



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 24, 2025 – 09:10 PM JST

PDB ID : 9J0W / pdb_00009j0w
Title : CRYSTAL STRUCTURE OF A NOVEL ALDEHYDE DEHYDROGENASE
FROM KLEBSIELLA PNEUMONIAE IN COMPLEX WITH COENZYME
Authors : Zhang, J.; Han, Y.; Liu, W.D.; Zhang, W.Y.
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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

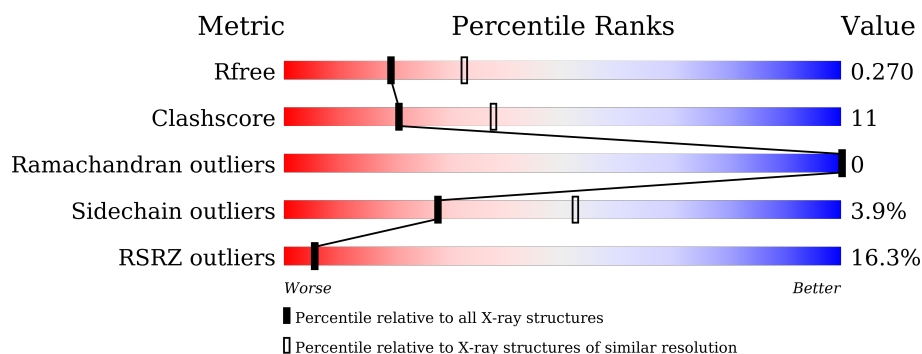
1 Overall quality at a glance

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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (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	<div> <div>5%</div> <div>78%</div> <div>21%</div> <div>..</div> </div>
1	B	489	<div> <div>43%</div> <div>63%</div> <div>30%</div> <div>..</div> </div>
1	C	489	<div> <div>10%</div> <div>77%</div> <div>18%</div> <div>..</div> </div>
1	D	489	<div> <div>5%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>

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.

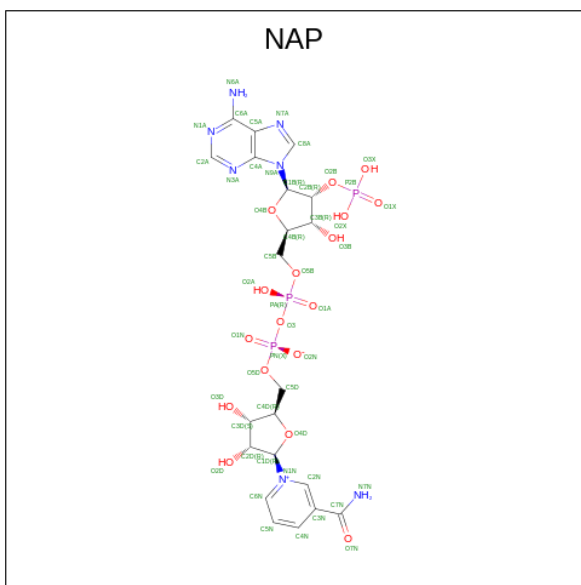
- Molecule 1 is a protein called Aldehyde dehydrogenase.

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 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

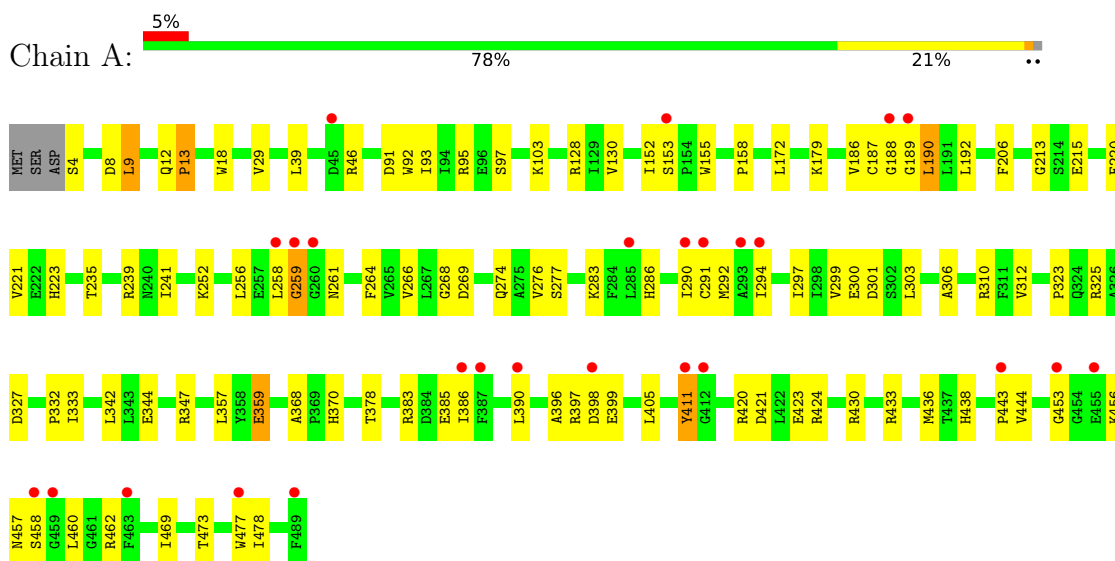
- Molecule 3 is water.

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

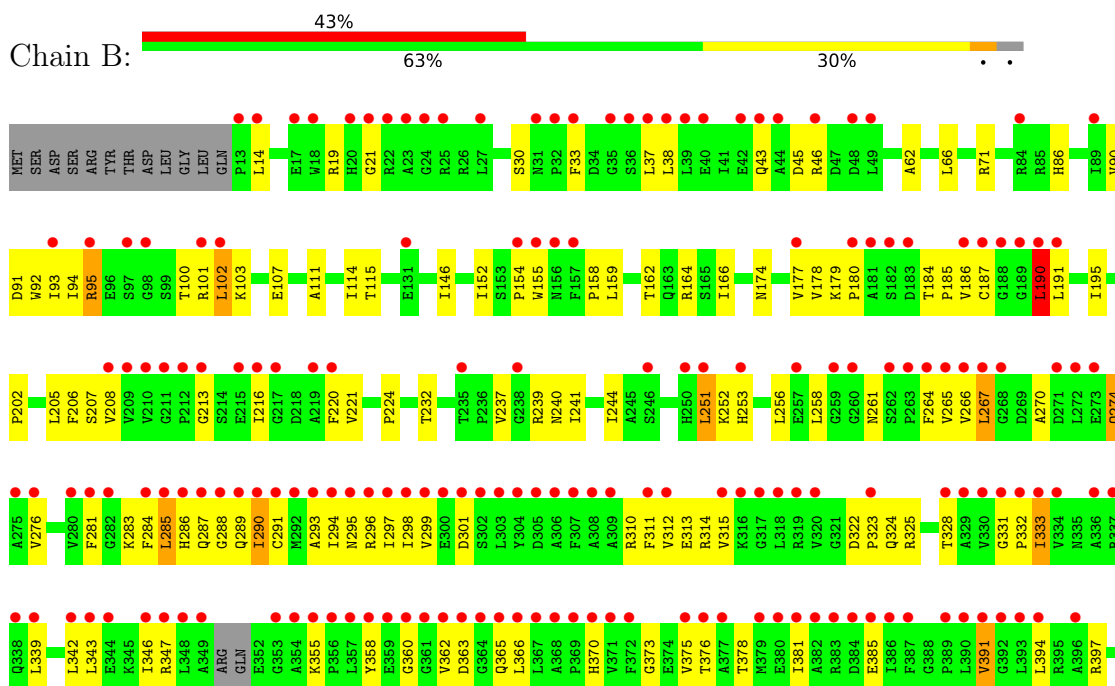
3 Residue-property plots

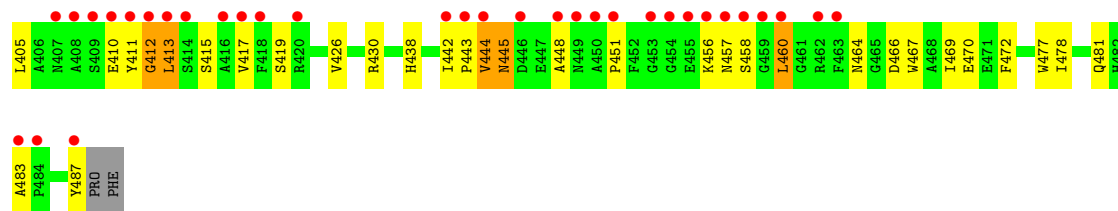
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

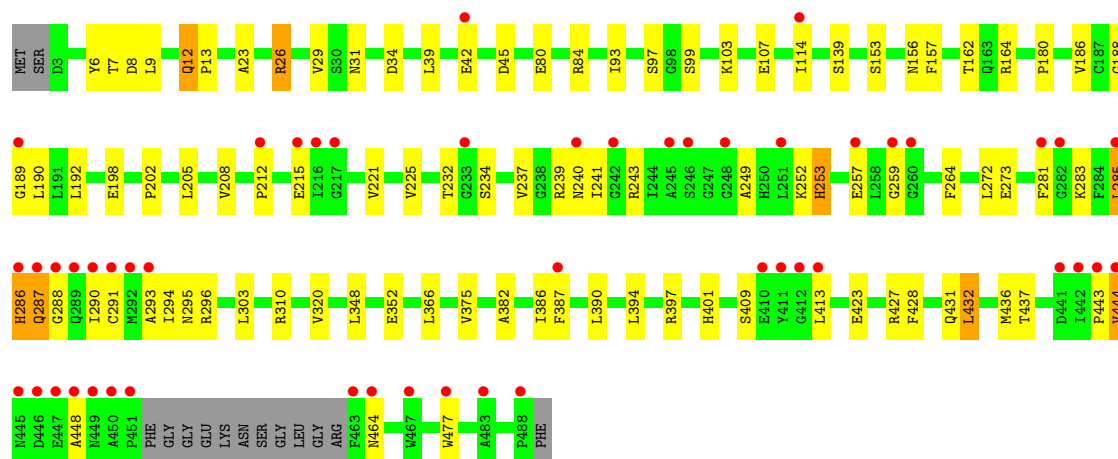
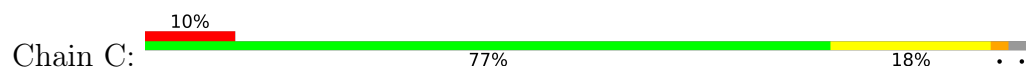


• Molecule 1: Aldehyde dehydrogenase

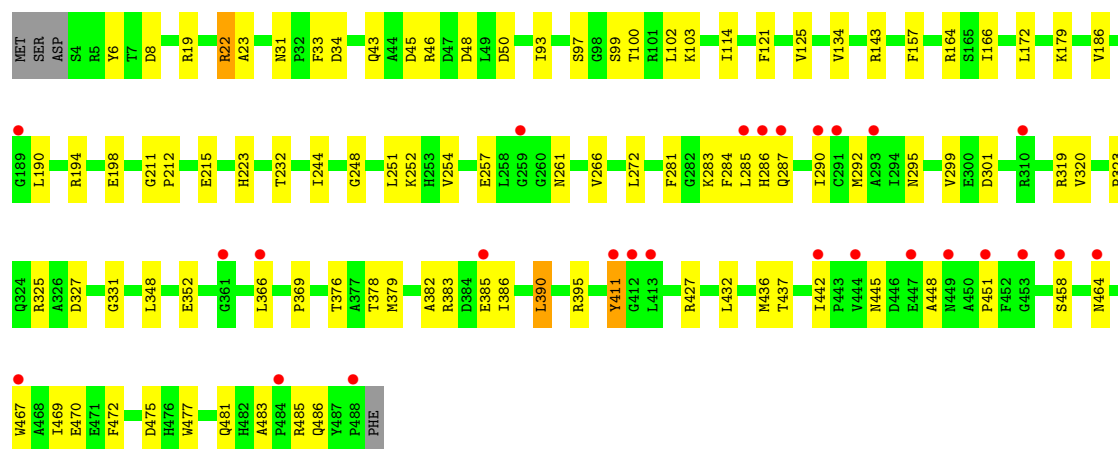
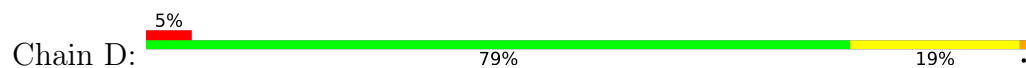




● Molecule 1: Aldehyde dehydrogenase



● 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 0.234 , 0.270	Depositor DCC
R_{free} test set	71693 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	484/489 (99%)	472 (98%)	12 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	469/489 (96%)	460 (98%)	9 (2%)	0	100	100
1	C	471/489 (96%)	462 (98%)	9 (2%)	0	100	100
1	D	483/489 (99%)	475 (98%)	8 (2%)	0	100	100
All	All	1907/1956 (98%)	1869 (98%)	38 (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	60
1	B	305/377 (81%)	278 (91%)	27 (9%)	8	17
1	C	362/377 (96%)	352 (97%)	10 (3%)	38	65
1	D	372/377 (99%)	366 (98%)	6 (2%)	58	80
All	All	1412/1508 (94%)	1357 (96%)	55 (4%)	27	52

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

Continued on next page...

Continued from previous page...

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	C	3001	-	27,33,52	1.85	3 (11%)	35,52,80	1.11	3 (8%)
2	NAP	B	3001	-	27,33,52	1.84	3 (11%)	35,52,80	1.45	6 (17%)
2	NAP	A	3001	-	45,52,52	1.46	3 (6%)	56,80,80	1.15	5 (8%)
2	NAP	D	3001	-	45,52,52	1.48	3 (6%)	56,80,80	1.03	4 (7%)

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	C	3001	-	-	5/17/37/67	0/3/3/5
2	NAP	B	3001	-	-	4/17/37/67	0/3/3/5
2	NAP	A	3001	-	-	6/31/67/67	0/5/5/5
2	NAP	D	3001	-	-	9/31/67/67	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3001	NAP	P2B-O2B	7.97	1.74	1.59
2	B	3001	NAP	P2B-O2B	7.94	1.74	1.59
2	D	3001	NAP	P2B-O2B	7.93	1.74	1.59
2	A	3001	NAP	P2B-O2B	7.78	1.74	1.59
2	C	3001	NAP	PN-O5D	2.77	1.65	1.54
2	B	3001	NAP	PN-O5D	2.75	1.65	1.54
2	A	3001	NAP	O4D-C1D	-2.50	1.37	1.41
2	D	3001	NAP	O4D-C1D	-2.39	1.37	1.41
2	C	3001	NAP	C8A-N7A	-2.28	1.30	1.34
2	A	3001	NAP	C8A-N7A	-2.24	1.30	1.34
2	D	3001	NAP	C8A-N7A	-2.18	1.30	1.34
2	B	3001	NAP	C8A-N7A	-2.13	1.30	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3001	NAP	PA-O3-PN	-3.57	120.58	132.83
2	B	3001	NAP	C1B-N9A-C4A	-3.16	121.09	126.64
2	C	3001	NAP	O2N-PN-O1N	3.10	122.80	110.68
2	A	3001	NAP	C1B-N9A-C4A	-3.08	121.24	126.64
2	D	3001	NAP	C1B-N9A-C4A	-3.03	121.32	126.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	NAP	C3D-C2D-C1D	2.71	105.06	100.98
2	B	3001	NAP	O2N-PN-O1N	2.70	121.27	110.68
2	B	3001	NAP	O5B-C5B-C4B	-2.69	99.72	108.99
2	A	3001	NAP	C3N-C7N-N7N	-2.23	115.07	117.75
2	C	3001	NAP	C1B-N9A-C4A	-2.21	122.75	126.64
2	D	3001	NAP	O3X-P2B-O2X	2.12	115.74	107.64
2	A	3001	NAP	O2N-PN-O1N	2.09	122.56	112.24
2	B	3001	NAP	O2A-PA-O1A	2.08	122.51	112.24
2	B	3001	NAP	O3X-P2B-O2X	2.06	115.52	107.64
2	D	3001	NAP	O2N-PN-O1N	2.05	122.39	112.24
2	D	3001	NAP	C3N-C7N-N7N	-2.05	115.29	117.75
2	C	3001	NAP	O3X-P2B-O2X	2.04	115.44	107.64
2	A	3001	NAP	O2A-PA-O1A	2.03	122.27	112.24

There are no chirality outliers.

All (24) torsion outliers are listed below:

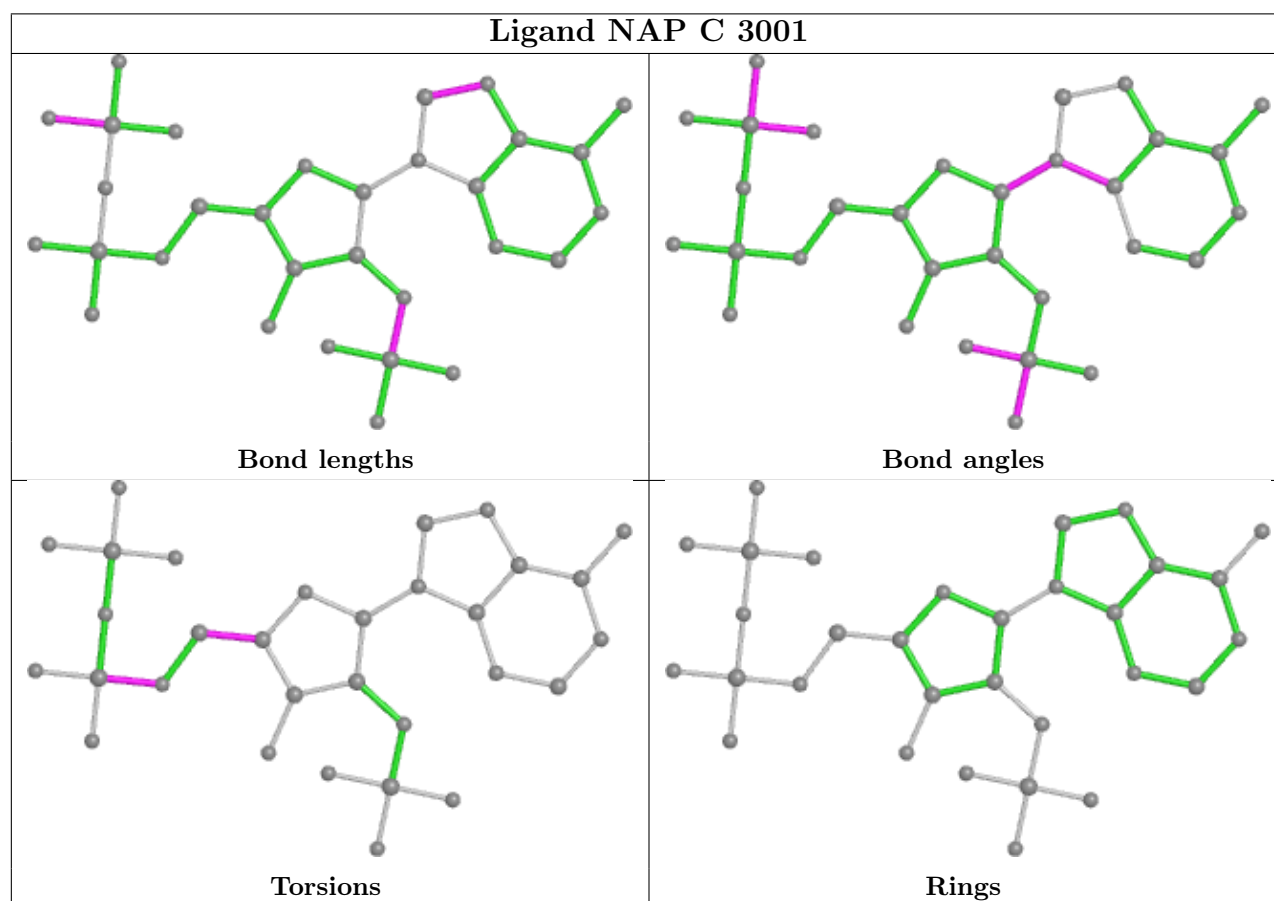
Mol	Chain	Res	Type	Atoms
2	A	3001	NAP	C5B-O5B-PA-O1A
2	A	3001	NAP	C5D-O5D-PN-O1N
2	A	3001	NAP	C5D-O5D-PN-O2N
2	C	3001	NAP	C5B-O5B-PA-O1A
2	D	3001	NAP	C5B-O5B-PA-O3
2	D	3001	NAP	C5D-O5D-PN-O1N
2	D	3001	NAP	C5D-O5D-PN-O2N
2	D	3001	NAP	C3B-C4B-C5B-O5B
2	B	3001	NAP	O4B-C4B-C5B-O5B
2	B	3001	NAP	C3B-C4B-C5B-O5B
2	C	3001	NAP	O4B-C4B-C5B-O5B
2	C	3001	NAP	C3B-C4B-C5B-O5B
2	D	3001	NAP	O4B-C4B-C5B-O5B
2	B	3001	NAP	C5B-O5B-PA-O3
2	C	3001	NAP	C5B-O5B-PA-O3
2	C	3001	NAP	C5B-O5B-PA-O2A
2	D	3001	NAP	C5B-O5B-PA-O1A
2	D	3001	NAP	C4B-C5B-O5B-PA
2	A	3001	NAP	C5D-O5D-PN-O3
2	D	3001	NAP	C5D-O5D-PN-O3
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	B	3001	NAP	C5B-O5B-PA-O1A

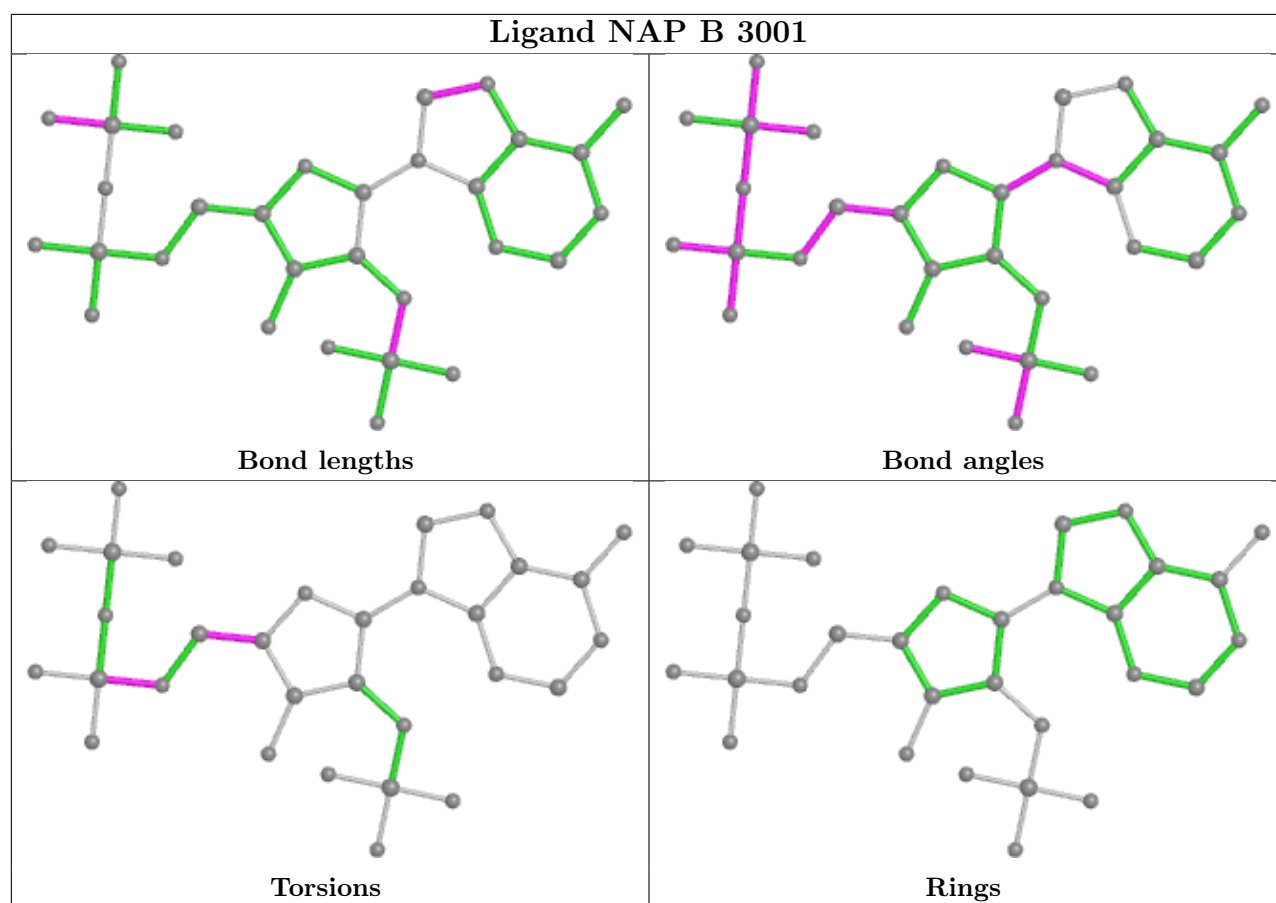
There are no ring outliers.

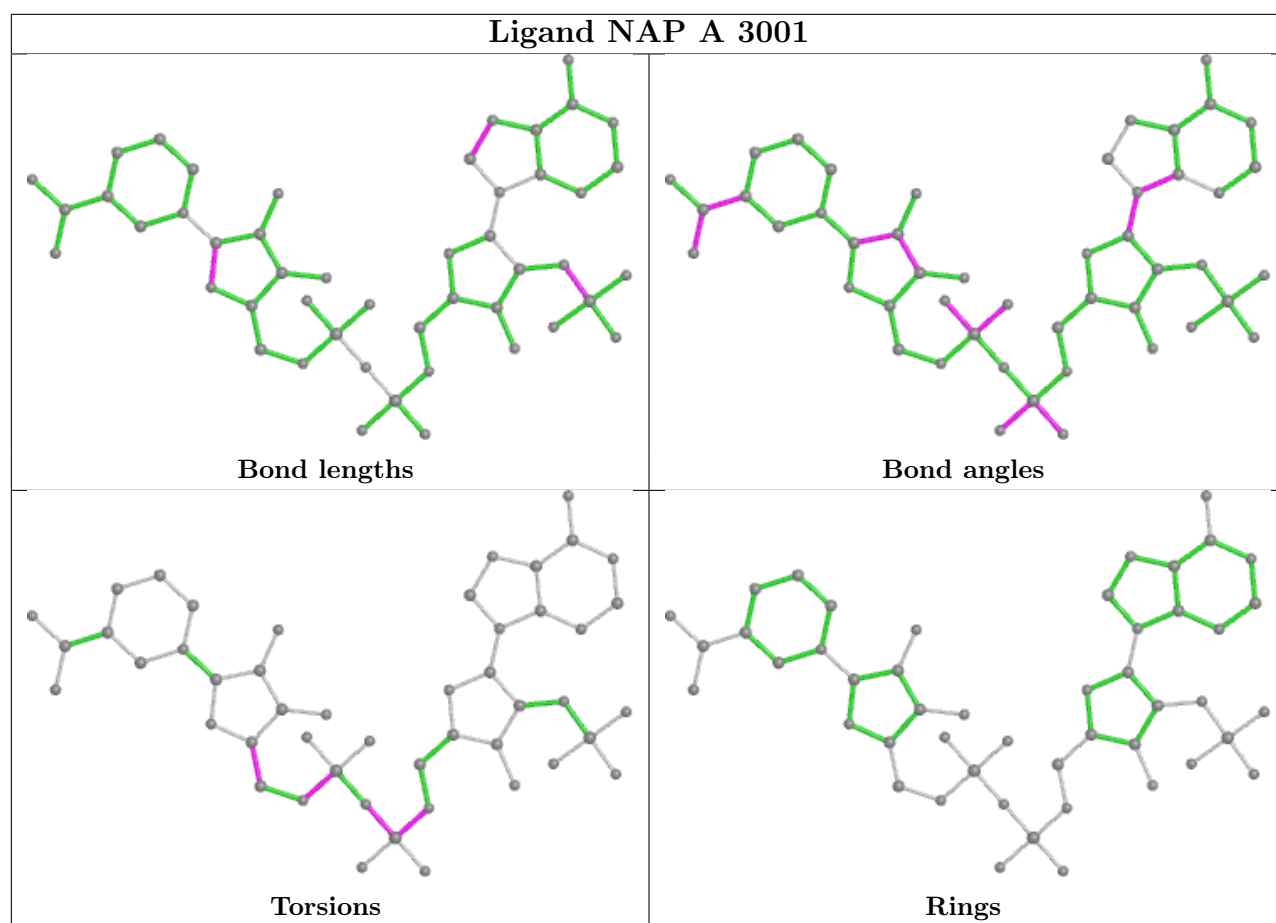
3 monomers are involved in 12 short contacts:

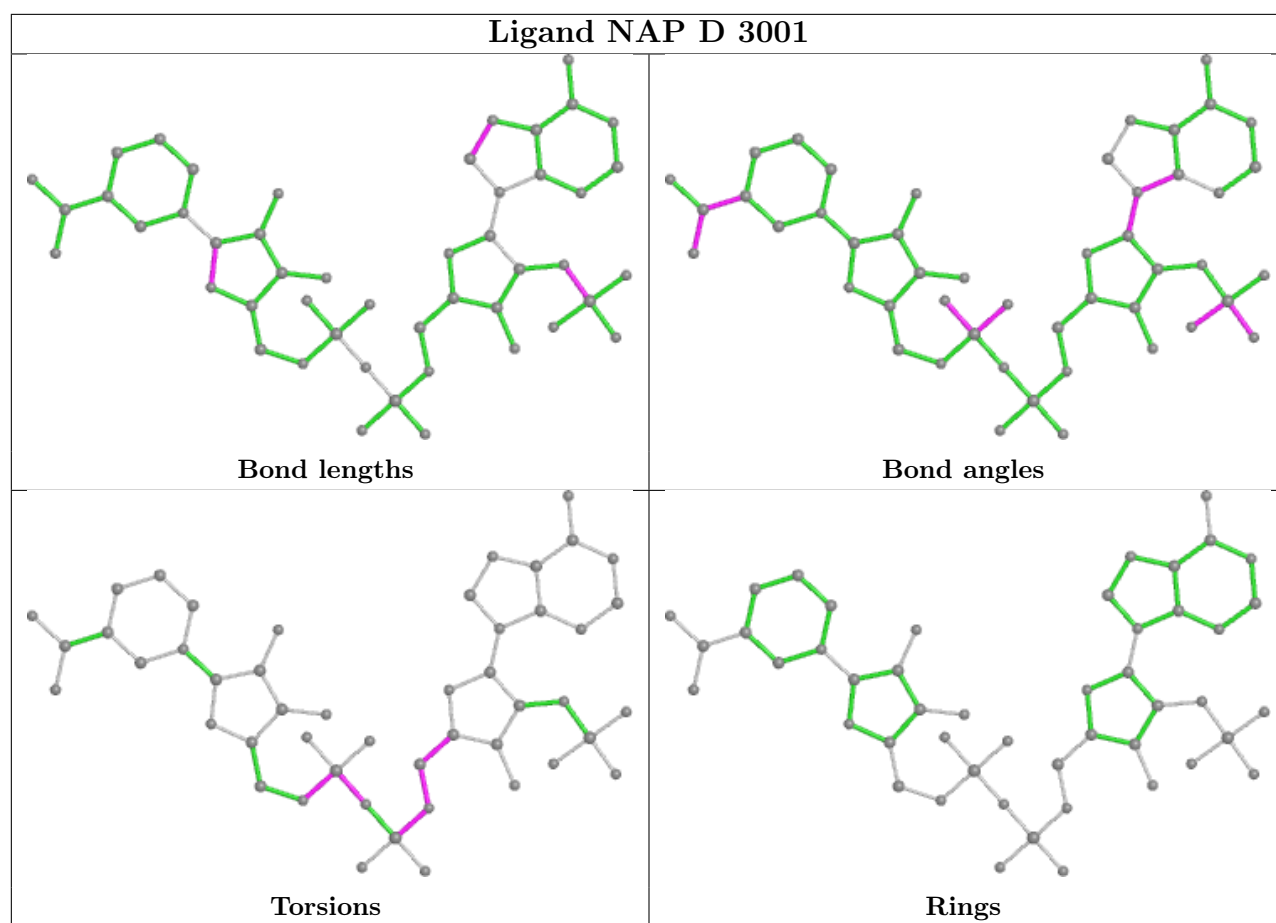
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3001	NAP	2	0
2	A	3001	NAP	7	0
2	D	3001	NAP	3	0

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 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	486/489 (99%)	0.32	26 (5%) 33 31	34, 54, 75, 91	0
1	B	473/489 (96%)	1.97	210 (44%) 1 1	48, 89, 112, 120	0
1	C	475/489 (97%)	0.52	50 (10%) 13 12	34, 51, 92, 108	0
1	D	485/489 (99%)	0.31	26 (5%) 32 30	36, 52, 77, 101	0
All	All	1919/1956 (98%)	0.77	312 (16%) 5 5	34, 58, 105, 120	0

All (312) 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	5.8
1	C	290	ILE	5.6
1	B	457	ASN	5.5
1	B	413	LEU	5.3
1	C	189	GLY	5.3
1	B	450	ALA	5.3
1	D	291	CYS	5.2
1	B	332	PRO	5.2
1	C	443	PRO	5.2
1	C	292	MET	5.1
1	B	210	VAL	5.0
1	B	362	VAL	5.0
1	B	190	LEU	5.0
1	C	463	PHE	4.9
1	B	483	ALA	4.9
1	B	349	ALA	4.8
1	B	331	GLY	4.8
1	B	371	VAL	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	183	ASP	4.7
1	B	307	PHE	4.7
1	B	289	GLN	4.6
1	B	272	LEU	4.5
1	B	459	GLY	4.5
1	B	43	GLN	4.5
1	C	448	ALA	4.4
1	B	381	ILE	4.4
1	B	253	HIS	4.4
1	B	367	LEU	4.4
1	B	387	PHE	4.4
1	B	455	GLU	4.4
1	B	386	ILE	4.3
1	B	366	LEU	4.3
1	B	329	ALA	4.3
1	C	288	GLY	4.3
1	B	484	PRO	4.2
1	B	389	PRO	4.2
1	C	451	PRO	4.2
1	B	330	VAL	4.1
1	B	275	ALA	4.1
1	C	445	ASN	4.1
1	B	365	GLN	4.1
1	B	98	GLY	4.0
1	B	410	GLU	4.0
1	B	101	ARG	4.0
1	B	453	GLY	4.0
1	C	444	VAL	4.0
1	B	357	LEU	3.9
1	D	451	PRO	3.9
1	D	189	GLY	3.9
1	B	449	ASN	3.9
1	B	265	VAL	3.9
1	B	301	ASP	3.9
1	B	328	THR	3.8
1	B	32	PRO	3.8
1	A	386	ILE	3.8
1	B	315	VAL	3.8
1	B	458	SER	3.8
1	C	287	GLN	3.8
1	B	318	LEU	3.8
1	B	375	VAL	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	338	GLN	3.8
1	B	285	LEU	3.7
1	C	412	GLY	3.7
1	B	382	ALA	3.7
1	B	333	ILE	3.7
1	B	364	GLY	3.7
1	B	384	ASP	3.7
1	C	285	LEU	3.7
1	B	323	PRO	3.7
1	B	456	LYS	3.7
1	B	296	ARG	3.7
1	B	462	ARG	3.7
1	B	372	PHE	3.6
1	C	450	ALA	3.6
1	D	290	ILE	3.6
1	B	293	ALA	3.6
1	B	216	ILE	3.6
1	A	459	GLY	3.6
1	B	311	PHE	3.5
1	D	361	GLY	3.5
1	B	25	ARG	3.5
1	A	259	GLY	3.5
1	B	188	GLY	3.5
1	B	390	LEU	3.5
1	B	263	PRO	3.5
1	B	380	GLU	3.5
1	C	260	GLY	3.5
1	B	339	LEU	3.5
1	B	418	PHE	3.5
1	B	219	ALA	3.5
1	B	308	ALA	3.4
1	B	37	LEU	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	3.3
1	B	42	GLU	3.3
1	D	411	TYR	3.3
1	B	213	GLY	3.3
1	B	312	VAL	3.3
1	B	347	ARG	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	293	ALA	3.3
1	B	271	ASP	3.3
1	B	284	PHE	3.3
1	B	358	TYR	3.3
1	B	260	GLY	3.3
1	A	489	PHE	3.3
1	C	387	PHE	3.3
1	B	411	TYR	3.3
1	B	303	LEU	3.3
1	B	414	SER	3.3
1	B	359	GLU	3.3
1	B	97	SER	3.2
1	B	320	VAL	3.2
1	B	377	ALA	3.2
1	B	211	GLY	3.2
1	B	186	VAL	3.2
1	B	131	GLU	3.2
1	B	317	GLY	3.2
1	C	289	GLN	3.2
1	B	268	GLY	3.1
1	B	360	GLY	3.1
1	B	299	VAL	3.1
1	B	443	PRO	3.1
1	B	379	MET	3.1
1	B	346	ILE	3.1
1	B	460	LEU	3.1
1	B	181	ALA	3.1
1	C	467	TRP	3.1
1	C	477	TRP	3.1
1	D	467	TRP	3.1
1	B	417	VAL	3.0
1	B	44	ALA	3.0
1	B	391	VAL	3.0
1	B	408	ALA	3.0
1	D	285	LEU	3.0
1	A	294	ILE	3.0
1	B	383	ARG	3.0
1	B	420	ARG	3.0
1	B	336	ALA	3.0
1	B	292	MET	3.0
1	B	217	GLY	2.9
1	B	259	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	392	GLY	2.9
1	B	451	PRO	2.9
1	B	46	ARG	2.9
1	B	48	ASP	2.9
1	B	444	VAL	2.9
1	C	441	ASP	2.9
1	C	447	GLU	2.9
1	B	155	TRP	2.9
1	A	293	ALA	2.9
1	B	267	LEU	2.9
1	B	154	PRO	2.9
1	B	212	PRO	2.9
1	B	287	GLN	2.9
1	B	276	VAL	2.9
1	B	13	PRO	2.8
1	B	376	THR	2.8
1	B	298	ILE	2.8
1	A	477	TRP	2.8
1	B	394	LEU	2.8
1	B	93	ILE	2.8
1	A	458	SER	2.8
1	B	487	TYR	2.8
1	B	177	VAL	2.8
1	B	294	ILE	2.7
1	C	216	ILE	2.7
1	B	273	GLU	2.7
1	B	182	SER	2.7
1	A	411	TYR	2.7
1	B	209	VAL	2.7
1	B	354	ALA	2.7
1	B	20	HIS	2.7
1	B	282	GLY	2.7
1	B	266	VAL	2.7
1	B	370	HIS	2.7
1	B	385	GLU	2.7
1	A	387	PHE	2.7
1	A	463	PHE	2.7
1	B	246	SER	2.7
1	B	448	ALA	2.6
1	B	369	PRO	2.6
1	C	442	ILE	2.6
1	B	257	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	49	LEU	2.6
1	B	342	LEU	2.6
1	C	411	TYR	2.6
1	B	319	ARG	2.6
1	D	413	LEU	2.6
1	B	156	ASN	2.6
1	D	287	GLN	2.6
1	B	348	LEU	2.6
1	B	262	SER	2.6
1	B	409	SER	2.6
1	B	286	HIS	2.6
1	B	297	ILE	2.6
1	B	288	GLY	2.6
1	B	407	ASN	2.6
1	B	102	LEU	2.5
1	B	304	TYR	2.5
1	B	291	CYS	2.5
1	B	95	ARG	2.5
1	B	281	PHE	2.5
1	C	413	LEU	2.5
1	D	366	LEU	2.5
1	B	368	ALA	2.5
1	B	180	PRO	2.5
1	C	42	GLU	2.5
1	B	363	ASP	2.5
1	A	291	CYS	2.5
1	B	14	LEU	2.5
1	B	27	LEU	2.5
1	A	153	SER	2.5
1	B	40	GLU	2.5
1	B	31	ASN	2.5
1	B	316	LYS	2.5
1	C	281	PHE	2.5
1	A	258	LEU	2.5
1	A	443	PRO	2.5
1	B	84	ARG	2.5
1	B	235	THR	2.5
1	D	412	GLY	2.5
1	B	24	GLY	2.4
1	C	217	GLY	2.4
1	B	295	ASN	2.4
1	D	488	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	455	GLU	2.4
1	B	17	GLU	2.4
1	C	215	GLU	2.4
1	C	245	ALA	2.4
1	D	458	SER	2.4
1	A	188	GLY	2.4
1	D	259	GLY	2.4
1	A	285	LEU	2.4
1	A	390	LEU	2.4
1	B	305	ASP	2.4
1	B	337	ARG	2.4
1	C	410	GLU	2.4
1	B	446	ASP	2.3
1	B	306	ALA	2.3
1	C	233	GLY	2.3
1	B	463	PHE	2.3
1	D	484	PRO	2.3
1	B	344	GLU	2.3
1	B	238	GLY	2.3
1	A	398	ASP	2.3
1	C	240	ASN	2.3
1	C	212	PRO	2.3
1	B	416	ALA	2.3
1	B	220	PHE	2.3
1	B	300	GLU	2.3
1	C	257	GLU	2.3
1	D	447	GLU	2.3
1	C	483	ALA	2.3
1	B	250	HIS	2.2
1	B	89	ILE	2.2
1	B	442	ILE	2.2
1	B	396	ALA	2.2
1	A	453	GLY	2.2
1	B	361	GLY	2.2
1	B	454	GLY	2.2
1	B	290	ILE	2.2
1	B	353	GLY	2.2
1	C	248	GLY	2.2
1	C	282	GLY	2.2
1	B	36	SER	2.2
1	B	22	ARG	2.2
1	C	446	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	38	LEU	2.2
1	A	189	GLY	2.2
1	B	187	CYS	2.2
1	B	33	PHE	2.2
1	C	246	SER	2.2
1	D	449	ASN	2.2
1	D	442	ILE	2.2
1	B	412	GLY	2.1
1	C	449	ASN	2.1
1	A	290	ILE	2.1
1	B	39	LEU	2.1
1	D	293	ALA	2.1
1	B	21	GLY	2.1
1	B	355	LYS	2.1
1	B	208	VAL	2.1
1	B	251	LEU	2.1
1	B	309	ALA	2.1
1	C	464	ASN	2.1
1	B	191	LEU	2.1
1	B	393	LEU	2.1
1	C	251	LEU	2.1
1	B	18	TRP	2.1
1	B	23	ALA	2.1
1	A	412	GLY	2.1
1	C	242	GLY	2.1
1	B	264	PHE	2.1
1	D	286	HIS	2.1
1	B	280	VAL	2.0
1	D	444	VAL	2.0
1	D	310	ARG	2.0
1	B	35	GLY	2.0
1	B	157	PHE	2.0
1	B	215	GLU	2.0
1	D	385	GLU	2.0
1	C	114	ILE	2.0
1	A	45	ASP	2.0
1	B	343	LEU	2.0
1	C	259	GLY	2.0
1	D	464	ASN	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](#)

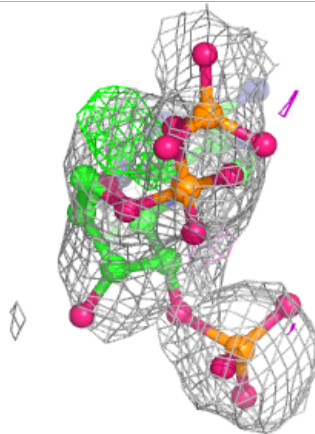
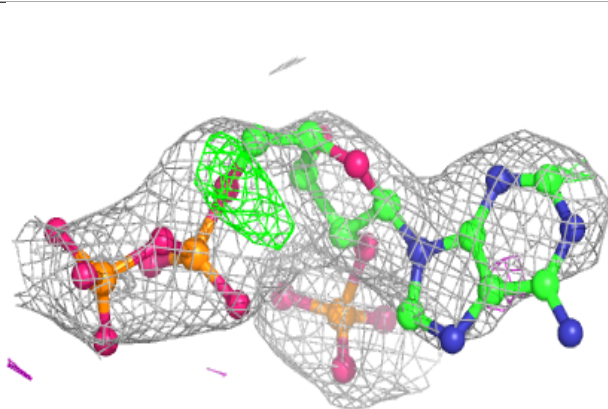
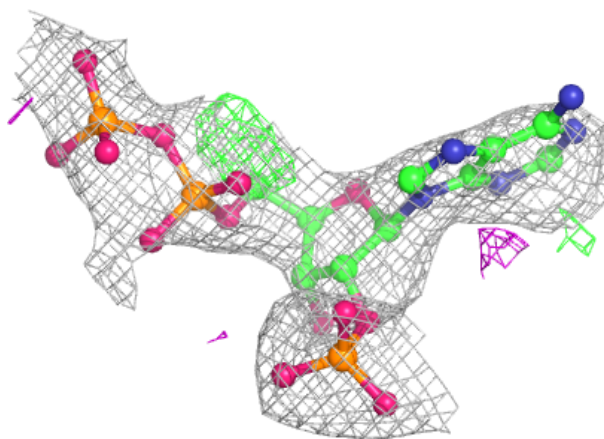
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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.

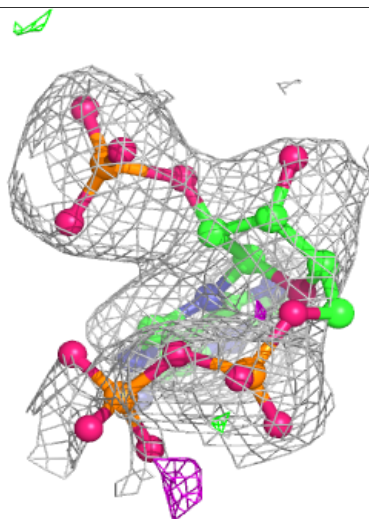
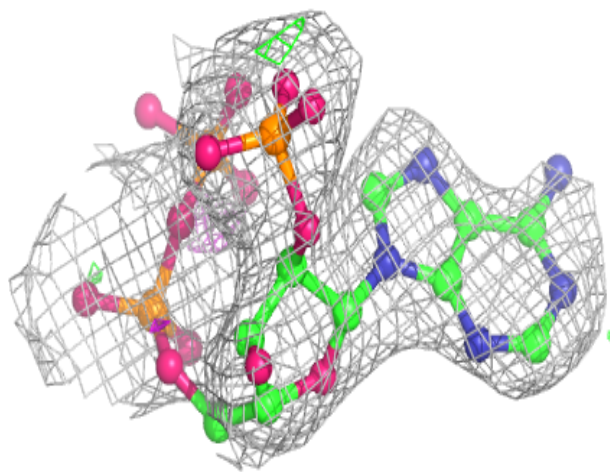
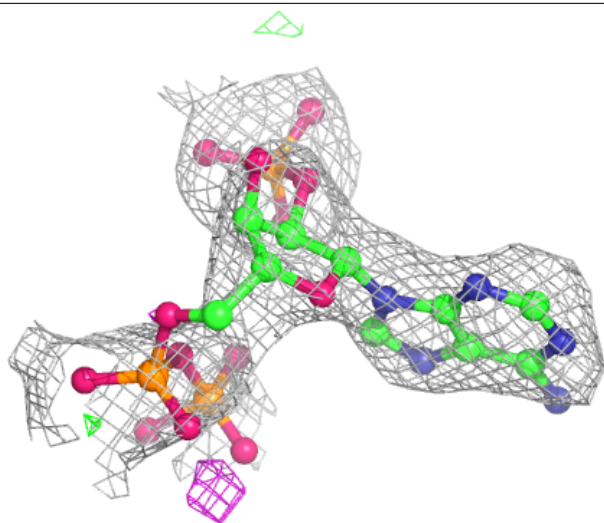
Electron density around NAP B 3001:

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



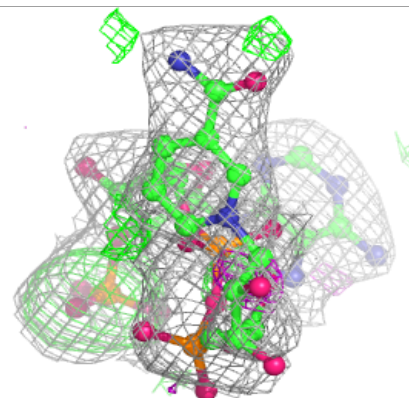
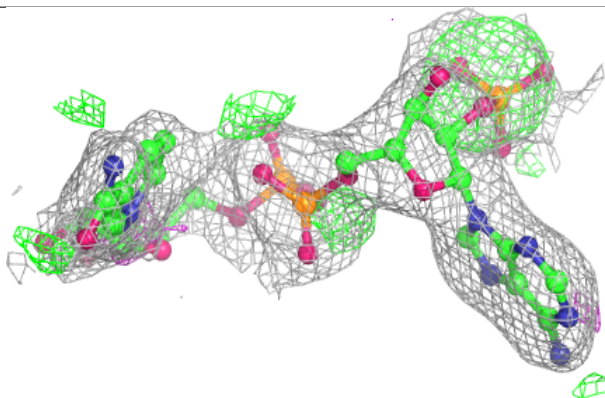
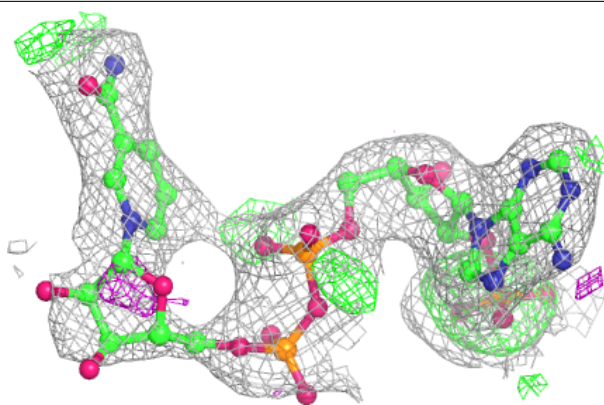
Electron density around NAP C 3001:

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

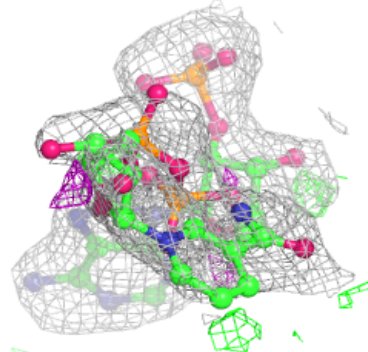
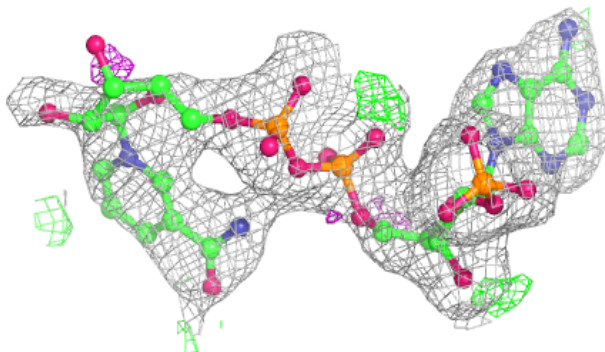
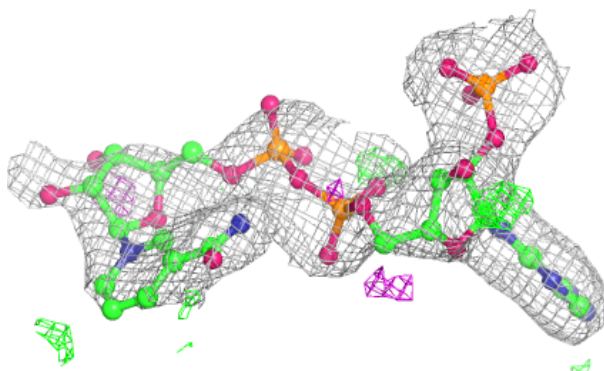


Electron density around NAP A 3001:

$2mF_o-DF_c$ (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.