



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:07 AM UTC

PDB ID : 1T0L / pdb_00001t0l
Title : Crystal structure of human cytosolic NADP(+)-dependent isocitrate dehydrogenase in complex with NADP, isocitrate, and calcium(2+)
Authors : Xu, X.; Zhao, J.; Peng, B.; Huang, Q.; Arnold, E.; Ding, J.
Deposited on : 2004-04-10
Resolution : 2.41 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

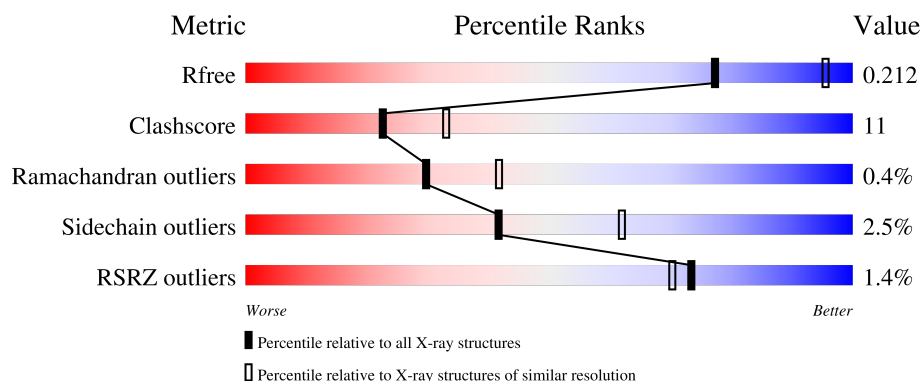
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	414	 78% 21% .
1	B	414	 79% 21% .
1	C	414	 79% 19% .
1	D	414	 79% 18% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14286 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.

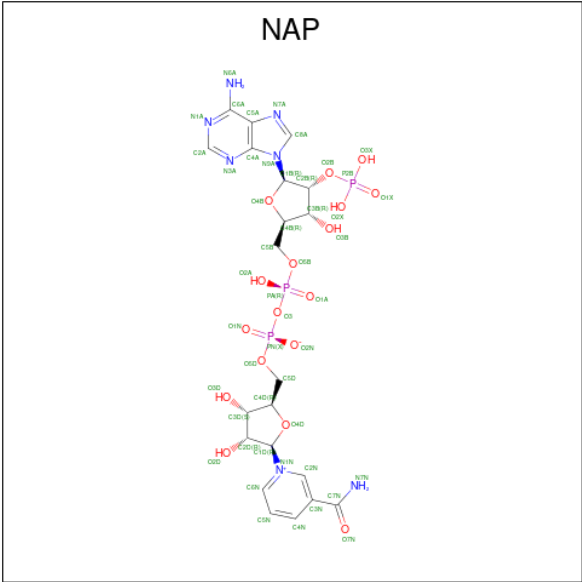
- Molecule 1 is a protein called Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3281	2085	556	621	19			
1	B	414	Total	C	N	O	S	0	0	0
			3281	2085	556	621	19			
1	C	414	Total	C	N	O	S	0	0	0
			3281	2085	556	621	19			
1	D	414	Total	C	N	O	S	0	0	0
			3281	2085	556	621	19			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

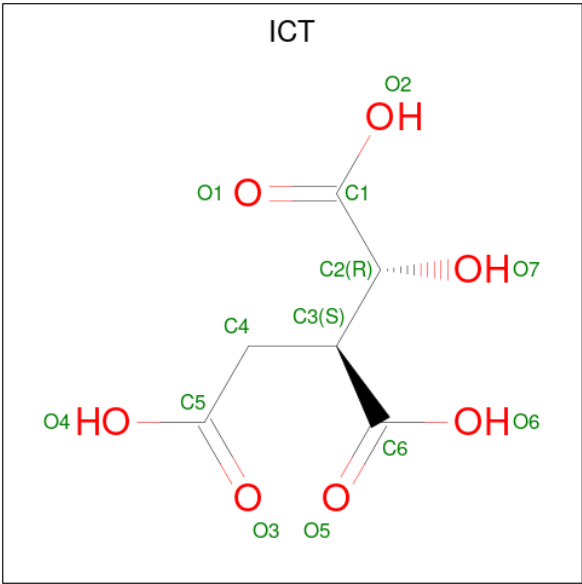
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

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



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

- Molecule 4 is ISOCITRIC ACID (CCD ID: ICT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0
4	C	1	Total C O 13 6 7	0	0
4	D	1	Total C O 13 6 7	0	0

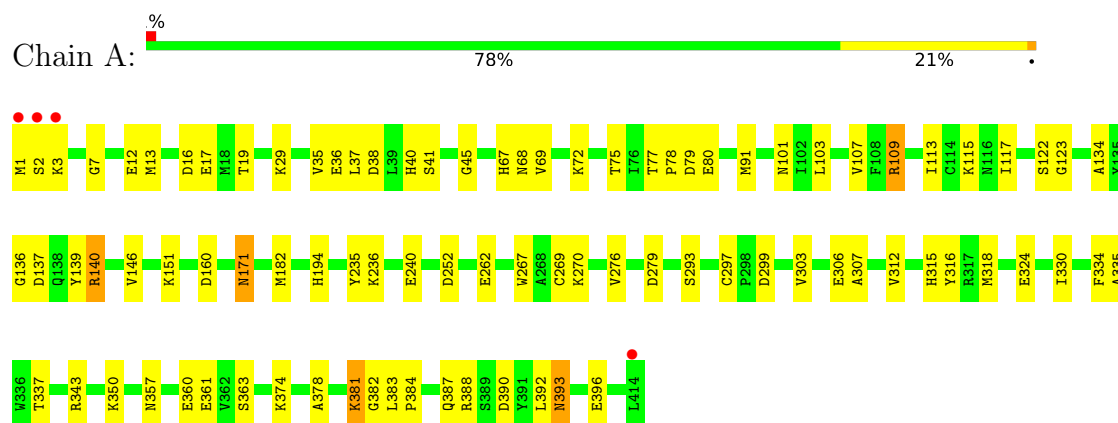
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	227	Total O 227 227	0	0
5	B	221	Total O 221 221	0	0
5	C	226	Total O 226 226	0	0
5	D	240	Total O 240 240	0	0

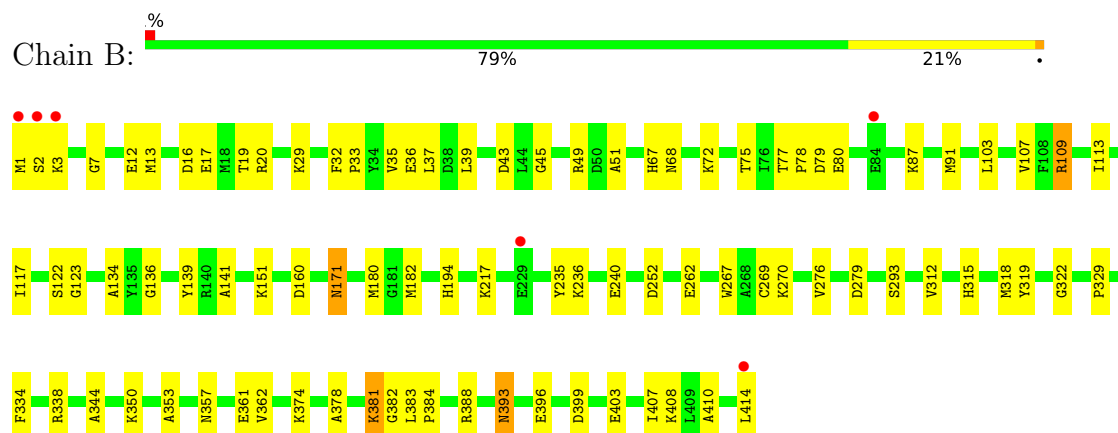
3 Residue-property plots

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.

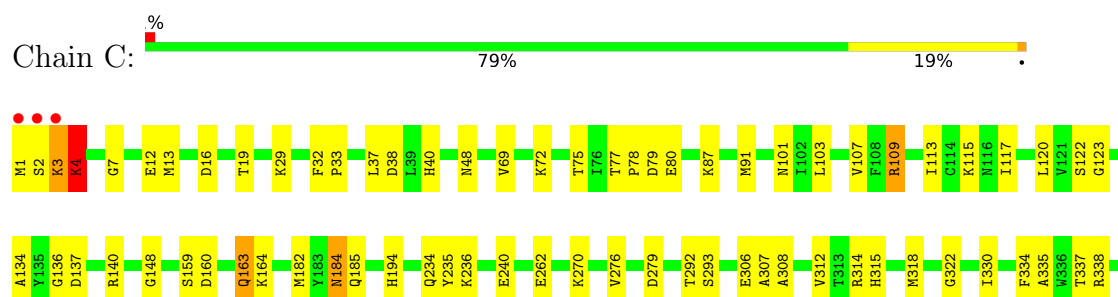
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

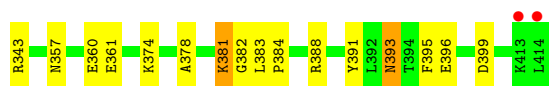


- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

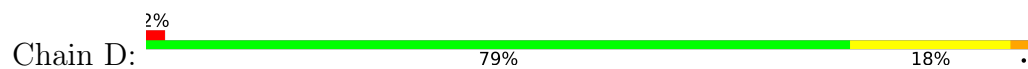


- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic





- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.30Å 86.74Å 115.77Å 90.00° 107.15° 90.00°	Depositor
Resolution (Å)	12.00 – 2.41 12.00 – 2.41	Depositor EDS
% Data completeness (in resolution range)	94.2 (12.00-2.41) 93.4 (12.00-2.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.40Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.253 0.216 , 0.212	Depositor DCC
R_{free} test set	3562 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 70.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14286	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ICT, 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	0.41	0/3349	0.98	24/4513 (0.5%)
1	B	0.40	0/3349	0.96	18/4513 (0.4%)
1	C	0.41	0/3349	0.98	23/4513 (0.5%)
1	D	0.41	0/3349	0.98	23/4513 (0.5%)
All	All	0.41	0/13396	0.98	88/18052 (0.5%)

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	D	0	1

There are no bond length outliers.

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	SER	N-CA-C	9.30	121.42	111.28
1	C	122	SER	N-CA-C	9.20	121.31	111.28
1	B	122	SER	N-CA-C	9.12	121.22	111.28
1	D	122	SER	N-CA-C	8.91	121.00	111.28
1	C	330	ILE	N-CA-C	7.69	118.43	110.36
1	D	113	ILE	N-CA-C	7.20	119.43	108.71
1	A	113	ILE	N-CA-C	7.14	119.34	108.71
1	C	113	ILE	N-CA-C	7.11	119.30	108.71
1	B	113	ILE	N-CA-C	7.06	119.24	108.71
1	A	117	ILE	N-CA-C	6.99	114.47	107.55
1	C	3	LYS	N-CA-C	6.84	116.36	108.49
1	B	117	ILE	N-CA-C	6.56	114.62	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	117	ILE	N-CA-C	6.54	114.59	107.60
1	D	78	PRO	N-CA-C	6.48	121.00	111.03
1	D	136	GLY	N-CA-C	6.40	123.45	111.80
1	C	77	THR	CA-C-N	6.38	126.34	119.76
1	C	77	THR	C-N-CA	6.38	126.34	119.76
1	B	78	PRO	N-CA-C	6.38	120.86	111.03
1	A	297	CYS	CA-C-N	6.32	125.81	119.24
1	A	297	CYS	C-N-CA	6.32	125.81	119.24
1	A	78	PRO	N-CA-C	6.26	120.67	111.03
1	C	117	ILE	N-CA-C	6.17	114.20	107.60
1	D	381	LYS	N-CA-C	-6.16	101.67	110.59
1	A	41	SER	N-CA-C	6.15	120.30	109.96
1	B	382	GLY	N-CA-C	-6.13	104.36	112.82
1	B	77	THR	CA-C-N	6.11	126.43	119.83
1	B	77	THR	C-N-CA	6.11	126.43	119.83
1	A	381	LYS	N-CA-C	-6.06	101.81	110.59
1	D	77	THR	CA-C-N	6.05	126.37	119.83
1	D	77	THR	C-N-CA	6.05	126.37	119.83
1	A	136	GLY	N-CA-C	5.99	122.70	111.80
1	C	78	PRO	N-CA-C	5.97	120.46	111.14
1	A	77	THR	CA-C-N	5.97	126.28	119.83
1	A	77	THR	C-N-CA	5.97	126.28	119.83
1	D	382	GLY	N-CA-C	-5.97	104.58	112.82
1	A	382	GLY	N-CA-C	-5.96	104.60	112.82
1	C	381	LYS	N-CA-C	-5.94	101.97	110.59
1	B	381	LYS	N-CA-C	-5.94	101.98	110.59
1	C	136	GLY	N-CA-C	5.90	122.99	112.02
1	D	406	LYS	N-CA-C	-5.89	104.68	112.34
1	D	276	VAL	N-CA-C	5.87	116.04	110.53
1	C	382	GLY	N-CA-C	-5.83	104.78	112.82
1	D	37	LEU	N-CA-C	5.79	118.65	109.50
1	C	72	LYS	N-CA-C	5.77	118.80	109.40
1	C	307	ALA	N-CA-C	-5.74	100.35	109.76
1	D	38	ASP	N-CA-C	-5.73	97.86	108.24
1	D	16	ASP	N-CA-C	5.72	118.56	109.81
1	D	146	VAL	CA-C-N	5.71	125.39	119.56
1	D	146	VAL	C-N-CA	5.71	125.39	119.56
1	B	374	LYS	N-CA-C	5.71	118.24	111.33
1	A	276	VAL	N-CA-C	5.69	115.88	110.53
1	C	335	ALA	N-CA-C	-5.69	105.16	111.36
1	A	72	LYS	N-CA-C	5.67	118.65	109.40
1	C	276	VAL	N-CA-C	5.64	115.83	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	VAL	CA-C-N	5.60	125.44	119.28
1	A	146	VAL	C-N-CA	5.60	125.44	119.28
1	B	276	VAL	N-CA-C	5.59	115.78	110.53
1	C	374	LYS	N-CA-C	5.56	118.06	111.33
1	B	16	ASP	N-CA-C	5.56	118.32	109.81
1	D	335	ALA	N-CA-C	-5.56	105.30	111.36
1	B	79	ASP	N-CA-C	-5.54	101.32	109.18
1	A	79	ASP	N-CA-C	-5.51	101.35	109.18
1	A	374	LYS	N-CA-C	5.48	117.97	111.33
1	D	374	LYS	N-CA-C	5.43	117.90	111.33
1	A	307	ALA	N-CA-C	-5.41	101.46	110.17
1	D	79	ASP	N-CA-C	-5.38	101.54	109.18
1	D	72	LYS	N-CA-C	5.38	118.16	109.40
1	D	270	LYS	N-CA-C	-5.37	103.44	110.53
1	C	79	ASP	N-CA-C	-5.35	101.58	109.18
1	B	72	LYS	N-CA-C	5.34	118.11	109.40
1	C	16	ASP	N-CA-C	5.32	117.94	109.81
1	A	45	GLY	N-CA-C	-5.27	105.87	111.93
1	C	115	LYS	N-CA-C	5.22	117.71	111.71
1	A	335	ALA	N-CA-C	-5.21	105.68	111.36
1	C	270	LYS	N-CA-C	-5.20	103.67	110.53
1	C	148	GLY	CA-C-N	5.18	126.32	119.84
1	C	148	GLY	C-N-CA	5.18	126.32	119.84
1	A	16	ASP	N-CA-C	5.17	117.72	109.81
1	B	39	LEU	N-CA-C	5.17	117.97	109.76
1	B	45	GLY	N-CA-C	-5.17	105.99	111.93
1	D	35	VAL	N-CA-C	5.17	115.56	108.12
1	B	270	LYS	N-CA-C	-5.10	103.80	110.53
1	C	391	TYR	N-CA-C	5.07	116.01	108.86
1	B	136	GLY	N-CA-C	5.06	123.10	112.17
1	A	270	LYS	N-CA-C	-5.06	103.86	110.53
1	B	217	LYS	N-CA-C	5.05	117.44	111.33
1	A	115	LYS	N-CA-C	5.05	117.52	111.71
1	D	45	GLY	N-CA-C	-5.04	106.13	111.93

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	183	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3281	0	3256	62	0
1	B	3281	0	3256	63	0
1	C	3281	0	3256	62	0
1	D	3281	0	3256	95	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	48	0	25	3	0
3	B	48	0	25	4	0
3	C	48	0	25	5	0
3	D	48	0	25	4	0
4	A	13	0	5	3	0
4	B	13	0	5	2	0
4	C	13	0	5	3	0
4	D	13	0	5	2	0
5	A	227	0	0	3	0
5	B	221	0	0	4	0
5	C	226	0	0	4	0
5	D	240	0	0	4	0
All	All	14286	0	13144	279	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (279) 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:407:ILE:HA	1:D:413:LYS:HB2	1.36	1.07
1:B:51:ALA:HB1	1:C:87:LYS:HG3	1.35	1.06
1:D:404:ASN:O	1:D:407:ILE:HB	1.55	1.05
1:B:315:HIS:HA	1:B:318:MET:HE3	1.42	1.01
1:C:393:ASN:ND2	1:C:396:GLU:H	1.66	0.94
1:D:412:ALA:O	1:D:413:LYS:HG3	1.68	0.93
1:A:393:ASN:C	1:A:393:ASN:HD22	1.78	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LYS:HD3	1:A:36:GLU:HG3	1.50	0.91
1:D:407:ILE:HA	1:D:413:LYS:CB	2.01	0.89
1:D:407:ILE:CA	1:D:413:LYS:HB2	2.02	0.88
1:C:3:LYS:HB3	5:C:1875:HOH:O	1.72	0.88
1:C:1:MET:HA	1:C:32:PHE:HB3	1.56	0.88
1:D:407:ILE:HG23	1:D:413:LYS:N	1.88	0.87
1:A:393:ASN:ND2	1:A:396:GLU:H	1.73	0.86
1:D:393:ASN:C	1:D:393:ASN:HD22	1.85	0.84
1:D:137:ASP:HA	1:D:182:MET:HE3	1.62	0.82
1:D:406:LYS:C	1:D:413:LYS:HD2	2.05	0.82
1:D:407:ILE:HG12	1:D:413:LYS:HB2	1.62	0.79
1:A:2:SER:O	1:A:3:LYS:HG3	1.83	0.79
1:A:3:LYS:HB3	1:A:36:GLU:HB2	1.65	0.77
1:D:404:ASN:HA	1:D:407:ILE:HG13	1.65	0.77
1:C:393:ASN:C	1:C:393:ASN:HD22	1.92	0.77
1:B:3:LYS:HG2	1:B:32:PHE:O	1.85	0.77
1:A:151:LYS:HE2	1:A:171:ASN:HD21	1.49	0.77
1:A:137:ASP:HA	1:A:182:MET:HE3	1.68	0.76
1:B:51:ALA:CB	1:C:87:LYS:HG3	2.14	0.76
1:B:393:ASN:HD22	1:B:393:ASN:C	1.94	0.74
1:C:393:ASN:HD21	1:C:396:GLU:H	1.33	0.73
1:D:393:ASN:ND2	1:D:396:GLU:H	1.85	0.73
1:D:407:ILE:HG12	1:D:413:LYS:CB	2.19	0.73
1:D:407:ILE:HG12	1:D:413:LYS:C	2.13	0.72
1:D:404:ASN:HA	1:D:407:ILE:CD1	2.21	0.70
1:C:292:THR:HG21	1:C:338:ARG:NH1	2.06	0.70
1:D:410:ALA:HB2	1:D:413:LYS:HZ1	1.54	0.70
1:B:151:LYS:HG3	1:B:171:ASN:ND2	2.07	0.70
1:C:3:LYS:O	1:C:4:LYS:HB2	1.91	0.70
1:B:3:LYS:HD3	1:B:36:GLU:HA	1.73	0.70
1:B:7:GLY:HA3	1:B:37:LEU:HD23	1.74	0.70
1:A:3:LYS:HE3	1:A:36:GLU:HA	1.73	0.69
1:D:404:ASN:O	1:D:407:ILE:CB	2.36	0.69
1:C:101:ASN:HB2	5:C:1908:HOH:O	1.92	0.69
1:D:406:LYS:HB3	1:D:413:LYS:HD2	1.74	0.68
1:D:404:ASN:HA	1:D:407:ILE:CG1	2.23	0.68
1:D:410:ALA:HB2	1:D:413:LYS:NZ	2.09	0.67
1:C:279:ASP:OD2	1:D:252:ASP:HB3	1.95	0.67
1:B:393:ASN:ND2	1:B:396:GLU:H	1.93	0.67
1:D:315:HIS:HA	1:D:318:MET:HE2	1.76	0.67
1:A:3:LYS:CD	1:A:36:GLU:HG3	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:LEU:HD23	5:D:1768:HOH:O	1.95	0.66
1:C:75:THR:H	3:C:1517:NAP:H71N	1.44	0.65
1:D:407:ILE:CG1	1:D:413:LYS:HB2	2.25	0.65
1:B:29:LYS:NZ	1:B:399:ASP:OD1	2.30	0.65
1:C:137:ASP:HA	1:C:182:MET:HE3	1.79	0.65
1:D:407:ILE:HG23	1:D:413:LYS:H	1.62	0.64
1:A:7:GLY:HA3	1:A:37:LEU:HD23	1.79	0.64
1:A:393:ASN:HD21	1:A:396:GLU:H	1.45	0.64
1:B:1:MET:N	1:B:3:LYS:HE3	2.11	0.64
1:D:101:ASN:HB2	5:D:1734:HOH:O	1.97	0.64
1:D:412:ALA:O	1:D:413:LYS:CG	2.44	0.63
1:B:151:LYS:HG3	1:B:171:ASN:HD21	1.65	0.62
1:B:3:LYS:CD	1:B:36:GLU:HA	2.30	0.62
1:C:75:THR:O	3:C:1517:NAP:H2N	2.00	0.62
1:C:2:SER:HB2	1:C:32:PHE:O	1.99	0.61
1:D:187:LYS:HE3	5:D:1954:HOH:O	2.00	0.61
1:C:38:ASP:OD2	1:C:40:HIS:HE1	1.82	0.61
1:B:75:THR:O	3:B:1516:NAP:H2N	2.00	0.61
1:D:156:TYR:CE2	1:D:158:PRO:HG3	2.36	0.61
1:B:3:LYS:HD2	1:B:36:GLU:CD	2.26	0.60
1:D:39:LEU:HD12	1:D:41:SER:OG	2.01	0.60
1:A:75:THR:H	3:A:1515:NAP:H71N	1.50	0.60
1:A:279:ASP:OD2	1:B:252:ASP:HB3	2.01	0.60
3:B:1516:NAP:C4N	4:B:1617:ICT:H2	2.31	0.60
1:C:315:HIS:HA	1:C:318:MET:HE3	1.83	0.60
1:C:2:SER:HB2	1:C:33:PRO:HA	1.84	0.60
1:D:407:ILE:HD13	1:D:414:LEU:C	2.27	0.60
1:B:75:THR:H	3:B:1516:NAP:H71N	1.49	0.58
1:D:29:LYS:NZ	1:D:399:ASP:OD1	2.28	0.58
1:A:315:HIS:HA	1:A:318:MET:CE	2.33	0.58
1:C:2:SER:CB	1:C:33:PRO:HA	2.33	0.58
1:D:406:LYS:O	1:D:413:LYS:HD2	2.02	0.58
1:C:383:LEU:HB3	1:C:384:PRO:HD3	1.86	0.58
1:A:194:HIS:HD2	1:A:235:TYR:OH	1.87	0.57
1:B:383:LEU:HB3	1:B:384:PRO:HD3	1.86	0.57
1:A:1:MET:HE1	1:A:3:LYS:NZ	2.20	0.57
1:B:350:LYS:HG2	5:B:1743:HOH:O	2.04	0.57
1:C:194:HIS:HD2	1:C:235:TYR:OH	1.87	0.57
1:B:1:MET:H3	1:B:3:LYS:HE3	1.67	0.57
1:D:393:ASN:ND2	1:D:396:GLU:HG3	2.19	0.57
1:D:194:HIS:HD2	1:D:235:TYR:OH	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:ASN:C	1:D:393:ASN:ND2	2.59	0.56
1:B:3:LYS:HD3	1:B:35:VAL:O	2.05	0.56
1:B:151:LYS:NZ	1:B:171:ASN:HD21	2.04	0.56
1:D:383:LEU:HB3	1:D:384:PRO:HD3	1.86	0.56
1:B:87:LYS:HE2	1:C:48:ASN:OD1	2.06	0.56
1:A:383:LEU:HB3	1:A:384:PRO:HD3	1.87	0.56
1:C:393:ASN:ND2	1:C:396:GLU:HG3	2.20	0.56
3:D:1518:NAP:C4N	4:D:1619:ICT:H2	2.36	0.55
1:C:123:GLY:O	1:C:262:GLU:HA	2.06	0.55
1:D:407:ILE:HG23	1:D:412:ALA:C	2.31	0.55
4:A:1616:ICT:H41	5:B:1886:HOH:O	2.07	0.55
1:C:69:VAL:HG11	1:C:343:ARG:HD2	1.88	0.55
1:A:1:MET:HE2	1:A:3:LYS:HD2	1.88	0.54
1:D:406:LYS:CB	1:D:413:LYS:HD2	2.38	0.54
1:C:2:SER:O	1:C:3:LYS:HG3	2.06	0.54
1:B:1:MET:N	1:B:1:MET:HE2	2.21	0.54
1:B:3:LYS:HB2	1:B:36:GLU:OE1	2.07	0.54
1:B:194:HIS:HD2	1:B:235:TYR:OH	1.90	0.54
1:C:29:LYS:NZ	1:C:399:ASP:OD1	2.30	0.54
1:D:407:ILE:HA	1:D:413:LYS:CG	2.37	0.54
1:D:407:ILE:O	1:D:408:LYS:C	2.51	0.54
1:D:407:ILE:O	1:D:412:ALA:O	2.26	0.53
1:A:393:ASN:C	1:A:393:ASN:ND2	2.52	0.53
1:B:180:MET:HE2	1:B:182:MET:HE2	1.89	0.53
1:A:69:VAL:HG11	1:A:343:ARG:HD2	1.90	0.53
1:A:75:THR:O	3:A:1515:NAP:H2N	2.09	0.53
1:A:393:ASN:ND2	1:A:396:GLU:HG3	2.24	0.53
1:B:3:LYS:HD2	1:B:36:GLU:OE2	2.09	0.53
1:D:107:VAL:HG23	1:D:134:ALA:HB2	1.90	0.53
1:D:383:LEU:HD13	1:D:383:LEU:C	2.34	0.53
1:D:407:ILE:HA	1:D:412:ALA:C	2.33	0.53
1:D:378:ALA:O	1:D:381:LYS:O	2.27	0.53
1:C:80:GLU:HG3	1:C:91:MET:CE	2.39	0.52
1:A:107:VAL:HG23	1:A:134:ALA:HB2	1.91	0.52
1:C:109:ARG:HD3	1:C:293:SER:OG	2.10	0.52
1:C:140:ARG:O	1:C:140:ARG:HG3	2.09	0.52
1:A:383:LEU:C	1:A:383:LEU:HD13	2.35	0.52
1:A:378:ALA:O	1:A:381:LYS:O	2.27	0.52
1:A:123:GLY:O	1:A:262:GLU:HA	2.09	0.52
3:C:1517:NAP:C4N	4:C:1618:ICT:H2	2.40	0.52
1:D:413:LYS:O	1:D:414:LEU:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:ALA:O	1:B:381:LYS:O	2.28	0.51
1:C:2:SER:OG	1:C:33:PRO:HA	2.10	0.51
1:D:407:ILE:HG22	1:D:412:ALA:HA	1.91	0.51
1:B:80:GLU:HG3	1:B:91:MET:CE	2.40	0.51
1:A:3:LYS:HD3	1:A:36:GLU:CG	2.34	0.51
1:B:141:ALA:HB1	1:B:180:MET:HE3	1.93	0.51
1:C:378:ALA:O	1:C:381:LYS:O	2.28	0.51
1:D:315:HIS:HA	1:D:318:MET:CE	2.40	0.51
1:D:80:GLU:HG3	1:D:91:MET:CE	2.41	0.51
1:B:107:VAL:HG23	1:B:134:ALA:HB2	1.92	0.51
1:B:267:TRP:CD1	1:B:269:CYS:HG	2.28	0.51
1:D:405:LEU:C	1:D:407:ILE:N	2.66	0.51
1:B:49:ARG:HD2	5:B:1736:HOH:O	2.11	0.51
1:C:383:LEU:C	1:C:383:LEU:HD13	2.35	0.51
1:D:39:LEU:CD1	1:D:41:SER:OG	2.58	0.51
1:A:324:GLU:CD	1:A:388:ARG:HH12	2.19	0.51
1:B:80:GLU:HG3	1:B:91:MET:HE1	1.92	0.51
1:A:267:TRP:CD1	1:A:269:CYS:HG	2.29	0.51
1:D:404:ASN:CA	1:D:407:ILE:HG13	2.39	0.51
1:B:109:ARG:HD3	1:B:293:SER:OG	2.12	0.50
1:C:80:GLU:HG3	1:C:91:MET:HE1	1.92	0.50
1:D:142:THR:HG23	1:D:142:THR:O	2.12	0.50
1:D:361:GLU:OE2	1:D:408:LYS:NZ	2.39	0.50
1:D:404:ASN:HD22	1:D:407:ILE:HD11	1.77	0.50
1:D:404:ASN:ND2	1:D:407:ILE:HD11	2.27	0.50
1:C:393:ASN:HD21	1:C:396:GLU:N	2.06	0.50
3:A:1515:NAP:C4N	4:A:1616:ICT:H2	2.41	0.50
1:C:315:HIS:HA	1:C:318:MET:CE	2.41	0.50
1:D:404:ASN:HA	1:D:407:ILE:HD12	1.92	0.50
1:D:407:ILE:HG22	1:D:408:LYS:N	2.27	0.50
1:A:80:GLU:HG3	1:A:91:MET:CE	2.42	0.49
1:B:2:SER:O	1:B:33:PRO:HA	2.12	0.49
1:D:75:THR:O	3:D:1518:NAP:H2N	2.12	0.49
1:A:383:LEU:N	1:A:384:PRO:CD	2.75	0.49
1:D:80:GLU:HG3	1:D:91:MET:HE1	1.94	0.49
1:B:362:VAL:HG23	1:B:408:LYS:HD2	1.95	0.49
1:B:383:LEU:HD13	1:B:383:LEU:C	2.37	0.49
1:D:383:LEU:N	1:D:384:PRO:CD	2.76	0.49
1:A:315:HIS:HA	1:A:318:MET:HE2	1.93	0.49
1:D:407:ILE:HA	1:D:412:ALA:O	2.13	0.49
1:A:1:MET:HE1	1:A:3:LYS:HZ3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:HG3	1:A:91:MET:HE1	1.94	0.48
1:D:407:ILE:HG12	1:D:413:LYS:CA	2.43	0.48
1:B:383:LEU:N	1:B:384:PRO:CD	2.77	0.48
1:B:410:ALA:O	1:B:414:LEU:HD13	2.13	0.48
1:C:334:PHE:CZ	1:C:360:GLU:HG2	2.47	0.48
1:A:393:ASN:HD22	1:A:396:GLU:H	1.59	0.48
1:C:107:VAL:HG23	1:C:134:ALA:HB2	1.95	0.48
1:B:139:TYR:CD1	1:B:139:TYR:N	2.82	0.48
1:A:324:GLU:OE1	1:A:388:ARG:NH1	2.46	0.48
1:B:1:MET:HE2	1:B:1:MET:H1	1.79	0.48
1:C:383:LEU:N	1:C:384:PRO:CD	2.76	0.48
1:D:406:LYS:O	1:D:413:LYS:NZ	2.46	0.48
1:B:334:PHE:O	1:B:338:ARG:HB2	2.14	0.47
1:C:7:GLY:HA3	1:C:37:LEU:HD23	1.96	0.47
1:B:3:LYS:HB3	1:B:35:VAL:C	2.38	0.47
1:D:7:GLY:HA3	1:D:37:LEU:HD23	1.97	0.47
1:D:406:LYS:HG2	1:D:413:LYS:HE2	1.96	0.47
1:D:137:ASP:CA	1:D:182:MET:HE3	2.41	0.47
1:D:294:VAL:CG1	1:D:303:VAL:HG13	2.44	0.47
1:C:184:ASN:HD22	1:C:185:GLN:H	1.63	0.47
1:A:393:ASN:HD21	1:A:396:GLU:N	2.12	0.47
1:B:20:ARG:NH2	1:B:43:ASP:OD1	2.47	0.47
1:A:140:ARG:O	1:A:140:ARG:HG3	2.15	0.47
1:A:330:ILE:HD12	1:A:363:SER:HB3	1.96	0.47
1:D:406:LYS:O	1:D:413:LYS:CD	2.63	0.47
1:A:109:ARG:HD3	1:A:293:SER:OG	2.15	0.47
1:A:3:LYS:HG2	1:A:35:VAL:O	2.15	0.46
1:A:252:ASP:HB3	1:B:279:ASP:OD2	2.14	0.46
1:A:388:ARG:HD2	1:A:388:ARG:O	2.15	0.46
1:D:12:GLU:HG2	1:D:13:MET:N	2.30	0.46
1:D:407:ILE:CG2	1:D:412:ALA:HA	2.46	0.46
1:C:163:GLN:H	1:C:163:GLN:HG3	1.39	0.46
1:D:393:ASN:HD21	1:D:396:GLU:HG3	1.79	0.46
1:B:123:GLY:O	1:B:262:GLU:HA	2.16	0.46
1:D:404:ASN:ND2	1:D:407:ILE:CD1	2.79	0.46
1:B:236:LYS:O	1:B:240:GLU:HG3	2.17	0.45
1:C:109:ARG:NH2	4:C:1618:ICT:O2	2.39	0.45
1:C:314:ARG:HD2	3:C:1517:NAP:O3B	2.17	0.45
1:D:75:THR:H	3:D:1518:NAP:H71N	1.64	0.45
1:A:334:PHE:HA	1:A:337:THR:OG1	2.17	0.45
1:A:387:GLN:O	1:A:390:ASP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:TYR:OH	1:C:322:GLY:HA2	2.17	0.44
1:C:334:PHE:HA	1:C:337:THR:OG1	2.16	0.44
1:D:292:THR:HA	5:D:1752:HOH:O	2.17	0.44
1:A:29:LYS:HE3	5:A:1789:HOH:O	2.17	0.44
1:D:407:ILE:HA	1:D:413:LYS:HG3	1.99	0.44
1:A:38:ASP:OD2	1:A:40:HIS:HE1	2.01	0.44
1:B:322:GLY:HA3	1:C:395:PHE:CD2	2.52	0.44
1:D:407:ILE:HG12	1:D:413:LYS:O	2.16	0.44
1:C:164:LYS:HE3	1:C:164:LYS:HB3	1.90	0.44
1:A:236:LYS:O	1:A:240:GLU:HG3	2.18	0.44
1:C:308:ALA:HB3	5:C:1909:HOH:O	2.17	0.44
1:B:160:ASP:C	1:B:160:ASP:OD1	2.60	0.44
1:A:101:ASN:HB2	5:A:1772:HOH:O	2.18	0.44
1:C:2:SER:HB2	1:C:33:PRO:CA	2.47	0.44
1:C:334:PHE:CE2	1:C:360:GLU:HG2	2.53	0.44
1:B:403:GLU:O	1:B:407:ILE:HG13	2.18	0.44
1:C:236:LYS:O	1:C:240:GLU:HG3	2.18	0.44
1:D:357:ASN:O	1:D:361:GLU:HG2	2.18	0.44
1:A:12:GLU:HG2	1:A:13:MET:N	2.33	0.43
1:B:12:GLU:HG2	1:B:13:MET:N	2.31	0.43
1:D:13:MET:HA	1:D:42:TYR:O	2.17	0.43
1:D:236:LYS:O	1:D:240:GLU:HG3	2.18	0.43
1:A:357:ASN:O	1:A:361:GLU:HG2	2.18	0.43
3:C:1517:NAP:H4N	4:C:1618:ICT:H2	2.01	0.43
1:A:350:LYS:HA	1:A:350:LYS:HD3	1.81	0.43
1:B:7:GLY:HA3	1:B:37:LEU:CD2	2.47	0.43
1:B:393:ASN:C	1:B:393:ASN:ND2	2.64	0.43
1:A:3:LYS:CE	1:A:36:GLU:HG3	2.48	0.43
1:A:252:ASP:HB2	5:B:1741:HOH:O	2.18	0.43
3:D:1518:NAP:H4N	4:D:1619:ICT:H2	2.01	0.43
1:D:123:GLY:O	1:D:262:GLU:HA	2.19	0.43
1:C:357:ASN:O	1:C:361:GLU:HG2	2.19	0.43
1:A:17:GLU:HB3	1:A:316:TYR:CG	2.54	0.42
1:A:160:ASP:OD2	1:A:160:ASP:C	2.62	0.42
1:A:315:HIS:HA	1:A:318:MET:HE3	2.01	0.42
1:D:183:TYR:CD1	1:D:184:ASN:N	2.87	0.42
1:B:344:ALA:HB1	1:B:353:ALA:HB2	2.00	0.42
1:C:393:ASN:HD21	1:C:396:GLU:HG3	1.84	0.42
1:A:334:PHE:CE2	1:A:360:GLU:HG2	2.54	0.42
1:C:120:LEU:HD13	1:D:259:MET:HG3	2.02	0.42
1:D:20:ARG:NH2	1:D:43:ASP:OD1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ASN:O	1:B:361:GLU:HG2	2.20	0.42
1:D:109:ARG:HD3	1:D:293:SER:OG	2.19	0.42
1:D:407:ILE:CA	1:D:412:ALA:C	2.93	0.42
1:C:120:LEU:CD1	1:D:259:MET:HG3	2.50	0.42
1:D:393:ASN:HD21	1:D:396:GLU:H	1.60	0.42
1:A:392:LEU:HB3	1:A:396:GLU:HB2	2.00	0.42
1:B:171:ASN:HD22	1:B:171:ASN:HA	1.62	0.41
1:C:393:ASN:HD22	1:C:396:GLU:H	1.59	0.41
1:A:299:ASP:HB3	5:A:1893:HOH:O	2.21	0.41
1:D:406:LYS:HB3	1:D:413:LYS:CD	2.46	0.41
1:C:234:GLN:HG2	5:C:1924:HOH:O	2.20	0.41
1:D:393:ASN:HD22	1:D:396:GLU:H	1.65	0.41
1:B:393:ASN:HD21	1:B:396:GLU:H	1.64	0.41
1:C:1:MET:HG3	1:C:32:PHE:CG	2.55	0.41
1:C:12:GLU:HG2	1:C:13:MET:N	2.35	0.41
1:C:160:ASP:OD1	1:C:160:ASP:C	2.63	0.41
1:D:101:ASN:ND2	1:D:140:ARG:HG3	2.36	0.41
1:A:139:TYR:HE1	4:A:1616:ICT:O5	2.04	0.41
1:B:151:LYS:HZ3	1:B:171:ASN:HD21	1.67	0.41
1:D:69:VAL:HG11	1:D:343:ARG:HD2	2.02	0.41
1:B:20:ARG:HH22	1:B:43:ASP:CG	2.28	0.40
1:B:67:HIS:O	1:B:68:ASN:HB2	2.21	0.40
1:C:159:SER:OG	1:D:149:PRO:HB2	2.21	0.40
3:B:1516:NAP:H4N	4:B:1617:ICT:H2	2.02	0.40
1:D:272:TYR:O	1:D:275:ASP:HB3	2.22	0.40
1:A:67:HIS:O	1:A:68:ASN:HB2	2.21	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	412/414 (100%)	392 (95%)	19 (5%)	1 (0%)	43	57
1	B	412/414 (100%)	396 (96%)	15 (4%)	1 (0%)	43	57
1	C	412/414 (100%)	390 (95%)	21 (5%)	1 (0%)	43	57
1	D	412/414 (100%)	388 (94%)	20 (5%)	4 (1%)	12	18
All	All	1648/1656 (100%)	1566 (95%)	75 (5%)	7 (0%)	30	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	411	GLN
1	D	413	LYS
1	C	4	LYS
1	D	407	ILE
1	D	412	ALA
1	A	140	ARG
1	B	17	GLU

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	350/350 (100%)	342 (98%)	8 (2%)	44	64
1	B	350/350 (100%)	342 (98%)	8 (2%)	44	64
1	C	350/350 (100%)	340 (97%)	10 (3%)	37	57
1	D	350/350 (100%)	341 (97%)	9 (3%)	40	61
All	All	1400/1400 (100%)	1365 (98%)	35 (2%)	42	62

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	103	LEU
1	A	109	ARG
1	A	171	ASN

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Mol	Chain	Res	Type
1	A	303	VAL
1	A	306	GLU
1	A	312	VAL
1	A	393	ASN
1	B	19	THR
1	B	103	LEU
1	B	109	ARG
1	B	171	ASN
1	B	312	VAL
1	B	329	PRO
1	B	388	ARG
1	B	393	ASN
1	C	4	LYS
1	C	19	THR
1	C	103	LEU
1	C	109	ARG
1	C	163	GLN
1	C	184	ASN
1	C	306	GLU
1	C	312	VAL
1	C	388	ARG
1	C	393	ASN
1	D	19	THR
1	D	39	LEU
1	D	103	LEU
1	D	109	ARG
1	D	140	ARG
1	D	312	VAL
1	D	329	PRO
1	D	388	ARG
1	D	393	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	53	ASN
1	A	90	GLN
1	A	171	ASN
1	A	185	GLN
1	A	194	HIS
1	A	198	GLN

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Mol	Chain	Res	Type
1	A	228	GLN
1	A	234	GLN
1	A	242	GLN
1	A	257	GLN
1	A	277	GLN
1	A	348	ASN
1	A	357	ASN
1	A	393	ASN
1	A	404	ASN
1	A	411	GLN
1	B	40	HIS
1	B	53	ASN
1	B	68	ASN
1	B	90	GLN
1	B	171	ASN
1	B	185	GLN
1	B	194	HIS
1	B	198	GLN
1	B	213	ASN
1	B	228	GLN
1	B	234	GLN
1	B	257	GLN
1	B	277	GLN
1	B	323	GLN
1	B	348	ASN
1	B	357	ASN
1	B	393	ASN
1	B	404	ASN
1	C	40	HIS
1	C	53	ASN
1	C	90	GLN
1	C	184	ASN
1	C	194	HIS
1	C	198	GLN
1	C	213	ASN
1	C	228	GLN
1	C	234	GLN
1	C	242	GLN
1	C	257	GLN
1	C	277	GLN
1	C	348	ASN
1	C	357	ASN

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Mol	Chain	Res	Type
1	C	393	ASN
1	C	404	ASN
1	C	411	GLN
1	D	40	HIS
1	D	53	ASN
1	D	90	GLN
1	D	101	ASN
1	D	185	GLN
1	D	194	HIS
1	D	198	GLN
1	D	228	GLN
1	D	234	GLN
1	D	242	GLN
1	D	257	GLN
1	D	277	GLN
1	D	283	GLN
1	D	323	GLN
1	D	393	ASN
1	D	404	ASN
1	D	411	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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
4	ICT	A	1616	2	12,12,12	3.00	6 (50%)	13,16,16	2.32	5 (38%)
4	ICT	C	1618	2	12,12,12	3.08	6 (50%)	13,16,16	2.30	5 (38%)
3	NAP	A	1515	-	50,52,52	3.21	14 (28%)	71,80,80	1.71	12 (16%)
3	NAP	B	1516	-	50,52,52	3.22	15 (30%)	71,80,80	1.68	13 (18%)
4	ICT	D	1619	2	12,12,12	3.20	7 (58%)	13,16,16	2.17	4 (30%)
3	NAP	C	1517	-	50,52,52	3.26	13 (26%)	71,80,80	1.72	12 (16%)
4	ICT	B	1617	2	12,12,12	3.04	7 (58%)	13,16,16	2.22	4 (30%)
3	NAP	D	1518	-	50,52,52	3.22	14 (28%)	71,80,80	1.65	13 (18%)

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
4	ICT	A	1616	2	-	4/16/16/16	-
4	ICT	C	1618	2	-	4/16/16/16	-
3	NAP	A	1515	-	-	7/35/67/67	0/5/5/5
3	NAP	B	1516	-	-	8/35/67/67	0/5/5/5
4	ICT	D	1619	2	-	4/16/16/16	-
3	NAP	C	1517	-	-	7/35/67/67	0/5/5/5
4	ICT	B	1617	2	-	4/16/16/16	-
3	NAP	D	1518	-	-	8/35/67/67	0/5/5/5

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1518	NAP	C2N-N1N	12.83	1.49	1.35
3	B	1516	NAP	C2N-N1N	12.19	1.48	1.35
3	C	1517	NAP	C2N-N1N	12.05	1.48	1.35
3	A	1515	NAP	C2N-N1N	11.44	1.47	1.35
3	A	1515	NAP	PA-O3	-9.89	1.48	1.59
3	C	1517	NAP	PA-O3	-9.54	1.49	1.59
3	B	1516	NAP	PA-O3	-9.27	1.49	1.59
3	D	1518	NAP	PA-O3	-8.97	1.49	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1517	NAP	C3N-C7N	7.78	1.62	1.50
3	B	1516	NAP	C3N-C7N	7.52	1.61	1.50
3	D	1518	NAP	C3N-C7N	7.37	1.61	1.50
4	D	1619	ICT	O3-C5	7.28	1.45	1.22
4	B	1617	ICT	O3-C5	7.05	1.45	1.22
3	A	1515	NAP	C3N-C7N	7.02	1.61	1.50
4	C	1618	ICT	O3-C5	6.88	1.44	1.22
4	A	1616	ICT	O3-C5	6.77	1.44	1.22
3	C	1517	NAP	C5N-C4N	6.73	1.50	1.38
3	A	1515	NAP	C5N-C4N	6.51	1.50	1.38
3	B	1516	NAP	C5N-C4N	6.42	1.49	1.38
3	A	1515	NAP	P2B-O2B	6.36	1.70	1.59
3	D	1518	NAP	C5N-C4N	6.25	1.49	1.38
3	D	1518	NAP	P2B-O2B	6.04	1.70	1.59
3	B	1516	NAP	P2B-O2B	5.75	1.69	1.59
3	A	1515	NAP	C4N-C3N	5.73	1.48	1.39
3	C	1517	NAP	P2B-O2B	5.67	1.69	1.59
3	C	1517	NAP	C4N-C3N	5.50	1.47	1.39
3	B	1516	NAP	C4N-C3N	5.25	1.47	1.39
3	D	1518	NAP	C4N-C3N	5.18	1.47	1.39
3	A	1515	NAP	PN-O3	-4.79	1.54	1.59
3	C	1517	NAP	PN-O3	-4.62	1.54	1.59
3	B	1516	NAP	PN-O3	-4.49	1.54	1.59
3	B	1516	NAP	C6N-N1N	4.12	1.44	1.35
3	A	1515	NAP	C6N-N1N	4.05	1.44	1.35
3	C	1517	NAP	C6N-N1N	3.97	1.44	1.35
4	C	1618	ICT	O4-C5	-3.94	1.17	1.30
4	A	1616	ICT	O4-C5	-3.92	1.17	1.30
3	D	1518	NAP	PN-O3	-3.87	1.55	1.59
4	D	1619	ICT	O4-C5	-3.85	1.18	1.30
4	B	1617	ICT	O4-C5	-3.83	1.18	1.30
3	D	1518	NAP	C6N-N1N	3.80	1.44	1.35
3	C	1517	NAP	C4A-N3A	3.78	1.41	1.34
4	D	1619	ICT	O2-C1	-3.74	1.18	1.30
4	C	1618	ICT	C3-C6	3.73	1.57	1.51
3	D	1518	NAP	C4A-N3A	3.70	1.41	1.34
4	C	1618	ICT	O2-C1	-3.61	1.19	1.30
4	B	1617	ICT	O2-C1	-3.51	1.19	1.30
3	C	1517	NAP	C2A-N1A	3.48	1.40	1.33
4	A	1616	ICT	O2-C1	-3.32	1.20	1.30
4	B	1617	ICT	O1-C1	3.32	1.31	1.22
4	D	1619	ICT	C3-C6	3.30	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1516	NAP	C4A-N3A	3.29	1.40	1.34
3	A	1515	NAP	C4A-N3A	3.24	1.40	1.34
4	C	1618	ICT	O1-C1	3.18	1.31	1.22
4	A	1616	ICT	O1-C1	3.13	1.31	1.22
4	D	1619	ICT	O1-C1	3.12	1.31	1.22
4	A	1616	ICT	C2-C1	3.11	1.57	1.52
3	D	1518	NAP	C2A-N1A	3.03	1.39	1.33
3	B	1516	NAP	C2A-N1A	2.94	1.39	1.33
3	A	1515	NAP	C2A-N1A	2.87	1.39	1.33
4	D	1619	ICT	C2-C1	2.69	1.56	1.52
4	B	1617	ICT	C2-C1	2.65	1.56	1.52
4	B	1617	ICT	C3-C6	2.60	1.55	1.51
4	C	1618	ICT	C2-C1	2.47	1.56	1.52
4	A	1616	ICT	C3-C6	2.36	1.55	1.51
3	B	1516	NAP	PA-O2A	-2.36	1.44	1.55
3	A	1515	NAP	C5A-C6A	2.33	1.47	1.41
3	B	1516	NAP	C3B-C2B	2.31	1.58	1.53
3	C	1517	NAP	PA-O2A	-2.30	1.44	1.55
3	D	1518	NAP	P2B-O3X	-2.30	1.46	1.54
3	D	1518	NAP	P2B-O2X	-2.29	1.46	1.54
3	D	1518	NAP	PA-O2A	-2.27	1.44	1.55
3	B	1516	NAP	C2N-C3N	2.23	1.42	1.39
3	A	1515	NAP	P2B-O2X	-2.21	1.46	1.54
3	A	1515	NAP	PA-O2A	-2.19	1.45	1.55
3	C	1517	NAP	P2B-O2X	-2.18	1.46	1.54
3	B	1516	NAP	P2B-O2X	-2.17	1.46	1.54
3	C	1517	NAP	P2B-O3X	-2.14	1.46	1.54
3	B	1516	NAP	P2B-O3X	-2.12	1.46	1.54
3	A	1515	NAP	C3B-C2B	2.10	1.57	1.53
4	D	1619	ICT	O5-C6	2.10	1.28	1.22
4	B	1617	ICT	O5-C6	2.09	1.28	1.22
3	D	1518	NAP	O4D-C1D	2.07	1.43	1.40

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1515	NAP	C5N-C4N-C3N	-6.22	114.25	120.36
3	C	1517	NAP	C5N-C4N-C3N	-5.96	114.51	120.36
3	D	1518	NAP	C5N-C4N-C3N	-5.61	114.84	120.36
3	B	1516	NAP	C5N-C4N-C3N	-5.61	114.85	120.36
3	A	1515	NAP	C2N-C3N-C4N	5.30	124.42	118.26
3	C	1517	NAP	C2N-C3N-C4N	5.10	124.19	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1518	NAP	C2N-C3N-C4N	5.01	124.09	118.26
3	B	1516	NAP	C2N-C3N-C4N	4.88	123.94	118.26
3	A	1515	NAP	C2N-N1N-C1D	-4.04	110.21	119.13
4	A	1616	ICT	O3-C5-C4	-3.96	110.67	122.84
4	C	1618	ICT	O3-C5-C4	-3.94	110.74	122.84
3	C	1517	NAP	C2N-N1N-C1D	-3.94	110.44	119.13
4	A	1616	ICT	O4-C5-C4	3.93	126.22	114.00
3	A	1515	NAP	C6N-N1N-C1D	3.85	127.29	119.73
3	B	1516	NAP	C2N-N1N-C1D	-3.82	110.71	119.13
4	B	1617	ICT	O3-C5-C4	-3.82	111.13	122.84
4	D	1619	ICT	O3-C5-C4	-3.77	111.26	122.84
4	C	1618	ICT	O2-C1-C2	3.76	123.77	113.31
4	C	1618	ICT	O4-C5-C4	3.76	125.68	114.00
4	D	1619	ICT	O4-C5-C4	3.75	125.66	114.00
4	A	1616	ICT	O2-C1-C2	3.73	123.67	113.31
3	C	1517	NAP	C6N-N1N-C1D	3.73	127.04	119.73
4	B	1617	ICT	O4-C5-C4	3.72	125.58	114.00
4	B	1617	ICT	O2-C1-C2	3.72	123.65	113.31
4	D	1619	ICT	O2-C1-C2	3.66	123.48	113.31
4	C	1618	ICT	O1-C1-C2	-3.64	111.93	121.62
3	B	1516	NAP	C6N-N1N-C1D	3.61	126.82	119.73
3	D	1518	NAP	C2N-N1N-C1D	-3.59	111.20	119.13
3	B	1516	NAP	O3B-C3B-C2B	3.55	121.12	111.19
4	B	1617	ICT	O1-C1-C2	-3.50	112.29	121.62
3	A	1515	NAP	O3B-C3B-C2B	3.47	120.91	111.19
3	C	1517	NAP	O3B-C3B-C2B	3.41	120.72	111.19
4	A	1616	ICT	O1-C1-C2	-3.37	112.65	121.62
3	D	1518	NAP	C6N-N1N-C1D	3.34	126.29	119.73
4	D	1619	ICT	O1-C1-C2	-3.30	112.83	121.62
3	D	1518	NAP	O3B-C3B-C2B	3.21	120.18	111.19
3	D	1518	NAP	O2B-P2B-O1X	-3.21	97.91	109.33
3	C	1517	NAP	C4A-C5A-N7A	3.09	114.11	110.58
3	D	1518	NAP	C6N-C5N-C4N	3.04	123.83	119.45
3	B	1516	NAP	C6N-C5N-C4N	3.04	123.83	119.45
3	A	1515	NAP	O2B-P2B-O1X	-3.02	98.56	109.33
3	C	1517	NAP	N6A-C6A-N1A	3.01	125.08	118.38
3	D	1518	NAP	N6A-C6A-N1A	2.92	124.89	118.38
3	A	1515	NAP	C6N-C5N-C4N	2.92	123.65	119.45
3	C	1517	NAP	C6N-C5N-C4N	2.91	123.64	119.45
3	C	1517	NAP	O2B-P2B-O1X	-2.90	99.00	109.33
3	B	1516	NAP	O2B-P2B-O1X	-2.88	99.06	109.33
3	D	1518	NAP	C4A-C5A-N7A	2.85	113.84	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1516	NAP	N6A-C6A-N1A	2.85	124.73	118.38
3	C	1517	NAP	C2B-C3B-C4B	-2.84	95.89	101.99
3	B	1516	NAP	C4A-C5A-N7A	2.84	113.83	110.58
3	B	1516	NAP	C2B-C3B-C4B	-2.78	96.01	101.99
3	A	1515	NAP	C4A-C5A-N7A	2.77	113.75	110.58
3	A	1515	NAP	C2B-C3B-C4B	-2.68	96.23	101.99
3	A	1515	NAP	N6A-C6A-N1A	2.61	124.19	118.38
3	D	1518	NAP	C2B-C3B-C4B	-2.52	96.58	101.99
3	B	1516	NAP	O3X-P2B-O2X	2.27	116.33	107.80
3	C	1517	NAP	O2X-P2B-O1X	2.22	119.50	110.83
3	C	1517	NAP	O3X-P2B-O2X	2.22	116.13	107.80
3	A	1515	NAP	O3X-P2B-O2X	2.20	116.04	107.80
3	D	1518	NAP	O3X-P2B-O2X	2.14	115.83	107.80
3	D	1518	NAP	O5B-C5B-C4B	-2.12	101.78	108.99
4	C	1618	ICT	O6-C6-C3	2.09	119.34	113.93
3	A	1515	NAP	O2X-P2B-O1X	2.08	118.95	110.83
3	D	1518	NAP	O2X-P2B-O1X	2.08	118.94	110.83
3	B	1516	NAP	O5B-C5B-C4B	-2.07	101.96	108.99
3	B	1516	NAP	O2X-P2B-O1X	2.06	118.85	110.83
4	A	1616	ICT	O5-C6-C3	-2.01	118.27	123.01

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1515	NAP	O4D-C1D-N1N-C2N
3	A	1515	NAP	O4D-C1D-N1N-C6N
3	B	1516	NAP	O4D-C1D-N1N-C2N
3	B	1516	NAP	O4D-C1D-N1N-C6N
3	B	1516	NAP	C2D-C1D-N1N-C2N
3	C	1517	NAP	O4D-C1D-N1N-C2N
3	C	1517	NAP	O4D-C1D-N1N-C6N
3	C	1517	NAP	C2D-C1D-N1N-C2N
3	C	1517	NAP	C2D-C1D-N1N-C6N
3	D	1518	NAP	O4D-C1D-N1N-C2N
3	D	1518	NAP	O4D-C1D-N1N-C6N
3	D	1518	NAP	C2D-C1D-N1N-C2N
3	D	1518	NAP	C2D-C1D-N1N-C6N
4	A	1616	ICT	C2-C3-C4-C5
4	A	1616	ICT	C6-C3-C4-C5
4	B	1617	ICT	C2-C3-C4-C5
4	B	1617	ICT	C6-C3-C4-C5

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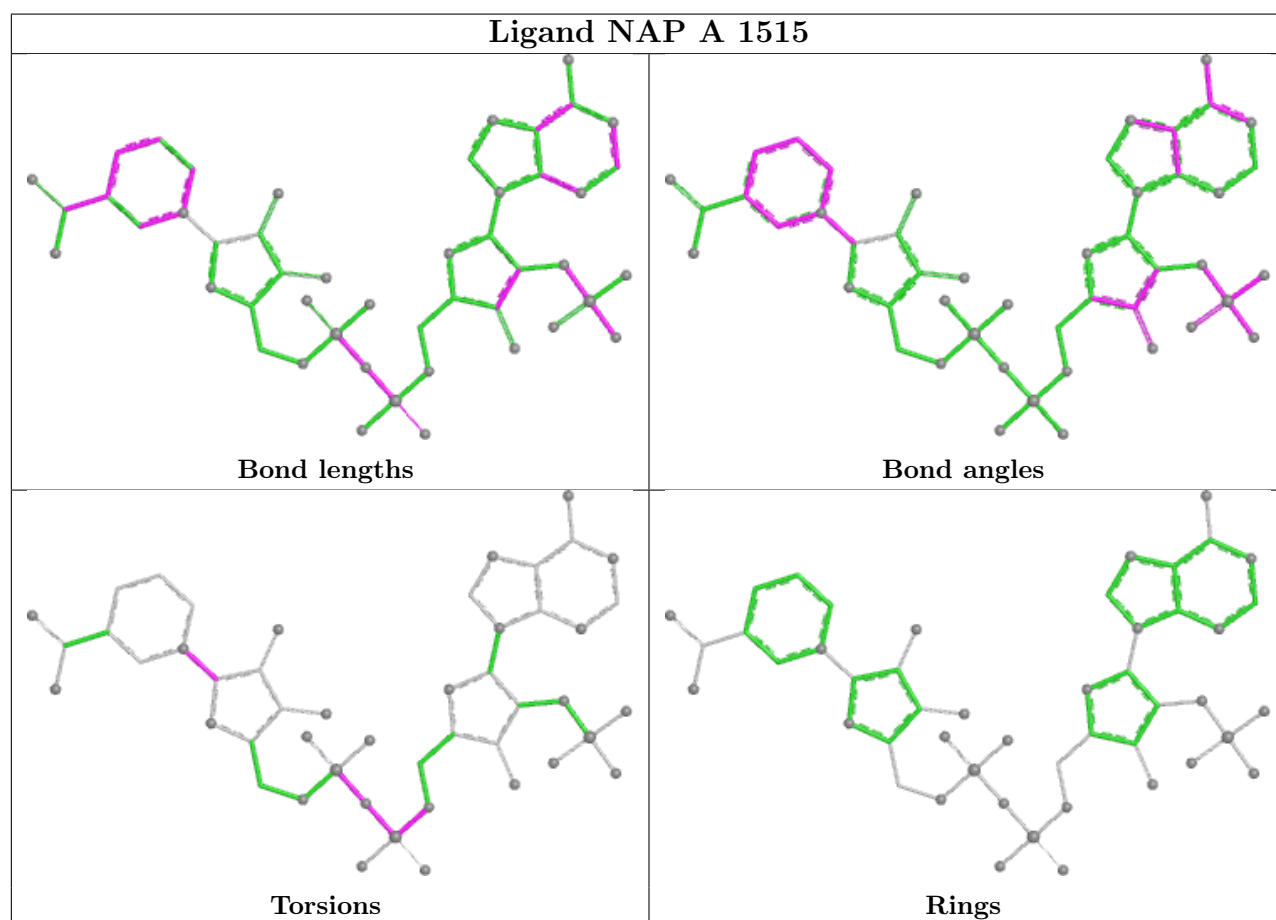
Mol	Chain	Res	Type	Atoms
4	C	1618	ICT	C4-C3-C6-O6
3	A	1515	NAP	PN-O3-PA-O1A
3	A	1515	NAP	PA-O3-PN-O1N
3	B	1516	NAP	PN-O3-PA-O1A
3	B	1516	NAP	PA-O3-PN-O1N
3	C	1517	NAP	PN-O3-PA-O1A
3	C	1517	NAP	PA-O3-PN-O1N
3	D	1518	NAP	PN-O3-PA-O1A
3	D	1518	NAP	PA-O3-PN-O1N
3	A	1515	NAP	C5B-O5B-PA-O1A
3	B	1516	NAP	C5B-O5B-PA-O1A
3	D	1518	NAP	C5B-O5B-PA-O1A
4	D	1619	ICT	C2-C3-C6-O5
4	C	1618	ICT	C4-C3-C6-O5
3	A	1515	NAP	C2D-C1D-N1N-C2N
3	B	1516	NAP	C2D-C1D-N1N-C6N
4	B	1617	ICT	C3-C4-C5-O4
4	B	1617	ICT	C3-C4-C5-O3
4	C	1618	ICT	C3-C4-C5-O4
4	D	1619	ICT	C2-C3-C6-O6
4	A	1616	ICT	C3-C4-C5-O4
3	A	1515	NAP	PN-O3-PA-O2A
3	B	1516	NAP	PN-O3-PA-O2A
3	C	1517	NAP	PN-O3-PA-O2A
3	D	1518	NAP	PN-O3-PA-O2A
4	A	1616	ICT	C3-C4-C5-O3
4	C	1618	ICT	C3-C4-C5-O3
4	D	1619	ICT	C4-C3-C6-O6
4	D	1619	ICT	C3-C4-C5-O3

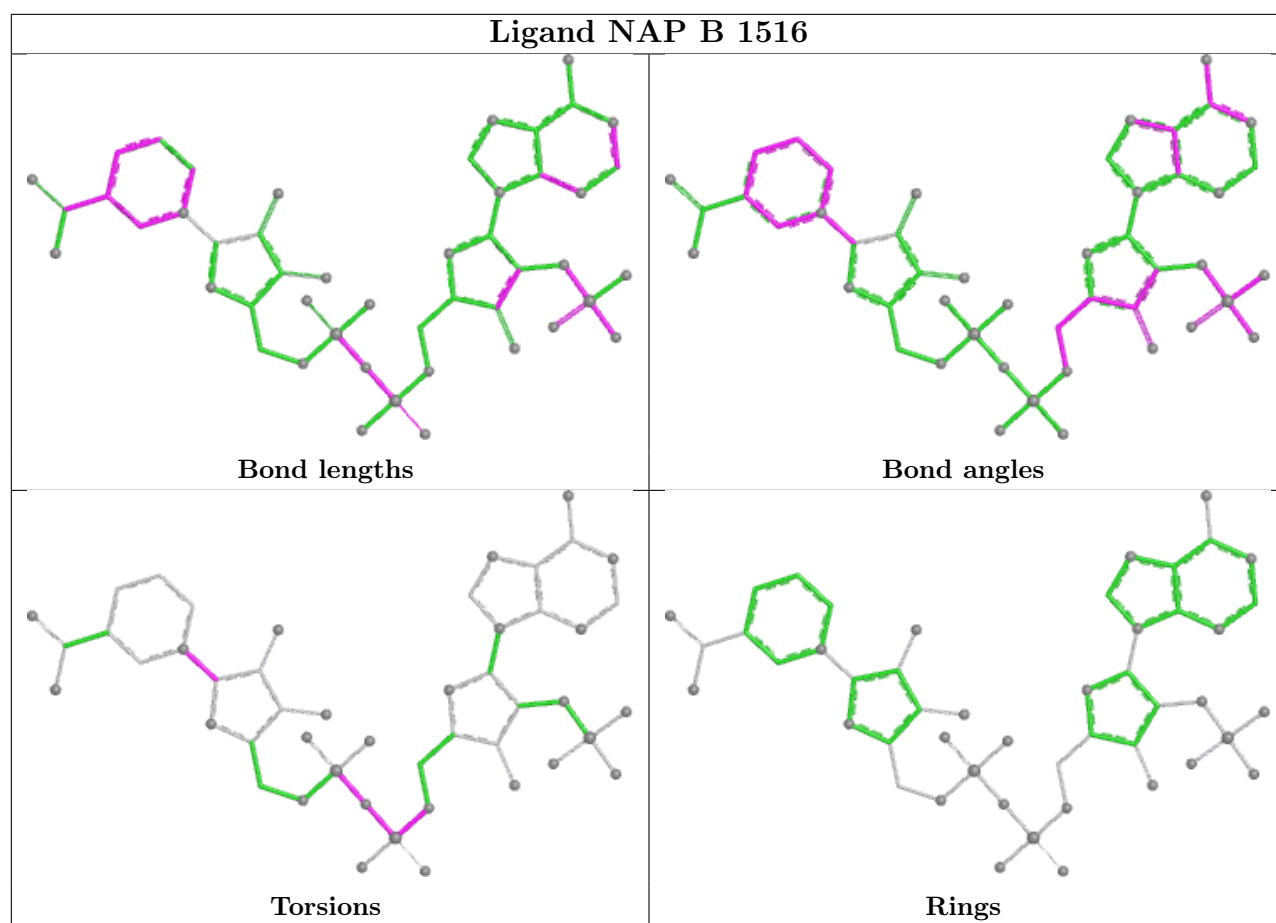
There are no ring outliers.

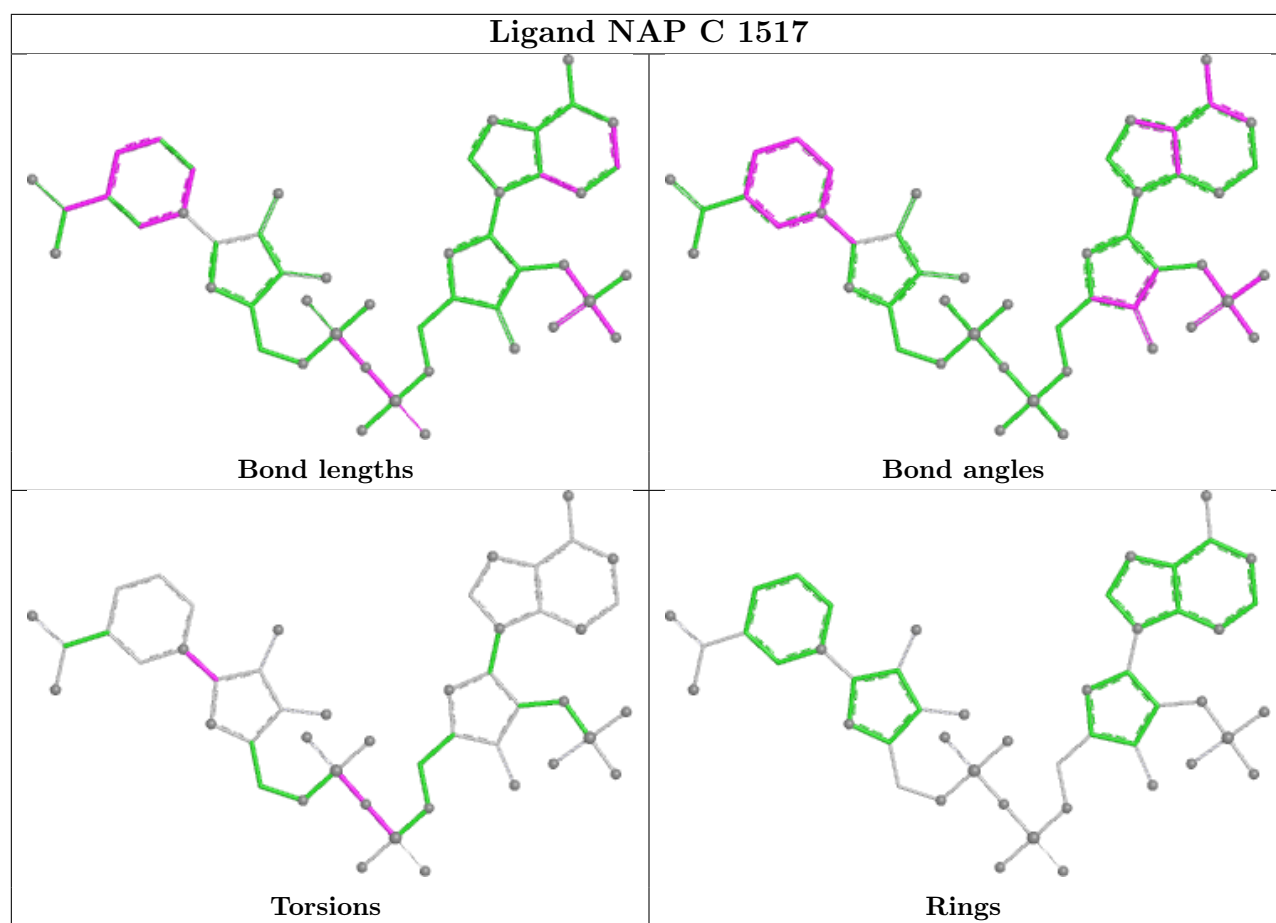
8 monomers are involved in 19 short contacts:

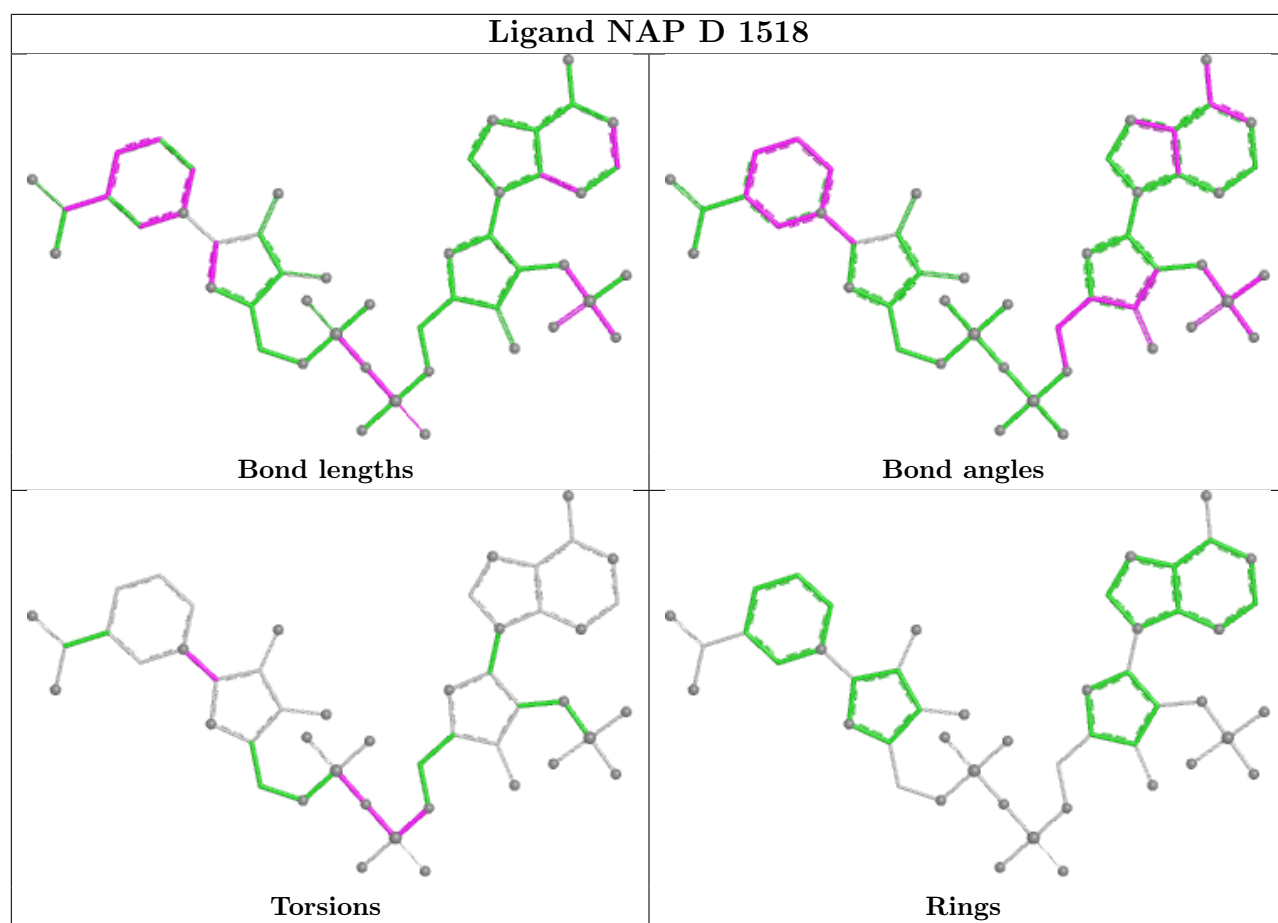
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1616	ICT	3	0
4	C	1618	ICT	3	0
3	A	1515	NAP	3	0
3	B	1516	NAP	4	0
4	D	1619	ICT	2	0
3	C	1517	NAP	5	0
4	B	1617	ICT	2	0
3	D	1518	NAP	4	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	414/414 (100%)	-0.27	4 (0%) 79 77	9, 20, 41, 103	0
1	B	414/414 (100%)	-0.21	6 (1%) 73 70	8, 22, 41, 97	0
1	C	414/414 (100%)	-0.24	5 (1%) 76 74	8, 19, 42, 97	0
1	D	414/414 (100%)	-0.13	9 (2%) 62 59	7, 21, 43, 114	0
All	All	1656/1656 (100%)	-0.21	24 (1%) 73 70	7, 20, 42, 114	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	412	ALA	12.0
1	D	413	LYS	10.5
1	C	2	SER	8.0
1	D	414	LEU	6.6
1	B	414	LEU	5.6
1	A	3	LYS	5.4
1	A	414	LEU	5.4
1	B	3	LYS	5.1
1	B	2	SER	5.0
1	D	407	ILE	4.6
1	D	1	MET	4.5
1	D	411	GLN	3.8
1	C	414	LEU	3.7
1	C	1	MET	3.3
1	C	3	LYS	3.3
1	D	28	GLU	3.2
1	B	1	MET	2.8
1	A	2	SER	2.6
1	D	159	SER	2.5
1	A	1	MET	2.5
1	B	84	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	229	GLU	2.4
1	D	84	GLU	2.3
1	C	413	LYS	2.3

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](#)

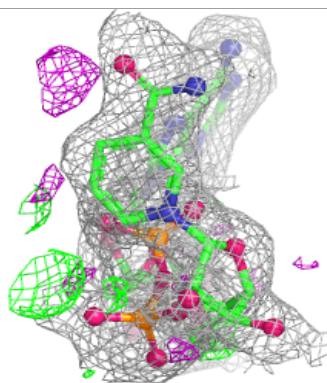
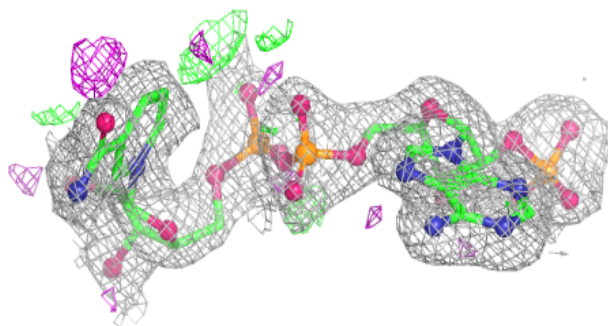
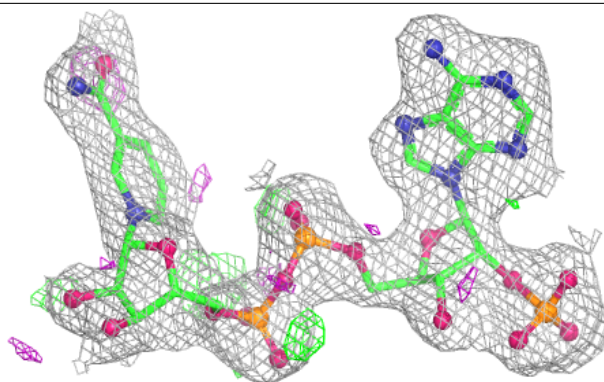
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CA	A	1717	1/1	0.69	0.12	45,45,45,45	0
4	ICT	A	1616	13/13	0.72	0.16	27,36,41,44	0
4	ICT	D	1619	13/13	0.75	0.20	30,36,39,41	0
4	ICT	B	1617	13/13	0.78	0.13	30,36,39,40	0
4	ICT	C	1618	13/13	0.80	0.14	28,31,36,38	0
2	CA	B	1718	1/1	0.80	0.10	38,38,38,38	0
2	CA	C	1719	1/1	0.92	0.06	29,29,29,29	0
3	NAP	D	1518	48/48	0.96	0.07	9,15,24,25	0
2	CA	D	1720	1/1	0.96	0.06	26,26,26,26	0
3	NAP	A	1515	48/48	0.96	0.06	10,16,24,28	0
3	NAP	B	1516	48/48	0.96	0.07	8,16,24,25	0
3	NAP	C	1517	48/48	0.96	0.07	8,15,23,24	0

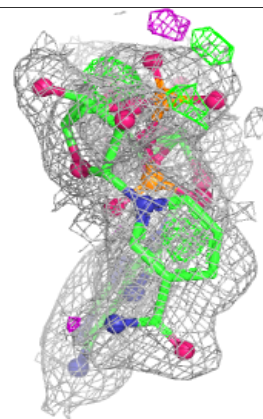
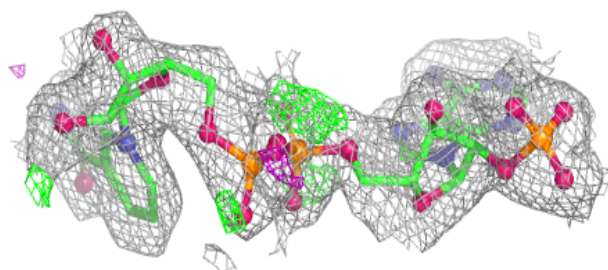
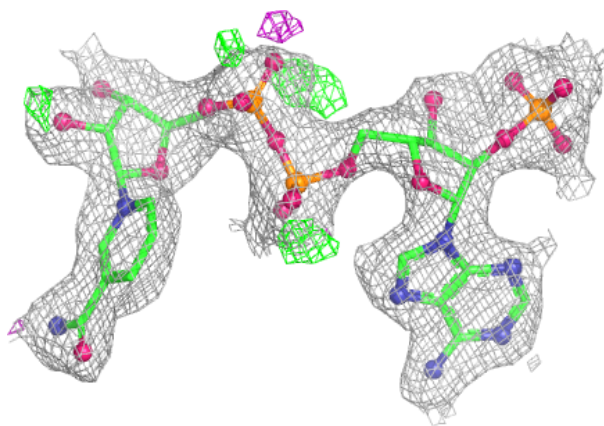
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP D 1518:

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

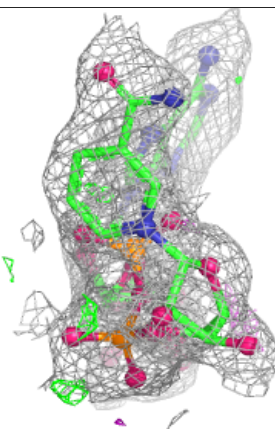
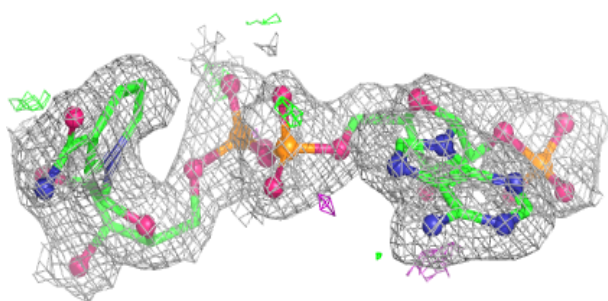
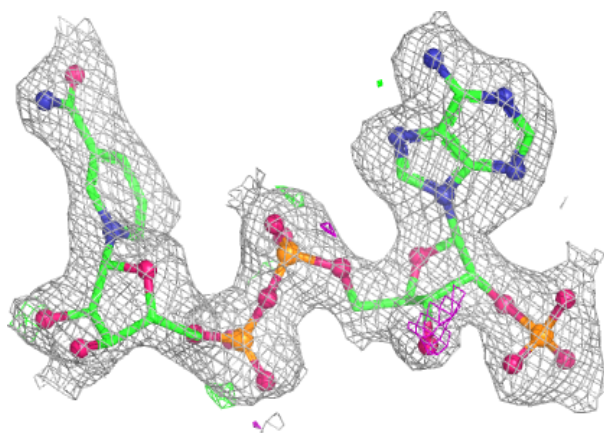
**Electron density around NAP A 1515:**

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



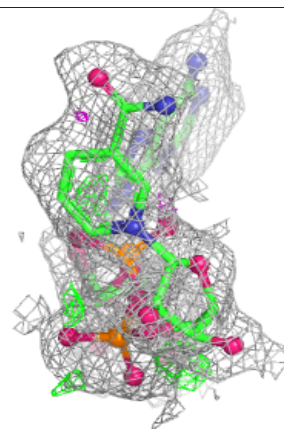
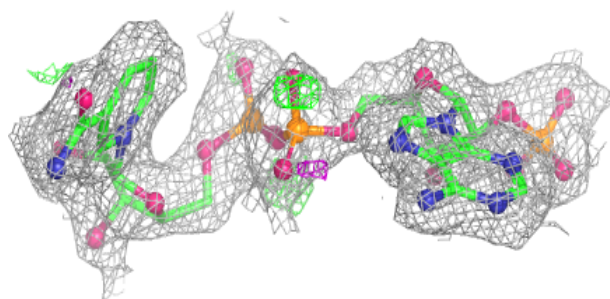
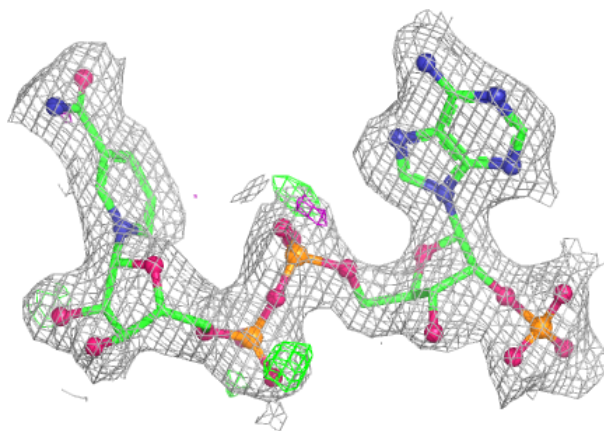
Electron density around NAP B 1516:

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



Electron density around NAP C 1517:

$2mF_o-DF_c$ (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.