Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2023 – 05:12 AM EDT

PDB ID	:	2ESD
Title	:	Crystal Structure of thioacylenzyme intermediate of an Nadp Dependent Aldehyde Dehydrogenase
Authors	:	D'Ambrosio, K.; Didierjean, C.; Benedetti, E.; Aubry, A.; Corbier, C.
Deposited on	:	2005-10-26
Resolution	:	2.55 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 (i) 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 (i)) were used in the production of this report:

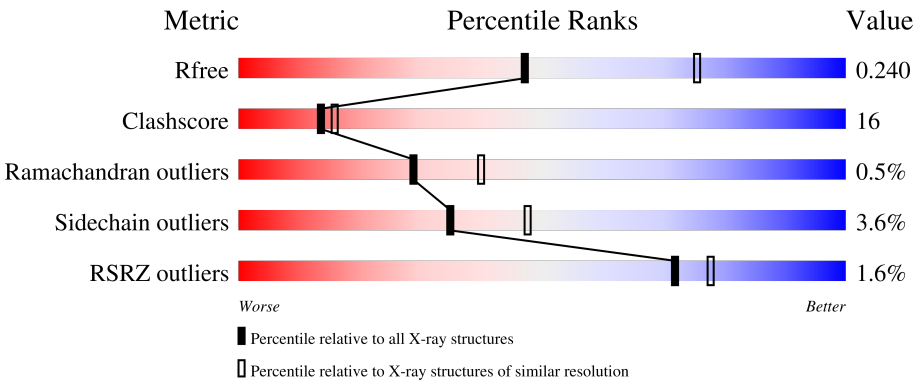
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.55 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	475	.% 70% 28% •
1	B	475	2% 68% 30% •
1	C	475	.% 73% 25% •
1	D	475	2% 65% 33% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	G3H	A	800	-	-	X	X
3	G3H	B	800	-	-	X	-
3	G3H	C	800	-	-	X	-
3	G3H	D	800	-	-	X	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15592 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.

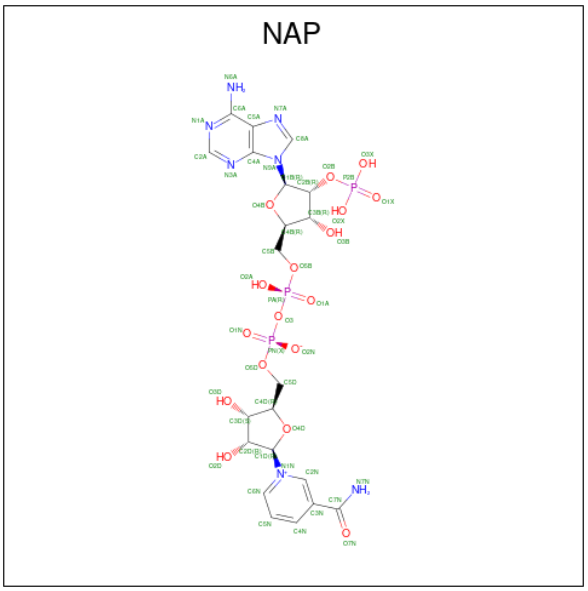
- Molecule 1 is a protein called NADP-dependent glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	474	3598	2287	601	698	12	0	1	0
1	B	474	3598	2287	601	698	12	0	1	0
1	C	474	3598	2287	601	698	12	0	1	0
1	D	474	3598	2287	601	698	12	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

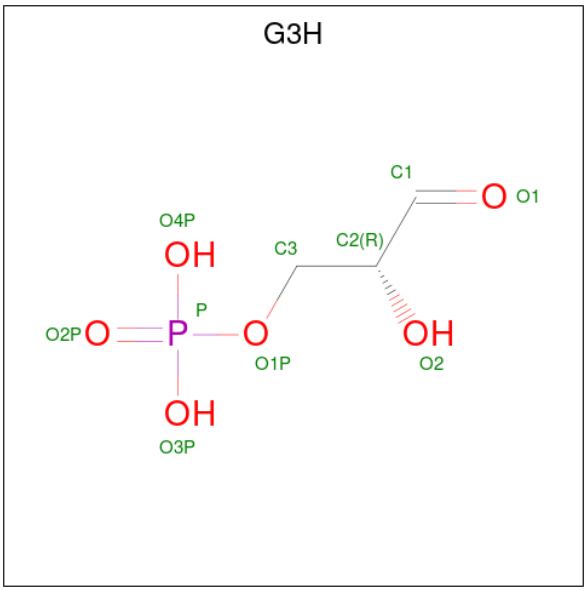
Chain	Residue	Modelled	Actual	Comment	Reference
A	250	ALA	GLU	engineered mutation	UNP Q59931
B	250	ALA	GLU	engineered mutation	UNP Q59931
C	250	ALA	GLU	engineered mutation	UNP Q59931
D	250	ALA	GLU	engineered mutation	UNP Q59931

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	96	42	14	34	6	0	1
2	B	1	96	42	14	34	6	0	1
2	C	1	96	42	14	34	6	0	1
2	D	1	96	42	14	34	6	0	1

- Molecule 3 is GLYCERALDEHYDE-3-PHOSPHATE (three-letter code: G3H) (formula: $C_3H_7O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	10	3	6	1	0	0
3	B	1	10	3	6	1	0	0
3	C	1	10	3	6	1	0	0
3	D	1	10	3	6	1	0	0

- Molecule 4 is water.

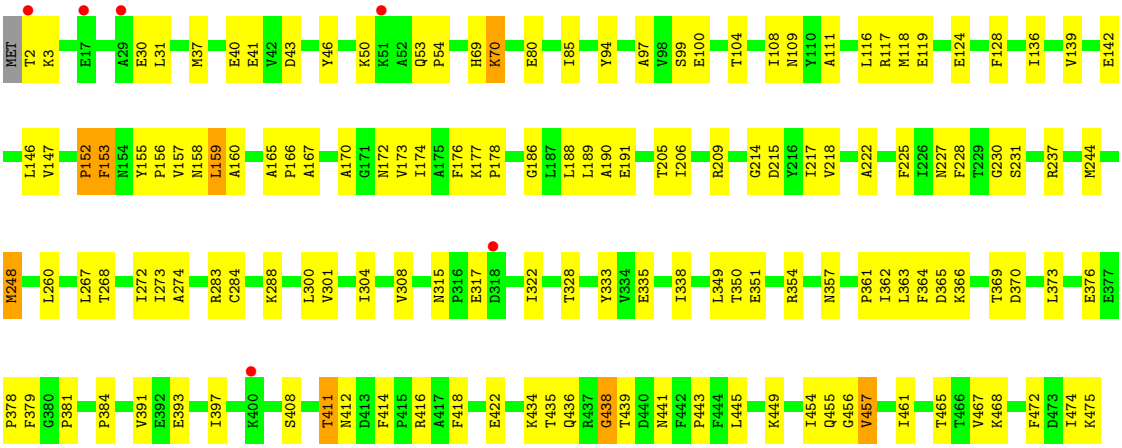
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	192	192	192	0	0
4	B	149	149	149	0	0
4	C	276	276	276	0	0
4	D	159	159	159	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

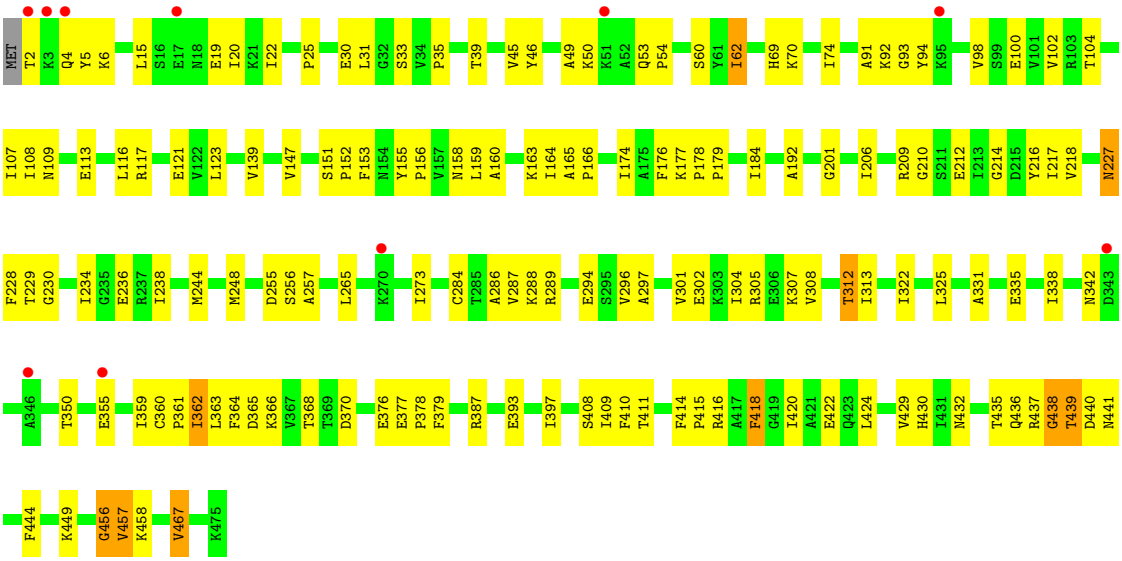
• Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain A:



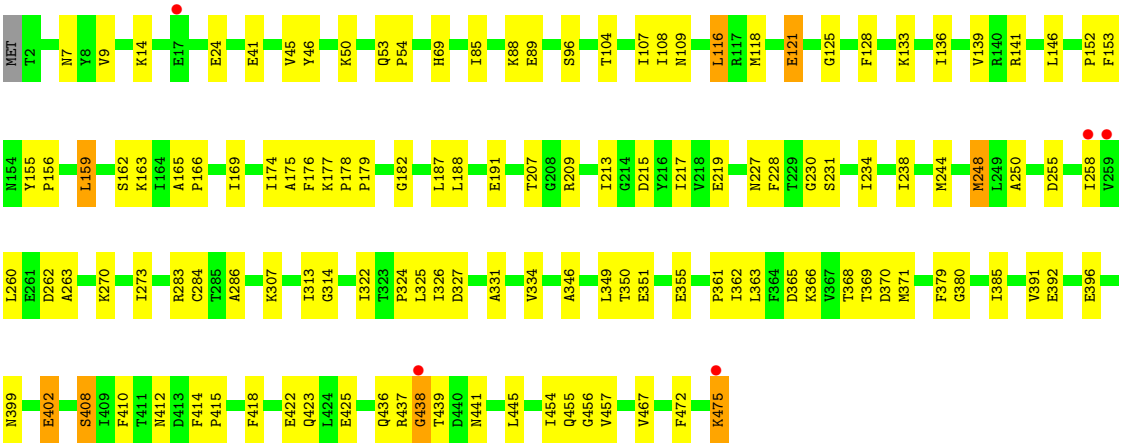
• Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain B:



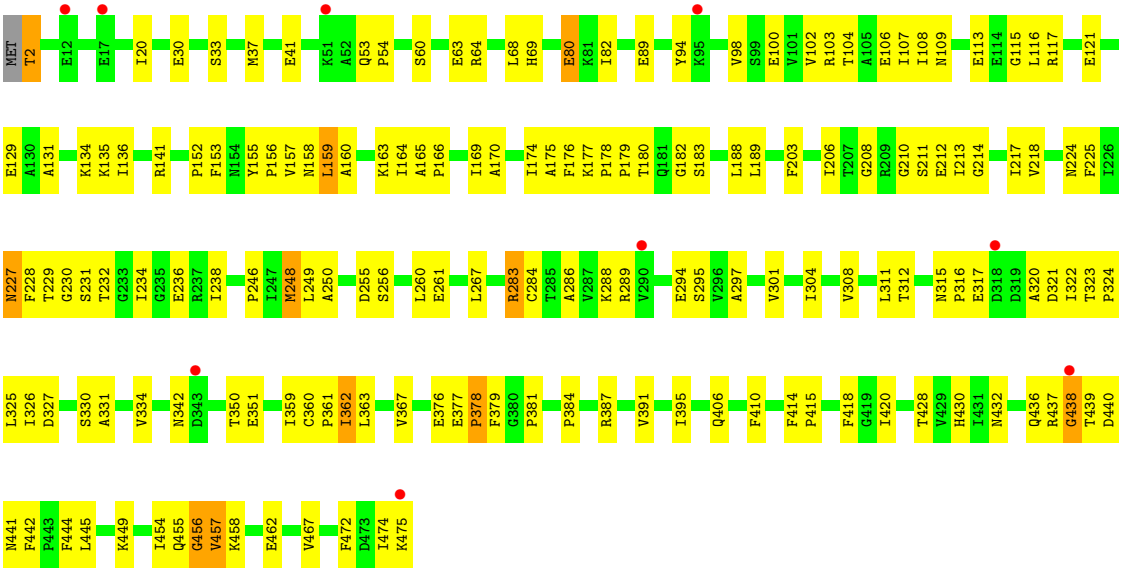
• Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain C:



• Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	142.50Å 154.90Å 112.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.55 20.03 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.9 (20.00-2.55) 97.1 (20.03-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 2.56Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.248 0.189 , 0.240	Depositor DCC
R_{free} test set	7952 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15592	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0667e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: G3H, 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	0.35	0/3656	0.62	1/4945 (0.0%)
1	B	0.34	0/3656	0.61	1/4945 (0.0%)
1	C	0.36	0/3656	0.64	1/4945 (0.0%)
1	D	0.34	0/3656	0.61	1/4945 (0.0%)
All	All	0.35	0/14624	0.62	4/19780 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	456	GLY	N-CA-C	-6.49	96.88	113.10
1	B	456	GLY	N-CA-C	-6.31	97.33	113.10
1	D	456	GLY	N-CA-C	-6.26	97.44	113.10
1	A	456	GLY	N-CA-C	-6.10	97.86	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3598	0	3651	118	0
1	B	3598	0	3651	139	0
1	C	3598	0	3651	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3598	0	3651	135	0
2	A	96	0	50	7	0
2	B	96	0	50	10	0
2	C	96	0	50	4	0
2	D	96	0	50	9	0
3	A	10	0	4	6	0
3	B	10	0	4	7	0
3	C	10	0	4	5	0
3	D	10	0	4	7	0
4	A	192	0	0	11	0
4	B	149	0	0	5	0
4	C	276	0	0	9	0
4	D	159	0	0	4	0
All	All	15592	0	14820	473	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 16.

All (473) 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:B:284[B]:CYS:SG	3:B:800:G3H:O1	2.23	0.96
1:D:284[B]:CYS:SG	3:D:800:G3H:O1	2.26	0.94
1:C:346:ALA:HB2	1:C:371:MET:HE1	1.60	0.83
1:B:147:VAL:HB	1:B:174:ILE:HD12	1.61	0.83
1:C:439:THR:HG23	1:C:441:ASN:OD1	1.78	0.83
1:B:439:THR:HG23	1:B:441:ASN:OD1	1.77	0.83
1:C:284[B]:CYS:HB2	3:C:800:G3H:C1	2.08	0.82
1:D:284[B]:CYS:SG	3:D:800:G3H:C1	2.67	0.82
1:C:436:GLN:HE21	1:C:438:GLY:HA3	1.44	0.82
1:A:369:THR:HB	4:A:1586:HOH:O	1.80	0.81
1:C:118:MET:HB2	4:C:3711:HOH:O	1.81	0.80
1:A:284[B]:CYS:SG	3:A:800:G3H:O1	2.39	0.80
1:B:164:ILE:HD13	1:B:174:ILE:HG12	1.61	0.80
1:B:284[B]:CYS:SG	3:B:800:G3H:C1	2.70	0.80
1:C:350:THR:HB	1:C:362:ILE:HD12	1.64	0.79
1:D:350:THR:HG21	1:D:361:PRO:O	1.83	0.79
1:D:107:ILE:HD12	1:D:158:ASN:HD21	1.47	0.78
1:C:104:THR:O	1:C:108:ILE:HG12	1.83	0.78
1:D:164:ILE:HD13	1:D:203:PHE:HE2	1.48	0.78
1:B:436:GLN:HE21	1:B:438:GLY:HA3	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284[B]:CYS:HB2	3:A:800:G3H:C1	2.17	0.74
1:B:288:LYS:HE2	1:B:377:GLU:HG3	1.69	0.74
1:D:436:GLN:NE2	1:D:438:GLY:HA3	2.03	0.73
1:D:80:GLU:HB2	4:D:4627:HOH:O	1.89	0.72
1:B:284[B]:CYS:HB2	3:B:800:G3H:C1	2.20	0.72
1:B:70:LYS:HA	1:B:70:LYS:HE3	1.72	0.71
1:C:475:LYS:HE3	1:C:475:LYS:HA	1.72	0.71
1:A:439:THR:HG23	1:A:441:ASN:OD1	1.90	0.71
1:A:104:THR:O	1:A:108:ILE:HG12	1.91	0.71
1:A:155:TYR:HB2	1:A:159:LEU:HD22	1.73	0.71
1:A:231:SER:HA	2:A:1476[B]:NAP:H2D	1.73	0.70
1:A:436:GLN:NE2	1:A:438:GLY:HA3	2.05	0.70
1:B:159:LEU:HD23	1:B:229:THR:HG21	1.73	0.70
1:B:209:ARG:HH11	1:B:209:ARG:HG3	1.56	0.70
1:C:436:GLN:NE2	1:C:438:GLY:HA3	2.06	0.70
1:C:9:VAL:HB	1:C:14:LYS:HD2	1.71	0.69
1:C:155:TYR:HB2	1:C:159:LEU:HD22	1.73	0.69
1:D:230:GLY:HA2	2:D:4476[B]:NAP:H52N	1.72	0.69
1:C:346:ALA:HB2	1:C:371:MET:CE	2.22	0.69
1:A:284[B]:CYS:SG	2:A:1476[B]:NAP:O3D	2.49	0.69
1:B:436:GLN:NE2	1:B:438:GLY:HA3	2.08	0.69
1:C:209:ARG:HG3	1:C:209:ARG:HH11	1.57	0.68
1:B:415:PRO:HG3	1:C:414:PHE:CZ	2.28	0.68
1:D:107:ILE:HD12	1:D:158:ASN:ND2	2.10	0.67
1:D:414:PHE:HB3	1:D:415:PRO:HD3	1.77	0.67
1:C:423:GLN:HG2	4:D:4616:HOH:O	1.94	0.67
1:D:261:GLU:HG2	1:D:295:SER:OG	1.95	0.67
1:A:209:ARG:HG3	1:A:209:ARG:HH11	1.60	0.67
1:D:2:THR:HB	1:D:30:GLU:OE2	1.94	0.67
1:D:165:ALA:HB3	1:D:166:PRO:HD3	1.75	0.67
1:A:349:LEU:HD12	1:A:363:LEU:HD23	1.77	0.66
1:B:284[B]:CYS:CB	3:B:800:G3H:C1	2.74	0.66
1:C:439:THR:CG2	1:C:441:ASN:OD1	2.43	0.66
1:A:139:VAL:HG13	1:A:467:VAL:HG13	1.76	0.66
1:B:362:ILE:HD12	1:B:363:LEU:N	2.11	0.66
1:B:415:PRO:HB2	1:D:475:LYS:HG3	1.77	0.66
1:B:415:PRO:HB2	1:D:475:LYS:CG	2.26	0.66
1:B:160:ALA:O	1:B:164:ILE:HG12	1.96	0.66
1:A:436:GLN:HE21	1:A:438:GLY:HA3	1.61	0.65
1:C:118:MET:HA	4:C:3675:HOH:O	1.97	0.65
1:B:362:ILE:HD11	1:B:364:PHE:CD1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ALA:HB2	1:C:455:GLN:HE22	1.61	0.64
1:A:53:GLN:HB3	1:A:54:PRO:HD3	1.80	0.64
1:D:362:ILE:HD12	1:D:363:LEU:N	2.12	0.64
1:A:273:ILE:HD11	1:A:304:ILE:HG23	1.80	0.64
1:D:304:ILE:O	1:D:308:VAL:HG23	1.98	0.64
1:A:416:ARG:HA	1:C:475:LYS:HB2	1.80	0.63
1:B:163:LYS:HE3	1:B:227:ASN:ND2	2.13	0.63
1:A:176:PHE:CZ	1:A:178:PRO:HB3	2.33	0.63
1:B:209:ARG:HB2	1:B:212:GLU:OE1	1.99	0.63
1:B:359:ILE:HD12	1:B:359:ILE:N	2.14	0.62
1:B:165:ALA:HB3	1:B:166:PRO:HD3	1.81	0.62
1:B:53:GLN:HB3	1:B:54:PRO:HD3	1.82	0.62
1:B:62:ILE:O	1:B:62:ILE:HD13	1.99	0.62
1:D:250:ALA:HB2	1:D:455:GLN:NE2	2.15	0.61
1:A:2:THR:HB	1:A:30:GLU:OE2	2.00	0.61
1:B:297:ALA:O	1:B:301:VAL:HG23	2.00	0.61
1:A:284[B]:CYS:CB	3:A:800:G3H:C1	2.78	0.61
1:D:391:VAL:O	1:D:395:ILE:HG12	2.01	0.61
1:A:273:ILE:CD1	1:A:304:ILE:HG23	2.30	0.60
1:B:409:ILE:HD13	1:B:429:VAL:CG1	2.31	0.60
1:B:437:ARG:HG3	1:B:444:PHE:CD1	2.36	0.60
1:D:250:ALA:HB2	1:D:455:GLN:HE22	1.67	0.60
1:D:163:LYS:HE3	1:D:227:ASN:ND2	2.17	0.60
1:C:128:PHE:HB2	1:D:441:ASN:OD1	2.01	0.59
1:B:228:PHE:CE1	2:B:2476[B]:NAP:H52A	2.37	0.59
1:A:70:LYS:HE3	1:A:70:LYS:HA	1.85	0.59
1:A:284[B]:CYS:SG	3:A:800:G3H:C1	2.90	0.59
1:D:445:LEU:HD13	1:D:454:ILE:HG12	1.84	0.59
1:D:153:PHE:O	1:D:156:PRO:HD3	2.02	0.59
1:C:165:ALA:HB3	1:C:166:PRO:HD3	1.84	0.59
1:D:315:ASN:HB3	1:D:317:GLU:OE1	2.03	0.59
1:C:118:MET:HG3	4:C:3709:HOH:O	2.03	0.59
1:D:211:SER:O	1:D:212:GLU:HG3	2.03	0.59
1:D:284[B]:CYS:SG	2:D:4476[B]:NAP:O3D	2.57	0.59
1:C:230:GLY:HA2	2:C:3476[B]:NAP:H52N	1.85	0.58
1:D:152:PRO:HD3	1:D:229:THR:HB	1.85	0.58
1:B:117:ARG:NH2	1:D:113:GLU:HB2	2.18	0.58
1:A:165:ALA:HB3	1:A:166:PRO:HD3	1.86	0.58
1:D:53:GLN:HB3	1:D:54:PRO:HD3	1.86	0.58
1:A:157:VAL:O	1:A:160:ALA:HB3	2.03	0.57
1:B:230:GLY:HA2	2:B:2476[B]:NAP:H52N	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:GLY:HA2	1:D:439:THR:HG21	1.84	0.57
1:C:159:LEU:O	1:C:163:LYS:HE2	2.04	0.57
1:C:53:GLN:HB3	1:C:54:PRO:HD3	1.86	0.57
1:B:350:THR:HG21	1:B:361:PRO:O	2.04	0.57
1:A:244:MET:HE1	1:B:449:LYS:HA	1.86	0.57
1:A:349:LEU:HD12	1:A:363:LEU:CD2	2.34	0.57
1:B:5:TYR:CE2	1:B:184:ILE:HG23	2.39	0.57
1:B:113:GLU:HB2	1:D:117:ARG:NH2	2.19	0.57
1:B:164:ILE:HD12	1:B:174:ILE:HG21	1.87	0.57
1:D:231:SER:HA	2:D:4476[B]:NAP:H2D	1.87	0.57
1:B:234:ILE:O	1:B:238:ILE:HG12	2.04	0.57
1:D:176:PHE:CZ	1:D:178:PRO:HB3	2.40	0.57
1:D:248:MET:HE1	1:D:454:ILE:N	2.20	0.57
1:A:268:THR:O	1:A:272:ILE:HG12	2.05	0.57
1:A:414:PHE:CZ	1:D:415:PRO:HG3	2.39	0.57
1:B:45:VAL:HG21	1:B:206:ILE:CD1	2.35	0.56
1:D:350:THR:HG22	1:D:351:GLU:N	2.20	0.56
1:D:436:GLN:HE21	1:D:438:GLY:HA3	1.69	0.56
1:A:350:THR:HB	1:A:362:ILE:HD12	1.88	0.56
1:B:284[B]:CYS:SG	2:B:2476[B]:NAP:O3D	2.59	0.56
1:A:85:ILE:HG13	1:A:188:LEU:HD11	1.88	0.55
1:A:118:MET:HB2	4:A:1555:HOH:O	2.07	0.55
1:C:46:TYR:O	1:C:50:LYS:HG2	2.06	0.55
1:C:176:PHE:CZ	1:C:178:PRO:HB3	2.41	0.55
1:B:230:GLY:O	2:B:2476[B]:NAP:H3D	2.07	0.55
1:D:439:THR:HG22	1:D:441:ASN:OD1	2.06	0.55
1:A:304:ILE:HG22	1:A:363:LEU:HD22	1.88	0.55
1:B:107:ILE:HD12	1:B:158:ASN:HD21	1.70	0.55
1:D:350:THR:HB	1:D:362:ILE:HA	1.90	0.54
1:C:136:ILE:HD11	1:C:472:PHE:CZ	2.41	0.54
1:A:439:THR:CG2	1:A:441:ASN:OD1	2.54	0.54
1:D:248:MET:O	1:D:249:LEU:HD23	2.07	0.54
1:C:244:MET:HE1	1:D:449:LYS:HA	1.90	0.54
1:B:69:HIS:ND1	1:B:109:ASN:ND2	2.55	0.54
1:B:236:GLU:HG3	4:B:2592:HOH:O	2.07	0.54
1:D:284[B]:CYS:HB2	3:D:800:G3H:C1	2.37	0.54
1:D:406:GLN:HG2	1:D:428:THR:HB	1.90	0.54
1:B:393:GLU:HG2	1:B:397:ILE:HD13	1.90	0.53
1:D:361:PRO:HA	1:D:381:PRO:HB2	1.90	0.53
1:A:284[B]:CYS:H	3:A:800:G3H:C1	2.21	0.53
1:D:288:LYS:HE2	1:D:377:GLU:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:MET:HA	1:A:41:GLU:OE2	2.08	0.53
1:A:328:THR:HA	1:A:357:ASN:OD1	2.09	0.53
1:C:41:GLU:O	1:C:45:VAL:HG23	2.09	0.53
1:B:22:ILE:HD12	1:B:22:ILE:N	2.23	0.53
1:B:104:THR:O	1:B:108:ILE:HG13	2.09	0.53
1:C:418:PHE:O	1:C:422:GLU:HG3	2.08	0.53
1:B:256:SER:HA	1:B:289:ARG:HG3	1.91	0.53
1:A:418:PHE:O	1:A:422:GLU:HG3	2.08	0.53
1:C:445:LEU:HD23	1:C:445:LEU:H	1.73	0.53
1:D:37:MET:SD	1:D:206:ILE:HA	2.48	0.53
1:A:301:VAL:HG13	1:A:349:LEU:CD1	2.39	0.53
4:A:1593:HOH:O	1:B:430:HIS:HD2	1.92	0.53
1:B:304:ILE:O	1:B:308:VAL:HG23	2.09	0.53
1:D:437:ARG:HG3	1:D:444:PHE:CD1	2.44	0.53
1:B:409:ILE:HD13	1:B:429:VAL:HG13	1.91	0.53
1:C:46:TYR:CD1	1:C:146:LEU:HD21	2.44	0.53
1:B:151:SER:O	1:B:179:PRO:HD3	2.10	0.52
1:C:250:ALA:HB2	1:C:455:GLN:NE2	2.25	0.52
1:D:284[B]:CYS:CB	3:D:800:G3H:C1	2.87	0.52
1:C:116:LEU:C	1:C:116:LEU:HD12	2.30	0.52
1:A:301:VAL:HG13	1:A:349:LEU:HD11	1.92	0.52
1:B:437:ARG:HG3	1:B:444:PHE:CG	2.45	0.52
1:B:4:GLN:NE2	1:B:19:GLU:OE1	2.43	0.52
1:B:153:PHE:O	1:B:156:PRO:HD3	2.10	0.51
1:B:236:GLU:OE1	1:B:449:LYS:HE3	2.10	0.51
1:B:284[B]:CYS:H	3:B:800:G3H:C1	2.23	0.51
1:C:258:ILE:N	1:C:258:ILE:HD12	2.25	0.51
1:C:365:ASP:HA	1:C:385:ILE:HB	1.92	0.51
1:A:209:ARG:HG3	1:A:209:ARG:NH1	2.25	0.51
1:C:437:ARG:HB3	3:C:800:G3H:O4P	2.10	0.51
1:C:445:LEU:HD23	1:C:445:LEU:N	2.24	0.51
1:C:475:LYS:HA	1:C:475:LYS:CE	2.39	0.51
1:D:107:ILE:CD1	1:D:158:ASN:HD21	2.18	0.51
1:D:325:LEU:HD12	1:D:331:ALA:HA	1.92	0.51
1:D:164:ILE:HD13	1:D:203:PHE:CE2	2.38	0.51
1:A:373:LEU:HG	1:A:384:PRO:HB3	1.92	0.51
1:C:325:LEU:HD12	1:C:331:ALA:HA	1.93	0.51
1:A:40:GLU:HA	1:A:43:ASP:OD2	2.10	0.51
1:A:153:PHE:CD1	1:A:153:PHE:C	2.84	0.50
1:C:350:THR:HG22	1:C:351:GLU:N	2.27	0.50
1:D:317:GLU:OE1	1:D:317:GLU:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:ALA:O	1:D:164:ILE:HG13	2.11	0.50
1:D:94:TYR:O	1:D:98:VAL:HG23	2.12	0.50
1:B:147:VAL:HB	1:B:174:ILE:CD1	2.38	0.50
1:B:360:CYS:O	1:B:362:ILE:HG22	2.12	0.50
1:C:365:ASP:OD1	1:C:366:LYS:N	2.44	0.50
1:B:244:MET:HG2	4:B:2600:HOH:O	2.12	0.50
1:D:437:ARG:HG3	1:D:444:PHE:CG	2.46	0.50
1:B:284[A]:CYS:H	3:B:800:G3H:C1	2.25	0.50
1:C:402:GLU:HB2	4:C:3495:HOH:O	2.12	0.50
1:A:284[A]:CYS:H	3:A:800:G3H:C1	2.25	0.50
1:B:139:VAL:HG13	1:B:467:VAL:HG13	1.92	0.50
1:B:294:GLU:OE1	1:B:387:ARG:NH1	2.44	0.50
1:C:96:SER:HB2	4:C:3683:HOH:O	2.11	0.50
1:C:334:VAL:HG21	1:C:380:GLY:HA3	1.94	0.50
1:A:300:LEU:O	1:A:304:ILE:HD13	2.12	0.49
1:B:74:ILE:HG21	1:B:192:ALA:HA	1.92	0.49
1:B:214:GLY:O	1:B:217:ILE:HG12	2.12	0.49
4:C:3707:HOH:O	1:D:135:LYS:HE3	2.12	0.49
1:A:147:VAL:HB	1:A:174:ILE:HD13	1.94	0.49
1:B:409:ILE:HD12	1:B:409:ILE:N	2.27	0.49
1:C:174:ILE:CG2	1:C:175:ALA:N	2.74	0.49
1:A:100:GLU:HG3	1:A:158:ASN:HB2	1.94	0.49
1:A:218:VAL:HG21	2:A:1476[B]:NAP:H2A	1.93	0.49
1:D:174:ILE:CG2	1:D:175:ALA:N	2.75	0.49
1:D:359:ILE:HD12	1:D:359:ILE:N	2.27	0.49
1:A:475:LYS:HG2	1:C:415:PRO:CB	2.42	0.49
1:B:6:LYS:HG2	1:B:15:LEU:HG	1.94	0.49
1:D:322:ILE:N	1:D:322:ILE:HD12	2.27	0.49
1:D:438:GLY:O	1:D:439:THR:HB	2.12	0.49
1:A:439:THR:HG22	1:A:439:THR:O	2.12	0.49
1:D:37:MET:HA	1:D:41:GLU:OE2	2.13	0.49
1:B:255:ASP:HB2	1:B:286:ALA:O	2.11	0.49
1:B:4:GLN:HG2	1:B:33:SER:OG	2.12	0.49
1:C:248:MET:HE3	1:C:455:GLN:HA	1.94	0.49
1:D:312:THR:O	1:D:320:ALA:HB1	2.13	0.49
1:B:325:LEU:HD12	1:B:331:ALA:HA	1.95	0.49
1:C:263:ALA:HB2	1:C:410:PHE:O	2.12	0.49
1:C:346:ALA:CB	1:C:371:MET:HE1	2.39	0.49
1:B:439:THR:CG2	1:B:441:ASN:OD1	2.57	0.48
1:D:129:GLU:OE2	1:D:131:ALA:HB3	2.13	0.48
1:B:60:SER:HB3	1:C:133:LYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:ILE:HG23	1:D:327:ASP:N	2.27	0.48
1:A:365:ASP:OD1	1:A:366:LYS:N	2.46	0.48
1:B:116:LEU:HD12	1:B:116:LEU:C	2.33	0.48
1:B:152:PRO:HD3	1:B:229:THR:HB	1.95	0.48
1:C:69:HIS:ND1	1:C:109:ASN:ND2	2.61	0.48
1:A:228:PHE:CZ	2:A:1476[B]:NAP:H52A	2.49	0.48
1:A:46:TYR:CD1	1:A:146:LEU:HD21	2.49	0.48
1:B:53:GLN:HG3	4:B:2521:HOH:O	2.13	0.48
1:D:103:ARG:NH1	4:D:4536:HOH:O	2.45	0.48
1:D:323:THR:HB	1:D:324:PRO:CD	2.43	0.48
1:A:408:SER:OG	1:A:435:THR:HG23	2.13	0.48
1:A:475:LYS:HG2	1:C:415:PRO:HB3	1.95	0.48
1:B:227:ASN:HA	1:B:248:MET:HB3	1.96	0.48
1:B:409:ILE:HG22	1:B:411:THR:HG22	1.95	0.48
1:C:284[B]:CYS:H	3:C:800:G3H:C1	2.27	0.48
1:D:104:THR:O	1:D:108:ILE:HG13	2.14	0.48
1:D:234:ILE:O	1:D:238:ILE:HG12	2.14	0.48
1:C:213:ILE:O	1:C:217:ILE:HG23	2.14	0.48
4:C:3654:HOH:O	1:D:430:HIS:HD2	1.96	0.48
1:D:136:ILE:HD11	1:D:472:PHE:CZ	2.49	0.48
1:D:134:LYS:HE3	1:D:474:ILE:HB	1.96	0.48
1:A:455:GLN:NE2	4:A:1548:HOH:O	2.47	0.48
1:B:164:ILE:CD1	1:B:174:ILE:HG12	2.38	0.48
1:C:153:PHE:O	1:C:156:PRO:HD3	2.13	0.48
1:C:244:MET:CE	1:D:449:LYS:HA	2.43	0.48
1:D:315:ASN:HB3	1:D:316:PRO:HD2	1.95	0.47
1:B:312:THR:O	1:B:313:ILE:HD13	2.14	0.47
1:C:188:LEU:O	1:C:191:GLU:HB2	2.14	0.47
1:B:335:GLU:HA	1:B:338:ILE:HD12	1.96	0.47
1:C:262:ASP:O	1:C:412:ASN:ND2	2.47	0.47
1:D:115:GLY:HA3	1:D:169:ILE:HG12	1.95	0.47
1:B:153:PHE:HD2	2:B:2476[B]:NAP:O1N	1.97	0.47
1:D:284[B]:CYS:H	3:D:800:G3H:C1	2.27	0.47
1:C:260:LEU:HD22	1:C:391:VAL:HG22	1.97	0.47
1:C:392:GLU:O	1:C:396:GLU:HG3	2.14	0.47
1:D:225:PHE:CD2	1:D:246:PRO:HB2	2.50	0.47
1:B:45:VAL:HG21	1:B:206:ILE:HD13	1.96	0.47
1:B:415:PRO:HB2	1:D:475:LYS:HG2	1.96	0.47
1:C:85:ILE:HD12	1:C:188:LEU:HD11	1.96	0.47
1:A:3:LYS:NZ	4:A:1549:HOH:O	2.35	0.47
1:B:45:VAL:HG21	1:B:206:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:LYS:HB2	4:B:2533:HOH:O	2.15	0.47
1:C:177:LYS:O	1:C:177:LYS:HG3	2.15	0.47
1:B:46:TYR:O	1:B:50:LYS:HG2	2.15	0.46
1:B:228:PHE:HE1	2:B:2476[B]:NAP:H52A	1.78	0.46
1:B:377:GLU:O	2:B:2476[B]:NAP:N7N	2.48	0.46
1:A:139:VAL:HG13	1:A:467:VAL:CG1	2.45	0.46
1:A:155:TYR:CB	1:A:159:LEU:HD22	2.43	0.46
1:B:5:TYR:O	1:B:35:PRO:HD3	2.15	0.46
1:A:267:LEU:C	1:A:267:LEU:HD23	2.36	0.46
1:B:94:TYR:O	1:B:98:VAL:HG23	2.15	0.46
1:B:409:ILE:HD11	1:B:424:LEU:HD11	1.98	0.46
1:C:166:PRO:O	1:C:169:ILE:HG22	2.15	0.46
1:D:227:ASN:C	1:D:227:ASN:HD22	2.19	0.46
1:D:439:THR:CG2	1:D:441:ASN:OD1	2.63	0.46
1:B:257:ALA:HB2	1:B:287:VAL:HG13	1.96	0.46
1:A:449:LYS:HD2	4:A:1659:HOH:O	2.14	0.46
1:B:159:LEU:HD11	1:B:437:ARG:NH2	2.31	0.46
1:C:228:PHE:CE1	2:C:3476[B]:NAP:H52A	2.50	0.46
1:A:186:GLY:O	1:A:189:LEU:HB3	2.16	0.46
1:B:273:ILE:HG13	1:B:307:LYS:CB	2.46	0.46
1:D:60:SER:HG	1:D:63:GLU:HG3	1.79	0.46
1:D:116:LEU:HD12	1:D:117:ARG:HG3	1.98	0.46
1:D:376:GLU:O	1:D:378:PRO:HD3	2.15	0.46
1:A:362:ILE:HD12	1:A:363:LEU:H	1.81	0.46
1:D:159:LEU:HD11	1:D:437:ARG:CZ	2.45	0.46
1:A:118:MET:CB	4:A:1555:HOH:O	2.63	0.46
1:A:315:ASN:HB3	1:A:317:GLU:OE1	2.15	0.46
1:C:284[A]:CYS:H	3:C:800:G3H:C1	2.29	0.46
1:D:232:THR:O	1:D:236:GLU:HG2	2.15	0.46
1:B:456:GLY:O	1:B:457:VAL:C	2.54	0.45
1:B:415:PRO:HG3	1:C:414:PHE:CE2	2.51	0.45
1:A:228:PHE:CZ	1:A:230:GLY:HA3	2.51	0.45
1:B:49:ALA:HA	1:B:201:GLY:O	2.15	0.45
1:B:210:GLY:O	1:B:214:GLY:HA3	2.16	0.45
1:D:103:ARG:NH1	1:D:440:ASP:OD2	2.50	0.45
1:A:228:PHE:CE1	2:A:1476[B]:NAP:H52A	2.51	0.45
1:D:230:GLY:HA2	2:D:4476[B]:NAP:C5D	2.42	0.45
1:A:136:ILE:HD11	1:A:472:PHE:CZ	2.52	0.45
1:A:142:GLU:CD	1:A:468:LYS:HB2	2.36	0.45
1:A:170:ALA:HB1	1:A:465:THR:CG2	2.46	0.45
1:A:393:GLU:HG2	1:A:397:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LYS:O	1:B:177:LYS:HG3	2.17	0.45
1:B:365:ASP:OD1	1:B:366:LYS:N	2.48	0.45
1:B:440:ASP:HA	4:B:2505:HOH:O	2.17	0.45
1:C:215:ASP:O	1:C:219:GLU:HG3	2.17	0.45
1:D:260:LEU:HB3	4:D:4628:HOH:O	2.16	0.45
1:A:449:LYS:HE3	4:A:1507:HOH:O	2.16	0.45
1:A:46:TYR:O	1:A:50:LYS:HG2	2.17	0.45
1:A:273:ILE:HD11	1:A:308:VAL:HG23	1.98	0.45
1:A:147:VAL:HG22	1:A:225:PHE:HB3	1.99	0.45
1:B:117:ARG:HH22	1:D:113:GLU:HB2	1.81	0.45
1:B:155:TYR:CB	1:B:159:LEU:HD13	2.47	0.45
1:B:302:GLU:OE2	1:B:305:ARG:NH1	2.50	0.45
1:C:139:VAL:HG13	1:C:467:VAL:HG13	1.99	0.45
1:D:69:HIS:ND1	1:D:109:ASN:ND2	2.64	0.45
1:B:408:SER:C	1:B:409:ILE:HD12	2.38	0.45
1:C:121:GLU:OE1	1:D:458:LYS:NZ	2.44	0.45
1:D:100:GLU:HG3	1:D:158:ASN:HB2	1.98	0.45
1:A:322:ILE:HD12	1:A:322:ILE:N	2.32	0.44
1:B:98:VAL:O	1:B:102:VAL:HG23	2.17	0.44
1:B:228:PHE:CZ	2:B:2476[B]:NAP:H52A	2.52	0.44
1:D:367:VAL:HG21	1:D:384:PRO:CB	2.47	0.44
1:A:153:PHE:O	1:A:156:PRO:HD3	2.17	0.44
1:B:218:VAL:CG2	2:B:2476[B]:NAP:H2A	2.47	0.44
1:D:82:ILE:HD12	1:D:188:LEU:HB3	1.98	0.44
1:D:228:PHE:CE1	2:D:4476[B]:NAP:H52A	2.52	0.44
1:C:326:ILE:HG23	1:C:327:ASP:N	2.32	0.44
1:D:297:ALA:HB3	1:D:387:ARG:NH1	2.31	0.44
1:C:231:SER:HA	2:C:3476[B]:NAP:H2D	2.00	0.44
1:C:273:ILE:HG13	1:C:307:LYS:HB2	1.99	0.44
1:D:283:ARG:HG2	3:D:800:G3H:H32	1.98	0.44
1:D:297:ALA:O	1:D:301:VAL:HG23	2.17	0.44
1:A:283:ARG:HD3	4:A:1527:HOH:O	2.18	0.44
1:C:24:GLU:HG2	1:C:88:LYS:HB3	2.00	0.44
1:D:260:LEU:HD22	1:D:391:VAL:HG22	2.00	0.44
1:A:178:PRO:HD2	1:A:206:ILE:O	2.17	0.44
1:A:445:LEU:N	1:A:445:LEU:HD23	2.32	0.44
1:B:408:SER:OG	1:B:435:THR:HG23	2.18	0.44
1:C:153:PHE:CD1	1:C:153:PHE:C	2.90	0.44
1:C:322:ILE:HG13	1:C:361:PRO:HD3	1.99	0.44
1:D:177:LYS:HE2	1:D:208:GLY:O	2.17	0.44
1:C:187:LEU:HD23	1:C:187:LEU:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ILE:O	1:D:217:ILE:HG23	2.18	0.44
1:D:311:LEU:HD13	1:D:322:ILE:HD11	1.98	0.44
1:A:128:PHE:HB2	1:B:441:ASN:OD1	2.18	0.44
1:A:146:LEU:HD23	1:A:222:ALA:O	2.18	0.44
1:D:360:CYS:O	1:D:362:ILE:HG22	2.18	0.44
1:D:331:ALA:HB1	1:D:359:ILE:HD11	2.00	0.43
1:D:439:THR:O	1:D:442:PHE:HB2	2.17	0.43
1:A:335:GLU:OE1	1:A:354:ARG:HD3	2.18	0.43
1:C:346:ALA:H	1:C:371:MET:HE3	1.83	0.43
1:D:102:VAL:O	1:D:106:GLU:HG3	2.18	0.43
1:A:124:GLU:HB3	4:A:1503:HOH:O	2.19	0.43
1:A:188:LEU:O	1:A:191:GLU:HB2	2.18	0.43
1:C:209:ARG:NH1	4:C:3643:HOH:O	2.41	0.43
1:D:89:GLU:CD	1:D:182:GLY:HA2	2.39	0.43
1:D:395:ILE:CD1	1:D:420:ILE:HG23	2.49	0.43
1:B:39:THR:HB	1:B:216:TYR:CZ	2.54	0.43
1:B:109:ASN:HD22	1:B:109:ASN:HA	1.72	0.43
1:C:89:GLU:CD	1:C:182:GLY:HA2	2.38	0.43
1:C:248:MET:HE1	1:C:454:ILE:O	2.18	0.43
1:C:314:GLY:O	1:C:324:PRO:HD3	2.19	0.43
1:A:116:LEU:C	1:A:116:LEU:HD12	2.38	0.43
1:B:414:PHE:CZ	1:C:415:PRO:HG3	2.52	0.43
1:D:20:ILE:O	1:D:33:SER:HA	2.18	0.43
1:D:159:LEU:HA	1:D:159:LEU:HD12	1.82	0.43
1:D:456:GLY:O	1:D:457:VAL:C	2.55	0.43
1:A:411:THR:OG1	1:A:412:ASN:N	2.49	0.43
1:C:234:ILE:O	1:C:238:ILE:HG12	2.18	0.43
1:D:157:VAL:HG13	1:D:189:LEU:HD22	2.00	0.43
1:D:410:PHE:HA	1:D:432:ASN:OD1	2.19	0.43
1:A:167:ALA:O	1:A:172:ASN:HB2	2.19	0.43
1:A:218:VAL:HG21	2:A:1476[A]:NAP:H2A	2.01	0.43
1:B:209:ARG:HH11	1:B:209:ARG:CG	2.25	0.43
1:C:408:SER:HB3	1:C:410:PHE:CE1	2.53	0.43
1:C:7:ASN:OD1	1:C:207:THR:HG23	2.18	0.43
1:D:152:PRO:O	1:D:179:PRO:HG3	2.19	0.43
1:B:2:THR:HB	1:B:30:GLU:OE2	2.19	0.42
1:B:20:ILE:HD13	1:B:209:ARG:HG2	2.01	0.42
1:B:176:PHE:CZ	1:B:178:PRO:HB3	2.54	0.42
1:D:230:GLY:O	2:D:4476[B]:NAP:H3D	2.19	0.42
1:C:107:ILE:HG21	1:C:162:SER:HA	2.00	0.42
1:C:209:ARG:NH1	1:C:209:ARG:CG	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ILE:HG22	1:A:274:ALA:N	2.33	0.42
1:A:376:GLU:HA	4:A:1583:HOH:O	2.19	0.42
1:B:322:ILE:HG12	1:B:361:PRO:HD3	2.01	0.42
1:B:437:ARG:HB2	3:B:800:G3H:O3P	2.19	0.42
1:A:128:PHE:CE2	1:B:440:ASP:HB2	2.53	0.42
1:A:333:TYR:CD1	2:A:1476[A]:NAP:H4N	2.53	0.42
1:A:350:THR:HG22	1:A:351:GLU:H	1.84	0.42
1:A:146:LEU:HA	1:A:173:VAL:HG23	2.02	0.42
1:B:151:SER:HB2	1:B:152:PRO:HD2	2.01	0.42
1:D:155:TYR:HB2	1:D:159:LEU:HD22	2.00	0.42
1:A:118:MET:HE1	1:A:461:ILE:HB	2.02	0.42
1:B:359:ILE:N	1:B:359:ILE:CD1	2.83	0.42
1:C:153:PHE:HA	1:C:179:PRO:HG3	2.01	0.42
1:D:330:SER:O	1:D:334:VAL:HG23	2.20	0.42
1:A:443:PRO:HD3	1:B:123:LEU:HD12	2.02	0.42
1:A:214:GLY:O	1:A:217:ILE:HG12	2.20	0.42
1:A:215:ASP:OD1	1:A:237:ARG:NH2	2.53	0.42
1:B:438:GLY:O	1:B:439:THR:HB	2.20	0.42
1:D:255:ASP:HB2	1:D:286:ALA:O	2.20	0.42
1:A:260:LEU:HD22	1:A:391:VAL:HG22	2.02	0.42
1:C:313:ILE:HD12	1:C:313:ILE:N	2.35	0.42
1:D:284[A]:CYS:H	3:D:800:G3H:C1	2.33	0.42
1:A:111:ALA:HA	1:A:457:VAL:CG1	2.50	0.41
1:A:152:PRO:HG3	1:A:159:LEU:HD23	2.02	0.41
1:A:338:ILE:HG23	1:A:364:PHE:CE1	2.55	0.41
1:C:209:ARG:HG3	1:C:209:ARG:NH1	2.30	0.41
1:C:349:LEU:HD12	1:C:363:LEU:HG	2.01	0.41
1:B:153:PHE:CD1	1:B:153:PHE:C	2.93	0.41
1:B:416:ARG:O	1:B:420:ILE:HG13	2.20	0.41
1:C:349:LEU:HD11	1:C:365:ASP:HB2	2.02	0.41
1:C:370:ASP:HB2	4:C:3501:HOH:O	2.20	0.41
1:D:169:ILE:HG23	1:D:170:ALA:N	2.35	0.41
1:D:288:LYS:CE	1:D:377:GLU:HG3	2.49	0.41
1:A:69:HIS:HA	1:A:109:ASN:ND2	2.35	0.41
1:B:25:PRO:HB2	1:B:91:ALA:HB2	2.01	0.41
1:C:162:SER:O	1:C:166:PRO:HG2	2.19	0.41
1:C:399:ASN:CG	1:C:425:GLU:HG3	2.41	0.41
1:A:94:TYR:O	1:A:97:ALA:HB3	2.21	0.41
1:A:117:ARG:HG3	1:A:117:ARG:HH11	1.84	0.41
1:A:361:PRO:HA	1:A:381:PRO:HB2	2.03	0.41
1:C:248:MET:CE	1:C:454:ILE:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ARG:O	1:D:68:LEU:HG	2.20	0.41
1:D:153:PHE:HD2	2:D:4476[B]:NAP:O1N	2.04	0.41
1:D:224:ASN:O	1:D:246:PRO:HD2	2.19	0.41
1:B:218:VAL:HG21	2:B:2476[B]:NAP:H2A	2.03	0.41
1:B:273:ILE:HG13	1:B:307:LYS:HB2	2.02	0.41
1:A:146:LEU:HD23	1:A:222:ALA:C	2.41	0.41
1:B:92:LYS:O	1:B:93:GLY:C	2.59	0.41
1:A:248:MET:HE3	1:A:454:ILE:O	2.21	0.41
1:A:474:ILE:HG23	1:C:418:PHE:HB3	2.03	0.41
1:C:283:ARG:HG2	3:C:800:G3H:H32	2.02	0.41
1:D:256:SER:HA	1:D:289:ARG:HG3	2.03	0.41
1:A:304:ILE:N	1:A:304:ILE:HD12	2.35	0.41
1:A:445:LEU:HD23	1:A:445:LEU:H	1.86	0.41
1:C:255:ASP:HB2	1:C:286:ALA:O	2.21	0.41
1:C:270:LYS:HE3	1:C:270:LYS:HB2	1.88	0.41
1:D:178:PRO:HD2	1:D:206:ILE:O	2.20	0.41
1:D:180:THR:HA	1:D:183:SER:OG	2.21	0.41
1:B:376:GLU:O	1:B:378:PRO:HD3	2.21	0.41
1:D:377:GLU:O	2:D:4476[B]:NAP:N7N	2.54	0.41
1:B:117:ARG:HH11	1:B:117:ARG:HG3	1.86	0.40
1:B:265:LEU:HD11	1:B:296:VAL:HB	2.02	0.40
1:C:174:ILE:HG23	1:C:175:ALA:N	2.36	0.40
1:D:60:SER:OG	1:D:63:GLU:HG3	2.21	0.40
1:A:190:ALA:HB2	1:A:205:THR:HG21	2.03	0.40
1:B:209:ARG:HG3	1:B:209:ARG:NH1	2.31	0.40
2:C:3476[A]:NAP:H8A	2:C:3476[A]:NAP:H2B	1.95	0.40
1:D:210:GLY:O	1:D:214:GLY:HA3	2.21	0.40
1:A:288:LYS:HD3	1:A:378:PRO:HD2	2.03	0.40
1:A:414:PHE:HB2	1:D:414:PHE:CB	2.51	0.40
1:B:227:ASN:HD22	1:B:227:ASN:C	2.25	0.40
1:B:313:ILE:HD13	1:B:322:ILE:HB	2.02	0.40
1:B:368:THR:C	1:B:370:ASP:H	2.24	0.40
1:B:410:PHE:HA	1:B:432:ASN:OD1	2.21	0.40
1:D:129:GLU:O	1:D:129:GLU:HG3	2.21	0.40
1:D:218:VAL:HG21	2:D:4476[B]:NAP:H2A	2.04	0.40
1:D:294:GLU:OE2	1:D:387:ARG:HD3	2.21	0.40
1:A:438:GLY:O	1:A:439:THR:HB	2.22	0.40
1:B:100:GLU:HG3	1:B:158:ASN:HB2	2.04	0.40
1:D:311:LEU:HA	1:D:321:ASP:OD1	2.21	0.40
1:A:177:LYS:O	1:A:177:LYS:HG3	2.22	0.40
1:A:350:THR:HG22	1:A:351:GLU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:PHE:O	1:B:422:GLU:HG3	2.21	0.40
1:C:368:THR:C	1:C:370:ASP:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	473/475 (100%)	452 (96%)	19 (4%)	2 (0%)	34	46
1	B	473/475 (100%)	452 (96%)	19 (4%)	2 (0%)	34	46
1	C	473/475 (100%)	453 (96%)	18 (4%)	2 (0%)	34	46
1	D	473/475 (100%)	443 (94%)	27 (6%)	3 (1%)	25	34
All	All	1892/1900 (100%)	1800 (95%)	83 (4%)	9 (0%)	29	40

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	438	GLY
1	B	438	GLY
1	C	438	GLY
1	D	438	GLY
1	D	457	VAL
1	B	457	VAL
1	C	457	VAL
1	A	457	VAL
1	D	378	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	378/378 (100%)	364 (96%)	14 (4%)	34	46
1	B	378/378 (100%)	366 (97%)	12 (3%)	39	53
1	C	378/378 (100%)	365 (97%)	13 (3%)	37	50
1	D	378/378 (100%)	363 (96%)	15 (4%)	31	43
All	All	1512/1512 (100%)	1458 (96%)	54 (4%)	35	47

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	70	LYS
1	A	80	GLU
1	A	99	SER
1	A	119	GLU
1	A	152	PRO
1	A	153	PHE
1	A	159	LEU
1	A	227	ASN
1	A	248	MET
1	A	370	ASP
1	A	379	PHE
1	A	411	THR
1	A	434	LYS
1	B	31	LEU
1	B	62	ILE
1	B	121	GLU
1	B	227	ASN
1	B	312	THR
1	B	342	ASN
1	B	355	GLU
1	B	362	ILE
1	B	379	PHE
1	B	418	PHE

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Mol	Chain	Res	Type
1	B	439	THR
1	B	467	VAL
1	C	116	LEU
1	C	121	GLU
1	C	141	ARG
1	C	152	PRO
1	C	159	LEU
1	C	227	ASN
1	C	248	MET
1	C	355	GLU
1	C	369	THR
1	C	379	PHE
1	C	402	GLU
1	C	408	SER
1	C	475	LYS
1	D	2	THR
1	D	80	GLU
1	D	121	GLU
1	D	141	ARG
1	D	159	LEU
1	D	227	ASN
1	D	248	MET
1	D	267	LEU
1	D	283	ARG
1	D	342	ASN
1	D	362	ILE
1	D	379	PHE
1	D	418	PHE
1	D	462	GLU
1	D	467	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	227	ASN
1	A	315	ASN
1	A	436	GLN
1	A	455	GLN
1	B	4	GLN
1	B	109	ASN
1	B	158	ASN

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Mol	Chain	Res	Type
1	B	227	ASN
1	B	315	ASN
1	B	342	ASN
1	B	430	HIS
1	B	433	ASN
1	C	109	ASN
1	C	227	ASN
1	C	315	ASN
1	C	342	ASN
1	C	430	HIS
1	C	436	GLN
1	C	455	GLN
1	D	109	ASN
1	D	158	ASN
1	D	227	ASN
1	D	315	ASN
1	D	342	ASN
1	D	430	HIS
1	D	455	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAP	C	3476[B]	1	45,52,52	2.19	11 (24%)	56,80,80	1.58	12 (21%)
3	G3H	D	800	1	8,9,9	1.53	1 (12%)	10,12,12	1.78	3 (30%)
2	NAP	A	1476[A]	-	45,52,52	2.14	13 (28%)	56,80,80	1.51	12 (21%)
2	NAP	A	1476[B]	-	45,52,52	2.16	11 (24%)	56,80,80	1.54	11 (19%)
3	G3H	A	800	1	8,9,9	1.56	1 (12%)	10,12,12	1.75	3 (30%)
3	G3H	B	800	1	8,9,9	1.50	1 (12%)	10,12,12	1.74	3 (30%)
2	NAP	D	4476[A]	-	45,52,52	2.11	11 (24%)	56,80,80	1.50	11 (19%)
2	NAP	B	2476[A]	-	45,52,52	2.09	11 (24%)	56,80,80	1.52	11 (19%)
2	NAP	C	3476[A]	-	45,52,52	2.06	11 (24%)	56,80,80	1.54	12 (21%)
2	NAP	B	2476[B]	-	45,52,52	2.13	11 (24%)	56,80,80	1.50	10 (17%)
3	G3H	C	800	1	8,9,9	1.64	1 (12%)	10,12,12	1.78	3 (30%)
2	NAP	D	4476[B]	-	45,52,52	2.15	11 (24%)	56,80,80	1.53	11 (19%)

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	3476[B]	1	-	4/31/67/67	0/5/5/5
3	G3H	D	800	1	-	3/7/8/8	-
2	NAP	A	1476[A]	-	-	7/31/67/67	0/5/5/5
2	NAP	A	1476[B]	-	-	8/31/67/67	0/5/5/5
3	G3H	A	800	1	-	2/7/8/8	-
3	G3H	B	800	1	-	0/7/8/8	-
2	NAP	D	4476[A]	-	-	9/31/67/67	0/5/5/5
2	NAP	B	2476[A]	-	-	9/31/67/67	0/5/5/5
2	NAP	C	3476[A]	-	-	11/31/67/67	0/5/5/5
2	NAP	B	2476[B]	-	-	4/31/67/67	0/5/5/5
3	G3H	C	800	1	-	3/7/8/8	-
2	NAP	D	4476[B]	-	-	7/31/67/67	0/5/5/5

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1476[A]	NAP	C2N-N1N	7.12	1.43	1.35
2	C	3476[B]	NAP	C2N-N1N	6.96	1.43	1.35
2	A	1476[B]	NAP	C2N-N1N	6.94	1.43	1.35
2	D	4476[B]	NAP	C2N-N1N	6.91	1.43	1.35
2	D	4476[A]	NAP	C2N-N1N	6.67	1.43	1.35
2	B	2476[B]	NAP	C2N-N1N	6.61	1.43	1.35
2	B	2476[A]	NAP	C2N-N1N	6.60	1.43	1.35
2	C	3476[A]	NAP	C2N-N1N	6.31	1.42	1.35
2	A	1476[A]	NAP	C4N-C3N	5.00	1.47	1.39
2	B	2476[B]	NAP	C4N-C3N	4.86	1.47	1.39
2	C	3476[A]	NAP	C4N-C3N	4.79	1.47	1.39
2	D	4476[A]	NAP	C4N-C3N	4.77	1.47	1.39
2	D	4476[B]	NAP	C4N-C3N	4.77	1.47	1.39
2	C	3476[B]	NAP	C4N-C3N	4.76	1.47	1.39
2	A	1476[B]	NAP	C4N-C3N	4.76	1.47	1.39
2	B	2476[A]	NAP	C4N-C3N	4.66	1.47	1.39
2	C	3476[B]	NAP	C2D-C1D	-4.57	1.46	1.53
2	C	3476[B]	NAP	O4D-C1D	4.46	1.47	1.41
2	D	4476[A]	NAP	O4D-C1D	4.46	1.47	1.41
2	B	2476[A]	NAP	C2A-N3A	4.40	1.39	1.32
2	B	2476[A]	NAP	O4D-C1D	4.35	1.47	1.41
2	A	1476[B]	NAP	O4D-C1D	4.33	1.47	1.41
2	B	2476[B]	NAP	C2D-C1D	-4.32	1.47	1.53
2	B	2476[B]	NAP	C2A-N3A	4.32	1.39	1.32
2	A	1476[B]	NAP	C2A-N3A	4.24	1.38	1.32
2	D	4476[B]	NAP	C2A-N3A	4.24	1.38	1.32
2	D	4476[B]	NAP	O4D-C1D	4.23	1.47	1.41
2	D	4476[A]	NAP	C2A-N3A	4.22	1.38	1.32
2	A	1476[A]	NAP	O4D-C1D	4.22	1.47	1.41
2	A	1476[A]	NAP	C2A-N3A	4.22	1.38	1.32
2	C	3476[A]	NAP	O4D-C1D	4.14	1.46	1.41
3	C	800	G3H	C3-C2	4.13	1.57	1.51
2	A	1476[B]	NAP	C2D-C1D	-4.09	1.47	1.53
2	B	2476[B]	NAP	O4D-C1D	4.06	1.46	1.41
2	D	4476[B]	NAP	C2D-C1D	-4.03	1.47	1.53
2	C	3476[A]	NAP	C2A-N3A	4.02	1.38	1.32
2	C	3476[B]	NAP	C2A-N3A	3.98	1.38	1.32
2	D	4476[B]	NAP	C2A-N1A	3.94	1.41	1.33
2	D	4476[A]	NAP	C2A-N1A	3.91	1.41	1.33
2	A	1476[A]	NAP	C2A-N1A	3.91	1.41	1.33
2	B	2476[B]	NAP	C2A-N1A	3.90	1.41	1.33
3	A	800	G3H	C3-C2	3.89	1.57	1.51
2	C	3476[B]	NAP	C2A-N1A	3.87	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1476[B]	NAP	C2A-N1A	3.87	1.41	1.33
3	D	800	G3H	C3-C2	3.84	1.56	1.51
2	B	2476[A]	NAP	C2A-N1A	3.84	1.41	1.33
2	C	3476[A]	NAP	C2A-N1A	3.83	1.41	1.33
2	D	4476[B]	NAP	C6N-N1N	3.78	1.44	1.35
3	B	800	G3H	C3-C2	3.76	1.56	1.51
2	A	1476[B]	NAP	C6N-N1N	3.75	1.44	1.35
2	B	2476[B]	NAP	C6N-N1N	3.74	1.44	1.35
2	D	4476[A]	NAP	C6N-N1N	3.74	1.44	1.35
2	B	2476[A]	NAP	C6N-N1N	3.73	1.44	1.35
2	C	3476[A]	NAP	C6N-N1N	3.68	1.44	1.35
2	C	3476[B]	NAP	C6N-N1N	3.60	1.44	1.35
2	C	3476[A]	NAP	C2D-C1D	-3.48	1.48	1.53
2	A	1476[A]	NAP	C6N-N1N	3.32	1.43	1.35
2	D	4476[A]	NAP	C2D-C1D	-3.26	1.48	1.53
2	B	2476[A]	NAP	C2D-C1D	-3.12	1.49	1.53
2	A	1476[A]	NAP	C3N-C7N	2.88	1.54	1.50
2	A	1476[A]	NAP	C2D-C1D	-2.79	1.49	1.53
2	D	4476[B]	NAP	PA-O1A	-2.76	1.41	1.50
2	A	1476[B]	NAP	PA-O1A	-2.73	1.41	1.50
2	C	3476[B]	NAP	PA-O1A	-2.72	1.41	1.50
2	C	3476[A]	NAP	PA-O1A	-2.71	1.41	1.50
2	A	1476[A]	NAP	PA-O1A	-2.70	1.41	1.50
2	B	2476[A]	NAP	PA-O1A	-2.67	1.41	1.50
2	D	4476[A]	NAP	PA-O1A	-2.61	1.41	1.50
2	A	1476[B]	NAP	P2B-O2B	2.61	1.64	1.59
2	B	2476[B]	NAP	PA-O1A	-2.60	1.41	1.50
2	C	3476[B]	NAP	P2B-O2B	2.58	1.64	1.59
2	B	2476[A]	NAP	P2B-O2B	2.58	1.64	1.59
2	D	4476[B]	NAP	P2B-O2B	2.56	1.64	1.59
2	A	1476[A]	NAP	P2B-O2B	2.55	1.64	1.59
2	D	4476[A]	NAP	P2B-O2B	2.54	1.64	1.59
2	D	4476[B]	NAP	C4A-N3A	2.52	1.39	1.35
2	B	2476[A]	NAP	C4A-N3A	2.46	1.39	1.35
2	B	2476[B]	NAP	P2B-O2B	2.46	1.64	1.59
2	C	3476[A]	NAP	P2B-O2B	2.45	1.63	1.59
2	A	1476[A]	NAP	C4A-N3A	2.45	1.39	1.35
2	D	4476[A]	NAP	C4A-N3A	2.44	1.39	1.35
2	A	1476[B]	NAP	C3N-C7N	2.43	1.54	1.50
2	B	2476[B]	NAP	C4A-N3A	2.36	1.38	1.35
2	C	3476[B]	NAP	C3N-C7N	2.36	1.54	1.50
2	D	4476[A]	NAP	C3N-C7N	2.36	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2476[A]	NAP	C3N-C7N	2.33	1.54	1.50
2	C	3476[A]	NAP	C3N-C7N	2.30	1.54	1.50
2	D	4476[B]	NAP	C3N-C7N	2.28	1.54	1.50
2	A	1476[B]	NAP	C4A-N3A	2.26	1.38	1.35
2	C	3476[A]	NAP	C4A-N3A	2.25	1.38	1.35
2	B	2476[B]	NAP	C3N-C7N	2.10	1.53	1.50
2	C	3476[B]	NAP	C4A-N3A	2.08	1.38	1.35
2	A	1476[A]	NAP	C5N-C4N	2.05	1.43	1.38
2	A	1476[A]	NAP	C6N-C5N	2.01	1.43	1.38

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3476[B]	NAP	C5A-C6A-N6A	4.51	127.21	120.35
2	C	3476[A]	NAP	C5A-C6A-N6A	4.45	127.11	120.35
2	A	1476[B]	NAP	C5A-C6A-N6A	4.44	127.09	120.35
2	C	3476[B]	NAP	O4B-C4B-C5B	-4.39	94.92	109.37
2	A	1476[A]	NAP	C5A-C6A-N6A	4.37	126.99	120.35
2	D	4476[B]	NAP	C5A-C6A-N6A	4.34	126.95	120.35
2	B	2476[B]	NAP	C5A-C6A-N6A	4.30	126.89	120.35
2	B	2476[A]	NAP	C5A-C6A-N6A	4.29	126.87	120.35
2	D	4476[A]	NAP	C5A-C6A-N6A	4.25	126.82	120.35
2	A	1476[B]	NAP	O4B-C4B-C5B	-3.81	96.82	109.37
2	D	4476[A]	NAP	N3A-C2A-N1A	-3.62	123.03	128.68
2	B	2476[A]	NAP	N3A-C2A-N1A	-3.60	123.05	128.68
2	D	4476[B]	NAP	N3A-C2A-N1A	-3.58	123.08	128.68
2	C	3476[A]	NAP	N3A-C2A-N1A	-3.55	123.12	128.68
2	A	1476[A]	NAP	N3A-C2A-N1A	-3.53	123.16	128.68
2	B	2476[B]	NAP	O4B-C4B-C5B	-3.49	97.88	109.37
2	C	3476[B]	NAP	N3A-C2A-N1A	-3.48	123.25	128.68
2	A	1476[B]	NAP	N3A-C2A-N1A	-3.47	123.25	128.68
2	D	4476[B]	NAP	O4B-C4B-C5B	-3.45	98.04	109.37
2	B	2476[B]	NAP	N3A-C2A-N1A	-3.44	123.31	128.68
2	A	1476[A]	NAP	O4B-C4B-C5B	-3.35	98.36	109.37
2	C	3476[A]	NAP	O4B-C4B-C5B	-3.24	98.73	109.37
3	A	800	G3H	O1P-C3-C2	3.11	116.58	108.33
3	B	800	G3H	O1P-C3-C2	3.11	116.57	108.33
3	D	800	G3H	O1P-C3-C2	3.11	116.56	108.33
3	C	800	G3H	O1P-C3-C2	3.07	116.46	108.33
2	B	2476[A]	NAP	C3N-C7N-N7N	3.00	121.35	117.75
2	B	2476[B]	NAP	C2N-C3N-C4N	2.99	121.65	118.26
2	C	3476[A]	NAP	C3N-C7N-N7N	2.98	121.32	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4476[A]	NAP	C3N-C7N-N7N	2.97	121.32	117.75
2	B	2476[A]	NAP	C2N-C3N-C4N	2.96	121.62	118.26
2	D	4476[B]	NAP	C3N-C7N-N7N	2.94	121.28	117.75
2	D	4476[A]	NAP	O4B-C4B-C5B	-2.94	99.70	109.37
2	C	3476[B]	NAP	C3N-C7N-N7N	2.91	121.25	117.75
2	B	2476[A]	NAP	O4B-C4B-C5B	-2.89	99.86	109.37
2	D	4476[B]	NAP	C2N-C3N-C4N	2.86	121.50	118.26
2	C	3476[B]	NAP	C2N-C3N-C4N	2.84	121.47	118.26
2	A	1476[A]	NAP	C3N-C7N-N7N	2.83	121.14	117.75
2	D	4476[A]	NAP	C2N-C3N-C4N	2.83	121.46	118.26
2	A	1476[B]	NAP	C2N-C3N-C4N	2.81	121.44	118.26
2	C	3476[A]	NAP	C2N-C3N-C4N	2.81	121.44	118.26
3	C	800	G3H	P-O1P-C3	2.80	126.02	118.30
2	B	2476[B]	NAP	O2A-PA-O1A	2.76	125.87	112.24
2	D	4476[B]	NAP	O2A-PA-O1A	2.74	125.79	112.24
2	B	2476[A]	NAP	O2A-PA-O1A	2.71	125.64	112.24
2	A	1476[A]	NAP	O2A-PA-O1A	2.71	125.62	112.24
2	D	4476[A]	NAP	O2A-PA-O1A	2.69	125.55	112.24
2	A	1476[B]	NAP	C3N-C7N-N7N	2.69	120.97	117.75
2	A	1476[B]	NAP	O2A-PA-O1A	2.68	125.51	112.24
2	D	4476[B]	NAP	O7N-C7N-C3N	-2.68	116.42	119.63
3	D	800	G3H	P-O1P-C3	2.67	125.65	118.30
2	B	2476[A]	NAP	O7N-C7N-C3N	-2.64	116.47	119.63
2	C	3476[A]	NAP	O2A-PA-O1A	2.64	125.30	112.24
2	D	4476[A]	NAP	O7N-C7N-C3N	-2.63	116.49	119.63
2	C	3476[B]	NAP	O2A-PA-O1A	2.60	125.07	112.24
3	A	800	G3H	P-O1P-C3	2.59	125.44	118.30
2	B	2476[B]	NAP	C3N-C7N-N7N	2.58	120.84	117.75
3	B	800	G3H	P-O1P-C3	2.54	125.30	118.30
3	D	800	G3H	O3P-P-O1P	2.53	113.46	106.73
2	C	3476[B]	NAP	O7N-C7N-C3N	-2.53	116.61	119.63
3	A	800	G3H	O3P-P-O1P	2.52	113.44	106.73
2	A	1476[B]	NAP	O7N-C7N-C3N	-2.48	116.66	119.63
2	B	2476[B]	NAP	O7N-C7N-C3N	-2.47	116.68	119.63
2	C	3476[A]	NAP	O7N-C7N-C3N	-2.46	116.69	119.63
3	B	800	G3H	O3P-P-O1P	2.44	113.24	106.73
3	C	800	G3H	O3P-P-O1P	2.44	113.22	106.73
2	A	1476[A]	NAP	C2N-C3N-C4N	2.43	121.02	118.26
2	C	3476[B]	NAP	O3B-C3B-C4B	-2.43	104.03	111.05
2	C	3476[B]	NAP	O4B-C1B-C2B	-2.36	102.49	106.59
2	C	3476[B]	NAP	O3X-P2B-O2X	2.35	116.60	107.64
2	C	3476[A]	NAP	O3B-C3B-C4B	-2.33	104.30	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4476[B]	NAP	O3X-P2B-O2X	2.33	116.56	107.64
2	B	2476[A]	NAP	C3N-C2N-N1N	-2.33	118.15	120.43
2	C	3476[A]	NAP	O3X-P2B-O2X	2.32	116.51	107.64
2	A	1476[B]	NAP	O3X-P2B-O2X	2.32	116.50	107.64
2	A	1476[A]	NAP	O3X-P2B-O2X	2.31	116.47	107.64
2	A	1476[B]	NAP	O3B-C3B-C4B	-2.31	104.36	111.05
2	B	2476[B]	NAP	O3X-P2B-O2X	2.30	116.43	107.64
2	D	4476[B]	NAP	C3N-C2N-N1N	-2.29	118.18	120.43
2	D	4476[A]	NAP	O3X-P2B-O2X	2.29	116.40	107.64
2	B	2476[B]	NAP	O3B-C3B-C4B	-2.27	104.47	111.05
2	B	2476[A]	NAP	O3X-P2B-O2X	2.27	116.30	107.64
2	C	3476[A]	NAP	C3N-C2N-N1N	-2.26	118.22	120.43
2	A	1476[A]	NAP	O3B-C3B-C4B	-2.25	104.56	111.05
2	B	2476[A]	NAP	O3B-C3B-C4B	-2.24	104.58	111.05
2	B	2476[B]	NAP	C3N-C2N-N1N	-2.20	118.28	120.43
2	D	4476[B]	NAP	C1B-N9A-C4A	-2.19	122.79	126.64
2	B	2476[A]	NAP	C2B-C3B-C4B	2.18	106.72	101.99
2	D	4476[B]	NAP	O3B-C3B-C4B	-2.18	104.76	111.05
2	C	3476[B]	NAP	C1B-N9A-C4A	-2.15	122.86	126.64
2	D	4476[A]	NAP	C1B-N9A-C4A	-2.15	122.86	126.64
2	D	4476[A]	NAP	O3B-C3B-C4B	-2.14	104.85	111.05
2	C	3476[A]	NAP	C1B-N9A-C4A	-2.14	122.89	126.64
2	A	1476[A]	NAP	O7N-C7N-C3N	-2.13	117.08	119.63
2	A	1476[A]	NAP	C1B-N9A-C4A	-2.12	122.91	126.64
2	A	1476[A]	NAP	C3N-C2N-N1N	-2.11	118.36	120.43
2	A	1476[A]	NAP	C2N-N1N-C1D	2.09	123.80	119.14
2	C	3476[B]	NAP	C3N-C2N-N1N	-2.08	118.40	120.43
2	D	4476[A]	NAP	C3N-C2N-N1N	-2.06	118.41	120.43
2	C	3476[A]	NAP	C2B-C3B-C4B	2.05	106.44	101.99
2	A	1476[B]	NAP	C3N-C2N-N1N	-2.04	118.43	120.43
2	A	1476[B]	NAP	C1B-N9A-C4A	-2.03	123.07	126.64

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1476[B]	NAP	C5D-O5D-PN-O3
2	A	1476[B]	NAP	C5D-O5D-PN-O1N
2	A	1476[B]	NAP	C5D-O5D-PN-O2N
2	B	2476[A]	NAP	C2B-O2B-P2B-O2X
2	B	2476[A]	NAP	O4D-C4D-C5D-O5D
2	B	2476[A]	NAP	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
2	B	2476[B]	NAP	O4D-C4D-C5D-O5D
2	B	2476[B]	NAP	C3D-C4D-C5D-O5D
2	C	3476[A]	NAP	O4D-C4D-C5D-O5D
2	C	3476[A]	NAP	C3D-C4D-C5D-O5D
2	C	3476[A]	NAP	O4D-C1D-N1N-C6N
2	C	3476[B]	NAP	C2B-O2B-P2B-O2X
2	C	3476[B]	NAP	O4D-C4D-C5D-O5D
2	C	3476[B]	NAP	C3D-C4D-C5D-O5D
2	D	4476[A]	NAP	C2B-O2B-P2B-O2X
2	D	4476[A]	NAP	O4D-C4D-C5D-O5D
2	D	4476[A]	NAP	C3D-C4D-C5D-O5D
2	D	4476[B]	NAP	C2B-O2B-P2B-O2X
2	D	4476[B]	NAP	C5D-O5D-PN-O3
2	D	4476[B]	NAP	C3D-C4D-C5D-O5D
3	A	800	G3H	C3-O1P-P-O2P
3	C	800	G3H	C3-O1P-P-O3P
3	C	800	G3H	C3-O1P-P-O4P
3	D	800	G3H	C3-O1P-P-O4P
2	D	4476[B]	NAP	O4D-C4D-C5D-O5D
2	C	3476[A]	NAP	C4D-C5D-O5D-PN
3	C	800	G3H	C3-O1P-P-O2P
3	D	800	G3H	C3-O1P-P-O2P
2	D	4476[A]	NAP	C4D-C5D-O5D-PN
2	B	2476[A]	NAP	C4D-C5D-O5D-PN
3	D	800	G3H	C3-O1P-P-O3P
2	A	1476[A]	NAP	C4D-C5D-O5D-PN
2	C	3476[A]	NAP	C2B-O2B-P2B-O2X
2	C	3476[A]	NAP	C2B-O2B-P2B-O3X
2	C	3476[A]	NAP	PN-O3-PA-O1A
2	D	4476[A]	NAP	PN-O3-PA-O1A
2	D	4476[A]	NAP	PN-O3-PA-O2A
2	A	1476[A]	NAP	C5B-O5B-PA-O2A
2	B	2476[A]	NAP	C5B-O5B-PA-O2A
2	C	3476[A]	NAP	C5B-O5B-PA-O2A
2	D	4476[A]	NAP	C5B-O5B-PA-O2A
2	D	4476[B]	NAP	C5B-O5B-PA-O2A
2	A	1476[B]	NAP	C3D-C4D-C5D-O5D
2	A	1476[A]	NAP	PN-O3-PA-O2A
2	C	3476[A]	NAP	PN-O3-PA-O2A
2	A	1476[B]	NAP	O4D-C4D-C5D-O5D
2	A	1476[A]	NAP	PN-O3-PA-O1A
2	B	2476[B]	NAP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	D	4476[B]	NAP	O4B-C4B-C5B-O5B
3	A	800	G3H	C3-O1P-P-O4P
2	A	1476[A]	NAP	O4B-C4B-C5B-O5B
2	A	1476[B]	NAP	O4B-C4B-C5B-O5B
2	B	2476[A]	NAP	O4B-C4B-C5B-O5B
2	C	3476[A]	NAP	O4B-C4B-C5B-O5B
2	C	3476[B]	NAP	O4B-C4B-C5B-O5B
2	D	4476[A]	NAP	O4B-C4B-C5B-O5B
2	A	1476[A]	NAP	C5B-O5B-PA-O3
2	A	1476[A]	NAP	C2B-O2B-P2B-O3X
2	A	1476[B]	NAP	C2B-O2B-P2B-O3X
2	B	2476[A]	NAP	C5B-O5B-PA-O3
2	B	2476[A]	NAP	C2B-O2B-P2B-O3X
2	B	2476[B]	NAP	C2B-O2B-P2B-O2X
2	C	3476[A]	NAP	C5B-O5B-PA-O3
2	D	4476[A]	NAP	C5B-O5B-PA-O3
2	B	2476[A]	NAP	PN-O3-PA-O2A
2	A	1476[B]	NAP	C5B-O5B-PA-O2A
2	D	4476[B]	NAP	C5D-O5D-PN-O1N

There are no ring outliers.

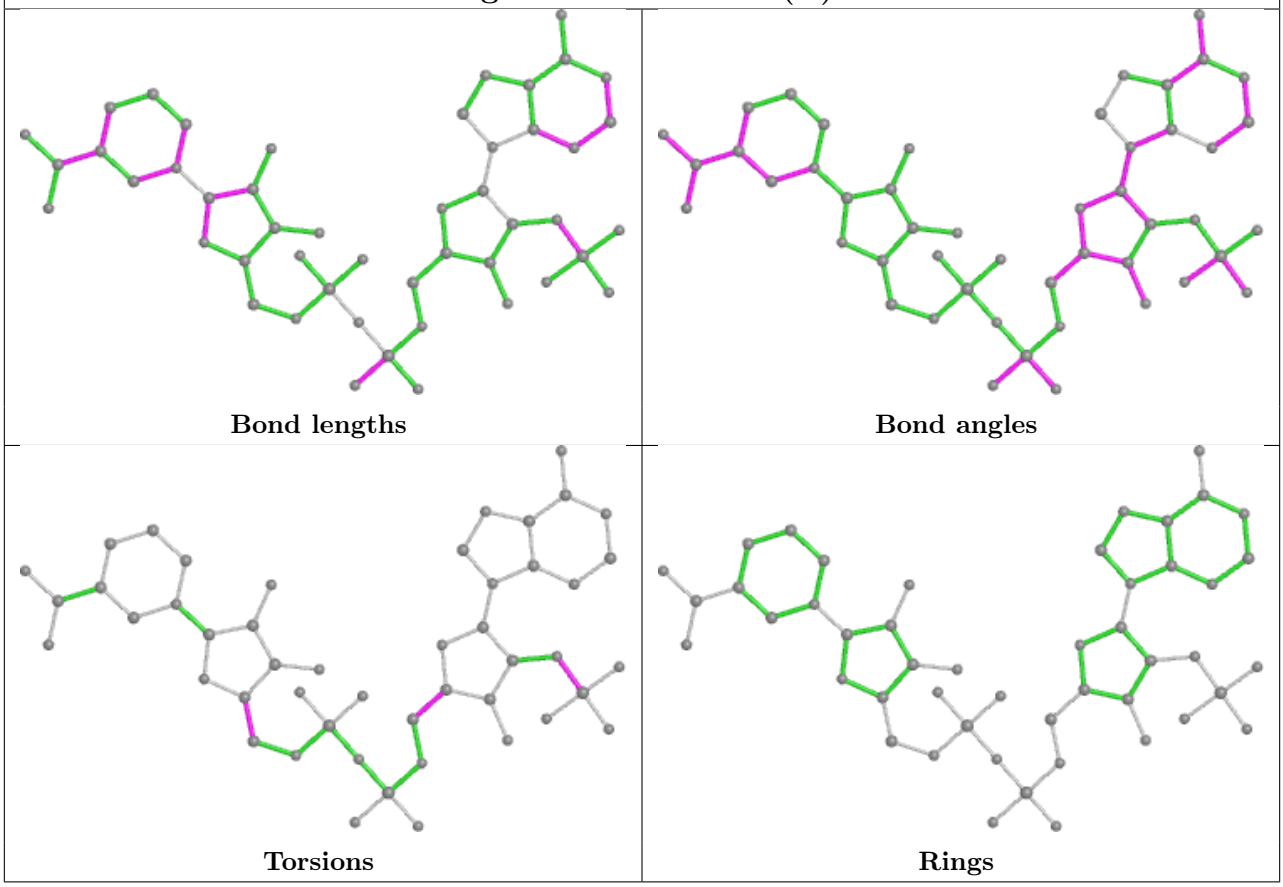
10 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3476[B]	NAP	3	0
3	D	800	G3H	7	0
2	A	1476[A]	NAP	2	0
2	A	1476[B]	NAP	5	0
3	A	800	G3H	6	0
3	B	800	G3H	7	0
2	C	3476[A]	NAP	1	0
2	B	2476[B]	NAP	10	0
3	C	800	G3H	5	0
2	D	4476[B]	NAP	9	0

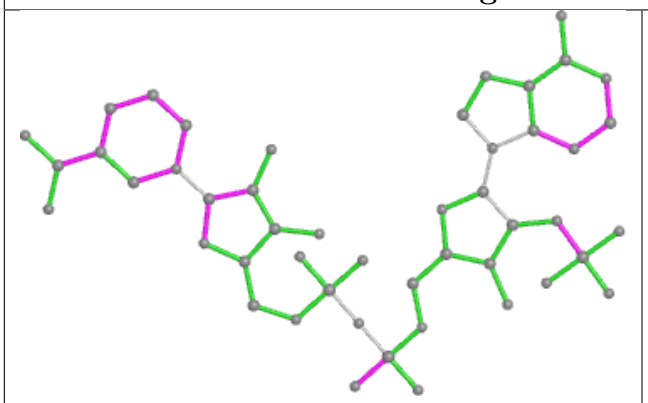
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

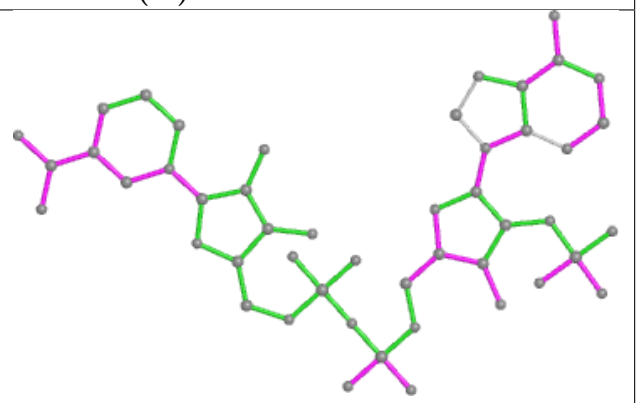
Ligand NAP C 3476 (B)



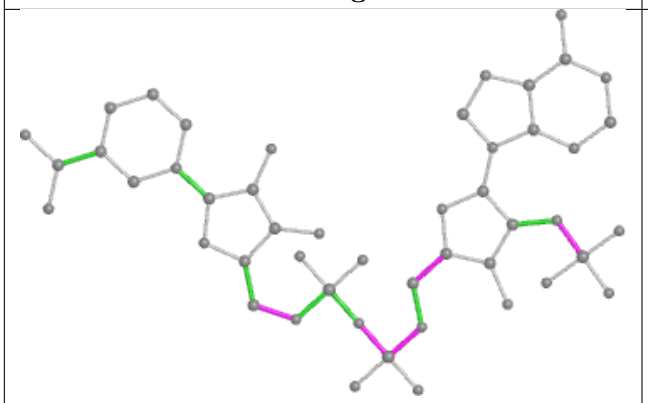
Ligand NAP A 1476 (A)



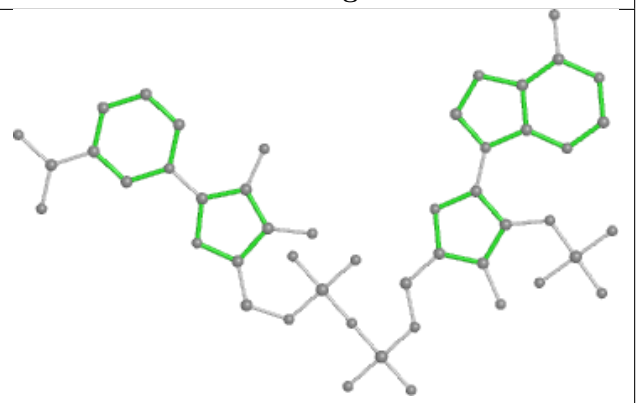
Bond lengths



Bond angles

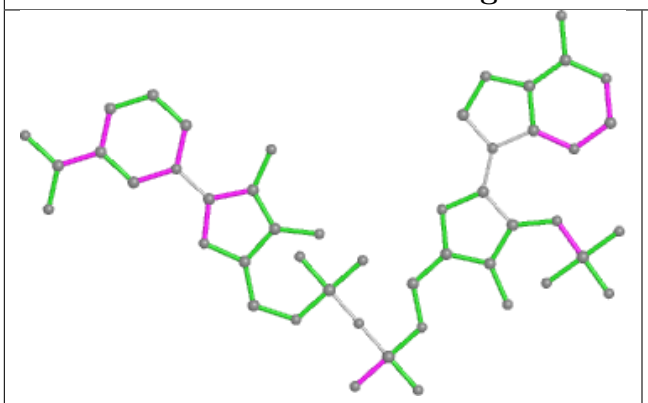


Torsions

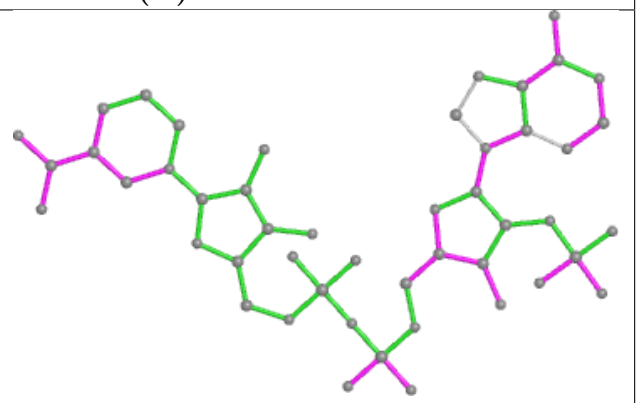


Rings

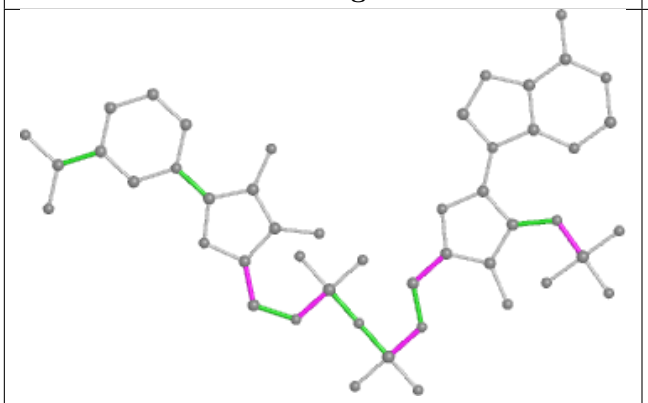
Ligand NAP A 1476 (B)



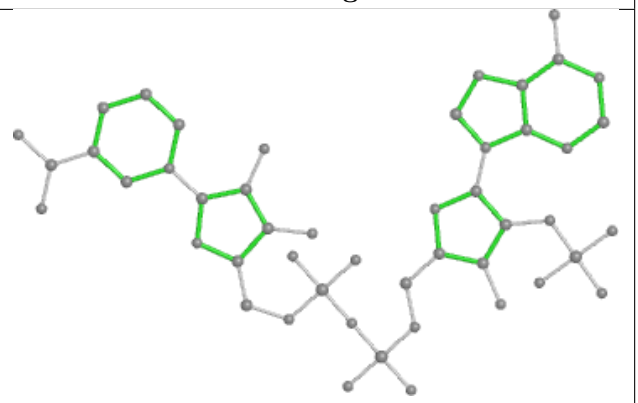
Bond lengths



Bond angles

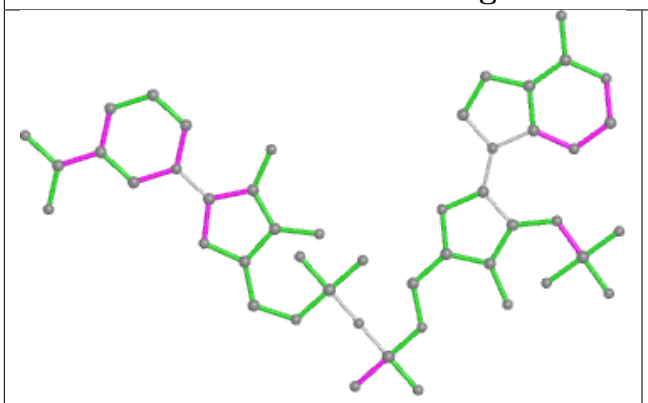


Torsions

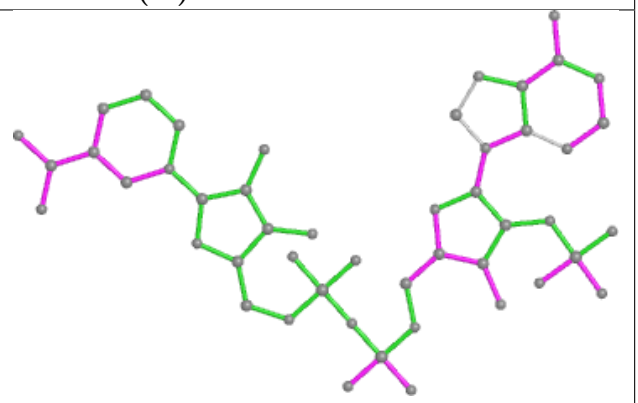


Rings

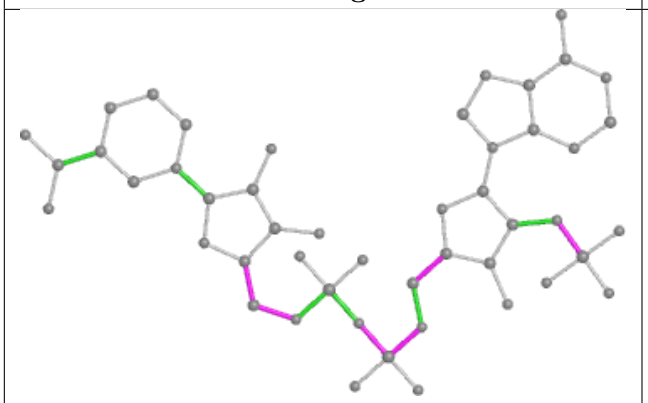
Ligand NAP D 4476 (A)



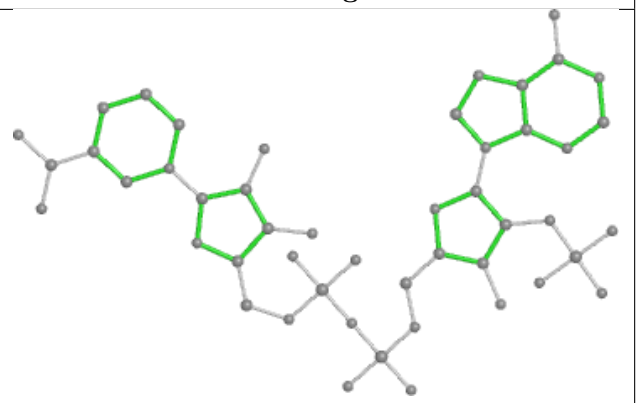
Bond lengths



Bond angles

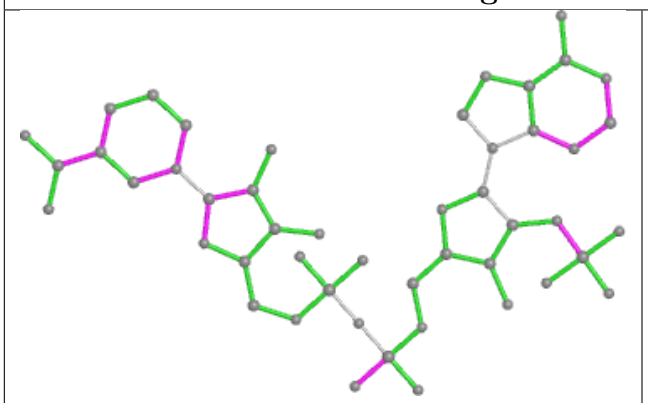


Torsions

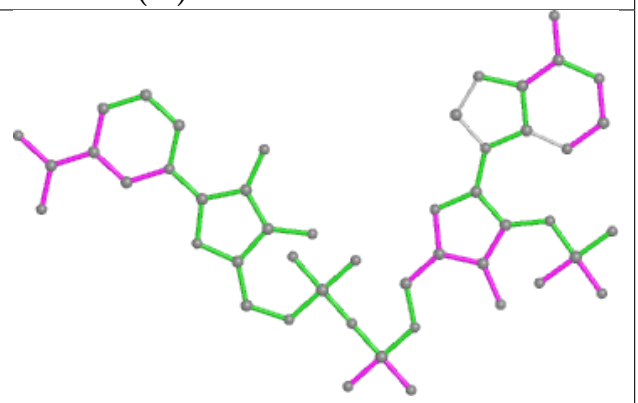


Rings

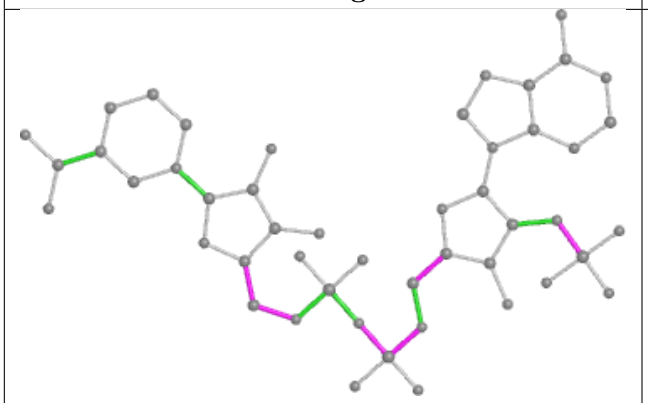
Ligand NAP B 2476 (A)



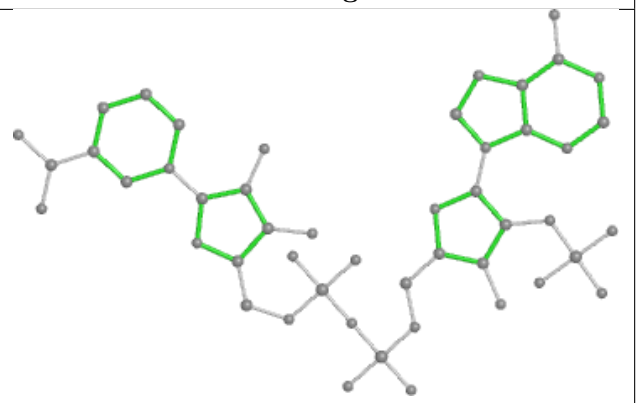
Bond lengths



Bond angles

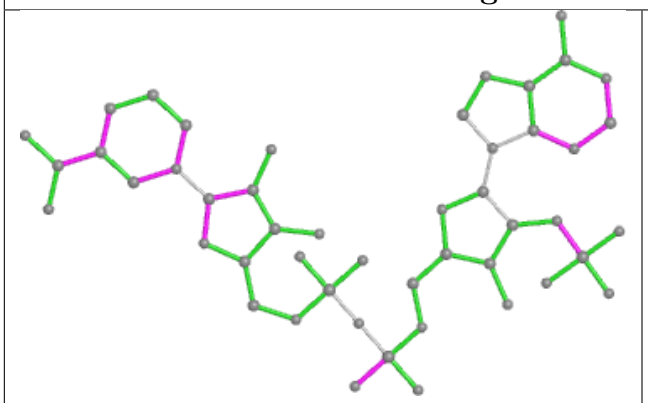


Torsions

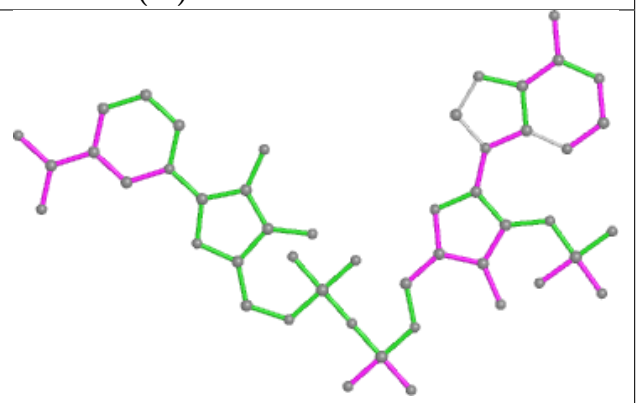


Rings

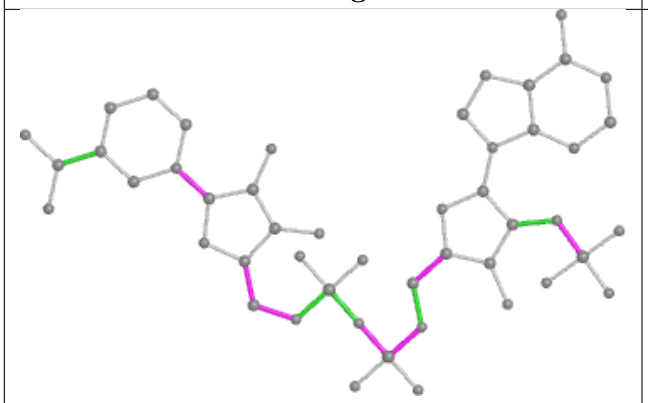
Ligand NAP C 3476 (A)



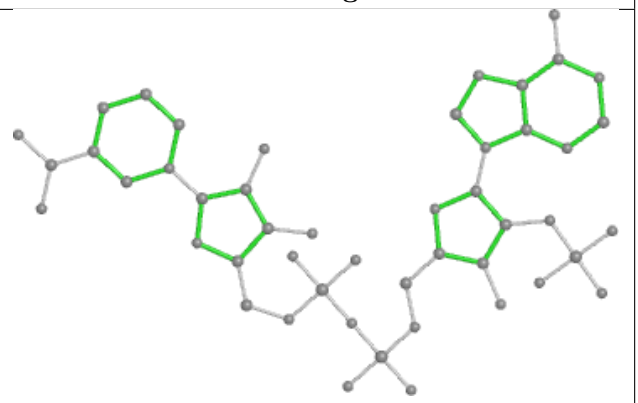
Bond lengths



Bond angles

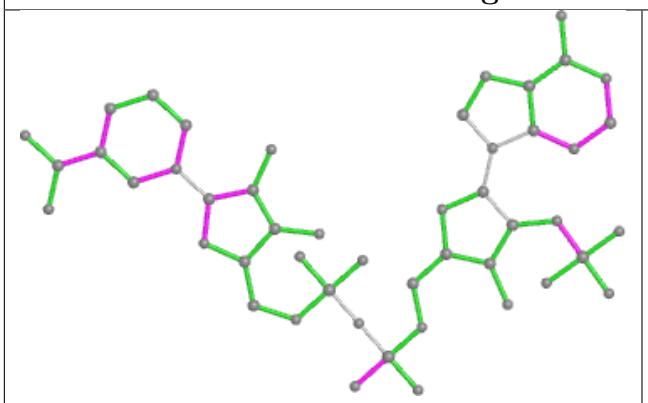


Torsions

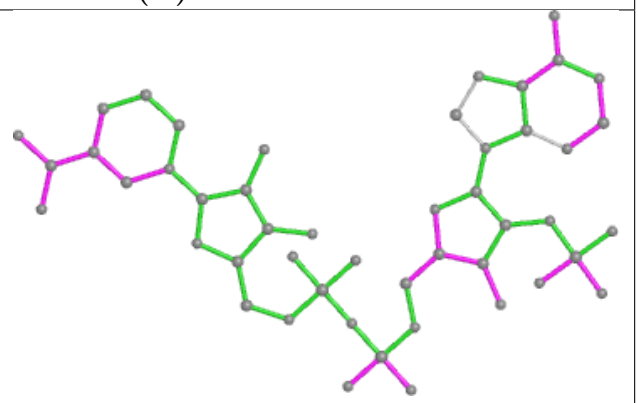


Rings

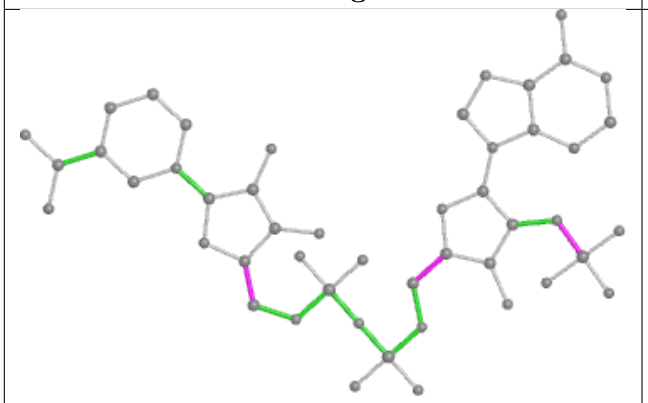
Ligand NAP B 2476 (B)



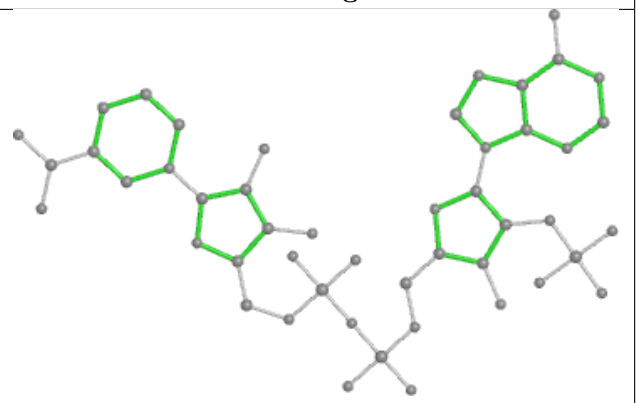
Bond lengths



Bond angles

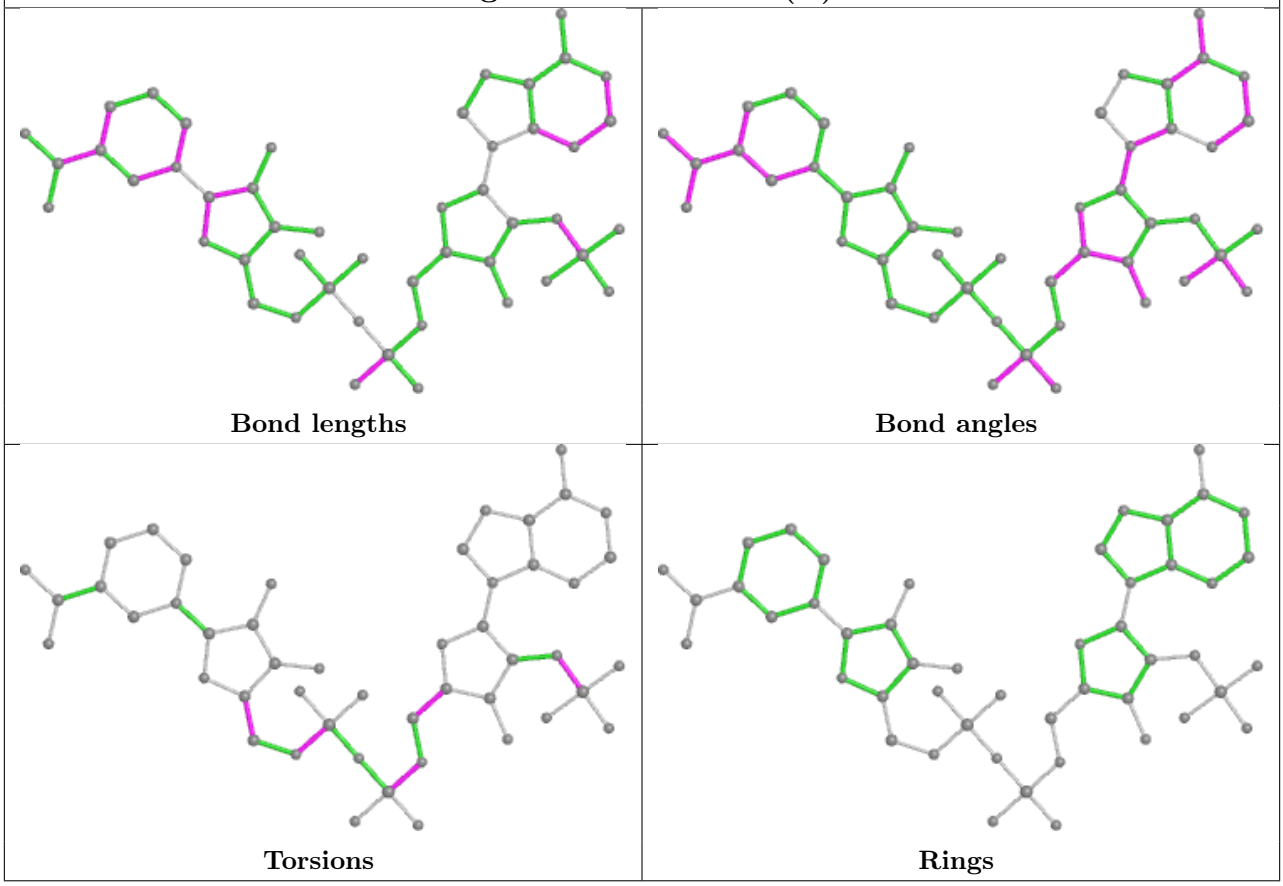


Torsions



Rings

Ligand NAP D 4476 (B)



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	474/475 (99%)	-0.24	6 (1%)	77	82	17, 32, 50, 73	0
1	B	474/475 (99%)	-0.16	10 (2%)	63	70	18, 38, 53, 83	0
1	C	474/475 (99%)	-0.38	5 (1%)	80	85	14, 26, 40, 51	0
1	D	474/475 (99%)	-0.15	9 (1%)	66	73	17, 35, 53, 64	0
All	All	1896/1900 (99%)	-0.23	30 (1%)	72	78	14, 33, 51, 83	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	THR	5.9
1	A	17	GLU	3.1
1	A	2	THR	3.1
1	B	17	GLU	3.0
1	D	95	LYS	2.9
1	C	259	VAL	2.6
1	B	51	LYS	2.6
1	A	400	LYS	2.5
1	D	318	ASP	2.5
1	C	475	LYS	2.5
1	D	343	ASP	2.5
1	B	4	GLN	2.4
1	D	290	VAL	2.4
1	B	95	LYS	2.4
1	B	355	GLU	2.4
1	B	270	LYS	2.3
1	A	29	ALA	2.3
1	D	438	GLY	2.3
1	D	475	LYS	2.2
1	C	438	GLY	2.2
1	A	318	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	12	GLU	2.2
1	B	343	ASP	2.2
1	D	51	LYS	2.2
1	B	346	ALA	2.2
1	D	17	GLU	2.2
1	A	51	LYS	2.1
1	B	3	LYS	2.1
1	C	17	GLU	2.1
1	C	258	ILE	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 monosaccharides in this entry.

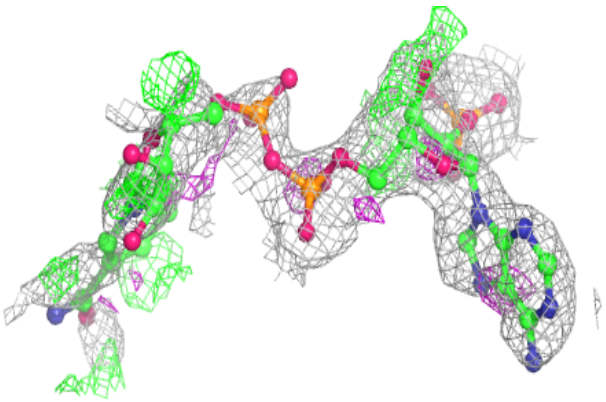
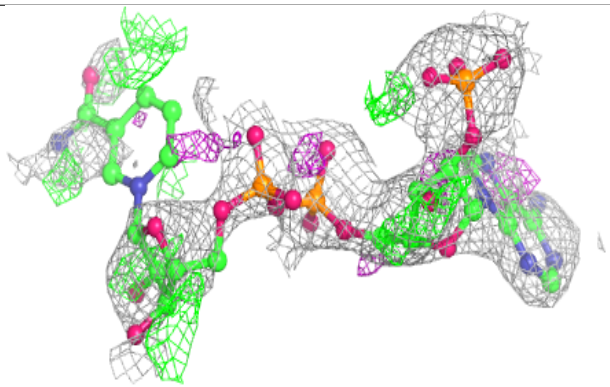
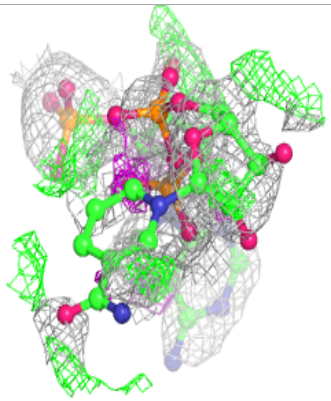
6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	G3H	D	800	10/10	0.73	0.41	42,44,46,46	10
3	G3H	A	800	10/10	0.78	0.44	35,36,38,38	10
3	G3H	B	800	10/10	0.79	0.39	46,48,51,52	10
2	NAP	B	2476[B]	48/48	0.80	0.36	38,50,53,53	48
2	NAP	B	2476[A]	48/48	0.80	0.36	53,56,61,63	48
2	NAP	D	4476[B]	48/48	0.85	0.30	42,47,51,52	48
2	NAP	D	4476[A]	48/48	0.85	0.30	43,52,58,60	48
2	NAP	A	1476[B]	48/48	0.86	0.34	37,43,49,49	48
2	NAP	A	1476[A]	48/48	0.86	0.34	23,33,39,40	48
2	NAP	C	3476[B]	48/48	0.89	0.26	31,38,42,45	48
2	NAP	C	3476[A]	48/48	0.89	0.26	42,46,55,57	48
3	G3H	C	800	10/10	0.92	0.32	25,27,30,30	10

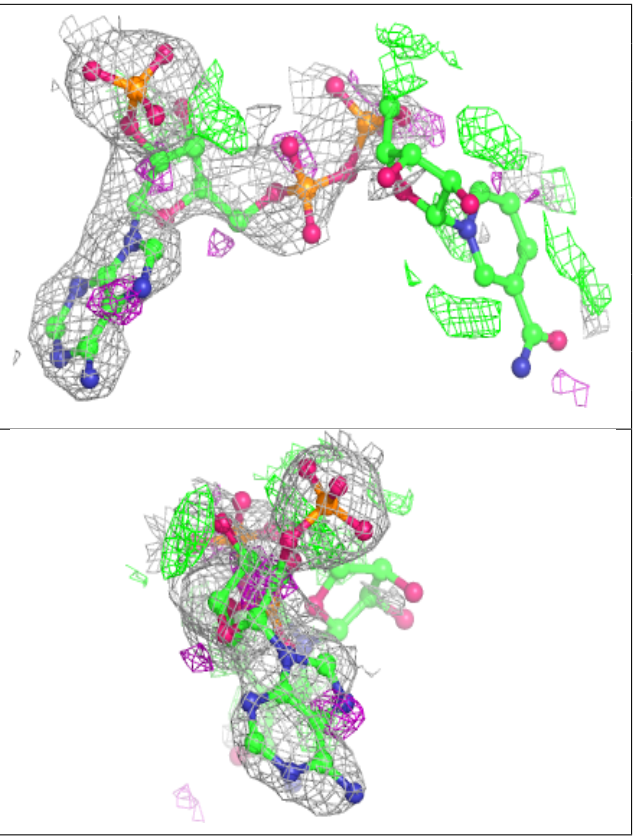
The following is a graphical depiction of the model fit to experimental electron density of all

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 2476 (B): 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

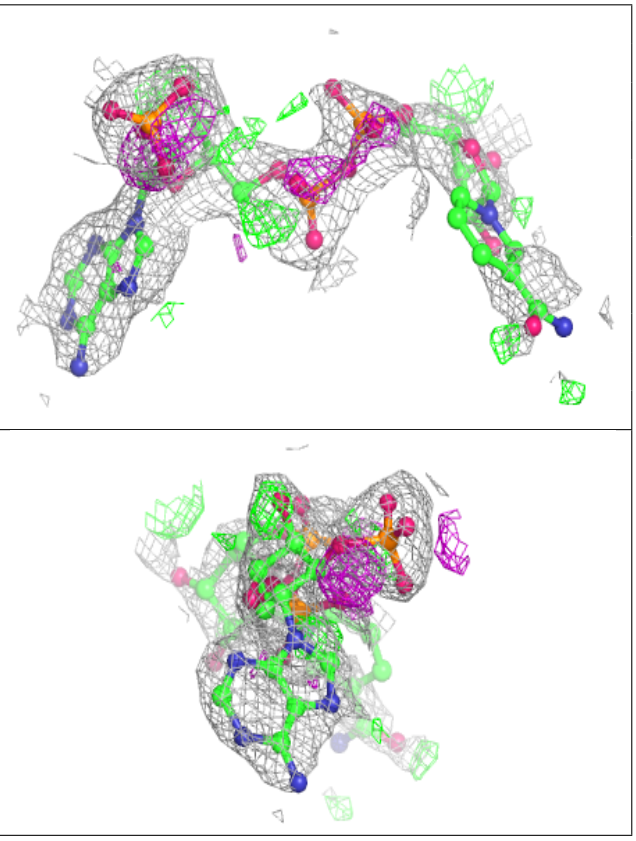
Electron density around NAP B 2476 (A):

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



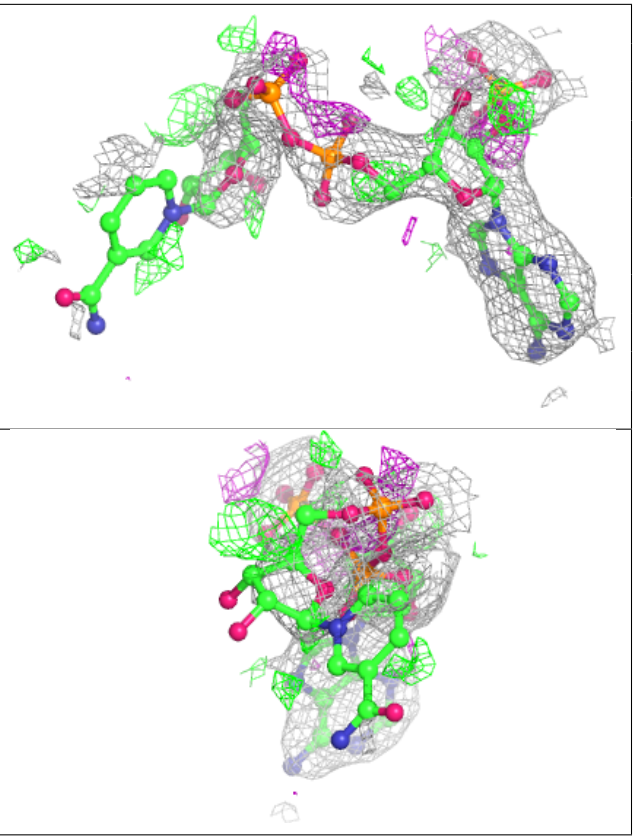
Electron density around NAP D 4476 (B):

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



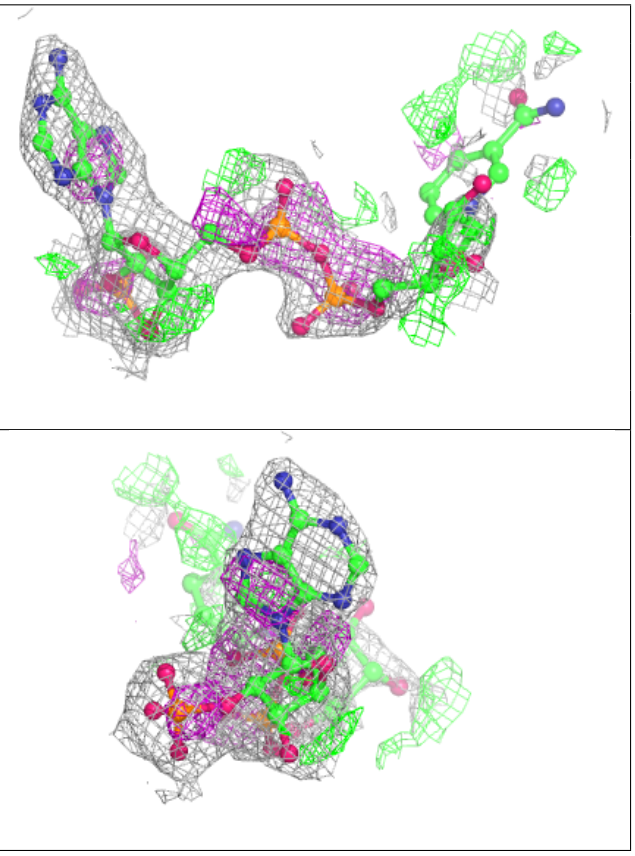
Electron density around NAP D 4476 (A):

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



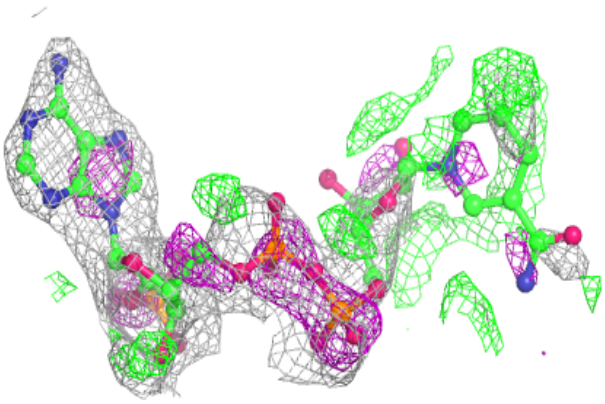
Electron density around NAP A 1476 (B):

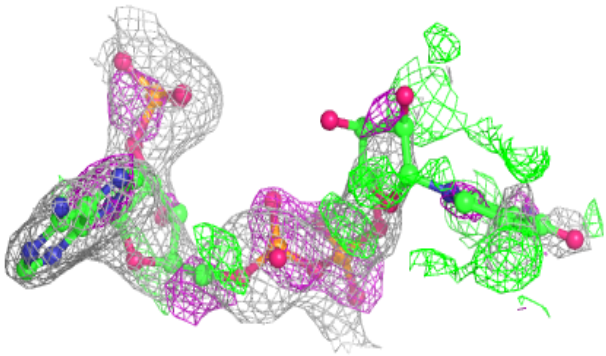
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

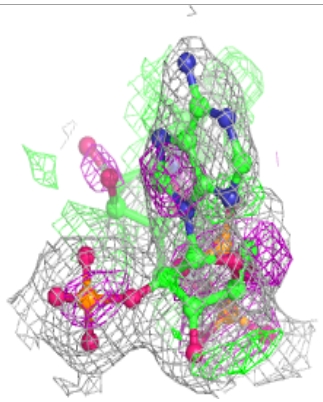


Electron density around NAP A 1476 (A):

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

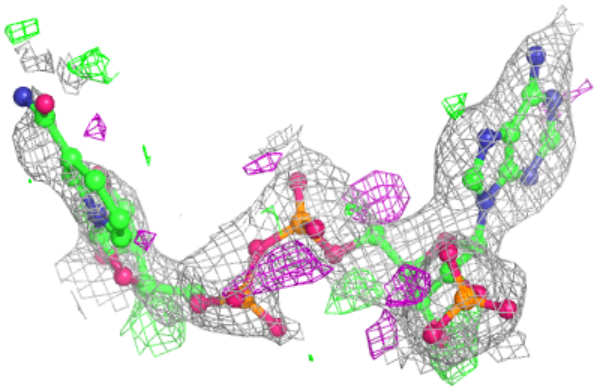


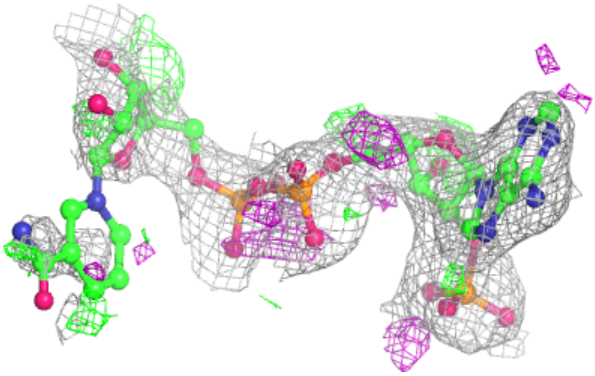


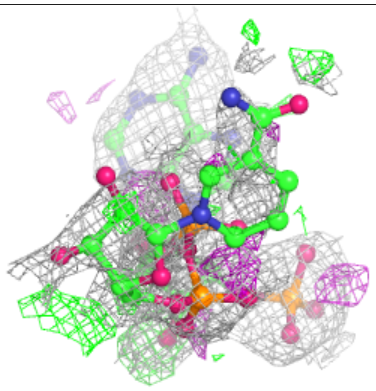


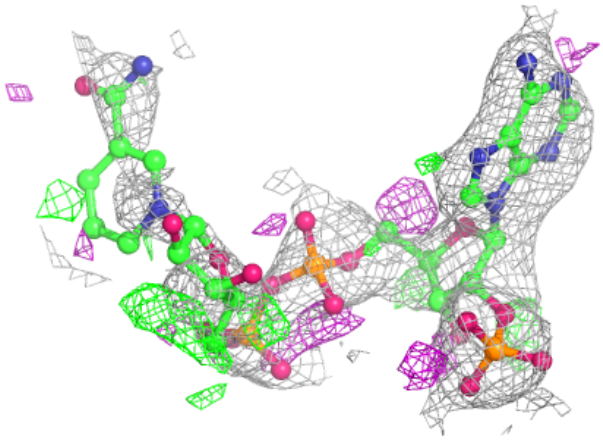
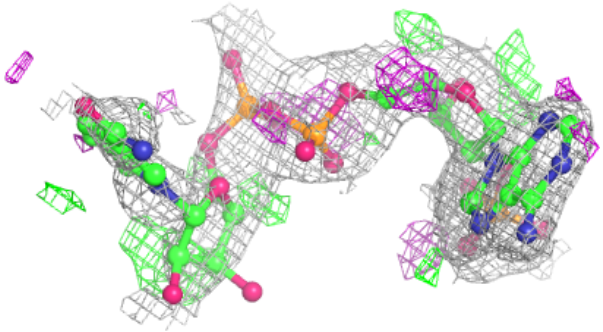
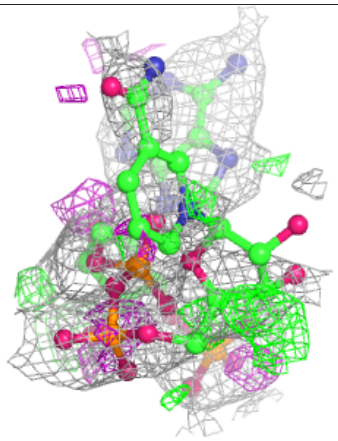
Electron density around NAP C 3476 (B):

$2mF_o$-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 3476 (A): $2mF_o$-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.