



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:01 AM UTC

PDB ID : 5J5Q / pdb_00005j5q
Title : AMP-PNP-stabilized ATPase domain of topoisomerase IV from *Streptococcus pneumoniae*, complex type II
Authors : Laponogov, I.; Pan, X.-S.; Skamrova, G.; Umrekar, T.; Fisher, L.M.; Sander-son, M.R.
Deposited on : 2016-04-03
Resolution : 2.83 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

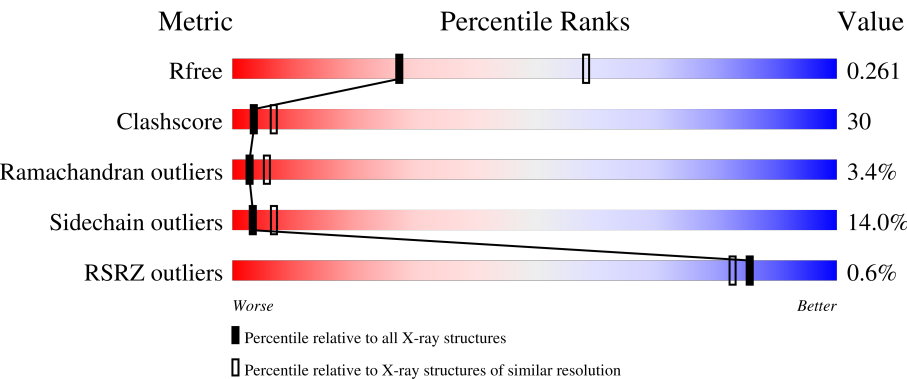
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.83 Å.

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



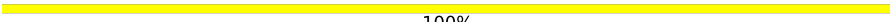
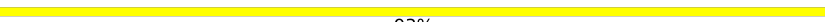
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	409	50%37%9% . .
1	B	409	% 49%38%8% . .
1	C	409	48%42%7% .
1	D	409	% 51%40%6% .

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Mol	Chain	Length	Quality of chain
2	E	14	 100%
2	F	14	 7%  93%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12219 atoms, of which 64 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 DNA topoisomerase 4 subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	4	0
			3016	1898	513	598	7			
1	B	396	Total	C	N	O	S	0	2	0
			2930	1836	508	580	6			
1	C	394	Total	C	N	O	S	0	3	0
			2847	1799	485	556	7			
1	D	395	Total	C	N	O	S	0	1	0
			2643	1666	461	512	4			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP Q59961
A	217	ASP	ASN	conflict	UNP Q59961
A	403	HIS	-	expression tag	UNP Q59961
A	404	HIS	-	expression tag	UNP Q59961
A	405	HIS	-	expression tag	UNP Q59961
A	406	HIS	-	expression tag	UNP Q59961
A	407	HIS	-	expression tag	UNP Q59961
A	408	HIS	-	expression tag	UNP Q59961
B	0	ALA	-	expression tag	UNP Q59961
B	217	ASP	ASN	conflict	UNP Q59961
B	403	HIS	-	expression tag	UNP Q59961
B	404	HIS	-	expression tag	UNP Q59961
B	405	HIS	-	expression tag	UNP Q59961
B	406	HIS	-	expression tag	UNP Q59961
B	407	HIS	-	expression tag	UNP Q59961
B	408	HIS	-	expression tag	UNP Q59961
C	0	ALA	-	expression tag	UNP Q59961
C	217	ASP	ASN	conflict	UNP Q59961
C	403	HIS	-	expression tag	UNP Q59961
C	404	HIS	-	expression tag	UNP Q59961
C	405	HIS	-	expression tag	UNP Q59961

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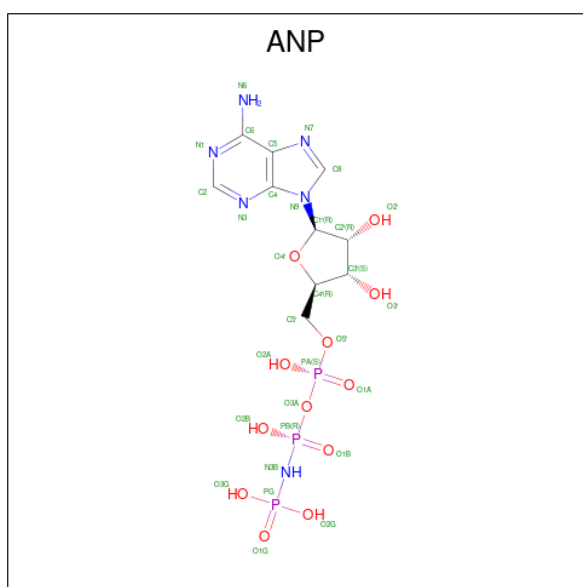
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Chain	Residue	Modelled	Actual	Comment	Reference
C	406	HIS	-	expression tag	UNP Q59961
C	407	HIS	-	expression tag	UNP Q59961
C	408	HIS	-	expression tag	UNP Q59961
D	0	ALA	-	expression tag	UNP Q59961
D	217	ASP	ASN	conflict	UNP Q59961
D	403	HIS	-	expression tag	UNP Q59961
D	404	HIS	-	expression tag	UNP Q59961
D	405	HIS	-	expression tag	UNP Q59961
D	406	HIS	-	expression tag	UNP Q59961
D	407	HIS	-	expression tag	UNP Q59961
D	408	HIS	-	expression tag	UNP Q59961

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*CP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	P	0	0	0
			284	138	51	82	13			
2	F	14	Total	C	N	O	P	0	0	0
			284	138	51	82	13			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
3	B	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
3	C	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
3	D	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
3	F	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		

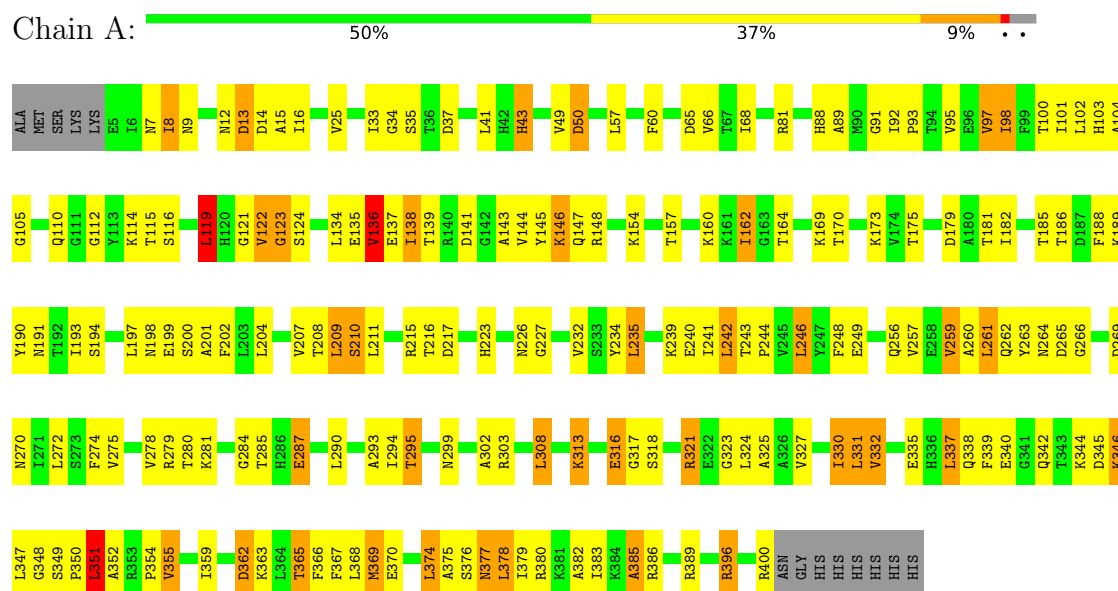
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

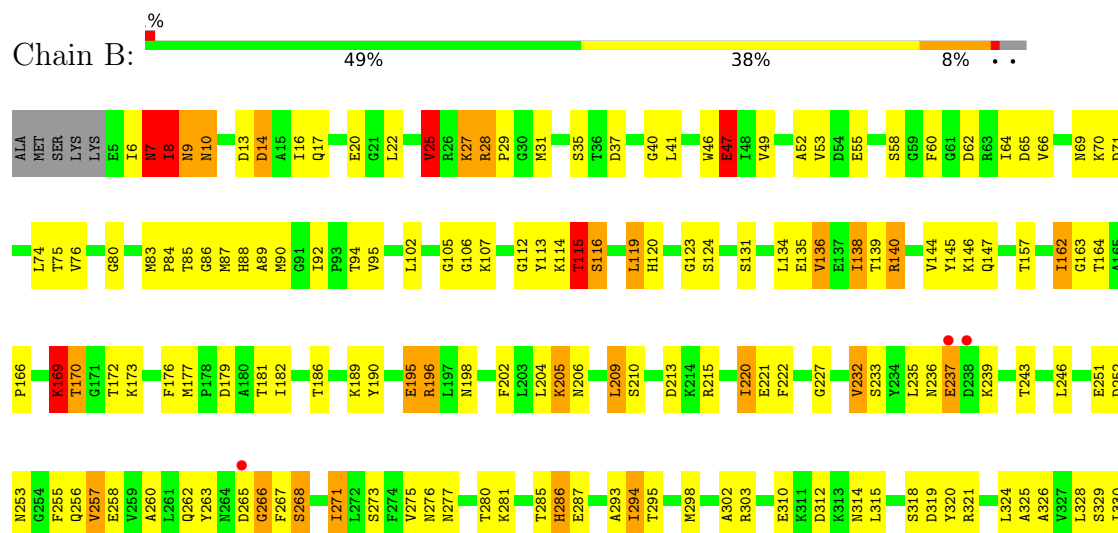
3 Residue-property plots

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

• Molecule 1: DNA topoisomerase 4 subunit B

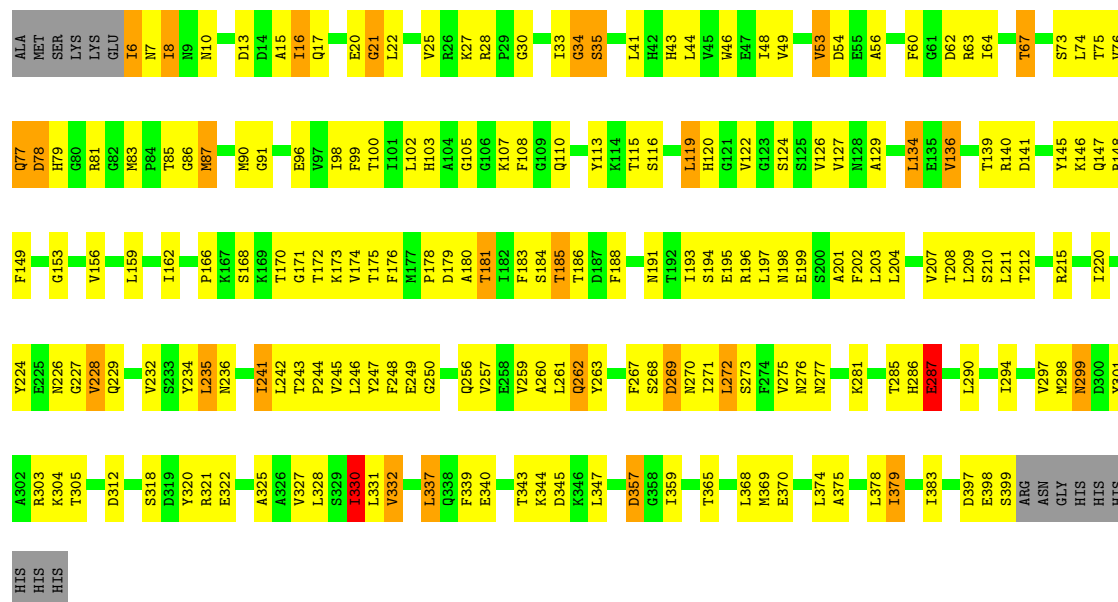


• Molecule 1: DNA topoisomerase 4 subunit B

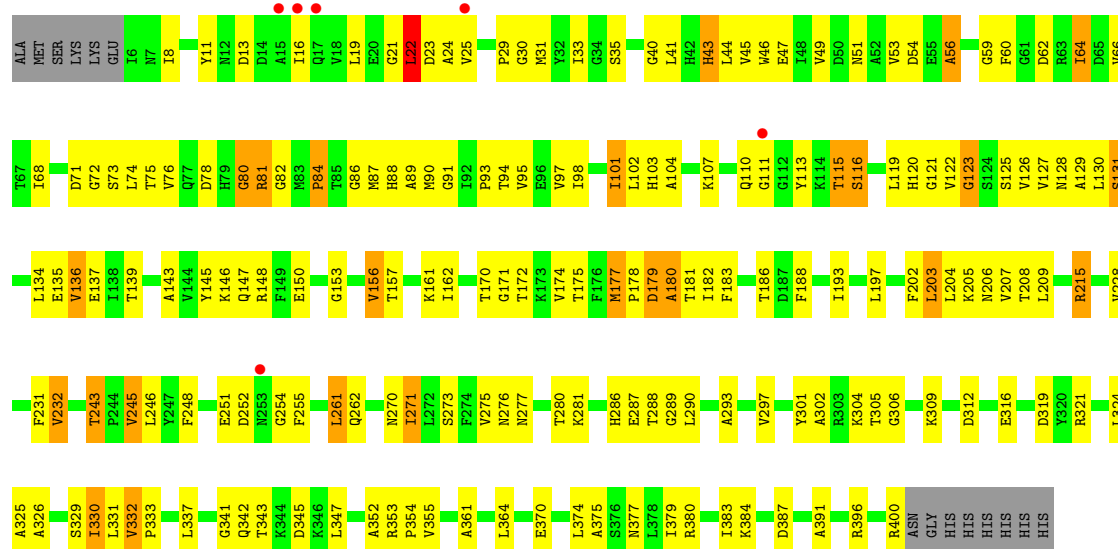




• Molecule 1: DNA topoisomerase 4 subunit B



• Molecule 1: DNA topoisomerase 4 subunit B



• Molecule 2: DNA (5'-D(*GP*CP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*GP*C)-3')



G1
C2
A3
T4
A5
T6
A7
T8
A9
T10
A11
T12
G13
C14

● Molecule 2: DNA (5'-D(*GP*CP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*GP*C)-3')



G1
C2
A3
T4
A5
T6
A7
T8
A9
T10
A11
T12
G13
C14

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.95Å 72.74Å 222.96Å 90.00° 91.89° 90.00°	Depositor
Resolution (Å)	60.76 – 2.83 60.76 – 2.83	Depositor EDS
% Data completeness (in resolution range)	99.7 (60.76-2.83) 99.7 (60.76-2.83)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.184 , 0.263 0.186 , 0.261	Depositor DCC
R_{free} test set	3189 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 80.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.015 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.025 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.023 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12219	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.41	7/3078 (0.2%)	1.56	31/4168 (0.7%)
1	B	1.38	16/2986 (0.5%)	1.46	22/4056 (0.5%)
1	C	1.04	1/2907 (0.0%)	1.26	10/3959 (0.3%)
1	D	0.88	0/2692	1.08	7/3690 (0.2%)
2	E	0.56	0/318	0.80	0/489
2	F	0.63	0/318	0.61	0/489
All	All	1.19	24/12299 (0.2%)	1.33	70/16851 (0.4%)

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

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	GLN	CD-OE1	6.79	1.36	1.23
1	B	25	VAL	CB-CG1	-6.59	1.30	1.52
1	A	226	ASN	CB-CG	-6.36	1.36	1.52
1	B	342	GLN	CA-C	6.31	1.61	1.52
1	A	313	LYS	CD-CE	6.08	1.70	1.52
1	B	340	GLU	C-O	-6.07	1.14	1.23
1	A	157	THR	C-O	-6.06	1.14	1.23
1	B	345	ASP	CG-OD2	5.90	1.36	1.25
1	B	62	ASP	CG-OD1	5.86	1.36	1.25
1	A	173	LYS	CE-NZ	5.66	1.66	1.49
1	B	169	LYS	CE-NZ	5.63	1.66	1.49
1	B	66	VAL	CA-CB	-5.57	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	170	THR	CB-CG2	-5.52	1.34	1.52
1	C	330	ILE	CB-CG2	5.48	1.70	1.52
1	B	102	LEU	C-N	-5.39	1.25	1.33
1	B	232	VAL	CB-CG2	-5.23	1.35	1.52
1	B	65	ASP	C-N	5.22	1.40	1.33
1	B	169	LYS	CD-CE	5.22	1.68	1.52
1	A	338	GLN	CB-CG	-5.20	1.36	1.52
1	B	37	ASP	CG-OD2	5.14	1.35	1.25
1	B	29	PRO	CA-C	-5.13	1.43	1.52
1	A	50	ASP	CB-CG	5.10	1.64	1.52
1	B	14	ASP	CB-CG	-5.06	1.39	1.52
1	B	176	PHE	CE2-CZ	5.03	1.53	1.38

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ILE	CB-CG1-CD1	-8.26	96.45	113.80
1	A	57	LEU	CA-C-N	-7.47	110.22	122.54
1	A	57	LEU	C-N-CA	-7.47	110.22	122.54
1	A	351	LEU	CA-C-N	-7.30	108.81	121.66
1	A	351	LEU	C-N-CA	-7.30	108.81	121.66
1	A	123	GLY	N-CA-C	7.18	121.33	112.64
1	B	13	ASP	CA-C-N	7.06	132.52	120.72
1	B	13	ASP	C-N-CA	7.06	132.52	120.72
1	A	355	VAL	CA-C-N	-7.06	108.72	120.30
1	A	355	VAL	C-N-CA	-7.06	108.72	120.30
1	B	352	ALA	CA-C-N	-6.95	104.84	121.80
1	B	352	ALA	C-N-CA	-6.95	104.84	121.80
1	B	281	LYS	CG-CD-CE	-6.83	95.58	111.30
1	B	8	ILE	CA-C-N	-6.74	110.63	122.62
1	B	8	ILE	C-N-CA	-6.74	110.63	122.62
1	A	226	ASN	CA-CB-CG	-6.69	105.91	112.60
1	A	34	GLY	CA-C-N	-6.60	109.54	121.62
1	A	34	GLY	C-N-CA	-6.60	109.54	121.62
1	A	154	LYS	CB-CG-CD	6.58	126.44	111.30
1	A	136	VAL	CB-CA-C	-6.45	102.35	111.38
1	C	299	ASN	CA-C-N	-6.25	111.94	120.44
1	C	299	ASN	C-N-CA	-6.25	111.94	120.44
1	B	6	ILE	CA-C-N	-6.22	115.04	122.44
1	B	6	ILE	C-N-CA	-6.22	115.04	122.44
1	C	91	GLY	N-CA-C	6.15	120.99	113.79
1	A	281	LYS	CD-CE-NZ	-6.14	92.25	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	SER	CA-C-N	-6.00	110.91	122.06
1	B	131	SER	C-N-CA	-6.00	110.91	122.06
1	D	81	ARG	NE-CZ-NH1	-5.98	115.52	121.50
1	D	30	GLY	N-CA-C	-5.95	105.45	113.24
1	A	396	ARG	NE-CZ-NH1	-5.91	115.59	121.50
1	D	81	ARG	NE-CZ-NH2	5.87	124.48	119.20
1	A	345	ASP	CB-CG-OD1	-5.82	105.03	118.40
1	B	47	GLU	CA-C-N	-5.67	112.36	120.42
1	B	47	GLU	C-N-CA	-5.67	112.36	120.42
1	A	272	LEU	CA-C-N	-5.67	113.30	122.82
1	A	272	LEU	C-N-CA	-5.67	113.30	122.82
1	B	28	ARG	NE-CZ-NH2	-5.66	114.11	119.20
1	A	340	GLU	CA-C-N	-5.62	113.81	122.69
1	A	340	GLU	C-N-CA	-5.62	113.81	122.69
1	A	321	ARG	NE-CZ-NH1	-5.61	115.89	121.50
1	A	232	VAL	CA-CB-CG1	-5.61	100.86	110.40
1	A	154	LYS	CB-CA-C	5.55	117.36	109.08
1	B	7	ASN	N-CA-C	5.55	119.46	111.02
1	A	14	ASP	CA-CB-CG	5.45	118.05	112.60
1	D	161	LYS	CA-C-N	5.44	131.76	121.97
1	D	161	LYS	C-N-CA	5.44	131.76	121.97
1	A	338	GLN	CA-CB-CG	-5.40	103.29	114.10
1	A	122	VAL	CA-C-N	-5.39	113.90	119.99
1	A	122	VAL	C-N-CA	-5.39	113.90	119.99
1	B	169	LYS	CB-CG-CD	5.38	123.67	111.30
1	B	14	ASP	N-CA-CB	-5.30	101.60	110.39
1	C	287[A]	GLU	CA-C-N	-5.30	112.26	120.31
1	C	287[A]	GLU	C-N-CA	-5.30	112.26	120.31
1	C	287[B]	GLU	CA-C-N	-5.30	112.26	120.31
1	C	287[B]	GLU	C-N-CA	-5.30	112.26	120.31
1	A	43	HIS	CA-CB-CG	-5.25	108.55	113.80
1	A	346	LYS	CB-CG-CD	-5.25	99.24	111.30
1	A	396	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	C	53	VAL	O-C-N	5.23	127.17	121.94
1	A	97	VAL	CA-CB-CG1	-5.22	101.53	110.40
1	D	101	ILE	CA-C-N	5.13	128.75	121.42
1	D	101	ILE	C-N-CA	5.13	128.75	121.42
1	C	41	LEU	CA-C-N	-5.11	112.54	120.31
1	C	41	LEU	C-N-CA	-5.11	112.54	120.31
1	B	294	ILE	CA-C-N	-5.10	113.45	120.28
1	B	294	ILE	C-N-CA	-5.10	113.45	120.28
1	B	80	GLY	N-CA-C	-5.05	103.66	112.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	383	ILE	CA-CB-CG2	-5.04	101.93	110.50
1	B	346	LYS	CA-CB-CG	5.02	124.14	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	7	ASN	Peptide
1	B	9	ASN	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	3016	0	2919	150	0
1	B	2930	0	2759	150	0
1	C	2847	0	2625	176	0
1	D	2643	0	2225	173	0
2	E	284	0	161	35	0
2	F	284	0	161	36	0
3	A	31	13	13	2	0
3	B	31	13	13	0	0
3	C	31	13	13	5	0
3	D	31	13	13	5	0
3	F	23	12	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	12155	64	10914	681	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 30.

All (681) 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:A:179:ASP:OD1	1:A:181:THR:HG22	1.49	1.12
1:C:53:VAL:HG13	1:C:204:LEU:HD11	1.32	1.12
1:B:7:ASN:HB2	1:B:10:ASN:HB3	1.14	1.07
2:E:7:DA:H2''	2:E:8:DT:H5'	1.37	1.05
1:C:83:MET:HE2	1:C:98:ILE:HG21	1.41	1.02
1:C:119:LEU:HD13	1:C:337:LEU:HD13	1.02	1.02
1:C:119:LEU:HD13	1:C:337:LEU:CD1	1.89	1.01
1:B:324:LEU:HD12	1:B:325:ALA:H	1.28	0.99
1:B:396:ARG:NH2	2:E:12:DT:OP2	1.95	0.98
1:B:7:ASN:O	1:B:8:ILE:HB	1.66	0.94
1:D:21:GLY:O	1:D:23:ASP:N	2.02	0.93
1:C:85:THR:HG23	1:C:140:ARG:HD2	1.52	0.92
1:B:243:THR:O	1:B:262:GLN:NE2	2.03	0.90
2:E:14:DC:H42	2:F:1:DG:H1	1.17	0.90
1:C:119:LEU:CD1	1:C:337:LEU:HD13	1.98	0.89
1:B:7:ASN:HB3	1:B:9:ASN:H	1.38	0.89
2:F:6:DT:H2''	2:F:7:DA:N7	1.87	0.89
1:D:374:LEU:O	1:D:377:ASN:N	2.07	0.87
1:C:257:VAL:HG22	1:C:330:ILE:HG22	1.56	0.87
1:C:74:LEU:HB2	1:C:188:PHE:CE2	2.10	0.86
2:E:7:DA:C2'	2:E:8:DT:H5'	2.07	0.84
1:B:7:ASN:HB3	1:B:9:ASN:N	1.90	0.84
1:B:220:ILE:HD13	1:B:222:PHE:CZ	2.12	0.84
1:C:243:THR:CG2	1:C:263:TYR:HB2	2.08	0.83
1:B:324:LEU:HD12	1:B:325:ALA:N	1.93	0.83
1:B:83:MET:HB2	1:B:138:ILE:HD12	1.57	0.83
2:F:11:DA:H1'	2:F:12:DT:H5'	1.61	0.83
1:D:341:GLY:O	1:D:343:THR:N	2.11	0.82
2:F:7:DA:H2''	2:F:8:DT:H5''	1.60	0.82
1:C:83:MET:CE	1:C:98:ILE:HG21	2.10	0.82
1:C:243:THR:CG2	1:C:263:TYR:H	1.92	0.81
1:A:112:GLY:O	1:B:8:ILE:HD12	1.81	0.80
1:A:376:SER:HB3	1:A:380:ARG:HH21	1.46	0.80
2:F:11:DA:H2''	2:F:12:DT:OP2	1.79	0.80
1:C:257:VAL:HG22	1:C:330:ILE:CG2	2.10	0.80
1:D:21:GLY:O	1:D:24:ALA:N	2.14	0.80
1:D:136:VAL:O	1:D:146:LYS:HA	1.80	0.80
1:C:298:MET:HB3	1:C:320:TYR:CE2	2.15	0.80
1:C:73:SER:HB2	1:C:176:PHE:O	1.80	0.80
1:D:128:ASN:HB2	1:D:134:LEU:HD13	1.65	0.79
1:A:396:ARG:HD3	1:A:400:ARG:NH2	1.98	0.79
1:D:301:TYR:O	1:D:305:THR:N	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:ASP:OD1	1:D:181:THR:OG1	2.03	0.77
1:D:341:GLY:C	1:D:343:THR:H	1.91	0.77
2:F:4:DT:H2''	2:F:5:DA:H5''	1.67	0.77
1:B:351:LEU:O	1:B:354:PRO:HD2	1.85	0.77
1:A:134:LEU:HD23	1:A:134:LEU:C	2.11	0.76
2:E:8:DT:H1'	2:E:9:DA:H5'	1.67	0.76
1:A:256[A]:GLN:HB3	1:A:331:LEU:HB2	1.68	0.76
1:B:303:ARG:NH2	1:B:312:ASP:O	2.17	0.76
1:B:213:ASP:OD1	1:B:215:ARG:HB2	1.85	0.76
1:A:400:ARG:HD3	1:B:267:PHE:CE1	2.21	0.76
1:D:182:ILE:HG22	1:D:183:PHE:CD1	2.21	0.75
1:B:115:THR:HG21	1:B:331:LEU:HG	1.67	0.75
1:A:190:TYR:CE2	1:A:211:LEU:HD23	2.22	0.75
1:C:27:LYS:O	1:C:28:ARG:HD3	1.86	0.75
1:D:332:VAL:CG2	1:D:337:LEU:HD13	2.16	0.75
1:C:67:THR:HG23	1:C:212:THR:HB	1.68	0.74
1:D:302:ALA:HB2	1:D:379:ILE:HD13	1.69	0.74
1:B:7:ASN:CB	1:B:10:ASN:HB3	2.06	0.74
2:E:3:DA:H4'	2:E:4:DT:OP1	1.87	0.74
1:A:146:LYS:HB3	1:A:162:ILE:HD13	1.69	0.74
1:C:299:ASN:OD1	1:C:320:TYR:OH	2.01	0.74
1:C:267:PHE:HZ	1:D:400:ARG:CB	1.99	0.74
1:A:65:ASP:OD1	1:A:210:SER:HB3	1.88	0.74
1:B:204:LEU:O	1:B:206:ASN:N	2.21	0.73
1:A:256[A]:GLN:CD	1:A:331:LEU:HD22	2.12	0.73
2:E:3:DA:H2''	2:E:4:DT:H72	1.69	0.73
1:A:179:ASP:CG	1:A:181:THR:HG22	2.14	0.72
1:D:89:ALA:O	1:D:91:GLY:N	2.22	0.72
1:B:58:SER:HA	1:B:114:LYS:HD3	1.70	0.72
1:C:62:ASP:HA	1:C:207:VAL:HG22	1.72	0.71
2:F:6:DT:H2''	2:F:7:DA:C8	2.24	0.71
1:D:49:VAL:O	1:D:53:VAL:HG23	1.90	0.71
1:A:134:LEU:HD23	1:A:135:GLU:N	2.06	0.71
1:A:239:LYS:HD3	1:A:264:ASN:ND2	2.06	0.71
1:C:301:TYR:CE1	1:C:375:ALA:HB1	2.26	0.71
2:E:8:DT:H1'	2:E:9:DA:C5'	2.21	0.70
1:A:376:SER:HB3	1:A:380:ARG:NH2	2.06	0.70
1:B:83:MET:HB2	1:B:138:ILE:CD1	2.21	0.70
1:A:243:THR:HG23	1:A:244:PRO:O	1.91	0.70
1:A:261:LEU:HD12	1:A:261:LEU:N	2.06	0.70
1:A:396:ARG:HD3	1:A:400:ARG:HH21	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ALA:HB1	1:A:308:LEU:HD22	1.75	0.69
1:D:281:LYS:HG2	1:D:345:ASP:OD1	1.93	0.69
1:C:243:THR:HG22	1:C:263:TYR:HB2	1.73	0.69
1:C:134:LEU:HD23	1:C:134:LEU:C	2.18	0.69
1:D:332:VAL:HG22	1:D:337:LEU:HD13	1.74	0.69
1:A:66:VAL:HG12	1:A:211:LEU:HD12	1.75	0.68
1:C:271:ILE:O	1:C:272:LEU:HD23	1.94	0.68
1:A:375:ALA:O	1:A:379:ILE:HG12	1.94	0.68
1:B:351:LEU:O	1:B:355:VAL:HG23	1.93	0.67
1:D:293:ALA:O	1:D:297:VAL:HG23	1.94	0.67
1:B:209:LEU:N	1:B:209:LEU:HD12	2.09	0.67
1:B:332:VAL:HG22	1:B:337:LEU:HD13	1.75	0.67
1:C:243:THR:HG21	1:C:263:TYR:HB2	1.76	0.67
1:A:362:ASP:C	1:A:362:ASP:OD1	2.37	0.67
2:F:7:DA:H2''	2:F:8:DT:O4'	1.95	0.67
1:A:241:ILE:HG21	1:A:262:GLN:NE2	2.10	0.67
1:C:13:ASP:OD2	1:D:84:PRO:HB3	1.94	0.67
1:C:83:MET:HE2	1:C:98:ILE:CG2	2.22	0.67
1:D:72:GLY:C	1:D:177:MET:HE1	2.20	0.66
1:D:180:ALA:HA	1:D:186:THR:HG21	1.77	0.66
1:A:8:ILE:HG23	1:B:60:PHE:HZ	1.61	0.66
1:A:347:LEU:HD12	1:A:348:GLY:H	1.59	0.66
1:B:246:LEU:HD22	1:B:367:PHE:CE1	2.31	0.66
1:C:275:VAL:HG21	1:C:347:LEU:HD22	1.78	0.66
1:D:248:PHE:CE2	1:D:364:LEU:HD13	2.31	0.66
1:D:243:THR:O	1:D:262:GLN:HG3	1.95	0.66
1:A:8:ILE:HG23	1:B:60:PHE:CZ	2.30	0.66
1:C:241:ILE:HD12	1:C:262:GLN:HE22	1.61	0.66
1:B:275:VAL:HG21	1:B:347:LEU:HD22	1.76	0.65
1:C:229:GLN:HB3	1:C:245:VAL:HG11	1.77	0.65
2:F:9:DA:C2'	2:F:10:DT:H5'	2.26	0.65
1:A:41:LEU:HD22	1:A:186:THR:HA	1.77	0.65
2:F:7:DA:H2''	2:F:8:DT:C5'	2.26	0.65
1:B:220:ILE:HG12	1:B:221:GLU:H	1.62	0.65
1:D:73:SER:HB3	1:D:177:MET:HE3	1.78	0.65
1:C:148:ARG:O	1:C:156:VAL:HG22	1.97	0.65
1:C:271:ILE:C	1:C:272:LEU:HD23	2.21	0.65
1:B:243:THR:CG2	1:B:263:TYR:H	2.10	0.65
1:B:275:VAL:CG2	1:B:347:LEU:HD22	2.27	0.65
1:B:302:ALA:HB2	1:B:379:ILE:HG13	1.78	0.65
2:F:4:DT:H2''	2:F:5:DA:C8	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ILE:HG22	1:C:10:ASN:O	1.97	0.64
1:C:246:LEU:O	1:C:260:ALA:HA	1.97	0.64
1:A:275:VAL:HG21	1:A:347:LEU:HD22	1.79	0.64
1:A:339:PHE:CE2	1:A:344:LYS:HG2	2.31	0.64
1:A:382:ALA:O	1:A:385:ALA:HB3	1.97	0.64
1:B:195:GLU:OE1	1:B:195:GLU:HA	1.98	0.64
1:C:236:ASN:ND2	1:C:262:GLN:HB3	2.12	0.64
1:D:275:VAL:HG21	1:D:347:LEU:HD13	1.80	0.64
1:C:107:LYS:HE3	1:C:113:TYR:CE1	2.32	0.64
1:A:16:ILE:HG23	1:B:105:GLY:HA2	1.79	0.63
1:A:339:PHE:CD2	1:A:344:LYS:HA	2.33	0.63
2:F:4:DT:C2'	2:F:5:DA:H5''	2.28	0.63
1:A:243:THR:HG22	1:A:263:TYR:H	1.63	0.63
1:A:302:ALA:CB	1:A:308:LEU:HD22	2.28	0.63
1:D:270:ASN:O	1:D:325:ALA:HA	1.98	0.63
1:B:343:THR:O	1:B:344:LYS:HG3	1.98	0.63
1:C:136:VAL:HG13	1:C:174:VAL:HG22	1.81	0.63
1:C:236:ASN:HD21	1:C:262:GLN:HB3	1.64	0.63
1:A:138:ILE:N	1:A:138:ILE:HD13	2.14	0.62
1:C:269:ASP:OD1	1:C:321:ARG:HD2	2.00	0.62
1:D:71:ASP:OD2	1:D:73:SER:OG	2.09	0.62
1:C:241:ILE:HD12	1:C:262:GLN:NE2	2.15	0.62
1:D:193:ILE:HG22	1:D:197:LEU:HD12	1.81	0.62
1:D:330:ILE:CD1	1:D:332:VAL:HG12	2.30	0.62
1:C:46:TRP:CZ3	1:C:196:ARG:HG2	2.34	0.61
1:D:19:LEU:HD13	1:D:24:ALA:HA	1.82	0.61
1:B:243:THR:HG22	1:B:263:TYR:H	1.63	0.61
1:D:94:THR:O	1:D:97:VAL:N	2.34	0.61
1:C:184:SER:C	1:C:185:THR:HG22	2.25	0.61
1:A:239:LYS:HD3	1:A:264:ASN:HD22	1.65	0.61
1:D:53:VAL:O	1:D:56:ALA:HB3	2.01	0.61
1:D:251:GLU:HA	1:D:255:PHE:O	2.00	0.61
1:B:303:ARG:HG2	1:B:303:ARG:HH11	1.66	0.61
1:A:91:GLY:O	1:A:92:ILE:HG23	2.01	0.61
1:B:257:VAL:HB	1:B:330:ILE:HG22	1.82	0.61
1:B:268:SER:OG	2:E:10:DT:OP2	2.18	0.61
1:C:77:GLN:HG3	1:C:78:ASP:N	2.16	0.61
1:A:41:LEU:HD11	1:A:188:PHE:CE1	2.36	0.60
1:C:179:ASP:OD1	1:C:181:THR:HG22	2.00	0.60
1:B:220:ILE:HD13	1:B:222:PHE:CE1	2.36	0.60
1:B:332:VAL:CG2	1:B:337:LEU:HD13	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:ASP:OD1	1:D:107:LYS:NZ	2.31	0.60
1:B:260:ALA:O	1:B:326:ALA:HA	2.02	0.60
1:C:96:GLU:O	1:C:100:THR:HG23	2.00	0.60
2:E:10:DT:H2'	2:E:11:DA:C8	2.37	0.60
1:A:386:ARG:HG3	1:A:389:ARG:HH21	1.66	0.60
1:C:83:MET:HG2	1:C:98:ILE:CD1	2.31	0.60
1:B:280:THR:HG22	1:B:344:LYS:O	2.01	0.60
1:D:60:PHE:HB3	1:D:80:GLY:HA2	1.82	0.60
1:B:139:THR:HG22	1:B:170:THR:HA	1.83	0.60
1:D:60:PHE:CE2	1:D:81:ARG:HD3	2.37	0.60
1:D:56:ALA:O	1:D:59:GLY:N	2.32	0.59
1:C:365:THR:HG23	1:C:369:MET:HE3	1.83	0.59
1:C:119:LEU:N	3:C:501:ANP:HNB1	2.00	0.59
1:D:273:SER:HB2	1:D:286:HIS:CD2	2.37	0.59
1:D:332:VAL:HG21	1:D:337:LEU:HD13	1.83	0.59
1:B:379:ILE:O	1:B:383:ILE:HG13	2.03	0.59
1:C:207:VAL:HG12	1:C:209:LEU:HD12	1.85	0.59
1:B:236:ASN:HD22	1:B:262:GLN:HG2	1.68	0.59
1:B:47:GLU:HA	1:B:47:GLU:OE2	2.03	0.59
1:C:267:PHE:CZ	1:D:400:ARG:CB	2.85	0.59
1:C:301:TYR:HD1	1:C:379:ILE:HD11	1.67	0.59
2:E:12:DT:H4'	2:E:12:DT:OP1	2.03	0.59
1:C:103:HIS:H	1:C:122:VAL:HG12	1.66	0.59
1:B:27:LYS:O	1:B:27:LYS:HG3	2.01	0.59
1:B:367:PHE:HD2	1:B:368:LEU:HD23	1.68	0.59
1:D:316:GLU:HB2	1:D:319:ASP:CB	2.33	0.59
1:A:137:GLU:HG3	1:A:146:LYS:HB2	1.85	0.58
1:A:143:ALA:HB3	1:A:145:TYR:CE1	2.38	0.58
1:D:228:VAL:O	1:D:232:VAL:HG23	2.03	0.58
1:B:7:ASN:O	1:B:8:ILE:CB	2.47	0.58
1:C:332:VAL:O	1:C:332:VAL:HG22	2.03	0.58
1:D:94:THR:O	1:D:97:VAL:HB	2.03	0.58
1:A:216:THR:O	1:A:217:ASP:HB2	2.03	0.58
1:C:197:LEU:CD2	1:C:209:LEU:HD23	2.33	0.58
1:D:40:GLY:O	1:D:43:HIS:HB2	2.03	0.58
1:D:119:LEU:CD2	1:D:120:HIS:CD2	2.86	0.58
1:A:8:ILE:HD12	1:B:112:GLY:O	2.03	0.58
1:A:121:GLY:H	3:A:501:ANP:HNB1	1.49	0.58
1:D:89:ALA:C	1:D:91:GLY:H	2.12	0.58
1:A:13:ASP:OD2	1:A:13:ASP:N	2.37	0.58
1:C:86:GLY:HA3	1:D:13:ASP:OD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:ALA:O	1:D:355:VAL:N	2.35	0.58
1:B:204:LEU:C	1:B:206:ASN:H	2.11	0.57
1:D:271:ILE:C	1:D:271:ILE:HD13	2.29	0.57
2:F:8:DT:H2''	2:F:9:DA:C8	2.40	0.57
1:A:316:GLU:HG3	1:A:389:ARG:CZ	2.34	0.57
1:B:144:VAL:N	1:B:163:GLY:O	2.35	0.57
1:B:190:TYR:CD1	1:B:190:TYR:C	2.82	0.57
1:B:202:PHE:O	1:B:227:GLY:HA2	2.05	0.57
1:B:303:ARG:NE	1:B:314:ASN:OD1	2.26	0.57
1:C:107:LYS:HG3	1:C:113:TYR:CD1	2.39	0.57
2:F:4:DT:C2'	2:F:5:DA:C8	2.87	0.57
1:B:198:ASN:HB2	1:B:222:PHE:CZ	2.40	0.56
1:D:341:GLY:C	1:D:343:THR:N	2.56	0.56
1:D:102:LEU:O	1:D:103:HIS:HB2	2.05	0.56
1:C:13:ASP:OD2	1:D:84:PRO:CB	2.53	0.56
1:C:147:GLN:HB2	1:C:159:LEU:CD1	2.35	0.56
1:D:286:HIS:HD1	1:D:286:HIS:H	1.53	0.56
1:D:301:TYR:CD1	1:D:379:ILE:HD11	2.40	0.56
1:A:240:GLU:HA	1:A:240:GLU:OE2	2.05	0.56
1:C:16:ILE:HG22	1:C:16:ILE:O	2.05	0.56
1:D:113:TYR:OH	3:D:501:ANP:H2'	2.05	0.56
1:A:396:ARG:CD	1:A:400:ARG:HH21	2.18	0.56
1:C:267:PHE:O	1:C:322:GLU:HG2	2.06	0.56
2:F:5:DA:H2''	2:F:6:DT:O4'	2.06	0.56
1:A:257:VAL:HA	1:A:330:ILE:HG22	1.88	0.56
1:A:386:ARG:HG3	1:A:389:ARG:NH2	2.21	0.56
1:C:124:SER:N	3:C:501:ANP:O1A	2.37	0.56
1:D:148:ARG:HD3	1:D:156:VAL:CG2	2.36	0.56
1:D:330:ILE:HD11	1:D:332:VAL:CG1	2.36	0.56
1:A:137:GLU:C	1:A:138:ILE:HD13	2.31	0.56
1:B:364:LEU:O	1:B:365:THR:C	2.47	0.56
1:C:17:GLN:HB2	1:D:110:GLN:HE21	1.71	0.56
1:C:134:LEU:HD22	1:C:149:PHE:HD1	1.70	0.56
1:B:315:LEU:CD2	1:B:386:ARG:HG2	2.37	0.55
1:A:257:VAL:CG2	1:A:359:ILE:HD12	2.36	0.55
1:A:299:ASN:O	1:A:302:ALA:HB3	2.05	0.55
1:B:179:ASP:OD1	1:B:181:THR:HB	2.07	0.55
1:C:83:MET:HG2	1:C:98:ILE:HD13	1.87	0.55
1:D:202:PHE:CE1	1:D:231:PHE:HA	2.41	0.55
2:E:14:DC:N3	2:F:1:DG:N2	2.54	0.55
1:B:134:LEU:C	1:B:134:LEU:HD23	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:LEU:C	1:D:206:ASN:H	2.14	0.55
1:A:275:VAL:CG2	1:A:347:LEU:HD22	2.37	0.55
2:E:9:DA:H1'	2:E:10:DT:C6	2.41	0.55
1:A:139:THR:HG21	1:A:169:LYS:HG2	1.89	0.55
1:C:178:PRO:HB2	1:C:186:THR:HG22	1.89	0.55
1:D:150:GLU:CD	1:D:156:VAL:HG11	2.32	0.55
1:A:347:LEU:HD11	1:A:349:SER:OG	2.07	0.55
1:D:309:LYS:O	1:D:312:ASP:N	2.40	0.55
1:C:146:LYS:C	1:C:159:LEU:HD12	2.31	0.55
1:D:261:LEU:N	1:D:261:LEU:HD12	2.21	0.55
1:B:233:SER:O	1:B:236:ASN:N	2.30	0.55
1:C:62:ASP:O	1:C:207:VAL:HA	2.06	0.55
1:C:298:MET:CB	1:C:320:TYR:CE2	2.89	0.55
1:D:116:SER:O	1:D:276:ASN:ND2	2.35	0.55
1:C:178:PRO:HB2	1:C:186:THR:CG2	2.37	0.55
1:A:144:VAL:O	1:A:162:ILE:HG12	2.07	0.54
1:D:66:VAL:HG22	1:D:76:VAL:HG13	1.90	0.54
1:D:148:ARG:HD3	1:D:156:VAL:HG21	1.89	0.54
1:B:87:MET:HE2	1:B:87:MET:HA	1.89	0.54
1:B:298:MET:HB3	1:B:320:TYR:CE2	2.43	0.54
1:D:113:TYR:CD1	1:D:113:TYR:N	2.75	0.54
2:E:1:DG:H2''	2:E:2:DC:C5	2.43	0.54
1:B:136:VAL:O	1:B:146:LYS:HA	2.07	0.54
1:C:13:ASP:OD1	1:D:86:GLY:HA3	2.08	0.54
1:C:245:VAL:C	1:C:246:LEU:HD23	2.32	0.54
1:C:275:VAL:CG2	1:C:347:LEU:HD22	2.37	0.54
1:C:178:PRO:HG2	1:C:186:THR:HB	1.89	0.54
1:C:343:THR:O	1:C:345:ASP:N	2.41	0.54
2:F:3:DA:N6	3:F:101:ANP:O2'	2.40	0.54
1:D:139:THR:O	1:D:170:THR:HA	2.07	0.54
1:D:51:ASN:HB3	3:D:501:ANP:N7	2.22	0.54
1:D:248:PHE:CZ	1:D:364:LEU:HD13	2.43	0.54
2:E:14:DC:N4	2:F:1:DG:H1	1.96	0.54
1:A:208:THR:HG23	1:A:223:HIS:HB2	1.91	0.53
1:D:137:GLU:HA	1:D:145:TYR:O	2.06	0.53
1:A:146:LYS:HG3	1:A:147:GLN:N	2.17	0.53
1:A:243:THR:CG2	1:A:263:TYR:H	2.20	0.53
1:C:368:LEU:O	1:C:370:GLU:N	2.41	0.53
1:D:21:GLY:O	1:D:22:LEU:C	2.51	0.53
1:A:190:TYR:CD2	1:A:211:LEU:CD2	2.91	0.53
2:F:5:DA:H5''	2:F:5:DA:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASP:HB3	1:A:321:ARG:O	2.09	0.53
1:B:85:THR:HG21	1:B:145:TYR:CD1	2.44	0.53
1:B:303:ARG:HG2	1:B:303:ARG:NH1	2.24	0.53
1:C:49:VAL:O	1:C:53:VAL:HG23	2.08	0.53
1:C:235:LEU:HD23	1:C:325:ALA:HB1	1.91	0.53
2:F:3:DA:C6	3:F:101:ANP:O2'	2.61	0.53
1:B:237:GLU:C	1:B:239:LYS:H	2.16	0.52
1:C:290:LEU:HD22	1:C:328:LEU:HD13	1.91	0.52
1:C:243:THR:OG1	1:C:374:LEU:HD21	2.09	0.52
1:B:232:VAL:HG21	1:B:260:ALA:CB	2.39	0.52
1:C:245:VAL:CG2	1:C:262:GLN:HG3	2.39	0.52
1:A:139:THR:O	1:A:170:THR:HA	2.10	0.52
1:D:245:VAL:HA	1:D:261:LEU:O	2.08	0.52
1:D:302:ALA:CB	1:D:379:ILE:HD13	2.38	0.52
1:A:8:ILE:CG2	1:B:60:PHE:HZ	2.22	0.52
1:B:146:LYS:CB	1:B:162:ILE:HD13	2.39	0.52
1:C:368:LEU:C	1:C:370:GLU:H	2.17	0.52
1:B:341:GLY:O	1:B:342:GLN:C	2.51	0.52
1:C:22:LEU:HD22	1:C:129:ALA:HB2	1.92	0.52
1:D:148:ARG:HG3	1:D:148:ARG:HH11	1.74	0.52
1:D:98:ILE:HG23	3:D:501:ANP:H5'1	1.92	0.51
1:B:55:GLU:OE1	1:B:113:TYR:CE2	2.62	0.51
1:C:257:VAL:HG22	1:C:330:ILE:HG21	1.91	0.51
1:D:204:LEU:O	1:D:206:ASN:N	2.43	0.51
1:D:45:VAL:HG22	1:D:74:LEU:HD13	1.92	0.51
1:D:193:ILE:HG22	1:D:197:LEU:CD1	2.41	0.51
1:A:190:TYR:CD2	1:A:211:LEU:HD23	2.45	0.51
2:E:5:DA:H4'	2:E:6:DT:OP1	2.11	0.51
1:A:257:VAL:HG21	1:A:359:ILE:HD12	1.93	0.51
1:A:7:ASN:OD1	1:A:9:ASN:N	2.41	0.51
1:B:146:LYS:HB2	1:B:162:ILE:HD13	1.91	0.51
1:B:285:THR:HG23	1:B:347:LEU:O	2.11	0.51
1:C:257:VAL:HA	1:C:330:ILE:HG22	1.92	0.51
1:B:393:ARG:O	1:B:394:LYS:C	2.54	0.51
1:B:204:LEU:C	1:B:206:ASN:N	2.69	0.50
1:D:206:ASN:C	1:D:207:VAL:HG23	2.35	0.50
1:D:275:VAL:CG2	1:D:347:LEU:HD22	2.42	0.50
2:E:10:DT:C2'	2:E:11:DA:C8	2.94	0.50
1:A:342:GLN:HA	1:B:31:MET:HG3	1.92	0.50
1:B:147:GLN:HG3	1:B:157:THR:O	2.10	0.50
1:B:357:ASP:OD2	1:B:357:ASP:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:LEU:HD22	1:C:209:LEU:HD23	1.93	0.50
2:F:5:DA:H8	2:F:5:DA:C5'	2.25	0.50
1:A:374:LEU:HA	1:A:377:ASN:OD1	2.10	0.50
1:D:304:LYS:C	1:D:306:GLY:H	2.20	0.50
1:A:12:ASN:OD1	1:B:140:ARG:NH1	2.44	0.50
1:C:85:THR:CG2	1:C:140:ARG:HD2	2.34	0.50
1:C:147:GLN:HB2	1:C:159:LEU:HD13	1.93	0.50
1:C:188:PHE:O	1:C:215:ARG:NH2	2.44	0.50
1:A:259:VAL:HA	1:A:327:VAL:O	2.12	0.50
1:B:328:LEU:HD12	1:B:329:SER:N	2.27	0.50
1:D:203:LEU:HB2	1:D:277:ASN:OD1	2.12	0.50
1:A:35:SER:OG	1:A:37:ASP:OD1	2.30	0.50
2:E:13:DG:H2''	2:E:14:DC:OP2	2.12	0.50
1:C:245:VAL:HG22	1:C:262:GLN:HG3	1.94	0.50
1:D:21:GLY:C	1:D:23:ASP:N	2.69	0.50
1:C:228:VAL:O	1:C:232:VAL:HG23	2.12	0.49
1:D:293:ALA:HB1	1:D:361:ALA:HB2	1.93	0.49
2:F:7:DA:C8	2:F:7:DA:H5'	2.46	0.49
2:E:5:DA:H2''	2:E:6:DT:H71	1.93	0.49
1:A:13:ASP:OD1	1:B:86:GLY:CA	2.60	0.49
1:B:232:VAL:O	1:B:233:SER:C	2.55	0.49
1:C:81:ARG:NH1	1:C:113:TYR:CE2	2.80	0.49
1:C:243:THR:HG22	1:C:263:TYR:H	1.76	0.49
1:D:180:ALA:CB	1:D:186:THR:HG21	2.43	0.49
1:A:287:GLU:O	1:A:290:LEU:HB3	2.12	0.49
1:C:140:ARG:O	1:C:141:ASP:C	2.55	0.49
1:D:135:GLU:HA	1:D:147:GLN:O	2.13	0.49
2:F:9:DA:H2'	2:F:10:DT:H5'	1.93	0.49
1:D:276:ASN:OD1	1:D:331:LEU:HD23	2.12	0.49
1:C:273:SER:OG	1:C:287[B]:GLU:OE2	2.22	0.49
1:D:45:VAL:CG2	1:D:74:LEU:HD13	2.42	0.49
1:D:93:PRO:O	1:D:94:THR:C	2.56	0.49
1:D:179:ASP:C	1:D:181:THR:H	2.21	0.49
1:D:180:ALA:CA	1:D:186:THR:HG21	2.42	0.49
1:D:273:SER:HB3	1:D:287[B]:GLU:HG3	1.94	0.49
1:A:275:VAL:HG13	1:A:332:VAL:CG1	2.43	0.49
1:B:315:LEU:HD21	1:B:386:ARG:HG2	1.94	0.49
1:C:228:VAL:HG12	1:C:327:VAL:HG11	1.94	0.49
1:D:206:ASN:O	1:D:207:VAL:CG2	2.60	0.49
2:F:5:DA:H5''	2:F:5:DA:H8	1.77	0.49
1:B:46:TRP:CZ3	1:B:196:ARG:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:GLY:O	1:B:343:THR:N	2.46	0.49
1:C:44:LEU:HD11	1:C:183:PHE:CZ	2.48	0.49
1:B:75:THR:HG22	1:B:76:VAL:N	2.28	0.48
1:B:166:PRO:HG2	1:B:169:LYS:HB2	1.94	0.48
1:C:203:LEU:HA	1:C:203:LEU:HD23	1.45	0.48
1:C:204:LEU:HD21	1:C:277:ASN:OD1	2.13	0.48
1:C:303:ARG:O	1:C:304:LYS:C	2.56	0.48
1:A:143:ALA:HB3	1:A:145:TYR:HE1	1.77	0.48
1:A:263:TYR:CZ	1:A:324:LEU:HD13	2.48	0.48
1:C:87:MET:HB2	1:C:87:MET:HE3	1.31	0.48
1:D:41:LEU:HD11	1:D:178:PRO:HG2	1.95	0.48
1:C:184:SER:C	1:C:185:THR:CG2	2.86	0.48
1:A:88:HIS:ND1	1:A:89:ALA:N	2.62	0.48
1:A:190:TYR:O	1:A:194:SER:HB2	2.13	0.48
1:D:62:ASP:O	1:D:207:VAL:HA	2.12	0.48
1:A:13:ASP:HB3	1:B:94:THR:OG1	2.14	0.48
1:A:60:PHE:CZ	1:A:81:ARG:HD3	2.48	0.48
1:B:265:ASP:O	1:B:266:GLY:O	2.31	0.48
1:D:122:VAL:O	1:D:123:GLY:C	2.55	0.48
1:B:49:VAL:O	1:B:53:VAL:HG23	2.14	0.48
1:D:45:VAL:HG23	1:D:188:PHE:HE1	1.77	0.48
1:D:103:HIS:N	1:D:121:GLY:O	2.46	0.48
1:D:119:LEU:HG	1:D:120:HIS:HD2	1.79	0.48
1:C:67:THR:CG2	1:C:212:THR:HB	2.41	0.48
1:C:74:LEU:HB2	1:C:188:PHE:HE2	1.69	0.48
1:C:105:GLY:HA2	1:D:16:ILE:HG23	1.96	0.48
1:D:44:LEU:HD22	1:D:127:VAL:HA	1.95	0.48
1:A:379:ILE:O	1:A:383:ILE:HG13	2.14	0.48
1:D:84:PRO:HB2	1:D:94:THR:HG21	1.96	0.48
1:A:102:LEU:O	1:A:103:HIS:HB2	2.13	0.48
1:B:71:ASP:O	1:B:177:MET:HE1	2.14	0.48
1:B:119:LEU:HD21	1:B:120:HIS:NE2	2.29	0.48
1:A:350:PRO:O	1:A:352:ALA:N	2.47	0.47
1:A:396:ARG:CG	1:A:400:ARG:HH21	2.27	0.47
1:B:74:LEU:C	1:B:74:LEU:HD23	2.39	0.47
1:B:298:MET:HE3	1:B:379:ILE:CD1	2.44	0.47
1:C:259:VAL:HG22	1:C:260:ALA:N	2.28	0.47
1:D:352:ALA:O	1:D:353:ARG:C	2.57	0.47
1:A:119:LEU:HD13	1:A:337:LEU:HD13	1.95	0.47
1:A:181:THR:HG23	1:A:182:ILE:HG12	1.95	0.47
1:A:274:PHE:CD1	1:A:279:ARG:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:VAL:HG22	1:B:332:VAL:O	2.13	0.47
1:D:123:GLY:HA3	3:D:501:ANP:O1A	2.14	0.47
2:E:1:DG:H2''	2:E:2:DC:C6	2.49	0.47
1:A:270:ASN:HB3	1:A:325:ALA:HA	1.95	0.47
1:B:246:LEU:CD2	1:B:367:PHE:CE1	2.98	0.47
1:C:22:LEU:CD1	1:C:153:GLY:HA3	2.43	0.47
1:D:130:LEU:O	1:D:179:ASP:HB2	2.15	0.47
1:D:134:LEU:C	1:D:134:LEU:HD23	2.39	0.47
1:C:201:ALA:O	1:C:202:PHE:C	2.57	0.47
1:D:252:ASP:C	1:D:254:GLY:N	2.70	0.47
1:A:66:VAL:CG1	1:A:211:LEU:HD12	2.43	0.47
1:A:112:GLY:O	1:B:8:ILE:CD1	2.57	0.47
1:C:168:SER:O	1:C:170:THR:HG23	2.15	0.47
1:C:241:ILE:HG21	1:C:241:ILE:HD13	1.47	0.47
1:C:328:LEU:HD12	1:C:328:LEU:HA	1.71	0.47
1:C:375:ALA:O	1:C:379:ILE:HG13	2.14	0.47
2:F:12:DT:H1'	2:F:13:DG:C8	2.49	0.47
1:A:91:GLY:O	1:A:92:ILE:CG2	2.63	0.47
1:B:35:SER:O	1:B:40:GLY:HA3	2.13	0.47
1:C:44:LEU:HD22	1:C:127:VAL:HA	1.97	0.47
1:D:115:THR:HG22	1:D:333:PRO:HA	1.97	0.47
2:E:1:DG:H22	2:F:14:DC:H42	1.63	0.47
1:A:248:PHE:CD1	1:A:363:LYS:HB3	2.50	0.47
1:C:62:ASP:OD1	1:C:62:ASP:N	2.46	0.47
1:D:72:GLY:C	1:D:177:MET:CE	2.88	0.47
1:C:79:HIS:HA	1:C:171:GLY:HA3	1.98	0.46
1:C:229:GLN:NE2	1:C:247:TYR:CG	2.82	0.46
1:A:92:ILE:O	1:A:93:PRO:C	2.57	0.46
1:D:374:LEU:O	1:D:375:ALA:C	2.58	0.46
1:A:201:ALA:O	1:A:202:PHE:C	2.55	0.46
1:C:301:TYR:CE1	1:C:305:THR:HG21	2.50	0.46
1:C:248:PHE:HB2	1:C:259:VAL:CG1	2.46	0.46
2:F:5:DA:C8	2:F:5:DA:C5'	2.99	0.46
1:D:45:VAL:HG23	1:D:188:PHE:CE1	2.50	0.46
1:D:66:VAL:HG13	1:D:74:LEU:HD21	1.97	0.46
1:D:94:THR:HG22	1:D:95:VAL:N	2.29	0.46
1:D:275:VAL:O	1:D:276:ASN:HB2	2.16	0.46
1:A:256[A]:GLN:OE1	1:A:331:LEU:HD22	2.15	0.46
1:A:339:PHE:CZ	1:A:344:LYS:HG2	2.51	0.46
1:A:246:LEU:HD11	1:A:367:PHE:CE2	2.50	0.46
1:C:119:LEU:HD21	1:C:120:HIS:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:LEU:HD12	1:A:378:LEU:HA	1.53	0.46
2:E:5:DA:C2	2:F:11:DA:C2	3.04	0.46
1:A:190:TYR:CD2	1:A:211:LEU:HD21	2.51	0.46
1:B:41:LEU:HD22	1:B:186:THR:HA	1.97	0.46
1:B:273:SER:HB3	1:B:287:GLU:OE2	2.15	0.46
1:D:203:LEU:CD2	1:D:329:SER:CB	2.94	0.46
1:A:95:VAL:CG1	1:A:136:VAL:HG21	2.46	0.46
1:B:14:ASP:O	1:B:14:ASP:OD1	2.34	0.46
1:B:331:LEU:HD12	1:B:331:LEU:HA	1.31	0.46
1:D:44:LEU:HA	1:D:127:VAL:HG22	1.98	0.46
1:A:98:ILE:HG12	3:A:501:ANP:O4'	2.15	0.45
1:A:241:ILE:HG21	1:A:262:GLN:CD	2.41	0.45
1:C:140:ARG:NH2	1:D:11:TYR:O	2.50	0.45
1:A:204:LEU:HD13	1:A:207:VAL:HG21	1.98	0.45
1:A:243:THR:HG22	1:A:262:GLN:HG3	1.98	0.45
1:A:8:ILE:HD12	1:A:8:ILE:HA	1.67	0.45
1:B:220:ILE:HG12	1:B:221:GLU:N	2.29	0.45
1:C:202:PHE:CE1	1:C:224:TYR:CE1	3.05	0.45
1:C:228:VAL:HG12	1:C:327:VAL:CG1	2.45	0.45
1:D:127:VAL:O	1:D:131:SER:OG	2.33	0.45
1:C:48:ILE:CG2	1:C:76:VAL:HB	2.46	0.45
1:C:63:ARG:HA	1:C:208:THR:O	2.16	0.45
1:C:78:ASP:C	1:C:78:ASP:OD1	2.59	0.45
1:C:172:THR:CG2	1:C:173:LYS:N	2.79	0.45
1:D:288:THR:O	1:D:289:GLY:C	2.58	0.45
1:C:242:LEU:O	1:C:243:THR:HB	2.16	0.45
1:D:275:VAL:HG11	1:D:337:LEU:HD11	1.98	0.45
1:A:351:LEU:H	1:A:351:LEU:HG	1.52	0.45
1:A:368:LEU:C	1:A:370:GLU:H	2.25	0.45
1:B:204:LEU:O	1:B:205:LYS:C	2.60	0.45
1:D:46:TRP:HE3	1:D:46:TRP:HA	1.82	0.45
1:D:87:MET:HA	1:D:93:PRO:HA	1.98	0.45
1:D:379:ILE:O	1:D:383:ILE:HG23	2.16	0.45
1:A:264:ASN:OD1	1:A:323:GLY:HA2	2.16	0.45
1:A:293:ALA:O	1:A:294:ILE:C	2.60	0.45
1:C:294:ILE:O	1:C:298:MET:HG2	2.17	0.45
2:E:5:DA:H1'	2:E:6:DT:H5'	1.99	0.45
1:A:88:HIS:CG	1:A:97:VAL:HG21	2.52	0.45
1:A:145:TYR:N	1:A:145:TYR:CD1	2.85	0.45
1:B:60:PHE:N	1:B:60:PHE:CD1	2.84	0.45
1:B:294:ILE:O	1:B:295:THR:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:LEU:C	1:C:134:LEU:CD2	2.89	0.45
1:C:147:GLN:N	1:C:159:LEU:HD12	2.32	0.45
1:C:339:PHE:CE1	1:C:344:LYS:HG2	2.52	0.45
1:B:271:ILE:HB	1:B:326:ALA:HB3	1.98	0.45
1:C:6:ILE:HG21	1:C:15:ALA:HB2	1.99	0.45
2:E:10:DT:H2''	2:E:11:DA:C5'	2.47	0.45
1:B:367:PHE:CD2	1:B:367:PHE:C	2.95	0.45
1:C:197:LEU:HD23	1:C:209:LEU:HD23	1.97	0.45
1:D:22:LEU:HD22	1:D:22:LEU:HA	1.58	0.45
1:D:125:SER:O	1:D:129:ALA:HB2	2.16	0.45
1:D:330:ILE:CD1	1:D:332:VAL:CG1	2.94	0.45
1:A:347:LEU:HD12	1:A:348:GLY:N	2.29	0.44
1:B:69:ASN:O	1:B:70:LYS:C	2.59	0.44
1:B:232:VAL:HG21	1:B:260:ALA:HB1	1.98	0.44
1:B:246:LEU:N	1:B:246:LEU:HD23	2.30	0.44
1:D:301:TYR:CE1	1:D:375:ALA:HB1	2.52	0.44
1:A:264:ASN:C	1:A:266:GLY:H	2.25	0.44
1:D:383:ILE:HG13	1:D:384:LYS:N	2.32	0.44
1:A:368:LEU:C	1:A:370:GLU:N	2.76	0.44
1:C:85:THR:HG21	1:C:145:TYR:CE1	2.52	0.44
1:C:191:ASN:O	1:C:194:SER:HB3	2.17	0.44
1:D:88:HIS:ND1	1:D:89:ALA:N	2.65	0.44
1:D:271:ILE:HD13	1:D:271:ILE:O	2.18	0.44
1:B:360:VAL:O	1:B:361:ALA:C	2.58	0.44
1:C:202:PHE:O	1:C:227:GLY:HA2	2.17	0.44
1:D:119:LEU:HD21	1:D:120:HIS:CD2	2.52	0.44
1:D:271:ILE:HB	1:D:326:ALA:HB3	2.00	0.44
1:A:199[B]:GLU:HG3	1:A:274:PHE:HZ	1.83	0.44
1:B:135:GLU:OE2	1:B:146:LYS:HE2	2.18	0.44
1:B:209:LEU:N	1:B:209:LEU:CD1	2.78	0.44
1:B:246:LEU:O	1:B:260:ALA:HA	2.17	0.44
1:B:343:THR:O	1:B:344:LYS:CB	2.66	0.44
1:A:110:GLN:HE21	1:B:17:GLN:HB2	1.83	0.44
1:B:276:ASN:OD1	1:B:331:LEU:HA	2.17	0.44
1:B:293:ALA:HB1	1:B:361:ALA:HB2	1.98	0.44
1:C:193:ILE:HG22	1:C:211:LEU:HD22	1.98	0.44
1:D:273:SER:HB3	1:D:287[B]:GLU:CG	2.47	0.44
1:A:365:THR:O	1:A:366:PHE:C	2.59	0.44
2:E:10:DT:H2''	2:E:11:DA:O5'	2.17	0.44
1:A:256[B]:GLN:HB2	1:A:331:LEU:HB2	2.00	0.44
1:B:88:HIS:HB2	1:B:94:THR:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:THR:HA	1:C:174:VAL:O	2.18	0.44
1:C:343:THR:O	1:C:344:LYS:C	2.59	0.44
1:D:206:ASN:O	1:D:207:VAL:HG23	2.17	0.44
1:C:275:VAL:O	1:C:276:ASN:C	2.60	0.43
1:B:220:ILE:CD1	1:B:222:PHE:CE1	3.01	0.43
1:C:243:THR:CG2	1:C:263:TYR:N	2.72	0.43
1:A:295:THR:OG1	1:A:317:GLY:HA2	2.17	0.43
1:C:397:ASP:C	1:C:399:SER:H	2.27	0.43
1:D:78:ASP:O	1:D:171:GLY:HA3	2.18	0.43
1:C:46:TRP:CH2	1:C:196:ARG:HG2	2.52	0.43
1:D:75:THR:HA	1:D:174:VAL:O	2.17	0.43
1:A:193:ILE:CG2	1:A:211:LEU:HD13	2.49	0.43
1:A:235:LEU:HD12	1:A:235:LEU:HA	1.65	0.43
1:D:246:LEU:O	1:D:261:LEU:HD12	2.19	0.43
2:E:3:DA:C2	2:F:13:DG:C2	3.06	0.43
1:A:15:ALA:O	1:B:106:GLY:HA2	2.19	0.43
1:B:52:ALA:HB1	1:B:64:ILE:HG12	2.01	0.43
1:C:107:LYS:HD2	3:C:501:ANP:O2B	2.19	0.43
1:C:115:THR:HG22	1:C:116:SER:N	2.33	0.43
1:C:172:THR:HG22	1:C:173:LYS:N	2.31	0.43
1:D:208:THR:C	1:D:209:LEU:HD12	2.44	0.43
1:A:396:ARG:CD	1:A:400:ARG:NH2	2.75	0.43
1:B:343:THR:O	1:B:344:LYS:CG	2.65	0.43
1:C:56:ALA:HA	1:C:60:PHE:O	2.18	0.43
1:C:62:ASP:O	1:C:208:THR:N	2.47	0.43
1:D:41:LEU:HD11	1:D:178:PRO:CG	2.49	0.43
2:E:9:DA:H2''	2:E:10:DT:O5'	2.19	0.43
2:F:4:DT:H2'	2:F:5:DA:C8	2.53	0.43
1:A:66:VAL:HG12	1:A:211:LEU:CD1	2.45	0.43
1:A:246:LEU:O	1:A:260:ALA:HA	2.18	0.43
1:D:46:TRP:CE3	1:D:46:TRP:CA	3.01	0.43
1:D:60:PHE:CB	1:D:80:GLY:HA2	2.48	0.43
1:C:74:LEU:O	1:C:175:THR:HA	2.19	0.42
1:C:195:GLU:O	1:C:199:GLU:HG3	2.18	0.42
1:C:368:LEU:C	1:C:370:GLU:N	2.73	0.42
1:D:21:GLY:CA	1:D:102:LEU:HD12	2.49	0.42
1:D:271:ILE:CG1	1:D:326:ALA:HB3	2.50	0.42
2:E:10:DT:H2''	2:E:11:DA:H5'	2.01	0.42
1:B:397:ASP:O	1:B:398:GLU:C	2.61	0.42
1:C:64:ILE:O	1:C:209:LEU:HA	2.19	0.42
1:D:380:ARG:HA	1:D:383:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:THR:HG23	1:B:116:SER:N	2.35	0.42
1:B:276:ASN:O	1:B:277:ASN:HB2	2.18	0.42
2:E:7:DA:C1'	2:E:8:DT:H5'	2.49	0.42
1:A:13:ASP:OD1	1:B:86:GLY:HA3	2.20	0.42
1:A:275:VAL:HG13	1:A:332:VAL:HG13	2.02	0.42
1:A:366:PHE:CE1	1:A:370:GLU:OE1	2.73	0.42
1:B:10:ASN:CG	1:B:10:ASN:O	2.62	0.42
1:B:310:GLU:CA	1:B:310:GLU:OE2	2.68	0.42
1:A:105:GLY:HA2	1:B:16:ILE:HG23	2.01	0.42
1:B:233:SER:O	1:B:235:LEU:N	2.52	0.42
1:C:105:GLY:CA	1:D:16:ILE:HG23	2.50	0.42
1:C:119:LEU:H	3:C:501:ANP:HNB1	1.66	0.42
1:D:33:ILE:O	1:D:35:SER:N	2.51	0.42
1:A:119:LEU:HD12	1:B:28:ARG:NE	2.35	0.42
1:B:315:LEU:HD23	1:B:315:LEU:HA	1.57	0.42
1:D:353:ARG:N	1:D:354:PRO:HD2	2.35	0.42
1:A:135:GLU:OE1	1:A:148:ARG:HD2	2.20	0.42
1:B:236:ASN:ND2	1:B:262:GLN:HG2	2.31	0.42
1:C:147:GLN:HB2	1:C:159:LEU:HD12	2.01	0.42
1:D:134:LEU:HD23	1:D:135:GLU:N	2.34	0.42
1:C:147:GLN:CB	1:C:159:LEU:HD13	2.50	0.42
1:A:103:HIS:N	1:A:121:GLY:O	2.50	0.42
1:C:20:GLU:O	1:C:21:GLY:C	2.63	0.42
1:C:204:LEU:CD2	1:C:277:ASN:OD1	2.67	0.42
1:C:250:GLY:C	1:C:359:ILE:HD13	2.45	0.42
1:D:89:ALA:C	1:D:91:GLY:N	2.71	0.42
1:D:74:LEU:O	1:D:175:THR:HA	2.20	0.41
1:A:41:LEU:CD2	1:A:186:THR:HA	2.47	0.41
1:A:100:THR:C	1:A:101:ILE:HD13	2.45	0.41
1:C:339:PHE:CD1	1:C:344:LYS:HG2	2.55	0.41
1:D:179:ASP:O	1:D:181:THR:N	2.53	0.41
1:D:252:ASP:C	1:D:254:GLY:H	2.26	0.41
2:E:3:DA:C2	2:F:13:DG:N2	2.88	0.41
1:A:33:ILE:HG21	1:A:33:ILE:HD13	1.77	0.41
1:A:60:PHE:CE1	1:A:81:ARG:HD3	2.55	0.41
1:A:324:LEU:HA	1:A:324:LEU:HD12	1.72	0.41
1:A:354:PRO:O	1:A:355:VAL:C	2.60	0.41
1:C:229:GLN:NE2	1:C:247:TYR:HB2	2.36	0.41
1:D:46:TRP:HA	1:D:46:TRP:CE3	2.55	0.41
2:E:5:DA:H2''	2:E:6:DT:C7	2.50	0.41
2:F:4:DT:C3'	2:F:5:DA:H5''	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:ASN:ND2	1:C:234:TYR:CZ	2.88	0.41
1:C:270:ASN:OD1	1:C:270:ASN:C	2.64	0.41
1:C:83:MET:HE3	3:C:501:ANP:C8	2.50	0.41
1:D:64:ILE:O	1:D:64:ILE:HG22	2.19	0.41
2:E:1:DG:H22	2:F:14:DC:N4	2.18	0.41
1:A:104:ALA:HA	1:B:17:GLN:O	2.19	0.41
1:A:122:VAL:O	1:A:123:GLY:C	2.62	0.41
1:B:107:LYS:HD3	1:B:116:SER:OG	2.20	0.41
1:B:310:GLU:C	1:B:312:ASP:H	2.28	0.41
1:C:7:ASN:O	1:C:8:ILE:C	2.63	0.41
1:C:33:ILE:HD12	1:C:35:SER:O	2.21	0.41
1:D:180:ALA:HA	1:D:186:THR:CG2	2.47	0.41
2:E:3:DA:C2'	2:E:4:DT:H72	2.46	0.41
1:A:68:ILE:HG21	1:A:215:ARG:CZ	2.50	0.41
1:A:242:LEU:O	1:A:243:THR:HB	2.19	0.41
1:C:256:GLN:HB3	1:C:331:LEU:HB2	2.02	0.41
1:C:259:VAL:CG2	1:C:260:ALA:N	2.82	0.41
1:A:49:VAL:O	1:A:50:ASP:C	2.59	0.41
1:B:356:VAL:O	1:B:357:ASP:C	2.64	0.41
1:C:301:TYR:CE1	1:C:375:ALA:CB	3.02	0.41
1:D:126:VAL:O	1:D:129:ALA:HB3	2.21	0.41
1:D:128:ASN:OD1	1:D:153:GLY:HA2	2.21	0.41
1:D:179:ASP:C	1:D:181:THR:N	2.78	0.41
1:A:275:VAL:O	1:A:278:VAL:HB	2.21	0.41
1:A:284:GLY:O	1:A:285:THR:C	2.63	0.41
1:A:376:SER:CB	1:A:380:ARG:NH2	2.82	0.41
1:B:251:GLU:HA	1:B:255:PHE:O	2.21	0.41
1:B:319:ASP:OD2	1:B:386:ARG:HB3	2.21	0.41
1:C:7:ASN:O	1:C:10:ASN:N	2.48	0.41
1:D:139:THR:HA	1:D:143:ALA:O	2.21	0.41
1:D:204:LEU:C	1:D:206:ASN:N	2.79	0.41
1:D:207:VAL:HG12	1:D:208:THR:N	2.36	0.41
1:D:273:SER:OG	1:D:280:THR:OG1	2.34	0.41
2:E:4:DT:O2	2:F:11:DA:H2	2.03	0.41
2:F:11:DA:C2'	2:F:12:DT:OP2	2.59	0.41
1:A:197:LEU:HD22	1:A:209:LEU:CD2	2.51	0.41
1:C:102:LEU:HD23	1:C:122:VAL:HB	2.03	0.41
1:C:108:PHE:N	1:C:110:GLN:OE1	2.50	0.41
1:D:101:ILE:HG22	1:D:104:ALA:HB2	2.03	0.41
1:D:119:LEU:N	3:D:501:ANP:O1G	2.49	0.41
2:E:7:DA:H1'	2:E:8:DT:H5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASN:O	1:A:201:ALA:HB3	2.21	0.40
1:A:202:PHE:O	1:A:227:GLY:HA2	2.21	0.40
1:B:27:LYS:HE3	1:B:28:ARG:NH1	2.35	0.40
1:B:315:LEU:HB2	1:B:320:TYR:CE1	2.57	0.40
1:B:331:LEU:N	1:B:331:LEU:HD13	2.35	0.40
1:C:30:GLY:O	1:C:34:GLY:HA2	2.21	0.40
1:D:72:GLY:O	1:D:177:MET:CE	2.69	0.40
1:B:368:LEU:HD23	1:B:368:LEU:HA	1.86	0.40
1:D:330:ILE:HD12	1:D:332:VAL:HG12	2.03	0.40
1:B:22:LEU:O	1:B:25:VAL:HG13	2.21	0.40
1:B:286:HIS:HB3	1:B:330:ILE:CD1	2.51	0.40
1:B:321:ARG:HG3	1:B:321:ARG:HH11	1.87	0.40
1:C:243:THR:OG1	1:C:244:PRO:HD2	2.21	0.40
1:D:321:ARG:O	1:D:324:LEU:HB3	2.21	0.40
1:B:166:PRO:O	1:B:169:LYS:HB3	2.22	0.40
1:C:83:MET:HE1	1:C:99:PHE:CE1	2.57	0.40
1:C:357:ASP:O	1:C:359:ILE:N	2.54	0.40
2:F:7:DA:H2''	2:F:8:DT:C4'	2.52	0.40
1:C:180:ALA:HA	1:C:186:THR:HG21	2.03	0.40
1:C:339:PHE:CD2	1:C:344:LYS:HA	2.57	0.40
1:D:29:PRO:C	1:D:31:MET:N	2.77	0.40
1:D:68:ILE:HG21	1:D:215:ARG:NH2	2.36	0.40
1:D:364:LEU:HD12	1:D:364:LEU:HA	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/409 (97%)	354 (89%)	37 (9%)	7 (2%)	6	14
1	B	396/409 (97%)	341 (86%)	37 (9%)	18 (4%)	2	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	395/409 (97%)	348 (88%)	38 (10%)	9 (2%)	5	10
1	D	394/409 (96%)	315 (80%)	60 (15%)	19 (5%)	2	3
All	All	1583/1636 (97%)	1358 (86%)	172 (11%)	53 (3%)	3	6

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	ILE
1	B	10	ASN
1	B	237	GLU
1	B	253	ASN
1	B	266	GLY
1	B	343	THR
1	B	344	LYS
1	B	355	VAL
1	D	22	LEU
1	D	90	MET
1	D	162	ILE
1	B	20	GLU
1	B	119	LEU
1	B	123	GLY
1	B	205	LYS
1	B	372	GLY
1	C	21	GLY
1	C	34	GLY
1	C	119	LEU
1	C	398	GLU
1	D	64	ILE
1	D	80	GLY
1	D	179	ASP
1	D	342	GLN
1	D	387	ASP
1	A	351	LEU
1	A	385	ALA
1	B	89	ALA
1	B	352	ALA
1	C	340	GLU
1	D	82	GLY
1	D	123	GLY
1	D	205	LYS
1	A	114	LYS

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Mol	Chain	Res	Type
1	A	119	LEU
1	A	265	ASP
1	A	365	THR
1	B	115	THR
1	B	252	ASP
1	D	84	PRO
1	D	180	ALA
1	D	245	VAL
1	D	370	GLU
1	D	391	ALA
1	C	8	ILE
1	D	56	ALA
1	A	369	MET
1	C	166	PRO
1	D	243	THR
1	C	220	ILE
1	C	162	ILE
1	B	349	SER
1	D	111	GLY

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	314/340 (92%)	266 (85%)	48 (15%)	3	5
1	B	292/340 (86%)	253 (87%)	39 (13%)	4	8
1	C	270/340 (79%)	227 (84%)	43 (16%)	2	4
1	D	208/340 (61%)	186 (89%)	22 (11%)	6	13
All	All	1084/1360 (80%)	932 (86%)	152 (14%)	3	7

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	13	ASP

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Mol	Chain	Res	Type
1	A	25	VAL
1	A	43	HIS
1	A	98	ILE
1	A	115	THR
1	A	116	SER
1	A	119	LEU
1	A	124	SER
1	A	136	VAL
1	A	138	ILE
1	A	141	ASP
1	A	146	LYS
1	A	160	LYS
1	A	162	ILE
1	A	164	THR
1	A	175	THR
1	A	185	THR
1	A	189	LYS
1	A	191	ASN
1	A	200	SER
1	A	209	LEU
1	A	210	SER
1	A	234	TYR
1	A	235	LEU
1	A	242	LEU
1	A	246	LEU
1	A	249	GLU
1	A	259	VAL
1	A	261	LEU
1	A	280	THR
1	A	287	GLU
1	A	295	THR
1	A	303	ARG
1	A	308	LEU
1	A	313	LYS
1	A	316	GLU
1	A	318	SER
1	A	331	LEU
1	A	332	VAL
1	A	335	GLU
1	A	337	LEU
1	A	346	LYS
1	A	362	ASP

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Mol	Chain	Res	Type
1	A	369	MET
1	A	374	LEU
1	A	377	ASN
1	A	378	LEU
1	B	8	ILE
1	B	25	VAL
1	B	27	LYS
1	B	47	GLU
1	B	84	PRO
1	B	90	MET
1	B	92	ILE
1	B	95	VAL
1	B	115	THR
1	B	116	SER
1	B	124	SER
1	B	136	VAL
1	B	138	ILE
1	B	140	ARG
1	B	162	ILE
1	B	164	THR
1	B	169	LYS
1	B	172	THR
1	B	173	LYS
1	B	182	ILE
1	B	189	LYS
1	B	195	GLU
1	B	196	ARG
1	B	209	LEU
1	B	210	SER
1	B	220	ILE
1	B	256	GLN
1	B	257	VAL
1	B	258	GLU
1	B	268	SER
1	B	271	ILE
1	B	286	HIS
1	B	318	SER
1	B	331	LEU
1	B	332	VAL
1	B	335	GLU
1	B	353	ARG
1	B	371	ASN

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Mol	Chain	Res	Type
1	B	386	ARG
1	C	6	ILE
1	C	16	ILE
1	C	25	VAL
1	C	35	SER
1	C	43	HIS
1	C	54	ASP
1	C	67	THR
1	C	77	GLN
1	C	78	ASP
1	C	87	MET
1	C	90	MET
1	C	126	VAL
1	C	134	LEU
1	C	136	VAL
1	C	139	THR
1	C	181	THR
1	C	185	THR
1	C	210	SER
1	C	226	ASN
1	C	228	VAL
1	C	235	LEU
1	C	241	ILE
1	C	249	GLU
1	C	261	LEU
1	C	262	GLN
1	C	268	SER
1	C	269	ASP
1	C	272	LEU
1	C	281	LYS
1	C	285	THR
1	C	286	HIS
1	C	287[A]	GLU
1	C	287[B]	GLU
1	C	297	VAL
1	C	312	ASP
1	C	318	SER
1	C	330	ILE
1	C	332	VAL
1	C	337	LEU
1	C	357	ASP
1	C	378	LEU

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Mol	Chain	Res	Type
1	C	379	ILE
1	C	383	ILE
1	D	8	ILE
1	D	22	LEU
1	D	25	VAL
1	D	43	HIS
1	D	47	GLU
1	D	115	THR
1	D	116	SER
1	D	131	SER
1	D	136	VAL
1	D	156	VAL
1	D	157	THR
1	D	172	THR
1	D	177	MET
1	D	203	LEU
1	D	215	ARG
1	D	232	VAL
1	D	261	LEU
1	D	271	ILE
1	D	290	LEU
1	D	330	ILE
1	D	332	VAL
1	D	396	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	264	ASN
1	B	9	ASN
1	B	338	GLN
1	C	9	ASN
1	C	10	ASN
1	C	69	ASN
1	C	79	HIS
1	C	103	HIS
1	C	147	GLN
1	C	314	ASN
1	D	147	GLN
1	D	338	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ANP	A	501	4	33,33,33	2.00	4 (12%)	45,52,52	2.80	9 (20%)
3	ANP	F	101	-	25,25,33	0.80	2 (8%)	37,38,52	0.85	1 (2%)
3	ANP	C	501	4	33,33,33	2.30	4 (12%)	45,52,52	1.88	5 (11%)
3	ANP	D	501	4	33,33,33	2.36	7 (21%)	45,52,52	2.55	6 (13%)
3	ANP	B	501	4	33,33,33	3.42	8 (24%)	45,52,52	1.88	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	501	4	-	5/18/38/38	0/3/3/3
3	ANP	F	101	-	-	8/10/26/38	0/3/3/3
3	ANP	C	501	4	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	D	501	4	-	7/18/38/38	0/3/3/3
3	ANP	B	501	4	-	7/18/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	ANP	PA-O3A	-13.09	1.45	1.59
3	C	501	ANP	PB-O1B	11.61	1.63	1.46
3	D	501	ANP	PB-O1B	9.30	1.60	1.46
3	B	501	ANP	PB-O1B	8.47	1.59	1.46
3	A	501	ANP	PA-O3A	-7.72	1.51	1.59
3	B	501	ANP	PB-O2B	-7.41	1.37	1.56
3	D	501	ANP	PG-O1G	6.89	1.56	1.46
3	B	501	ANP	PB-O3A	-6.44	1.51	1.59
3	A	501	ANP	PB-O1B	5.63	1.54	1.46
3	B	501	ANP	PG-O1G	4.62	1.53	1.46
3	A	501	ANP	PG-O1G	4.35	1.52	1.46
3	C	501	ANP	PB-O3A	-3.67	1.54	1.59
3	D	501	ANP	PG-N3B	3.64	1.72	1.63
3	C	501	ANP	PB-O2B	-3.55	1.47	1.56
3	D	501	ANP	PB-O3A	-3.36	1.54	1.59
3	D	501	ANP	PB-O2B	-3.08	1.48	1.56
3	B	501	ANP	PG-N3B	2.87	1.70	1.63
3	C	501	ANP	PG-N3B	2.37	1.69	1.63
3	B	501	ANP	PG-O3G	2.36	1.63	1.56
3	D	501	ANP	PA-O3A	-2.33	1.57	1.59
3	B	501	ANP	PG-O2G	2.21	1.62	1.56
3	F	101	ANP	O5'-C5'	2.15	1.52	1.44
3	D	501	ANP	PG-O2G	-2.09	1.51	1.56
3	F	101	ANP	PA-O5'	2.07	1.66	1.60
3	A	501	ANP	PB-N3B	2.05	1.68	1.63

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	ANP	O1G-PG-N3B	-12.60	93.22	111.77
3	A	501	ANP	O1G-PG-N3B	-11.61	94.67	111.77
3	C	501	ANP	O3G-PG-O1G	-8.35	92.51	113.45
3	D	501	ANP	O1B-PB-N3B	-8.29	99.56	111.77
3	B	501	ANP	O3G-PG-O1G	-6.50	97.15	113.45
3	A	501	ANP	O2G-PG-O3G	-6.37	90.47	107.59
3	A	501	ANP	O3G-PG-O1G	6.27	129.18	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	ANP	O2A-PA-O3A	6.27	124.23	107.27
3	B	501	ANP	O2B-PB-O3A	5.50	122.99	104.64
3	A	501	ANP	O3A-PA-O1A	-5.00	95.65	110.70
3	A	501	ANP	O1B-PB-N3B	-4.81	104.68	111.77
3	A	501	ANP	O2A-PA-O3A	4.47	119.36	107.27
3	D	501	ANP	O2G-PG-O1G	4.37	124.41	113.45
3	B	501	ANP	O1G-PG-N3B	4.23	118.00	111.77
3	A	501	ANP	O2B-PB-O1B	4.20	118.89	109.87
3	B	501	ANP	O2B-PB-O1B	-4.14	100.99	109.87
3	A	501	ANP	O2A-PA-O5'	3.95	125.48	107.57
3	C	501	ANP	O2B-PB-O1B	-3.85	101.61	109.87
3	A	501	ANP	O2G-PG-O1G	-3.65	104.29	113.45
3	D	501	ANP	O2B-PB-O1B	3.43	117.23	109.87
3	B	501	ANP	O2G-PG-O1G	3.23	121.54	113.45
3	F	101	ANP	O2A-PA-O5'	3.20	115.02	106.67
3	B	501	ANP	O2G-PG-O3G	3.03	115.72	107.59
3	C	501	ANP	O2B-PB-O3A	2.92	114.40	104.64
3	B	501	ANP	O3A-PA-O1A	2.92	119.49	110.70
3	D	501	ANP	O3G-PG-O1G	-2.59	106.95	113.45
3	B	501	ANP	O1B-PB-N3B	-2.52	108.06	111.77
3	D	501	ANP	O3A-PA-O1A	2.39	117.88	110.70
3	B	501	ANP	O2A-PA-O1A	-2.16	102.42	112.44
3	C	501	ANP	O1B-PB-N3B	-2.02	108.80	111.77

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	ANP	PB-N3B-PG-O1G
3	A	501	ANP	PG-N3B-PB-O3A
3	A	501	ANP	PA-O3A-PB-O2B
3	B	501	ANP	PB-N3B-PG-O1G
3	B	501	ANP	PG-N3B-PB-O1B
3	B	501	ANP	PA-O3A-PB-O2B
3	B	501	ANP	PB-O3A-PA-O5'
3	C	501	ANP	PB-N3B-PG-O1G
3	C	501	ANP	PG-N3B-PB-O1B
3	D	501	ANP	PB-N3B-PG-O1G
3	D	501	ANP	PG-N3B-PB-O1B
3	D	501	ANP	PA-O3A-PB-O1B
3	D	501	ANP	PA-O3A-PB-O2B
3	F	101	ANP	C5'-O5'-PA-O2A

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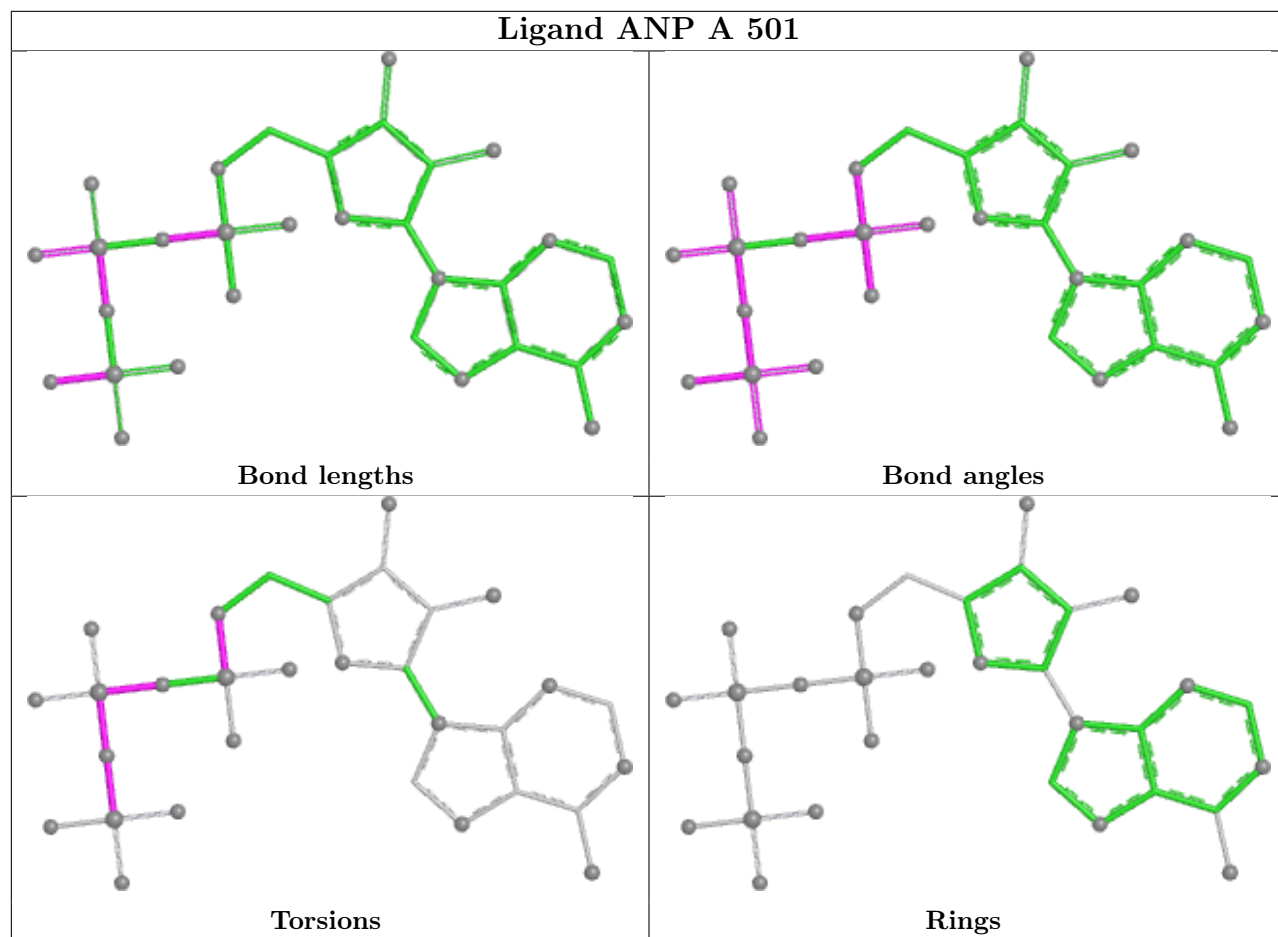
Mol	Chain	Res	Type	Atoms
3	F	101	ANP	C5'-O5'-PA-O3A
3	F	101	ANP	O4'-C4'-C5'-O5'
3	F	101	ANP	C3'-C4'-C5'-O5'
3	B	501	ANP	O4'-C4'-C5'-O5'
3	F	101	ANP	C2'-C1'-N9-C4
3	B	501	ANP	C3'-C4'-C5'-O5'
3	D	501	ANP	O4'-C4'-C5'-O5'
3	D	501	ANP	PB-O3A-PA-O5'
3	F	101	ANP	C4'-C5'-O5'-PA
3	F	101	ANP	C2'-C1'-N9-C8
3	A	501	ANP	C5'-O5'-PA-O3A
3	D	501	ANP	C3'-C4'-C5'-O5'
3	C	501	ANP	PA-O3A-PB-O2B
3	F	101	ANP	C5'-O5'-PA-O1A
3	A	501	ANP	PA-O3A-PB-O1B
3	B	501	ANP	PA-O3A-PB-O1B
3	C	501	ANP	PA-O3A-PB-O1B

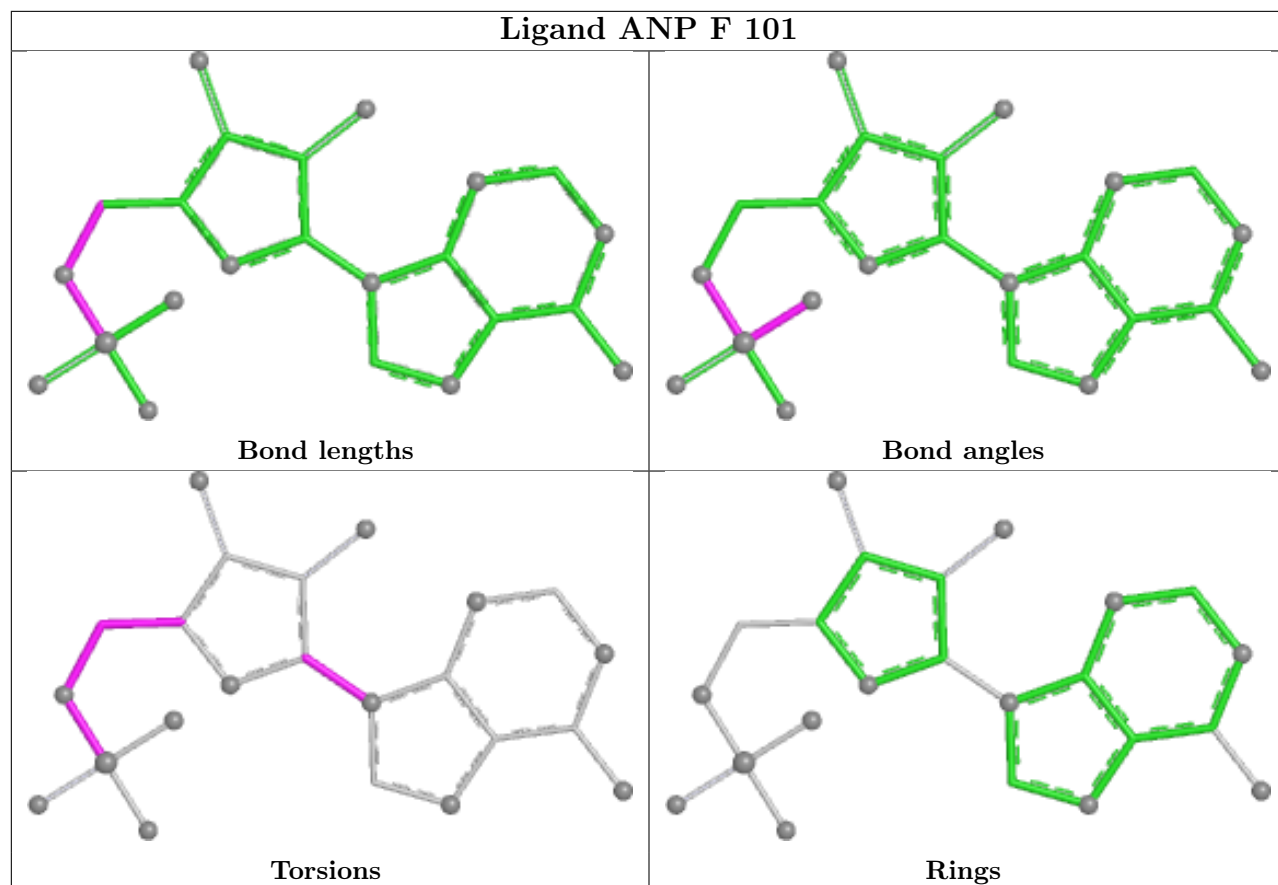
There are no ring outliers.

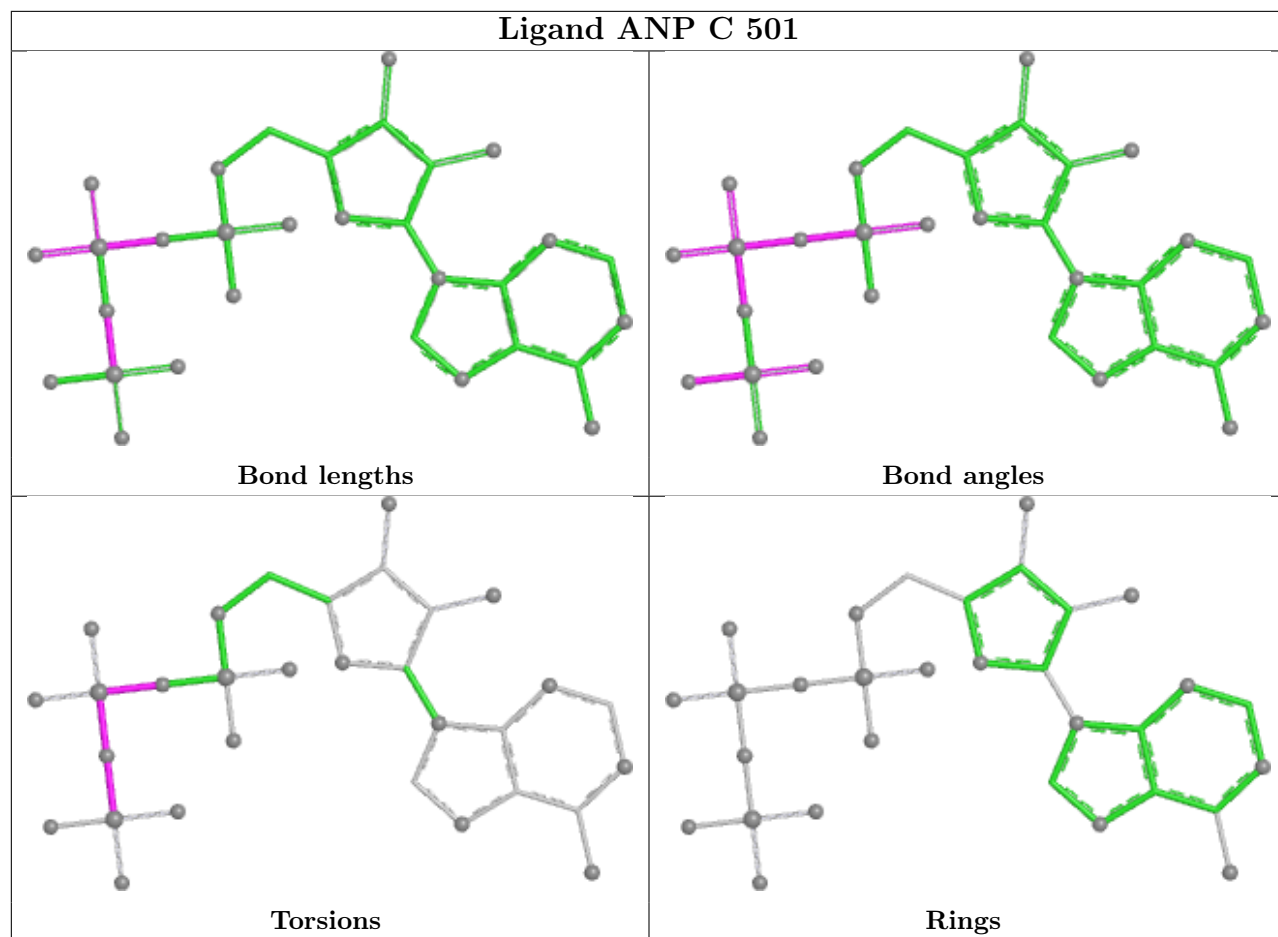
4 monomers are involved in 14 short contacts:

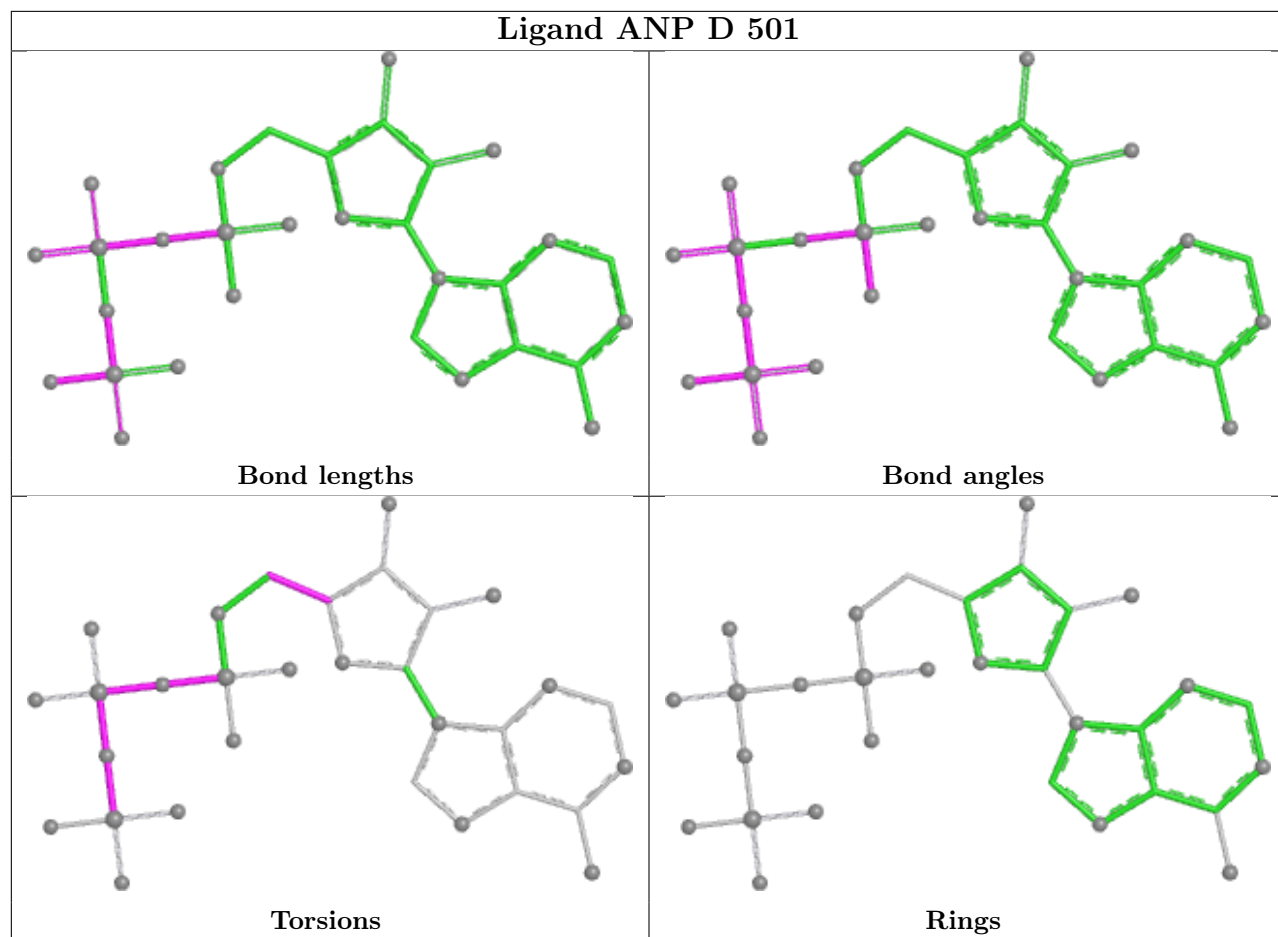
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	ANP	2	0
3	F	101	ANP	2	0
3	C	501	ANP	5	0
3	D	501	ANP	5	0

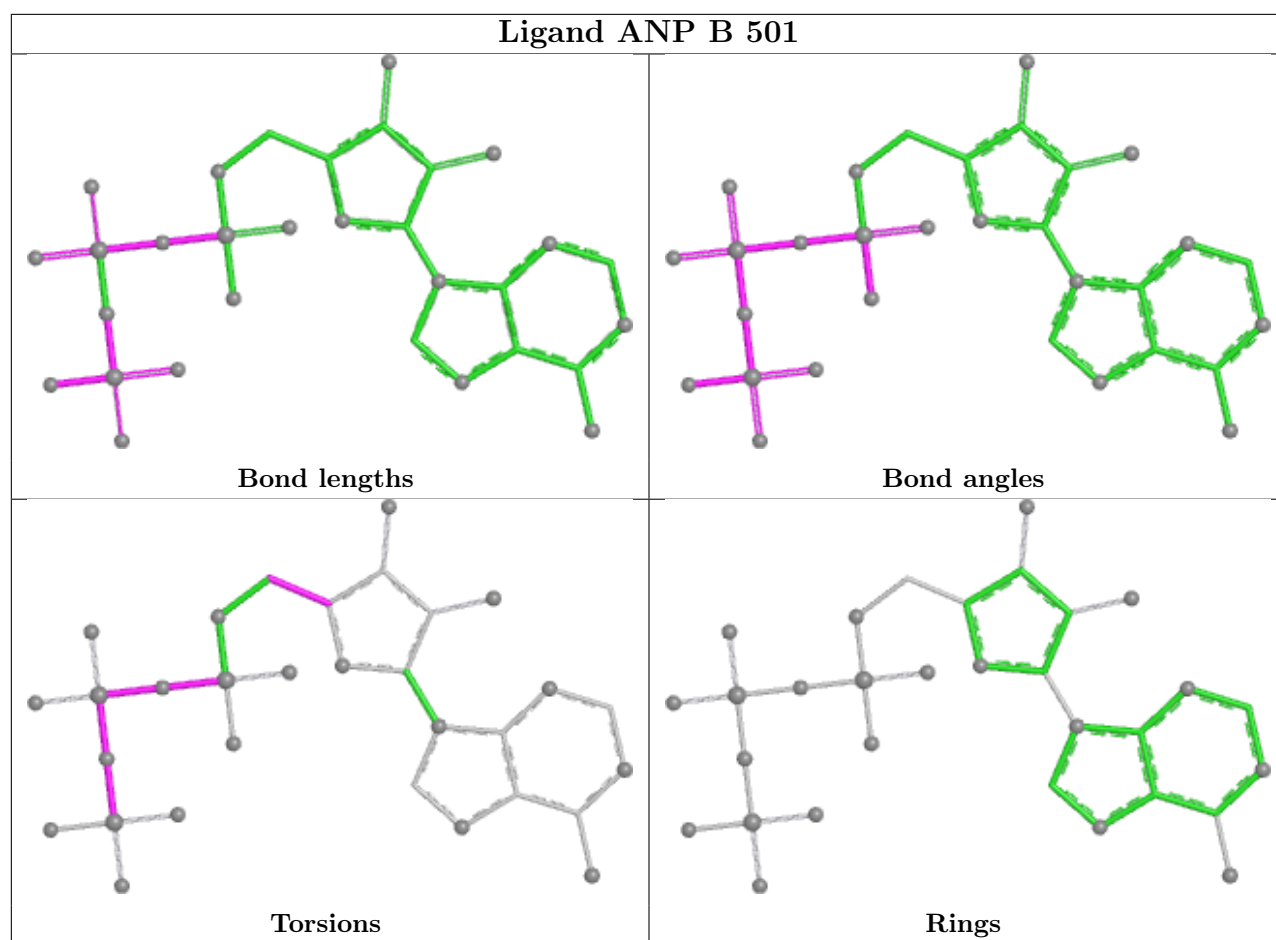
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	396/409 (96%)	-0.50	0 100 100	24, 56, 85, 116	4 (1%)
1	B	396/409 (96%)	-0.48	3 (0%) 82 78	32, 61, 102, 142	2 (0%)
1	C	394/409 (96%)	-0.30	0 100 100	33, 84, 132, 206	3 (0%)
1	D	395/409 (96%)	0.04	6 (1%) 72 65	49, 105, 156, 203	1 (0%)
2	E	14/14 (100%)	0.64	0 100 100	161, 199, 338, 344	0
2	F	14/14 (100%)	0.82	0 100 100	179, 198, 252, 256	0
All	All	1609/1664 (96%)	-0.29	9 (0%) 85 83	24, 75, 140, 344	10 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	15	ALA	3.6
1	B	238	ASP	2.8
1	D	253	ASN	2.5
1	D	111	GLY	2.3
1	D	17	GLN	2.3
1	D	16	ILE	2.2
1	B	265	ASP	2.2
1	B	237	GLU	2.2
1	D	25	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

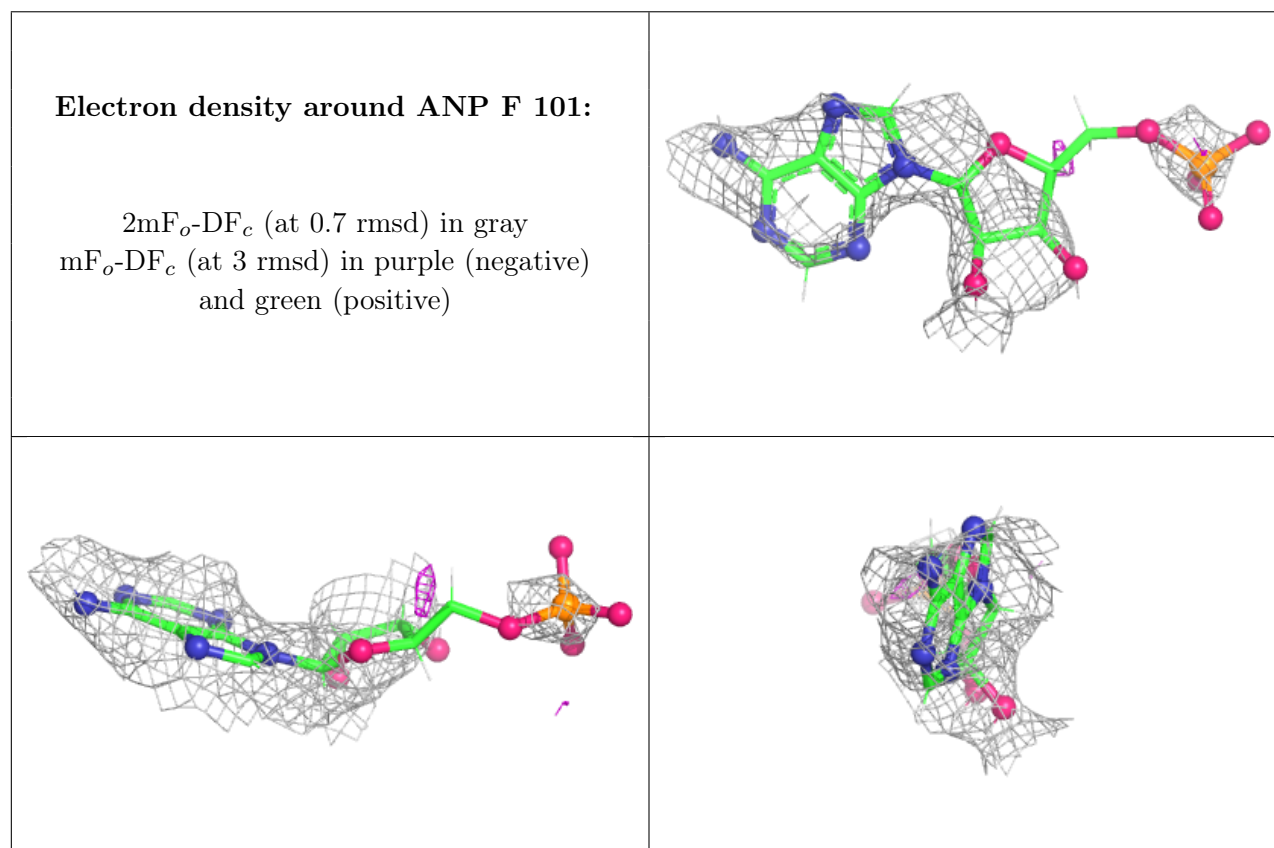
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

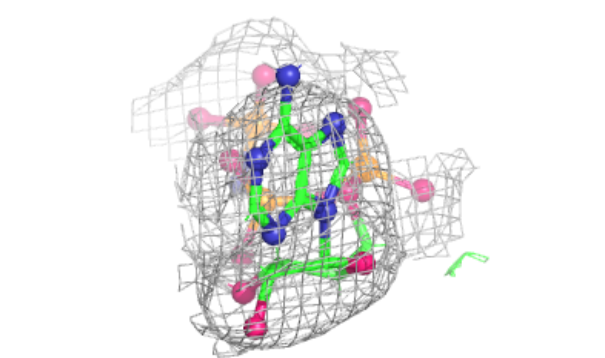
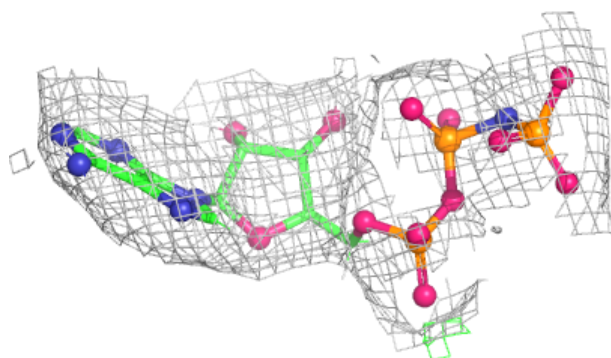
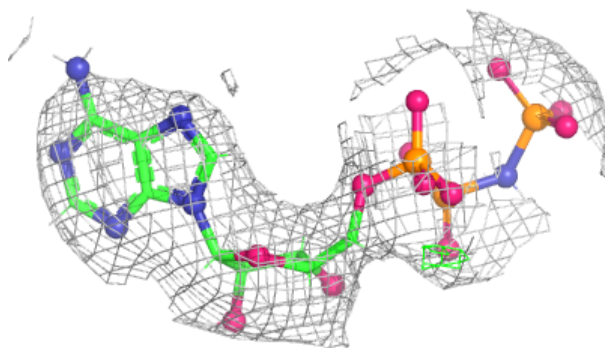
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ANP	F	101	23/31	0.66	0.12	9,200,209,211	0
4	MG	B	502	1/1	0.90	0.14	49,49,49,49	0
4	MG	A	502	1/1	0.94	0.08	36,36,36,36	0
4	MG	C	502	1/1	0.94	0.06	64,64,64,64	0
4	MG	D	502	1/1	0.96	0.10	71,71,71,71	0
3	ANP	D	501	31/31	0.97	0.06	76,92,115,128	0
3	ANP	A	501	31/31	0.98	0.05	32,42,54,63	0
3	ANP	B	501	31/31	0.98	0.05	39,50,69,95	0
3	ANP	C	501	31/31	0.98	0.05	61,78,115,128	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.

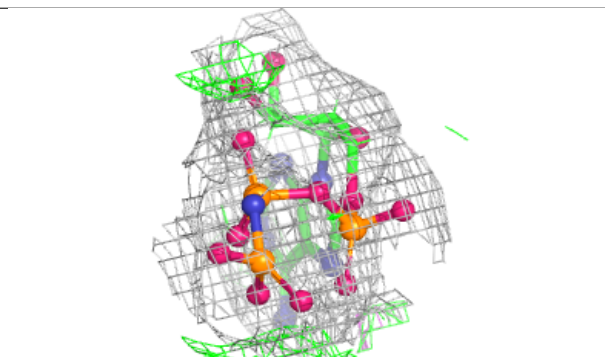
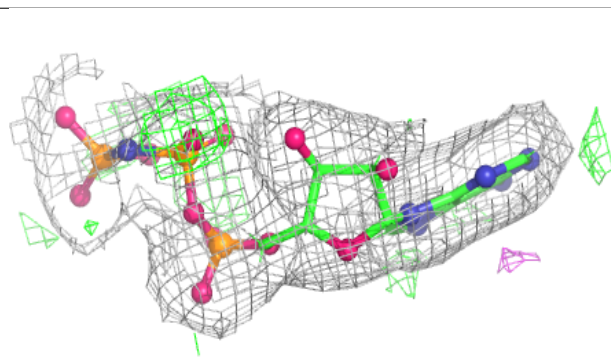
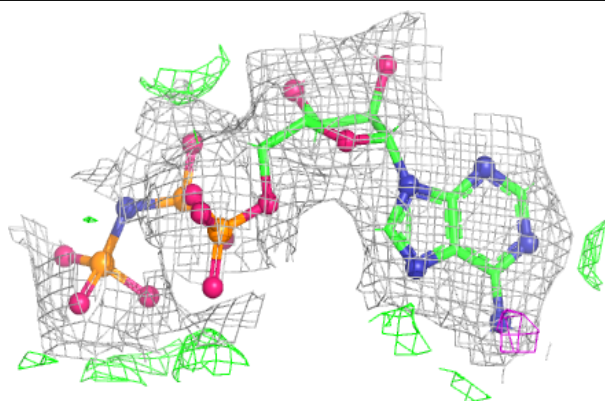


Electron density around ANP D 501:

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

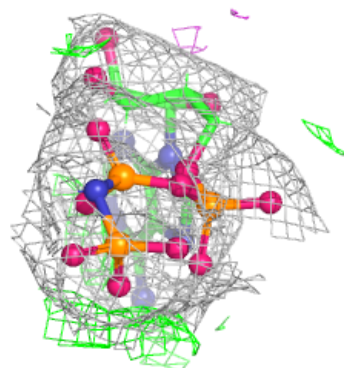
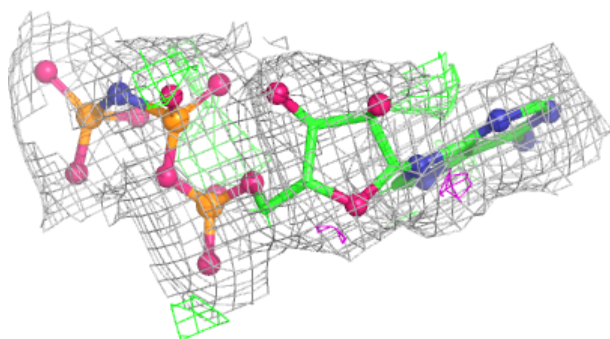
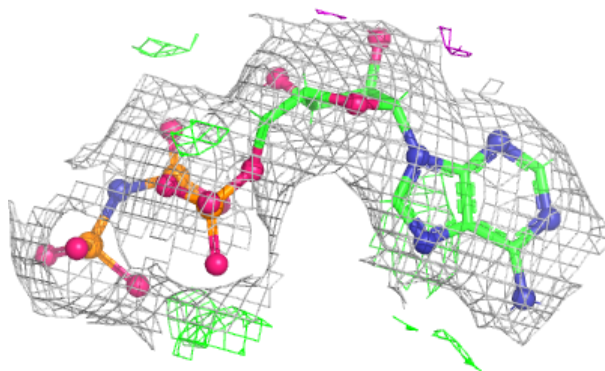
**Electron density around ANP A 501:**

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

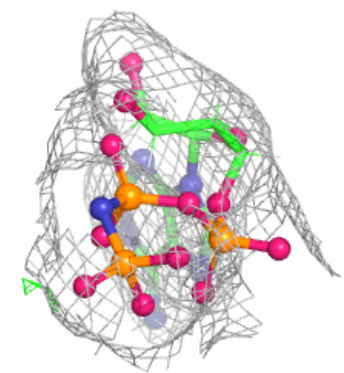
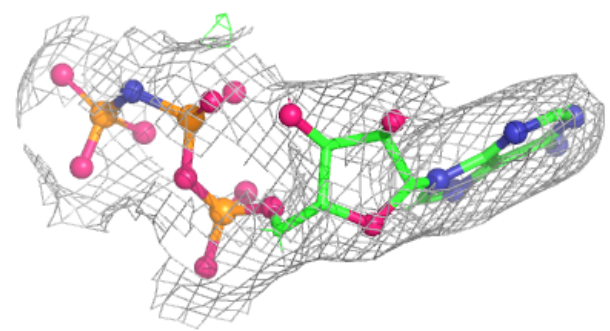
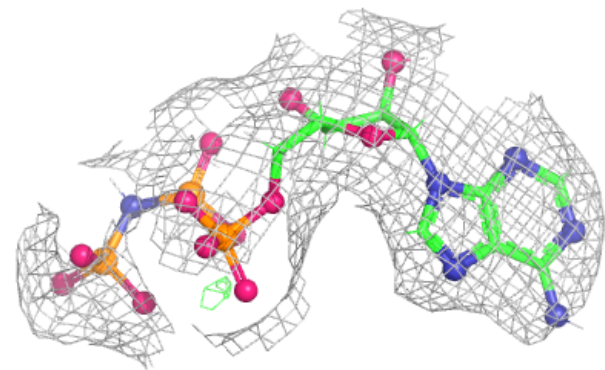


Electron density around ANP B 501:

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

**Electron density around ANP C 501:**

$2mF_o-DF_c$ (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.