



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:21 PM UTC

PDB ID : 9J0W / pdb_00009j0w
Title : CRYSTAL STRUCTURE OF A NOVEL ALDEHYDE DEHYDROGENASE
FROM KLEBSIELLA PNEUMONIAE IN COMPLEX WITH COENZYME
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Deposited on : 2024-08-03
Resolution : 2.51 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

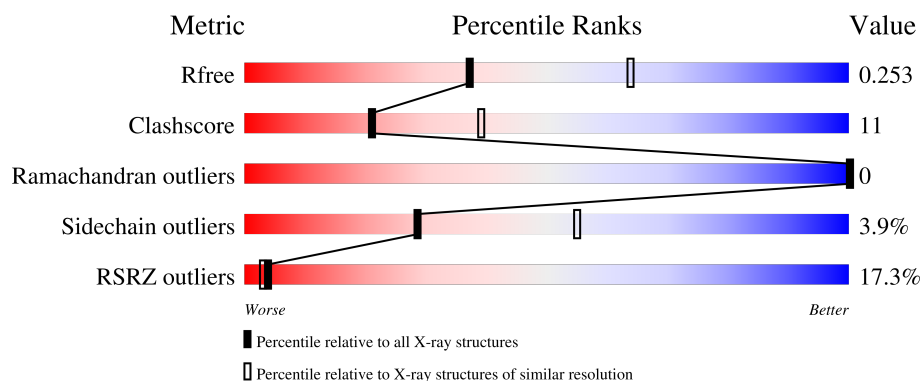
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	489	6% 78% 21% ..
1	B	489	46% 63% 30% ..
1	C	489	11% 77% 18% ..
1	D	489	6% 79% 19% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14639 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.

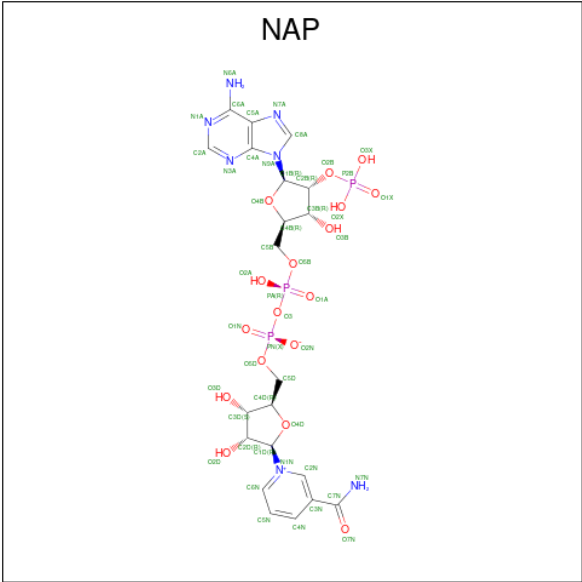
- Molecule 1 is a protein called Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3695	2336	669	685	5			
1	B	473	Total	C	N	O	S	0	0	0
			3333	2118	587	625	3			
1	C	475	Total	C	N	O	S	0	0	0
			3598	2274	655	665	4			
1	D	485	Total	C	N	O	S	0	0	0
			3685	2328	671	681	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	SER	ASN	conflict	UNP A0A069Q1D5
B	277	SER	ASN	conflict	UNP A0A069Q1D5
C	277	SER	ASN	conflict	UNP A0A069Q1D5
D	277	SER	ASN	conflict	UNP A0A069Q1D5

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (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
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

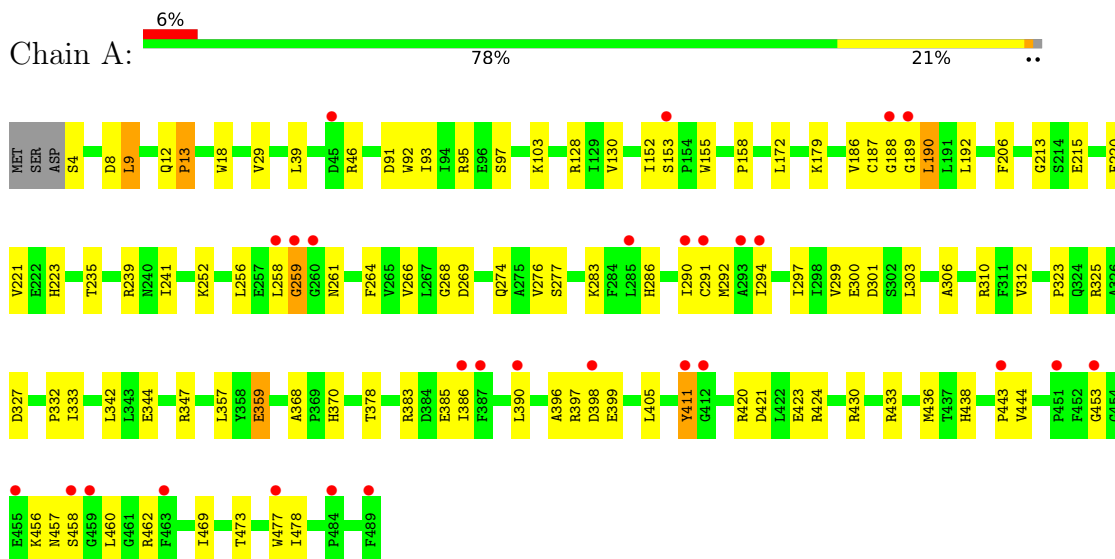
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total	O	0	0
			44	44		
3	B	13	Total	O	0	0
			13	13		
3	C	52	Total	O	0	0
			52	52		
3	D	61	Total	O	0	0
			61	61		

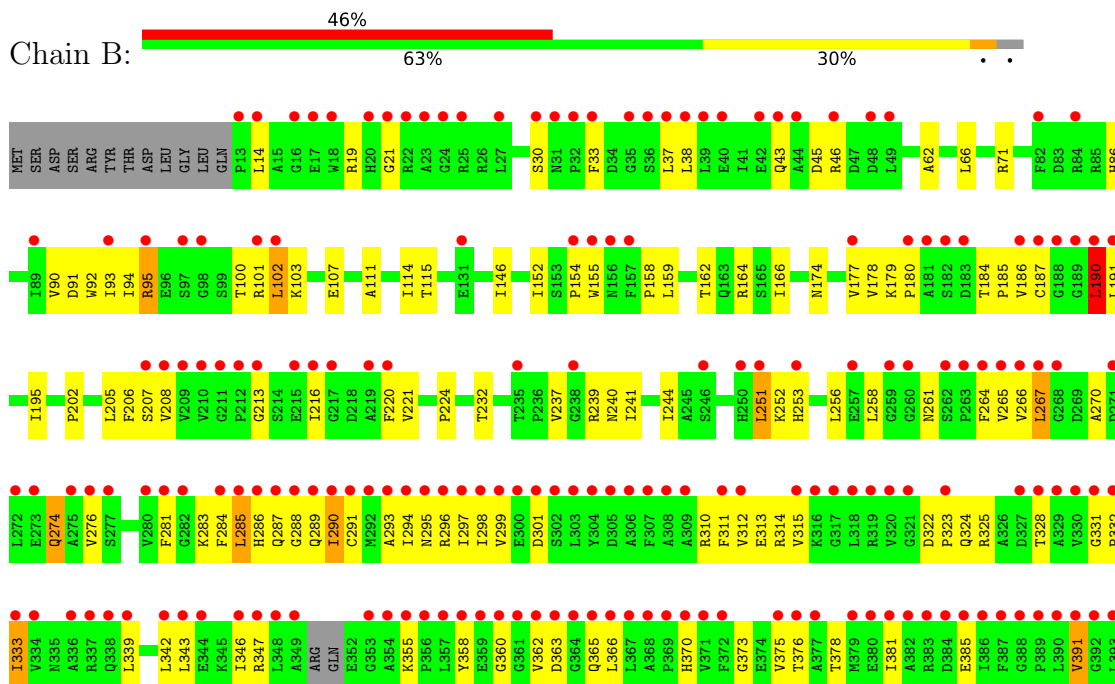
3 Residue-property plots

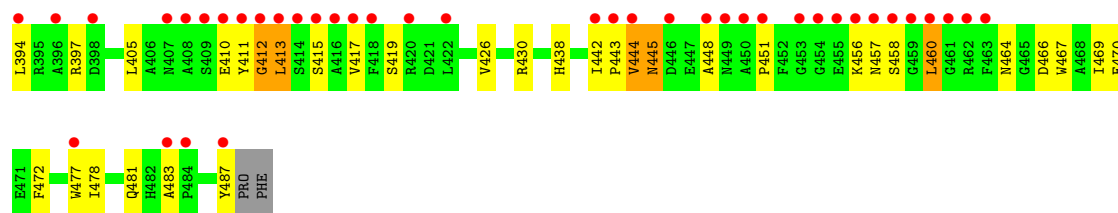
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Aldehyde dehydrogenase

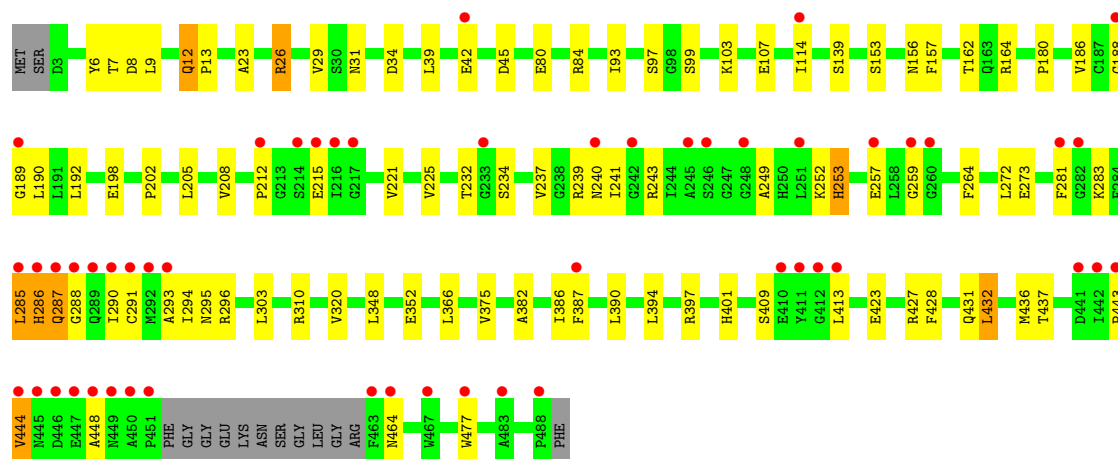
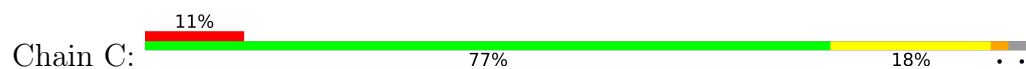


• Molecule 1: Aldehyde dehydrogenase

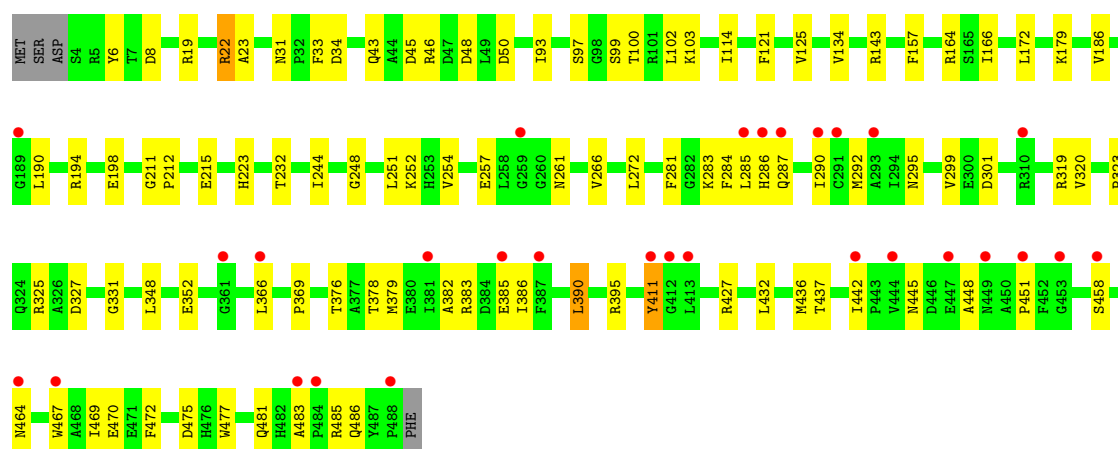
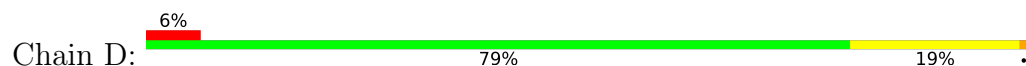




● Molecule 1: Aldehyde dehydrogenase



● Molecule 1: Aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.11Å 144.25Å 150.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.92 – 2.51 47.92 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.92-2.51) 99.8 (47.92-2.51)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, R_{free}	0.224 , 0.265 (Not available) , 0.253	Depositor DCC
R_{free} test set	3780 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14639	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.28	0/3776	0.50	5/5129 (0.1%)
1	B	0.64	0/3407	0.98	15/4664 (0.3%)
1	C	0.36	1/3675 (0.0%)	0.58	2/4997 (0.0%)
1	D	0.26	0/3765	0.47	0/5115
All	All	0.41	1/14623 (0.0%)	0.65	22/19905 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	225	VAL	CA-CB	6.90	1.63	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	ARG	CB-CA-C	-6.18	101.14	110.90
1	A	259	GLY	N-CA-C	5.86	119.77	112.73
1	B	220	PHE	N-CA-CB	-5.79	101.61	110.12
1	C	190	LEU	N-CA-C	-5.74	105.02	111.28
1	B	347	ARG	N-CA-CB	5.63	118.39	110.12
1	B	190	LEU	N-CA-C	5.61	117.40	111.28
1	B	411	TYR	CA-C-N	5.61	126.17	120.00
1	B	411	TYR	C-N-CA	5.61	126.17	120.00
1	B	284	PHE	CA-CB-CG	-5.52	108.28	113.80
1	B	412	GLY	N-CA-C	5.46	119.75	112.77
1	B	296	ARG	CB-CA-C	5.45	119.07	109.80
1	B	284	PHE	CB-CA-C	5.43	119.17	110.09
1	A	13	PRO	N-CA-C	-5.30	102.87	111.03
1	B	220	PHE	CA-CB-CG	5.23	119.03	113.80
1	B	413	LEU	N-CA-C	5.22	116.97	111.28
1	C	286	HIS	CA-CB-CG	-5.18	108.62	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	410	GLU	CA-C-N	-5.13	115.87	123.05
1	B	410	GLU	C-N-CA	-5.13	115.87	123.05
1	A	399	GLU	N-CA-C	-5.12	105.70	111.28
1	A	190	LEU	N-CA-C	-5.10	105.72	111.28
1	A	187	CYS	N-CA-C	-5.07	107.12	113.15
1	B	224	PRO	N-CA-CB	-5.02	97.81	103.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3695	0	3657	73	0
1	B	3333	0	3118	115	0
1	C	3598	0	3561	66	0
1	D	3685	0	3655	68	0
2	A	48	0	25	7	0
2	B	31	0	11	2	0
2	C	31	0	11	0	0
2	D	48	0	25	3	0
3	A	44	0	0	3	0
3	B	13	0	0	1	0
3	C	52	0	0	0	0
3	D	61	0	0	2	0
All	All	14639	0	14063	314	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 11.

All (314) 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:258:LEU:HB2	1:A:458:SER:HA	1.41	1.02
1:A:283:LYS:HB2	1:A:294:ILE:HD11	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ARG:HH12	1:C:249:ALA:HA	1.36	0.88
1:A:189:GLY:HA2	1:A:192:LEU:HB2	1.57	0.86
1:A:411:TYR:HB2	1:A:458:SER:HB3	1.62	0.79
1:D:261:ASN:HB2	1:D:411:TYR:HE1	1.47	0.79
1:D:386:ILE:HD12	1:D:390:LEU:HB3	1.65	0.79
1:B:94:ILE:HD11	1:B:101:ARG:HG2	1.66	0.77
1:A:386:ILE:HG21	1:A:390:LEU:HB2	1.67	0.77
1:A:436:MET:HG2	1:D:477:TRP:HE3	1.52	0.75
1:A:294:ILE:HG23	1:A:443:PRO:HG3	1.70	0.74
1:B:295:ASN:ND2	1:B:385:GLU:HA	2.03	0.72
1:D:103:LYS:HG3	1:D:286:HIS:HB2	1.70	0.72
1:C:99:SER:OG	1:C:103:LYS:HD2	1.91	0.70
1:B:154:PRO:HD3	1:B:232:THR:HG23	1.74	0.70
1:B:103:LYS:NZ	1:B:107:GLU:OE1	2.25	0.69
1:D:223:HIS:O	1:D:252:LYS:NZ	2.25	0.68
1:A:259:GLY:HA2	2:A:3001:NAP:O7N	1.94	0.68
1:C:232:THR:HG23	1:C:257:GLU:HB3	1.76	0.67
1:D:411:TYR:HB2	1:D:458:SER:HB2	1.76	0.67
1:B:114:ILE:HG21	1:B:164:ARG:HA	1.76	0.67
1:D:295:ASN:ND2	1:D:386:ILE:HG12	2.09	0.67
1:C:294:ILE:HG12	1:C:443:PRO:HG2	1.77	0.67
1:B:186:VAL:HA	1:B:190:LEU:HD12	1.76	0.66
1:B:312:VAL:HG13	1:B:358:TYR:HB2	1.77	0.66
1:C:26:ARG:HG3	1:C:42:GLU:OE1	1.95	0.66
1:B:261:ASN:HD22	1:B:295:ASN:HD22	1.41	0.66
1:A:46:ARG:NH2	1:A:215:GLU:O	2.29	0.65
1:B:261:ASN:HD22	1:B:295:ASN:ND2	1.93	0.65
1:C:164:ARG:NH1	1:C:257:GLU:OE1	2.28	0.65
1:B:239:ARG:NH1	1:C:249:ALA:HA	2.10	0.65
1:A:477:TRP:HE3	1:D:436:MET:HG2	1.62	0.64
1:A:290:ILE:HG22	1:A:292:MET:H	1.62	0.64
1:B:155:TRP:NE1	2:B:3001:NAP:O1A	2.28	0.64
1:A:306:ALA:O	1:A:310:ARG:HG2	1.98	0.64
1:C:295:ASN:HD22	1:C:386:ILE:H	1.44	0.63
1:B:294:ILE:HG21	1:B:297:ILE:HG13	1.81	0.63
1:D:186:VAL:HA	1:D:190:LEU:HB2	1.81	0.63
1:A:438:HIS:HD2	1:A:443:PRO:HA	1.64	0.63
1:C:273:GLU:HG2	1:C:310:ARG:HH12	1.63	0.63
1:B:438:HIS:CE1	1:B:445:ASN:HB2	2.34	0.63
1:B:283:LYS:O	1:B:288:GLY:HA2	1.99	0.62
1:B:264:PHE:CD2	1:B:294:ILE:HG12	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:VAL:HB	1:C:39:LEU:HD23	1.82	0.62
1:D:261:ASN:ND2	1:D:295:ASN:OD1	2.33	0.62
1:B:30:SER:HB3	1:B:37:LEU:HA	1.81	0.61
1:B:237:VAL:HG21	2:B:3001:NAP:H51A	1.81	0.61
1:B:94:ILE:HG23	1:B:323:PRO:HB2	1.83	0.61
1:B:91:ASP:OD2	1:B:324:GLN:NE2	2.32	0.61
1:A:344:GLU:OE2	1:A:347:ARG:NH2	2.33	0.61
1:A:186:VAL:HA	1:A:190:LEU:HB2	1.82	0.60
1:B:100:THR:OG1	1:B:102:LEU:HD23	2.02	0.60
1:B:14:LEU:HD23	1:B:19:ARG:HG3	1.82	0.60
1:A:378:THR:O	1:A:383:ARG:NH1	2.35	0.60
1:C:264:PHE:HB2	1:C:294:ILE:HG23	1.84	0.59
1:C:286:HIS:HB3	1:C:290:ILE:HD13	1.85	0.59
1:C:286:HIS:HB3	1:C:290:ILE:CD1	2.33	0.59
1:C:103:LYS:HE2	1:C:157:PHE:CZ	2.37	0.59
1:C:189:GLY:HA2	1:C:192:LEU:HB2	1.84	0.59
1:A:269:ASP:O	1:A:420:ARG:HG3	2.03	0.58
1:B:94:ILE:CD1	1:B:101:ARG:HG2	2.32	0.58
1:B:322:ASP:HB3	1:B:325:ARG:HD3	1.85	0.58
1:C:237:VAL:O	1:C:241:ILE:HG13	2.03	0.58
1:B:481:GLN:NE2	1:B:483:ALA:O	2.36	0.58
1:C:103:LYS:NZ	1:C:107:GLU:OE1	2.34	0.58
1:C:281:PHE:HA	1:C:285:LEU:HD23	1.86	0.58
1:A:261:ASN:HB2	1:A:411:TYR:CE1	2.39	0.58
1:B:30:SER:HB3	1:B:37:LEU:HD12	1.84	0.58
1:A:291:CYS:SG	3:A:3125:HOH:O	2.57	0.58
1:C:272:LEU:HD13	1:C:303:LEU:HD22	1.85	0.58
1:D:19:ARG:NH2	1:D:22:ARG:HD3	2.19	0.58
1:A:91:ASP:OD1	1:A:95:ARG:NH1	2.38	0.57
1:A:235:THR:HG23	1:A:258:LEU:HD13	1.86	0.56
1:B:33:PHE:HB2	1:B:332:PRO:HG3	1.87	0.56
1:D:43:GLN:HG2	1:D:211:GLY:HA2	1.87	0.56
1:B:152:ILE:HD13	1:B:179:LYS:HB3	1.86	0.56
1:B:343:LEU:HA	1:B:346:ILE:HD12	1.87	0.56
1:C:6:TYR:HB3	1:C:9:LEU:HD21	1.88	0.56
1:D:481:GLN:NE2	1:D:483:ALA:O	2.34	0.56
1:C:293:ALA:HA	1:C:444:VAL:HG22	1.88	0.56
2:A:3001:NAP:H52N	2:A:3001:NAP:H6N	1.87	0.56
1:B:442:ILE:HD12	1:B:444:VAL:HG23	1.88	0.55
1:B:264:PHE:HD2	1:B:294:ILE:HG12	1.70	0.55
1:A:430:ARG:NH1	3:A:3103:HOH:O	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:LEU:O	1:B:71:ARG:NH1	2.38	0.55
1:D:448:ALA:O	1:D:464:ASN:HB3	2.06	0.55
1:C:240:ASN:HA	1:C:243:ARG:HG2	1.88	0.55
1:A:436:MET:HG2	1:D:477:TRP:CE3	2.38	0.55
1:B:90:VAL:O	1:B:94:ILE:HG13	2.07	0.55
1:A:438:HIS:CD2	1:A:443:PRO:HA	2.42	0.55
1:A:93:ILE:O	1:A:97:SER:OG	2.25	0.55
1:A:179:LYS:NZ	2:A:3001:NAP:O2B	2.39	0.55
1:D:212:PRO:HB2	1:D:215:GLU:HB2	1.88	0.55
1:B:38:LEU:HD21	1:B:95:ARG:CB	2.38	0.54
1:B:251:LEU:HD11	1:C:239:ARG:HG2	1.90	0.53
1:A:268:GLY:N	1:A:300:GLU:OE1	2.37	0.53
1:B:294:ILE:HD12	1:B:294:ILE:H	1.73	0.53
1:C:237:VAL:HG22	1:C:241:ILE:HD11	1.90	0.53
1:D:100:THR:HG22	1:D:102:LEU:H	1.74	0.53
1:D:134:VAL:HG11	1:D:485:ARG:HD2	1.90	0.53
1:A:261:ASN:HB2	1:A:411:TYR:HE1	1.74	0.53
1:D:103:LYS:HE2	1:D:157:PHE:CE2	2.44	0.52
1:D:46:ARG:NH1	1:D:50:ASP:OD1	2.42	0.52
1:B:477:TRP:HE3	1:C:436:MET:HG2	1.73	0.52
1:B:451:PRO:HB3	1:B:467:TRP:CE2	2.45	0.52
1:B:466:ASP:HA	1:B:469:ILE:HD12	1.92	0.52
1:B:266:VAL:HB	1:B:299:VAL:HG13	1.92	0.52
1:D:325:ARG:NH2	1:D:327:ASP:OD2	2.32	0.52
1:A:478:ILE:HD13	1:D:437:THR:HB	1.92	0.52
1:A:155:TRP:O	1:A:158:PRO:HD3	2.09	0.52
1:A:323:PRO:HG3	1:A:332:PRO:HD3	1.92	0.52
1:D:99:SER:O	1:D:323:PRO:HB2	2.10	0.52
1:D:266:VAL:HB	1:D:299:VAL:HG13	1.91	0.52
1:A:264:PHE:HB2	1:A:294:ILE:HG21	1.91	0.51
1:B:426:VAL:O	1:B:430:ARG:HG2	2.10	0.51
1:C:114:ILE:HG21	1:C:164:ARG:HA	1.92	0.51
1:C:186:VAL:C	1:C:188:GLY:H	2.18	0.51
1:D:292:MET:HE1	1:D:445:ASN:O	2.10	0.51
1:B:103:LYS:HG3	1:B:286:HIS:HB2	1.91	0.51
1:C:103:LYS:HE2	1:C:157:PHE:CE1	2.46	0.51
1:A:213:GLY:H	2:A:3001:NAP:P2B	2.32	0.51
1:D:295:ASN:HD22	1:D:386:ILE:HG12	1.76	0.51
1:C:295:ASN:ND2	1:C:386:ILE:H	2.09	0.51
1:B:287:GLN:HB3	1:B:331:GLY:H	1.76	0.51
1:B:448:ALA:O	1:B:464:ASN:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ASN:OD1	1:C:157:PHE:N	2.41	0.51
1:C:448:ALA:O	1:C:464:ASN:HB3	2.10	0.51
1:A:4:SER:N	3:A:3104:HOH:O	2.45	0.50
1:C:23:ALA:HA	1:C:45:ASP:HB3	1.94	0.50
1:B:289:GLN:C	1:B:290:ILE:HG12	2.36	0.50
1:D:23:ALA:HA	1:D:45:ASP:HB3	1.94	0.50
1:D:261:ASN:HB2	1:D:411:TYR:CE1	2.37	0.50
1:B:256:LEU:HB2	1:B:460:LEU:HB2	1.94	0.50
1:C:202:PRO:HD2	1:C:205:LEU:HD12	1.93	0.50
1:D:284:PHE:CE1	1:D:369:PRO:HB3	2.46	0.50
1:A:294:ILE:CG2	1:A:443:PRO:HG3	2.41	0.50
1:A:223:HIS:O	1:A:252:LYS:NZ	2.28	0.50
1:B:191:LEU:O	1:B:195:ILE:HG13	2.12	0.50
1:B:333:ILE:CD1	1:B:339:LEU:HB2	2.41	0.50
1:D:261:ASN:ND2	1:D:382:ALA:O	2.45	0.50
1:C:221:VAL:HG21	1:C:241:ILE:HG23	1.94	0.50
1:C:283:LYS:HE3	1:C:390:LEU:O	2.10	0.50
1:C:296:ARG:HD3	1:C:382:ALA:HB1	1.93	0.49
1:D:114:ILE:HG21	1:D:164:ARG:HA	1.93	0.49
1:B:346:ILE:HD13	1:B:370:HIS:CE1	2.47	0.49
1:C:12:GLN:NE2	1:C:42:GLU:O	2.45	0.49
1:A:421:ASP:OD2	1:A:424:ARG:HB2	2.12	0.49
1:B:267:LEU:HB2	1:B:419:SER:HB2	1.94	0.49
1:D:19:ARG:HH22	1:D:48:ASP:CG	2.20	0.49
1:C:80:GLU:OE1	1:C:84:ARG:NH2	2.46	0.49
1:A:213:GLY:N	2:A:3001:NAP:O3X	2.35	0.49
1:C:93:ILE:O	1:C:97:SER:OG	2.29	0.49
1:A:276:VAL:HG21	1:A:310:ARG:HB2	1.93	0.48
1:D:320:VAL:HG12	1:D:366:LEU:HD22	1.95	0.48
1:A:13:PRO:HD3	1:A:18:TRP:CZ3	2.48	0.48
1:A:294:ILE:HD12	1:A:294:ILE:O	2.13	0.48
1:B:276:VAL:HG21	1:B:310:ARG:HB2	1.95	0.48
1:B:258:LEU:HB2	1:B:458:SER:HA	1.95	0.48
1:D:292:MET:HE3	1:D:445:ASN:H	1.78	0.48
1:B:111:ALA:O	1:B:115:THR:OG1	2.28	0.48
1:B:333:ILE:HG13	1:B:365:GLN:O	2.14	0.47
1:D:99:SER:HB3	1:D:103:LYS:HD2	1.96	0.47
1:D:100:THR:HG22	1:D:102:LEU:N	2.29	0.47
1:C:286:HIS:O	1:C:287:GLN:HB2	2.13	0.47
1:D:172:LEU:HD12	1:D:472:PHE:HB2	1.96	0.47
1:C:320:VAL:HG12	1:C:366:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:THR:O	1:D:383:ARG:NH1	2.43	0.47
1:D:385:GLU:N	1:D:411:TYR:OH	2.46	0.47
1:D:486:GLN:HE21	1:D:486:GLN:HA	1.80	0.47
1:B:412:GLY:HA3	1:B:456:LYS:H	1.80	0.47
1:B:62:ALA:O	1:B:66:LEU:HD23	2.14	0.47
1:C:375:VAL:HB	1:C:394:LEU:HG	1.97	0.47
1:A:453:GLY:HA3	1:A:462:ARG:HD3	1.97	0.47
1:B:240:ASN:O	1:B:244:ILE:HG13	2.15	0.47
1:A:128:ARG:HG2	1:A:130:VAL:HG23	1.97	0.46
1:D:283:LYS:NZ	3:D:3101:HOH:O	2.44	0.46
1:D:386:ILE:O	3:D:3101:HOH:O	2.20	0.46
1:B:477:TRP:CE3	1:C:436:MET:HG2	2.50	0.46
1:A:266:VAL:HB	1:A:299:VAL:HG13	1.97	0.46
1:D:33:PHE:HE1	1:D:366:LEU:HD11	1.81	0.46
1:A:172:LEU:HD13	1:A:473:THR:HG23	1.98	0.46
1:B:206:PHE:CD1	1:B:206:PHE:C	2.93	0.46
1:B:294:ILE:HG13	1:B:443:PRO:HG3	1.96	0.46
1:D:121:PHE:HB3	1:D:172:LEU:HD21	1.98	0.46
1:B:221:VAL:HG21	1:B:241:ILE:HG12	1.96	0.46
1:B:267:LEU:HD13	1:B:267:LEU:HA	1.79	0.46
1:B:33:PHE:CD1	1:B:322:ASP:HA	2.51	0.46
1:B:184:THR:O	1:B:184:THR:OG1	2.26	0.46
1:A:301:ASP:N	1:A:396:ALA:O	2.49	0.45
1:C:139:SER:HB3	1:C:477:TRP:HE1	1.82	0.45
1:D:232:THR:HA	1:D:257:GLU:O	2.17	0.45
1:B:313:GLU:OE2	1:B:314:ARG:NH1	2.49	0.45
1:D:31:ASN:HB3	1:D:34:ASP:OD1	2.16	0.45
1:A:256:LEU:HD12	1:A:460:LEU:HD22	1.98	0.45
1:B:332:PRO:HA	1:B:366:LEU:HA	1.98	0.45
1:C:153:SER:OG	1:C:162:THR:OG1	2.23	0.45
1:A:312:VAL:HG21	1:A:357:LEU:HB3	1.98	0.45
1:B:285:LEU:HB3	1:B:290:ILE:HD11	1.99	0.45
1:B:375:VAL:HB	1:B:394:LEU:HG	1.99	0.45
1:C:348:LEU:O	1:C:352:GLU:HG2	2.17	0.45
1:D:8:ASP:O	1:D:194:ARG:NH2	2.49	0.45
1:A:186:VAL:C	1:A:188:GLY:H	2.24	0.45
1:B:270:ALA:HB2	1:B:419:SER:HA	1.99	0.45
1:B:290:ILE:HB	1:B:293:ALA:HB2	1.99	0.45
1:D:93:ILE:O	1:D:97:SER:OG	2.32	0.45
1:B:478:ILE:HD13	1:C:437:THR:HB	1.98	0.44
1:B:487:TYR:HB3	1:C:281:PHE:CG	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:SER:HB2	1:C:180:PRO:HA	1.98	0.44
1:D:179:LYS:NZ	2:D:3001:NAP:O2X	2.50	0.44
1:A:46:ARG:HE	1:A:46:ARG:HB2	1.59	0.44
1:B:332:PRO:HB3	1:B:366:LEU:HG	1.99	0.44
1:B:360:GLY:O	1:B:370:HIS:NE2	2.50	0.44
1:D:272:LEU:HD23	1:D:272:LEU:HA	1.78	0.44
1:C:427:ARG:O	1:C:431:GLN:HG3	2.17	0.44
1:A:172:LEU:HD11	1:A:469:ILE:HA	2.00	0.44
1:A:325:ARG:HB3	1:A:327:ASP:OD1	2.17	0.44
1:B:179:LYS:HE3	1:B:213:GLY:HA2	1.99	0.44
1:D:6:TYR:OH	1:D:198:GLU:OE1	2.26	0.44
1:B:33:PHE:C	1:B:33:PHE:CD2	2.95	0.44
1:B:155:TRP:O	1:B:158:PRO:HD3	2.17	0.44
1:D:287:GLN:CG	1:D:331:GLY:H	2.30	0.44
1:A:292:MET:HE3	1:A:444:VAL:HG13	2.00	0.44
1:C:428:PHE:CE1	1:C:432:LEU:HD11	2.53	0.44
1:D:319:ARG:HD2	1:D:327:ASP:O	2.17	0.44
1:A:368:ALA:O	1:A:370:HIS:HD2	2.01	0.43
1:C:397:ARG:HG2	1:C:401:HIS:ND1	2.32	0.43
1:A:433:ARG:O	1:A:456:LYS:HD2	2.18	0.43
1:B:274:GLN:H	1:B:274:GLN:HG2	1.53	0.43
1:A:359:GLU:HG3	1:A:370:HIS:ND1	2.33	0.43
1:D:164:ARG:NH2	1:D:232:THR:OG1	2.52	0.43
2:D:3001:NAP:H52N	2:D:3001:NAP:H2N	2.01	0.43
1:B:166:ILE:HD11	1:B:178:VAL:HG22	2.00	0.43
1:B:190:LEU:O	1:B:191:LEU:C	2.62	0.43
1:B:265:VAL:HB	1:B:417:VAL:HG22	2.00	0.43
1:B:445:ASN:HD22	1:B:445:ASN:HA	1.71	0.43
1:B:180:PRO:HB2	1:B:185:PRO:HA	1.99	0.43
1:B:285:LEU:HD12	1:B:285:LEU:HA	1.69	0.43
1:B:287:GLN:CB	1:B:331:GLY:H	2.32	0.43
1:B:206:PHE:HD1	1:B:207:SER:N	2.16	0.43
1:D:432:LEU:HD23	1:D:432:LEU:HA	1.81	0.43
1:B:159:LEU:HD12	1:B:187:CYS:O	2.17	0.43
1:B:190:LEU:HG	1:B:208:VAL:HG11	2.00	0.43
1:B:179:LYS:HD3	1:B:179:LYS:C	2.43	0.43
1:C:7:THR:HG23	1:C:8:ASP:OD2	2.19	0.43
1:C:428:PHE:O	1:C:432:LEU:HD13	2.19	0.43
1:A:405:LEU:HD23	1:A:405:LEU:HA	1.87	0.43
1:C:283:LYS:HE2	1:C:294:ILE:O	2.19	0.43
1:A:221:VAL:HG21	1:A:241:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:TYR:OH	1:C:198:GLU:OE1	2.29	0.43
1:A:291:CYS:HB3	2:A:3001:NAP:O7N	2.19	0.42
1:A:333:ILE:HD12	1:A:342:LEU:CD1	2.49	0.42
1:B:202:PRO:HD2	1:B:205:LEU:HD12	2.01	0.42
1:D:427:ARG:NH1	1:D:427:ARG:HB3	2.34	0.42
1:B:103:LYS:HE2	1:B:286:HIS:CD2	2.54	0.42
1:C:234:SER:OG	1:C:237:VAL:HG12	2.19	0.42
1:C:288:GLY:O	1:C:387:PHE:HA	2.19	0.42
1:A:385:GLU:OE1	2:A:3001:NAP:O2D	2.31	0.42
1:B:270:ALA:HB2	1:B:419:SER:CA	2.50	0.42
1:C:253:HIS:ND1	1:C:253:HIS:N	2.67	0.42
1:B:21:GLY:HA3	1:B:43:GLN:O	2.19	0.42
1:B:311:PHE:CE2	1:B:391:VAL:HG21	2.53	0.42
1:B:274:GLN:HE21	1:B:274:GLN:HB3	1.65	0.42
1:B:397:ARG:NE	3:B:3101:HOH:O	2.44	0.42
1:D:143:ARG:NE	1:D:475:ASP:OD1	2.49	0.42
1:D:442:ILE:HG13	1:D:445:ASN:HD21	1.84	0.42
1:B:86:HIS:C	1:B:86:HIS:CD2	2.98	0.42
1:B:298:ILE:HG12	1:B:405:LEU:HB3	2.01	0.42
1:D:301:ASP:OD1	1:D:395:ARG:HD3	2.19	0.42
1:A:411:TYR:CB	1:A:458:SER:HB3	2.41	0.42
1:B:45:ASP:OD1	1:B:46:ARG:N	2.51	0.42
1:B:146:ILE:HG13	1:B:472:PHE:C	2.45	0.42
1:B:311:PHE:O	1:B:315:VAL:HG23	2.20	0.42
1:D:451:PRO:HB3	1:D:467:TRP:CE2	2.55	0.42
1:A:103:LYS:HD2	1:A:286:HIS:CG	2.54	0.42
1:A:323:PRO:HG3	1:A:332:PRO:CD	2.50	0.42
1:D:348:LEU:O	1:D:352:GLU:HG2	2.20	0.42
1:D:157:PHE:HE1	1:D:290:ILE:HG12	1.85	0.42
1:B:190:LEU:HG	1:B:190:LEU:H	1.43	0.41
1:B:328:THR:O	1:B:328:THR:CG2	2.67	0.41
1:B:342:LEU:O	1:B:346:ILE:HG13	2.20	0.41
1:A:179:LYS:HB2	1:A:220:PHE:CE2	2.54	0.41
1:B:281:PHE:HD2	1:B:442:ILE:HG21	1.85	0.41
1:B:333:ILE:HD12	1:B:333:ILE:O	2.20	0.41
1:C:285:LEU:HD13	1:C:285:LEU:HA	1.67	0.41
1:A:206:PHE:C	1:A:206:PHE:CD1	2.98	0.41
1:A:239:ARG:HH12	1:A:457:ASN:ND2	2.18	0.41
1:B:355:LYS:O	1:B:373:GLY:N	2.38	0.41
1:C:252:LYS:HB3	1:C:252:LYS:HE3	1.69	0.41
1:A:301:ASP:C	1:A:303:LEU:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PHE:HB2	1:A:294:ILE:CG2	2.51	0.41
1:B:93:ILE:HA	1:B:187:CYS:SG	2.61	0.41
1:B:310:ARG:NH1	1:B:314:ARG:HH22	2.18	0.41
1:C:186:VAL:C	1:C:188:GLY:N	2.79	0.41
1:B:322:ASP:O	1:B:325:ARG:HG2	2.20	0.41
1:C:13:PRO:HD2	1:C:208:VAL:HB	2.03	0.41
1:B:177:VAL:HG13	1:B:207:SER:HB2	2.01	0.41
1:A:9:LEU:HD12	1:A:92:TRP:CZ2	2.56	0.41
1:A:29:VAL:HB	1:A:39:LEU:HD23	2.03	0.41
1:B:146:ILE:N	1:B:174:ASN:OD1	2.54	0.41
1:C:31:ASN:HB3	1:C:34:ASP:OD1	2.21	0.41
1:C:259:GLY:HA2	1:C:291:CYS:SG	2.61	0.41
1:D:281:PHE:CE1	1:D:285:LEU:HD13	2.56	0.41
1:D:376:THR:HG23	1:D:379:MET:HE3	2.03	0.41
1:D:166:ILE:HD13	1:D:166:ILE:HA	1.81	0.41
2:D:3001:NAP:H2N	2:D:3001:NAP:C5D	2.51	0.41
1:B:146:ILE:HG13	1:B:472:PHE:O	2.20	0.40
1:A:359:GLU:HG3	1:A:370:HIS:CE1	2.57	0.40
1:B:206:PHE:C	1:B:206:PHE:HD1	2.30	0.40
1:D:125:VAL:HG12	1:D:469:ILE:HG23	2.03	0.40
1:D:287:GLN:HG2	1:D:331:GLY:O	2.20	0.40
1:B:162:THR:HG22	1:B:166:ILE:HG13	2.02	0.40
1:C:212:PRO:HB2	1:C:215:GLU:HB2	2.03	0.40
1:A:264:PHE:HD2	1:A:297:ILE:HG23	1.87	0.40
1:D:244:ILE:O	1:D:248:GLY:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	191/489 (39%)	188 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	232/489 (47%)	224 (97%)	8 (3%)	0	100	100
1	C	193/489 (40%)	190 (98%)	3 (2%)	0	100	100
1	D	438/489 (90%)	431 (98%)	7 (2%)	0	100	100
All	All	1054/1956 (54%)	1033 (98%)	21 (2%)	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	373/377 (99%)	361 (97%)	12 (3%)	34	62
1	B	305/377 (81%)	278 (91%)	27 (9%)	9	20
1	C	362/377 (96%)	352 (97%)	10 (3%)	38	66
1	D	372/377 (99%)	366 (98%)	6 (2%)	55	79
All	All	1412/1508 (94%)	1357 (96%)	55 (4%)	28	55

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	9	LEU
1	A	12	GLN
1	A	152	ILE
1	A	153	SER
1	A	274	GLN
1	A	277	SER
1	A	359	GLU
1	A	397	ARG
1	A	398	ASP
1	A	411	TYR
1	A	423	GLU
1	B	92	TRP

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Mol	Chain	Res	Type
1	B	102	LEU
1	B	190	LEU
1	B	216	ILE
1	B	251	LEU
1	B	252	LYS
1	B	253	HIS
1	B	267	LEU
1	B	274	GLN
1	B	285	LEU
1	B	290	ILE
1	B	291	CYS
1	B	301	ASP
1	B	333	ILE
1	B	362	VAL
1	B	363	ASP
1	B	376	THR
1	B	378	THR
1	B	381	ILE
1	B	391	VAL
1	B	413	LEU
1	B	415	SER
1	B	444	VAL
1	B	445	ASN
1	B	457	ASN
1	B	460	LEU
1	B	470	GLU
1	C	12	GLN
1	C	26	ARG
1	C	253	HIS
1	C	285	LEU
1	C	287	GLN
1	C	409	SER
1	C	413	LEU
1	C	423	GLU
1	C	432	LEU
1	C	444	VAL
1	D	22	ARG
1	D	251	LEU
1	D	254	VAL
1	D	390	LEU
1	D	411	TYR
1	D	470	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	287	GLN
1	B	261	ASN
1	B	274	GLN
1	C	126	HIS
1	C	250	HIS
1	C	274	GLN
1	C	295	ASN
1	C	431	GLN
1	D	250	HIS
1	D	365	GLN
1	D	486	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](#)

4 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	3001	-	50,52,52	1.72	4 (8%)	71,80,80	0.98	5 (7%)
2	NAP	B	3001	-	32,33,52	1.97	3 (9%)	50,52,80	1.23	7 (14%)
2	NAP	C	3001	-	32,33,52	1.94	3 (9%)	50,52,80	1.01	3 (6%)
2	NAP	A	3001	-	50,52,52	1.72	4 (8%)	71,80,80	1.16	9 (12%)

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	D	3001	-	-	12/35/67/67	0/5/5/5
2	NAP	B	3001	-	-	5/21/37/67	0/3/3/5
2	NAP	C	3001	-	-	8/21/37/67	0/3/3/5
2	NAP	A	3001	-	-	8/35/67/67	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3001	NAP	P2B-O2B	8.47	1.74	1.59
2	B	3001	NAP	P2B-O2B	8.44	1.74	1.59
2	D	3001	NAP	P2B-O2B	8.42	1.74	1.59
2	A	3001	NAP	P2B-O2B	8.26	1.74	1.59
2	B	3001	NAP	PA-O3	5.52	1.65	1.59
2	A	3001	NAP	PN-O3	5.08	1.65	1.59
2	A	3001	NAP	PA-O3	5.06	1.65	1.59
2	C	3001	NAP	PA-O3	5.02	1.64	1.59
2	D	3001	NAP	PA-O3	4.93	1.64	1.59
2	D	3001	NAP	PN-O3	4.68	1.64	1.59
2	C	3001	NAP	PN-O5D	2.88	1.65	1.54
2	B	3001	NAP	PN-O5D	2.86	1.65	1.54
2	A	3001	NAP	O4D-C1D	-2.52	1.37	1.40
2	D	3001	NAP	O4D-C1D	-2.39	1.37	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	NAP	C4D-O4D-C1D	3.42	113.06	109.92
2	C	3001	NAP	O2N-PN-O1N	3.07	122.80	110.83
2	B	3001	NAP	O5B-C5B-C4B	-2.72	99.72	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3001	NAP	O2N-PN-O1N	2.68	121.27	110.83
2	B	3001	NAP	C1B-N9A-C8A	2.62	132.90	127.09
2	A	3001	NAP	P2B-O2B-C2B	-2.45	116.89	123.43
2	A	3001	NAP	C1B-N9A-C8A	2.43	132.49	127.09
2	D	3001	NAP	C1B-N9A-C8A	2.38	132.37	127.09
2	B	3001	NAP	C4A-N9A-C1B	-2.37	121.09	126.63
2	D	3001	NAP	P2B-O2B-C2B	-2.34	117.19	123.43
2	A	3001	NAP	C4A-N9A-C1B	-2.31	121.24	126.63
2	D	3001	NAP	C4A-N9A-C1B	-2.27	121.32	126.63
2	C	3001	NAP	P2B-O2B-C2B	-2.25	117.43	123.43
2	B	3001	NAP	P2B-O2B-C2B	-2.24	117.45	123.43
2	A	3001	NAP	O4B-C1B-N9A	2.24	112.39	108.09
2	A	3001	NAP	O2N-PN-O1N	2.17	122.56	112.44
2	A	3001	NAP	C3N-C7N-N7N	-2.17	115.07	117.74
2	B	3001	NAP	O2A-PA-O1A	2.16	122.51	112.44
2	D	3001	NAP	O2N-PN-O1N	2.14	122.39	112.44
2	D	3001	NAP	O3X-P2B-O2X	2.12	115.74	107.80
2	A	3001	NAP	O2A-PA-O1A	2.11	122.27	112.44
2	B	3001	NAP	O3X-P2B-O2X	2.06	115.52	107.80
2	A	3001	NAP	C6N-N1N-C1D	-2.05	115.71	119.73
2	C	3001	NAP	O3X-P2B-O2X	2.04	115.44	107.80

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3001	NAP	C5B-O5B-PA-O1A
2	A	3001	NAP	C5D-O5D-PN-O3
2	A	3001	NAP	C5D-O5D-PN-O1N
2	A	3001	NAP	C5D-O5D-PN-O2N
2	C	3001	NAP	C5B-O5B-PA-O1A
2	C	3001	NAP	C5B-O5B-PA-O3
2	D	3001	NAP	C5B-O5B-PA-O3
2	D	3001	NAP	C5D-O5D-PN-O3
2	D	3001	NAP	C5D-O5D-PN-O1N
2	D	3001	NAP	C5D-O5D-PN-O2N
2	D	3001	NAP	C3B-C4B-C5B-O5B
2	B	3001	NAP	O4B-C4B-C5B-O5B
2	B	3001	NAP	C3B-C4B-C5B-O5B
2	C	3001	NAP	O4B-C4B-C5B-O5B
2	C	3001	NAP	C3B-C4B-C5B-O5B
2	D	3001	NAP	O4B-C4B-C5B-O5B

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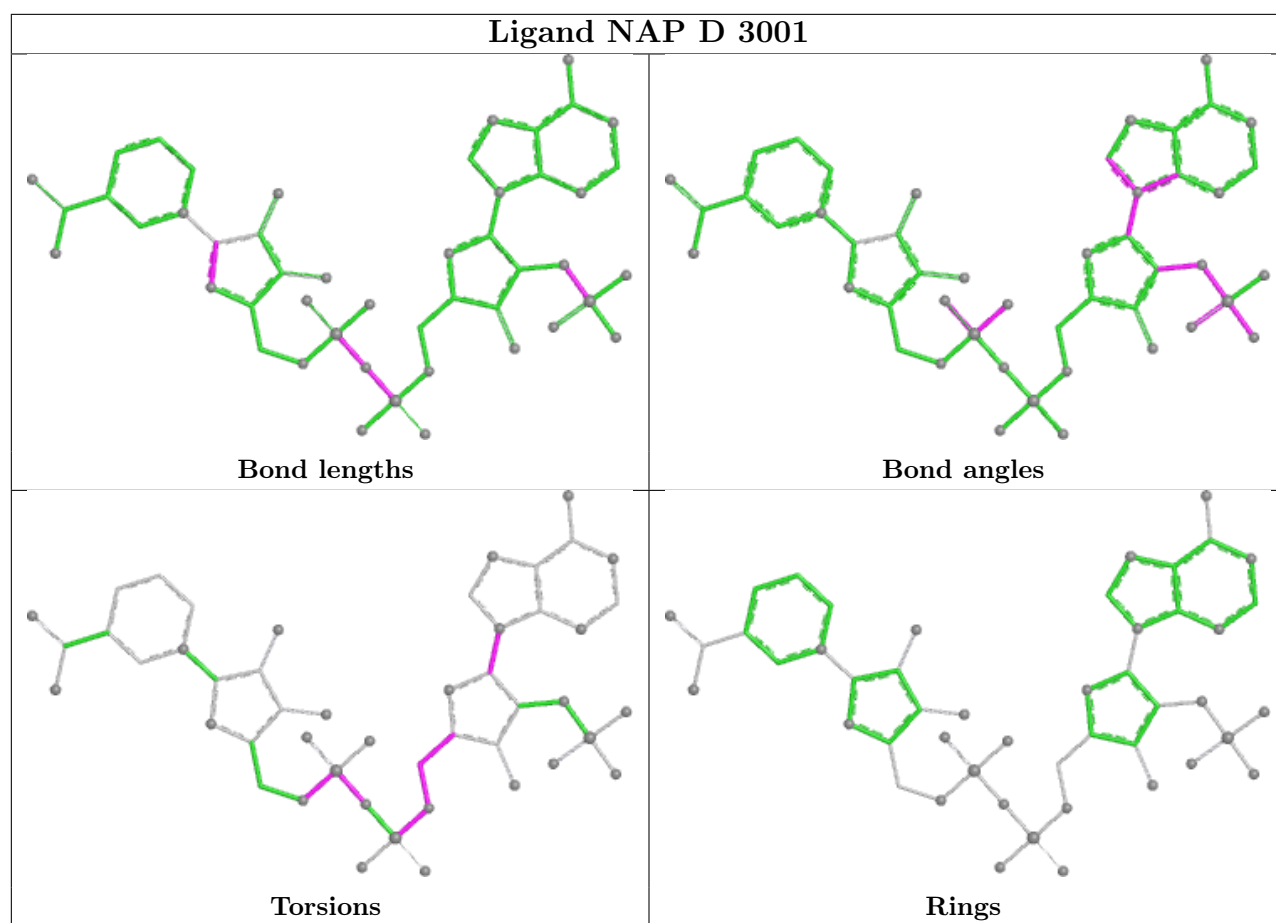
Mol	Chain	Res	Type	Atoms
2	A	3001	NAP	C2B-C1B-N9A-C8A
2	B	3001	NAP	C2B-C1B-N9A-C8A
2	C	3001	NAP	C2B-C1B-N9A-C8A
2	D	3001	NAP	C2B-C1B-N9A-C8A
2	B	3001	NAP	C5B-O5B-PA-O3
2	C	3001	NAP	C5B-O5B-PA-O2A
2	D	3001	NAP	C5B-O5B-PA-O1A
2	A	3001	NAP	O4B-C1B-N9A-C8A
2	C	3001	NAP	O4B-C1B-N9A-C8A
2	D	3001	NAP	C4B-C5B-O5B-PA
2	B	3001	NAP	O4B-C1B-N9A-C8A
2	D	3001	NAP	O4B-C1B-N9A-C8A
2	A	3001	NAP	C3D-C4D-C5D-O5D
2	A	3001	NAP	PN-O3-PA-O2A
2	D	3001	NAP	PA-O3-PN-O1N
2	C	3001	NAP	C2B-C1B-N9A-C4A
2	D	3001	NAP	C2B-C1B-N9A-C4A

There are no ring outliers.

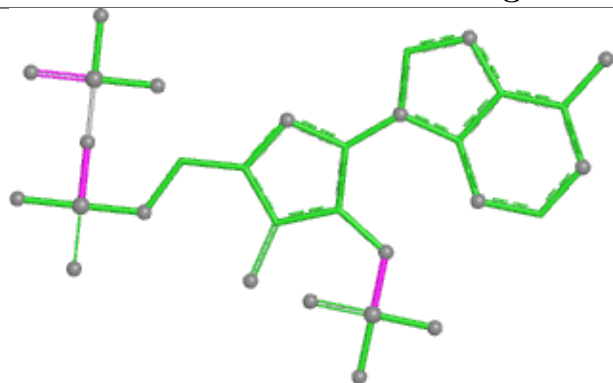
3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3001	NAP	3	0
2	B	3001	NAP	2	0
2	A	3001	NAP	7	0

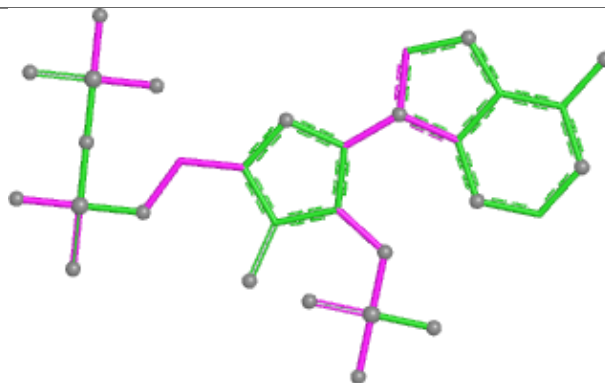
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



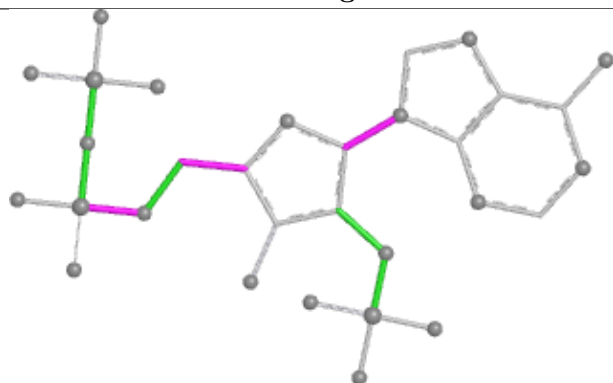
Ligand NAP B 3001



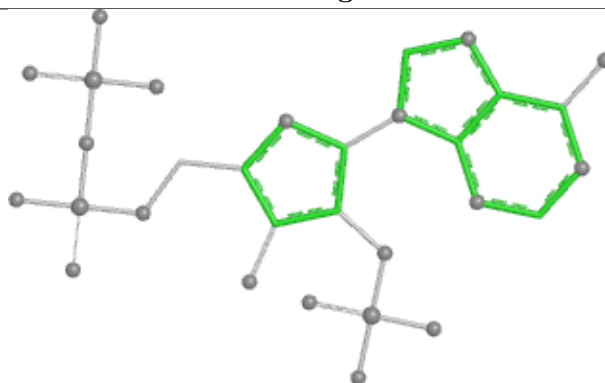
Bond lengths



Bond angles

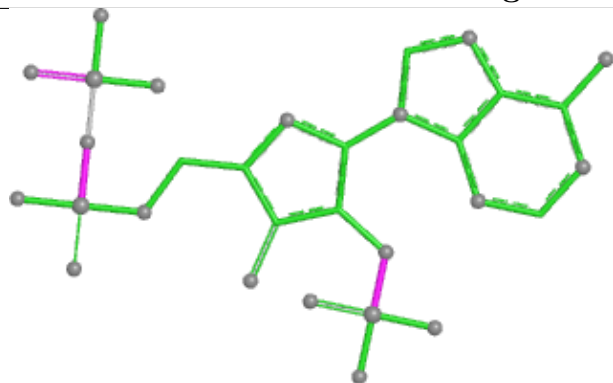


Torsions

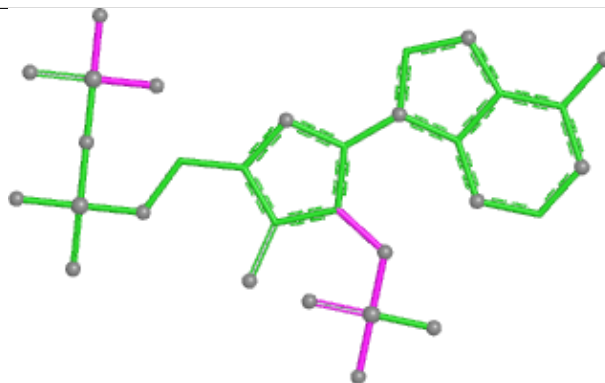


Rings

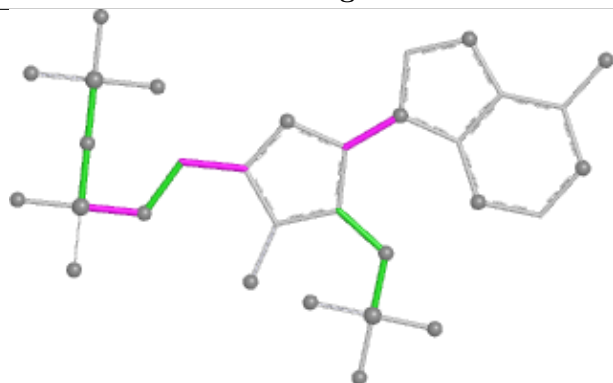
Ligand NAP C 3001



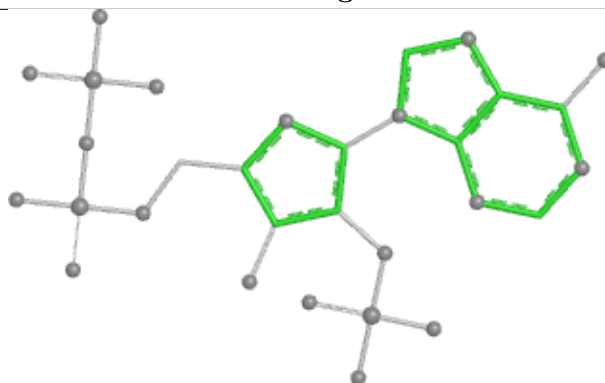
Bond lengths



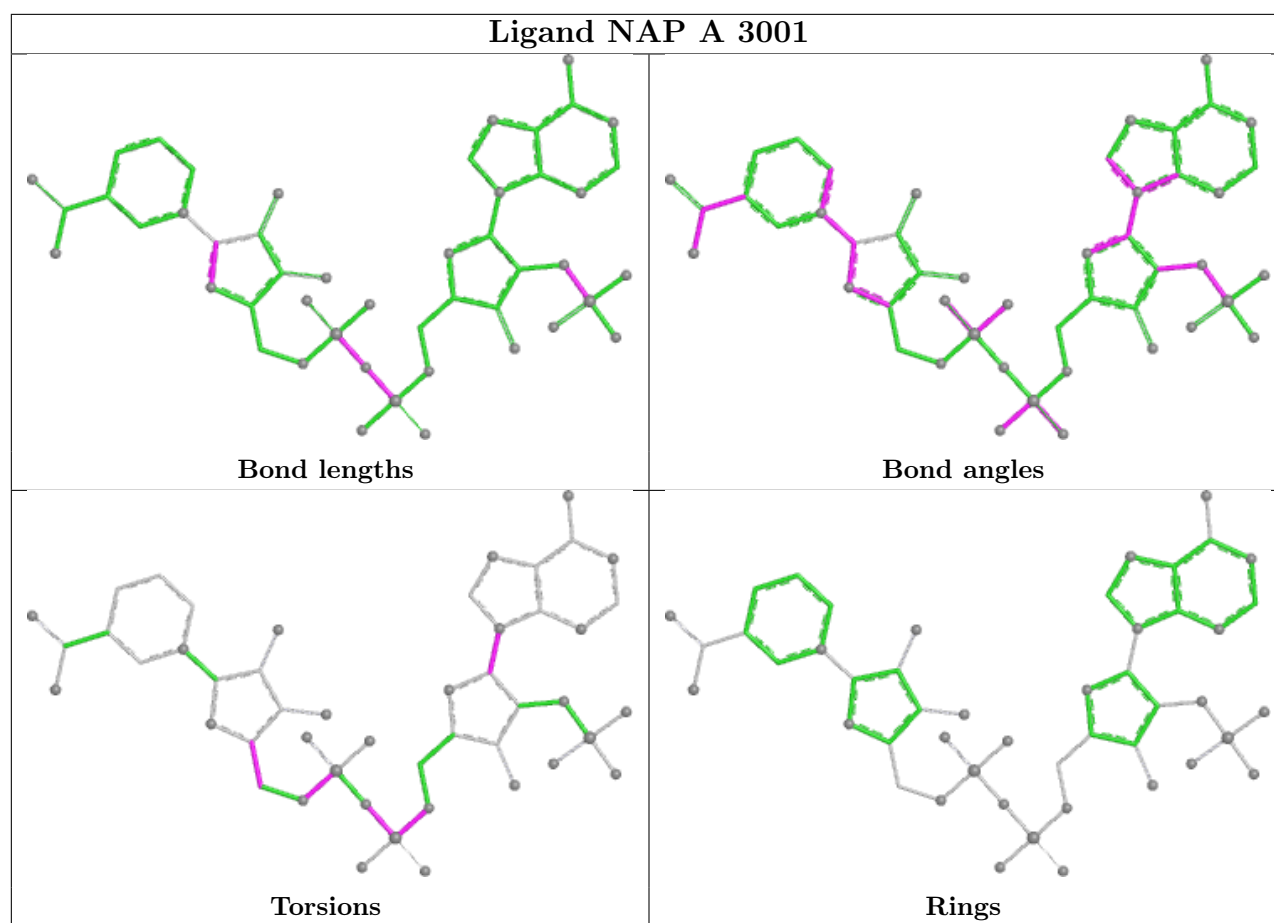
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	486/489 (99%)	0.42	28 (5%) 29 25	34, 54, 75, 91	0
1	B	473/489 (96%)	2.04	223 (47%) 0 0	48, 89, 112, 120	0
1	C	475/489 (97%)	0.61	52 (10%) 10 9	34, 51, 92, 108	0
1	D	485/489 (99%)	0.40	29 (5%) 27 24	36, 52, 77, 101	0
All	All	1919/1956 (98%)	0.86	332 (17%) 4 3	34, 58, 105, 120	0

All (332) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	286	HIS	8.4
1	B	189	GLY	6.9
1	B	334	VAL	6.8
1	C	291	CYS	6.0
1	C	290	ILE	5.7
1	B	457	ASN	5.5
1	B	413	LEU	5.4
1	D	291	CYS	5.3
1	C	189	GLY	5.3
1	B	450	ALA	5.3
1	B	332	PRO	5.2
1	C	443	PRO	5.2
1	C	292	MET	5.1
1	B	190	LEU	5.1
1	B	210	VAL	5.1
1	B	362	VAL	5.1
1	C	463	PHE	5.0
1	B	483	ALA	4.9
1	B	349	ALA	4.9
1	B	371	VAL	4.9
1	B	331	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	307	PHE	4.8
1	B	183	ASP	4.6
1	B	272	LEU	4.6
1	B	289	GLN	4.6
1	B	459	GLY	4.5
1	B	387	PHE	4.5
1	B	381	ILE	4.5
1	C	448	ALA	4.5
1	B	367	LEU	4.5
1	B	43	GLN	4.5
1	B	253	HIS	4.4
1	B	386	ILE	4.4
1	B	366	LEU	4.4
1	B	329	ALA	4.3
1	C	288	GLY	4.3
1	B	484	PRO	4.3
1	B	455	GLU	4.3
1	B	389	PRO	4.2
1	C	451	PRO	4.2
1	B	330	VAL	4.2
1	B	275	ALA	4.2
1	C	445	ASN	4.1
1	B	98	GLY	4.1
1	B	365	GLN	4.1
1	B	357	LEU	4.0
1	B	453	GLY	4.0
1	C	444	VAL	4.0
1	D	451	PRO	4.0
1	D	189	GLY	4.0
1	B	410	GLU	3.9
1	B	265	VAL	3.9
1	B	449	ASN	3.9
1	B	328	THR	3.9
1	A	386	ILE	3.9
1	B	101	ARG	3.9
1	B	32	PRO	3.9
1	B	318	LEU	3.9
1	B	315	VAL	3.9
1	B	301	ASP	3.8
1	B	285	LEU	3.8
1	B	458	SER	3.8
1	B	375	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	287	GLN	3.8
1	B	333	ILE	3.8
1	B	338	GLN	3.8
1	B	372	PHE	3.8
1	B	382	ALA	3.8
1	C	412	GLY	3.8
1	C	285	LEU	3.8
1	B	364	GLY	3.7
1	D	290	ILE	3.7
1	B	323	PRO	3.7
1	C	450	ALA	3.7
1	B	311	PHE	3.7
1	B	216	ILE	3.7
1	B	384	ASP	3.7
1	B	293	ALA	3.6
1	B	456	LYS	3.6
1	A	459	GLY	3.6
1	B	296	ARG	3.6
1	B	390	LEU	3.6
1	B	418	PHE	3.6
1	B	462	ARG	3.6
1	D	361	GLY	3.6
1	A	259	GLY	3.6
1	B	188	GLY	3.6
1	B	339	LEU	3.6
1	C	260	GLY	3.5
1	B	263	PRO	3.5
1	B	219	ALA	3.5
1	B	37	LEU	3.5
1	B	308	ALA	3.5
1	B	25	ARG	3.4
1	D	411	TYR	3.4
1	B	284	PHE	3.4
1	B	380	GLU	3.4
1	B	356	PRO	3.4
1	C	488	PRO	3.4
1	A	260	GLY	3.4
1	D	453	GLY	3.4
1	B	302	SER	3.4
1	B	358	TYR	3.4
1	A	489	PHE	3.4
1	C	387	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	312	VAL	3.4
1	B	213	GLY	3.4
1	C	293	ALA	3.4
1	B	411	TYR	3.4
1	B	303	LEU	3.4
1	B	260	GLY	3.4
1	B	414	SER	3.3
1	B	97	SER	3.3
1	B	271	ASP	3.3
1	B	320	VAL	3.3
1	B	42	GLU	3.3
1	B	377	ALA	3.3
1	B	347	ARG	3.3
1	B	186	VAL	3.3
1	B	211	GLY	3.3
1	B	317	GLY	3.2
1	C	467	TRP	3.2
1	C	477	TRP	3.2
1	B	359	GLU	3.2
1	B	299	VAL	3.2
1	B	268	GLY	3.2
1	B	360	GLY	3.2
1	D	467	TRP	3.2
1	C	289	GLN	3.2
1	B	443	PRO	3.2
1	B	460	LEU	3.2
1	B	346	ILE	3.2
1	B	379	MET	3.2
1	B	181	ALA	3.1
1	B	131	GLU	3.1
1	B	417	VAL	3.1
1	B	44	ALA	3.1
1	D	285	LEU	3.1
1	B	391	VAL	3.1
1	A	294	ILE	3.1
1	B	408	ALA	3.1
1	B	336	ALA	3.0
1	B	155	TRP	3.0
1	B	292	MET	3.0
1	B	217	GLY	3.0
1	B	259	GLY	3.0
1	B	392	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	451	PRO	3.0
1	B	444	VAL	3.0
1	B	267	LEU	3.0
1	A	293	ALA	2.9
1	A	477	TRP	2.9
1	B	383	ARG	2.9
1	B	420	ARG	2.9
1	B	276	VAL	2.9
1	B	154	PRO	2.9
1	B	212	PRO	2.9
1	B	48	ASP	2.9
1	C	441	ASP	2.9
1	B	287	GLN	2.9
1	B	298	ILE	2.9
1	B	46	ARG	2.9
1	B	376	THR	2.9
1	B	13	PRO	2.9
1	B	394	LEU	2.9
1	B	93	ILE	2.9
1	B	487	TYR	2.9
1	C	447	GLU	2.9
1	A	458	SER	2.8
1	A	411	TYR	2.8
1	B	294	ILE	2.8
1	C	216	ILE	2.8
1	B	177	VAL	2.8
1	B	182	SER	2.8
1	B	209	VAL	2.8
1	B	354	ALA	2.8
1	A	387	PHE	2.8
1	A	463	PHE	2.8
1	B	20	HIS	2.8
1	B	282	GLY	2.8
1	B	266	VAL	2.7
1	B	370	HIS	2.7
1	C	442	ILE	2.7
1	B	246	SER	2.7
1	C	411	TYR	2.7
1	B	49	LEU	2.7
1	B	342	LEU	2.7
1	B	448	ALA	2.7
1	B	273	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	369	PRO	2.7
1	D	413	LEU	2.7
1	B	291	CYS	2.7
1	B	348	LEU	2.7
1	A	291	CYS	2.6
1	B	281	PHE	2.6
1	B	297	ILE	2.6
1	B	156	ASN	2.6
1	B	102	LEU	2.6
1	B	262	SER	2.6
1	B	385	GLU	2.6
1	B	409	SER	2.6
1	B	304	TYR	2.6
1	D	287	GLN	2.6
1	B	286	HIS	2.6
1	B	288	GLY	2.6
1	B	407	ASN	2.6
1	C	413	LEU	2.6
1	D	366	LEU	2.6
1	B	257	GLU	2.6
1	C	281	PHE	2.6
1	B	14	LEU	2.6
1	B	27	LEU	2.6
1	B	368	ALA	2.6
1	B	180	PRO	2.6
1	B	319	ARG	2.6
1	A	258	LEU	2.6
1	A	153	SER	2.6
1	B	31	ASN	2.5
1	B	235	THR	2.5
1	A	443	PRO	2.5
1	B	363	ASP	2.5
1	D	412	GLY	2.5
1	B	95	ARG	2.5
1	B	24	GLY	2.5
1	C	217	GLY	2.5
1	C	42	GLU	2.5
1	B	316	LYS	2.5
1	B	295	ASN	2.5
1	D	488	PRO	2.5
1	B	40	GLU	2.5
1	A	285	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	390	LEU	2.5
1	C	245	ALA	2.5
1	D	458	SER	2.5
1	A	188	GLY	2.4
1	D	259	GLY	2.4
1	B	463	PHE	2.4
1	B	84	ARG	2.4
1	B	306	ALA	2.4
1	A	455	GLU	2.4
1	B	17	GLU	2.4
1	C	233	GLY	2.4
1	B	305	ASP	2.4
1	B	220	PHE	2.4
1	C	215	GLU	2.4
1	D	484	PRO	2.4
1	B	238	GLY	2.4
1	B	446	ASP	2.4
1	C	240	ASN	2.4
1	B	416	ALA	2.4
1	C	410	GLU	2.4
1	C	212	PRO	2.3
1	B	337	ARG	2.3
1	C	483	ALA	2.3
1	B	89	ILE	2.3
1	B	250	HIS	2.3
1	B	442	ILE	2.3
1	A	398	ASP	2.3
1	B	187	CYS	2.3
1	B	344	GLU	2.3
1	B	396	ALA	2.3
1	A	453	GLY	2.3
1	B	361	GLY	2.3
1	B	454	GLY	2.3
1	B	290	ILE	2.3
1	B	33	PHE	2.3
1	B	353	GLY	2.3
1	C	248	GLY	2.3
1	C	282	GLY	2.3
1	B	36	SER	2.3
1	B	38	LEU	2.3
1	B	300	GLU	2.3
1	C	257	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	447	GLU	2.3
1	A	189	GLY	2.2
1	C	246	SER	2.2
1	D	442	ILE	2.2
1	D	449	ASN	2.2
1	B	412	GLY	2.2
1	B	39	LEU	2.2
1	A	290	ILE	2.2
1	C	446	ASP	2.2
1	B	18	TRP	2.2
1	C	449	ASN	2.2
1	D	293	ALA	2.2
1	B	21	GLY	2.2
1	B	251	LEU	2.2
1	B	22	ARG	2.2
1	B	264	PHE	2.2
1	B	208	VAL	2.2
1	B	309	ALA	2.2
1	B	191	LEU	2.2
1	B	393	LEU	2.2
1	C	251	LEU	2.2
1	B	157	PHE	2.2
1	B	23	ALA	2.1
1	C	464	ASN	2.1
1	A	412	GLY	2.1
1	C	242	GLY	2.1
1	B	355	LYS	2.1
1	B	280	VAL	2.1
1	D	286	HIS	2.1
1	D	444	VAL	2.1
1	B	35	GLY	2.1
1	B	343	LEU	2.1
1	C	114	ILE	2.1
1	C	259	GLY	2.1
1	D	387	PHE	2.1
1	D	483	ALA	2.1
1	B	477	TRP	2.1
1	D	464	ASN	2.1
1	B	16	GLY	2.1
1	B	321	GLY	2.1
1	A	45	ASP	2.1
1	B	207	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	310	ARG	2.0
1	B	422	LEU	2.0
1	B	215	GLU	2.0
1	B	388	GLY	2.0
1	B	461	GLY	2.0
1	C	188	GLY	2.0
1	D	385	GLU	2.0
1	B	327	ASP	2.0
1	B	398	ASP	2.0
1	A	451	PRO	2.0
1	B	30	SER	2.0
1	C	214	SER	2.0
1	B	82	PHE	2.0
1	D	381	ILE	2.0
1	A	484	PRO	2.0
1	B	277	SER	2.0
1	B	415	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 [i](#)

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

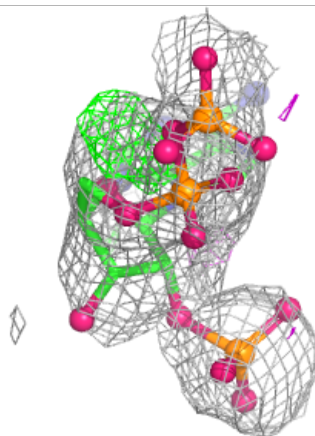
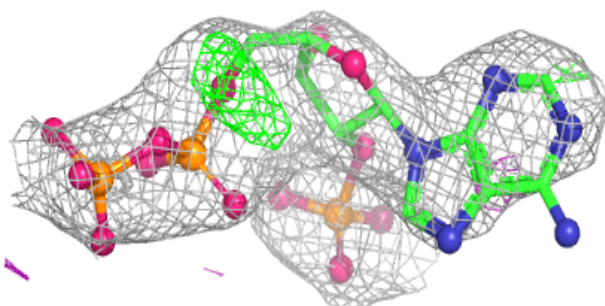
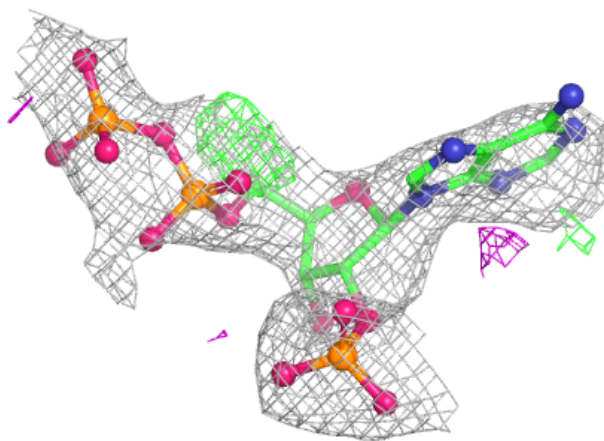
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	B	3001	31/48	0.70	0.16	93,112,122,258	0
2	NAP	C	3001	31/48	0.80	0.16	79,104,206,281	0
2	NAP	A	3001	48/48	0.81	0.18	38,77,130,343	0
2	NAP	D	3001	48/48	0.84	0.14	54,84,110,172	0

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.

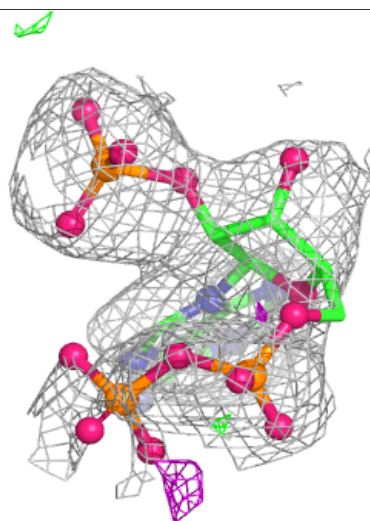
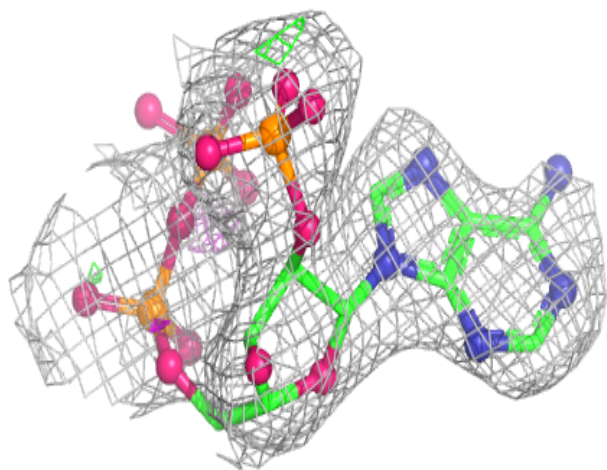
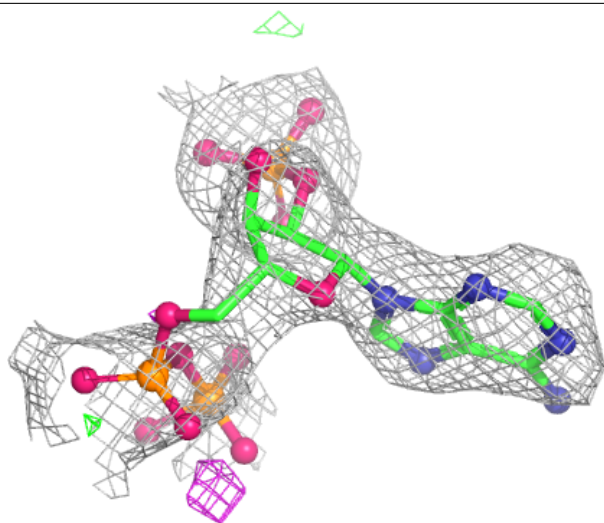
Electron density around NAP B 3001:

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



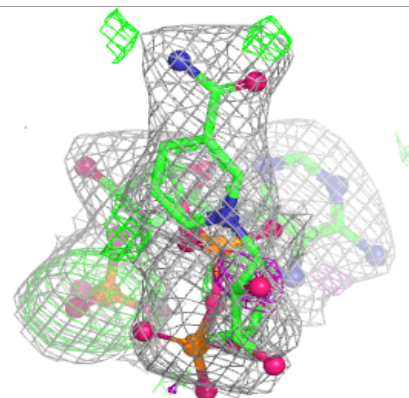
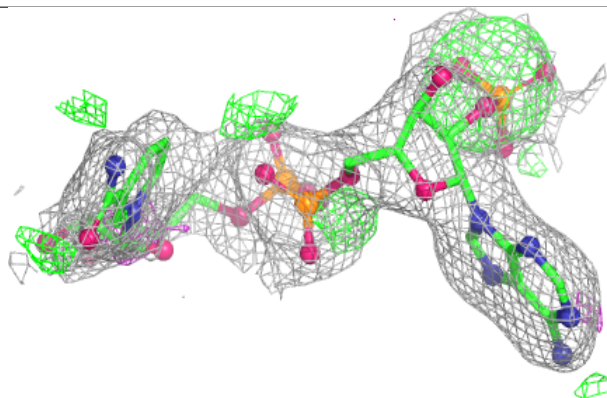
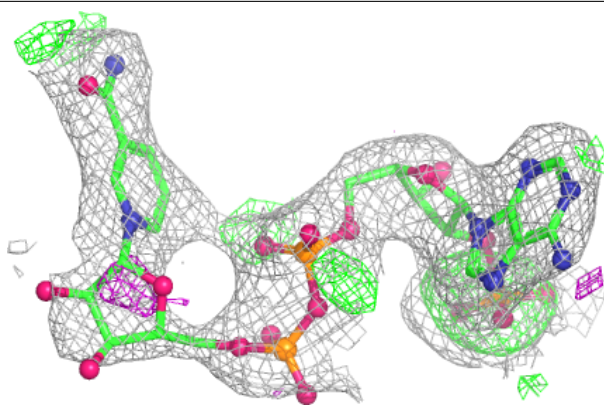
Electron density around NAP C 3001:

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

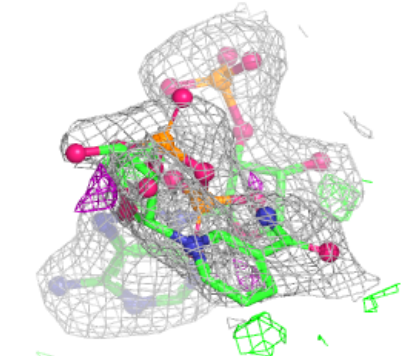
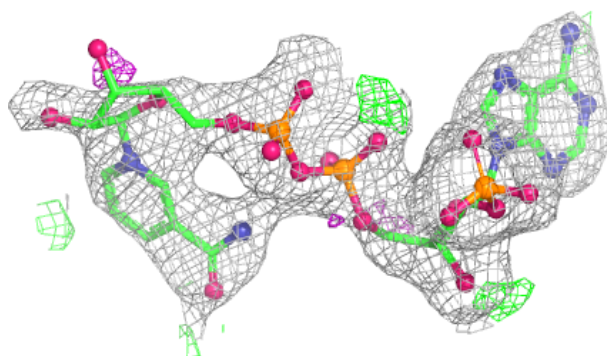
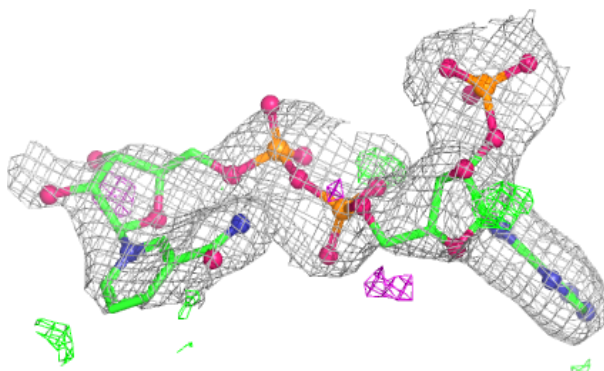


Electron density around NAP A 3001:

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

**Electron density around NAP D 3001:**

$2mF_o-DF_c$ (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.