



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:14 am BST

PDB ID : 3SZG
Title : Crystal structure of C176A glutamine-dependent NAD⁺ synthetase from M. tuberculosis bound to AMP/PPi and NaAD⁺
Authors : Chuenchor, W.; Doukov, T.; Gerratana, B.
Deposited on : 2011-07-19
Resolution : 2.25 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

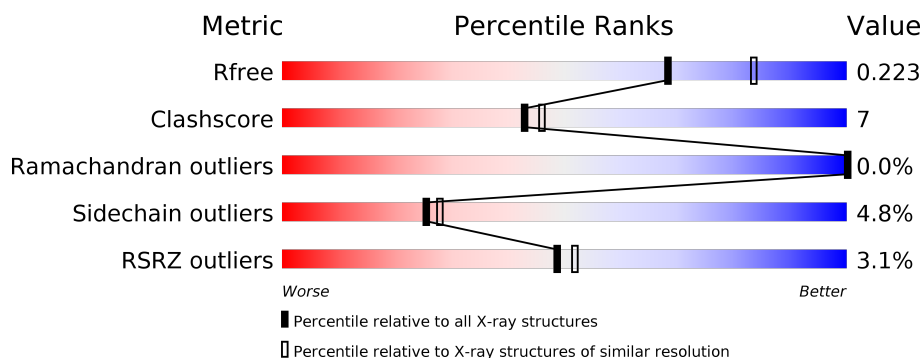
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 on 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	680	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• •</div> </div> </div>
1	B	680	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	C	680	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>• •</div> </div> </div>
1	D	680	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21381 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.

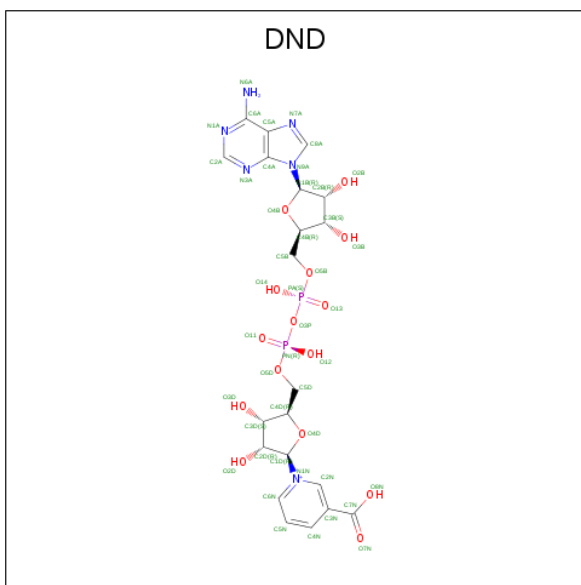
- Molecule 1 is a protein called Glutamine-dependent NAD(+) synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	0	0	0
			5040	3191	902	932	15			
1	B	649	Total	C	N	O	S	0	0	0
			5039	3188	902	934	15			
1	C	660	Total	C	N	O	S	0	0	0
			5119	3243	913	948	15			
1	D	658	Total	C	N	O	S	0	0	0
			5116	3242	912	947	15			

There are 8 discrepancies between the modelled and reference sequences:

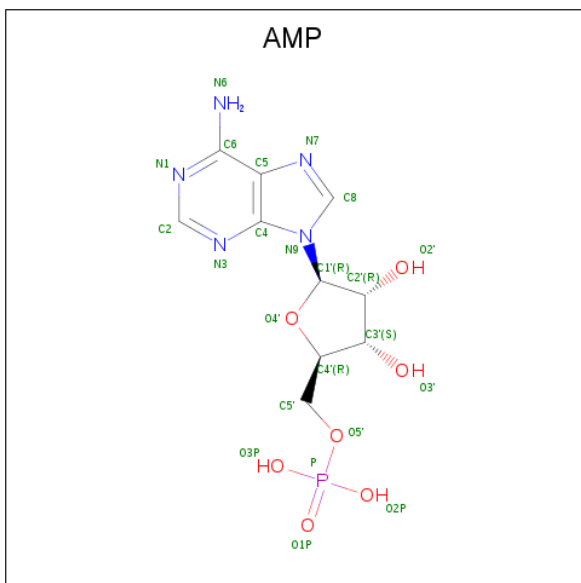
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P0A5L6
A	176	ALA	CYS	engineered mutation	UNP P0A5L6
B	0	SER	-	expression tag	UNP P0A5L6
B	176	ALA	CYS	engineered mutation	UNP P0A5L6
C	0	SER	-	expression tag	UNP P0A5L6
C	176	ALA	CYS	engineered mutation	UNP P0A5L6
D	0	SER	-	expression tag	UNP P0A5L6
D	176	ALA	CYS	engineered mutation	UNP P0A5L6

- Molecule 2 is NICOTINIC ACID ADENINE DINUCLEOTIDE (three-letter code: DND) (formula: C₂₁H₂₇N₆O₁₅P₂).



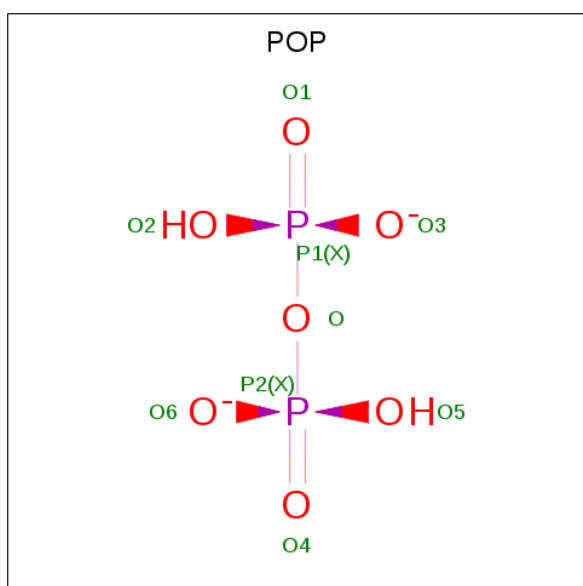
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 6	O 15	P 2	0	0
2	B	1	Total 44	C 21	N 6	O 15	P 2	0	0
2	C	1	Total 44	C 21	N 6	O 15	P 2	0	0
2	D	1	Total 44	C 21	N 6	O 15	P 2	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			9	7	2		
4	B	1	Total	O	P	0	0
			9	7	2		
4	C	1	Total	O	P	0	0
			9	7	2		
4	D	1	Total	O	P	0	0
			9	7	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

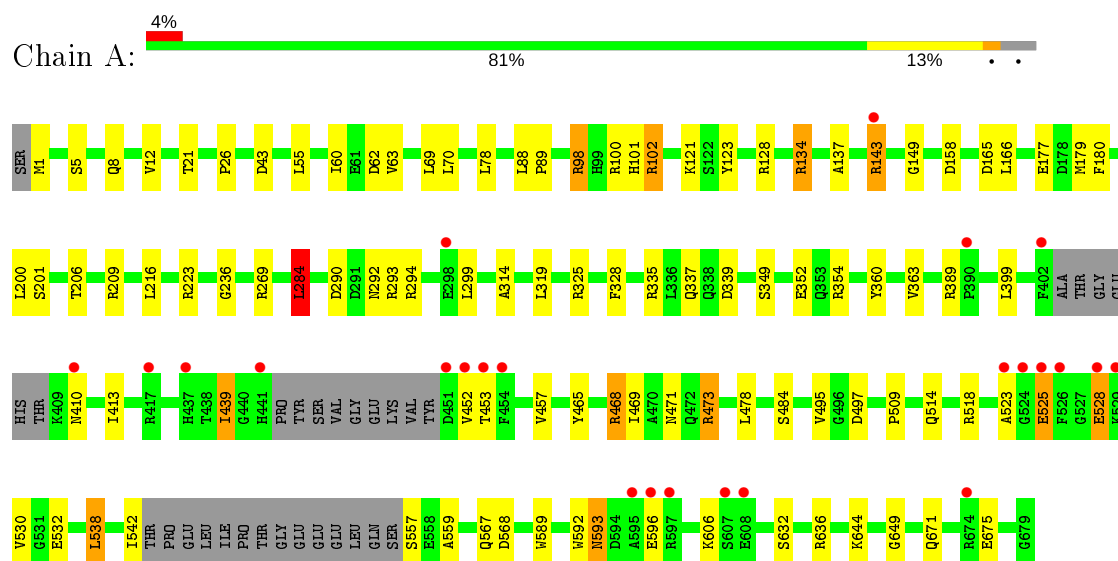
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	162	Total	O	0	0
			162	162		
6	B	190	Total	O	0	0
			190	190		
6	C	216	Total	O	0	0
			216	216		
6	D	177	Total	O	0	0
			177	177		

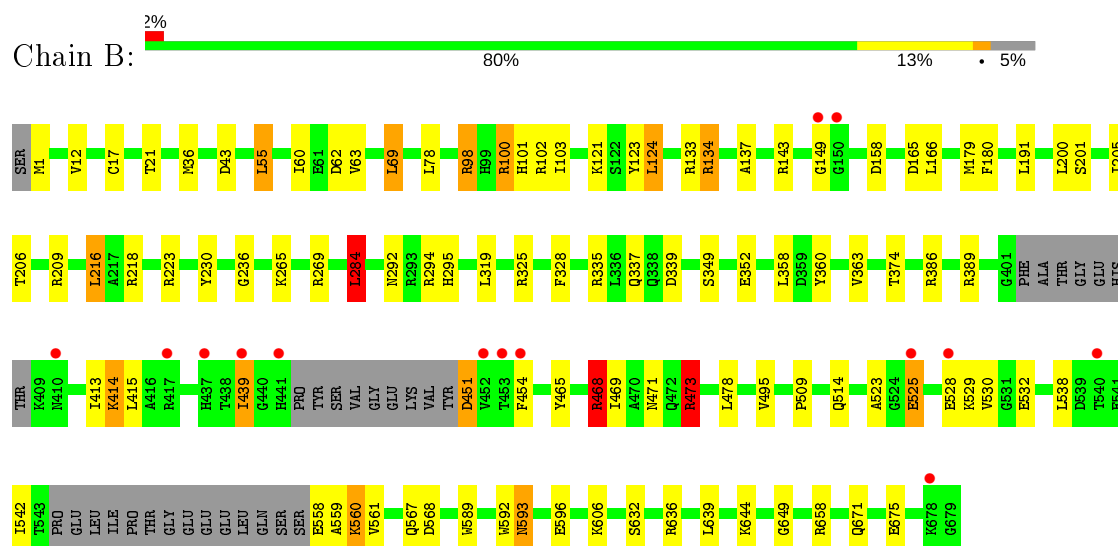
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

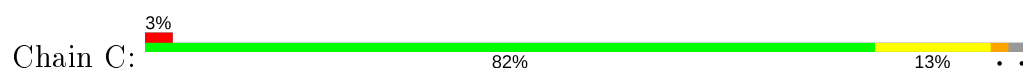
- Molecule 1: Glutamine-dependent NAD(+) synthetase

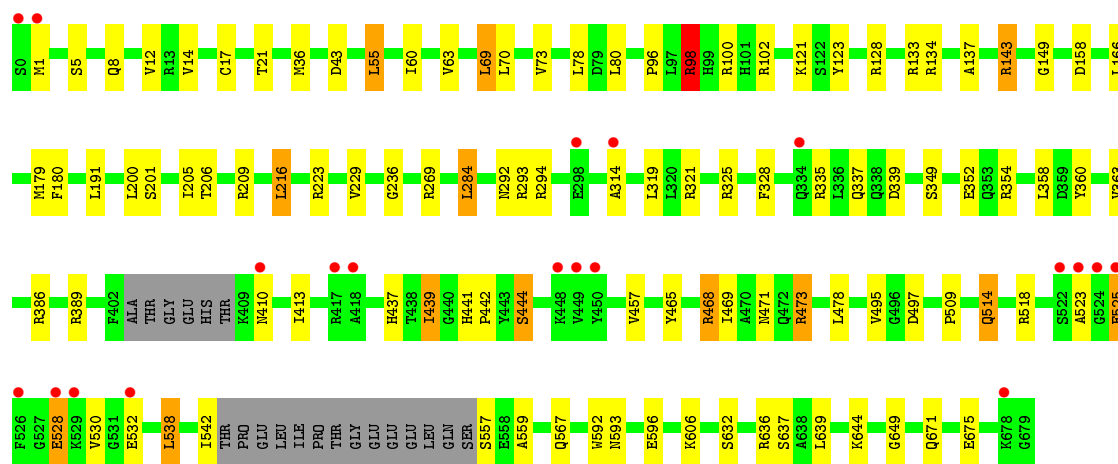


- Molecule 1: Glutamine-dependent NAD(+) synthetase

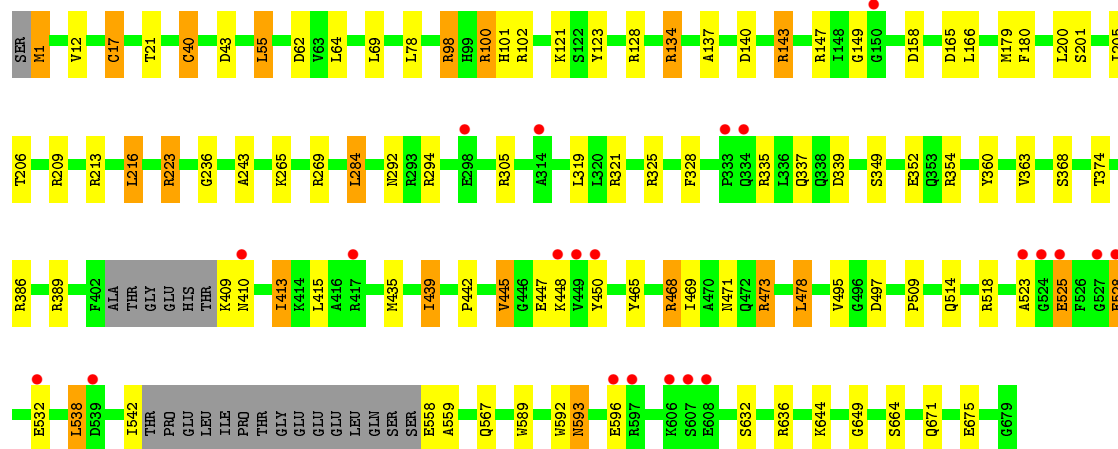
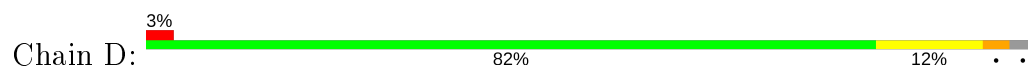


- Molecule 1: Glutamine-dependent NAD(+) synthetase





• Molecule 1: Glutamine-dependent NAD(+) synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	177.94Å 177.94Å 214.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.12 – 2.25 39.12 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.12-2.25) 99.4 (39.12-2.25)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.192 , 0.229 0.184 , 0.223	Depositor DCC
R_{free} test set	8068 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	1.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21381	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.58% 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: DND, GOL, POP, AMP

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	0.82	2/5156 (0.0%)	0.95	15/7003 (0.2%)
1	B	0.85	2/5154 (0.0%)	0.91	14/6999 (0.2%)
1	C	0.85	2/5239 (0.0%)	0.91	14/7118 (0.2%)
1	D	0.90	6/5236 (0.1%)	0.92	14/7112 (0.2%)
All	All	0.85	12/20785 (0.1%)	0.92	57/28232 (0.2%)

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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	40	CYS	CB-SG	20.02	2.16	1.82
1	D	17	CYS	CB-SG	12.07	2.02	1.82
1	C	284	LEU	CG-CD2	-7.48	1.24	1.51
1	A	284	LEU	CG-CD2	-6.98	1.26	1.51
1	B	284	LEU	CG-CD2	-6.83	1.26	1.51
1	C	292	ASN	CG-ND2	-6.73	1.16	1.32
1	D	292	ASN	CG-OD1	-6.43	1.09	1.24
1	A	292	ASN	CG-ND2	-6.05	1.17	1.32
1	D	284	LEU	CG-CD1	-5.92	1.29	1.51
1	B	292	ASN	CG-OD1	-5.21	1.12	1.24
1	D	284	LEU	CG-CD2	-5.17	1.32	1.51
1	D	292	ASN	CG-ND2	-5.12	1.20	1.32

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ARG	NE-CZ-NH1	-18.65	110.98	120.30
1	A	134	ARG	NE-CZ-NH2	-18.09	111.26	120.30
1	A	100	ARG	NE-CZ-NH2	17.31	128.96	120.30
1	D	134	ARG	NE-CZ-NH2	-16.60	112.00	120.30
1	C	134	ARG	NE-CZ-NH1	-16.36	112.12	120.30
1	B	134	ARG	NE-CZ-NH2	-15.87	112.36	120.30
1	C	134	ARG	NE-CZ-NH2	15.79	128.19	120.30
1	D	134	ARG	NE-CZ-NH1	15.09	127.84	120.30
1	A	134	ARG	NE-CZ-NH1	14.19	127.40	120.30
1	B	134	ARG	NE-CZ-NH1	12.30	126.45	120.30
1	A	294	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	B	294	ARG	NE-CZ-NH2	-9.91	115.34	120.30
1	D	98	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	A	100	ARG	CD-NE-CZ	8.48	135.47	123.60
1	D	40	CYS	CA-CB-SG	8.09	128.56	114.00
1	C	100	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	B	98	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	D	100	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	D	321	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	C	294	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	100	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	C	98	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	B	473	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	C	134	ARG	CD-NE-CZ	6.84	133.18	123.60
1	C	321	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	B	100	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	C	293	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	C	321	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	D	134	ARG	CD-NE-CZ	6.25	132.35	123.60
1	A	294	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	354	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	B	284	LEU	CD1-CG-CD2	-6.12	92.13	110.50
1	B	134	ARG	CD-NE-CZ	6.11	132.15	123.60
1	D	294	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	D	100	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	134	ARG	CD-NE-CZ	5.69	131.57	123.60
1	B	468	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	D	305	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	218	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	284	LEU	CD1-CG-CD2	-5.57	93.78	110.50
1	A	284	LEU	CA-CB-CG	-5.51	102.62	115.30
1	D	17	CYS	CA-CB-SG	5.49	123.88	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	414	LYS	CG-CD-CE	5.46	128.29	111.90
1	D	354	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	128	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	102	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	C	128	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	C	98	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	D	128	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	354	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	98	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	D	284	LEU	CD1-CG-CD2	-5.21	94.86	110.50
1	B	124	LEU	CB-CG-CD2	-5.21	102.15	111.00
1	B	658	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	299	LEU	CB-CG-CD2	-5.12	102.31	111.00
1	C	284	LEU	CD1-CG-CD2	-5.03	95.40	110.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	559	ALA	Peptide
1	D	559	ALA	Peptide

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	5040	0	4938	69	0
1	B	5039	0	4949	79	0
1	C	5119	0	5014	75	0
1	D	5116	0	5021	70	0
2	A	44	0	25	0	0
2	B	44	0	25	1	0
2	C	44	0	25	1	0
2	D	44	0	25	0	0
3	A	23	0	12	2	0
3	B	23	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	23	0	12	0	0
3	D	23	0	12	0	0
4	A	9	0	0	0	0
4	B	9	0	0	1	0
4	C	9	0	0	0	0
4	D	9	0	0	1	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	162	0	0	5	0
6	B	190	0	0	6	0
6	C	216	0	0	10	0
6	D	177	0	0	4	0
All	All	21381	0	20094	276	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 7.

All (276) 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:17:CYS:SG	1:D:17:CYS:CB	2.02	1.47
1:D:40:CYS:SG	1:D:40:CYS:CB	2.16	1.33
1:B:69:LEU:HD12	1:B:69:LEU:C	1.76	1.06
1:D:143:ARG:HH11	1:D:143:ARG:HG2	1.27	0.98
1:C:143:ARG:HG2	1:C:143:ARG:HH11	1.32	0.93
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.33	0.93
1:B:143:ARG:HG2	1:B:143:ARG:HH11	1.34	0.91
1:A:206:THR:HG22	1:A:209:ARG:HB2	1.52	0.89
1:D:206:THR:HG22	1:D:209:ARG:HB2	1.56	0.88
1:B:206:THR:HG22	1:B:209:ARG:HB2	1.56	0.88
1:C:69:LEU:C	1:C:69:LEU:HD12	1.94	0.86
1:A:43:ASP:OD2	1:A:269:ARG:NH2	2.08	0.86
1:C:206:THR:HG22	1:C:209:ARG:HB2	1.55	0.85
1:A:468:ARG:NH2	1:D:495:VAL:O	2.09	0.85
1:A:495:VAL:O	1:D:468:ARG:NH2	2.12	0.82
1:B:495:VAL:O	1:C:468:ARG:NH2	2.13	0.82
1:D:525:GLU:CD	1:D:525:GLU:H	1.81	0.82
1:C:469:ILE:HG23	1:C:473:ARG:HD3	1.60	0.81
1:A:525:GLU:H	1:A:525:GLU:CD	1.82	0.81
1:B:43:ASP:OD2	1:B:269:ARG:NH2	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:ASP:OD2	1:C:269:ARG:NH2	2.14	0.80
1:B:560:LYS:HE3	1:B:560:LYS:O	1.81	0.79
1:C:525:GLU:H	1:C:525:GLU:CD	1.84	0.78
1:D:43:ASP:OD2	1:D:269:ARG:NH2	2.16	0.78
1:A:335:ARG:NH1	1:A:339:ASP:OD1	2.17	0.78
1:B:69:LEU:CD1	1:B:69:LEU:C	2.52	0.77
1:A:606:LYS:N	1:A:606:LYS:HD3	2.00	0.77
1:D:335:ARG:NH1	1:D:339:ASP:OD1	2.18	0.77
1:D:469:ILE:HG23	1:D:473:ARG:HD3	1.66	0.77
1:B:469:ILE:HG23	1:B:473:ARG:HD3	1.67	0.75
1:A:469:ILE:HG23	1:A:473:ARG:HD3	1.69	0.75
1:B:525:GLU:H	1:B:525:GLU:CD	1.89	0.74
1:B:468:ARG:NH2	1:C:495:VAL:O	2.21	0.73
1:C:335:ARG:NH1	1:C:339:ASP:OD1	2.22	0.73
1:C:437:HIS:HA	1:C:444:SER:OG	1.89	0.73
1:A:514:GLN:HB3	6:A:820:HOH:O	1.88	0.72
1:C:143:ARG:HG2	1:C:143:ARG:NH1	2.01	0.72
1:B:632:SER:OG	1:B:636:ARG:NH2	2.22	0.72
1:C:69:LEU:C	1:C:69:LEU:CD1	2.57	0.71
1:D:1:MET:N	6:D:831:HOH:O	2.22	0.71
1:B:62:ASP:OD1	1:B:134:ARG:HD3	1.91	0.69
1:C:98:ARG:HG2	6:C:861:HOH:O	1.92	0.69
1:D:143:ARG:HG2	1:D:143:ARG:NH1	1.98	0.69
1:A:632:SER:OG	1:A:636:ARG:NH2	2.26	0.69
1:B:335:ARG:NH1	1:B:339:ASP:OD1	2.26	0.69
1:A:530:VAL:HG23	6:A:813:HOH:O	1.92	0.69
1:A:62:ASP:OD1	1:A:134:ARG:HD3	1.94	0.68
1:B:529:LYS:HB2	6:B:765:HOH:O	1.92	0.68
1:D:632:SER:OG	1:D:636:ARG:NH2	2.26	0.68
1:B:143:ARG:HG2	1:B:143:ARG:NH1	2.03	0.68
1:B:69:LEU:HD12	1:B:69:LEU:O	1.93	0.68
1:C:514:GLN:HB3	6:C:895:HOH:O	1.94	0.68
1:A:143:ARG:NH1	1:A:143:ARG:HG2	2.04	0.67
1:D:62:ASP:OD1	1:D:134:ARG:HD3	1.94	0.67
1:A:399:LEU:N	3:A:681:AMP:C2	2.63	0.66
1:A:325:ARG:HB3	1:A:592:TRP:CZ2	2.31	0.66
1:D:525:GLU:CD	1:D:525:GLU:N	2.49	0.64
1:B:542:ILE:HG22	1:B:542:ILE:O	1.98	0.63
1:B:528:GLU:O	1:B:532:GLU:HG3	1.99	0.63
1:B:325:ARG:HB3	1:B:592:TRP:CZ2	2.33	0.62
1:B:644:LYS:HE3	1:B:649:GLY:HA2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:GLU:CD	1:C:525:GLU:N	2.51	0.62
1:A:525:GLU:CD	1:A:525:GLU:N	2.52	0.62
1:B:78:LEU:HD21	1:B:149:GLY:HA3	1.82	0.61
1:C:200:LEU:N	1:C:200:LEU:HD12	2.15	0.61
1:C:632:SER:OG	1:C:636:ARG:NH2	2.34	0.61
1:D:528:GLU:O	1:D:532:GLU:HG3	2.00	0.61
1:C:542:ILE:HG22	1:C:542:ILE:O	2.01	0.61
1:C:441:HIS:O	1:C:444:SER:HB2	2.01	0.60
1:D:671:GLN:NE2	1:D:675:GLU:HG3	2.16	0.60
1:D:165:ASP:O	1:D:166:LEU:HD12	2.01	0.60
1:B:671:GLN:NE2	1:B:675:GLU:HG3	2.16	0.60
1:D:325:ARG:HB3	1:D:592:TRP:CZ2	2.37	0.59
1:A:671:GLN:NE2	1:A:675:GLU:HG3	2.17	0.59
1:C:671:GLN:NE2	1:C:675:GLU:HG3	2.18	0.59
1:B:525:GLU:N	1:B:525:GLU:CD	2.56	0.59
1:A:528:GLU:O	1:A:532:GLU:HG3	2.02	0.59
1:B:205:ILE:HD11	6:B:690:HOH:O	2.01	0.59
1:A:180:PHE:CD2	1:A:216:LEU:HD13	2.39	0.58
1:B:558:GLU:N	1:B:558:GLU:OE1	2.36	0.58
1:D:542:ILE:O	1:D:542:ILE:HG22	2.04	0.58
1:B:121:LYS:HE2	1:B:123:TYR:O	2.03	0.57
1:C:528:GLU:O	1:C:532:GLU:HG3	2.04	0.57
1:D:102:ARG:HD3	1:D:137:ALA:HB2	1.86	0.57
1:B:558:GLU:O	1:B:561:VAL:HG22	2.05	0.57
1:C:671:GLN:HE21	1:C:675:GLU:HG3	1.69	0.57
1:A:21:THR:O	1:A:236:GLY:HA3	2.05	0.57
1:D:368:SER:OG	4:D:682:POP:O4	2.18	0.56
1:C:102:ARG:HD3	1:C:137:ALA:HB2	1.86	0.56
1:B:671:GLN:HE21	1:B:675:GLU:HG3	1.70	0.56
1:C:386:ARG:NH2	6:C:893:HOH:O	2.38	0.56
1:A:452:VAL:HG13	1:A:453:THR:N	2.21	0.55
1:A:78:LEU:HD21	1:A:149:GLY:HA3	1.88	0.55
1:B:465:TYR:HD1	1:C:439:ILE:HD11	1.72	0.55
1:D:671:GLN:HE21	1:D:675:GLU:HG3	1.70	0.55
1:D:205:ILE:HD11	6:D:762:HOH:O	2.06	0.55
1:D:64:LEU:HA	1:D:69:LEU:HD23	1.88	0.55
1:D:78:LEU:HD21	1:D:149:GLY:HA3	1.89	0.55
1:C:121:LYS:HE2	1:C:123:TYR:O	2.07	0.54
1:A:102:ARG:NH2	6:A:776:HOH:O	2.39	0.54
1:B:102:ARG:HD3	1:B:137:ALA:HB2	1.90	0.54
1:C:17:CYS:HB3	1:C:36:MET:CE	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LYS:HE2	1:A:123:TYR:O	2.08	0.54
1:A:671:GLN:HE21	1:A:675:GLU:HG3	1.71	0.53
1:B:589:TRP:O	1:B:593:ASN:HB3	2.09	0.53
1:C:389:ARG:HD3	6:C:864:HOH:O	2.08	0.53
1:C:78:LEU:HD21	1:C:149:GLY:HA3	1.91	0.53
1:A:542:ILE:O	1:A:542:ILE:HG22	2.08	0.53
1:C:557:SER:C	1:C:559:ALA:H	2.12	0.53
1:D:180:PHE:CD2	1:D:216:LEU:HD13	2.43	0.52
1:D:468:ARG:NH1	1:D:471:ASN:OD1	2.42	0.52
1:B:468:ARG:NH1	1:B:471:ASN:OD1	2.41	0.52
1:B:530:VAL:HG23	6:B:765:HOH:O	2.10	0.52
1:C:200:LEU:HD12	1:C:200:LEU:H	1.74	0.52
1:A:60:ILE:HD11	1:A:69:LEU:CD2	2.40	0.52
1:B:102:ARG:NH2	6:B:844:HOH:O	2.43	0.52
1:A:206:THR:HG22	1:A:209:ARG:CB	2.34	0.51
1:A:589:TRP:O	1:A:593:ASN:HB3	2.09	0.51
1:B:523:ALA:HB3	1:B:525:GLU:OE2	2.10	0.51
1:D:121:LYS:HE2	1:D:123:TYR:O	2.11	0.51
1:C:530:VAL:HG23	6:C:812:HOH:O	2.10	0.51
1:D:644:LYS:HE3	1:D:649:GLY:HA2	1.91	0.51
1:C:180:PHE:CD2	1:C:216:LEU:HD13	2.46	0.51
1:C:349:SER:HA	1:C:352:GLU:OE1	2.10	0.51
1:B:468:ARG:HG3	1:C:457:VAL:HG22	1.92	0.51
1:C:523:ALA:HB3	1:C:525:GLU:OE2	2.10	0.51
1:D:363:VAL:HG13	1:D:478:LEU:HD13	1.91	0.51
1:B:363:VAL:HG13	1:B:478:LEU:HD13	1.93	0.51
1:A:12:VAL:HG22	1:A:166:LEU:HD23	1.94	0.50
1:A:143:ARG:NH1	1:A:143:ARG:CG	2.73	0.50
1:B:439:ILE:HD11	1:C:465:TYR:HD1	1.76	0.50
1:C:12:VAL:HG22	1:C:166:LEU:HD23	1.94	0.50
1:B:60:ILE:HD11	1:B:69:LEU:HD21	1.93	0.50
1:C:143:ARG:HH12	1:C:158:ASP:CG	2.15	0.50
1:C:17:CYS:HB3	1:C:36:MET:HE2	1.93	0.50
1:D:102:ARG:NH2	6:D:755:HOH:O	2.44	0.50
1:A:644:LYS:HE3	1:A:649:GLY:HA2	1.93	0.50
1:A:165:ASP:O	1:A:166:LEU:HD12	2.13	0.49
1:B:17:CYS:HB3	1:B:36:MET:CE	2.41	0.49
1:B:567:GLN:OE1	1:B:567:GLN:HA	2.12	0.49
1:D:200:LEU:N	1:D:200:LEU:HD12	2.27	0.49
1:C:328:PHE:CD2	1:C:509:PRO:HG3	2.48	0.49
2:B:680:DND:N6A	1:C:358:LEU:HD21	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:LEU:N	1:B:200:LEU:HD12	2.27	0.49
1:B:386:ARG:HH21	1:D:265:LYS:HE2	1.78	0.48
1:D:143:ARG:CG	1:D:143:ARG:NH1	2.69	0.48
1:D:349:SER:HA	1:D:352:GLU:OE1	2.12	0.48
1:D:445:VAL:O	1:D:445:VAL:HG13	2.13	0.48
1:B:180:PHE:CD2	1:B:216:LEU:HD13	2.49	0.48
1:C:21:THR:O	1:C:236:GLY:HA3	2.13	0.48
1:A:468:ARG:NH1	1:A:471:ASN:OD1	2.44	0.48
1:A:328:PHE:CG	1:A:509:PRO:HG3	2.49	0.48
1:C:55:LEU:HA	1:C:55:LEU:HD12	1.57	0.48
1:D:525:GLU:OE1	1:D:525:GLU:N	2.47	0.48
1:B:349:SER:HA	1:B:352:GLU:OE1	2.14	0.48
1:B:560:LYS:HD2	1:B:560:LYS:HA	1.34	0.48
1:A:349:SER:HA	1:A:352:GLU:OE1	2.13	0.47
1:A:518:ARG:HG3	1:A:538:LEU:HD11	1.96	0.47
1:B:17:CYS:HB3	1:B:36:MET:HE2	1.96	0.47
1:B:468:ARG:HD3	1:B:468:ARG:HA	1.45	0.47
1:B:63:VAL:HG12	1:B:69:LEU:HD23	1.96	0.47
1:D:243:ALA:N	6:D:712:HOH:O	2.33	0.47
1:D:328:PHE:CD2	1:D:509:PRO:HG3	2.50	0.47
1:A:102:ARG:HD3	1:A:137:ALA:HB2	1.96	0.47
1:D:12:VAL:HG22	1:D:166:LEU:HD23	1.95	0.47
1:B:335:ARG:NH2	6:B:819:HOH:O	2.47	0.47
1:B:386:ARG:HH21	1:D:265:LYS:CE	2.27	0.47
1:A:63:VAL:O	1:A:69:LEU:HD23	2.14	0.47
1:C:468:ARG:HA	1:C:468:ARG:HD3	1.57	0.47
1:C:69:LEU:HD12	1:C:70:LEU:N	2.29	0.47
1:D:328:PHE:CG	1:D:509:PRO:HG3	2.50	0.47
1:C:567:GLN:OE1	1:C:567:GLN:HA	2.15	0.47
1:D:589:TRP:O	1:D:593:ASN:HB3	2.15	0.47
1:B:216:LEU:HD21	1:D:223:ARG:HG3	1.96	0.46
1:A:363:VAL:HG13	1:A:478:LEU:HD13	1.98	0.46
1:C:473:ARG:HG2	6:C:869:HOH:O	2.15	0.46
1:D:55:LEU:HD12	1:D:55:LEU:HA	1.63	0.46
1:D:442:PRO:HB2	1:D:447:GLU:HB2	1.96	0.46
1:B:328:PHE:CD2	1:B:509:PRO:HG3	2.51	0.46
1:C:325:ARG:HB3	1:C:592:TRP:CZ2	2.50	0.46
1:C:363:VAL:HG13	1:C:478:LEU:HD13	1.97	0.46
1:D:523:ALA:HB3	1:D:525:GLU:OE2	2.16	0.46
1:A:439:ILE:HD11	1:D:465:TYR:HD1	1.79	0.46
1:A:525:GLU:OE1	1:A:525:GLU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ARG:HH12	1:B:158:ASP:CG	2.19	0.46
1:B:143:ARG:CG	1:B:143:ARG:NH1	2.74	0.46
1:A:457:VAL:HG22	1:D:468:ARG:HG3	1.97	0.46
1:C:360:TYR:HB3	1:C:389:ARG:HD2	1.97	0.46
1:A:101:HIS:ND1	6:A:839:HOH:O	2.36	0.45
1:A:5:SER:HB2	1:A:314:ALA:O	2.16	0.45
1:C:73:VAL:HG11	1:C:96:PRO:HD2	1.97	0.45
1:D:567:GLN:OE1	1:D:567:GLN:HA	2.17	0.45
1:A:88:LEU:HB3	1:A:89:PRO:HD3	1.98	0.45
1:C:468:ARG:NH1	1:C:471:ASN:OD1	2.43	0.45
1:D:360:TYR:HB3	1:D:389:ARG:HD2	1.98	0.45
1:B:55:LEU:HA	1:B:55:LEU:HD12	1.62	0.45
1:B:21:THR:O	1:B:236:GLY:HA3	2.17	0.45
1:D:21:THR:O	1:D:236:GLY:HA3	2.16	0.45
1:D:445:VAL:CG1	1:D:445:VAL:O	2.64	0.45
1:A:328:PHE:CD2	1:A:509:PRO:HG3	2.52	0.45
1:B:358:LEU:HD21	2:C:680:DND:N6A	2.31	0.45
1:B:328:PHE:CG	1:B:509:PRO:HG3	2.52	0.45
1:C:14:VAL:HG11	1:C:229:VAL:HG21	1.98	0.45
1:D:206:THR:HG22	1:D:209:ARG:CB	2.38	0.45
1:B:60:ILE:CD1	1:B:69:LEU:HD21	2.47	0.45
1:C:63:VAL:HG12	1:C:69:LEU:HD23	1.97	0.45
1:D:448:LYS:HE3	1:D:450:TYR:OH	2.17	0.45
1:A:399:LEU:N	3:A:681:AMP:H2	2.11	0.44
1:B:133:ARG:HA	1:B:133:ARG:HD2	1.83	0.44
1:A:143:ARG:HH12	1:A:158:ASP:CG	2.20	0.44
1:A:557:SER:C	1:A:559:ALA:H	2.19	0.44
1:C:328:PHE:CG	1:C:509:PRO:HG3	2.53	0.44
1:A:523:ALA:HB3	1:A:525:GLU:OE2	2.17	0.44
1:A:60:ILE:HD11	1:A:69:LEU:HD21	1.98	0.44
1:B:606:LYS:HA	1:B:606:LYS:HD3	1.92	0.44
1:C:205:ILE:HD11	6:C:724:HOH:O	2.18	0.44
1:A:325:ARG:HB3	1:A:592:TRP:CE2	2.52	0.44
1:A:557:SER:C	1:A:559:ALA:N	2.71	0.44
1:D:209:ARG:O	1:D:213:ARG:HG3	2.18	0.44
1:C:606:LYS:HA	1:C:606:LYS:HD3	1.84	0.44
1:B:451:ASP:OD1	1:B:454:PHE:HB3	2.18	0.44
1:C:441:HIS:CD2	1:C:442:PRO:HD2	2.53	0.44
1:C:133:ARG:HD2	1:C:133:ARG:HA	1.80	0.44
1:C:102:ARG:NH2	6:C:744:HOH:O	2.51	0.43
1:D:100:ARG:HG2	1:D:101:HIS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:LYS:CE	1:D:386:ARG:HH21	2.31	0.43
1:B:165:ASP:O	1:B:166:LEU:HD12	2.19	0.43
1:B:374:THR:HG23	1:B:415:LEU:HD22	1.99	0.43
1:C:5:SER:HB2	1:C:314:ALA:O	2.18	0.43
1:B:100:ARG:HG2	1:B:101:HIS:N	2.34	0.43
1:C:437:HIS:CA	1:C:444:SER:OG	2.62	0.43
1:C:525:GLU:OE1	1:C:525:GLU:N	2.51	0.43
1:D:518:ARG:HG3	1:D:538:LEU:HD11	1.99	0.43
1:B:509:PRO:HB2	1:B:568:ASP:OD2	2.18	0.43
1:C:518:ARG:HG3	1:C:538:LEU:HD11	2.01	0.43
1:D:143:ARG:HH12	1:D:158:ASP:CG	2.22	0.43
1:A:468:ARG:HA	1:A:468:ARG:HD3	1.37	0.43
1:C:143:ARG:CG	1:C:143:ARG:NH1	2.72	0.43
1:A:284:LEU:HD11	1:B:103:ILE:HG23	2.00	0.42
1:A:465:TYR:HD1	1:D:439:ILE:HD11	1.84	0.42
1:B:284:LEU:HA	1:B:284:LEU:HD23	1.77	0.42
1:D:200:LEU:H	1:D:200:LEU:HD12	1.83	0.42
1:A:180:PHE:CE2	1:A:216:LEU:HD13	2.54	0.42
1:D:468:ARG:HA	1:D:468:ARG:HD3	1.40	0.42
1:A:200:LEU:N	1:A:200:LEU:HD12	2.34	0.42
1:C:386:ARG:CZ	6:C:893:HOH:O	2.67	0.42
1:C:636:ARG:O	1:C:639:LEU:HB2	2.20	0.42
1:B:636:ARG:O	1:B:639:LEU:HB2	2.20	0.42
4:B:682:POP:O2	4:B:682:POP:O5	2.37	0.42
1:B:12:VAL:HG22	1:B:166:LEU:HD23	2.00	0.42
1:C:69:LEU:O	1:C:69:LEU:HD12	2.19	0.42
1:A:452:VAL:CG1	1:A:453:THR:N	2.81	0.42
1:C:191:LEU:HD23	1:C:191:LEU:HA	1.85	0.42
1:C:80:LEU:HA	1:C:80:LEU:HD23	1.83	0.42
1:A:465:TYR:CE1	1:D:435:MET:HG3	2.55	0.42
1:D:469:ILE:HG23	1:D:473:ARG:CD	2.45	0.42
1:A:360:TYR:HB3	1:A:389:ARG:HD2	2.02	0.42
1:B:230:TYR:C	1:B:230:TYR:CD1	2.93	0.42
1:C:60:ILE:HD11	1:C:69:LEU:HD21	2.02	0.41
1:A:5:SER:OG	1:A:8:GLN:HG3	2.20	0.41
1:C:5:SER:OG	1:C:8:GLN:HG3	2.20	0.41
1:B:295:HIS:HD2	1:D:140:ASP:OD2	2.03	0.41
1:B:191:LEU:HD23	1:B:191:LEU:HA	1.91	0.41
1:D:374:THR:HG23	1:D:415:LEU:HD22	2.01	0.41
1:B:325:ARG:HB3	1:B:592:TRP:CE2	2.55	0.41
1:B:386:ARG:HE	1:D:265:LYS:HE3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LYS:HG2	1:B:124:LEU:HD12	2.01	0.41
1:A:484:SER:OG	1:A:568:ASP:OD1	2.37	0.40
1:A:290:ASP:OD1	6:A:691:HOH:O	2.22	0.40
1:B:360:TYR:HB3	1:B:389:ARG:HD2	2.02	0.40
1:C:389:ARG:CD	6:C:864:HOH:O	2.67	0.40
1:D:413:ILE:HG13	1:D:413:ILE:O	2.20	0.40
1:A:70:LEU:HA	1:A:70:LEU:HD23	1.89	0.40
1:C:644:LYS:HE3	1:C:649:GLY:HA2	2.02	0.40
1:A:293:ARG:NH2	6:B:710:HOH:O	2.54	0.40
1:A:567:GLN:OE1	1:A:567:GLN:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	642/680 (94%)	615 (96%)	26 (4%)	1 (0%)	47	55
1	B	641/680 (94%)	616 (96%)	25 (4%)	0	100	100
1	C	654/680 (96%)	624 (95%)	30 (5%)	0	100	100
1	D	652/680 (96%)	626 (96%)	26 (4%)	0	100	100
All	All	2589/2720 (95%)	2481 (96%)	107 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	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	519/548 (95%)	497 (96%)	22 (4%)	30	34
1	B	521/548 (95%)	498 (96%)	23 (4%)	28	32
1	C	528/548 (96%)	502 (95%)	26 (5%)	25	27
1	D	529/548 (96%)	500 (94%)	29 (6%)	21	21
All	All	2097/2192 (96%)	1997 (95%)	100 (5%)	25	28

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	26	PRO
1	A	55	LEU
1	A	98	ARG
1	A	143	ARG
1	A	179	MET
1	A	201	SER
1	A	223	ARG
1	A	284	LEU
1	A	319	LEU
1	A	337	GLN
1	A	410	ASN
1	A	413	ILE
1	A	439	ILE
1	A	468	ARG
1	A	473	ARG
1	A	497	ASP
1	A	525	GLU
1	A	528	GLU
1	A	538	LEU
1	A	593	ASN
1	A	596	GLU
1	B	1	MET
1	B	55	LEU

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Mol	Chain	Res	Type
1	B	69	LEU
1	B	98	ARG
1	B	179	MET
1	B	201	SER
1	B	216	LEU
1	B	223	ARG
1	B	284	LEU
1	B	319	LEU
1	B	337	GLN
1	B	413	ILE
1	B	414	LYS
1	B	439	ILE
1	B	451	ASP
1	B	468	ARG
1	B	473	ARG
1	B	514	GLN
1	B	525	GLU
1	B	538	LEU
1	B	560	LYS
1	B	593	ASN
1	B	596	GLU
1	C	1	MET
1	C	55	LEU
1	C	69	LEU
1	C	98	ARG
1	C	143	ARG
1	C	179	MET
1	C	201	SER
1	C	216	LEU
1	C	223	ARG
1	C	284	LEU
1	C	319	LEU
1	C	337	GLN
1	C	410	ASN
1	C	413	ILE
1	C	439	ILE
1	C	444	SER
1	C	468	ARG
1	C	473	ARG
1	C	497	ASP
1	C	514	GLN
1	C	525	GLU

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Mol	Chain	Res	Type
1	C	528	GLU
1	C	538	LEU
1	C	593	ASN
1	C	596	GLU
1	C	637	SER
1	D	1	MET
1	D	55	LEU
1	D	98	ARG
1	D	143	ARG
1	D	147	ARG
1	D	179	MET
1	D	201	SER
1	D	216	LEU
1	D	223	ARG
1	D	284	LEU
1	D	319	LEU
1	D	337	GLN
1	D	409	LYS
1	D	410	ASN
1	D	413	ILE
1	D	439	ILE
1	D	445	VAL
1	D	468	ARG
1	D	473	ARG
1	D	478	LEU
1	D	497	ASP
1	D	514	GLN
1	D	525	GLU
1	D	528	GLU
1	D	538	LEU
1	D	558	GLU
1	D	593	ASN
1	D	596	GLU
1	D	664	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	295	HIS
1	C	515	HIS
1	C	626	GLN
1	D	295	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

15 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$
5	GOL	C	683	-	5,5,5	0.55	0	5,5,5	1.04	0
3	AMP	C	681	-	22,25,25	0.78	0	25,38,38	1.50	4 (16%)
3	AMP	D	681	-	22,25,25	0.83	0	25,38,38	1.55	3 (12%)
3	AMP	A	681	-	22,25,25	0.68	0	25,38,38	1.39	2 (8%)
3	AMP	B	681	-	22,25,25	0.92	0	25,38,38	1.53	3 (12%)
4	POP	D	682	-	6,8,8	0.71	0	13,13,13	1.21	1 (7%)
5	GOL	D	683	-	5,5,5	0.63	0	5,5,5	0.57	0
4	POP	C	682	-	6,8,8	0.62	0	13,13,13	1.29	1 (7%)
4	POP	A	682	-	6,8,8	0.81	0	13,13,13	0.95	0
4	POP	B	682	-	6,8,8	0.93	0	13,13,13	1.18	1 (7%)
2	DND	D	680	-	40,48,48	1.11	3 (7%)	47,73,73	1.22	4 (8%)
2	DND	B	680	-	40,48,48	1.17	2 (5%)	47,73,73	1.35	7 (14%)
5	GOL	B	683	-	5,5,5	0.53	0	5,5,5	0.71	0
2	DND	C	680	-	40,48,48	1.25	2 (5%)	47,73,73	1.16	2 (4%)
2	DND	A	680	-	40,48,48	1.15	1 (2%)	47,73,73	1.30	4 (8%)

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
5	GOL	C	683	-	-	2/4/4/4	-
3	AMP	C	681	-	-	1/6/26/26	0/3/3/3
3	AMP	D	681	-	-	2/6/26/26	0/3/3/3
3	AMP	A	681	-	-	2/6/26/26	0/3/3/3
3	AMP	B	681	-	-	5/6/26/26	0/3/3/3
4	POP	D	682	-	-	0/6/6/6	-
5	GOL	D	683	-	-	2/4/4/4	-
4	POP	C	682	-	-	0/6/6/6	-
4	POP	A	682	-	-	0/6/6/6	-
4	POP	B	682	-	-	3/6/6/6	-
2	DND	D	680	-	-	4/22/62/62	0/5/5/5
2	DND	B	680	-	-	6/22/62/62	0/5/5/5
5	GOL	B	683	-	-	4/4/4/4	-
2	DND	C	680	-	-	3/22/62/62	0/5/5/5
2	DND	A	680	-	-	4/22/62/62	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	680	DND	C3N-C7N	5.62	1.52	1.47
2	B	680	DND	C3N-C7N	5.46	1.52	1.47
2	A	680	DND	C3N-C7N	4.89	1.52	1.47
2	D	680	DND	C3N-C7N	3.64	1.51	1.47
2	C	680	DND	O4B-C1B	3.29	1.45	1.41
2	D	680	DND	O4B-C1B	3.16	1.45	1.41
2	B	680	DND	O4D-C1D	2.50	1.44	1.41
2	D	680	DND	C2A-N3A	2.40	1.36	1.32

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	681	AMP	N3-C2-N1	-5.65	119.85	128.68
2	B	680	DND	N3A-C2A-N1A	-5.59	119.94	128.68
2	D	680	DND	N3A-C2A-N1A	-5.06	120.77	128.68
3	B	681	AMP	N3-C2-N1	-4.87	121.07	128.68
3	C	681	AMP	N3-C2-N1	-4.45	121.73	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	680	DND	N3A-C2A-N1A	-4.23	122.07	128.68
3	A	681	AMP	N3-C2-N1	-4.20	122.11	128.68
2	A	680	DND	N3A-C2A-N1A	-3.88	122.61	128.68
2	A	680	DND	C3D-C2D-C1D	3.44	106.16	100.98
4	D	682	POP	P2-O-P1	-2.90	122.86	132.83
2	D	680	DND	N6A-C6A-N1A	2.90	124.60	118.57
4	C	682	POP	P2-O-P1	-2.77	123.31	132.83
3	C	681	AMP	C4-C5-N7	-2.77	106.52	109.40
3	D	681	AMP	O3P-P-O2P	2.73	118.07	107.64
3	C	681	AMP	O3P-P-O2P	2.72	118.05	107.64
3	B	681	AMP	O5'-P-O1P	-2.72	98.84	106.47
3	B	681	AMP	O3P-P-O2P	2.66	117.81	107.64
2	C	680	DND	N6A-C6A-N1A	2.54	123.85	118.57
2	B	680	DND	O4B-C4B-C5B	2.46	117.46	109.37
2	D	680	DND	C5A-C6A-N6A	-2.40	116.70	120.35
3	C	681	AMP	C5-C6-N6	2.38	123.96	120.35
2	D	680	DND	O2B-C2B-C3B	2.35	119.43	111.82
3	A	681	AMP	O3P-P-O5'	-2.35	100.48	106.73
2	A	680	DND	O4B-C4B-C5B	2.30	116.94	109.37
2	B	680	DND	O3B-C3B-C4B	-2.26	104.52	111.05
2	B	680	DND	C2A-N1A-C6A	2.24	122.59	118.75
4	B	682	POP	P2-O-P1	-2.24	125.15	132.83
3	D	681	AMP	C2-N1-C6	2.14	122.41	118.75
2	A	680	DND	O3D-C3D-C2D	-2.13	104.94	111.82
2	B	680	DND	C3D-C2D-C1D	2.07	104.09	100.98
2	B	680	DND	C1B-N9A-C4A	-2.06	123.01	126.64
2	B	680	DND	N6A-C6A-N1A	2.01	122.74	118.57

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	683	GOL	O1-C1-C2-C3
3	C	681	AMP	C5'-O5'-P-O3P
3	D	681	AMP	C5'-O5'-P-O3P
3	A	681	AMP	C5'-O5'-P-O1P
3	B	681	AMP	C5'-O5'-P-O1P
3	B	681	AMP	C5'-O5'-P-O2P
3	B	681	AMP	C5'-O5'-P-O3P
5	D	683	GOL	O1-C1-C2-O2
5	D	683	GOL	O1-C1-C2-C3
4	B	682	POP	P1-O-P2-O5

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Mol	Chain	Res	Type	Atoms
2	B	680	DND	O4D-C1D-N1N-C6N
5	B	683	GOL	C1-C2-C3-O3
2	C	680	DND	PN-O3P-PA-O5B
2	A	680	DND	PN-O3P-PA-O5B
3	B	681	AMP	O4'-C4'-C5'-O5'
3	B	681	AMP	C3'-C4'-C5'-O5'
2	B	680	DND	O4D-C4D-C5D-O5D
5	B	683	GOL	O2-C2-C3-O3
2	A	680	DND	O4D-C4D-C5D-O5D
5	B	683	GOL	O1-C1-C2-C3
5	C	683	GOL	O1-C1-C2-O2
5	B	683	GOL	O1-C1-C2-O2
2	C	680	DND	C4B-C5B-O5B-PA
2	D	680	DND	PN-O3P-PA-O5B
2	B	680	DND	PN-O3P-PA-O5B
2	C	680	DND	O4D-C4D-C5D-O5D
2	A	680	DND	C4B-C5B-O5B-PA
2	D	680	DND	O4D-C4D-C5D-O5D
2	D	680	DND	C4B-C5B-O5B-PA
2	B	680	DND	C4B-C5B-O5B-PA
2	B	680	DND	PN-O3P-PA-O13
3	D	681	AMP	C4'-C5'-O5'-P
2	B	680	DND	C3D-C4D-C5D-O5D
3	A	681	AMP	C5'-O5'-P-O3P
4	B	682	POP	P1-O-P2-O6
2	D	680	DND	C3D-C4D-C5D-O5D
2	A	680	DND	C3D-C4D-C5D-O5D
4	B	682	POP	P1-O-P2-O4

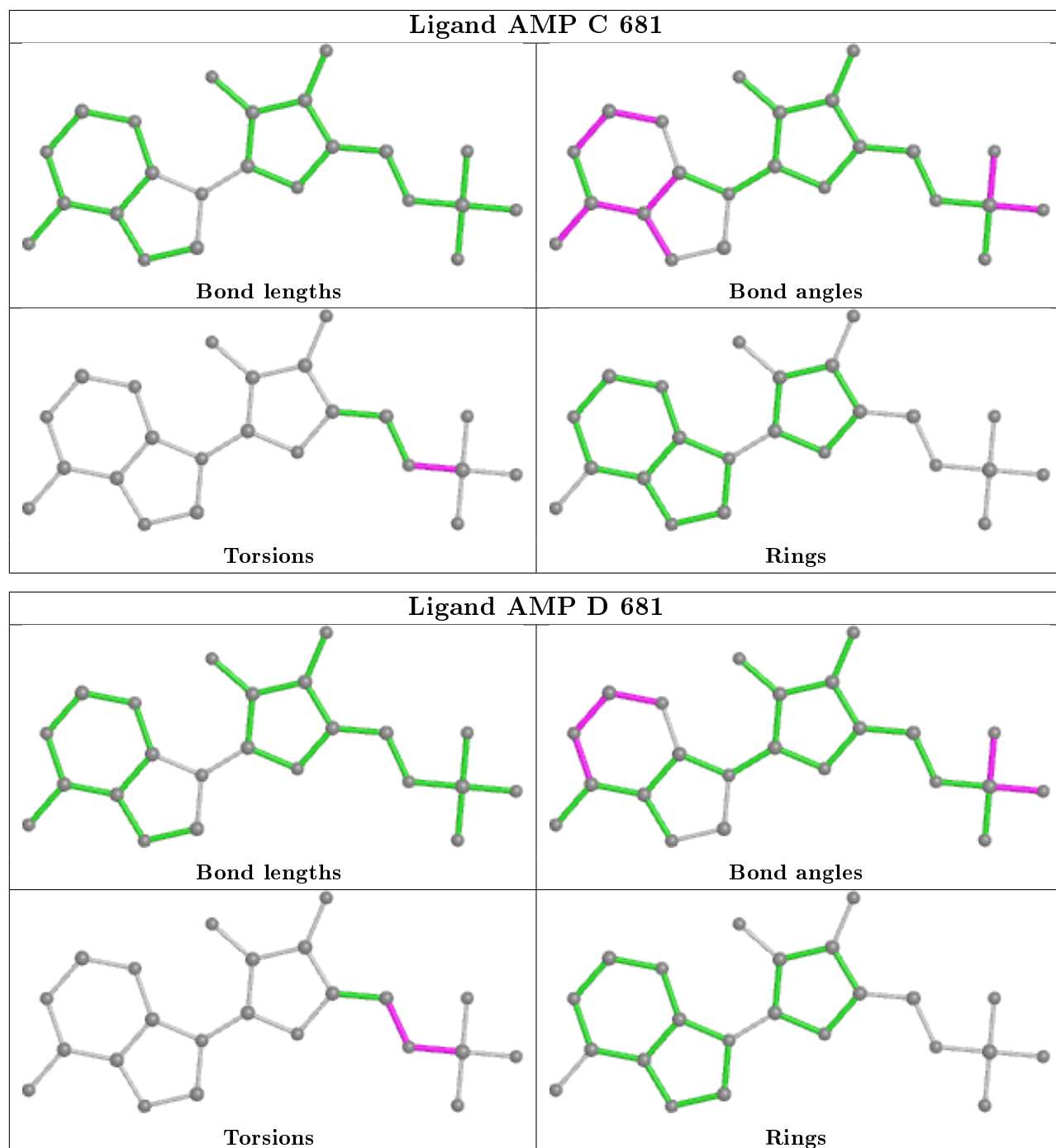
There are no ring outliers.

5 monomers are involved in 6 short contacts:

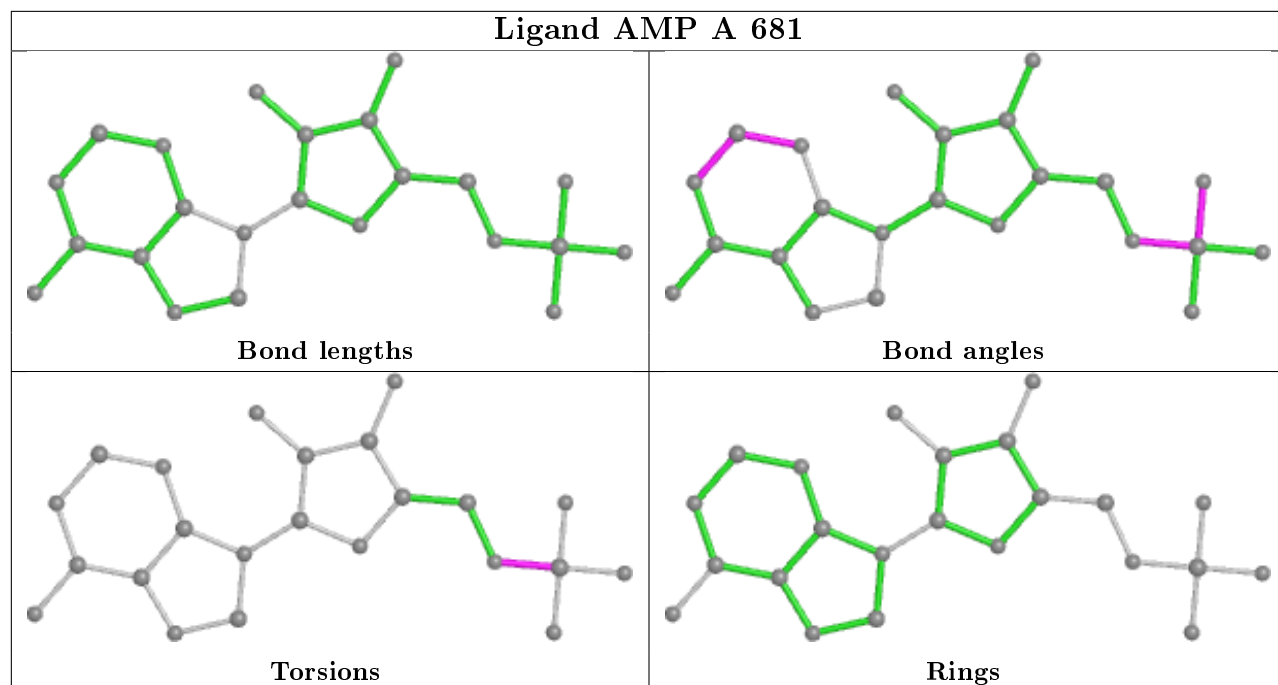
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	681	AMP	2	0
4	D	682	POP	1	0
4	B	682	POP	1	0
2	B	680	DND	1	0
2	C	680	DND	1	0

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

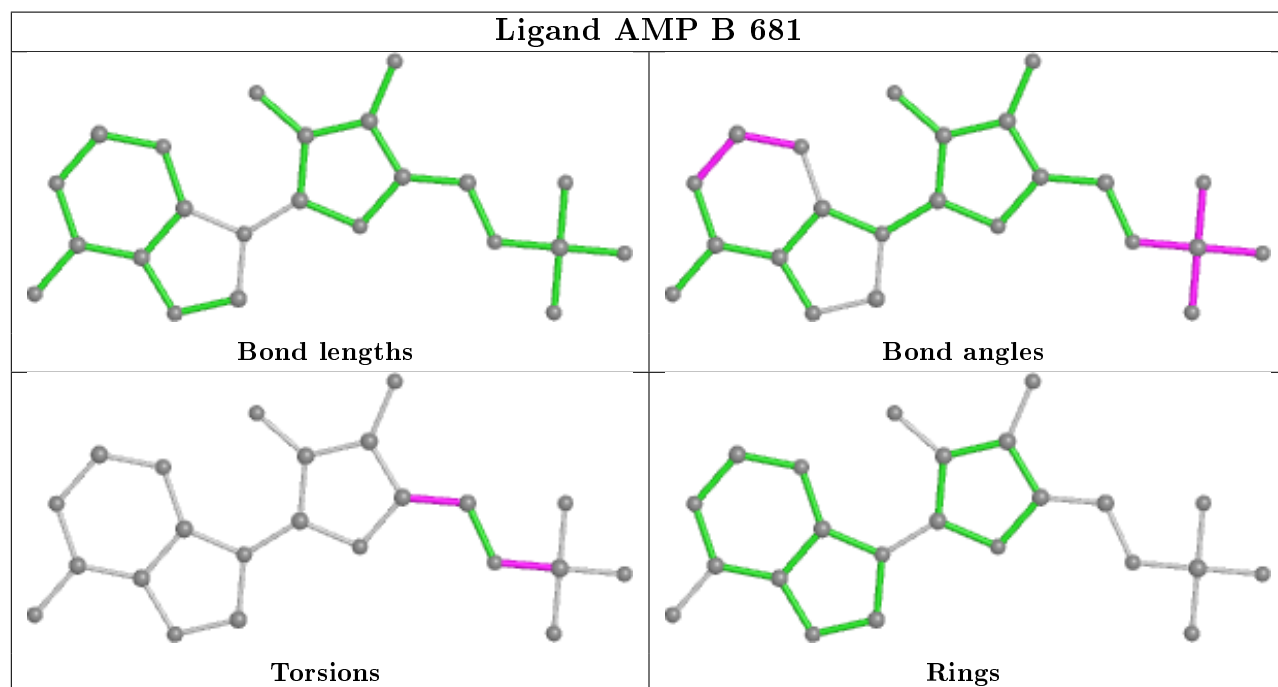
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

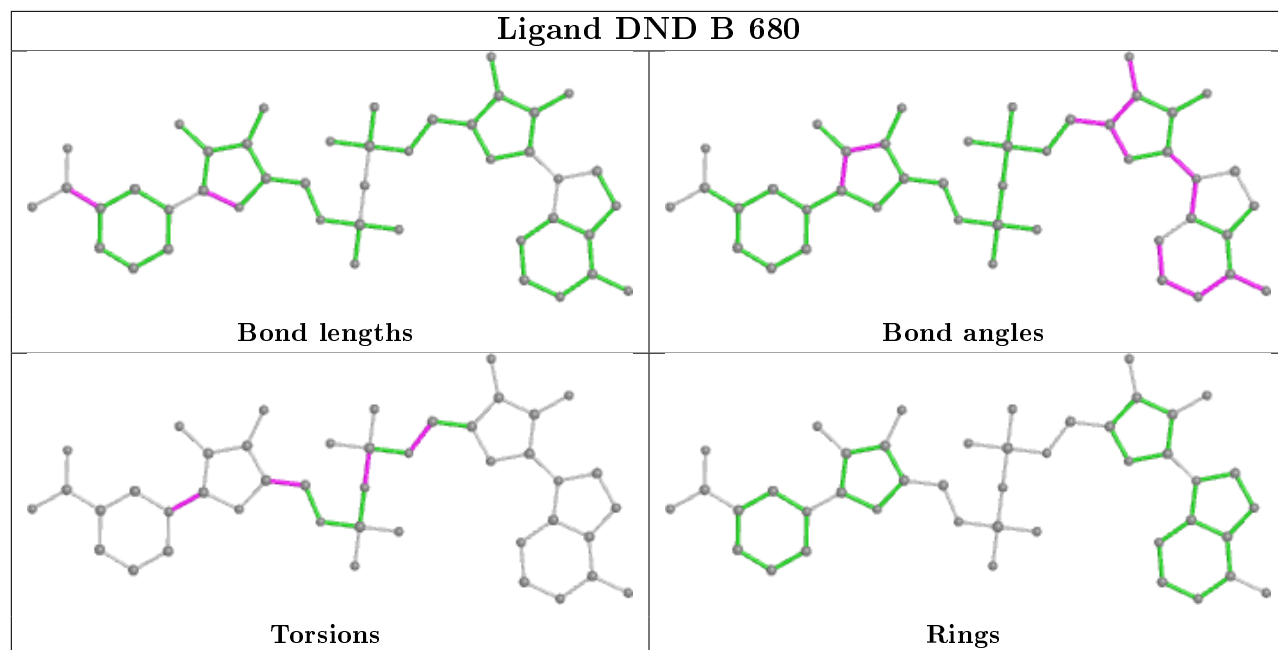
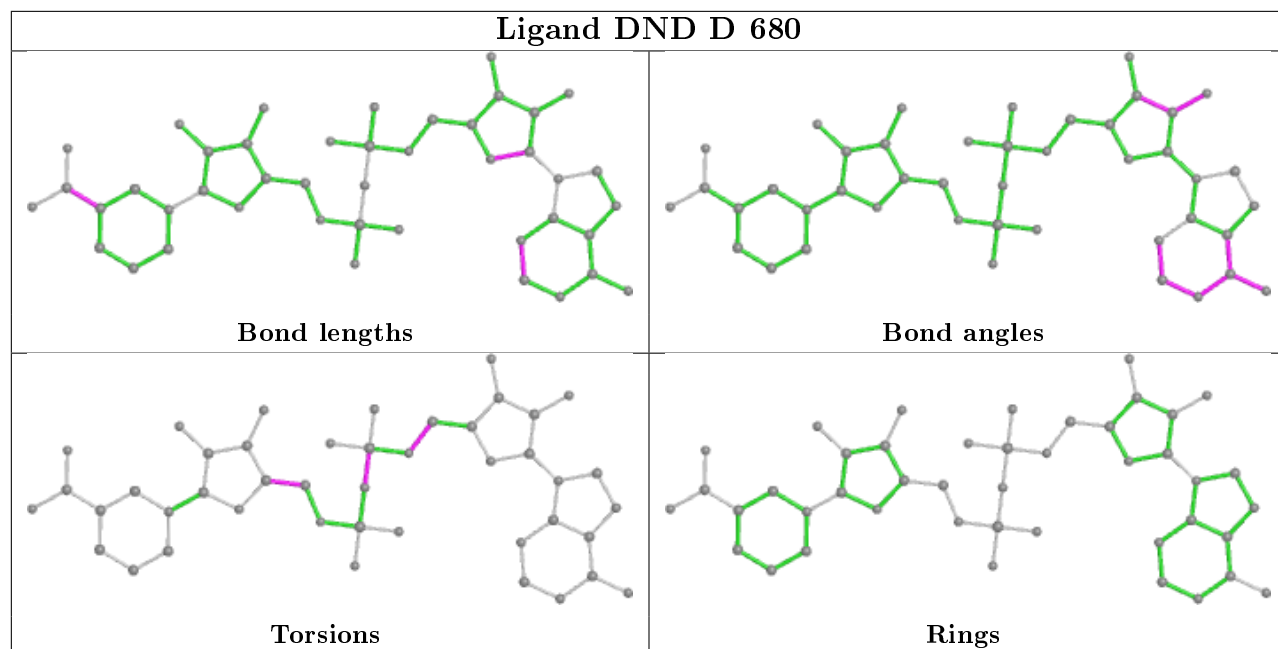


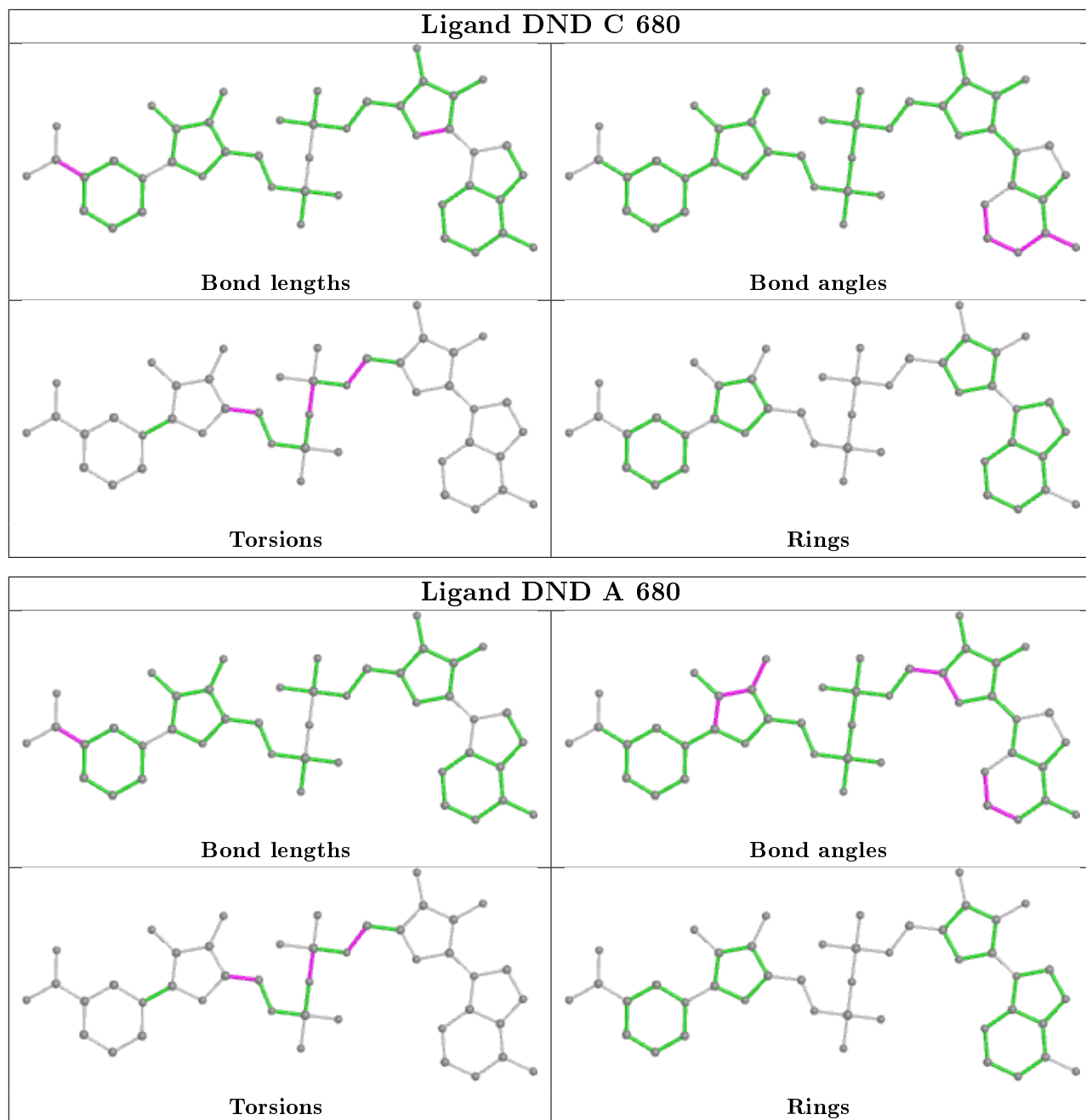
Ligand AMP A 681



Ligand AMP B 681







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	650/680 (95%)	-0.07	24 (3%) 41 44	26, 42, 71, 108	0
1	B	649/680 (95%)	-0.12	14 (2%) 62 65	23, 38, 68, 108	0
1	C	660/680 (97%)	-0.07	20 (3%) 50 53	22, 38, 68, 108	0
1	D	658/680 (96%)	-0.05	22 (3%) 46 48	23, 40, 71, 109	0
All	All	2617/2720 (96%)	-0.08	80 (3%) 49 52	22, 40, 70, 109	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	448	LYS	5.0
1	D	410	ASN	4.6
1	C	449	VAL	4.6
1	C	524	GLY	4.4
1	A	452	VAL	4.4
1	C	417	ARG	4.4
1	A	417	ARG	4.3
1	C	410	ASN	4.2
1	D	448	LYS	4.1
1	C	450	TYR	4.0
1	A	441	HIS	3.9
1	D	528	GLU	3.9
1	C	0	SER	3.8
1	D	417	ARG	3.8
1	A	402	PHE	3.7
1	C	526	PHE	3.7
1	A	410	ASN	3.7
1	B	417	ARG	3.6
1	D	450	TYR	3.6
1	C	525	GLU	3.6
1	D	524	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	525	GLU	3.5
1	B	410	ASN	3.4
1	B	441	HIS	3.4
1	A	596	GLU	3.4
1	C	532	GLU	3.4
1	A	523	ALA	3.3
1	B	150	GLY	3.3
1	D	525	GLU	3.2
1	A	524	GLY	3.2
1	C	523	ALA	3.1
1	D	596	GLU	3.1
1	A	528	GLU	3.1
1	A	298	GLU	3.1
1	C	334	GLN	3.0
1	A	529	LYS	3.0
1	A	597	ARG	3.0
1	B	525	GLU	3.0
1	D	527	GLY	3.0
1	D	298	GLU	2.9
1	B	452	VAL	2.9
1	B	528	GLU	2.9
1	C	529	LYS	2.9
1	D	449	VAL	2.9
1	A	608	GLU	2.8
1	C	528	GLU	2.8
1	C	314	ALA	2.8
1	A	454	PHE	2.8
1	D	523	ALA	2.8
1	D	314	ALA	2.7
1	D	597	ARG	2.8
1	D	607	SER	2.7
1	A	674	ARG	2.7
1	A	607	SER	2.7
1	A	526	PHE	2.7
1	D	539	ASP	2.7
1	A	451	ASP	2.6
1	C	298	GLU	2.6
1	B	453	THR	2.6
1	C	1	MET	2.6
1	A	390	PRO	2.5
1	A	453	THR	2.4
1	A	437	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	439	ILE	2.4
1	B	540	THR	2.4
1	B	678	LYS	2.3
1	C	678	LYS	2.3
1	D	532	GLU	2.3
1	D	334	GLN	2.3
1	B	454	PHE	2.3
1	D	608	GLU	2.2
1	A	595	ALA	2.2
1	D	606	LYS	2.2
1	A	143	ARG	2.2
1	D	150	GLY	2.1
1	D	333	PRO	2.1
1	C	418	ALA	2.1
1	B	437	HIS	2.1
1	C	522	SER	2.0
1	B	149	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AMP	C	681	23/23	0.69	0.30	58,93,202,206	0
3	AMP	B	681	23/23	0.72	0.25	51,80,139,151	0
3	AMP	A	681	23/23	0.80	0.22	55,89,150,153	0
3	AMP	D	681	23/23	0.80	0.23	44,80,192,196	0
4	POP	B	682	9/9	0.87	0.20	40,77,168,292	0
4	POP	A	682	9/9	0.88	0.19	53,83,179,264	0

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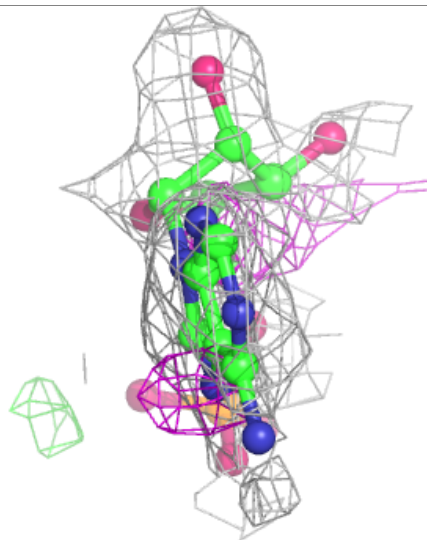
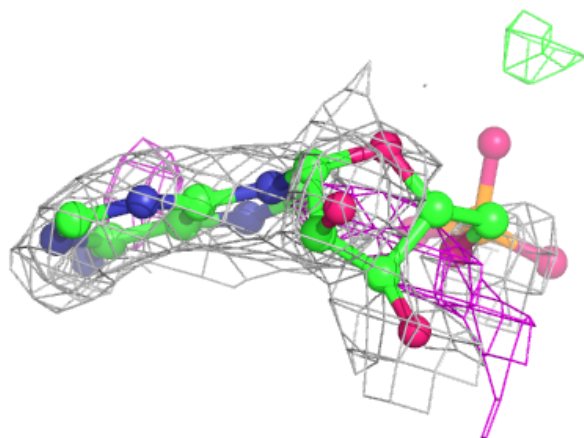
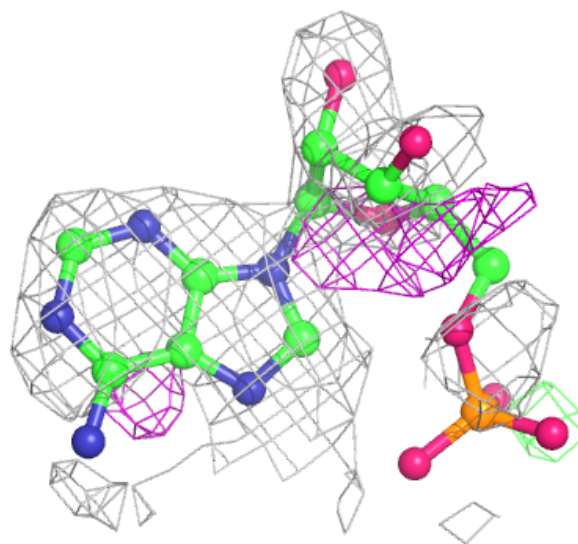
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	D	683	6/6	0.89	0.21	34,49,54,56	0
5	GOL	C	683	6/6	0.90	0.17	33,47,62,62	0
4	POP	C	682	9/9	0.91	0.16	49,103,170,272	0
5	GOL	B	683	6/6	0.92	0.14	30,45,52,57	0
4	POP	D	682	9/9	0.93	0.13	68,95,173,228	0
2	DND	D	680	44/44	0.95	0.13	34,52,87,121	0
2	DND	B	680	44/44	0.96	0.12	32,45,103,132	0
2	DND	C	680	44/44	0.96	0.11	25,46,76,87	0
2	DND	A	680	44/44	0.96	0.13	27,49,112,127	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.

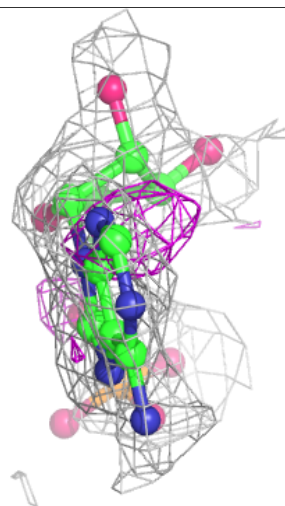
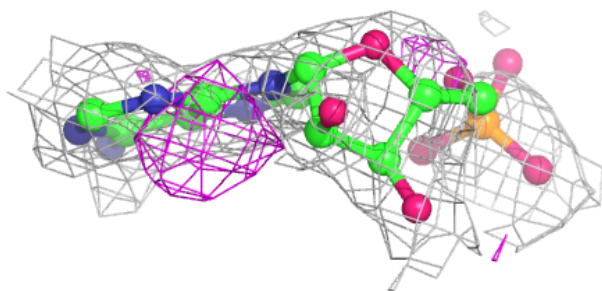
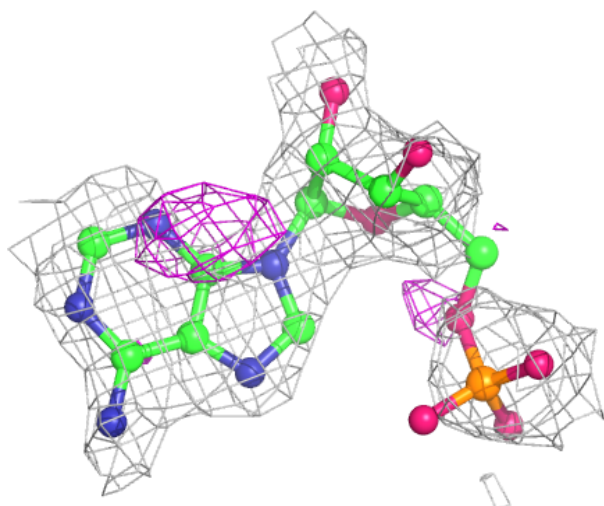
Electron density around AMP C 681:

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



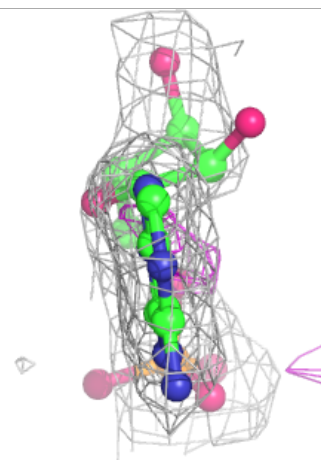
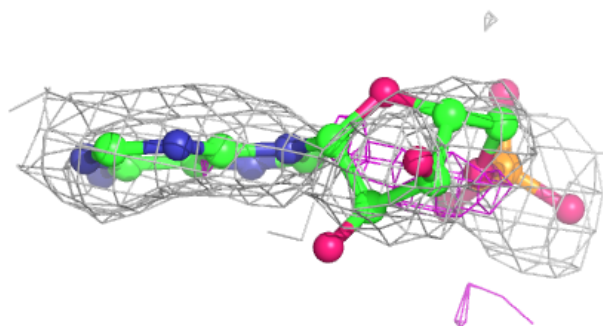
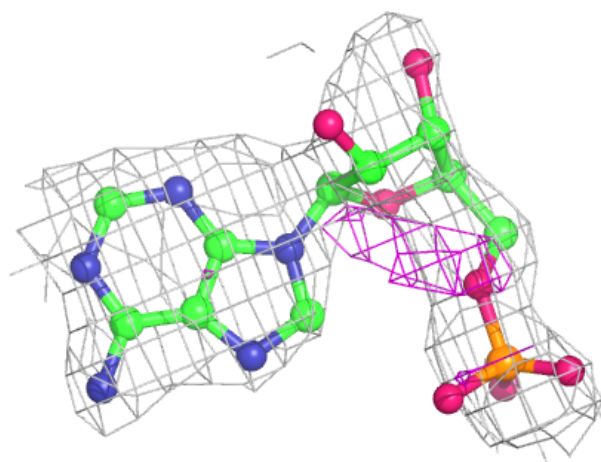
Electron density around AMP B 681:

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



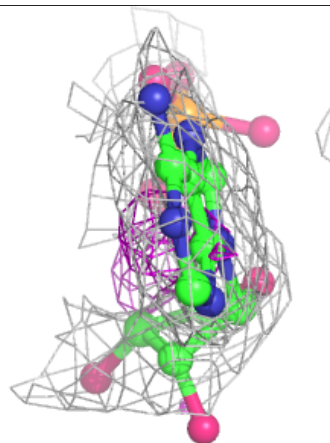
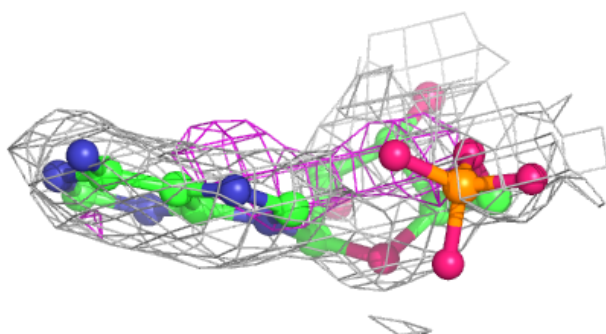
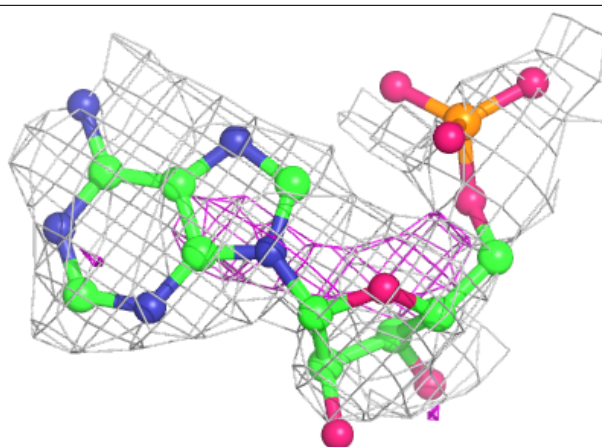
Electron density around AMP A 681:

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

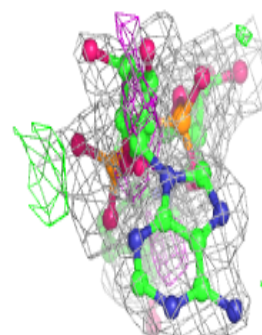
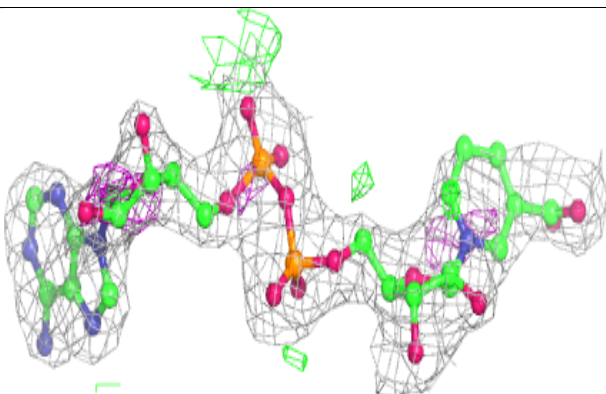
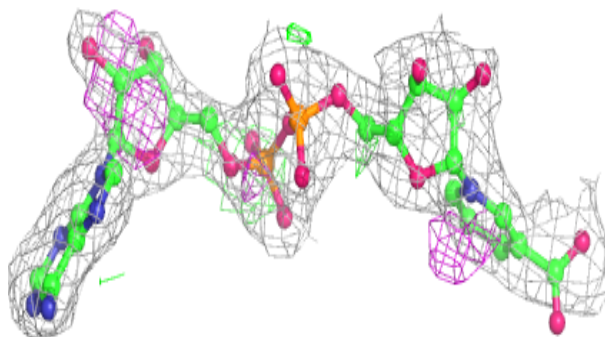


Electron density around AMP D 681:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

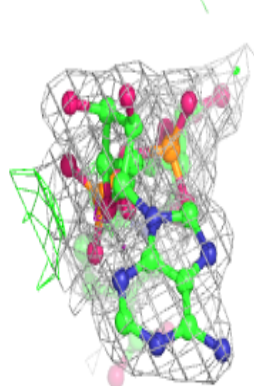
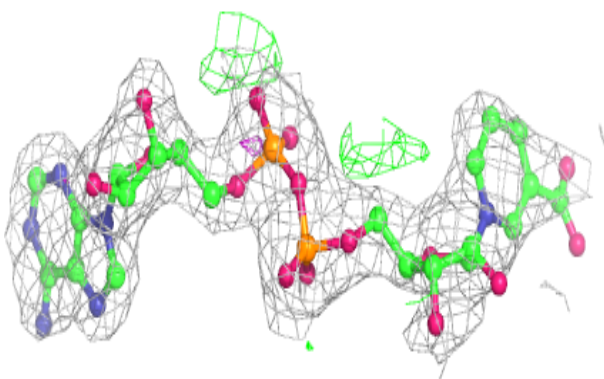
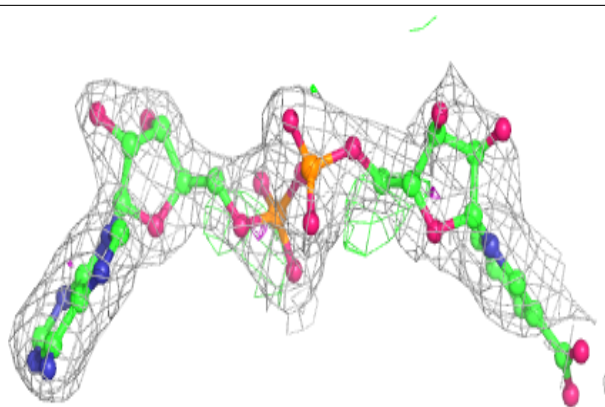
**Electron density around DND D 680:**

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

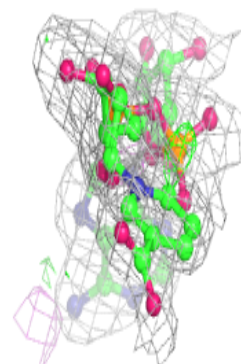
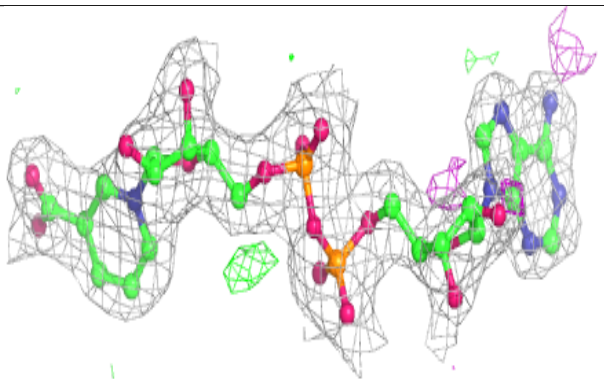
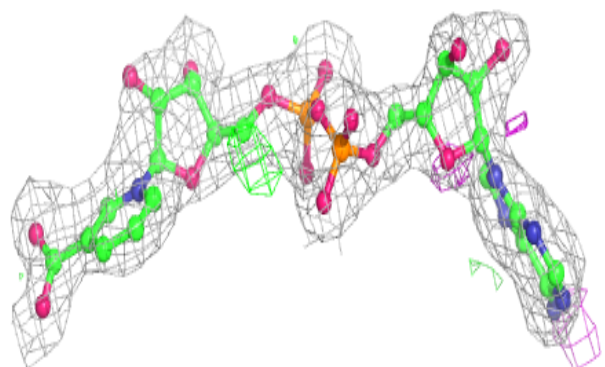


Electron density around DND B 680:

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

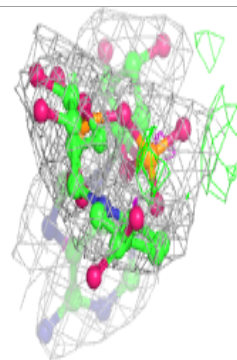
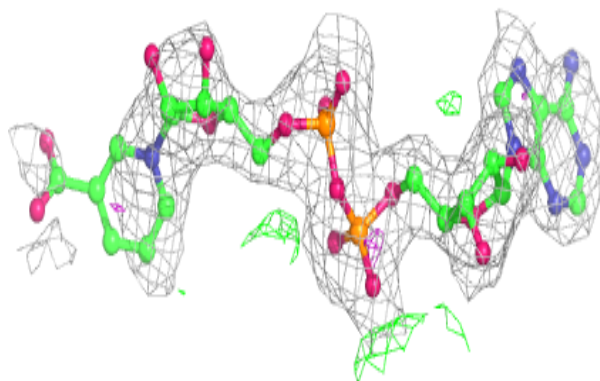
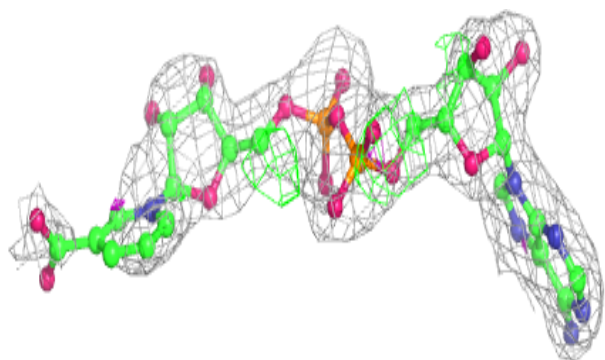
**Electron density around DND C 680:**

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



Electron density around DND A 680:

$2mF_o-DF_c$ (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.