Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:33 PM UTC

PDB ID	:	8BK1 / pdb_00008bk1
Title	:	Mutant Imine Reductase IR007-143 from Amycolatopsis azurea, E120A, M197W, M206S, A213P, D238G, I240L
Authors	:	Gilio, A.K.; Grogan, G.J.
Deposited on	:	2022-11-08
Resolution	:	2.70 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:

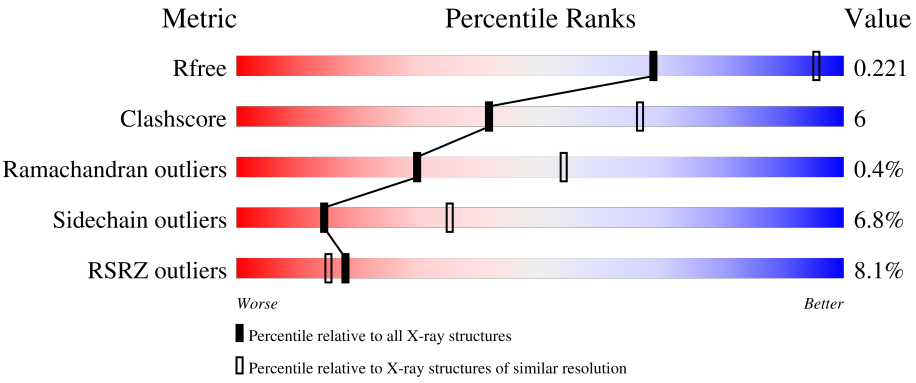
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	288	2% 87% 11%
1	B	288	3% 86% 11%
1	C	288	19% 83% 14%
1	D	288	8% 89% 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9070 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 Mutant Imine Reductase IR007-143 from Amycolatopsis azurea, E120A, M197W, M206S, A213P, D238G, I240L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	2	0
			2182	1384	375	414	9			
1	B	287	Total	C	N	O	S	0	1	0
			2164	1375	370	410	9			
1	C	287	Total	C	N	O	S	0	0	0
			2111	1339	358	405	9			
1	D	288	Total	C	N	O	S	0	2	0
			2149	1365	371	404	9			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLU	-	expression tag	UNP M2QI47
A	0	SER	-	expression tag	UNP M2QI47
A	120	ALA	GLU	engineered mutation	UNP M2QI47
A	197	TRP	MET	engineered mutation	UNP M2QI47
A	206	SER	MET	engineered mutation	UNP M2QI47
A	213	PRO	ALA	engineered mutation	UNP M2QI47
A	238	GLY	ASP	engineered mutation	UNP M2QI47
A	240	LEU	ILE	engineered mutation	UNP M2QI47
B	-1	GLU	-	expression tag	UNP M2QI47
B	0	SER	-	expression tag	UNP M2QI47
B	120	ALA	GLU	engineered mutation	UNP M2QI47
B	197	TRP	MET	engineered mutation	UNP M2QI47
B	206	SER	MET	engineered mutation	UNP M2QI47
B	213	PRO	ALA	engineered mutation	UNP M2QI47
B	238	GLY	ASP	engineered mutation	UNP M2QI47
B	240	LEU	ILE	engineered mutation	UNP M2QI47
C	-1	GLU	-	expression tag	UNP M2QI47
C	0	SER	-	expression tag	UNP M2QI47
C	120	ALA	GLU	engineered mutation	UNP M2QI47
C	197	TRP	MET	engineered mutation	UNP M2QI47

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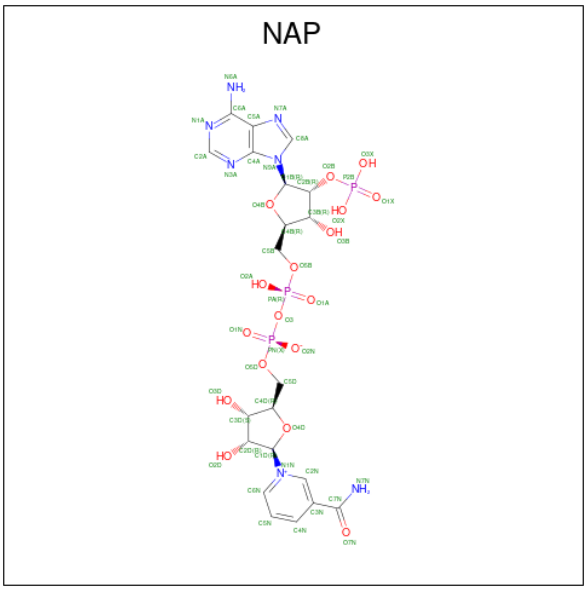
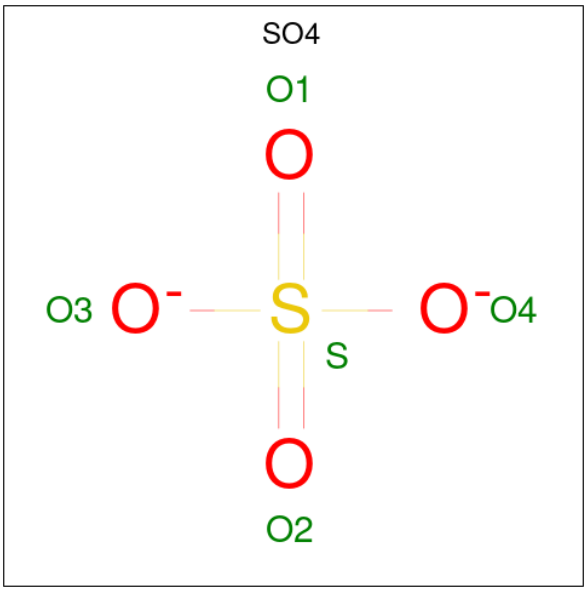
Chain	Residue	Modelled	Actual	Comment	Reference
C	206	SER	MET	engineered mutation	UNP M2QI47
C	213	PRO	ALA	engineered mutation	UNP M2QI47
C	238	GLY	ASP	engineered mutation	UNP M2QI47
C	240	LEU	ILE	engineered mutation	UNP M2QI47
D	-1	GLU	-	expression tag	UNP M2QI47
D	0	SER	-	expression tag	UNP M2QI47
D	120	ALA	GLU	engineered mutation	UNP M2QI47
D	197	TRP	MET	engineered mutation	UNP M2QI47
D	206	SER	MET	engineered mutation	UNP M2QI47
D	213	PRO	ALA	engineered mutation	UNP M2QI47
D	238	GLY	ASP	engineered mutation	UNP M2QI47
D	240	LEU	ILE	engineered mutation	UNP M2QI47

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

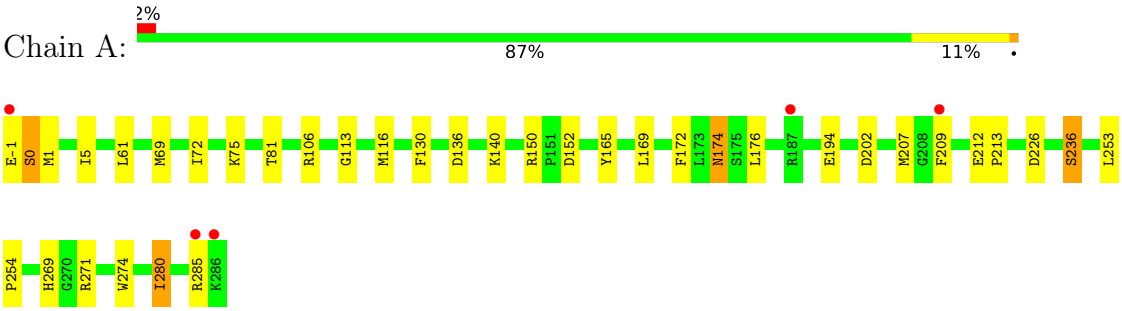
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	93	Total O 93 93	0	0
4	B	71	Total O 71 71	0	0
4	C	25	Total O 25 25	0	0
4	D	43	Total O 43 43	0	0

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.

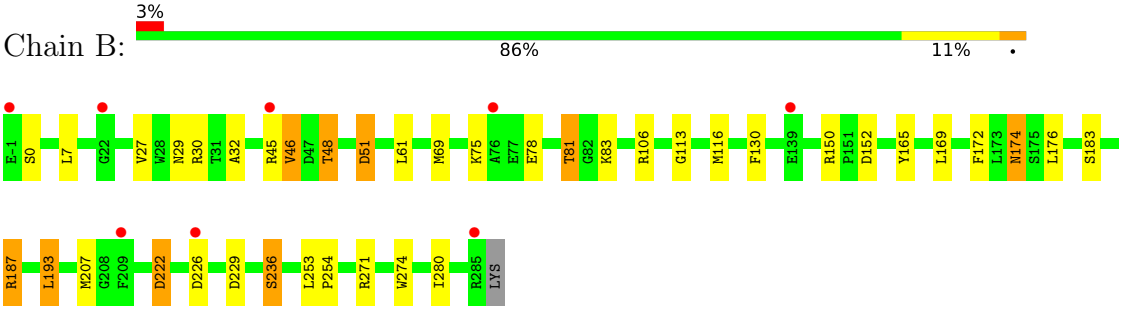
• Molecule 1: Mutant Imine Reductase IR007-143 from Amycolatopsis azurea, E120A, M197W, M206S, A213P, D238G, I240L

Chain A:



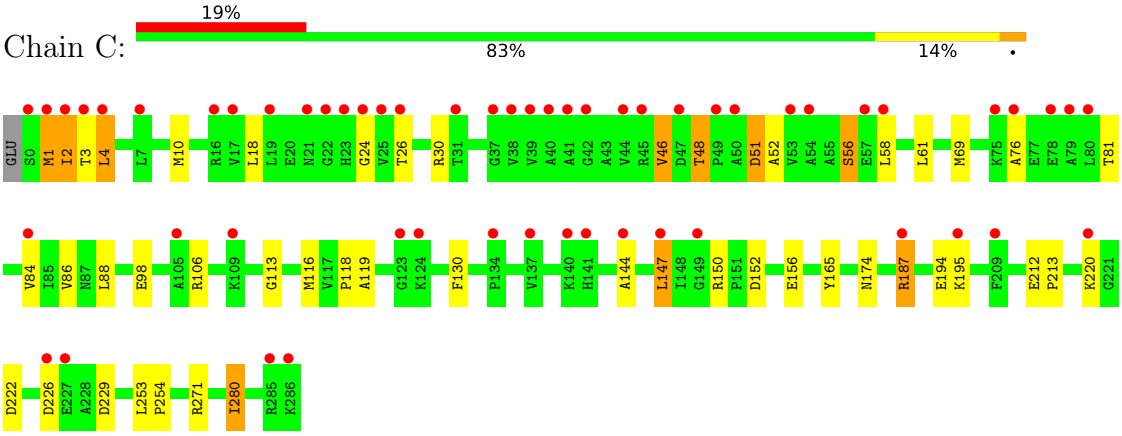
• Molecule 1: Mutant Imine Reductase IR007-143 from Amycolatopsis azurea, E120A, M197W, M206S, A213P, D238G, I240L

Chain B:



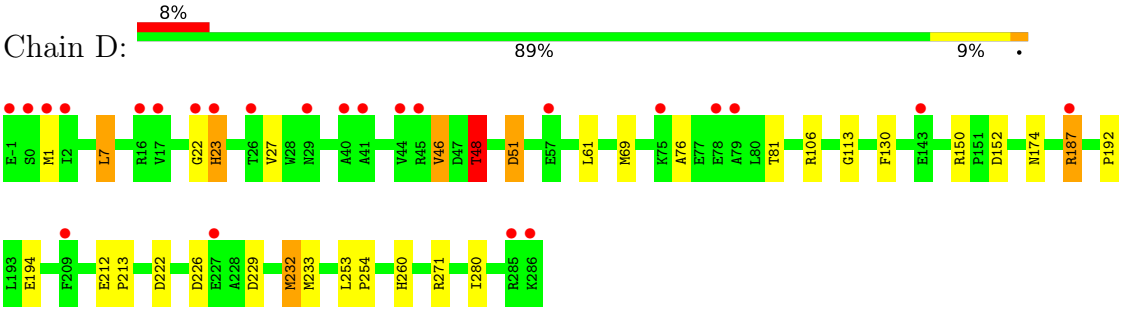
• Molecule 1: Mutant Imine Reductase IR007-143 from Amycolatopsis azurea, E120A, M197W, M206S, A213P, D238G, I240L

Chain C:



• Molecule 1: Mutant Imine Reductase IR007-143 from Amycolatopsis azurea, E120A, M197W, M206S, A213P, D238G, I240L

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	186.03Å 186.03Å 373.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.32 – 2.70 62.32 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.32-2.70) 99.9 (62.32-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, R_{free}	0.188 , 0.211 0.202 , 0.221	Depositor DCC
R_{free} test set	3396 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	55.9	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9070	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: SO4, NAP

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	1.09	2/2226 (0.1%)	1.43	6/3020 (0.2%)
1	B	1.07	1/2208 (0.0%)	1.45	4/2996 (0.1%)
1	C	1.11	0/2155	1.47	3/2934 (0.1%)
1	D	1.12	1/2196 (0.0%)	1.46	4/2985 (0.1%)
All	All	1.10	4/8785 (0.0%)	1.45	17/11935 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	229	ASP	C-N	-6.88	1.25	1.33
1	A	269	HIS	CE1-NE2	6.25	1.38	1.32
1	D	260	HIS	CE1-NE2	5.61	1.38	1.32
1	A	140	LYS	C-O	-5.09	1.17	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	81	THR	CB-CA-C	7.59	120.61	110.06
1	D	229	ASP	CA-CB-CG	6.82	119.42	112.60
1	D	222	ASP	CA-CB-CG	6.79	119.39	112.60
1	C	229	ASP	CA-CB-CG	6.68	119.28	112.60
1	B	51	ASP	CA-CB-CG	6.45	119.05	112.60
1	C	51	ASP	CA-CB-CG	6.44	119.04	112.60
1	B	229	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	81	THR	CB-CA-C	6.04	118.46	110.06
1	B	222	ASP	CA-CB-CG	5.95	118.55	112.60
1	D	51	ASP	CA-CB-CG	5.90	118.50	112.60
1	C	222	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	209	PHE	CA-C-O	-5.28	115.28	120.82
1	D	48	THR	CB-CA-C	5.21	116.94	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	202	ASP	CA-C-N	5.15	127.44	120.65
1	A	202	ASP	C-N-CA	5.15	127.44	120.65
1	A	136	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	285	ARG	N-CA-C	-5.02	105.94	111.71

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	2182	0	2147	25	0
1	B	2164	0	2133	31	0
1	C	2111	0	2022	41	0
1	D	2149	0	2091	23	0
2	A	48	0	25	0	0
2	B	48	0	25	2	0
2	C	48	0	25	3	0
2	D	48	0	25	0	0
3	A	15	0	0	1	0
3	B	10	0	0	1	0
3	C	10	0	0	0	0
3	D	5	0	0	0	0
4	A	93	0	0	1	0
4	B	71	0	0	1	0
4	C	25	0	0	3	0
4	D	43	0	0	1	0
All	All	9070	0	8493	111	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 6.

All (111) 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:3:THR:HG22	1:C:26:THR:HB	1.53	0.88
1:D:232:MET:HE2	1:D:232:MET:C	2.04	0.83
1:C:10:MET:CE	1:C:119:ALA:N	2.45	0.79
1:A:169:LEU:HD21	1:B:236:SER:HB3	1.63	0.79
1:A:236:SER:HB3	1:B:169:LEU:HD21	1.66	0.78
1:A:172:PHE:CD1	1:B:207:MET:HE1	2.21	0.75
1:A:116:MET:CE	1:A:165:TYR:CD1	2.70	0.74
1:C:10:MET:HE1	1:C:119:ALA:N	2.03	0.73
1:C:10:MET:HE1	1:C:118:PRO:C	2.13	0.73
1:C:86:VAL:HG12	1:C:88:LEU:HD11	1.73	0.70
1:A:207:MET:HE1	1:B:172:PHE:CD1	2.26	0.70
1:C:24:GLY:C	4:C:403:HOH:O	2.35	0.69
1:B:46:VAL:CG1	1:B:51:ASP:HB2	2.23	0.69
1:C:3:THR:HG23	1:C:56:SER:HB2	1.74	0.69
1:D:46:VAL:CG1	1:D:51:ASP:HB2	2.24	0.68
1:B:30:ARG:HH21	2:B:301:NAP:P2B	2.17	0.68
1:A:172:PHE:HD1	1:B:207:MET:HE1	1.57	0.68
1:C:46:VAL:CG1	1:C:51:ASP:HB2	2.24	0.67
1:B:187:ARG:NH1	4:B:401:HOH:O	2.29	0.65
1:B:116:MET:CE	1:B:165:TYR:CD1	2.81	0.64
1:A:207:MET:HE1	1:B:172:PHE:HD1	1.62	0.64
1:C:116:MET:CE	1:C:165:TYR:CD1	2.80	0.64
1:A:174:ASN:ND2	1:B:174:ASN:OD1	2.31	0.64
1:A:280:ILE:HD12	1:A:280:ILE:C	2.23	0.63
1:D:187[A]:ARG:NH1	4:D:401:HOH:O	2.34	0.61
1:C:86:VAL:HG12	1:C:88:LEU:CD1	2.30	0.61
1:C:10:MET:HE2	1:C:119:ALA:N	2.15	0.60
1:C:58:LEU:HA	1:C:84:VAL:HG23	1.83	0.60
1:C:280:ILE:C	1:C:280:ILE:HD12	2.26	0.60
1:C:1:MET:HA	4:C:403:HOH:O	2.02	0.60
1:C:30:ARG:HH21	2:C:301:NAP:P2B	2.27	0.57
1:B:32:ALA:N	3:B:303:SO4:O4	2.38	0.56
1:A:61:LEU:CD1	1:A:69:MET:HG3	2.36	0.56
1:A:150:ARG:NH1	1:A:152:ASP:OD1	2.40	0.55
1:D:61:LEU:CD1	1:D:69:MET:HG3	2.38	0.54
1:B:46:VAL:HG13	1:B:51:ASP:HB2	1.90	0.54
1:C:150:ARG:NH1	1:C:152:ASP:OD1	2.42	0.53
1:D:232:MET:HE2	1:D:232:MET:O	2.08	0.52
1:C:187:ARG:NH2	4:C:401:HOH:O	2.42	0.52
1:C:10:MET:HE2	1:C:119:ALA:CA	2.39	0.52
3:A:303:SO4:O2	4:A:401:HOH:O	2.15	0.52
1:B:150:ARG:NH1	1:B:152:ASP:OD1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LEU:CD1	1:C:69:MET:HG3	2.40	0.52
1:D:46:VAL:HG13	1:D:51:ASP:HB2	1.92	0.52
1:C:4:LEU:C	1:C:4:LEU:CD1	2.83	0.51
1:D:150:ARG:NH1	1:D:152:ASP:OD1	2.43	0.51
1:B:30:ARG:NE	2:B:301:NAP:O2X	2.38	0.51
1:B:113:GLY:HA2	1:B:130:PHE:O	2.11	0.51
1:D:187[B]:ARG:NH1	1:D:192:PRO:HA	2.25	0.50
1:D:232:MET:HE2	1:D:233:MET:N	2.25	0.50
1:D:22:GLY:O	1:D:23:HIS:C	2.54	0.50
1:D:232:MET:HE2	1:D:233:MET:HA	1.94	0.50
1:A:116:MET:HE3	1:A:165:TYR:CD1	2.45	0.50
1:B:46:VAL:CG1	1:B:51:ASP:CB	2.90	0.49
1:A:113:GLY:HA2	1:A:130:PHE:O	2.12	0.49
1:B:48:THR:HG22	1:B:51:ASP:CG	2.38	0.49
1:C:10:MET:HE2	1:C:119:ALA:HB2	1.95	0.49
1:B:7:LEU:HD11	1:B:27:VAL:HB	1.95	0.48
1:D:113:GLY:HA2	1:D:130:PHE:O	2.12	0.48
1:C:113:GLY:HA2	1:C:130:PHE:O	2.13	0.48
1:D:7:LEU:HD21	1:D:27:VAL:HB	1.96	0.48
1:C:48:THR:HG22	1:C:51:ASP:CG	2.38	0.48
1:B:183:SER:HB3	1:B:193:LEU:HD11	1.95	0.48
1:B:187:ARG:HH11	1:B:187:ARG:HB3	1.79	0.48
1:D:187[A]:ARG:HH11	1:D:187[A]:ARG:HB3	1.79	0.48
1:D:46:VAL:CG1	1:D:51:ASP:CB	2.91	0.48
1:C:144:ALA:O	1:C:147:LEU:HD22	2.13	0.48
1:A:61:LEU:HD13	1:A:69:MET:HG3	1.94	0.47
1:D:48:THR:HG22	1:D:51:ASP:CG	2.39	0.47
1:C:30:ARG:NE	2:C:301:NAP:O2X	2.35	0.47
1:C:150:ARG:NH1	1:C:152:ASP:OD2	2.48	0.47
1:B:46:VAL:HG13	1:B:51:ASP:CB	2.45	0.47
1:D:150:ARG:NH1	1:D:152:ASP:OD2	2.47	0.47
1:C:61:LEU:HD13	1:C:69:MET:HG3	1.97	0.46
1:B:253:LEU:HB3	1:B:254:PRO:HD3	1.98	0.46
1:A:212:GLU:HB3	1:A:213:PRO:HD3	1.98	0.46
1:C:10:MET:HE3	2:C:301:NAP:C7N	2.46	0.46
1:A:116:MET:CE	1:A:165:TYR:CE1	3.00	0.45
1:A:253:LEU:HB3	1:A:254:PRO:HD3	1.98	0.45
1:D:46:VAL:HG13	1:D:51:ASP:CB	2.46	0.45
1:D:212:GLU:HB3	1:D:213:PRO:HD3	1.99	0.45
1:B:45:ARG:HG2	1:B:46:VAL:N	2.32	0.45
1:C:46:VAL:CG1	1:C:51:ASP:CB	2.92	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:VAL:HG13	1:C:51:ASP:HB2	1.97	0.45
1:B:150:ARG:NH1	1:B:152:ASP:OD2	2.48	0.44
1:A:5:ILE:HG21	1:A:72:ILE:HG21	2.00	0.44
1:A:176:LEU:HD13	1:B:274:TRP:CD2	2.53	0.44
1:C:212:GLU:HB3	1:C:213:PRO:HD3	2.00	0.44
1:D:232:MET:HE2	1:D:233:MET:CA	2.47	0.44
1:D:61:LEU:HD13	1:D:69:MET:HG3	2.00	0.44
1:A:1:MET:HE2	1:A:1:MET:HB2	1.91	0.44
1:B:150:ARG:NH1	1:B:152:ASP:CG	2.76	0.43
1:C:3:THR:HG21	1:C:52:ALA:O	2.18	0.43
1:B:7:LEU:HD12	1:B:29:ASN:HB2	2.01	0.42
1:B:61:LEU:HD13	1:B:69:MET:HG3	2.01	0.42
1:C:58:LEU:HA	1:C:84:VAL:CG2	2.47	0.42
1:C:147:LEU:HD13	1:C:147:LEU:N	2.34	0.42
1:A:150:ARG:NH1	1:A:152:ASP:CG	2.78	0.42
1:C:150:ARG:NH1	1:C:152:ASP:CG	2.77	0.42
1:C:4:LEU:C	1:C:4:LEU:HD12	2.43	0.42
1:D:150:ARG:NH1	1:D:152:ASP:CG	2.78	0.41
1:D:253:LEU:HB3	1:D:254:PRO:HD3	2.02	0.41
1:A:116:MET:HE3	1:A:165:TYR:HD1	1.84	0.41
1:C:116:MET:HE3	1:C:165:TYR:CD1	2.55	0.41
1:C:253:LEU:HB3	1:C:254:PRO:HD3	2.00	0.41
1:A:-1:GLU:O	1:A:0:SER:C	2.62	0.41
1:C:46:VAL:HG11	1:C:51:ASP:HB2	2.00	0.41
1:C:1:MET:O	1:C:2:ILE:C	2.64	0.40
1:A:207:MET:HE1	1:B:172:PHE:HA	2.04	0.40
1:A:274:TRP:CD2	1:B:176:LEU:HD13	2.57	0.40
1:C:46:VAL:HG13	1:C:51:ASP:CB	2.50	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	288/288 (100%)	276 (96%)	12 (4%)	0	100	100
1	B	286/288 (99%)	276 (96%)	10 (4%)	0	100	100
1	C	285/288 (99%)	274 (96%)	9 (3%)	2 (1%)	18	41
1	D	288/288 (100%)	277 (96%)	9 (3%)	2 (1%)	18	41
All	All	1147/1152 (100%)	1103 (96%)	40 (4%)	4 (0%)	30	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2	ILE
1	D	23	HIS
1	D	76	ALA
1	C	76	ALA

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	218/219 (100%)	209 (96%)	9 (4%)	27	56
1	B	216/219 (99%)	200 (93%)	16 (7%)	13	32
1	C	204/219 (93%)	185 (91%)	19 (9%)	8	21
1	D	209/219 (95%)	195 (93%)	14 (7%)	15	36
All	All	847/876 (97%)	789 (93%)	58 (7%)	14	35

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	75	LYS
1	A	106	ARG
1	A	174	ASN
1	A	194	GLU
1	A	226	ASP
1	A	236	SER

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Mol	Chain	Res	Type
1	A	271	ARG
1	A	280	ILE
1	B	0	SER
1	B	46	VAL
1	B	48	THR
1	B	75	LYS
1	B	78	GLU
1	B	81	THR
1	B	83	LYS
1	B	106	ARG
1	B	174	ASN
1	B	187	ARG
1	B	193	LEU
1	B	222	ASP
1	B	226	ASP
1	B	236	SER
1	B	271	ARG
1	B	280	ILE
1	C	1	MET
1	C	4	LEU
1	C	18	LEU
1	C	46	VAL
1	C	48	THR
1	C	56	SER
1	C	81	THR
1	C	98	GLU
1	C	106	ARG
1	C	147	LEU
1	C	156	GLU
1	C	174	ASN
1	C	187	ARG
1	C	194	GLU
1	C	195	LYS
1	C	220	LYS
1	C	226	ASP
1	C	271	ARG
1	C	280	ILE
1	D	1	MET
1	D	7	LEU
1	D	46	VAL
1	D	48	THR
1	D	81	THR

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Mol	Chain	Res	Type
1	D	106	ARG
1	D	174	ASN
1	D	187[A]	ARG
1	D	187[B]	ARG
1	D	194	GLU
1	D	226	ASP
1	D	232	MET
1	D	271	ARG
1	D	280	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	23	HIS
1	B	141	HIS
1	B	162	GLN
1	C	23	HIS
1	C	141	HIS
1	C	166	GLN
1	D	141	HIS
1	D	162	GLN
1	D	166	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)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAP	D	301	-	50,52,52	0.57	1 (2%)	71,80,80	0.81	2 (2%)
3	SO4	C	303	-	4,4,4	0.25	0	6,6,6	0.13	0
2	NAP	B	301	-	50,52,52	0.60	1 (2%)	71,80,80	0.81	2 (2%)
3	SO4	C	302	-	4,4,4	0.25	0	6,6,6	0.21	0
3	SO4	A	303	-	4,4,4	0.22	0	6,6,6	0.14	0
2	NAP	A	301	-	50,52,52	0.96	1 (2%)	71,80,80	1.06	3 (4%)
3	SO4	D	302	-	4,4,4	0.21	0	6,6,6	0.14	0
3	SO4	A	304	-	4,4,4	0.32	0	6,6,6	0.08	0
3	SO4	B	303	-	4,4,4	0.25	0	6,6,6	0.13	0
3	SO4	B	302	-	4,4,4	0.34	0	6,6,6	0.17	0
3	SO4	A	302	-	4,4,4	0.37	0	6,6,6	0.24	0
2	NAP	C	301	-	50,52,52	0.55	0	71,80,80	0.83	2 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	A	301	-	-	4/35/67/67	0/5/5/5
2	NAP	D	301	-	-	5/35/67/67	0/5/5/5
2	NAP	B	301	-	-	11/35/67/67	0/5/5/5
2	NAP	C	301	-	-	8/35/67/67	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAP	C2N-N1N	5.71	1.41	1.35
2	B	301	NAP	C2N-N1N	2.54	1.37	1.35
2	D	301	NAP	C2N-N1N	2.01	1.37	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	NAP	P2B-O2B-C2B	-4.99	110.09	123.43
2	D	301	NAP	P2B-O2B-C2B	-4.76	110.73	123.43
2	B	301	NAP	P2B-O2B-C2B	-4.36	111.78	123.43
2	A	301	NAP	P2B-O2B-C2B	-4.33	111.87	123.43
2	A	301	NAP	C6N-N1N-C2N	-3.25	119.11	121.88
2	B	301	NAP	C6N-N1N-C2N	-2.44	119.80	121.88
2	D	301	NAP	C6N-N1N-C2N	-2.32	119.90	121.88
2	C	301	NAP	C6N-N1N-C2N	-2.25	119.97	121.88
2	A	301	NAP	O2A-PA-O3	2.11	112.98	107.27

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAP	O4D-C1D-N1N-C2N
2	A	301	NAP	O4D-C1D-N1N-C6N
2	A	301	NAP	C2D-C1D-N1N-C6N
2	B	301	NAP	C5D-O5D-PN-O3
2	B	301	NAP	C5D-O5D-PN-O1N
2	B	301	NAP	C5D-O5D-PN-O2N
2	B	301	NAP	O4D-C1D-N1N-C2N
2	B	301	NAP	O4D-C1D-N1N-C6N
2	B	301	NAP	C2D-C1D-N1N-C2N
2	B	301	NAP	C2D-C1D-N1N-C6N
2	C	301	NAP	C5B-O5B-PA-O1A
2	C	301	NAP	C5B-O5B-PA-O2A
2	C	301	NAP	O4D-C1D-N1N-C2N
2	C	301	NAP	O4D-C1D-N1N-C6N
2	C	301	NAP	C2D-C1D-N1N-C2N
2	C	301	NAP	C2D-C1D-N1N-C6N
2	D	301	NAP	O4D-C1D-N1N-C2N
2	D	301	NAP	O4D-C1D-N1N-C6N
2	D	301	NAP	C2D-C1D-N1N-C2N
2	D	301	NAP	C2D-C1D-N1N-C6N
2	B	301	NAP	O4D-C4D-C5D-O5D
2	B	301	NAP	PA-O3-PN-O5D
2	D	301	NAP	PA-O3-PN-O5D
2	B	301	NAP	C3D-C4D-C5D-O5D
2	C	301	NAP	C5B-O5B-PA-O3
2	A	301	NAP	C2D-C1D-N1N-C2N
2	C	301	NAP	C2B-O2B-P2B-O1X
2	B	301	NAP	PA-O3-PN-O2N

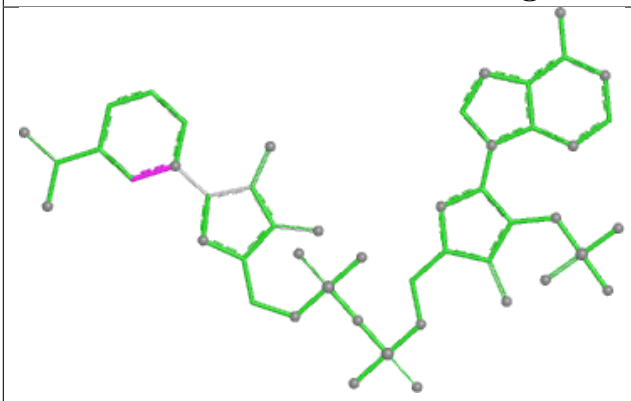
There are no ring outliers.

4 monomers are involved in 7 short contacts:

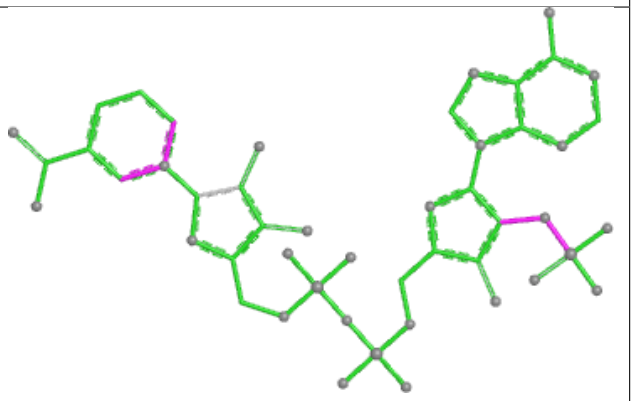
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	NAP	2	0
3	A	303	SO4	1	0
3	B	303	SO4	1	0
2	C	301	NAP	3	0

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.

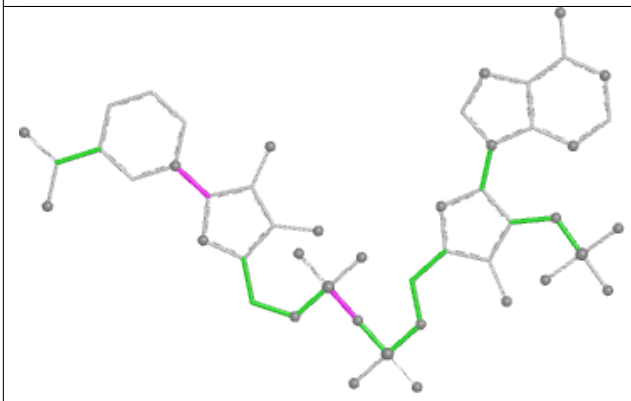
Ligand NAP D 301



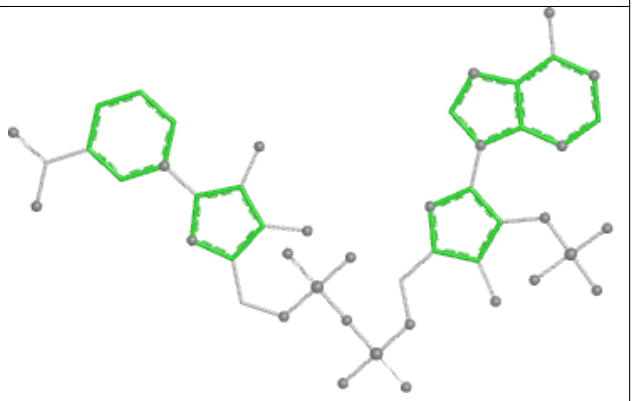
Bond lengths



Bond angles

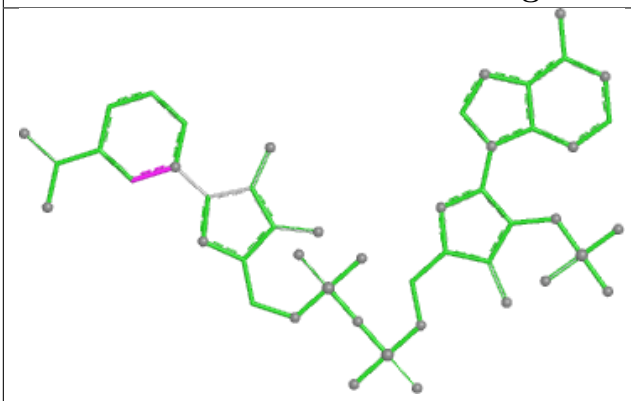


Torsions

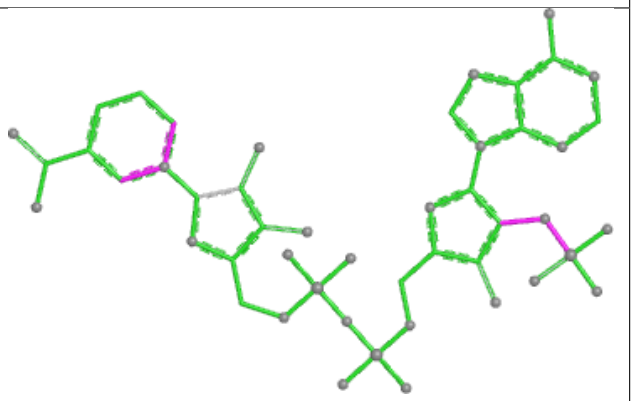


Rings

Ligand NAP B 301



Bond lengths



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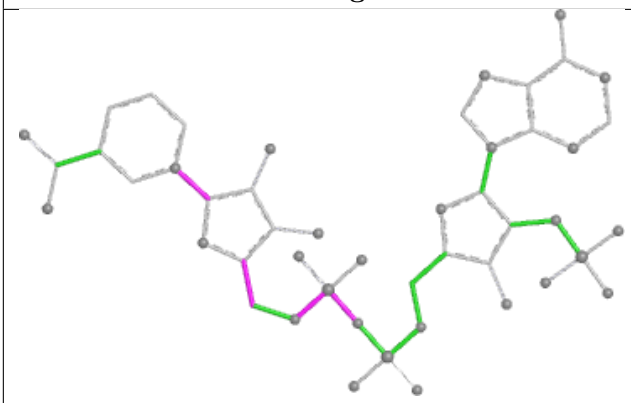

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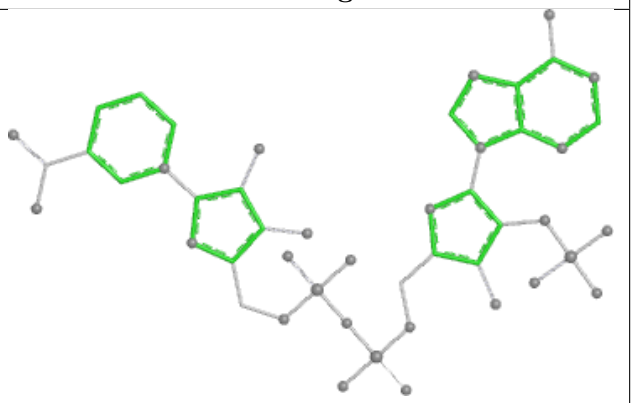
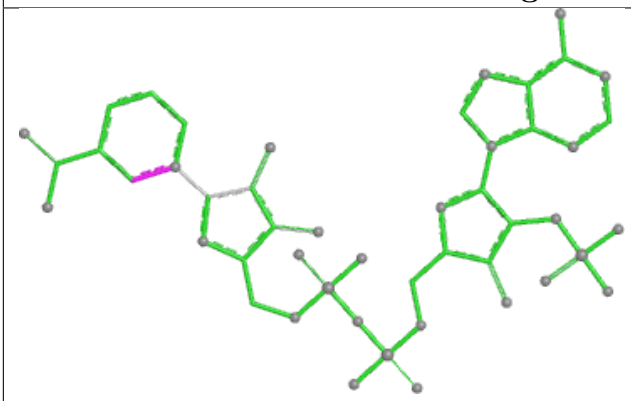
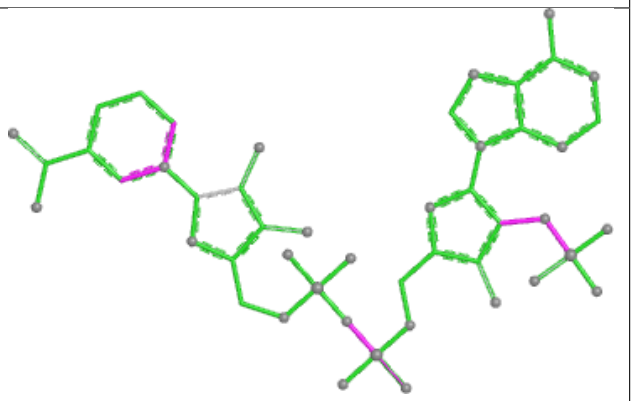


Rings

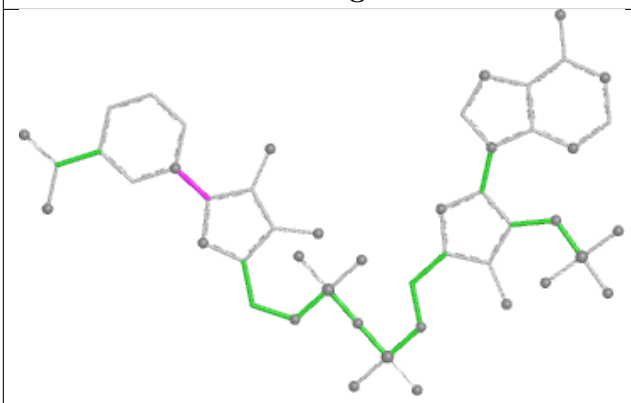
Ligand NAP A 301



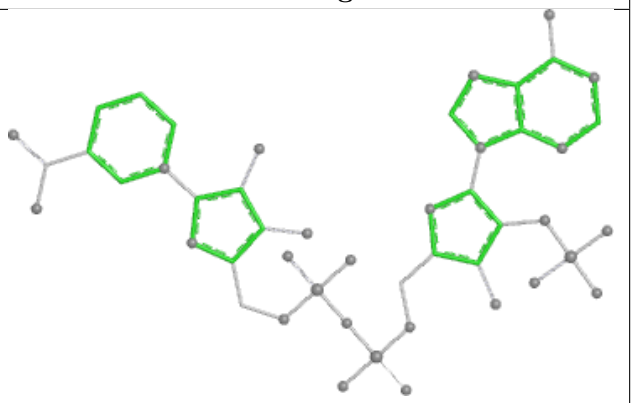
Bond lengths



Bond angles

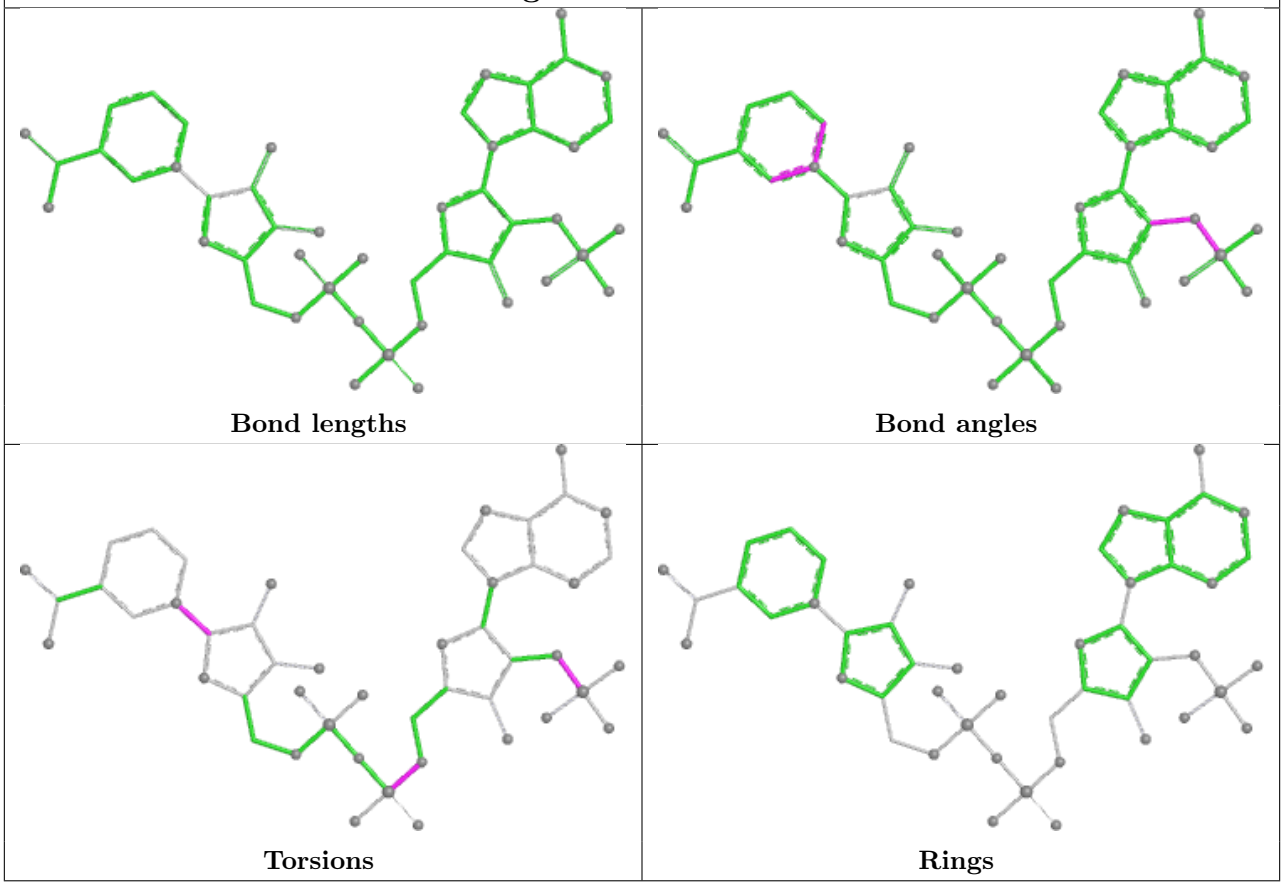


Torsions



Rings

Ligand NAP C 301



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	288/288 (100%)	-0.27	5 (1%) 69 67	26, 47, 69, 116	2 (0%)
1	B	287/288 (99%)	0.05	8 (2%) 55 51	22, 54, 83, 120	1 (0%)
1	C	287/288 (99%)	1.05	56 (19%) 3 2	41, 83, 123, 139	0
1	D	288/288 (100%)	0.55	24 (8%) 17 14	20, 71, 102, 118	2 (0%)
All	All	1150/1152 (99%)	0.34	93 (8%) 18 15	20, 58, 110, 139	5 (0%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	285	ARG	8.1
1	C	2	ILE	5.8
1	A	286	LYS	5.6
1	D	2	ILE	5.4
1	C	0	SER	5.3
1	D	286	LYS	4.6
1	D	187[A]	ARG	4.4
1	C	57	GLU	4.3
1	C	37	GLY	4.2
1	C	19	LEU	4.2
1	D	285	ARG	4.0
1	C	23	HIS	3.8
1	C	285	ARG	3.8
1	C	78	GLU	3.8
1	C	209	PHE	3.7
1	A	-1	GLU	3.7
1	B	-1	GLU	3.7
1	C	47	ASP	3.7
1	C	80	LEU	3.7
1	C	140	LYS	3.6
1	D	75	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	143	GLU	3.5
1	C	75	LYS	3.5
1	C	79	ALA	3.5
1	D	0	SER	3.5
1	C	195	LYS	3.4
1	C	40	ALA	3.3
1	C	141	HIS	3.3
1	C	3	THR	3.3
1	C	41	ALA	3.2
1	C	50	ALA	3.2
1	B	22	GLY	3.1
1	C	84	VAL	3.1
1	A	285	ARG	3.1
1	C	44	VAL	3.1
1	C	1	MET	3.1
1	D	26	THR	3.1
1	A	187[A]	ARG	3.1
1	C	286	LYS	3.0
1	C	53	VAL	3.0
1	B	139	GLU	3.0
1	C	25	VAL	2.9
1	D	23	HIS	2.9
1	C	144	ALA	2.8
1	D	209	PHE	2.8
1	C	147	LEU	2.8
1	C	137	VAL	2.8
1	D	-1	GLU	2.7
1	C	220	LYS	2.7
1	C	58	LEU	2.6
1	C	76	ALA	2.6
1	B	226	ASP	2.6
1	C	45	ARG	2.6
1	D	227	GLU	2.6
1	C	54	ALA	2.6
1	D	57	GLU	2.5
1	C	42	GLY	2.5
1	B	76	ALA	2.5
1	C	31	THR	2.5
1	A	209	PHE	2.5
1	C	134	PRO	2.5
1	D	1	MET	2.5
1	C	16	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	109	LYS	2.4
1	D	17	VAL	2.4
1	C	7	LEU	2.4
1	C	26	THR	2.4
1	C	39	VAL	2.4
1	D	22	GLY	2.4
1	C	17	VAL	2.4
1	D	79	ALA	2.4
1	C	123	GLY	2.3
1	B	209	PHE	2.3
1	C	4	LEU	2.3
1	C	105	ALA	2.3
1	C	227	GLU	2.3
1	C	21	ASN	2.3
1	D	41	ALA	2.2
1	C	124	LYS	2.2
1	C	187	ARG	2.2
1	C	149	GLY	2.2
1	D	44	VAL	2.2
1	D	40	ALA	2.2
1	C	49	PRO	2.1
1	D	29	ASN	2.1
1	C	38	VAL	2.1
1	C	226	ASP	2.1
1	D	78	GLU	2.1
1	D	16	ARG	2.1
1	D	45	ARG	2.1
1	C	22	GLY	2.1
1	B	45	ARG	2.1
1	C	24	GLY	2.1

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

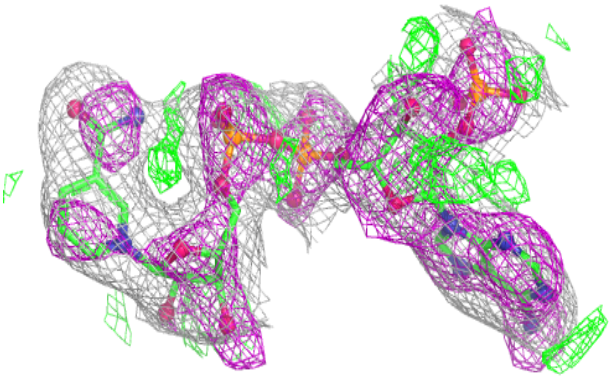
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

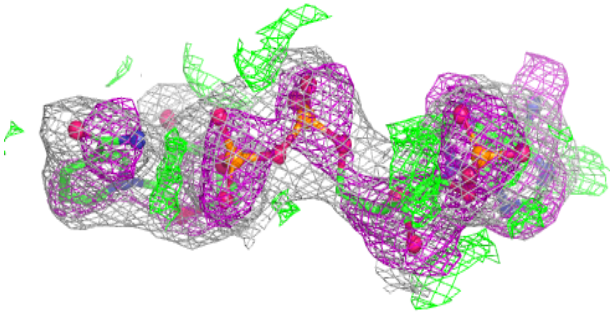
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	C	302	5/5	0.61	0.12	99,131,137,151	0
3	SO4	C	303	5/5	0.79	0.11	119,128,150,151	0
3	SO4	B	303	5/5	0.80	0.11	111,118,148,161	0
3	SO4	D	302	5/5	0.80	0.07	104,106,113,125	0
3	SO4	A	303	5/5	0.84	0.11	87,103,127,130	0
3	SO4	A	302	5/5	0.85	0.21	79,82,97,112	0
2	NAP	C	301	48/48	0.88	0.13	35,41,49,53	0
3	SO4	B	302	5/5	0.88	0.17	77,90,106,118	0
3	SO4	A	304	5/5	0.91	0.17	123,123,143,152	0
2	NAP	D	301	48/48	0.92	0.11	35,41,49,53	0
2	NAP	B	301	48/48	0.95	0.09	40,50,61,69	0
2	NAP	A	301	48/48	0.98	0.05	35,41,49,53	0

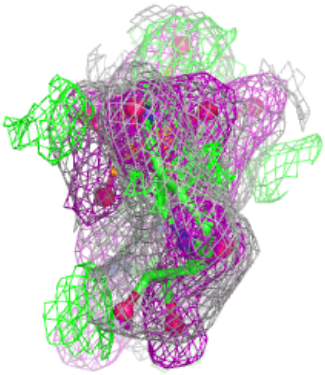
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP C 301:

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

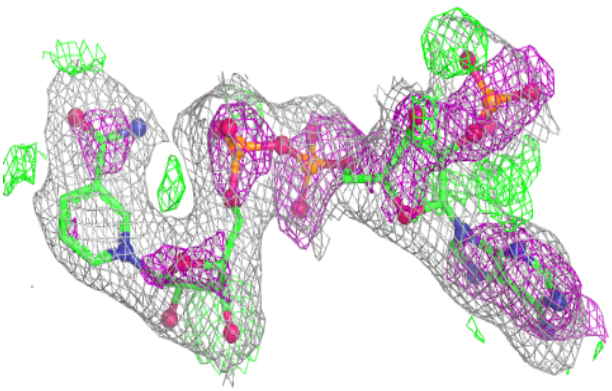


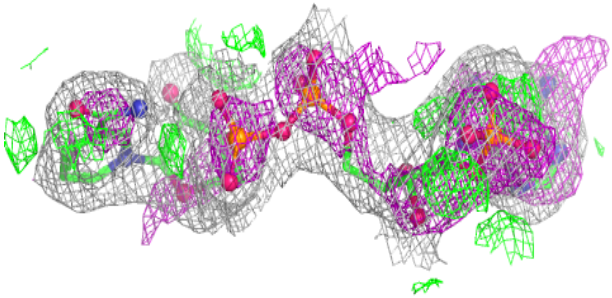


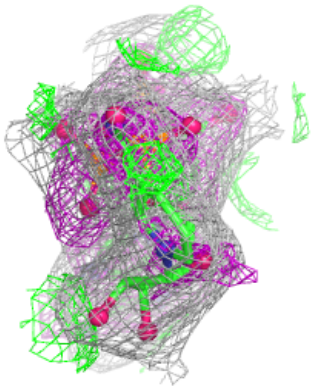


Electron density around NAP D 301:

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

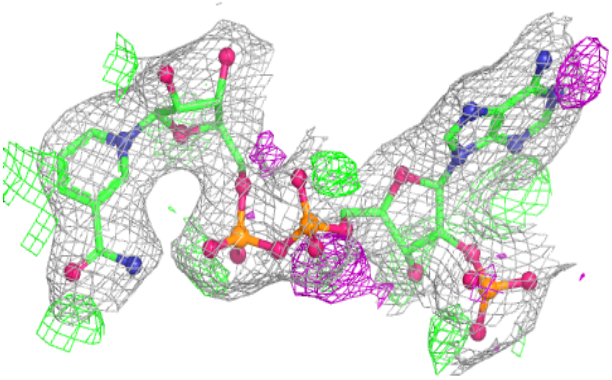


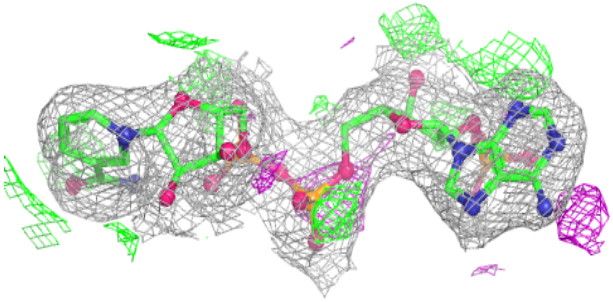


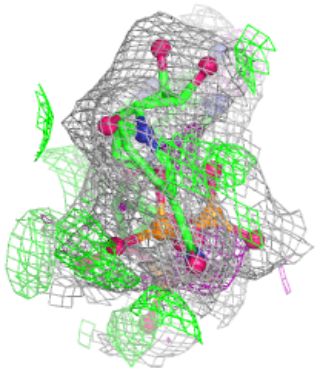


Electron density around NAP B 301:

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

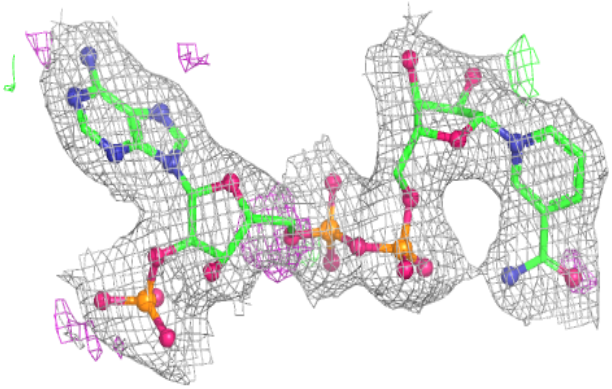


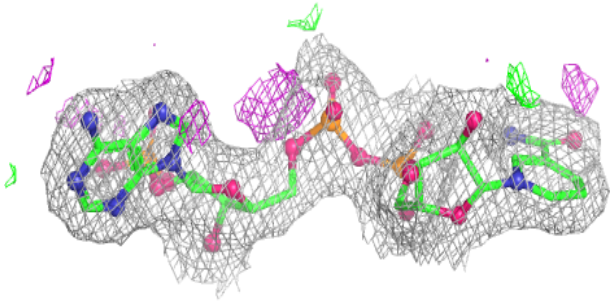


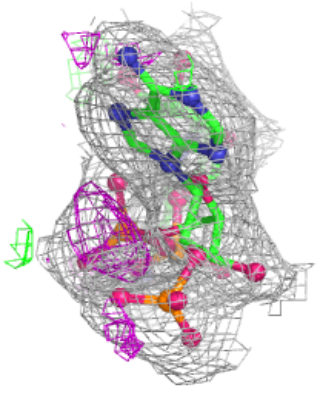


Electron density around NAP A 301:

$2mF_o$-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.