Full wwPDB X-ray Structure Validation Report (i)

Sep 3, 2023 – 07:29 PM EDT

PDB ID	:	3SEZ
Title	:	Crystal structure of C176A mutant of glutamine-dependent NAD+ synthetase from M. tuberculosis in complex with ATP and NaAD+
Authors	:	Chuenchor, W.; Gerratana, B.
Deposited on	:	2011-06-11
Resolution	:	2.65 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

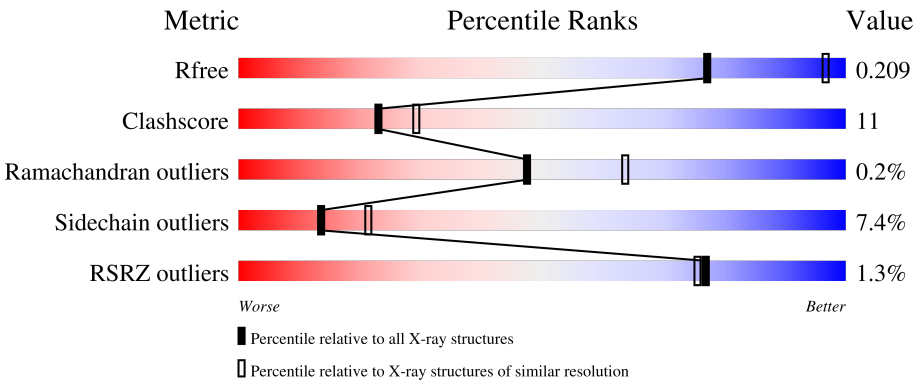
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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

Mol	Chain	Length	Quality of chain
1	A	680	.% 74% 20% • •
1	B	680	2% 74% 19% • •
1	C	680	.% 73% 19% • 5%
1	D	680	.% 71% 21% • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20820 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.

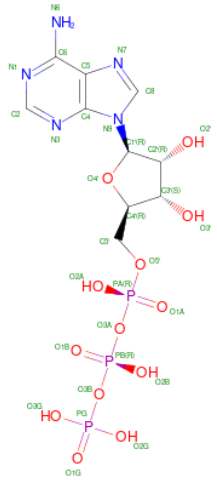
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	658	5104	3234	909	946	15	0	0	0
1	B	657	5096	3230	907	944	15	0	0	0
1	C	648	5014	3175	898	926	15	0	0	0
1	D	649	5030	3185	898	932	15	0	0	0

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 ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

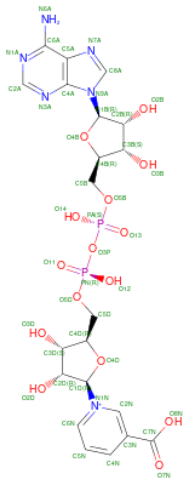
ATP



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
2	B	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
2	C	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
2	D	1	31	10	5	13	3	0	0

- Molecule 3 is NICOTINIC ACID ADENINE DINUCLEOTIDE (three-letter code: DND) (formula: $C_{21}H_{27}N_6O_{15}P_2$).

DND



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

- Molecule 4 is water.

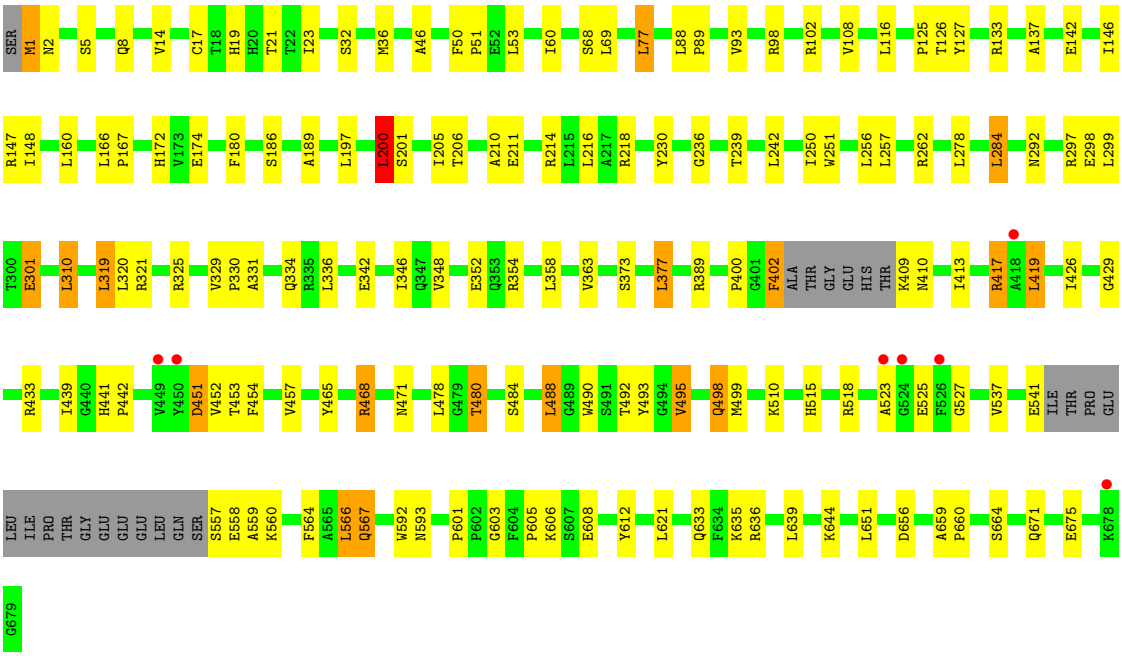
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	79	79	79	0	0
4	B	67	67	67	0	0
4	C	51	51	51	0	0
4	D	79	79	79	0	0

3 Residue-property plots (i)

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

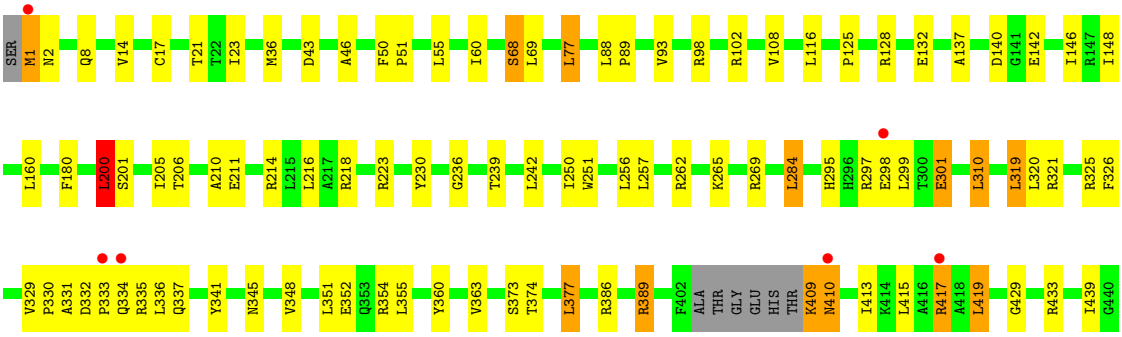
• Molecule 1: Glutamine-dependent NAD(+) synthetase

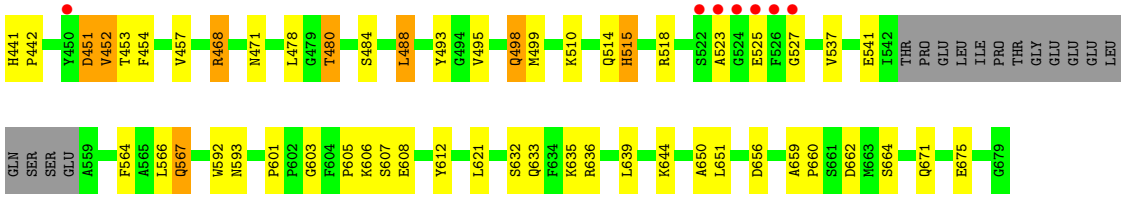
Chain A:



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

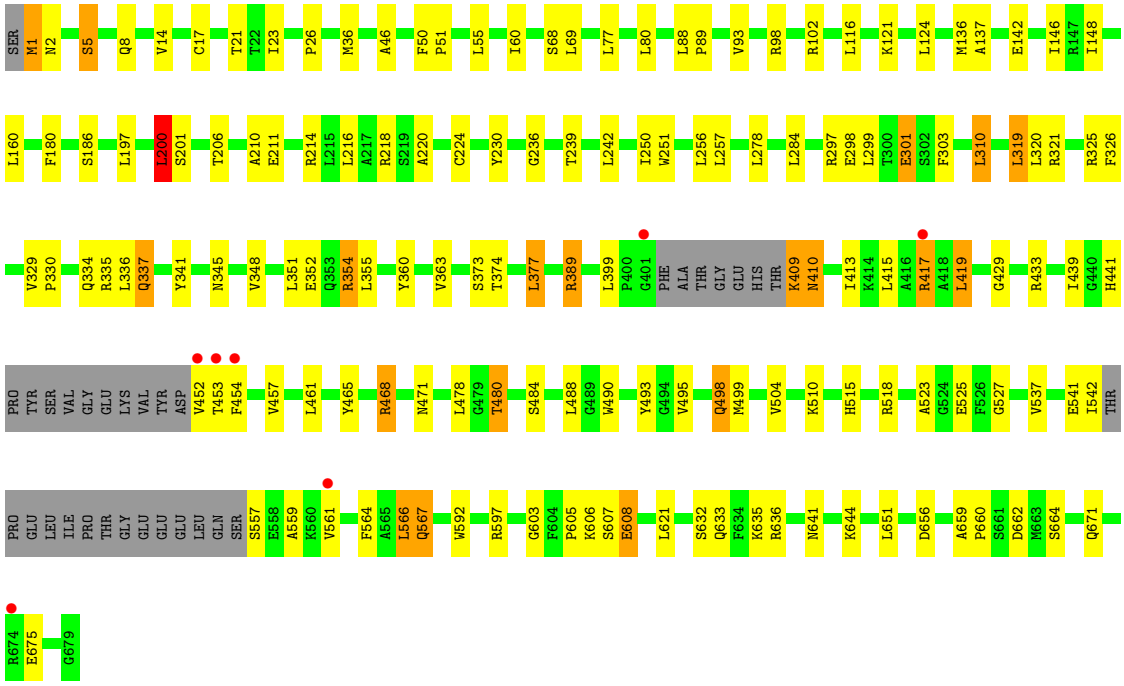
Chain B:





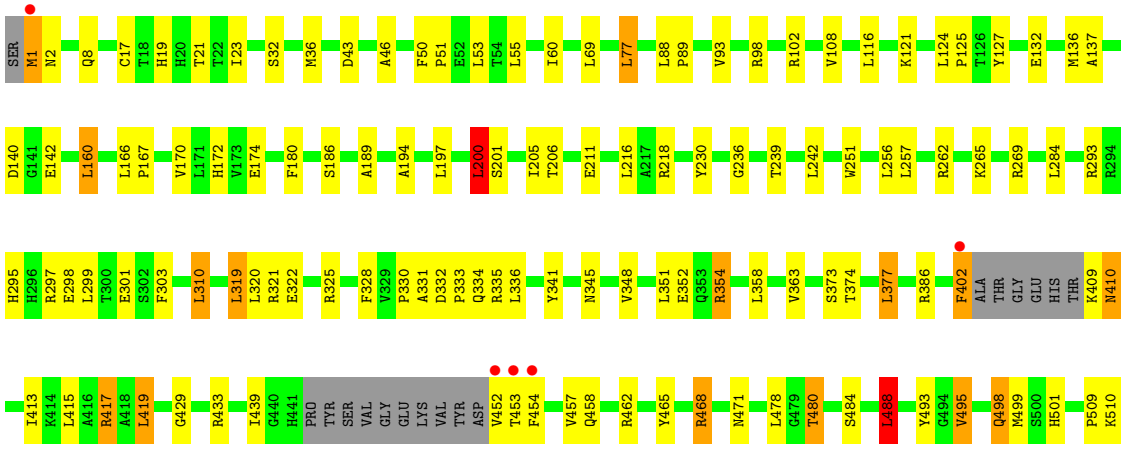
• Molecule 1: Glutamine-dependent NAD(+) synthetase

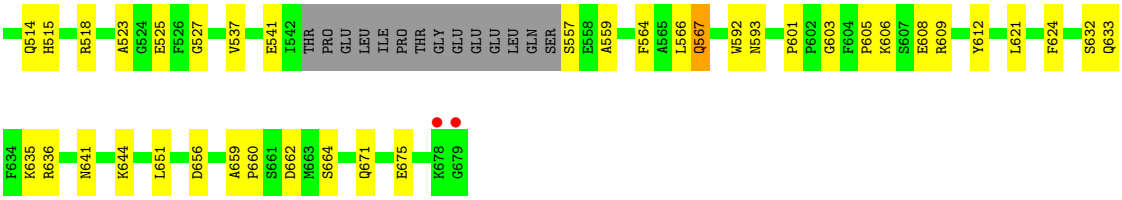
Chain C:



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

Chain D:




Q514
H515
R518
A523
G524
E525
F526
G527
V537
E541
I542
THR
PRO
GLU
LEU
ILE
PRO
THR
GLY
GLU
GLU
GLU
LEU
GLN
SER
S557
E558
A559
F564
A565
L566
Q567
W592
N593
P601
P602
G603
F604
P605
K606
S607
E608
R609
Y612
L621
F624
S632
Q633
F634
K635
R636
N641
K644
L651
D656
A659
P660
S661
D662
M663
S664
Q671
E675
K678
G679

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	178.41Å 178.41Å 216.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.33 – 2.65 34.33 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.0 (34.33-2.65) 90.4 (34.33-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	4.92 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.172 , 0.214 0.167 , 0.209	Depositor DCC
R_{free} test set	4946 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	37.7	Xtriage
Anisotropy	1.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20820	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, DND

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	0.66	2/5224 (0.0%)	0.76	4/7097 (0.1%)
1	B	0.66	0/5216	0.78	4/7088 (0.1%)
1	C	0.66	0/5129	0.76	3/6967 (0.0%)
1	D	0.66	0/5146	0.78	8/6990 (0.1%)
All	All	0.66	2/20715 (0.0%)	0.77	19/28142 (0.1%)

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	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	ASN	CG-ND2	-8.20	1.12	1.32
1	A	292	ASN	CG-OD1	-7.95	1.06	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	417	ARG	NE-CZ-NH1	-7.85	116.37	120.30
1	C	417	ARG	NE-CZ-NH2	7.59	124.09	120.30
1	D	200	LEU	CA-CB-CG	7.42	132.37	115.30
1	D	55	LEU	CB-CG-CD1	-7.35	98.50	111.00
1	B	200	LEU	CA-CB-CG	7.20	131.87	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	335	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	D	417	ARG	NE-CZ-NH2	6.93	123.77	120.30
1	C	200	LEU	CA-CB-CG	6.85	131.05	115.30
1	A	417	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	B	417	ARG	NE-CZ-NH2	6.45	123.53	120.30
1	A	200	LEU	CA-CB-CG	6.16	129.46	115.30
1	D	417	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	A	284	LEU	CA-CB-CG	5.83	128.71	115.30
1	D	293	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	D	609	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	417	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	B	284	LEU	CA-CB-CG	5.23	127.34	115.30
1	D	335	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	D	488	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	451	ASP	Peptide
1	B	451	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5104	0	4997	117	1
1	B	5096	0	4989	119	1
1	C	5014	0	4916	128	1
1	D	5030	0	4925	117	1
2	A	31	0	12	2	0
2	B	31	0	12	1	0
2	C	31	0	12	2	0
2	D	31	0	12	1	0
3	A	44	0	25	6	0
3	B	44	0	25	0	0
3	C	44	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	44	0	25	1	0
4	A	79	0	0	1	0
4	B	67	0	0	4	0
4	C	51	0	0	3	0
4	D	79	0	0	1	0
All	All	20820	0	19975	462	2

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 (462) 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:518:ARG:NH1	1:D:603:GLY:HA3	1.68	1.07
1:B:567:GLN:HA	1:B:567:GLN:HE21	1.17	1.06
1:A:567:GLN:HA	1:A:567:GLN:HE21	1.20	1.02
1:D:567:GLN:HE21	1:D:567:GLN:HA	1.19	1.02
1:C:567:GLN:HE21	1:C:567:GLN:HA	1.21	0.99
1:D:518:ARG:HH12	1:D:603:GLY:HA3	0.83	0.99
1:D:633:GLN:OE1	1:D:636:ARG:NH1	1.97	0.97
1:A:633:GLN:OE1	1:A:636:ARG:NH1	1.98	0.96
1:D:518:ARG:HH12	1:D:603:GLY:CA	1.79	0.95
1:C:633:GLN:OE1	1:C:636:ARG:NH1	1.99	0.94
1:C:46:ALA:HB1	1:C:310:LEU:HD21	1.54	0.89
1:B:633:GLN:OE1	1:B:636:ARG:NH1	2.05	0.89
1:D:46:ALA:HB1	1:D:310:LEU:HD21	1.55	0.88
1:A:46:ALA:HB1	1:A:310:LEU:HD21	1.55	0.87
1:A:172:HIS:CD2	1:A:189:ALA:HB2	2.11	0.86
1:C:518:ARG:HH22	1:C:603:GLY:HA3	1.42	0.85
1:C:329:VAL:HG11	1:C:515:HIS:CD2	2.12	0.84
1:A:329:VAL:HG11	1:A:515:HIS:CD2	2.13	0.83
1:A:671:GLN:NE2	1:A:675:GLU:HG3	1.92	0.83
1:B:493:TYR:CD1	1:B:498:GLN:NE2	2.47	0.83
1:C:518:ARG:HH22	1:C:603:GLY:CA	1.92	0.81
1:A:172:HIS:CD2	1:A:189:ALA:CB	2.64	0.80
1:B:1:MET:HG3	1:B:2:ASN:N	1.94	0.80
1:C:671:GLN:NE2	1:C:675:GLU:HG3	1.95	0.80
1:C:493:TYR:CD1	1:C:498:GLN:NE2	2.51	0.79
1:A:1:MET:HG3	1:A:2:ASN:N	1.98	0.79
1:B:671:GLN:NE2	1:B:675:GLU:HG3	1.97	0.79
1:D:319:LEU:HD13	1:D:321:ARG:HB3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:493:TYR:CD1	1:D:498:GLN:NE2	2.51	0.79
1:B:46:ALA:HB1	1:B:310:LEU:HD21	1.64	0.78
1:D:671:GLN:NE2	1:D:675:GLU:HG3	1.97	0.78
1:C:363:VAL:HG13	1:C:478:LEU:HG	1.63	0.78
1:A:493:TYR:CD1	1:A:498:GLN:NE2	2.51	0.78
1:D:363:VAL:HG13	1:D:478:LEU:HG	1.67	0.76
1:C:1:MET:HG3	1:C:2:ASN:N	1.99	0.75
1:C:518:ARG:NH2	1:C:603:GLY:HA3	2.01	0.74
1:A:297:ARG:NH2	1:B:142:GLU:OE2	2.20	0.74
1:B:363:VAL:HG13	1:B:478:LEU:HG	1.70	0.73
1:D:1:MET:HG3	1:D:2:ASN:N	2.01	0.73
1:B:493:TYR:HD1	1:B:498:GLN:HE21	1.34	0.73
1:B:567:GLN:HA	1:B:567:GLN:NE2	1.99	0.73
1:A:671:GLN:HE21	1:A:675:GLU:HG3	1.52	0.72
1:C:329:VAL:CG1	1:C:515:HIS:HD2	2.01	0.72
1:D:336:LEU:HD21	1:D:515:HIS:HD2	1.55	0.72
1:D:567:GLN:HE21	1:D:567:GLN:CA	2.00	0.72
1:A:329:VAL:CG1	1:A:515:HIS:HD2	2.02	0.72
1:A:363:VAL:HG13	1:A:478:LEU:HG	1.71	0.71
1:D:567:GLN:HA	1:D:567:GLN:NE2	2.02	0.71
1:C:329:VAL:CG1	1:C:515:HIS:CD2	2.73	0.71
1:C:297:ARG:NH2	1:D:142:GLU:OE2	2.24	0.70
1:C:671:GLN:HE21	1:C:675:GLU:HG3	1.56	0.70
1:C:377:LEU:HD13	1:C:419:LEU:HD23	1.73	0.70
1:A:329:VAL:CG1	1:A:515:HIS:CD2	2.75	0.69
1:C:98:ARG:HG3	4:C:702:HOH:O	1.90	0.69
1:A:319:LEU:HD13	1:A:321:ARG:HB3	1.75	0.69
1:D:671:GLN:HE21	1:D:675:GLU:HG3	1.58	0.69
1:A:567:GLN:HA	1:A:567:GLN:NE2	2.02	0.68
1:A:567:GLN:HE21	1:A:567:GLN:CA	2.01	0.68
1:C:480:THR:HG21	2:C:680:ATP:O3'	1.94	0.68
1:B:441:HIS:ND1	1:B:442:PRO:CD	2.57	0.68
1:A:480:THR:HG21	2:A:680:ATP:O3'	1.94	0.67
1:C:493:TYR:HD1	1:C:498:GLN:HE21	1.40	0.67
1:C:46:ALA:CB	1:C:310:LEU:HD21	2.23	0.67
1:A:468:ARG:NH2	1:D:495:VAL:HG22	2.10	0.67
1:B:671:GLN:HE21	1:B:675:GLU:HG3	1.60	0.67
1:B:441:HIS:ND1	1:B:442:PRO:HD2	2.10	0.66
1:C:319:LEU:HD13	1:C:321:ARG:HB3	1.77	0.66
1:D:493:TYR:HD1	1:D:498:GLN:HE21	1.43	0.66
1:A:377:LEU:HD13	1:A:419:LEU:HD23	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:GLU:CD	1:C:525:GLU:H	1.98	0.65
1:B:319:LEU:HD13	1:B:321:ARG:HB3	1.78	0.65
1:D:402:PHE:N	1:D:402:PHE:CD2	2.63	0.65
1:D:644:LYS:HE3	1:D:656:ASP:OD1	1.97	0.65
1:C:329:VAL:HG13	1:C:515:HIS:HD2	1.62	0.65
1:D:50:PHE:O	1:D:200:LEU:HB3	1.97	0.65
1:A:441:HIS:ND1	1:A:442:PRO:CD	2.60	0.64
1:A:493:TYR:HD1	1:A:498:GLN:HE21	1.44	0.64
1:D:468:ARG:NH1	1:D:471:ASN:OD1	2.30	0.64
1:D:525:GLU:CD	1:D:525:GLU:H	2.02	0.64
1:B:377:LEU:HD13	1:B:419:LEU:HD23	1.79	0.64
1:C:567:GLN:HA	1:C:567:GLN:NE2	2.05	0.63
1:A:525:GLU:CD	1:A:525:GLU:H	2.01	0.63
1:C:468:ARG:NH1	1:C:471:ASN:OD1	2.31	0.63
1:A:493:TYR:HB2	1:A:635:LYS:HG2	1.80	0.63
1:A:297:ARG:O	1:A:301:GLU:HG2	1.99	0.63
1:D:46:ALA:CB	1:D:310:LEU:HD21	2.29	0.62
1:A:495:VAL:HG22	1:D:468:ARG:NH2	2.14	0.62
1:D:480:THR:HG21	2:D:680:ATP:O3'	1.99	0.62
1:C:490:TRP:NE1	3:C:681:DND:H13	2.15	0.62
1:B:525:GLU:H	1:B:525:GLU:CD	2.02	0.62
1:B:413:ILE:HD13	1:B:417:ARG:HH21	1.65	0.62
1:A:441:HIS:CE1	1:A:442:PRO:HG2	2.35	0.62
1:D:297:ARG:O	1:D:301:GLU:HG2	1.99	0.61
1:D:336:LEU:HD21	1:D:515:HIS:CD2	2.36	0.61
1:C:644:LYS:HE3	1:C:656:ASP:OD1	2.01	0.61
1:D:493:TYR:HB2	1:D:635:LYS:HG2	1.83	0.61
1:D:402:PHE:N	1:D:402:PHE:HD2	1.97	0.61
1:D:514:GLN:HG3	1:D:515:HIS:ND1	2.17	0.60
1:C:493:TYR:HB2	1:C:635:LYS:HG2	1.83	0.60
1:B:413:ILE:CD1	1:B:417:ARG:HH21	2.14	0.60
1:D:377:LEU:HD13	1:D:419:LEU:HD23	1.82	0.60
1:A:402:PHE:CD2	1:A:402:PHE:N	2.70	0.59
1:C:567:GLN:HE21	1:C:567:GLN:CA	2.01	0.59
1:A:441:HIS:ND1	1:A:442:PRO:HD2	2.17	0.59
1:B:567:GLN:HE21	1:B:567:GLN:CA	1.99	0.59
1:A:329:VAL:HG13	1:A:515:HIS:HD2	1.66	0.59
1:B:441:HIS:CE1	1:B:442:PRO:HG2	2.36	0.59
1:B:2:ASN:HB3	1:B:8:GLN:NE2	2.18	0.59
1:B:514:GLN:HG3	1:B:515:HIS:ND1	2.18	0.59
1:B:644:LYS:HE3	1:B:656:ASP:OD1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:CYS:HB3	1:D:36:MET:HE2	1.85	0.59
1:A:330:PRO:HG2	1:A:336:LEU:HA	1.85	0.58
1:A:468:ARG:NH1	1:A:471:ASN:OD1	2.35	0.58
1:B:310:LEU:C	1:B:310:LEU:HD12	2.24	0.58
1:A:98:ARG:HD2	4:A:712:HOH:O	2.03	0.58
1:A:495:VAL:HG22	1:D:468:ARG:HH21	1.68	0.58
1:B:452:VAL:HG12	1:B:453:THR:N	2.19	0.58
1:C:50:PHE:O	1:C:200:LEU:HB3	2.04	0.57
1:B:50:PHE:O	1:B:200:LEU:HB3	2.05	0.57
1:A:17:CYS:HB3	1:A:36:MET:HE2	1.85	0.57
1:A:146:ILE:HG23	1:A:148:ILE:HD13	1.85	0.57
1:B:330:PRO:HG2	1:B:336:LEU:HA	1.85	0.57
1:B:468:ARG:NH2	1:C:495:VAL:HG22	2.20	0.57
1:B:46:ALA:CB	1:B:310:LEU:HD21	2.32	0.57
1:A:50:PHE:O	1:A:200:LEU:HB3	2.04	0.56
1:A:510:LYS:HD2	1:A:564:PHE:CD2	2.40	0.56
1:A:468:ARG:HH21	1:D:495:VAL:HG22	1.69	0.56
1:C:490:TRP:CD1	3:C:681:DND:H13	2.40	0.56
1:A:17:CYS:HB3	1:A:36:MET:CE	2.36	0.56
1:C:413:ILE:HD11	1:C:417:ARG:HH21	1.70	0.56
1:C:632:SER:OG	1:C:636:ARG:NH2	2.38	0.56
1:B:468:ARG:NH1	1:B:471:ASN:OD1	2.38	0.56
1:A:46:ALA:CB	1:A:310:LEU:HD21	2.30	0.56
1:D:69:LEU:C	1:D:69:LEU:HD13	2.26	0.56
1:D:98:ARG:HD2	4:D:696:HOH:O	2.05	0.56
1:B:336:LEU:HD21	1:B:515:HIS:CD2	2.40	0.55
1:D:17:CYS:HB3	1:D:36:MET:CE	2.36	0.55
1:A:363:VAL:CG1	1:A:478:LEU:HG	2.36	0.55
1:D:325:ARG:HB3	1:D:592:TRP:CZ2	2.42	0.55
1:A:492:THR:OG1	3:A:681:DND:H11	2.07	0.55
1:D:330:PRO:HG2	1:D:336:LEU:HA	1.89	0.55
1:B:325:ARG:HB3	1:B:592:TRP:CZ2	2.42	0.55
1:C:46:ALA:HB1	1:C:310:LEU:CD2	2.33	0.55
1:B:495:VAL:HG22	1:C:468:ARG:NH2	2.22	0.55
1:C:341:TYR:CE1	1:C:345:ASN:ND2	2.75	0.55
1:B:223:ARG:HD3	4:B:710:HOH:O	2.06	0.55
1:C:330:PRO:HG2	1:C:336:LEU:HA	1.89	0.55
1:C:452:VAL:HG12	1:C:453:THR:N	2.22	0.55
1:B:363:VAL:CG1	1:B:478:LEU:HG	2.36	0.55
1:C:98:ARG:HD2	4:C:718:HOH:O	2.07	0.54
1:C:557:SER:O	1:C:561:VAL:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:VAL:CG1	1:C:478:LEU:HG	2.35	0.54
1:B:386:ARG:HH21	1:D:265:LYS:HG2	1.72	0.54
1:B:480:THR:HG21	2:B:680:ATP:O3'	2.08	0.54
1:A:77:LEU:HD11	1:A:108:VAL:HG21	1.90	0.54
1:B:98:ARG:HD2	4:B:708:HOH:O	2.08	0.54
1:B:441:HIS:HE2	1:B:451:ASP:HB2	1.73	0.53
1:A:659:ALA:HB1	1:A:660:PRO:CD	2.38	0.53
1:D:439:ILE:CG2	1:D:439:ILE:O	2.57	0.53
1:A:413:ILE:HD11	1:A:417:ARG:HH21	1.72	0.53
1:C:510:LYS:HD2	1:C:564:PHE:CD2	2.44	0.53
1:B:140:ASP:HB2	1:D:295:HIS:CD2	2.43	0.53
1:C:325:ARG:HB3	1:C:592:TRP:CZ2	2.44	0.53
1:B:14:VAL:HG23	1:B:250:ILE:HD13	1.91	0.52
1:B:297:ARG:O	1:B:301:GLU:HG2	2.09	0.52
1:B:146:ILE:HG23	1:B:148:ILE:HD13	1.91	0.52
1:B:21:THR:O	1:B:236:GLY:HA3	2.10	0.52
1:B:510:LYS:HD2	1:B:564:PHE:CD2	2.45	0.52
1:C:351:LEU:HD22	1:C:355:LEU:HD11	1.92	0.52
1:D:632:SER:OG	1:D:636:ARG:NH2	2.43	0.52
1:A:510:LYS:HE3	1:A:564:PHE:CE2	2.45	0.52
1:A:23:ILE:HB	1:A:60:ILE:HG22	1.91	0.51
1:A:453:THR:O	1:A:457:VAL:HG23	2.10	0.51
1:A:441:HIS:HE2	1:A:451:ASP:HB2	1.75	0.51
1:B:495:VAL:HG22	1:C:468:ARG:HH21	1.76	0.51
1:D:429:GLY:O	1:D:433:ARG:HG3	2.10	0.51
3:A:681:DND:H24	1:D:501:HIS:HB3	1.91	0.51
1:B:493:TYR:HB2	1:B:635:LYS:HG2	1.92	0.51
1:C:2:ASN:HB3	1:C:8:GLN:NE2	2.26	0.51
1:D:410:ASN:OD1	1:D:410:ASN:N	2.41	0.51
1:B:265:LYS:HG2	1:D:386:ARG:HH21	1.76	0.51
1:B:336:LEU:HD21	1:B:515:HIS:HD2	1.75	0.51
1:B:632:SER:OG	1:B:636:ARG:NH2	2.44	0.51
1:C:329:VAL:HG11	1:C:515:HIS:NE2	2.26	0.51
1:B:429:GLY:O	1:B:433:ARG:HG3	2.11	0.51
1:D:23:ILE:HB	1:D:60:ILE:HG22	1.93	0.51
1:B:484:SER:O	1:B:488:LEU:HD22	2.10	0.51
1:A:14:VAL:HG23	1:A:250:ILE:HD13	1.93	0.50
1:D:510:LYS:HD2	1:D:564:PHE:CD2	2.46	0.50
1:C:218:ARG:HD2	1:C:251:TRP:CZ3	2.46	0.50
1:D:2:ASN:HB3	1:D:8:GLN:NE2	2.26	0.50
1:C:518:ARG:HH12	1:C:603:GLY:HA3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ASN:HB3	1:B:8:GLN:HE22	1.76	0.50
1:B:180:PHE:CD2	1:B:216:LEU:CD1	2.95	0.50
1:B:636:ARG:HD3	1:B:651:LEU:HB3	1.93	0.50
1:C:102:ARG:HD3	1:C:137:ALA:HB2	1.94	0.50
1:D:239:THR:HA	1:D:242:LEU:O	2.12	0.50
1:A:413:ILE:CD1	1:A:417:ARG:HH21	2.25	0.50
1:B:659:ALA:HB1	1:B:660:PRO:CD	2.41	0.50
1:D:21:THR:O	1:D:236:GLY:HA3	2.12	0.50
1:C:146:ILE:HG23	1:C:148:ILE:HD13	1.92	0.50
1:C:439:ILE:O	1:C:439:ILE:CG2	2.59	0.50
1:A:172:HIS:HD2	1:A:189:ALA:HB2	1.72	0.50
1:B:348:VAL:O	1:B:352:GLU:HG3	2.12	0.50
1:B:537:VAL:O	1:B:541:GLU:HG2	2.12	0.50
1:C:297:ARG:O	1:C:301:GLU:HG2	2.12	0.50
1:C:659:ALA:HB1	1:C:660:PRO:CD	2.42	0.49
1:B:452:VAL:CG1	1:B:453:THR:N	2.76	0.49
1:C:17:CYS:HB3	1:C:36:MET:CE	2.42	0.49
1:B:523:ALA:HB1	1:B:525:GLU:OE1	2.11	0.49
1:D:523:ALA:HB1	1:D:525:GLU:OE1	2.12	0.49
1:D:230:TYR:CD1	1:D:230:TYR:C	2.85	0.49
1:D:453:THR:O	1:D:457:VAL:HG23	2.12	0.49
1:A:441:HIS:ND1	1:A:442:PRO:N	2.60	0.49
1:A:358:LEU:HD21	3:D:681:DND:N6A	2.27	0.49
1:B:88:LEU:N	1:B:89:PRO:HD2	2.28	0.49
1:C:510:LYS:HE3	1:C:564:PHE:CE2	2.48	0.49
1:A:523:ALA:HB1	1:A:525:GLU:OE1	2.13	0.49
1:A:329:VAL:HG11	1:A:515:HIS:NE2	2.28	0.49
1:B:523:ALA:HB3	1:B:525:GLU:OE2	2.13	0.49
1:C:21:THR:O	1:C:236:GLY:HA3	2.12	0.49
1:D:484:SER:O	1:D:488:LEU:HD22	2.13	0.49
1:A:88:LEU:N	1:A:89:PRO:HD2	2.28	0.48
1:B:659:ALA:HB1	1:B:660:PRO:HD2	1.94	0.48
1:D:348:VAL:O	1:D:352:GLU:HG3	2.13	0.48
1:B:329:VAL:HG11	1:B:515:HIS:CD2	2.48	0.48
1:B:510:LYS:HE3	1:B:564:PHE:CE2	2.48	0.48
1:C:518:ARG:NH1	1:C:603:GLY:HA3	2.27	0.48
1:D:557:SER:C	1:D:559:ALA:N	2.64	0.48
1:A:490:TRP:NE1	3:A:681:DND:H13	2.29	0.48
1:C:23:ILE:HB	1:C:60:ILE:HG22	1.95	0.48
1:A:484:SER:O	1:A:488:LEU:HD22	2.13	0.48
1:C:186:SER:HB2	1:C:197:LEU:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:523:ALA:HB1	1:C:525:GLU:OE1	2.14	0.48
3:A:681:DND:C2A	1:D:501:HIS:HB3	2.43	0.48
1:A:644:LYS:HE3	1:A:656:ASP:OD1	2.14	0.48
1:B:468:ARG:NH2	1:C:495:VAL:O	2.47	0.48
1:C:14:VAL:HG23	1:C:250:ILE:HD13	1.95	0.48
1:A:2:ASN:HB3	1:A:8:GLN:NE2	2.29	0.48
1:A:125:PRO:HB3	1:A:127:TYR:CE2	2.49	0.48
1:B:441:HIS:ND1	1:B:442:PRO:N	2.62	0.48
1:C:518:ARG:CZ	1:C:603:GLY:HA3	2.43	0.48
1:D:659:ALA:HB1	1:D:660:PRO:CD	2.44	0.48
1:B:230:TYR:CD1	1:B:230:TYR:C	2.88	0.47
1:B:518:ARG:NH1	1:B:603:GLY:HA3	2.29	0.47
1:C:180:PHE:CD2	1:C:216:LEU:CD1	2.96	0.47
1:C:518:ARG:NH2	1:C:603:GLY:CA	2.65	0.47
1:D:523:ALA:CB	1:D:525:GLU:OE1	2.62	0.47
1:A:537:VAL:O	1:A:541:GLU:HG2	2.14	0.47
1:B:23:ILE:HB	1:B:60:ILE:HG22	1.95	0.47
1:B:69:LEU:C	1:B:69:LEU:HD13	2.34	0.47
1:B:146:ILE:HG23	1:B:148:ILE:CD1	2.43	0.47
1:C:605:PRO:HD2	1:C:608:GLU:HG3	1.97	0.47
1:C:337:GLN:OE1	1:C:337:GLN:C	2.53	0.47
1:A:200:LEU:H	1:A:200:LEU:HD23	1.80	0.47
1:A:439:ILE:HD11	1:D:465:TYR:CD1	2.50	0.47
1:B:210:ALA:O	1:B:214:ARG:HG3	2.15	0.47
1:B:360:TYR:HB3	1:B:389:ARG:HD2	1.97	0.47
1:C:88:LEU:HD11	1:C:310:LEU:HD11	1.96	0.47
1:C:537:VAL:O	1:C:541:GLU:HG2	2.14	0.47
1:D:605:PRO:HD2	1:D:608:GLU:HG3	1.97	0.47
1:B:498:GLN:OE1	1:B:499:MET:HE2	2.15	0.47
1:C:2:ASN:HB3	1:C:8:GLN:HE22	1.80	0.47
1:C:413:ILE:CD1	1:C:417:ARG:HH21	2.27	0.47
1:A:566:LEU:HD12	1:A:566:LEU:HA	1.76	0.47
1:A:348:VAL:O	1:A:352:GLU:HG3	2.15	0.47
1:B:17:CYS:HB3	1:B:36:MET:CE	2.45	0.47
1:C:452:VAL:CG1	1:C:453:THR:N	2.78	0.47
1:D:2:ASN:HB3	1:D:8:GLN:HE22	1.79	0.47
1:D:510:LYS:HE3	1:D:564:PHE:CE2	2.50	0.47
1:B:77:LEU:HD11	1:B:108:VAL:HG21	1.97	0.46
1:C:410:ASN:OD1	1:C:410:ASN:N	2.40	0.46
1:A:310:LEU:C	1:A:310:LEU:HD12	2.35	0.46
1:B:218:ARG:HD2	1:B:251:TRP:CZ3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:523:ALA:HB3	1:D:525:GLU:OE2	2.15	0.46
1:A:605:PRO:HD2	1:A:608:GLU:HG3	1.98	0.46
1:B:295:HIS:CD2	1:D:140:ASP:HB2	2.51	0.46
1:C:210:ALA:O	1:C:214:ARG:HG3	2.16	0.46
1:D:363:VAL:CG1	1:D:478:LEU:HG	2.40	0.46
1:D:557:SER:C	1:D:559:ALA:H	2.18	0.46
1:A:468:ARG:NH2	1:D:495:VAL:O	2.49	0.46
1:C:453:THR:O	1:C:457:VAL:HG23	2.16	0.46
1:D:331:ALA:HA	1:D:601:PRO:HA	1.97	0.46
1:A:146:ILE:HG23	1:A:148:ILE:CD1	2.45	0.46
1:A:636:ARG:HD3	1:A:651:LEU:HB3	1.98	0.46
1:B:125:PRO:HD2	1:B:132:GLU:CD	2.36	0.46
1:B:341:TYR:CE1	1:B:345:ASN:ND2	2.84	0.46
1:C:1:MET:CG	1:C:2:ASN:N	2.73	0.46
1:D:218:ARG:HD2	1:D:251:TRP:CZ3	2.51	0.46
1:A:21:THR:O	1:A:236:GLY:HA3	2.16	0.46
1:A:298:GLU:HG3	1:A:299:LEU:N	2.31	0.45
1:B:523:ALA:CB	1:B:525:GLU:OE1	2.64	0.45
1:B:1:MET:CG	1:B:2:ASN:N	2.71	0.45
1:B:351:LEU:HD22	1:B:355:LEU:HD11	1.96	0.45
1:A:523:ALA:CB	1:A:525:GLU:OE1	2.64	0.45
1:B:98:ARG:HG3	4:B:744:HOH:O	2.16	0.45
1:B:310:LEU:HD12	1:B:310:LEU:O	2.17	0.45
3:A:681:DND:H24	1:D:501:HIS:O	2.16	0.45
1:A:180:PHE:CD2	1:A:216:LEU:CD1	3.00	0.45
1:A:518:ARG:CZ	1:A:603:GLY:HA3	2.46	0.45
1:C:429:GLY:O	1:C:433:ARG:HG3	2.17	0.45
1:B:310:LEU:C	1:B:310:LEU:CD1	2.85	0.45
1:B:495:VAL:O	1:C:468:ARG:NH2	2.50	0.45
1:D:19:HIS:HB2	1:D:32:SER:OG	2.17	0.45
1:D:310:LEU:C	1:D:310:LEU:HD12	2.36	0.45
1:B:468:ARG:HH21	1:C:495:VAL:HG22	1.80	0.45
1:C:484:SER:O	1:C:488:LEU:HD22	2.16	0.45
1:C:662:ASP:OD1	1:C:662:ASP:N	2.50	0.45
1:C:160:LEU:HD13	1:C:303:PHE:CD2	2.51	0.45
1:D:186:SER:HB2	1:D:197:LEU:HD13	1.99	0.45
1:A:172:HIS:HD2	1:A:189:ALA:CB	2.24	0.44
1:A:200:LEU:HD23	1:A:200:LEU:N	2.32	0.44
1:A:239:THR:HA	1:A:242:LEU:O	2.17	0.44
1:B:650:ALA:O	1:B:656:ASP:HB2	2.17	0.44
1:B:662:ASP:N	1:B:662:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:LEU:N	1:D:89:PRO:HD2	2.33	0.44
1:C:17:CYS:HB3	1:C:36:MET:HE2	1.99	0.44
1:A:126:THR:OG1	1:A:133:ARG:HB2	2.17	0.44
1:A:278:LEU:C	1:A:278:LEU:HD23	2.38	0.44
1:B:514:GLN:O	1:B:518:ARG:HG3	2.17	0.44
1:C:523:ALA:HB3	1:C:525:GLU:OE2	2.18	0.44
1:C:566:LEU:HD12	1:C:566:LEU:HA	1.81	0.44
1:C:636:ARG:HD3	1:C:651:LEU:HB3	1.99	0.44
1:D:166:LEU:N	1:D:167:PRO:HD3	2.32	0.44
1:A:218:ARG:HD2	1:A:251:TRP:CZ3	2.52	0.44
1:A:523:ALA:HB3	1:A:525:GLU:OE2	2.17	0.44
1:A:557:SER:C	1:A:559:ALA:N	2.71	0.44
1:C:310:LEU:C	1:C:310:LEU:CD1	2.86	0.44
1:C:523:ALA:CB	1:C:525:GLU:OE1	2.66	0.44
1:D:205:ILE:HD11	1:D:262:ARG:NH2	2.32	0.44
1:C:88:LEU:HD11	1:C:310:LEU:CD1	2.48	0.44
1:C:230:TYR:CD1	1:C:230:TYR:C	2.90	0.44
1:A:23:ILE:HB	1:A:60:ILE:CG2	2.48	0.44
1:A:468:ARG:HA	1:A:468:ARG:HD3	1.42	0.44
1:D:174:GLU:CD	1:D:186:SER:HB3	2.38	0.44
1:D:659:ALA:HB1	1:D:660:PRO:HD2	2.00	0.44
1:A:325:ARG:HB3	1:A:592:TRP:CZ2	2.53	0.44
1:C:121:LYS:HG2	1:C:124:LEU:HD12	2.00	0.44
1:B:50:PHE:HB3	1:B:51:PRO:CD	2.48	0.43
1:B:205:ILE:HD11	1:B:262:ARG:NH2	2.33	0.43
1:B:453:THR:O	1:B:457:VAL:HG23	2.18	0.43
1:B:593:ASN:HA	1:B:612:TYR:O	2.18	0.43
1:C:239:THR:HA	1:C:242:LEU:O	2.18	0.43
1:B:298:GLU:HG3	1:B:299:LEU:N	2.33	0.43
1:C:351:LEU:HD12	1:C:504:VAL:HG11	2.00	0.43
1:D:537:VAL:O	1:D:541:GLU:HG2	2.17	0.43
1:A:19:HIS:HB2	1:A:32:SER:OG	2.18	0.43
1:A:498:GLN:OE1	1:A:499:MET:HE2	2.18	0.43
1:B:332:ASP:HA	1:B:333:PRO:HD3	1.90	0.43
1:C:88:LEU:N	1:C:89:PRO:HD2	2.33	0.43
1:A:210:ALA:O	1:A:214:ARG:HG3	2.19	0.43
1:C:200:LEU:N	1:C:200:LEU:HD23	2.34	0.43
1:C:278:LEU:C	1:C:278:LEU:HD23	2.38	0.43
1:C:298:GLU:HG3	1:C:299:LEU:N	2.34	0.43
1:C:498:GLN:OE1	1:C:499:MET:HE2	2.18	0.43
1:A:147:ARG:C	1:A:148:ILE:HD12	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:N	1:B:89:PRO:CD	2.81	0.43
1:D:102:ARG:HD3	1:D:137:ALA:HB2	2.01	0.43
1:D:498:GLN:OE1	1:D:499:MET:HE2	2.19	0.43
1:D:53:LEU:HD23	1:D:53:LEU:HA	1.80	0.43
1:D:77:LEU:HD11	1:D:108:VAL:HG21	2.01	0.43
1:A:2:ASN:HB3	1:A:8:GLN:HE22	1.84	0.43
1:C:310:LEU:C	1:C:310:LEU:HD12	2.38	0.43
1:D:567:GLN:HE22	1:D:624:PHE:HB2	1.84	0.43
1:D:662:ASP:N	1:D:662:ASP:OD1	2.52	0.43
1:C:360:TYR:HB3	1:C:389:ARG:HD2	2.01	0.43
1:A:186:SER:HB2	1:A:197:LEU:HD13	2.02	0.42
1:A:230:TYR:CD1	1:A:230:TYR:C	2.91	0.42
1:C:220:ALA:O	1:C:224:CYS:HB2	2.19	0.42
1:C:468:ARG:HA	1:C:468:ARG:HD3	1.50	0.42
1:D:125:PRO:HD2	1:D:132:GLU:CD	2.38	0.42
1:B:439:ILE:O	1:B:439:ILE:CG2	2.67	0.42
1:C:326:PHE:HB3	1:C:329:VAL:HB	2.01	0.42
1:B:239:THR:HA	1:B:242:LEU:O	2.20	0.42
1:B:331:ALA:HA	1:B:601:PRO:HA	2.01	0.42
1:C:297:ARG:HG2	1:C:301:GLU:OE2	2.19	0.42
1:C:337:GLN:OE1	1:C:337:GLN:O	2.36	0.42
1:D:170:VAL:HG12	1:D:194:ALA:HA	2.01	0.42
1:D:468:ARG:HA	1:D:468:ARG:HD3	1.52	0.42
1:D:636:ARG:HD3	1:D:651:LEU:HB3	2.01	0.42
1:A:659:ALA:HB1	1:A:660:PRO:HD2	2.01	0.42
1:B:636:ARG:O	1:B:639:LEU:HB2	2.19	0.42
1:A:377:LEU:HD13	1:A:419:LEU:CD2	2.47	0.42
1:D:172:HIS:CD2	1:D:189:ALA:HB2	2.54	0.42
1:D:180:PHE:CD2	1:D:216:LEU:CD1	3.03	0.42
1:A:50:PHE:HB3	1:A:51:PRO:CD	2.49	0.42
1:A:205:ILE:HD11	1:A:262:ARG:NH2	2.35	0.42
1:B:68:SER:HB2	4:B:698:HOH:O	2.20	0.42
1:C:557:SER:C	1:C:559:ALA:H	2.20	0.42
1:B:102:ARG:HD3	1:B:137:ALA:HB2	2.01	0.42
1:A:174:GLU:CD	1:A:186:SER:HB3	2.40	0.42
1:A:402:PHE:N	1:A:402:PHE:HD2	2.14	0.42
1:B:330:PRO:HG3	1:B:335:ARG:HG3	2.01	0.42
1:C:180:PHE:CD2	1:C:216:LEU:HD13	2.55	0.42
1:A:439:ILE:O	1:A:439:ILE:CG2	2.68	0.42
2:A:680:ATP:O2A	3:A:681:DND:O8N	2.38	0.42
1:C:80:LEU:HD23	1:C:80:LEU:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:557:SER:C	1:C:559:ALA:N	2.72	0.42
1:D:413:ILE:HD11	1:D:417:ARG:HH21	1.84	0.42
1:A:331:ALA:HA	1:A:601:PRO:HA	2.01	0.41
1:D:354:ARG:HH22	1:D:641:ASN:CG	2.22	0.41
1:A:557:SER:C	1:A:559:ALA:H	2.24	0.41
1:C:461:LEU:HD23	1:C:461:LEU:HA	1.94	0.41
1:A:166:LEU:N	1:A:167:PRO:HD3	2.35	0.41
1:C:50:PHE:HB3	1:C:51:PRO:CD	2.51	0.41
1:C:567:GLN:NE2	4:C:687:HOH:O	2.47	0.41
1:D:121:LYS:HG2	1:D:124:LEU:HD12	2.02	0.41
1:D:332:ASP:OD1	1:D:333:PRO:HD2	2.20	0.41
1:D:374:THR:HG23	1:D:415:LEU:CD2	2.50	0.41
1:A:342:GLU:O	1:A:346:ILE:HG13	2.20	0.41
1:A:429:GLY:O	1:A:433:ARG:HG3	2.20	0.41
1:B:605:PRO:HD2	1:B:608:GLU:HG3	2.02	0.41
1:C:348:VAL:O	1:C:352:GLU:HG3	2.19	0.41
1:C:377:LEU:HD13	1:C:419:LEU:CD2	2.45	0.41
1:D:593:ASN:HA	1:D:612:TYR:O	2.20	0.41
1:B:88:LEU:HD11	1:B:310:LEU:HD11	2.02	0.41
1:B:337:GLN:C	1:B:337:GLN:OE1	2.58	0.41
1:C:69:LEU:HD13	1:C:69:LEU:C	2.40	0.41
1:A:102:ARG:HD3	1:A:137:ALA:HB2	2.03	0.41
1:B:409:LYS:CG	1:B:410:ASN:H	2.33	0.41
1:C:441:HIS:ND1	1:C:441:HIS:C	2.73	0.41
1:C:542:ILE:N	1:C:542:ILE:HD12	2.36	0.41
1:D:310:LEU:HD12	1:D:310:LEU:O	2.21	0.41
1:B:43:ASP:OD2	1:B:269:ARG:NH2	2.54	0.41
1:C:5:SER:OG	1:C:8:GLN:HG3	2.21	0.41
1:D:160:LEU:HD13	1:D:303:PHE:CD2	2.56	0.41
1:D:358:LEU:HA	1:D:358:LEU:HD23	1.79	0.41
1:D:567:GLN:NE2	1:D:624:PHE:HB2	2.35	0.41
1:C:399:LEU:N	2:C:680:ATP:C2	2.89	0.41
1:D:50:PHE:HB3	1:D:51:PRO:CD	2.51	0.41
1:A:69:LEU:HD13	1:A:69:LEU:C	2.40	0.41
1:A:593:ASN:HA	1:A:612:TYR:O	2.20	0.41
1:B:374:THR:HG23	1:B:415:LEU:CD2	2.51	0.41
1:B:468:ARG:HA	1:B:468:ARG:HD3	1.44	0.41
1:C:354:ARG:HH22	1:C:641:ASN:CG	2.23	0.41
1:C:374:THR:HG23	1:C:415:LEU:CD2	2.51	0.41
1:C:659:ALA:HB1	1:C:660:PRO:HD2	2.01	0.41
1:D:341:TYR:CE1	1:D:345:ASN:ND2	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:SER:OG	1:A:8:GLN:HG3	2.21	0.41
1:B:55:LEU:HD12	1:B:55:LEU:HA	1.82	0.41
1:B:297:ARG:HG2	1:B:301:GLU:OE2	2.21	0.41
1:B:326:PHE:HB3	1:B:329:VAL:HB	2.03	0.41
1:D:298:GLU:HG3	1:D:299:LEU:N	2.35	0.41
1:B:439:ILE:HD11	1:C:465:TYR:CD1	2.57	0.40
1:C:490:TRP:CE2	3:C:681:DND:H13	2.56	0.40
1:D:23:ILE:HB	1:D:60:ILE:CG2	2.51	0.40
1:D:125:PRO:HB3	1:D:127:TYR:CE2	2.55	0.40
1:D:374:THR:HG23	1:D:415:LEU:HD22	2.03	0.40
1:D:458:GLN:O	1:D:462:ARG:HG3	2.21	0.40
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.89	0.40
1:A:297:ARG:HG2	1:A:301:GLU:OE2	2.21	0.40
1:B:128:ARG:HH11	1:B:128:ARG:HD2	1.71	0.40
1:B:265:LYS:HD3	1:B:265:LYS:HA	1.87	0.40
1:D:478:LEU:HD23	1:D:478:LEU:HA	1.84	0.40
1:A:400:PRO:HD2	1:A:426:ILE:O	2.21	0.40
1:A:465:TYR:CD1	1:D:439:ILE:HD11	2.57	0.40
1:C:409:LYS:CG	1:C:410:ASN:H	2.33	0.40
1:A:636:ARG:O	1:A:639:LEU:HB2	2.21	0.40
1:C:26:PRO:HA	1:C:55:LEU:O	2.22	0.40
1:D:43:ASP:OD2	1:D:269:ARG:NH2	2.53	0.40
1:D:328:PHE:CG	1:D:509:PRO:HG3	2.57	0.40
1:D:514:GLN:O	1:D:518:ARG:HG3	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ARG:NH2	1:C:142:GLU:OE2[8_555]	2.18	0.02
1:A:142:GLU:OE2	1:D:297:ARG:NH2[8_555]	2.19	0.01

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	652/680 (96%)	624 (96%)	27 (4%)	1 (0%)	47	64
1	B	651/680 (96%)	626 (96%)	24 (4%)	1 (0%)	47	64
1	C	640/680 (94%)	614 (96%)	25 (4%)	1 (0%)	47	64
1	D	641/680 (94%)	616 (96%)	24 (4%)	1 (0%)	47	64
All	All	2584/2720 (95%)	2480 (96%)	100 (4%)	4 (0%)	47	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	GLY
1	B	527	GLY
1	C	527	GLY
1	D	527	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	527/548 (96%)	487 (92%)	40 (8%)	13	21
1	B	525/548 (96%)	487 (93%)	38 (7%)	14	22
1	C	515/548 (94%)	476 (92%)	39 (8%)	13	21
1	D	518/548 (94%)	480 (93%)	38 (7%)	14	21
All	All	2085/2192 (95%)	1930 (93%)	155 (7%)	13	21

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	68	SER
1	A	77	LEU
1	A	93	VAL

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Mol	Chain	Res	Type
1	A	116	LEU
1	A	160	LEU
1	A	200	LEU
1	A	201	SER
1	A	206	THR
1	A	211	GLU
1	A	256	LEU
1	A	257	LEU
1	A	284	LEU
1	A	301	GLU
1	A	310	LEU
1	A	319	LEU
1	A	320	LEU
1	A	334	GLN
1	A	354	ARG
1	A	373	SER
1	A	377	LEU
1	A	389	ARG
1	A	402	PHE
1	A	409	LYS
1	A	410	ASN
1	A	419	LEU
1	A	452	VAL
1	A	454	PHE
1	A	468	ARG
1	A	480	THR
1	A	488	LEU
1	A	495	VAL
1	A	498	GLN
1	A	558	GLU
1	A	560	LYS
1	A	566	LEU
1	A	567	GLN
1	A	606	LYS
1	A	621	LEU
1	A	664	SER
1	B	1	MET
1	B	68	SER
1	B	77	LEU
1	B	93	VAL
1	B	116	LEU
1	B	160	LEU

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Mol	Chain	Res	Type
1	B	200	LEU
1	B	201	SER
1	B	206	THR
1	B	211	GLU
1	B	256	LEU
1	B	257	LEU
1	B	284	LEU
1	B	301	GLU
1	B	310	LEU
1	B	319	LEU
1	B	320	LEU
1	B	334	GLN
1	B	354	ARG
1	B	373	SER
1	B	377	LEU
1	B	389	ARG
1	B	409	LYS
1	B	410	ASN
1	B	419	LEU
1	B	452	VAL
1	B	454	PHE
1	B	468	ARG
1	B	480	THR
1	B	488	LEU
1	B	498	GLN
1	B	515	HIS
1	B	566	LEU
1	B	567	GLN
1	B	606	LYS
1	B	607	SER
1	B	621	LEU
1	B	664	SER
1	C	1	MET
1	C	5	SER
1	C	68	SER
1	C	77	LEU
1	C	93	VAL
1	C	116	LEU
1	C	136	MET
1	C	200	LEU
1	C	201	SER
1	C	206	THR

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Mol	Chain	Res	Type
1	C	211	GLU
1	C	256	LEU
1	C	257	LEU
1	C	284	LEU
1	C	301	GLU
1	C	310	LEU
1	C	319	LEU
1	C	320	LEU
1	C	334	GLN
1	C	337	GLN
1	C	354	ARG
1	C	373	SER
1	C	377	LEU
1	C	389	ARG
1	C	409	LYS
1	C	410	ASN
1	C	419	LEU
1	C	454	PHE
1	C	468	ARG
1	C	480	THR
1	C	498	GLN
1	C	566	LEU
1	C	567	GLN
1	C	597	ARG
1	C	606	LYS
1	C	607	SER
1	C	608	GLU
1	C	621	LEU
1	C	664	SER
1	D	1	MET
1	D	77	LEU
1	D	93	VAL
1	D	116	LEU
1	D	136	MET
1	D	160	LEU
1	D	200	LEU
1	D	201	SER
1	D	206	THR
1	D	211	GLU
1	D	256	LEU
1	D	257	LEU
1	D	284	LEU

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Mol	Chain	Res	Type
1	D	310	LEU
1	D	319	LEU
1	D	320	LEU
1	D	322	GLU
1	D	334	GLN
1	D	351	LEU
1	D	354	ARG
1	D	373	SER
1	D	377	LEU
1	D	402	PHE
1	D	409	LYS
1	D	410	ASN
1	D	419	LEU
1	D	452	VAL
1	D	454	PHE
1	D	468	ARG
1	D	480	THR
1	D	488	LEU
1	D	495	VAL
1	D	498	GLN
1	D	566	LEU
1	D	567	GLN
1	D	606	LYS
1	D	621	LEU
1	D	664	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	HIS
1	A	345	ASN
1	A	515	HIS
1	A	567	GLN
1	B	8	GLN
1	B	172	HIS
1	B	295	HIS
1	B	345	ASN
1	B	567	GLN
1	C	172	HIS
1	C	345	ASN
1	C	515	HIS
1	C	567	GLN

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Mol	Chain	Res	Type
1	D	8	GLN
1	D	295	HIS
1	D	345	ASN
1	D	567	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ATP	B	680	-	26,33,33	0.85	1 (3%)	31,52,52	1.27	1 (3%)
3	DND	B	681	-	42,48,48	0.92	1 (2%)	50,73,73	1.20	3 (6%)
3	DND	D	681	-	42,48,48	0.83	2 (4%)	50,73,73	1.25	4 (8%)
2	ATP	A	680	-	26,33,33	0.84	1 (3%)	31,52,52	1.46	5 (16%)
2	ATP	C	680	-	26,33,33	0.79	1 (3%)	31,52,52	1.37	4 (12%)
3	DND	C	681	-	42,48,48	0.81	1 (2%)	50,73,73	1.19	2 (4%)
3	DND	A	681	-	42,48,48	0.86	2 (4%)	50,73,73	1.40	5 (10%)
2	ATP	D	680	-	26,33,33	0.94	2 (7%)	31,52,52	1.25	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	B	680	-	-	11/18/38/38	0/3/3/3
3	DND	B	681	-	-	9/26/62/62	0/5/5/5
3	DND	D	681	-	-	12/26/62/62	0/5/5/5
2	ATP	A	680	-	-	0/18/38/38	0/3/3/3
2	ATP	C	680	-	-	4/18/38/38	0/3/3/3
3	DND	C	681	-	-	8/26/62/62	0/5/5/5
3	DND	A	681	-	-	9/26/62/62	0/5/5/5
2	ATP	D	680	-	-	2/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	680	ATP	O4'-C1'	2.89	1.45	1.41
3	A	681	DND	O4B-C1B	2.88	1.45	1.41
3	B	681	DND	O4B-C1B	2.88	1.45	1.41
2	A	680	ATP	O4'-C1'	2.47	1.44	1.41
2	B	680	ATP	O4'-C1'	2.45	1.44	1.41
3	C	681	DND	O4D-C1D	2.20	1.44	1.41
3	D	681	DND	O4D-C1D	2.13	1.44	1.41
2	C	680	ATP	O4'-C1'	2.09	1.44	1.41
3	A	681	DND	C2A-N3A	2.07	1.35	1.32
2	D	680	ATP	C2-N3	2.02	1.35	1.32
3	D	681	DND	O4B-C1B	2.02	1.43	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	681	DND	N3A-C2A-N1A	-5.31	120.38	128.68
3	C	681	DND	N3A-C2A-N1A	-5.01	120.85	128.68
3	A	681	DND	N3A-C2A-N1A	-4.92	120.99	128.68
2	A	680	ATP	N3-C2-N1	-4.76	121.23	128.68
2	D	680	ATP	N3-C2-N1	-4.56	121.55	128.68
2	B	680	ATP	N3-C2-N1	-4.55	121.57	128.68
2	C	680	ATP	N3-C2-N1	-4.41	121.78	128.68
3	B	681	DND	N3A-C2A-N1A	-4.22	122.08	128.68
3	A	681	DND	C3D-C2D-C1D	3.50	106.24	100.98
3	D	681	DND	C3D-C2D-C1D	3.27	105.91	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	681	DND	C3D-C2D-C1D	3.08	105.62	100.98
2	C	680	ATP	PB-O3B-PG	-3.04	122.41	132.83
3	B	681	DND	C3D-C2D-C1D	3.01	105.51	100.98
3	A	681	DND	N6A-C6A-N1A	2.85	124.50	118.57
3	D	681	DND	O4D-C4D-C3D	2.55	110.16	105.11
2	D	680	ATP	C4-C5-N7	-2.46	106.84	109.40
3	B	681	DND	C3B-C2B-C1B	2.44	104.64	100.98
3	A	681	DND	C5A-C6A-N6A	-2.43	116.65	120.35
3	A	681	DND	C2N-C3N-C4N	2.41	120.99	118.26
2	A	680	ATP	PB-O3B-PG	-2.32	124.86	132.83
2	A	680	ATP	C2-N1-C6	2.22	122.56	118.75
3	D	681	DND	C4A-C5A-N7A	-2.11	107.20	109.40
2	C	680	ATP	O3G-PG-O2G	2.07	115.53	107.64
2	A	680	ATP	PA-O3A-PB	-2.06	125.74	132.83
2	A	680	ATP	O2B-PB-O1B	2.06	122.44	112.24
2	C	680	ATP	C2-N1-C6	2.02	122.21	118.75

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	680	ATP	PB-O3B-PG-O2G
3	A	681	DND	O4D-C1D-N1N-C6N
3	A	681	DND	C2N-C3N-C7N-O7N
3	A	681	DND	C2N-C3N-C7N-O8N
3	B	681	DND	O4D-C1D-N1N-C6N
3	B	681	DND	O4D-C1D-N1N-C2N
3	B	681	DND	C2D-C1D-N1N-C6N
3	B	681	DND	C2D-C1D-N1N-C2N
3	C	681	DND	O4D-C4D-C5D-O5D
3	C	681	DND	C2N-C3N-C7N-O7N
3	C	681	DND	C2N-C3N-C7N-O8N
3	D	681	DND	O4D-C1D-N1N-C6N
3	D	681	DND	O4D-C1D-N1N-C2N
3	D	681	DND	C2D-C1D-N1N-C6N
3	D	681	DND	C2D-C1D-N1N-C2N
3	A	681	DND	C4N-C3N-C7N-O7N
3	A	681	DND	C4N-C3N-C7N-O8N
3	C	681	DND	C4N-C3N-C7N-O8N
3	C	681	DND	C4N-C3N-C7N-O7N
3	B	681	DND	O4D-C4D-C5D-O5D
3	C	681	DND	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
3	D	681	DND	O4D-C4D-C5D-O5D
2	B	680	ATP	O4'-C4'-C5'-O5'
3	B	681	DND	C3D-C4D-C5D-O5D
2	B	680	ATP	PA-O3A-PB-O1B
2	C	680	ATP	PG-O3B-PB-O1B
3	A	681	DND	PN-O3P-PA-O13
3	B	681	DND	PN-O3P-PA-O13
3	D	681	DND	C4N-C3N-C7N-O8N
3	A	681	DND	C4B-C5B-O5B-PA
3	D	681	DND	C4B-C5B-O5B-PA
3	D	681	DND	C4N-C3N-C7N-O7N
3	B	681	DND	C4B-C5B-O5B-PA
3	D	681	DND	C2N-C3N-C7N-O8N
3	A	681	DND	PN-O3P-PA-O5B
3	B	681	DND	PN-O3P-PA-O5B
3	D	681	DND	PN-O3P-PA-O5B
2	B	680	ATP	C3'-C4'-C5'-O5'
2	B	680	ATP	PB-O3B-PG-O3G
2	B	680	ATP	C5'-O5'-PA-O3A
3	A	681	DND	O4D-C4D-C5D-O5D
2	C	680	ATP	PB-O3A-PA-O1A
3	C	681	DND	C4B-C5B-O5B-PA
3	D	681	DND	C2N-C3N-C7N-O7N
2	B	680	ATP	PA-O3A-PB-O2B
2	C	680	ATP	PG-O3B-PB-O2B
3	D	681	DND	C3D-C4D-C5D-O5D
2	D	680	ATP	PG-O3B-PB-O1B
2	B	680	ATP	PB-O3B-PG-O1G
2	B	680	ATP	PG-O3B-PB-O2B
2	C	680	ATP	PB-O3A-PA-O2A
2	D	680	ATP	PG-O3B-PB-O2B
2	B	680	ATP	C5'-O5'-PA-O1A
2	B	680	ATP	C5'-O5'-PA-O2A
3	C	681	DND	C5B-O5B-PA-O13

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	680	ATP	1	0
3	D	681	DND	1	0
2	A	680	ATP	2	0

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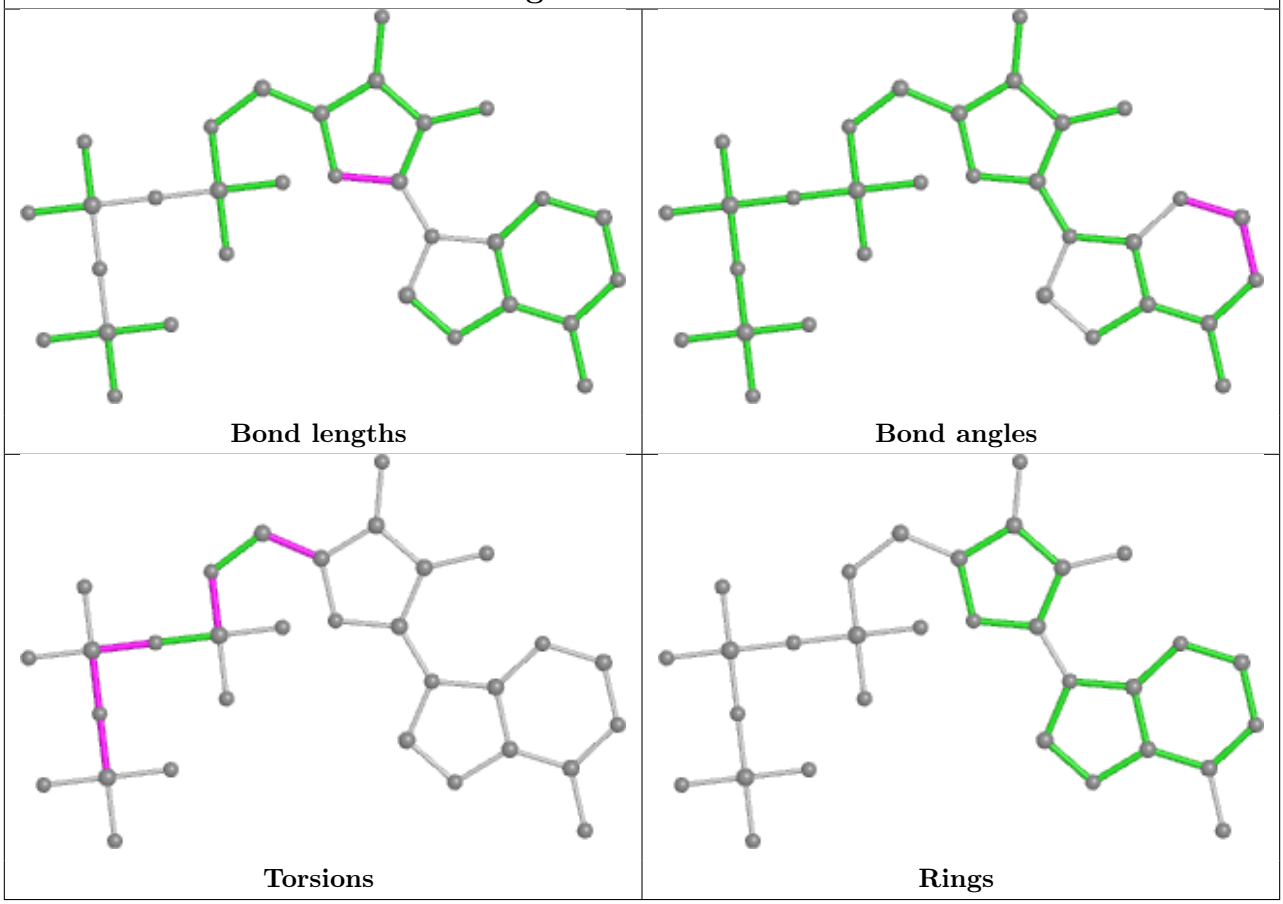
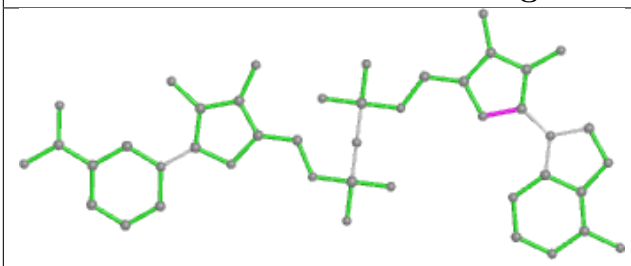
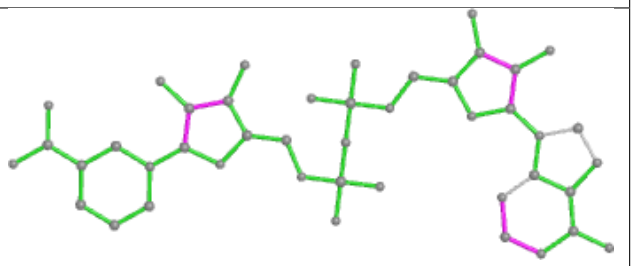
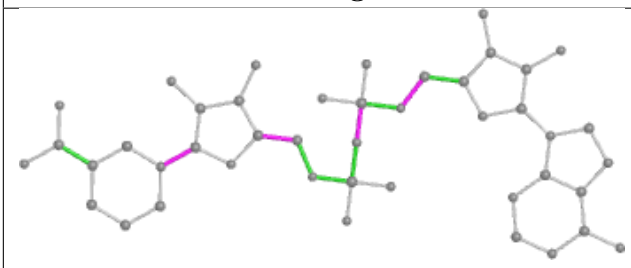
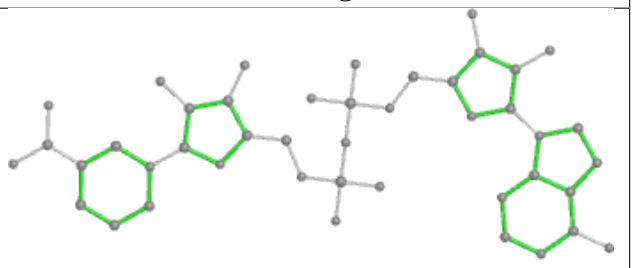
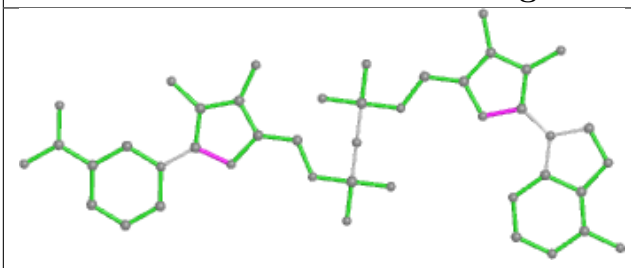
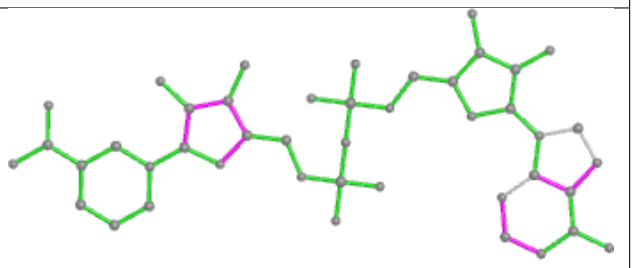
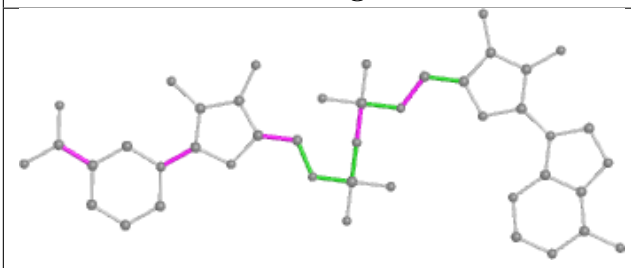
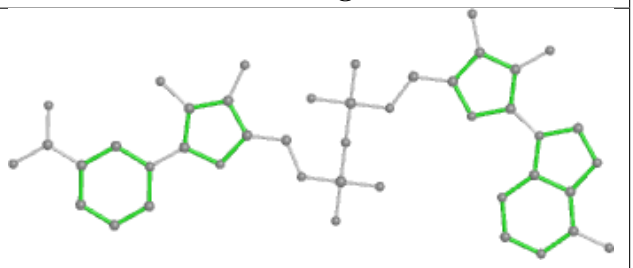
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	680	ATP	2	0
3	C	681	DND	3	0
3	A	681	DND	6	0
2	D	680	ATP	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

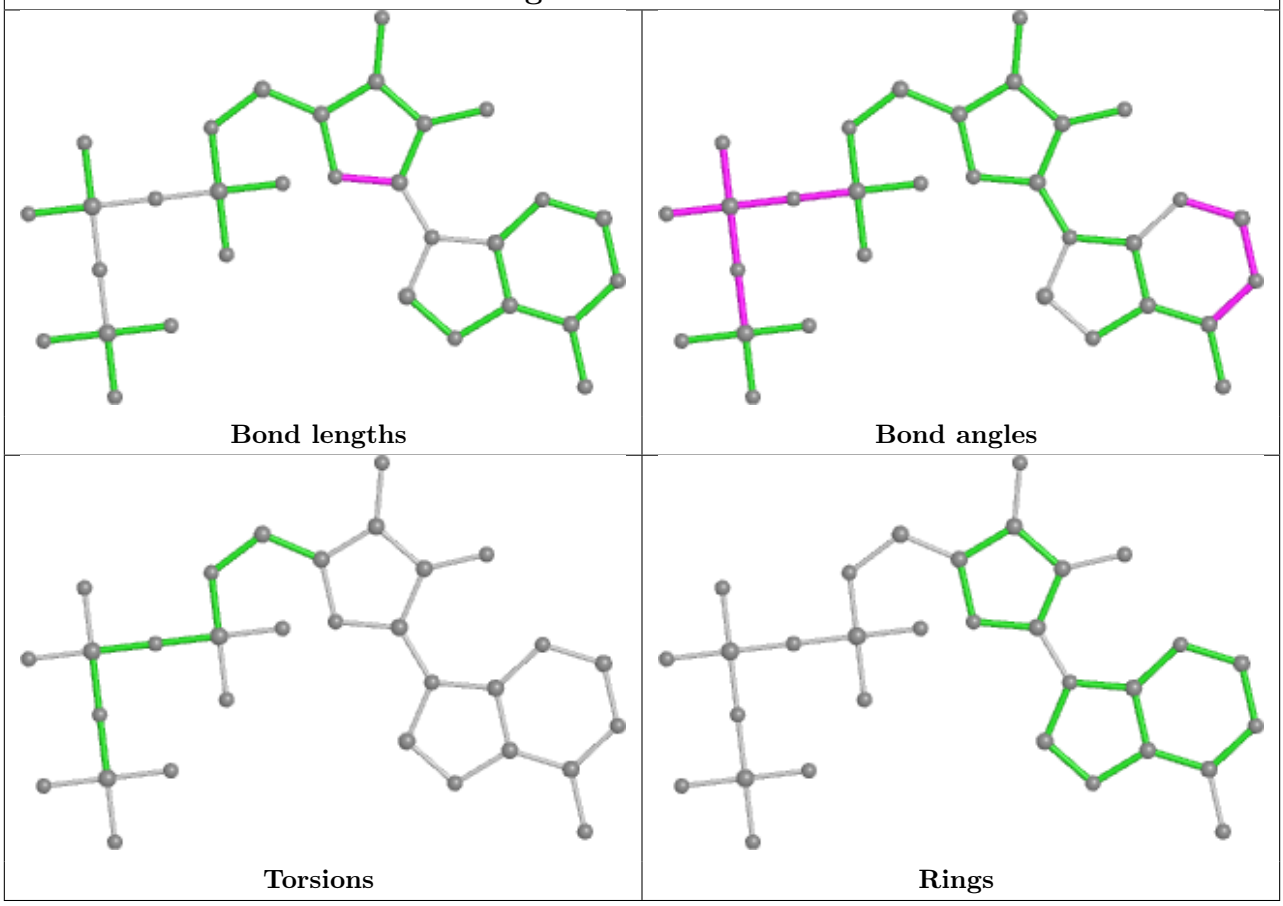
Ligand ATP B 680



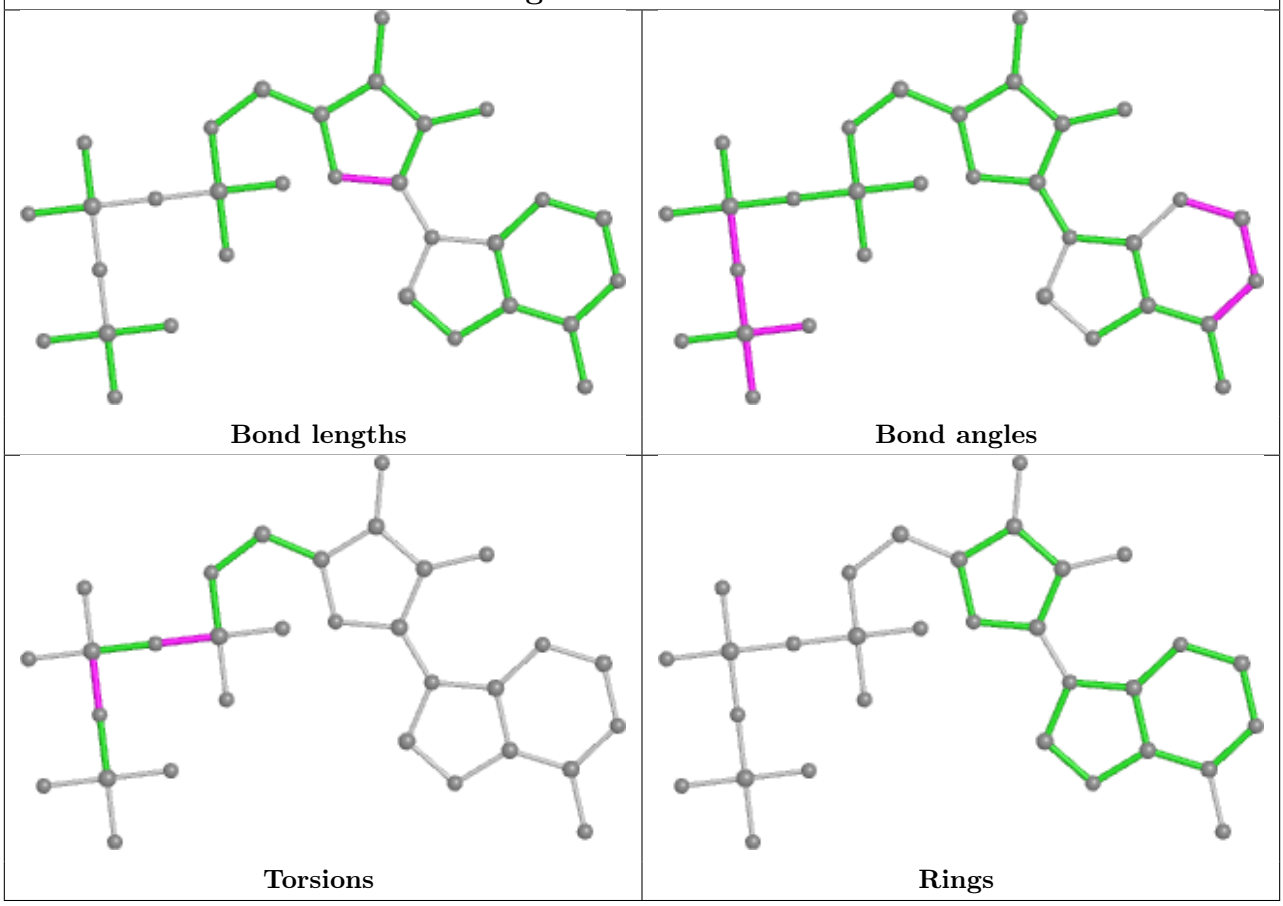
Ligand DND B 681	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DND D 681	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP A 680



Ligand ATP C 680



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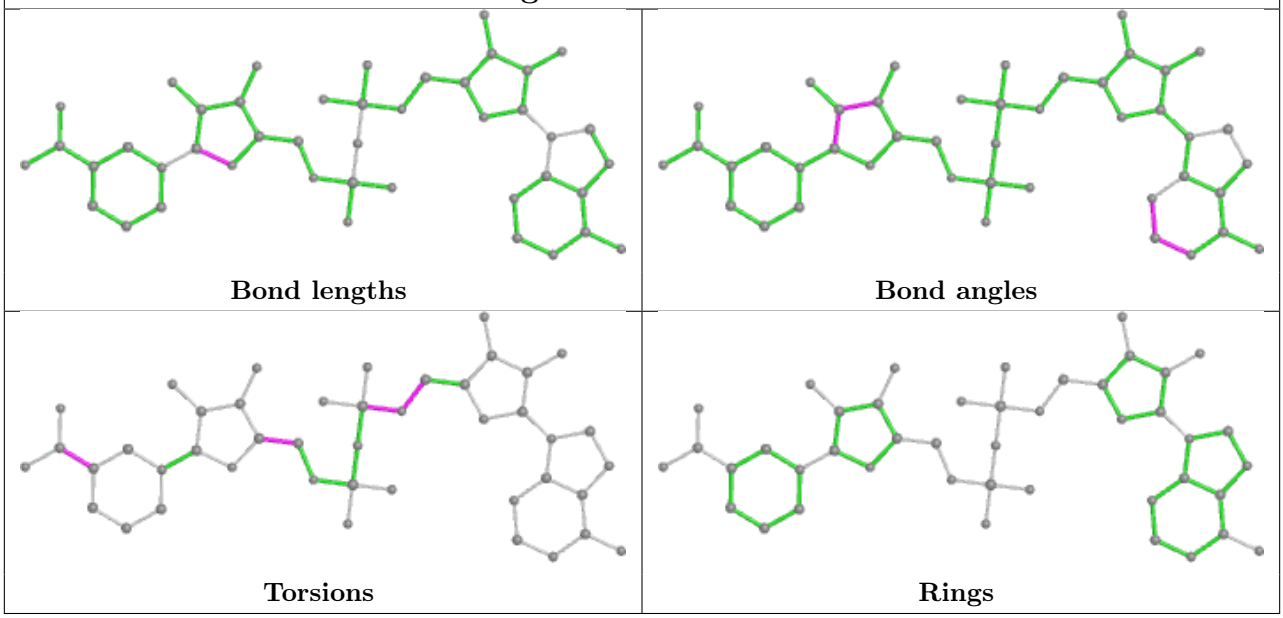
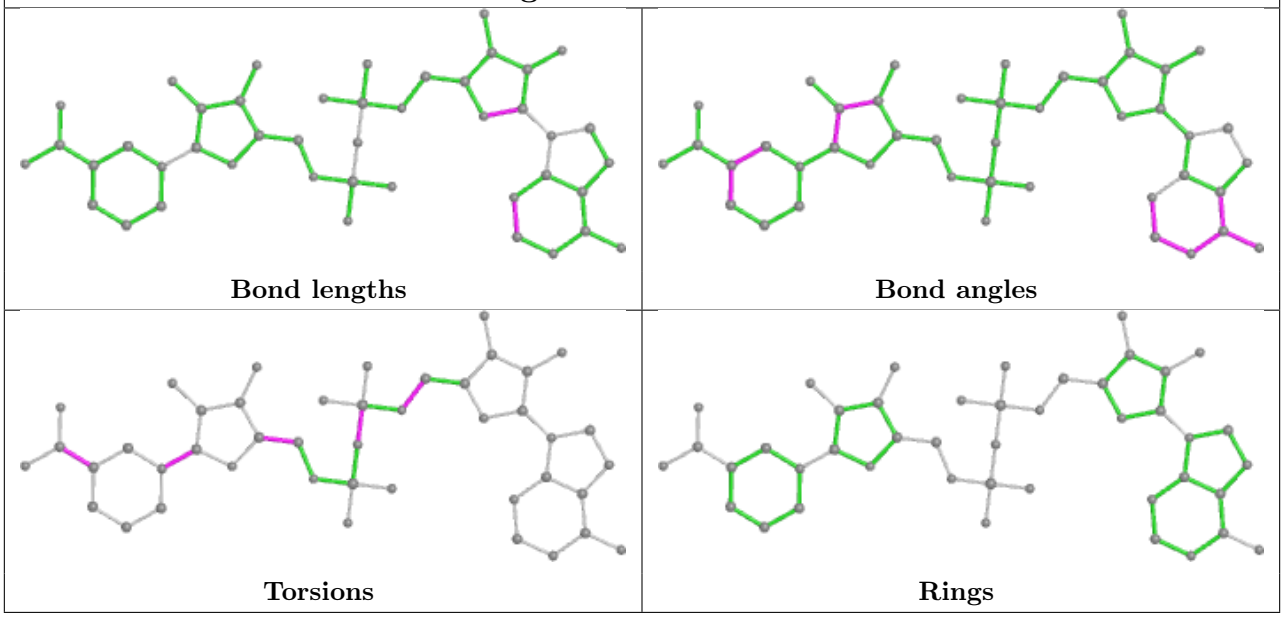
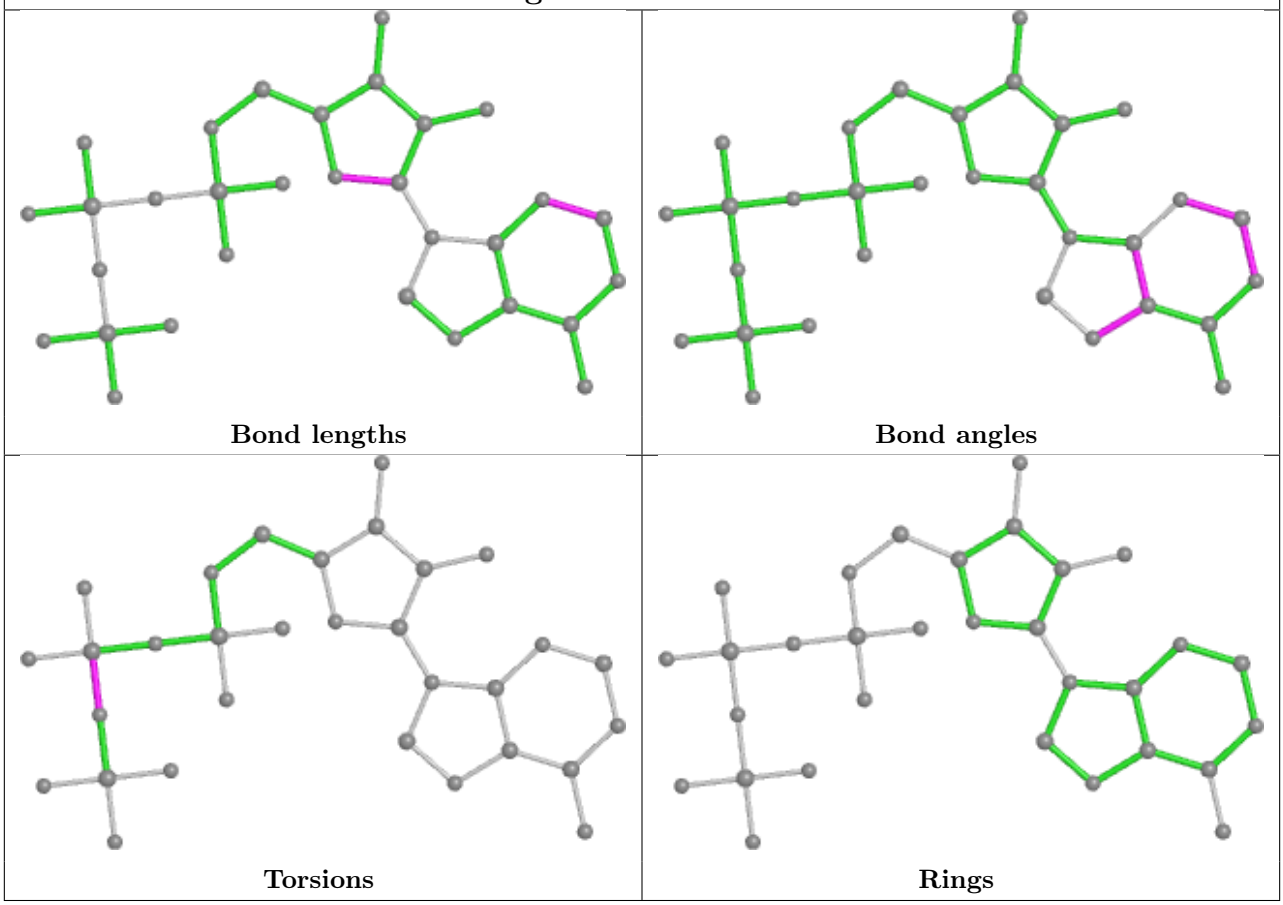


Ligand DND A 681



Ligand ATP D 680



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	658/680 (96%)	-0.45	7 (1%)	80	79	30, 49, 85, 147	0
1	B	657/680 (96%)	-0.42	13 (1%)	65	60	30, 50, 85, 147	0
1	C	648/680 (95%)	-0.44	7 (1%)	80	79	33, 52, 85, 148	0
1	D	649/680 (95%)	-0.45	7 (1%)	80	79	33, 49, 86, 146	0
All	All	2612/2720 (96%)	-0.44	34 (1%)	77	75	30, 50, 86, 148	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	453	THR	4.0
1	C	453	THR	4.0
1	C	454	PHE	3.6
1	C	452	VAL	3.3
1	B	523	ALA	3.2
1	A	524	GLY	3.1
1	D	452	VAL	3.1
1	B	450	TYR	3.1
1	A	450	TYR	3.1
1	B	524	GLY	2.9
1	A	449	VAL	2.9
1	A	678	LYS	2.8
1	B	417	ARG	2.8
1	D	402	PHE	2.8
1	B	298	GLU	2.7
1	C	417	ARG	2.7
1	D	678	LYS	2.6
1	A	523	ALA	2.5
1	A	418	ALA	2.4
1	C	561	VAL	2.4
1	D	454	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	525	GLU	2.4
1	D	679	GLY	2.3
1	C	401	GLY	2.3
1	D	1	MET	2.3
1	B	333	PRO	2.2
1	B	526	PHE	2.2
1	B	522	SER	2.2
1	C	674	ARG	2.1
1	B	334	GLN	2.1
1	A	526	PHE	2.1
1	B	410	ASN	2.1
1	B	527	GLY	2.1
1	B	1	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

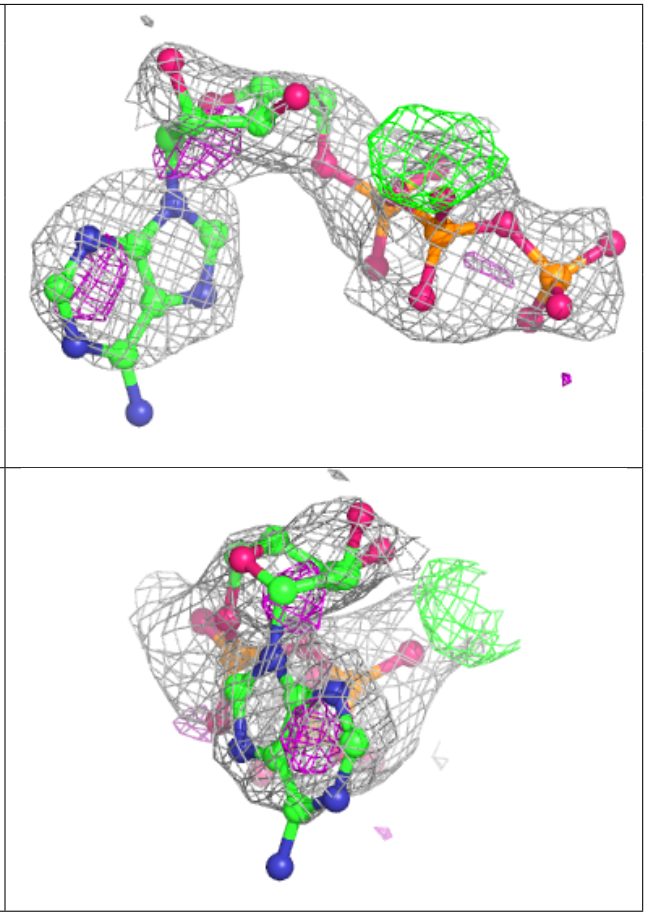
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ATP	A	680	31/31	0.88	0.24	59,98,151,255	0
2	ATP	D	680	31/31	0.88	0.18	61,85,130,136	0
2	ATP	B	680	31/31	0.91	0.21	55,81,185,260	0
3	DND	C	681	44/44	0.91	0.26	61,90,139,166	0
3	DND	D	681	44/44	0.91	0.23	57,86,153,164	0
2	ATP	C	680	31/31	0.92	0.14	53,90,153,230	0
3	DND	A	681	44/44	0.94	0.16	43,77,118,140	0
3	DND	B	681	44/44	0.94	0.19	48,78,161,169	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.

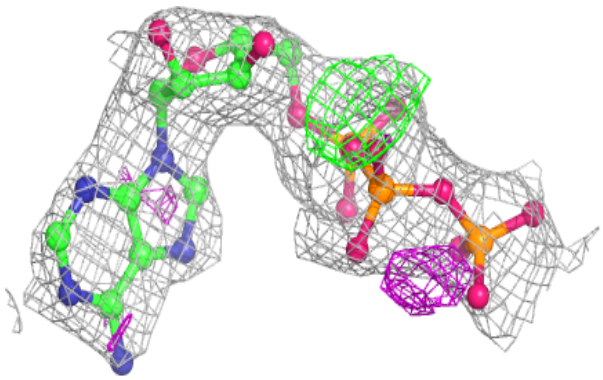
Electron density around ATP A 680:

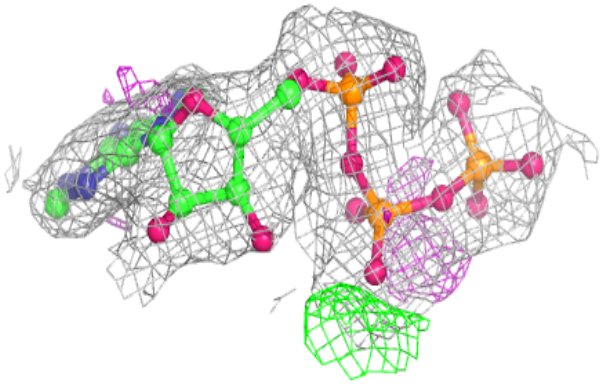
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

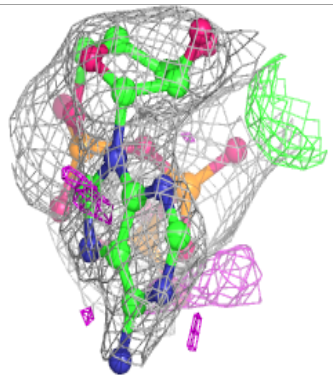


Electron density around ATP D 680:

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

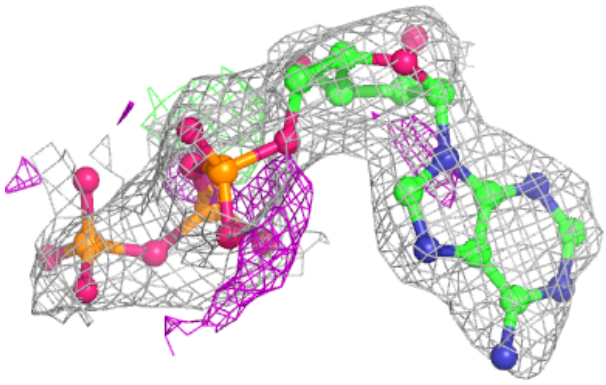


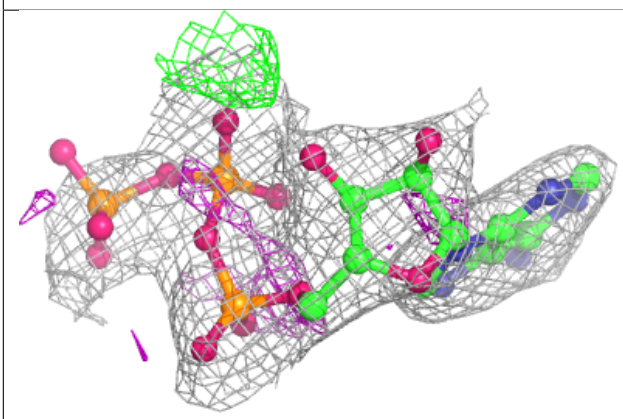


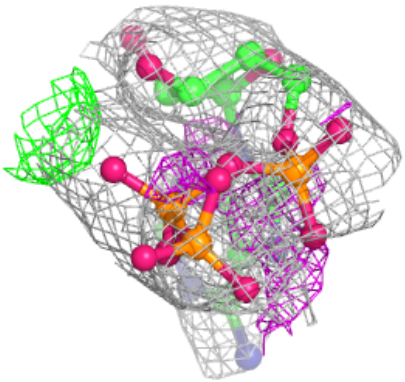


Electron density around ATP B 680:

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

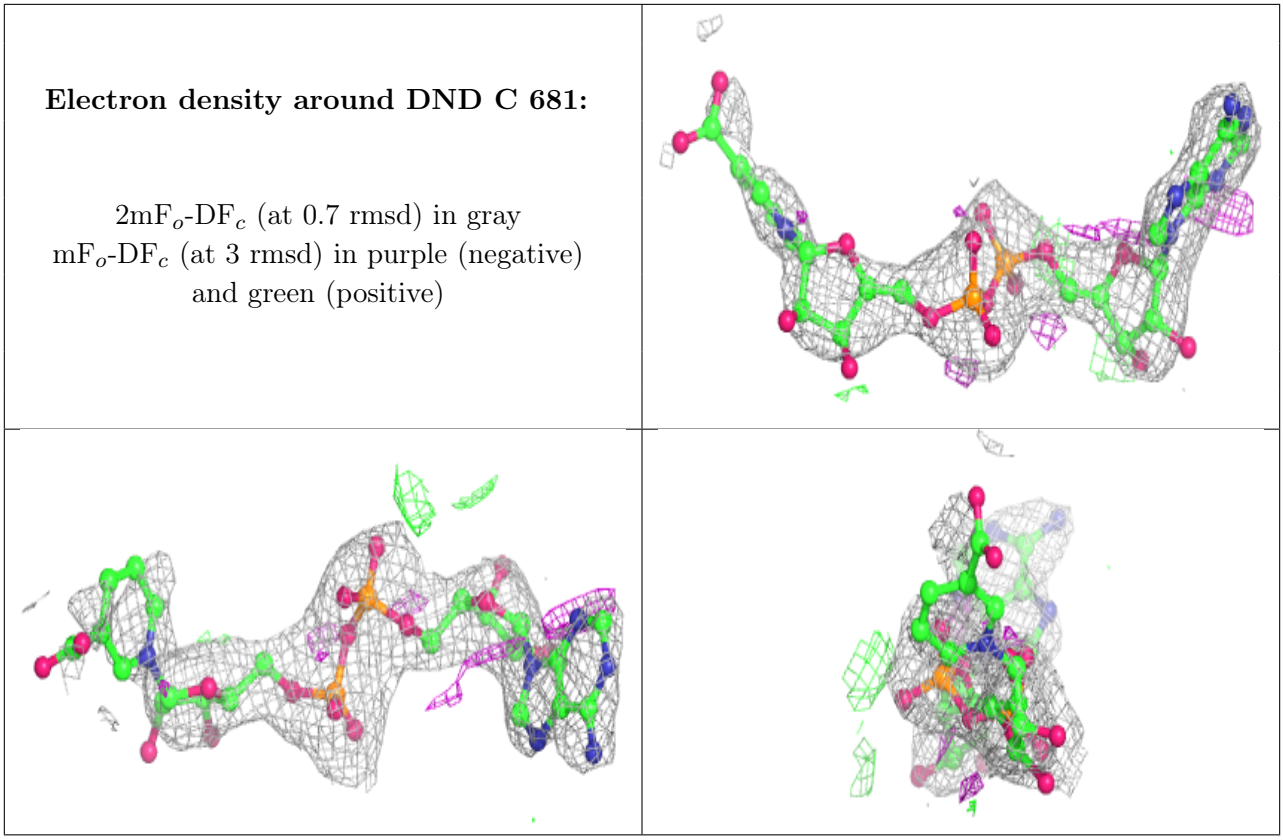






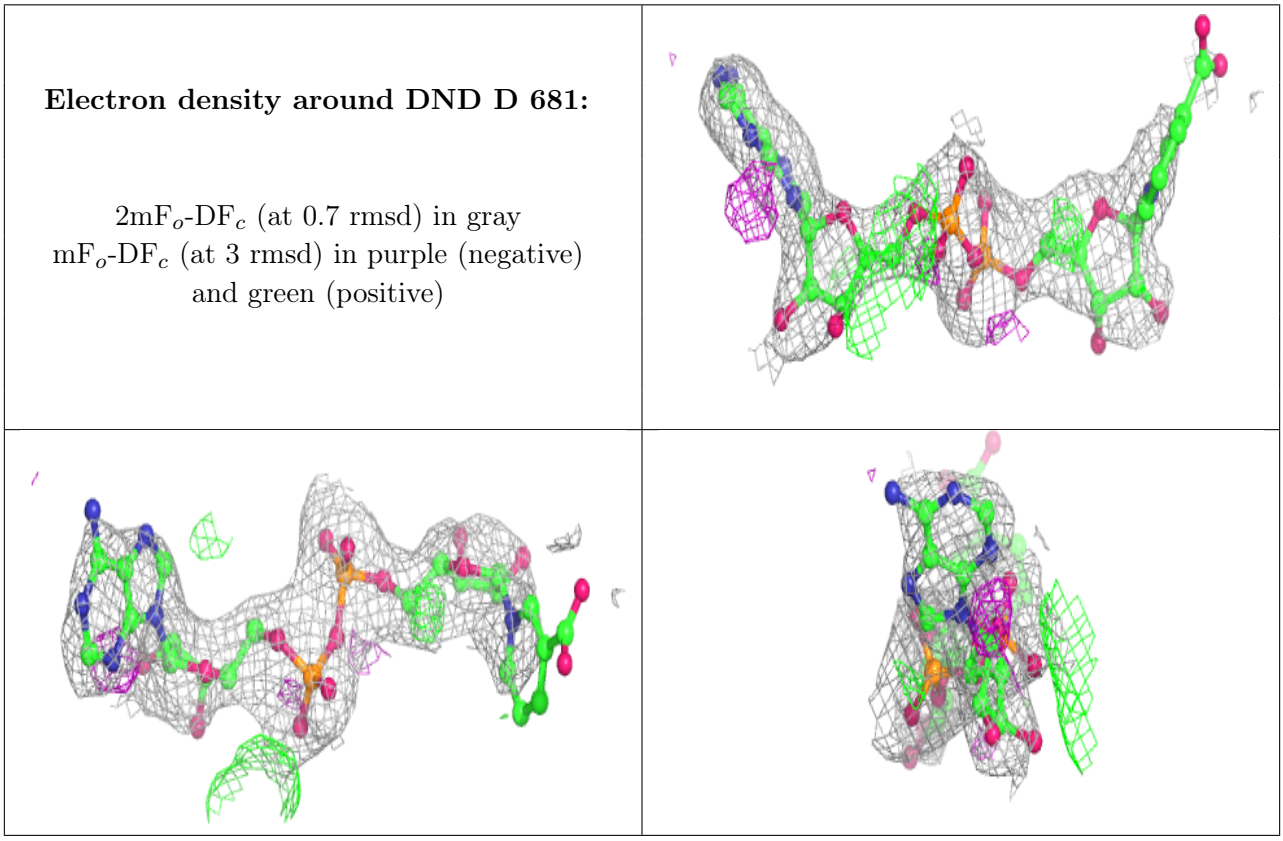
Electron density around DND C 681:

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



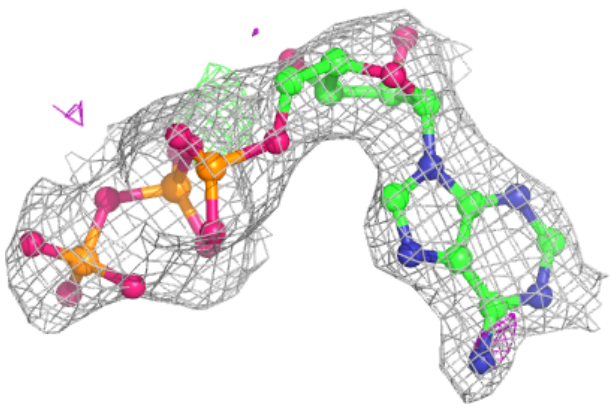
Electron density around DND D 681:

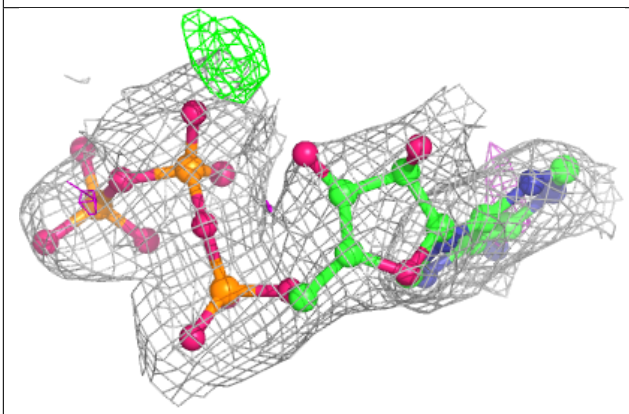
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

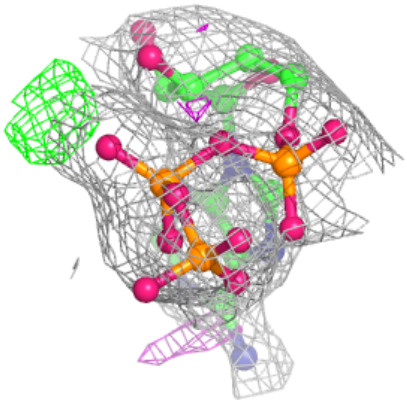


Electron density around ATP C 680:

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

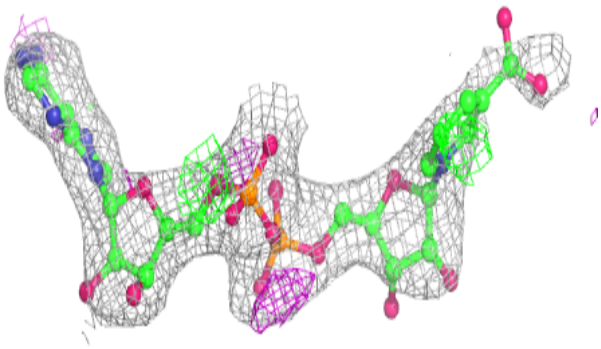


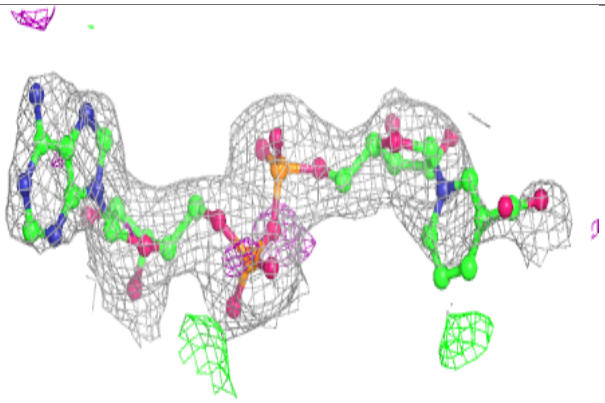


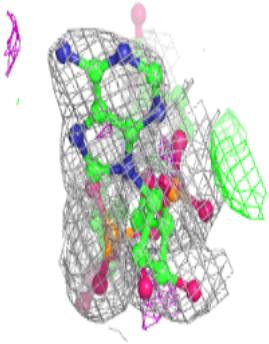


Electron density around DND A 681:

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

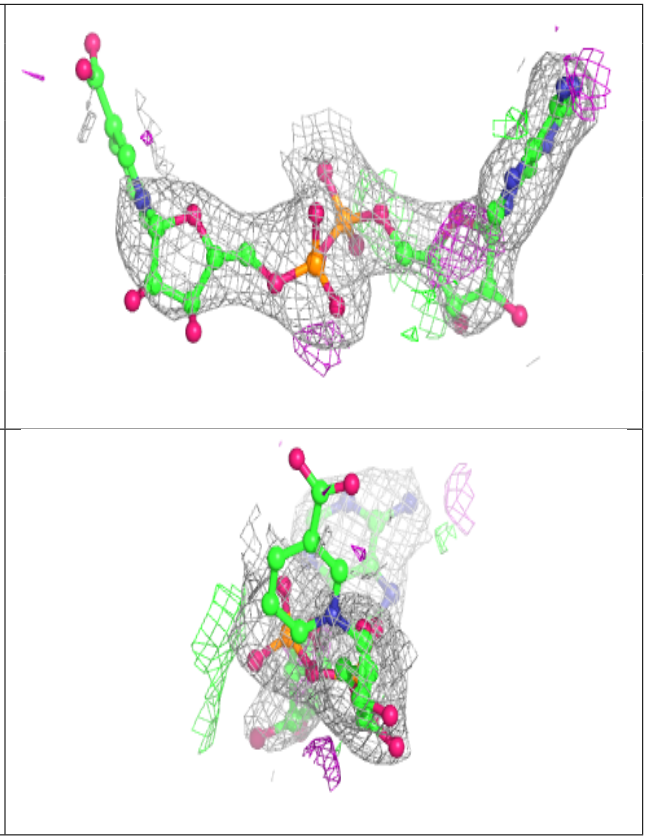






Electron density around DND B 681:

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



6.5 Other polymers (i)

There are no such residues in this entry.