



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:32 AM UTC

PDB ID : 2QE0 / pdb_00002qe0
Title : Thioacylenzyme Intermediate of GAPN from S. Mutans, New Data Integration and Refinement.
Authors : Corbier, C.; Didierjean, C.; Bricogne, G.; Branlant, G.; D'Ambrosio, K.; Vonrhein, C.
Deposited on : 2007-06-22
Resolution : 2.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

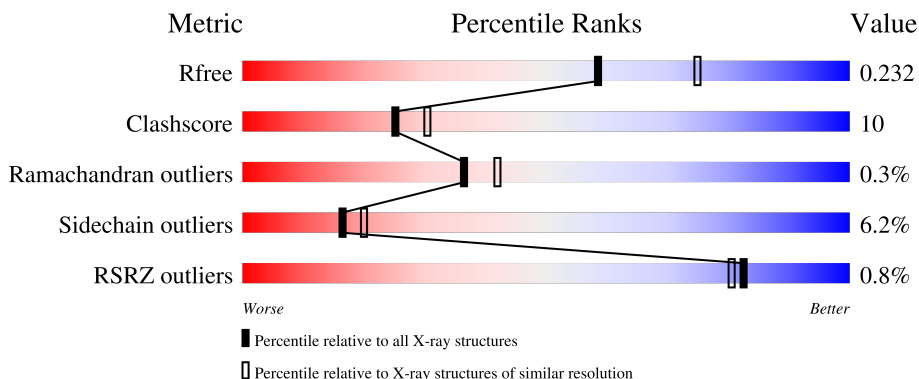
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	475	% 77% 19% .
1	B	475	% 77% 20% .
1	C	475	80% 17% .
1	D	475	% 73% 24% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16008 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.

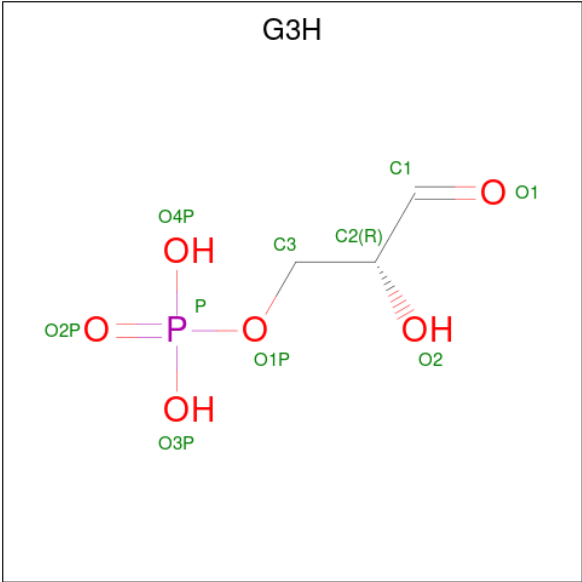
- Molecule 1 is a protein called NADP-dependent glyceraldehyde-3-phosphate dehydrogenase.

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

There are 16 discrepancies between the modelled and reference sequences:

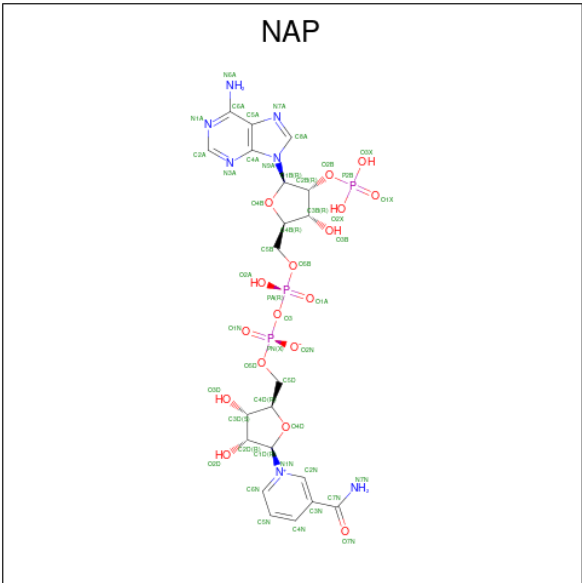
Chain	Residue	Modelled	Actual	Comment	Reference
A	58	ALA	SER	variant	UNP Q59931
A	85	ILE	VAL	variant	UNP Q59931
A	250	ALA	GLU	engineered mutation	UNP Q59931
A	347	THR	ALA	variant	UNP Q59931
B	58	ALA	SER	variant	UNP Q59931
B	85	ILE	VAL	variant	UNP Q59931
B	250	ALA	GLU	engineered mutation	UNP Q59931
B	347	THR	ALA	variant	UNP Q59931
C	58	ALA	SER	variant	UNP Q59931
C	85	ILE	VAL	variant	UNP Q59931
C	250	ALA	GLU	engineered mutation	UNP Q59931
C	347	THR	ALA	variant	UNP Q59931
D	58	ALA	SER	variant	UNP Q59931
D	85	ILE	VAL	variant	UNP Q59931
D	250	ALA	GLU	engineered mutation	UNP Q59931
D	347	THR	ALA	variant	UNP Q59931

- Molecule 2 is GLYCERALDEHYDE-3-PHOSPHATE (CCD ID: G3H) (formula: C₃H₇O₆P).



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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

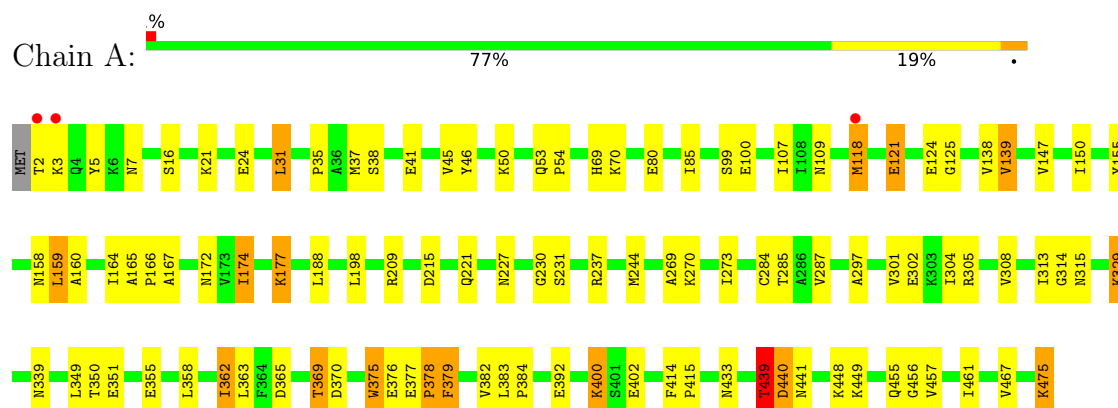
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	368	Total 368	O 368	0	0
4	B	300	Total 300	O 300	0	0
4	C	403	Total 403	O 403	0	0
4	D	313	Total 313	O 313	0	0

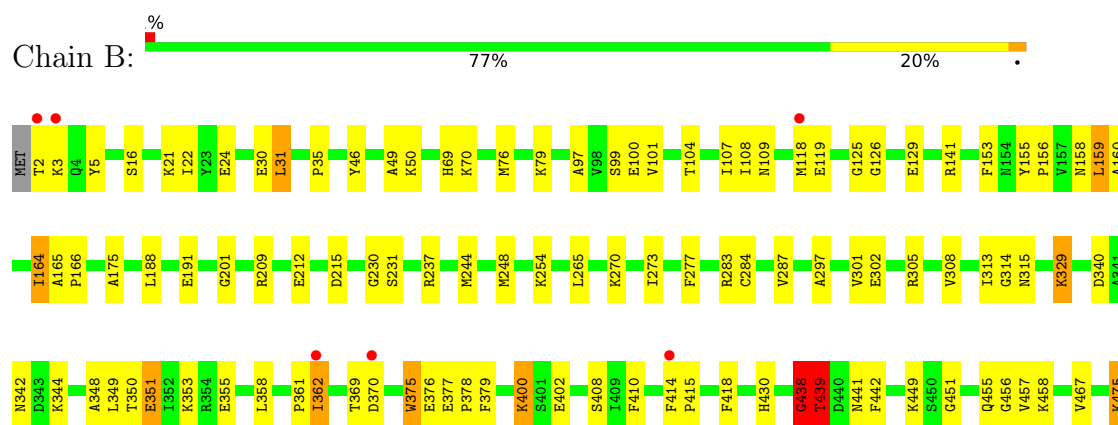
3 Residue-property plots

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.

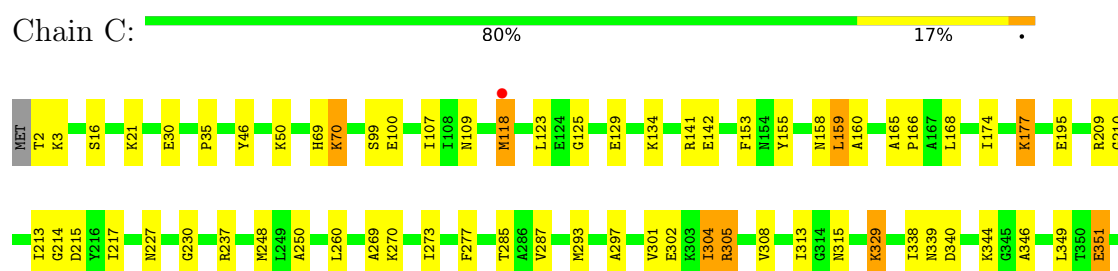
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



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

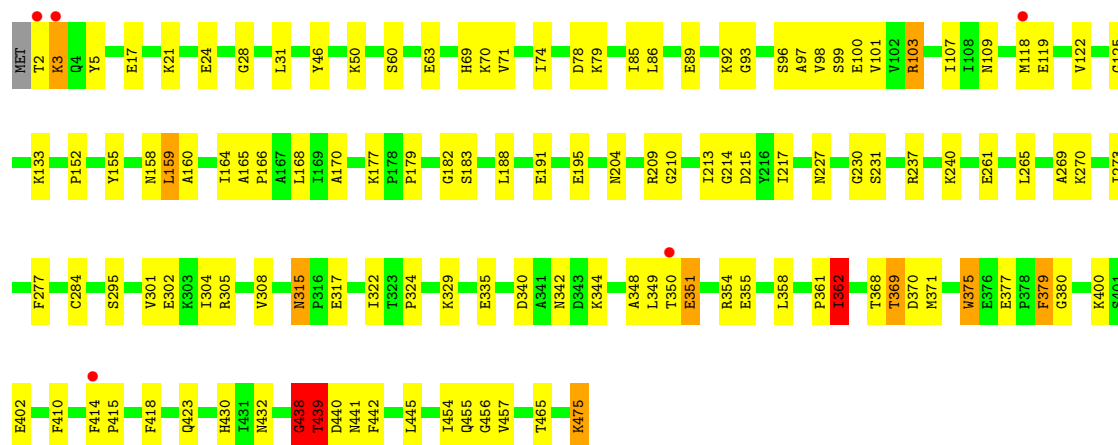


- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	142.47Å 155.21Å 113.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.78 – 2.19 19.78 – 2.21	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.78-2.19) 99.6 (19.78-2.21)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.21Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.184 , 0.230 0.187 , 0.232	Depositor DCC
R_{free} test set	12452 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16008	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 38.04 % 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 3.9128e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, G3H

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	0.76	0/3656	1.07	18/4945 (0.4%)
1	B	0.71	0/3656	1.06	17/4945 (0.3%)
1	C	0.84	0/3656	1.10	22/4945 (0.4%)
1	D	0.79	1/3656 (0.0%)	1.09	20/4945 (0.4%)
All	All	0.78	1/14624 (0.0%)	1.08	77/19780 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	71	VAL	CA-CB	5.05	1.60	1.54

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	456	GLY	N-CA-C	-11.55	96.70	112.18
1	B	456	GLY	N-CA-C	-10.67	97.88	112.18
1	D	315	ASN	CA-C-N	10.41	129.80	118.97
1	D	315	ASN	C-N-CA	10.41	129.80	118.97
1	D	456	GLY	N-CA-C	-10.22	98.49	112.18
1	A	315	ASN	CA-C-N	9.78	129.41	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	ASN	C-N-CA	9.78	129.41	119.24
1	B	315	ASN	CA-C-N	9.35	128.69	118.97
1	B	315	ASN	C-N-CA	9.35	128.69	118.97
1	C	315	ASN	CA-C-N	8.38	127.95	119.24
1	C	315	ASN	C-N-CA	8.38	127.95	119.24
1	D	439	THR	CB-CA-C	8.09	126.51	110.42
1	B	438	GLY	CA-C-N	7.92	136.67	121.54
1	B	438	GLY	C-N-CA	7.92	136.67	121.54
1	D	380	GLY	CA-C-N	7.86	129.66	119.84
1	D	380	GLY	C-N-CA	7.86	129.66	119.84
1	B	439	THR	CB-CA-C	7.85	126.05	110.42
1	C	160	ALA	N-CA-C	-7.53	102.67	112.68
1	C	440	ASP	N-CA-C	6.99	121.25	112.87
1	A	160	ALA	N-CA-C	-6.83	103.59	112.68
1	A	440	ASP	N-CA-C	6.79	121.02	112.87
1	D	438	GLY	CA-C-N	6.71	134.35	121.54
1	D	438	GLY	C-N-CA	6.71	134.35	121.54
1	D	362	ILE	N-CA-C	6.58	117.96	108.48
1	B	175	ALA	N-CA-C	-6.42	97.81	108.34
1	B	265	LEU	N-CA-C	6.22	118.06	111.28
1	C	439	THR	N-CA-CB	-6.22	100.93	111.50
1	A	456	GLY	N-CA-C	-6.18	98.53	113.18
1	C	168	LEU	N-CA-C	6.04	117.53	111.07
1	D	160	ALA	N-CA-C	-5.97	104.74	112.68
1	B	375	TRP	N-CA-C	5.90	120.27	112.72
1	A	457	VAL	N-CA-C	5.78	121.37	109.34
1	D	277	PHE	N-CA-C	5.75	120.30	113.28
1	C	457	VAL	N-CA-C	5.72	121.24	109.34
1	A	164	ILE	N-CA-C	5.66	115.85	110.53
1	C	174	ILE	N-CA-C	5.61	116.82	108.46
1	D	375	TRP	N-CA-C	5.59	119.87	112.72
1	C	142	GLU	CA-C-N	-5.58	114.85	120.31
1	C	142	GLU	C-N-CA	-5.58	114.85	120.31
1	C	375	TRP	N-CA-C	5.55	119.83	112.72
1	A	375	TRP	N-CA-C	5.51	120.37	113.43
1	C	277	PHE	N-CA-C	5.49	120.14	113.38
1	C	177	LYS	CA-C-N	-5.49	114.72	120.38
1	C	177	LYS	C-N-CA	-5.49	114.72	120.38
1	D	168	LEU	N-CA-C	5.45	117.22	111.28
1	D	98	VAL	N-CA-C	-5.45	105.06	111.00
1	A	198	LEU	CA-C-N	-5.42	114.19	119.78
1	A	198	LEU	C-N-CA	-5.42	114.19	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	ILE	N-CA-C	5.42	117.20	108.85
1	D	265	LEU	N-CA-C	5.42	117.89	111.33
1	D	164	ILE	N-CA-C	5.40	115.61	110.42
1	B	314	GLY	N-CA-C	5.36	117.15	110.29
1	C	414	PHE	N-CA-C	5.35	120.03	112.75
1	B	277	PHE	N-CA-C	5.35	119.96	113.38
1	A	439	THR	N-CA-CB	-5.33	102.43	111.50
1	B	451	GLY	N-CA-C	5.33	118.53	110.75
1	D	79	LYS	N-CA-C	5.31	117.75	111.33
1	B	287	VAL	N-CA-C	-5.26	101.89	108.84
1	A	287	VAL	N-CA-C	-5.26	101.90	108.84
1	C	287	VAL	N-CA-C	-5.25	101.84	108.93
1	D	457	VAL	N-CA-C	5.24	120.25	109.34
1	C	297	ALA	N-CA-C	5.22	116.66	111.07
1	A	314	GLY	N-CA-C	5.21	116.96	110.29
1	D	133	LYS	N-CA-C	5.20	117.69	111.71
1	B	164	ILE	N-CA-C	5.20	115.41	110.53
1	A	297	ALA	N-CA-C	5.14	116.57	111.07
1	C	412	ASN	N-CA-C	-5.14	106.41	113.30
1	B	254	LYS	N-CA-C	-5.12	102.52	109.54
1	B	457	VAL	N-CA-C	5.12	119.99	109.34
1	C	346	ALA	N-CA-C	-5.09	103.81	110.53
1	C	250	ALA	N-CA-C	-5.07	100.14	108.41
1	C	456	GLY	CA-C-O	-5.07	117.93	121.88
1	A	177	LYS	CA-C-N	-5.06	115.17	120.38
1	A	177	LYS	C-N-CA	-5.06	115.17	120.38
1	D	78	ASP	N-CA-C	5.06	119.14	112.92
1	A	139	VAL	N-CA-C	5.04	115.11	107.80
1	B	297	ALA	N-CA-C	5.03	117.15	111.11

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	438	GLY	Mainchain
1	D	438	GLY	Mainchain

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	82	0
1	B	3598	0	3651	71	0
1	C	3598	0	3651	69	1
1	D	3598	0	3651	83	0
2	A	10	0	4	1	0
2	B	10	0	4	1	0
2	C	10	0	4	1	0
2	D	10	0	4	1	0
3	A	48	0	25	8	0
3	B	48	0	25	7	0
3	C	48	0	24	8	0
3	D	48	0	25	9	0
4	A	368	0	0	14	0
4	B	300	0	0	4	0
4	C	403	0	0	12	0
4	D	313	0	0	11	0
All	All	16008	0	14719	284	1

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 10.

All (284) 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:D:230:GLY:HA2	3:D:4476:NAP:H51N	1.31	1.07
1:D:439:THR:HG23	1:D:441:ASN:OD1	1.62	0.98
1:C:439:THR:HG23	1:C:441:ASN:OD1	1.66	0.94
1:A:439:THR:HG23	1:A:441:ASN:OD1	1.68	0.92
1:B:439:THR:HG23	1:B:441:ASN:OD1	1.70	0.91
1:A:125:GLY:HA2	1:B:439:THR:HG21	1.60	0.83
1:B:415:PRO:HB2	1:D:475:LYS:HG3	1.59	0.83
1:A:475:LYS:HG3	1:C:415:PRO:HB2	1.60	0.81
1:A:415:PRO:HB2	1:C:475:LYS:HG3	1.63	0.80
1:B:119:GLU:HG2	1:C:123:LEU:HD23	1.64	0.80
1:B:230:GLY:HA2	3:B:2476:NAP:H52N	1.63	0.79
1:D:305:ARG:HD2	4:D:4635:HOH:O	1.82	0.79
1:B:2:THR:HG21	1:B:21:LYS:HE2	1.65	0.79
1:C:70:LYS:HE3	4:C:3787:HOH:O	1.84	0.78
1:A:302:GLU:OE2	1:A:305:ARG:NH1	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:THR:HG22	4:A:1580:HOH:O	1.84	0.78
1:C:155:TYR:HB2	1:C:159:LEU:HD22	1.69	0.75
1:C:125:GLY:HA2	1:D:439:THR:HG21	1.69	0.74
1:D:107:ILE:HD12	1:D:158:ASN:HD21	1.51	0.74
1:A:375:TRP:CH2	1:A:400:LYS:HG2	2.23	0.72
1:C:118:MET:HB3	4:C:3667:HOH:O	1.88	0.72
1:B:283:ARG:HD3	4:B:2580:HOH:O	1.90	0.72
1:C:302:GLU:OE2	1:C:305:ARG:NH1	2.24	0.71
1:D:155:TYR:HB2	1:D:159:LEU:HD22	1.72	0.71
1:B:302:GLU:OE2	1:B:305:ARG:NH1	2.24	0.71
1:D:230:GLY:CA	3:D:4476:NAP:H51N	2.15	0.71
1:B:475:LYS:HG3	1:D:415:PRO:HB2	1.73	0.70
1:C:439:THR:HG21	1:D:125:GLY:HA2	1.73	0.69
1:C:2:THR:HG22	1:C:30:GLU:OE2	1.92	0.69
1:A:329:LYS:HE2	4:A:1806:HOH:O	1.94	0.68
1:B:377:GLU:O	3:B:2476:NAP:N7N	2.27	0.68
1:B:212:GLU:HB3	4:B:2661:HOH:O	1.94	0.68
1:C:375:TRP:CH2	1:C:400:LYS:HG2	2.30	0.67
1:A:230:GLY:HA2	3:A:1476:NAP:H51N	1.77	0.67
1:B:119:GLU:HG2	1:C:123:LEU:CD2	2.24	0.67
1:C:118:MET:HG2	4:C:3665:HOH:O	1.94	0.67
1:D:100:GLU:HG3	1:D:158:ASN:HB2	1.77	0.66
1:C:215:ASP:OD2	1:C:237:ARG:NH2	2.29	0.66
1:A:118:MET:HG2	4:A:1551:HOH:O	1.93	0.66
1:B:155:TYR:HB2	1:B:159:LEU:HD22	1.79	0.65
1:D:230:GLY:O	3:D:4476:NAP:H3D	1.97	0.65
1:D:350:THR:HG21	1:D:361:PRO:O	1.97	0.65
1:B:340:ASP:O	1:B:344:LYS:HG3	1.98	0.64
1:A:414:PHE:HB3	4:A:1841:HOH:O	1.98	0.63
1:B:100:GLU:HG3	1:B:158:ASN:HB2	1.81	0.63
1:B:375:TRP:CH2	1:B:400:LYS:HG2	2.32	0.63
1:D:69:HIS:ND1	1:D:109:ASN:ND2	2.46	0.63
1:B:16:SER:HB2	1:B:35:PRO:HB3	1.81	0.62
1:B:69:HIS:ND1	1:B:109:ASN:ND2	2.48	0.62
1:C:362:ILE:HG13	1:C:363:LEU:N	2.13	0.61
1:D:439:THR:HG22	1:D:442:PHE:CD2	2.36	0.61
1:A:155:TYR:HB2	1:A:159:LEU:HD22	1.82	0.61
1:A:475:LYS:CG	1:C:415:PRO:HB2	2.29	0.61
1:D:2:THR:HG23	4:D:4773:HOH:O	2.01	0.60
1:C:339:ASN:ND2	4:C:3520:HOH:O	2.24	0.60
1:C:379:PHE:CZ	3:C:3476:NAP:H4D	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ALA:HB1	1:A:304:ILE:HD13	1.85	0.58
1:C:373:LEU:O	1:C:373:LEU:HG	2.03	0.58
1:D:375:TRP:CH2	1:D:400:LYS:HG2	2.38	0.58
1:A:439:THR:HG21	1:B:125:GLY:HA2	1.86	0.58
1:A:7:ASN:ND2	1:A:37:MET:HE3	2.18	0.58
1:A:231:SER:HA	3:A:1476:NAP:H2D	1.85	0.58
1:A:177:LYS:HG3	1:A:177:LYS:O	2.03	0.57
1:A:16:SER:HB2	1:A:35:PRO:HB3	1.86	0.57
1:D:24:GLU:HG2	1:D:31:LEU:HG	1.86	0.57
1:C:2:THR:HG21	1:C:21:LYS:HE2	1.87	0.56
1:A:215:ASP:OD2	1:A:237:ARG:NH2	2.39	0.56
1:B:76:MET:O	1:B:79:LYS:HG2	2.04	0.56
1:A:244:MET:HG2	4:B:2624:HOH:O	2.05	0.56
1:D:261:GLU:HG2	1:D:295:SER:OG	2.06	0.56
1:A:362:ILE:HG13	1:A:363:LEU:N	2.20	0.56
1:C:107:ILE:HD12	1:C:158:ASN:HD21	1.70	0.56
1:D:46:TYR:O	1:D:50:LYS:HG2	2.06	0.56
1:B:475:LYS:CG	1:D:415:PRO:HB2	2.35	0.56
1:D:377:GLU:O	3:D:4476:NAP:N7N	2.37	0.56
1:D:3:LYS:HD2	1:D:5:TYR:CE2	2.41	0.56
1:C:269:ALA:HA	1:C:304:ILE:HD11	1.88	0.55
1:A:269:ALA:CB	1:A:304:ILE:HD13	2.37	0.55
1:A:215:ASP:OD1	1:A:237:ARG:NH2	2.40	0.54
1:D:445:LEU:HD13	1:D:454:ILE:HG12	1.89	0.54
1:A:369:THR:HG23	4:A:1762:HOH:O	2.06	0.54
1:C:369:THR:HG22	4:C:3477:HOH:O	2.07	0.54
1:B:231:SER:HA	3:B:2476:NAP:H2D	1.91	0.53
1:B:377:GLU:OE1	3:B:2476:NAP:O2D	2.26	0.53
1:B:2:THR:HG21	1:B:21:LYS:CE	2.36	0.53
1:A:449:LYS:HA	1:B:244:MET:CE	2.39	0.53
1:B:230:GLY:O	3:B:2476:NAP:H3D	2.08	0.53
1:D:369:THR:HG23	4:D:4552:HOH:O	2.08	0.53
1:A:305:ARG:HG3	1:A:349:LEU:HB3	1.89	0.53
1:C:351:GLU:HB3	4:C:3824:HOH:O	2.09	0.53
1:A:5:TYR:O	1:A:35:PRO:HD3	2.08	0.53
1:A:100:GLU:HG3	1:A:158:ASN:HB2	1.91	0.52
1:C:273:ILE:HD11	1:C:308:VAL:HG23	1.92	0.52
1:D:107:ILE:HD12	1:D:158:ASN:ND2	2.23	0.52
1:D:152:PRO:C	1:D:179:PRO:HG3	2.34	0.52
1:D:368:THR:OG1	1:D:371:MET:HE3	2.09	0.52
1:B:230:GLY:CA	3:B:2476:NAP:H52N	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ILE:HG22	1:A:358:LEU:HD21	1.90	0.52
1:A:379:PHE:CE1	3:A:1476:NAP:H1D	2.43	0.52
1:B:414:PHE:HB2	1:C:414:PHE:HB2	1.91	0.52
1:A:414:PHE:HB2	1:D:414:PHE:HB2	1.90	0.52
1:A:221:GLN:HG3	4:A:1813:HOH:O	2.09	0.51
1:B:353:LYS:NZ	4:B:2601:HOH:O	2.42	0.51
1:B:230:GLY:HA2	3:B:2476:NAP:C5D	2.37	0.51
4:C:3622:HOH:O	1:D:430:HIS:HD2	1.93	0.51
1:B:2:THR:HG22	1:B:30:GLU:OE2	2.10	0.51
1:C:46:TYR:O	1:C:50:LYS:HG2	2.10	0.51
1:C:313:ILE:HG22	1:C:358:LEU:HD21	1.91	0.51
3:C:3476:NAP:H5N	4:C:3694:HOH:O	2.10	0.51
1:A:244:MET:HE1	1:B:449:LYS:HA	1.92	0.51
1:B:97:ALA:O	1:B:101:VAL:HG23	2.10	0.51
1:D:340:ASP:O	1:D:344:LYS:HG3	2.11	0.51
1:A:46:TYR:O	1:A:50:LYS:HG2	2.11	0.51
1:D:210:GLY:O	1:D:214:GLY:HA3	2.11	0.51
1:B:415:PRO:HB2	1:D:475:LYS:CG	2.36	0.50
1:A:2:THR:HG21	1:A:21:LYS:HE2	1.93	0.50
1:A:165:ALA:HB3	1:A:166:PRO:HD3	1.93	0.50
1:D:231:SER:HA	3:D:4476:NAP:H2D	1.94	0.50
1:C:329:LYS:HE2	4:C:3748:HOH:O	2.11	0.50
1:A:215:ASP:CG	1:A:237:ARG:HH21	2.19	0.50
1:A:244:MET:HE2	1:B:449:LYS:HD3	1.93	0.49
1:C:69:HIS:ND1	1:C:109:ASN:ND2	2.61	0.49
1:D:170:ALA:HB1	1:D:465:THR:CG2	2.42	0.49
1:A:383:LEU:HD12	1:A:384:PRO:HD2	1.94	0.49
1:C:230:GLY:HA2	3:C:3476:NAP:H52N	1.94	0.49
1:D:335:GLU:OE1	1:D:354:ARG:HD3	2.12	0.49
1:B:439:THR:HG22	1:B:442:PHE:CD2	2.48	0.49
1:D:85:ILE:HD12	1:D:188:LEU:HD11	1.95	0.49
1:B:215:ASP:OD2	1:B:237:ARG:NH2	2.46	0.48
1:A:230:GLY:HA2	3:A:1476:NAP:C5D	2.43	0.48
1:A:339:ASN:ND2	4:A:1549:HOH:O	2.46	0.48
1:D:60:SER:OG	1:D:63:GLU:HG3	2.12	0.48
1:C:376:GLU:O	1:C:378:PRO:HD3	2.13	0.48
1:D:269:ALA:HA	1:D:304:ILE:CD1	2.44	0.48
1:D:301:VAL:CG1	1:D:349:LEU:CD1	2.91	0.48
1:D:28:GLY:HA2	4:D:4524:HOH:O	2.12	0.48
1:A:53:GLN:HB3	1:A:54:PRO:HD3	1.95	0.48
1:B:408:SER:HB3	1:B:410:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ILE:O	1:D:217:ILE:HG23	2.13	0.48
3:D:4476:NAP:H5N	4:D:4757:HOH:O	2.13	0.48
1:A:449:LYS:HA	1:B:244:MET:HE1	1.96	0.48
1:D:3:LYS:HD2	1:D:5:TYR:CZ	2.49	0.48
1:D:103:ARG:HD2	1:D:440:ASP:OD2	2.13	0.48
1:A:230:GLY:HA3	3:A:1476:NAP:H51A	1.95	0.47
1:B:215:ASP:CG	1:B:237:ARG:HH21	2.22	0.47
1:A:376:GLU:O	1:A:378:PRO:HD3	2.14	0.47
1:C:293:MET:HE3	4:C:3836:HOH:O	2.14	0.47
1:D:379:PHE:CE1	3:D:4476:NAP:H1D	2.50	0.47
1:B:350:THR:HG22	1:B:351:GLU:N	2.30	0.47
1:A:273:ILE:HD11	1:A:308:VAL:HG23	1.97	0.47
1:B:5:TYR:O	1:B:35:PRO:HD3	2.14	0.47
1:C:2:THR:HG21	1:C:21:LYS:CE	2.44	0.47
1:D:97:ALA:O	1:D:101:VAL:HG23	2.15	0.47
1:A:244:MET:CE	1:B:449:LYS:HA	2.44	0.47
1:B:165:ALA:HB3	1:B:166:PRO:HD3	1.96	0.47
1:D:348:ALA:HB1	1:D:362:ILE:CD1	2.45	0.47
1:D:302:GLU:OE2	1:D:305:ARG:NH1	2.30	0.47
1:D:315:ASN:HB3	1:D:317:GLU:OE1	2.15	0.47
1:A:269:ALA:HA	1:A:304:ILE:HD11	1.97	0.47
1:C:304:ILE:N	1:C:304:ILE:HD13	2.30	0.47
1:C:338:ILE:HD11	1:C:382:VAL:HG21	1.97	0.47
1:D:439:THR:HG22	1:D:442:PHE:CG	2.49	0.47
1:A:215:ASP:CG	1:A:237:ARG:NH2	2.73	0.46
1:A:269:ALA:HA	1:A:304:ILE:CD1	2.45	0.46
1:B:376:GLU:O	1:B:378:PRO:HD3	2.15	0.46
1:B:126:GLY:HA3	4:C:3538:HOH:O	2.14	0.46
1:C:338:ILE:HD11	1:C:382:VAL:CG2	2.44	0.46
1:A:362:ILE:HG23	1:A:382:VAL:HG13	1.96	0.46
1:D:103:ARG:HG2	1:D:158:ASN:ND2	2.29	0.46
1:A:80:GLU:HB2	4:A:1622:HOH:O	2.14	0.46
1:C:269:ALA:HA	1:C:304:ILE:CD1	2.45	0.46
1:A:38:SER:OG	1:A:41:GLU:HG3	2.16	0.46
1:D:3:LYS:NZ	4:D:4492:HOH:O	2.37	0.46
1:D:301:VAL:CG1	1:D:349:LEU:HD11	2.46	0.46
1:B:24:GLU:HG2	1:B:31:LEU:HG	1.98	0.45
1:B:284[A]:CYS:H	2:B:800:G3H:C1	2.28	0.45
1:B:348:ALA:HB1	1:B:362:ILE:CD1	2.46	0.45
1:D:159:LEU:HD12	1:D:159:LEU:HA	1.77	0.45
1:B:49:ALA:HA	1:B:201:GLY:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ALA:HB3	1:C:166:PRO:HD3	1.99	0.45
1:A:227:ASN:C	1:A:227:ASN:HD22	2.22	0.45
1:C:2:THR:HG21	1:C:21:LYS:NZ	2.32	0.45
1:C:329:LYS:HB3	1:C:329:LYS:HE3	1.77	0.45
1:C:377:GLU:OE1	3:C:3476:NAP:O2D	2.34	0.45
1:C:379:PHE:CE1	3:C:3476:NAP:H1D	2.51	0.45
1:D:89:GLU:CD	1:D:182:GLY:HA2	2.42	0.45
1:D:209:ARG:HG3	1:D:209:ARG:HH11	1.81	0.45
1:D:400:LYS:O	1:D:400:LYS:HG3	2.16	0.45
1:B:215:ASP:OD1	1:B:237:ARG:NH2	2.50	0.45
1:A:301:VAL:HG13	1:A:349:LEU:CD1	2.47	0.45
1:A:209:ARG:HG3	1:A:209:ARG:HH11	1.80	0.45
1:B:248:MET:SD	1:B:455:GLN:HG3	2.56	0.45
1:D:227:ASN:C	1:D:227:ASN:HD22	2.25	0.45
3:C:3476:NAP:H2B	3:C:3476:NAP:H51A	1.61	0.44
1:B:313:ILE:HG22	1:B:358:LEU:HD21	1.99	0.44
1:A:41:GLU:O	1:A:45:VAL:HG23	2.17	0.44
1:A:377:GLU:OE1	3:A:1476:NAP:O2D	2.27	0.44
1:B:107:ILE:HD12	1:B:158:ASN:HD21	1.82	0.44
1:C:301:VAL:HG13	1:C:349:LEU:CD1	2.48	0.44
1:C:340:ASP:O	1:C:344:LYS:HG3	2.18	0.44
1:D:215:ASP:OD2	1:D:237:ARG:NH2	2.50	0.44
1:D:240:LYS:HE3	4:D:4647:HOH:O	2.16	0.44
1:B:21:LYS:C	1:B:22:ILE:HD12	2.42	0.44
1:C:305:ARG:HG3	1:C:349:LEU:HB3	1.98	0.44
1:A:69:HIS:ND1	1:A:109:ASN:ND2	2.64	0.44
1:C:301:VAL:CG1	1:C:349:LEU:CD1	2.95	0.44
1:D:165:ALA:HB3	1:D:166:PRO:HD3	1.99	0.44
1:D:455:GLN:NE2	4:D:4775:HOH:O	2.50	0.44
1:B:159:LEU:HA	1:B:159:LEU:HD12	1.65	0.44
1:D:350:THR:HG22	1:D:351:GLU:N	2.33	0.44
1:C:269:ALA:CB	1:C:304:ILE:CD1	2.96	0.44
1:A:121:GLU:HG3	1:A:139:VAL:HB	1.99	0.43
1:C:260:LEU:HD22	1:C:391:VAL:HG22	1.99	0.43
1:D:322:ILE:HG13	1:D:361:PRO:HD3	1.99	0.43
1:D:379:PHE:CZ	3:D:4476:NAP:H1D	2.53	0.43
1:C:134:LYS:NZ	4:C:3653:HOH:O	2.25	0.43
1:D:423:GLN:HG2	4:D:4666:HOH:O	2.18	0.43
1:D:3:LYS:NZ	4:D:4599:HOH:O	2.50	0.43
1:A:107:ILE:HD11	1:A:440:ASP:CG	2.44	0.43
1:A:209:ARG:NH1	4:A:1491:HOH:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:TYR:O	1:B:50:LYS:HG2	2.19	0.43
1:B:400:LYS:O	1:B:400:LYS:HG3	2.19	0.43
1:A:138:VAL:HG13	1:D:122:VAL:HG21	2.00	0.43
1:B:273:ILE:HD11	1:B:308:VAL:HG23	2.00	0.43
1:B:188:LEU:O	1:B:191:GLU:HB2	2.18	0.43
1:D:261:GLU:HG2	1:D:295:SER:HG	1.83	0.43
1:B:301:VAL:CG1	1:B:349:LEU:CD1	2.96	0.43
1:C:227:ASN:HD22	1:C:227:ASN:C	2.26	0.43
4:A:1587:HOH:O	1:B:430:HIS:HD2	2.01	0.42
1:C:155:TYR:CB	1:C:159:LEU:HD22	2.45	0.42
1:A:349:LEU:HD11	1:A:365:ASP:HB2	2.01	0.42
1:D:74:ILE:HD13	1:D:195:GLU:HB3	2.01	0.42
1:B:104:THR:O	1:B:108:ILE:HG13	2.19	0.42
1:B:209:ARG:HH11	1:B:209:ARG:HG3	1.84	0.42
1:C:213:ILE:O	1:C:217:ILE:HG23	2.18	0.42
1:D:188:LEU:O	1:D:191:GLU:HB2	2.19	0.42
1:A:284[A]:CYS:SG	1:A:285:THR:HG23	2.60	0.42
1:C:362:ILE:HG23	1:C:382:VAL:HG22	2.00	0.42
1:A:301:VAL:HG13	1:A:349:LEU:HD13	2.00	0.42
1:A:24:GLU:HG2	1:A:31:LEU:HG	2.01	0.42
1:A:415:PRO:HB2	1:C:475:LYS:CG	2.41	0.42
1:A:415:PRO:HG3	1:D:414:PHE:CZ	2.55	0.42
1:D:410:PHE:HA	1:D:432:ASN:OD1	2.19	0.42
1:A:147:VAL:HB	1:A:174:ILE:HD13	2.01	0.42
1:B:458:LYS:NZ	1:D:119:GLU:OE1	2.52	0.42
1:B:439:THR:CG2	1:B:441:ASN:OD1	2.57	0.42
1:B:160:ALA:O	1:B:164:ILE:HG13	2.19	0.42
1:C:100:GLU:HG3	1:C:158:ASN:HB2	2.02	0.41
1:C:379:PHE:CD1	3:C:3476:NAP:H1D	2.54	0.41
1:A:124:GLU:HB3	4:A:1502:HOH:O	2.20	0.41
1:A:150:ILE:HG22	3:A:1476:NAP:H4B	2.02	0.41
1:C:230:GLY:C	3:C:3476:NAP:H3D	2.45	0.41
1:C:285:THR:OG1	2:C:800:G3H:H31	2.21	0.41
1:B:153:PHE:CD1	1:B:153:PHE:C	2.98	0.41
1:C:159:LEU:HD12	1:C:159:LEU:HA	1.95	0.41
1:B:329:LYS:HE3	1:B:329:LYS:HB3	1.60	0.41
1:A:85:ILE:HD12	1:A:188:LEU:HD11	2.03	0.41
1:A:284[A]:CYS:H	2:A:800:G3H:C1	2.33	0.41
1:A:455:GLN:NE2	4:A:1545:HOH:O	2.53	0.41
1:A:433:ASN:HB3	4:A:1670:HOH:O	2.20	0.41
1:B:350:THR:HG21	1:B:361:PRO:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:THR:HG21	1:D:21:LYS:HE2	2.02	0.41
1:A:167:ALA:O	1:A:172:ASN:HB2	2.20	0.41
1:A:230:GLY:O	3:A:1476:NAP:H3D	2.20	0.41
1:B:153:PHE:O	1:B:156:PRO:HD3	2.20	0.41
1:D:284[A]:CYS:H	2:D:800:G3H:C1	2.34	0.41
1:C:134:LYS:HA	1:C:134:LYS:HD2	1.89	0.41
1:C:177:LYS:O	1:C:177:LYS:HG3	2.16	0.41
1:D:439:THR:CG2	1:D:441:ASN:OD1	2.50	0.41
1:A:269:ALA:CB	1:A:304:ILE:CD1	2.99	0.41
1:C:210:GLY:O	1:C:214:GLY:HA3	2.21	0.41
1:D:92:LYS:O	1:D:93:GLY:C	2.64	0.41
1:D:273:ILE:HD11	1:D:308:VAL:HG23	2.03	0.41
1:A:350:THR:HG22	4:A:1818:HOH:O	2.20	0.40
1:C:16:SER:HB2	1:C:35:PRO:HB3	2.03	0.40
1:D:31:LEU:HD23	1:D:31:LEU:HA	1.91	0.40
1:C:248:MET:HG3	1:C:455:GLN:HE21	1.87	0.40
1:C:209:ARG:HG3	1:C:209:ARG:HH11	1.86	0.40
1:D:324:PRO:HD3	1:D:358:LEU:HD13	2.02	0.40
1:D:377:GLU:OE1	3:D:4476:NAP:O2D	2.38	0.40
1:A:118:MET:HE2	1:A:461:ILE:HG22	2.02	0.40
1:C:248:MET:CG	1:C:455:GLN:HE21	2.35	0.40
1:C:153:PHE:CD1	1:C:153:PHE:C	2.99	0.40
1:D:227:ASN:ND2	4:D:4775:HOH:O	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:LYS:NZ	1:C:195:GLU:OE1[2_355]	2.16	0.04

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	473/475 (100%)	463 (98%)	9 (2%)	1 (0%)	43	51
1	B	473/475 (100%)	456 (96%)	15 (3%)	2 (0%)	30	34
1	C	473/475 (100%)	461 (98%)	12 (2%)	0	100	100
1	D	473/475 (100%)	454 (96%)	17 (4%)	2 (0%)	30	34
All	All	1892/1900 (100%)	1834 (97%)	53 (3%)	5 (0%)	36	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	438	GLY
1	D	438	GLY
1	B	439	THR
1	D	439	THR
1	A	378	PRO

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	378/378 (100%)	356 (94%)	22 (6%)	18	22
1	B	378/378 (100%)	355 (94%)	23 (6%)	17	20
1	C	378/378 (100%)	355 (94%)	23 (6%)	17	20
1	D	378/378 (100%)	353 (93%)	25 (7%)	15	18
All	All	1512/1512 (100%)	1419 (94%)	93 (6%)	16	20

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	31	LEU
1	A	70	LYS
1	A	99	SER
1	A	118	MET
1	A	121	GLU

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Mol	Chain	Res	Type
1	A	159	LEU
1	A	270	LYS
1	A	329	LYS
1	A	351	GLU
1	A	355	GLU
1	A	362	ILE
1	A	369	THR
1	A	370	ASP
1	A	379	PHE
1	A	392	GLU
1	A	400	LYS
1	A	402	GLU
1	A	439	THR
1	A	448	LYS
1	A	467	VAL
1	A	475	LYS
1	B	3	LYS
1	B	31	LEU
1	B	70	LYS
1	B	99	SER
1	B	118	MET
1	B	129	GLU
1	B	141	ARG
1	B	159	LEU
1	B	270	LYS
1	B	329	LYS
1	B	342	ASN
1	B	351	GLU
1	B	355	GLU
1	B	362	ILE
1	B	369	THR
1	B	370	ASP
1	B	379	PHE
1	B	400	LYS
1	B	402	GLU
1	B	418	PHE
1	B	439	THR
1	B	467	VAL
1	B	475	LYS
1	C	70	LYS
1	C	99	SER
1	C	118	MET

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Mol	Chain	Res	Type
1	C	129	GLU
1	C	141	ARG
1	C	159	LEU
1	C	270	LYS
1	C	304	ILE
1	C	305	ARG
1	C	329	LYS
1	C	351	GLU
1	C	355	GLU
1	C	362	ILE
1	C	369	THR
1	C	370	ASP
1	C	379	PHE
1	C	400	LYS
1	C	402	GLU
1	C	408	SER
1	C	439	THR
1	C	448	LYS
1	C	467	VAL
1	C	475	LYS
1	D	3	LYS
1	D	17	GLU
1	D	70	LYS
1	D	86	LEU
1	D	96	SER
1	D	99	SER
1	D	103	ARG
1	D	118	MET
1	D	159	LEU
1	D	177	LYS
1	D	183	SER
1	D	204	ASN
1	D	270	LYS
1	D	329	LYS
1	D	342	ASN
1	D	351	GLU
1	D	355	GLU
1	D	362	ILE
1	D	369	THR
1	D	370	ASP
1	D	379	PHE
1	D	402	GLU

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Mol	Chain	Res	Type
1	D	418	PHE
1	D	439	THR
1	D	475	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	227	ASN
1	A	342	ASN
1	A	455	GLN
1	B	109	ASN
1	B	227	ASN
1	B	342	ASN
1	B	430	HIS
1	B	433	ASN
1	C	18	ASN
1	C	109	ASN
1	C	227	ASN
1	C	455	GLN
1	D	109	ASN
1	D	227	ASN
1	D	342	ASN
1	D	430	HIS
1	D	436	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry

8 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$
3	NAP	A	1476	-	50,52,52	1.81	10 (20%)	71,80,80	1.46	14 (19%)
3	NAP	C	3476	-	50,52,52	2.35	18 (36%)	71,80,80	2.36	24 (33%)
3	NAP	B	2476	-	50,52,52	1.61	12 (24%)	71,80,80	1.79	16 (22%)
2	G3H	D	800	-	8,9,9	2.96	4 (50%)	7,12,12	4.57	4 (57%)
2	G3H	B	800	-	8,9,9	3.07	4 (50%)	7,12,12	4.85	5 (71%)
2	G3H	A	800	-	8,9,9	3.07	5 (62%)	7,12,12	4.11	4 (57%)
3	NAP	D	4476	-	50,52,52	1.99	10 (20%)	71,80,80	1.89	17 (23%)
2	G3H	C	800	-	8,9,9	3.24	4 (50%)	7,12,12	4.72	3 (42%)

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
3	NAP	A	1476	-	-	10/35/67/67	0/5/5/5
3	NAP	C	3476	-	-	19/35/67/67	0/5/5/5
3	NAP	B	2476	-	-	12/35/67/67	0/5/5/5
2	G3H	D	800	-	-	1/7/8/8	-
2	G3H	B	800	-	-	1/7/8/8	-
2	G3H	A	800	-	-	1/7/8/8	-
3	NAP	D	4476	-	-	10/35/67/67	0/5/5/5
2	G3H	C	800	-	-	1/7/8/8	-

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3476	NAP	C2N-N1N	8.93	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4476	NAP	PN-O3	6.83	1.66	1.59
3	D	4476	NAP	O4D-C1D	5.79	1.48	1.40
3	D	4476	NAP	PA-O3	5.76	1.65	1.59
2	D	800	G3H	P-O1P	5.65	1.78	1.60
2	C	800	G3H	P-O1P	5.22	1.76	1.60
2	A	800	G3H	P-O1P	5.09	1.76	1.60
2	B	800	G3H	P-O1P	5.07	1.76	1.60
3	A	1476	NAP	C2N-N1N	4.99	1.40	1.35
2	A	800	G3H	O1P-C3	4.95	1.63	1.44
3	C	3476	NAP	O4D-C1D	4.93	1.47	1.40
3	A	1476	NAP	P2B-O2B	4.67	1.67	1.59
3	B	2476	NAP	PN-O3	4.57	1.64	1.59
2	C	800	G3H	O1P-C3	4.56	1.61	1.44
2	C	800	G3H	O2-C2	4.25	1.51	1.43
3	B	2476	NAP	P2B-O2B	4.20	1.66	1.59
3	C	3476	NAP	C7N-N7N	4.05	1.40	1.33
2	D	800	G3H	O1P-C3	4.03	1.59	1.44
2	B	800	G3H	O1P-C3	3.98	1.59	1.44
3	A	1476	NAP	C7N-N7N	3.89	1.40	1.33
3	B	2476	NAP	C3N-C7N	-3.80	1.44	1.50
3	C	3476	NAP	PA-O3	3.73	1.63	1.59
2	B	800	G3H	O2-C2	3.72	1.50	1.43
3	A	1476	NAP	PN-O3	3.68	1.63	1.59
3	C	3476	NAP	C8A-N9A	3.60	1.43	1.37
2	B	800	G3H	P-O3P	-3.52	1.41	1.54
2	C	800	G3H	P-O3P	-3.48	1.41	1.54
3	A	1476	NAP	C2N-C3N	3.48	1.44	1.39
3	C	3476	NAP	C3N-C7N	3.34	1.55	1.50
3	B	2476	NAP	C2N-N1N	3.20	1.38	1.35
2	D	800	G3H	O2-C2	3.13	1.49	1.43
3	C	3476	NAP	O2D-C2D	-3.11	1.35	1.43
3	D	4476	NAP	C3N-C7N	-3.06	1.46	1.50
3	C	3476	NAP	PN-O3	3.06	1.62	1.59
3	A	1476	NAP	C3N-C7N	3.00	1.55	1.50
3	B	2476	NAP	O4B-C1B	2.88	1.48	1.42
3	C	3476	NAP	O7N-C7N	2.87	1.29	1.24
3	C	3476	NAP	P2B-O2B	2.86	1.64	1.59
2	A	800	G3H	P-O3P	-2.85	1.44	1.54
3	C	3476	NAP	P2B-O2X	-2.71	1.44	1.54
3	B	2476	NAP	C7N-N7N	2.69	1.37	1.33
3	D	4476	NAP	P2B-O2B	2.68	1.64	1.59
3	A	1476	NAP	C5A-C4A	2.67	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	G3H	P-O2P	-2.59	1.42	1.50
3	C	3476	NAP	C8A-N7A	2.57	1.36	1.31
3	C	3476	NAP	O5B-C5B	-2.56	1.34	1.44
3	C	3476	NAP	PN-O1N	2.53	1.59	1.50
3	C	3476	NAP	C6A-N6A	2.51	1.40	1.34
2	D	800	G3H	P-O3P	-2.46	1.45	1.54
3	B	2476	NAP	O7N-C7N	2.46	1.28	1.24
3	B	2476	NAP	PA-O3	2.44	1.62	1.59
3	D	4476	NAP	C3D-C4D	2.44	1.59	1.53
3	B	2476	NAP	PN-O5D	2.41	1.68	1.59
3	A	1476	NAP	PA-O3	2.40	1.62	1.59
3	B	2476	NAP	O4D-C1D	2.36	1.44	1.40
3	B	2476	NAP	O4B-C4B	2.35	1.50	1.45
2	A	800	G3H	O2-C2	2.31	1.48	1.43
3	A	1476	NAP	O7N-C7N	2.20	1.28	1.24
3	A	1476	NAP	PN-O5D	2.16	1.67	1.59
3	D	4476	NAP	PN-O5D	2.15	1.67	1.59
3	B	2476	NAP	C3D-C4D	2.14	1.58	1.53
3	C	3476	NAP	C5N-C4N	2.14	1.42	1.38
3	D	4476	NAP	P2B-O2X	-2.13	1.46	1.54
3	C	3476	NAP	O4D-C4D	2.12	1.49	1.45
3	D	4476	NAP	C3B-C4B	2.04	1.58	1.53
3	D	4476	NAP	PA-O2A	-2.04	1.45	1.55
3	C	3476	NAP	C4A-N3A	-2.04	1.30	1.34

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	G3H	O1P-P-O2P	-9.52	80.71	106.44
2	C	800	G3H	O4P-P-O1P	8.41	128.59	106.67
3	D	4476	NAP	O3D-C3D-C2D	-8.35	85.05	111.82
2	D	800	G3H	O1P-P-O2P	-8.23	84.20	106.44
2	C	800	G3H	O1P-P-O2P	-8.05	84.69	106.44
3	C	3476	NAP	C3N-C7N-N7N	7.88	127.44	117.74
2	A	800	G3H	O1P-P-O2P	-7.45	86.32	106.44
3	C	3476	NAP	O4B-C4B-C5B	-7.03	86.81	109.33
2	D	800	G3H	O4P-P-O1P	6.98	124.86	106.67
2	B	800	G3H	O4P-P-O1P	6.84	124.50	106.67
2	A	800	G3H	O4P-P-O1P	6.49	123.59	106.67
3	C	3476	NAP	O3-PN-O1N	-6.33	91.67	110.70
3	B	2476	NAP	O4D-C4D-C5D	-5.28	92.41	109.33
3	B	2476	NAP	O7N-C7N-N7N	4.36	128.92	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4476	NAP	O3-PN-O1N	-4.31	97.74	110.70
3	B	2476	NAP	C2N-C3N-C4N	3.94	122.84	118.26
2	D	800	G3H	O3P-P-O1P	3.93	116.91	106.67
3	C	3476	NAP	O7N-C7N-N7N	-3.86	117.03	122.62
2	B	800	G3H	O3P-P-O1P	3.85	116.70	106.67
3	B	2476	NAP	O3D-C3D-C2D	-3.82	99.57	111.82
3	C	3476	NAP	C5B-C4B-C3B	-3.81	101.51	115.21
3	A	1476	NAP	O2X-P2B-O1X	3.73	125.37	110.83
3	C	3476	NAP	O2D-C2D-C3D	-3.67	100.06	111.82
3	D	4476	NAP	C4D-O4D-C1D	-3.65	106.58	109.92
3	C	3476	NAP	C2B-C1B-N9A	3.64	119.74	113.75
3	B	2476	NAP	C3N-C7N-N7N	-3.62	113.27	117.74
2	C	800	G3H	O2-C2-C1	3.60	116.77	109.03
3	B	2476	NAP	C4D-O4D-C1D	-3.58	106.64	109.92
2	A	800	G3H	O3P-P-O1P	3.57	115.98	106.67
3	C	3476	NAP	C5N-C4N-C3N	3.49	123.80	120.36
3	D	4476	NAP	O4D-C4D-C3D	-3.39	98.42	105.15
3	C	3476	NAP	C2N-C3N-C4N	-3.34	114.37	118.26
3	C	3476	NAP	O7N-C7N-C3N	-3.33	115.52	119.60
3	D	4476	NAP	N9A-C8A-N7A	-3.31	109.24	113.94
3	C	3476	NAP	C2D-C3D-C4D	3.27	108.93	102.61
3	C	3476	NAP	O3X-P2B-O1X	-3.25	98.16	110.83
3	B	2476	NAP	C2D-C3D-C4D	3.03	108.46	102.61
2	D	800	G3H	O2-C2-C1	3.02	115.53	109.03
3	D	4476	NAP	C5A-N7A-C8A	3.01	108.19	103.45
3	B	2476	NAP	C4A-N9A-C8A	2.97	108.85	105.74
3	B	2476	NAP	O2A-PA-O3	2.87	115.02	107.27
3	D	4476	NAP	C4A-N9A-C8A	2.86	108.74	105.74
3	C	3476	NAP	O2N-PN-O1N	2.71	125.05	112.44
3	C	3476	NAP	C2N-C3N-C7N	2.69	127.24	119.46
3	A	1476	NAP	O5B-C5B-C4B	-2.63	100.04	108.99
3	C	3476	NAP	O4D-C4D-C3D	-2.60	99.99	105.15
3	A	1476	NAP	O3D-C3D-C2D	-2.60	103.48	111.82
3	B	2476	NAP	O3-PN-O1N	-2.58	102.95	110.70
3	A	1476	NAP	O2B-C2B-C3B	2.53	120.73	111.68
3	D	4476	NAP	O2N-PN-O1N	2.52	124.19	112.44
3	C	3476	NAP	O5D-PN-O1N	-2.49	99.07	108.94
3	C	3476	NAP	O2A-PA-O3	2.45	113.89	107.27
3	C	3476	NAP	O3D-C3D-C4D	-2.44	104.08	111.08
3	D	4476	NAP	C3N-C7N-N7N	-2.43	114.75	117.74
3	A	1476	NAP	C6N-N1N-C1D	-2.43	114.96	119.73
3	A	1476	NAP	C5A-C6A-N6A	2.38	129.18	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1476	NAP	O2B-P2B-O1X	-2.37	100.88	109.33
3	C	3476	NAP	C2B-C3B-C4B	-2.36	96.93	101.99
2	B	800	G3H	O3P-P-O2P	2.34	119.96	110.83
3	A	1476	NAP	C2N-N1N-C1D	2.34	124.30	119.13
3	D	4476	NAP	O2A-PA-O3	2.33	113.57	107.27
3	D	4476	NAP	C2N-C3N-C7N	-2.32	112.78	119.46
3	A	1476	NAP	O4B-C1B-C2B	-2.31	102.61	106.59
3	B	2476	NAP	O2N-PN-O1N	2.31	123.20	112.44
2	B	800	G3H	O4P-P-O2P	-2.28	101.95	110.83
3	B	2476	NAP	C6N-C5N-C4N	-2.27	116.17	119.45
3	C	3476	NAP	O2A-PA-O5B	2.25	117.78	107.57
3	D	4476	NAP	C4A-C5A-N7A	-2.24	108.03	110.58
3	A	1476	NAP	O2B-C2B-C1B	2.23	117.89	110.05
3	C	3476	NAP	O2X-P2B-O1X	2.23	119.51	110.83
3	C	3476	NAP	C2A-N1A-C6A	2.21	122.36	118.73
3	D	4476	NAP	O3B-C3B-C4B	-2.21	104.73	111.08
3	A	1476	NAP	O3-PN-O1N	-2.21	104.07	110.70
3	B	2476	NAP	N9A-C8A-N7A	-2.19	110.83	113.94
3	C	3476	NAP	O2N-PN-O3	2.18	113.16	107.27
3	D	4476	NAP	C4N-C3N-C7N	2.18	126.98	121.06
3	A	1476	NAP	C5N-C4N-C3N	2.15	122.48	120.36
3	B	2476	NAP	N3A-C2A-N1A	-2.15	125.32	128.58
3	A	1476	NAP	O2N-PN-O1N	2.10	122.22	112.44
3	C	3476	NAP	O5B-PA-O1A	-2.08	100.71	108.94
3	D	4476	NAP	O2D-C2D-C3D	-2.07	105.18	111.82
2	A	800	G3H	O2-C2-C1	2.04	113.43	109.03
3	A	1476	NAP	O4D-C4D-C5D	-2.04	102.80	109.33
3	B	2476	NAP	O2B-P2B-O1X	-2.03	102.09	109.33
3	B	2476	NAP	C5N-C6N-N1N	2.02	123.13	120.38
3	D	4476	NAP	O5B-C5B-C4B	-2.01	102.15	108.99
3	D	4476	NAP	C2D-C3D-C4D	2.01	106.49	102.61

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	G3H	C3-O1P-P-O2P
3	A	1476	NAP	C5D-O5D-PN-O3
3	A	1476	NAP	C5D-O5D-PN-O1N
3	A	1476	NAP	C5D-O5D-PN-O2N
3	A	1476	NAP	C2D-C1D-N1N-C2N
3	A	1476	NAP	C2D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	B	2476	NAP	C5B-O5B-PA-O1A
3	B	2476	NAP	O4D-C4D-C5D-O5D
3	B	2476	NAP	O4D-C1D-N1N-C2N
3	B	2476	NAP	C2D-C1D-N1N-C6N
3	C	3476	NAP	C5B-O5B-PA-O3
3	C	3476	NAP	O4B-C4B-C5B-O5B
3	C	3476	NAP	C3B-C4B-C5B-O5B
3	C	3476	NAP	C5D-O5D-PN-O3
3	C	3476	NAP	C5D-O5D-PN-O1N
3	C	3476	NAP	C5D-O5D-PN-O2N
3	C	3476	NAP	O4D-C4D-C5D-O5D
3	C	3476	NAP	C2D-C1D-N1N-C2N
3	C	3476	NAP	C2D-C1D-N1N-C6N
3	D	4476	NAP	C5B-O5B-PA-O1A
3	D	4476	NAP	C5D-O5D-PN-O3
3	D	4476	NAP	C5D-O5D-PN-O2N
3	B	2476	NAP	C3D-C4D-C5D-O5D
3	C	3476	NAP	C3D-C4D-C5D-O5D
3	D	4476	NAP	C3D-C4D-C5D-O5D
3	C	3476	NAP	C2N-C3N-C7N-O7N
3	C	3476	NAP	C2N-C3N-C7N-N7N
3	C	3476	NAP	C4N-C3N-C7N-N7N
3	C	3476	NAP	C4N-C3N-C7N-O7N
3	D	4476	NAP	O4D-C4D-C5D-O5D
2	B	800	G3H	C3-O1P-P-O2P
2	D	800	G3H	C3-O1P-P-O2P
3	A	1476	NAP	PN-O3-PA-O5B
3	D	4476	NAP	PN-O3-PA-O5B
3	A	1476	NAP	C2B-C1B-N9A-C8A
3	B	2476	NAP	C2B-C1B-N9A-C8A
3	C	3476	NAP	C2B-C1B-N9A-C8A
3	D	4476	NAP	C2B-C1B-N9A-C8A
3	A	1476	NAP	C5B-O5B-PA-O1A
3	B	2476	NAP	C5B-O5B-PA-O3
3	B	2476	NAP	C5D-O5D-PN-O3
3	B	2476	NAP	C5D-O5D-PN-O1N
3	C	3476	NAP	C5B-O5B-PA-O1A
3	D	4476	NAP	C5D-O5D-PN-O1N
2	C	800	G3H	C3-O1P-P-O2P
3	B	2476	NAP	C2D-C1D-N1N-C2N
3	B	2476	NAP	C2B-C1B-N9A-C4A
3	D	4476	NAP	O4B-C1B-N9A-C8A

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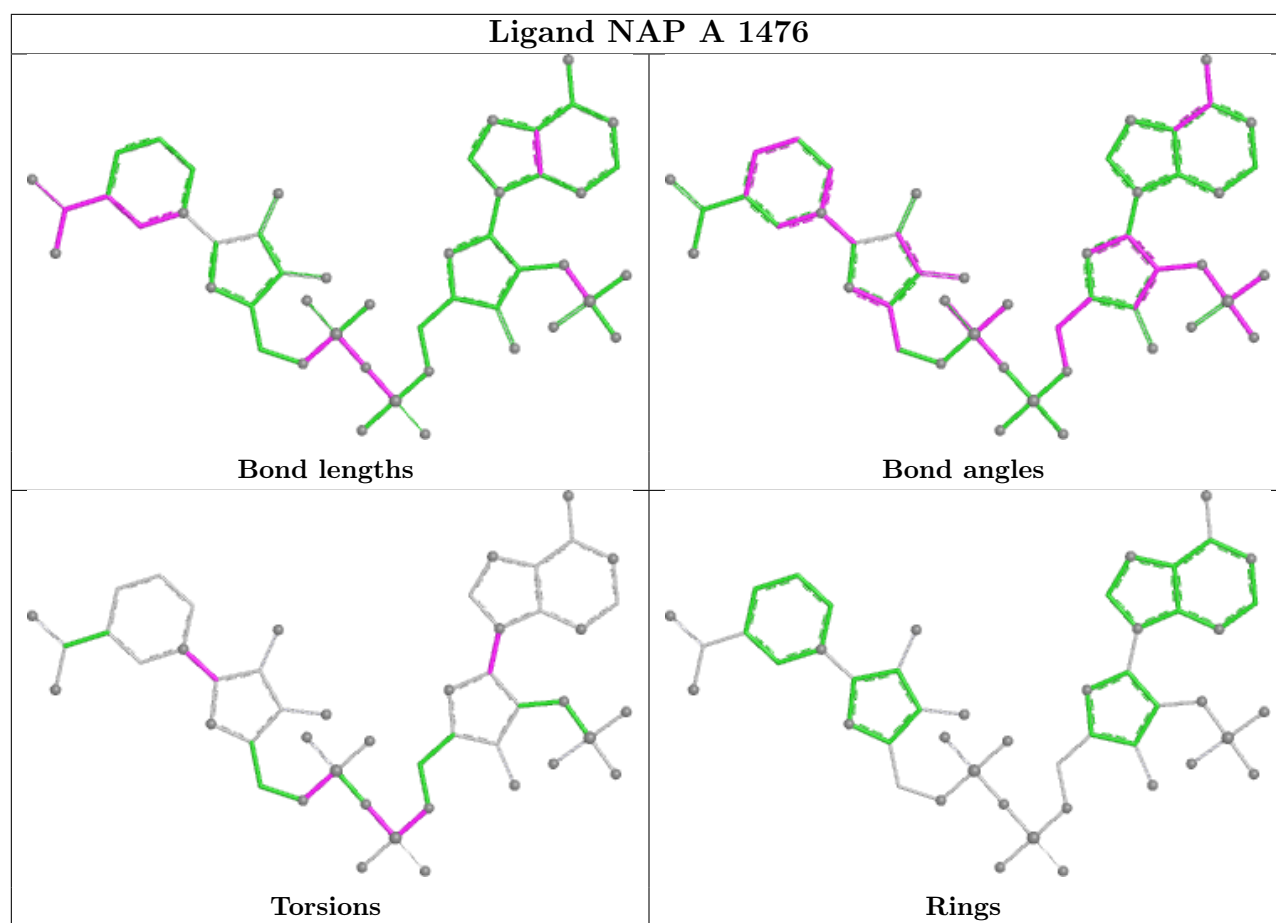
Mol	Chain	Res	Type	Atoms
3	B	2476	NAP	O4B-C1B-N9A-C8A
3	C	3476	NAP	O4B-C1B-N9A-C8A
3	C	3476	NAP	C2B-O2B-P2B-O2X
3	A	1476	NAP	C2B-C1B-N9A-C4A
3	C	3476	NAP	C2B-C1B-N9A-C4A
3	D	4476	NAP	C2B-C1B-N9A-C4A
3	A	1476	NAP	O4B-C1B-N9A-C8A

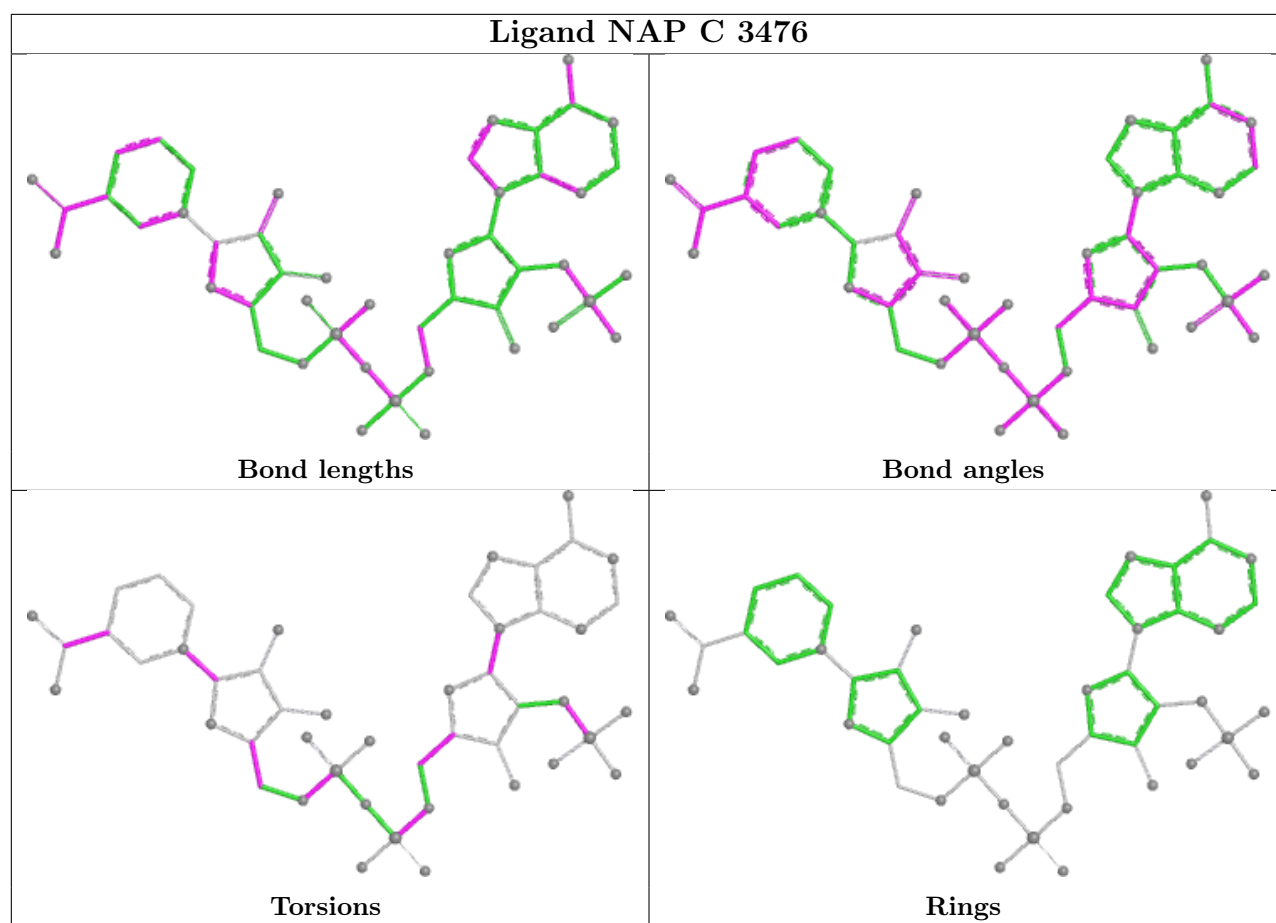
There are no ring outliers.

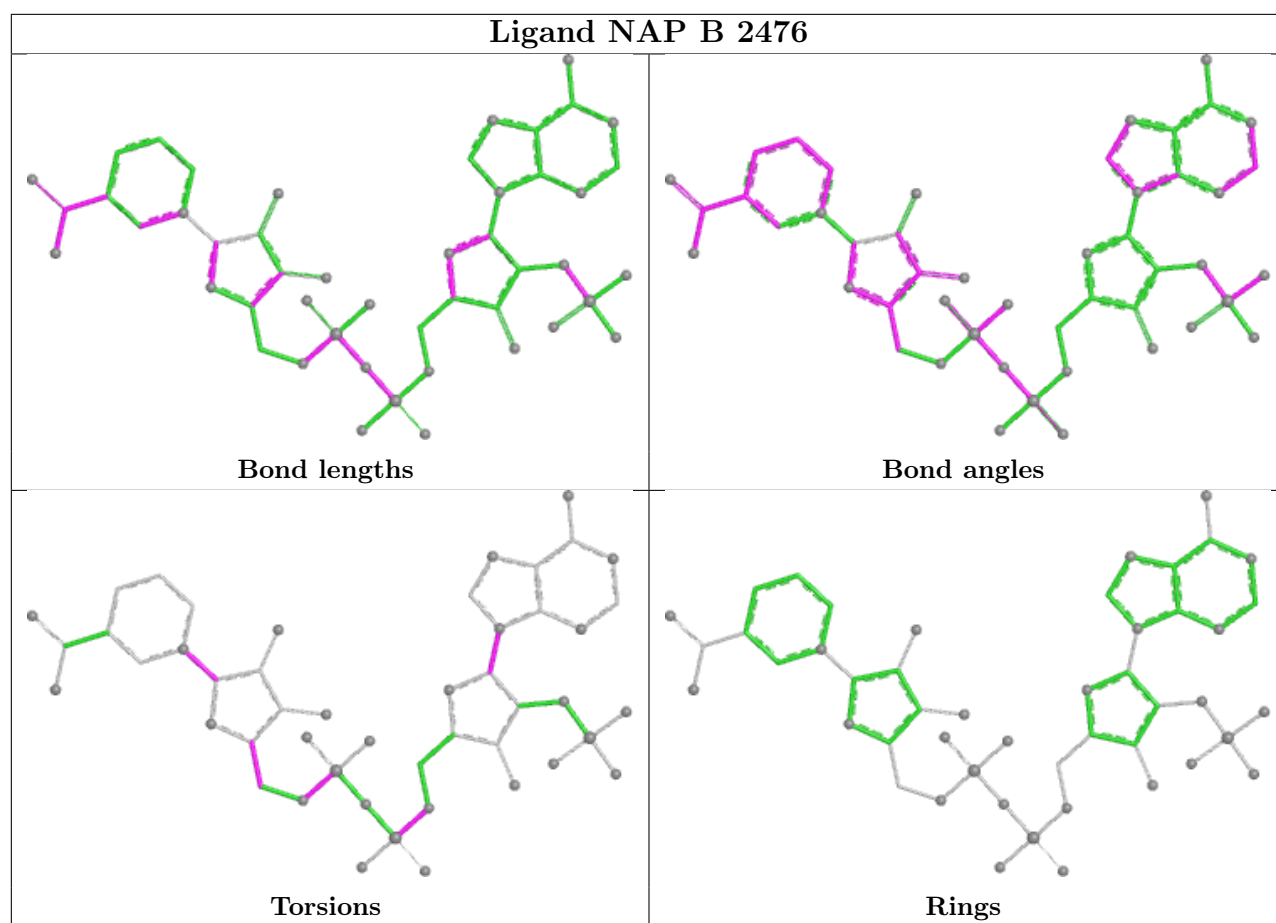
8 monomers are involved in 36 short contacts:

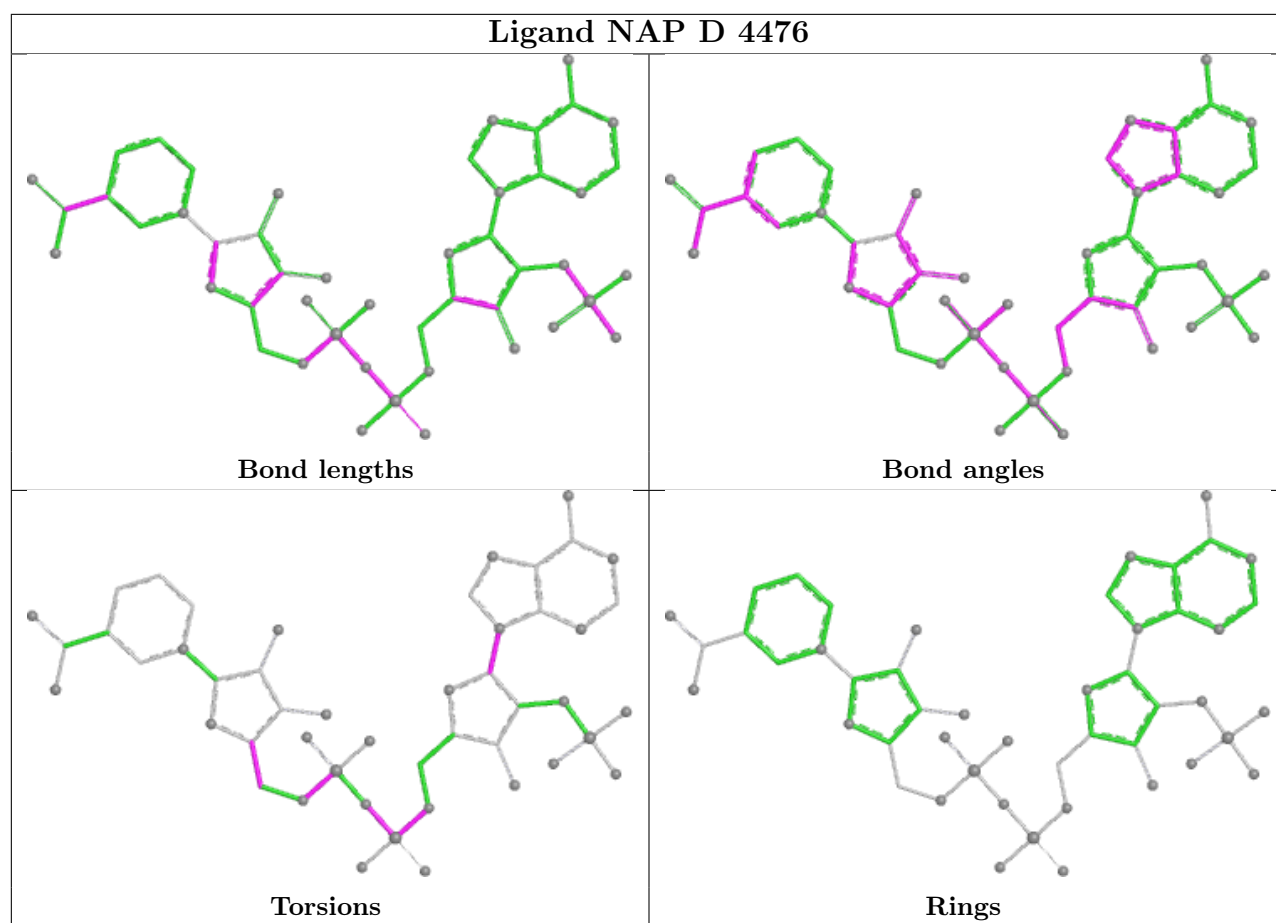
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1476	NAP	8	0
3	C	3476	NAP	8	0
3	B	2476	NAP	7	0
2	D	800	G3H	1	0
2	B	800	G3H	1	0
2	A	800	G3H	1	0
3	D	4476	NAP	9	0
2	C	800	G3H	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.33	3 (0%) 85 83	14, 29, 49, 79	1 (0%)
1	B	474/475 (99%)	-0.05	6 (1%) 75 73	16, 33, 53, 87	1 (0%)
1	C	474/475 (99%)	-0.56	2 (0%) 88 87	11, 23, 43, 63	1 (0%)
1	D	474/475 (99%)	-0.09	5 (1%) 78 76	15, 31, 51, 73	1 (0%)
All	All	1896/1900 (99%)	-0.26	16 (0%) 82 80	11, 29, 50, 87	4 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	THR	5.3
1	B	2	THR	3.7
1	D	2	THR	3.5
1	D	414	PHE	3.2
1	B	414	PHE	3.1
1	A	3	LYS	2.9
1	B	3	LYS	2.8
1	D	3	LYS	2.8
1	B	370	ASP	2.6
1	A	118	MET	2.3
1	D	118	MET	2.2
1	D	350	THR	2.2
1	B	362	ILE	2.1
1	B	118	MET	2.1
1	C	118	MET	2.1
1	C	414	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

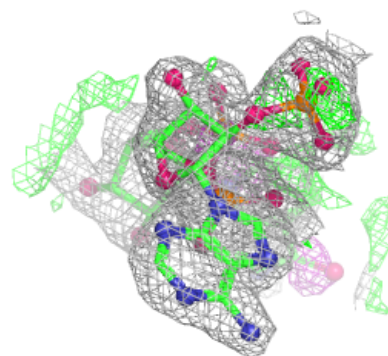
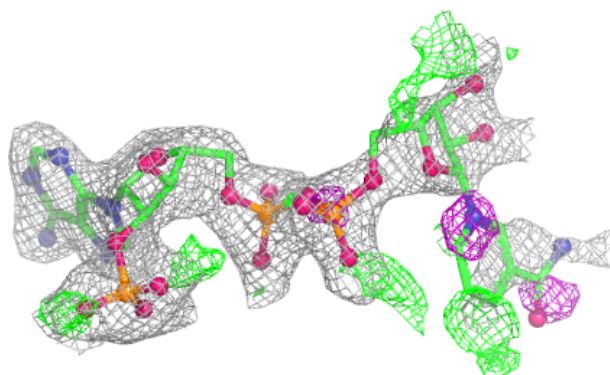
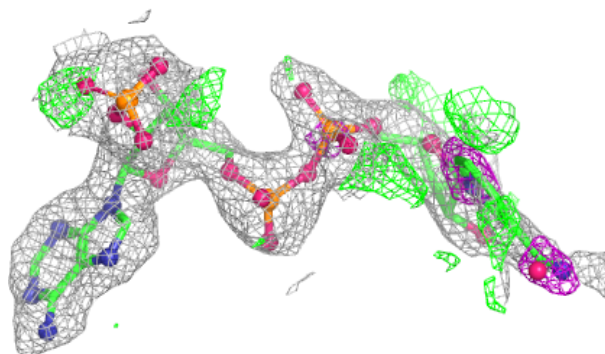
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	G3H	D	800	10/10	0.86	0.16	30,36,38,40	10
3	NAP	B	2476	48/48	0.86	0.15	33,39,41,43	48
2	G3H	A	800	10/10	0.87	0.14	29,34,35,36	10
2	G3H	B	800	10/10	0.87	0.15	31,38,39,41	10
3	NAP	A	1476	48/48	0.88	0.15	33,38,41,43	48
3	NAP	D	4476	48/48	0.88	0.15	34,41,45,47	48
3	NAP	C	3476	48/48	0.90	0.13	23,30,36,38	48
2	G3H	C	800	10/10	0.93	0.14	24,29,29,32	10

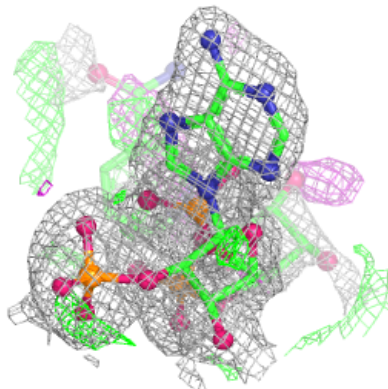
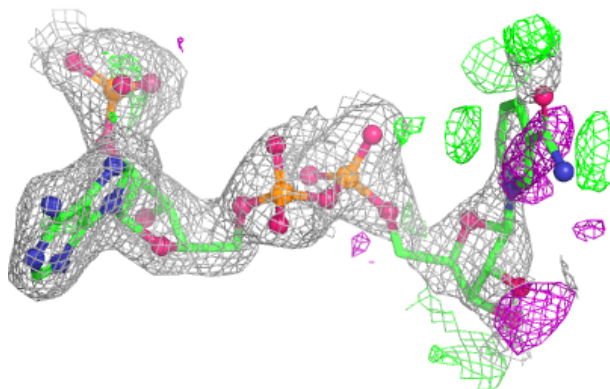
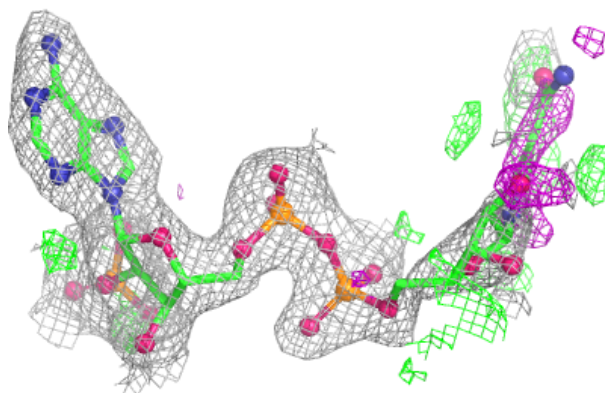
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP B 2476:

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

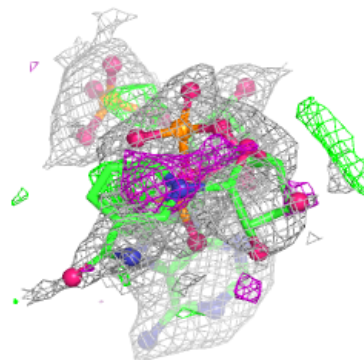
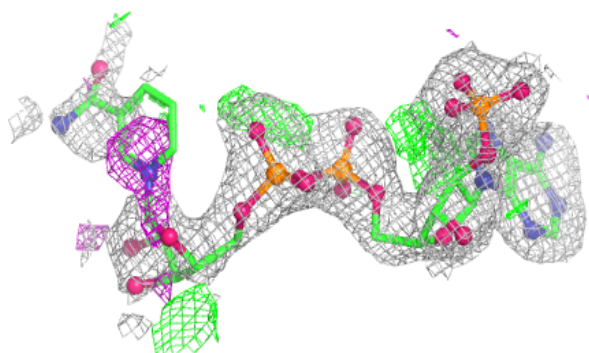
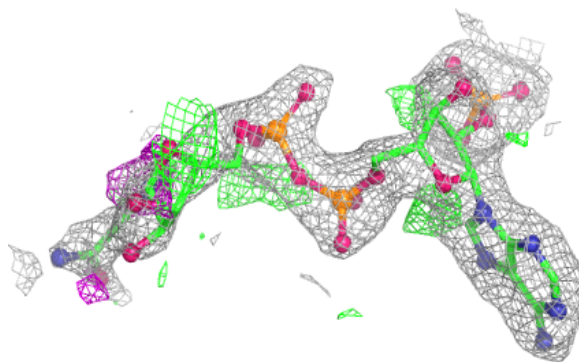
**Electron density around NAP A 1476:**

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

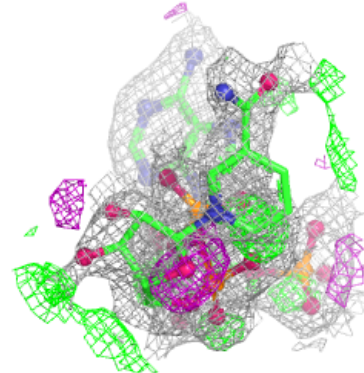
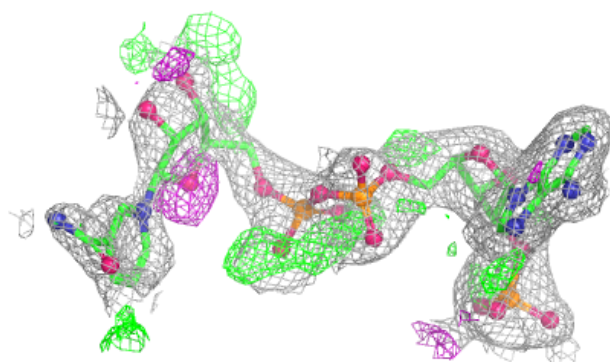
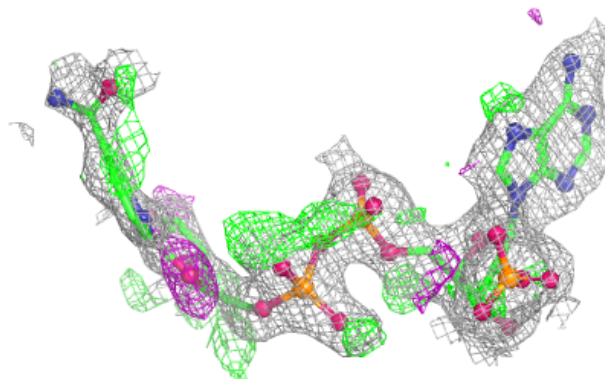


Electron density around NAP D 4476:

$2mF_o-DF_c$ (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:**

$2mF_o-DF_c$ (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.