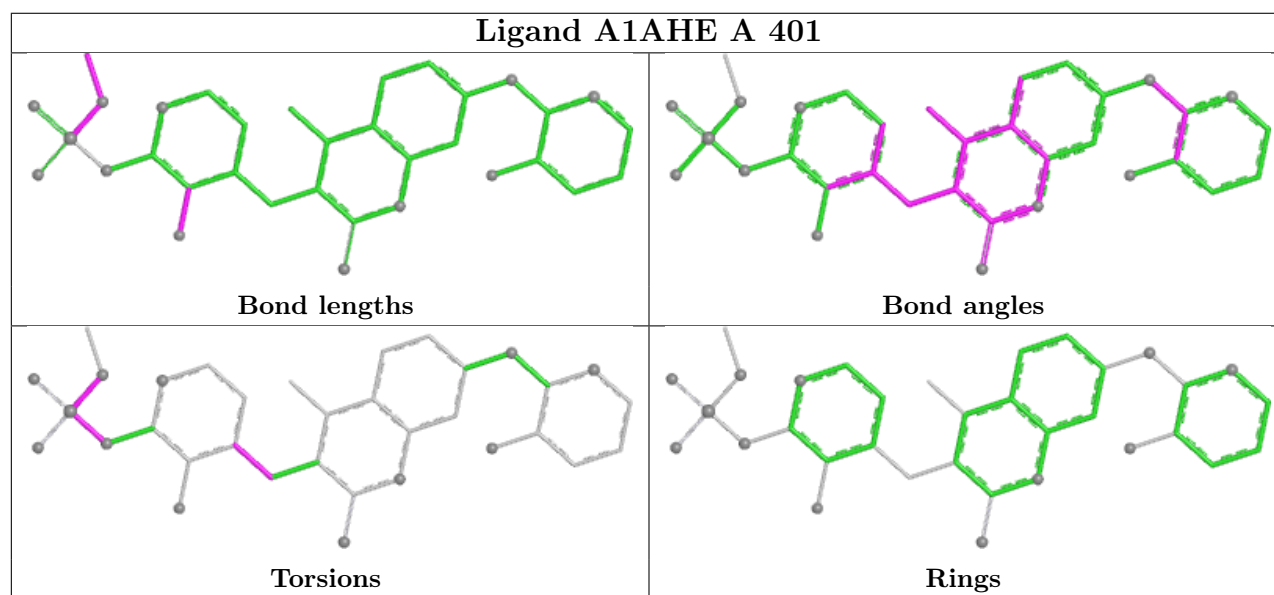
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	804	EDO	1	0
6	C	404	EDO	2	0

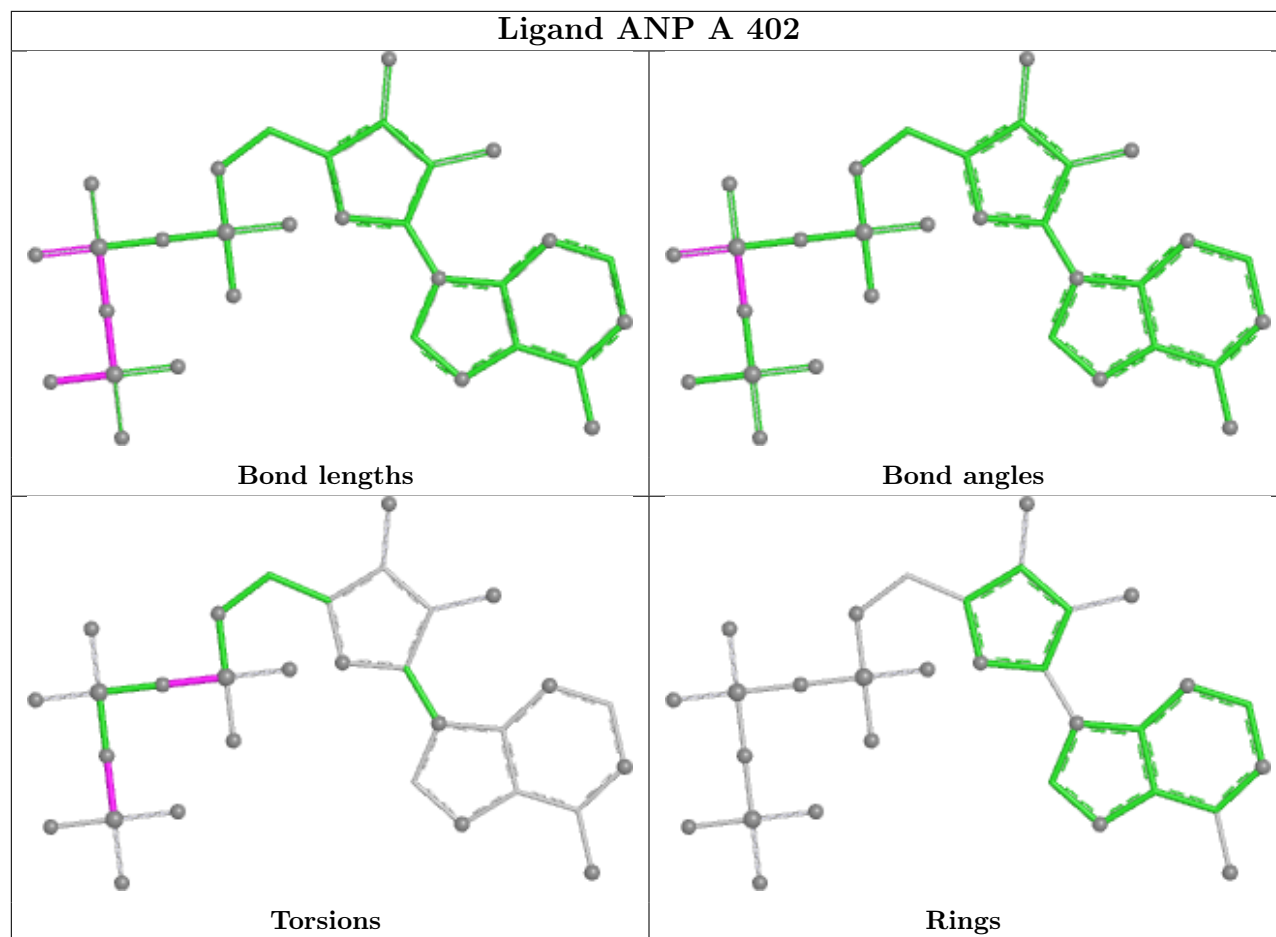
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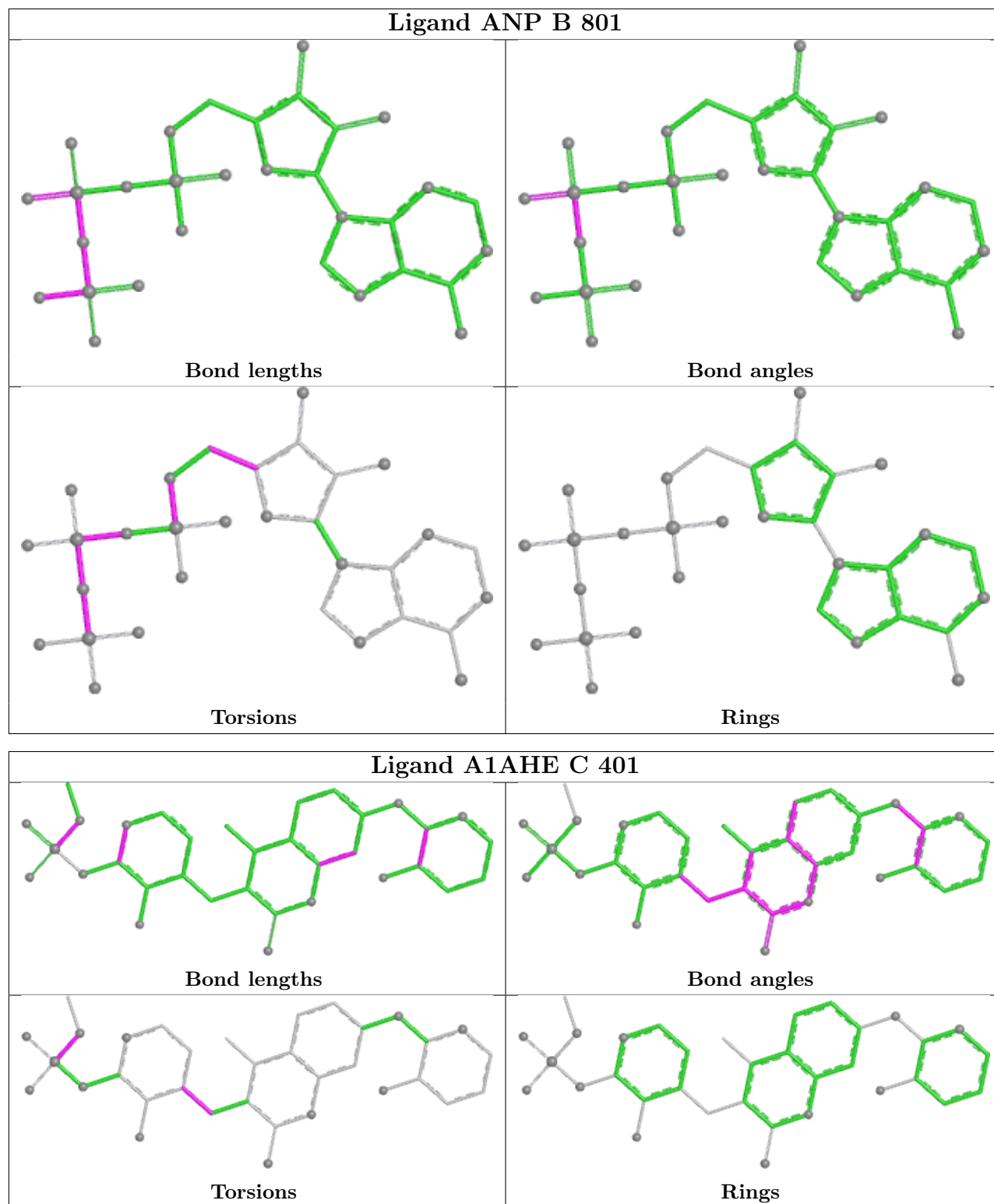
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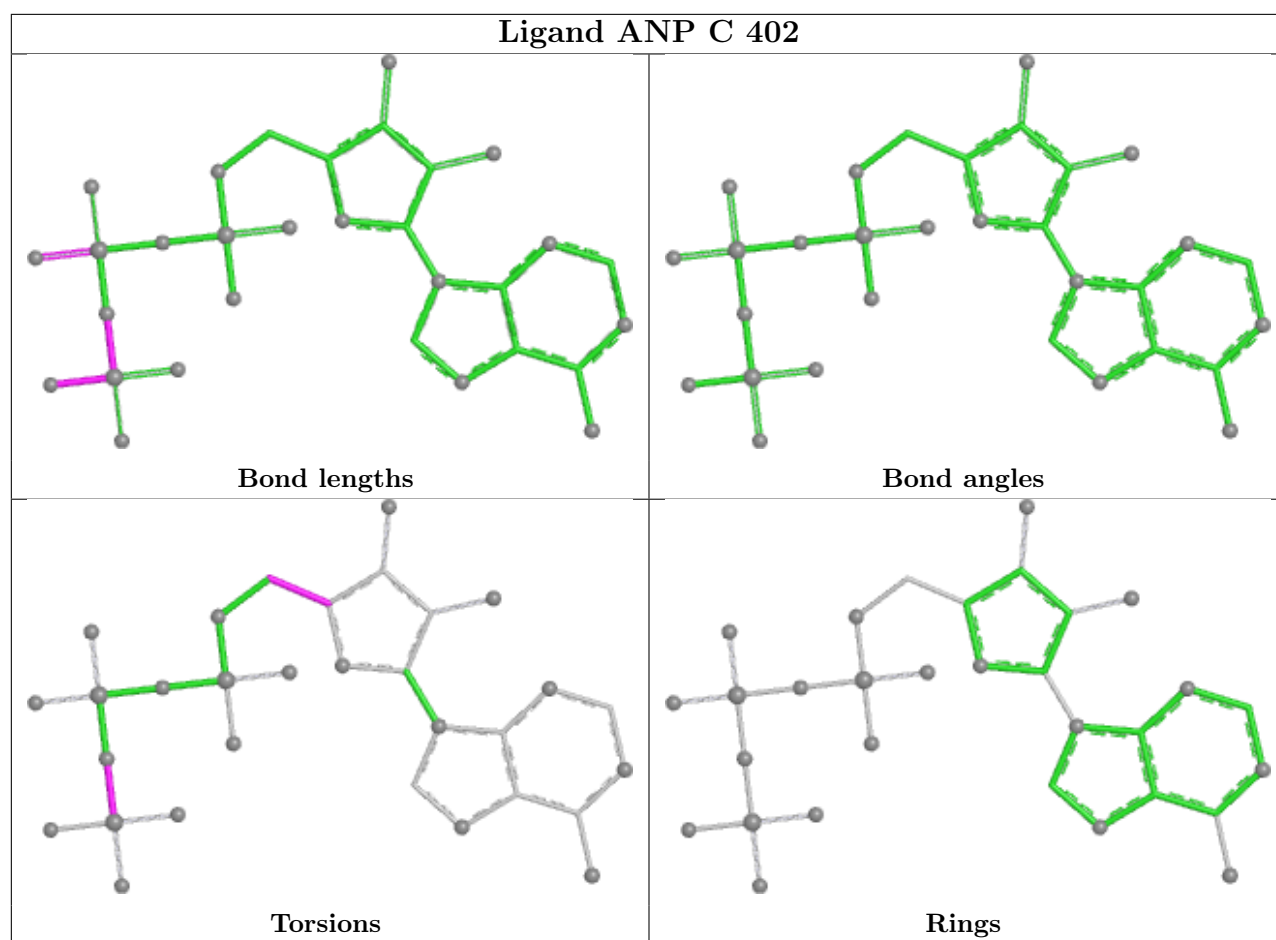
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	801	ANP	1	0
6	D	804	EDO	1	0

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.









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	300/310 (96%)	0.66	35 (11%) 9 9	24, 53, 96, 125	1 (0%)
1	C	299/310 (96%)	1.29	61 (20%) 3 2	46, 80, 112, 127	0
2	B	261/280 (93%)	0.57	28 (10%) 11 11	21, 50, 88, 114	1 (0%)
2	D	272/280 (97%)	0.19	6 (2%) 62 64	29, 46, 70, 107	0
All	All	1132/1180 (95%)	0.69	130 (11%) 9 9	21, 56, 103, 127	2 (0%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	224	VAL	7.2
2	D	588	LEU	6.6
1	C	76	ALA	5.5
1	C	223	PHE	4.9
1	A	92	LEU	4.9
1	C	158	ALA	4.8
2	B	487	VAL	4.1
1	C	112	ILE	4.0
1	A	264	GLY	4.0
1	C	372	ALA	3.9
1	C	155	LEU	3.9
1	C	378	THR	3.9
2	B	604	TRP	3.8
2	B	611	GLU	3.8
2	B	485	LEU	3.7
1	A	86	SER	3.7
1	C	40	LEU	3.6
2	B	500	ASN	3.6
1	C	81	VAL	3.5
1	A	49	ARG	3.5
1	C	161	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	75	GLY	3.4
2	B	495	LEU	3.4
1	C	44	GLU	3.4
1	A	42	LEU	3.4
1	C	374	TRP	3.3
2	B	488	THR	3.3
2	B	492	PRO	3.3
1	C	52	ALA	3.3
1	C	375	LEU	3.2
1	A	53	PHE	3.2
1	C	366	ALA	3.2
2	B	545	GLU	3.1
2	B	454	ASP	3.1
1	A	179	TYR	3.1
1	A	91	GLY	3.1
1	C	222	ALA	3.1
2	B	523	PRO	3.0
1	C	80	GLY	3.0
1	A	307	SER	3.0
1	C	77	GLY	3.0
1	A	183	LYS	3.0
1	A	117	VAL	2.9
1	A	41	GLU	2.9
1	A	90	SER	2.9
1	A	129	PHE	2.9
1	C	68	PHE	2.9
1	C	78	ASN	2.8
1	C	50	LEU	2.8
1	C	37	LEU	2.8
1	C	369	VAL	2.8
1	C	137	GLY	2.7
1	C	136	ASP	2.7
1	A	52	ALA	2.7
1	C	309	ALA	2.7
1	A	55	THR	2.7
1	A	121	CYS	2.7
2	B	489	ALA	2.6
1	A	89	PRO	2.6
1	A	43	ASP	2.6
1	C	154	VAL	2.6
2	B	615	GLY	2.6
1	A	68	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	721	LEU	2.6
1	C	361	ILE	2.5
1	C	54	LEU	2.5
1	C	92	LEU	2.5
1	C	198	VAL	2.5
2	B	496	GLN	2.5
1	C	47	ARG	2.5
2	B	603	ARG	2.5
2	B	662	ARG	2.5
2	B	486	ASN	2.5
1	A	78	ASN	2.5
1	A	118	LEU	2.4
1	C	133	PHE	2.4
2	B	463	ILE	2.4
2	B	612	GLN	2.4
1	C	377	SER	2.4
1	C	325	LEU	2.4
2	B	471	VAL	2.4
2	D	585	HIS	2.4
1	C	332	LEU	2.4
1	C	204	ILE	2.4
2	B	459	VAL	2.4
2	D	465	SER	2.4
1	C	63	LEU	2.3
1	C	74	LEU	2.3
1	C	225	GLY	2.3
1	A	88	LYS	2.3
2	B	614	SER	2.3
1	C	310	ILE	2.3
1	C	124	PRO	2.3
2	D	488	THR	2.3
1	A	382	ASN	2.3
1	C	264	GLY	2.3
1	A	85	VAL	2.2
2	B	600	VAL	2.2
1	C	207	CYS	2.2
2	D	464	GLY	2.2
1	A	87	HIS	2.2
1	A	119	HIS	2.2
1	C	53	PHE	2.2
1	C	171	ILE	2.2
2	B	491	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	82	VAL	2.2
1	A	237	GLY	2.2
1	A	180	LEU	2.2
1	C	151	LEU	2.2
2	B	588	LEU	2.2
1	A	178	THR	2.2
1	C	371	PHE	2.1
2	B	522	LYS	2.1
1	A	125	TYR	2.1
1	C	85	VAL	2.1
2	B	462	ARG	2.1
1	C	42	LEU	2.1
1	C	140	SER	2.1
1	C	125	TYR	2.1
1	A	186	ILE	2.1
1	C	83	PHE	2.1
1	C	93	VAL	2.1
1	C	258	VAL	2.1
1	C	67	ASP	2.1
1	A	130	TYR	2.1
1	A	185	LYS	2.1
1	C	329	VAL	2.1
1	A	60	VAL	2.0
2	D	468	PHE	2.0
1	C	156	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

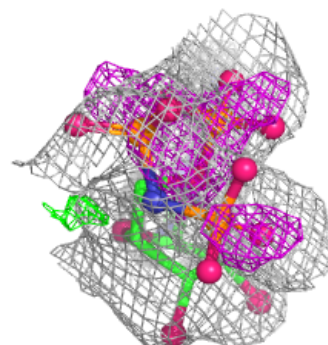
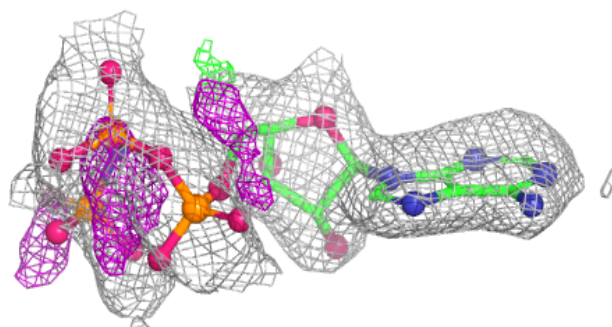
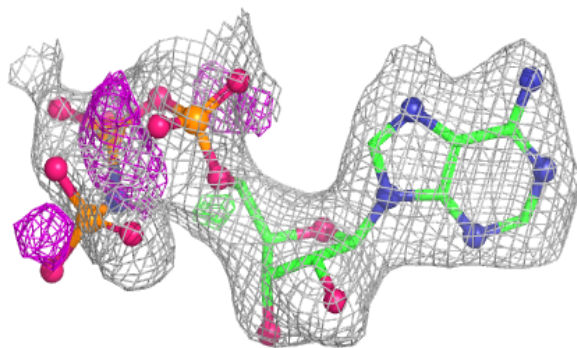
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ANP	B	801	31/31	0.74	0.13	49,84,134,141	0
7	TRS	B	802	8/8	0.74	0.16	52,61,67,72	0
5	MG	C	403	1/1	0.77	0.11	65,65,65,65	0
6	EDO	D	803	4/4	0.82	0.20	62,63,64,65	0
6	EDO	B	806	4/4	0.82	0.17	46,47,49,52	0
6	EDO	D	804	4/4	0.83	0.23	48,53,56,61	0
6	EDO	A	404	4/4	0.84	0.17	42,49,54,55	0
6	EDO	B	803	4/4	0.84	0.16	57,59,62,70	0
6	EDO	D	805	4/4	0.86	0.20	53,56,58,58	0
6	EDO	B	805	4/4	0.86	0.17	80,80,81,85	0
6	EDO	C	404	4/4	0.88	0.21	56,59,59,61	0
5	MG	A	403	1/1	0.89	0.09	42,42,42,42	0
4	ANP	C	402	31/31	0.90	0.11	69,81,87,91	0
6	EDO	D	802	4/4	0.91	0.12	42,43,48,52	0
6	EDO	B	804	4/4	0.93	0.11	44,47,47,52	0
3	A1AHE	C	401	34/34	0.94	0.11	39,47,65,68	0
3	A1AHE	A	401	34/34	0.94	0.10	36,45,52,54	0
6	EDO	D	801	4/4	0.95	0.09	34,39,40,42	0
4	ANP	A	402	31/31	0.95	0.08	37,47,52,59	0

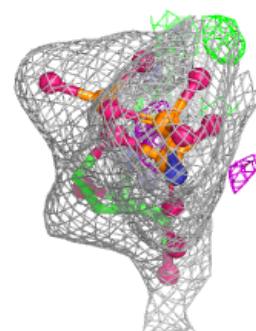
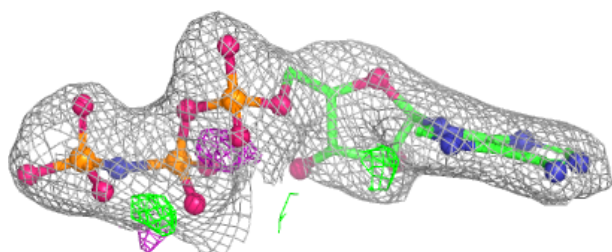
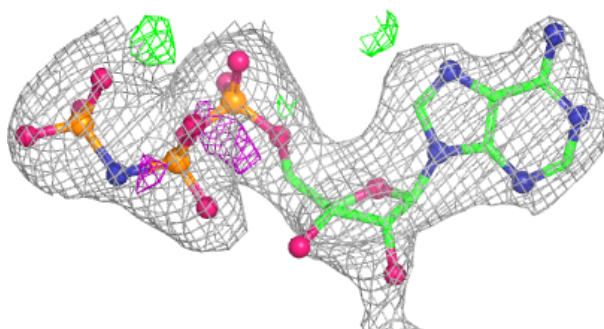
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

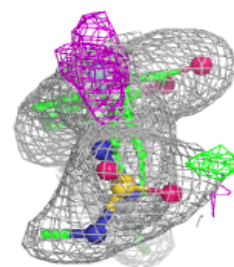
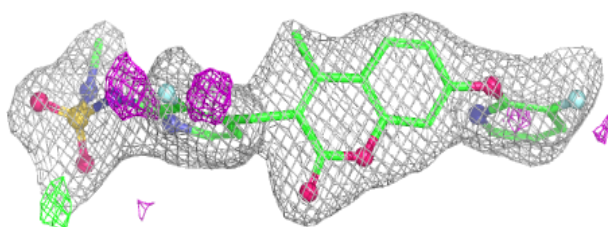
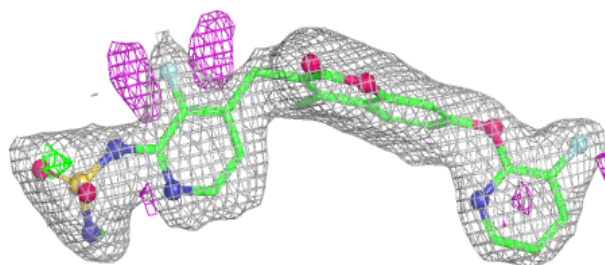
**Electron density around ANP C 402:**

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

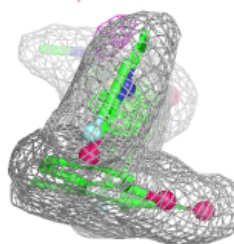
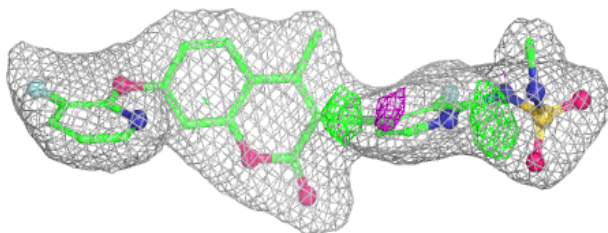
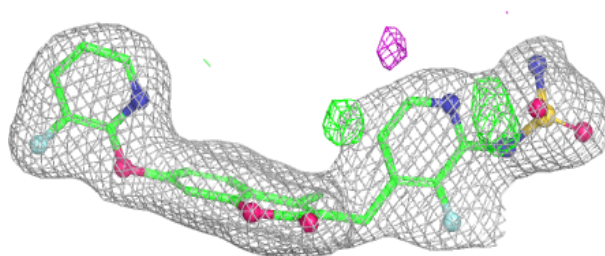


Electron density around A1AHE C 401:

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

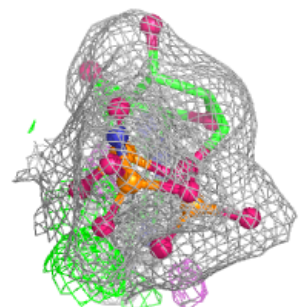
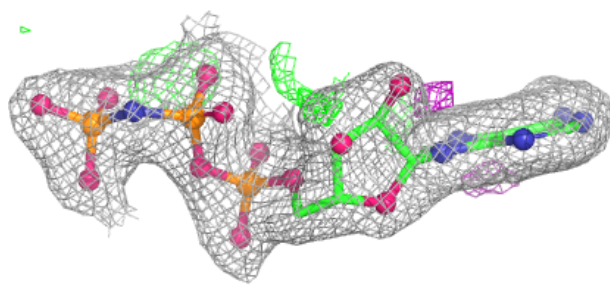
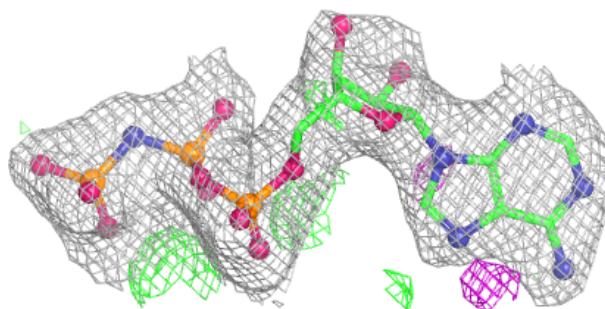
**Electron density around A1AHE A 401:**

$2mF_o-DF_c$ (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.