Full wwPDB X-ray Structure Validation Report (i)

Jan 5, 2024 – 12:23 am GMT

PDB ID	:	5J5Q
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.; Sanderson, 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 (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:

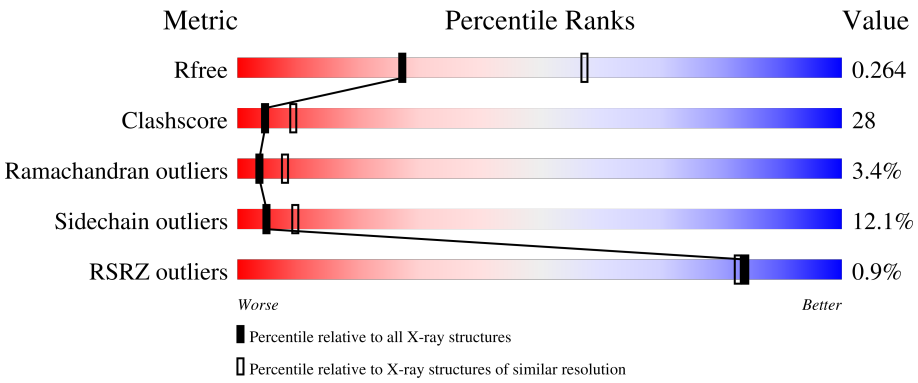
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (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 <=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	47% 39% 9% • •
1	B	409	48% 36% 10% • •
1	C	409	% 50% 38% 8% •
1	D	409	% 52% 38% 6% •

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Mol	Chain	Length	Quality of chain
2	E	14	14% 86% 14%
2	F	14	14% 7% 64% 29%

2 Entry composition (i)

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

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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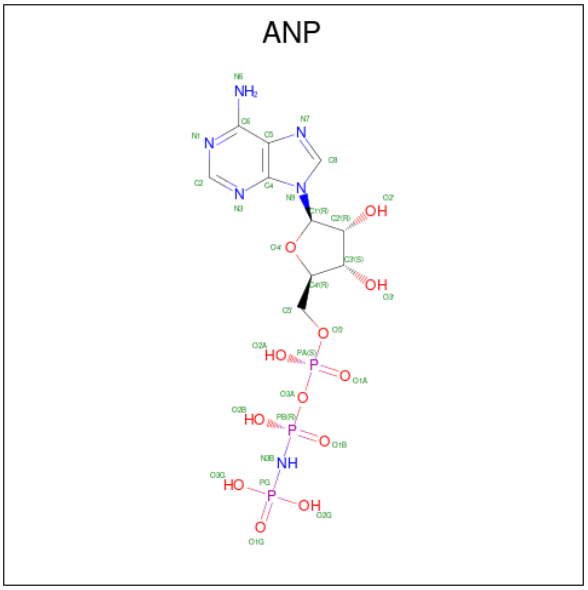
Chain	Residue	Modelled	Actual	Comment	Reference
C	406	HIS	-	expression tag	UNP Q59961
C	407	HIS	-	expression tag	UNP Q59961
C	408	HIS	-	expression tag	UNP Q59961
D	0	ALA	-	expression tag	UNP Q59961
D	217	ASP	ASN	conflict	UNP Q59961
D	403	HIS	-	expression tag	UNP Q59961
D	404	HIS	-	expression tag	UNP 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
			Total	C	N	O	P			
2	E	14	284	138	51	82	13	0	0	0
			Total	C	N	O	P			
2	F	14	284	138	51	82	13	0	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

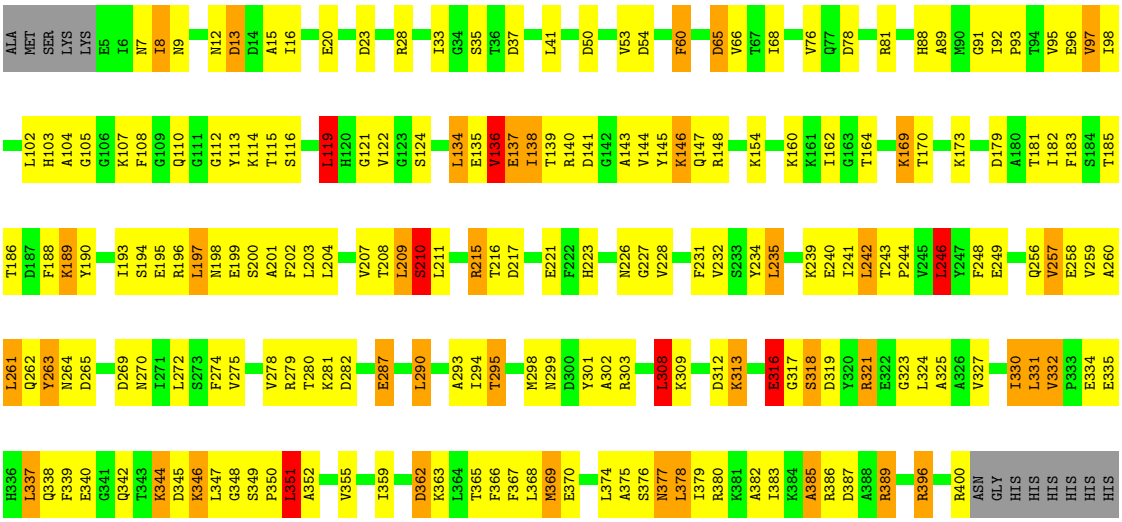
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0
4	B	1	1	1	0	0
4	C	1	1	1	0	0
4	D	1	1	1	0	0

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.

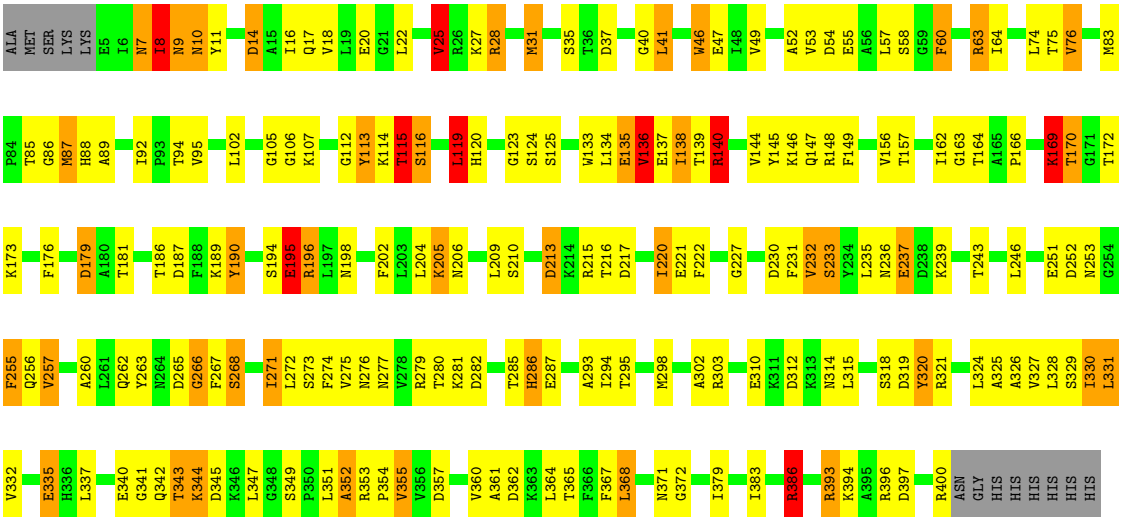
• Molecule 1: DNA topoisomerase 4 subunit B

Chain A: 47% 39% 9%



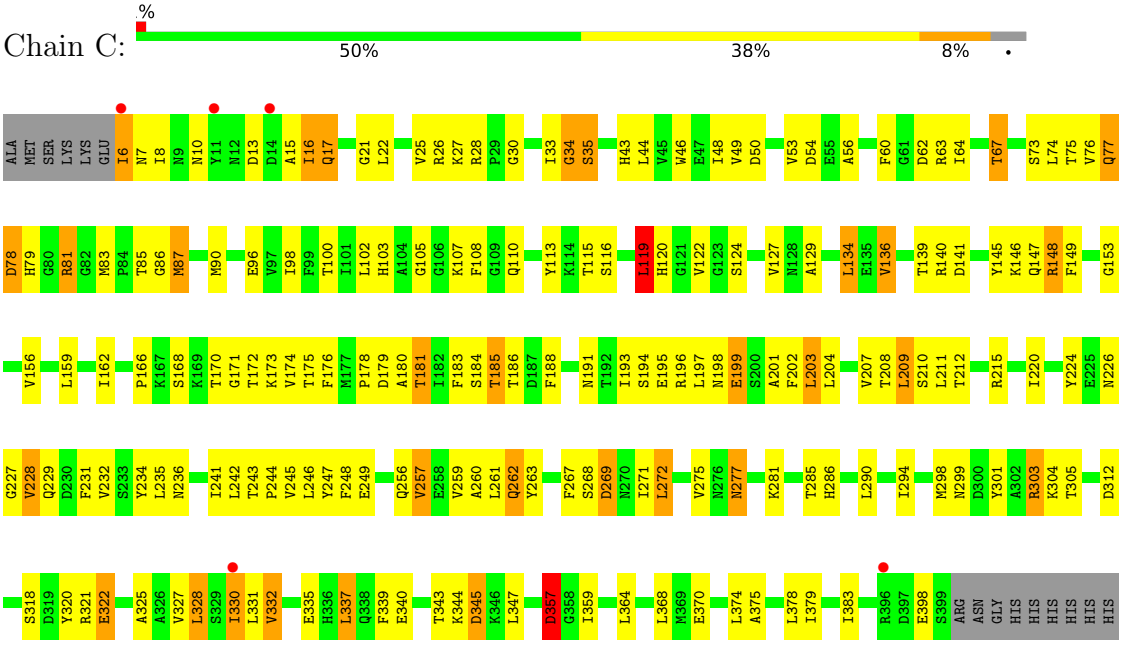
• Molecule 1: DNA topoisomerase 4 subunit B

Chain B: 48% 36% 10%



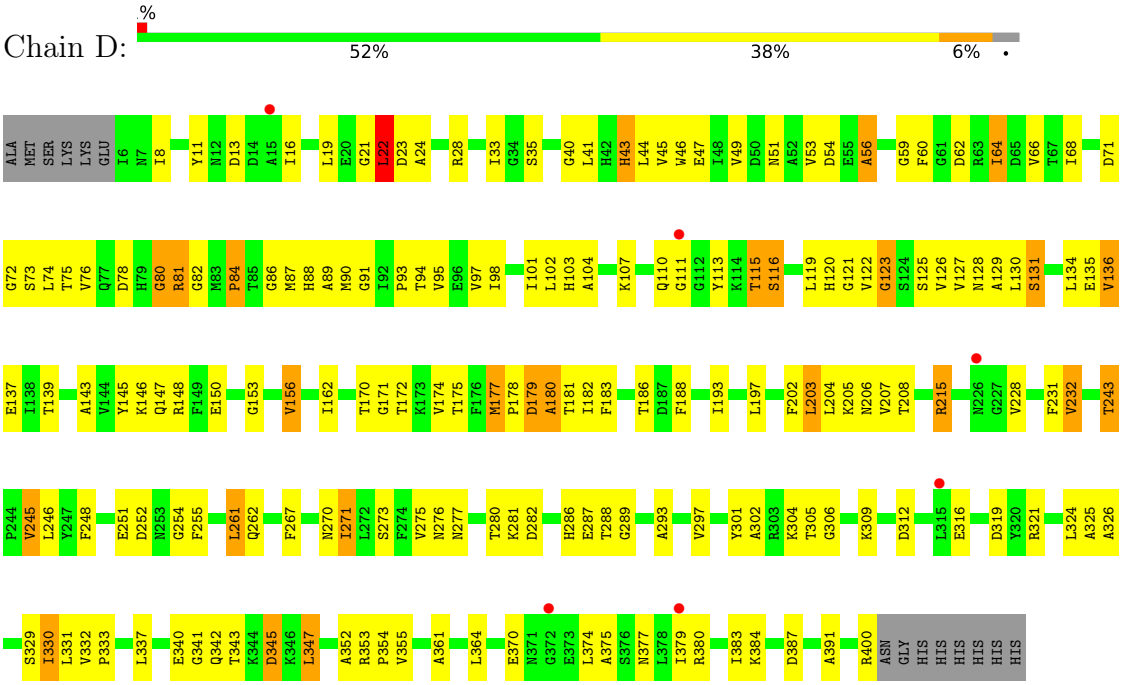
• Molecule 1: DNA topoisomerase 4 subunit B

Chain C:



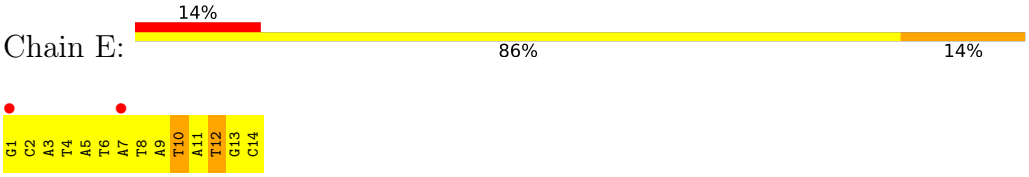
• Molecule 1: DNA topoisomerase 4 subunit B

Chain D:



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

Chain E:



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

Chain F:

4 Data and refinement statistics (i)

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 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.7 (60.76-2.83) 99.7 (60.76-2.57)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.184 , 0.263 0.184 , 0.264	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)	0.27 , 69.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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: 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	1.40	38/3078 (1.2%)	1.47	44/4168 (1.1%)
1	B	1.39	35/2986 (1.2%)	1.41	44/4056 (1.1%)
1	C	1.03	6/2907 (0.2%)	1.13	14/3959 (0.4%)
1	D	0.81	1/2692 (0.0%)	0.96	7/3690 (0.2%)
2	E	1.25	2/318 (0.6%)	1.30	2/489 (0.4%)
2	F	1.41	3/318 (0.9%)	1.16	5/489 (1.0%)
All	All	1.20	85/12299 (0.7%)	1.27	116/16851 (0.7%)

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 (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	25	VAL	CB-CG1	-10.49	1.30	1.52
2	F	3	DA	C3'-O3'	10.44	1.57	1.44
1	B	176	PHE	CE2-CZ	8.62	1.53	1.37
1	B	232	VAL	CB-CG2	-8.37	1.35	1.52
1	B	137	GLU	CD-OE2	8.19	1.34	1.25
1	A	313	LYS	CD-CE	7.78	1.70	1.51
1	A	232	VAL	CB-CG1	-7.72	1.36	1.52
1	B	137	GLU	CD-OE1	7.57	1.33	1.25
1	B	195	GLU	CD-OE1	7.33	1.33	1.25
1	A	258	GLU	CD-OE1	7.15	1.33	1.25
1	B	125	SER	CB-OG	-7.08	1.33	1.42
1	A	137	GLU	CB-CG	-7.06	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	LYS	CE-NZ	6.91	1.66	1.49
1	A	301	TYR	CB-CG	-6.90	1.41	1.51
1	B	169	LYS	CE-NZ	6.88	1.66	1.49
1	A	108	PHE	CD1-CE1	6.82	1.52	1.39
1	B	169	LYS	CD-CE	6.75	1.68	1.51
1	B	194	SER	CB-OG	6.62	1.50	1.42
1	A	226	ASN	CB-CG	-6.48	1.36	1.51
2	F	3	DA	N9-C4	6.48	1.41	1.37
1	A	316	GLU	CB-CG	-6.46	1.39	1.52
1	C	335	GLU	CD-OE1	6.45	1.32	1.25
1	B	156	VAL	CB-CG1	-6.43	1.39	1.52
1	A	355	VAL	CB-CG2	6.42	1.66	1.52
1	B	335	GLU	CD-OE1	6.41	1.32	1.25
1	A	113	TYR	CD2-CE2	-6.39	1.29	1.39
1	C	199	GLU	CD-OE2	6.37	1.32	1.25
1	B	176	PHE	CG-CD1	6.33	1.48	1.38
2	F	8	DT	C1'-N1	6.29	1.57	1.49
1	B	60	PHE	CD2-CE2	-6.25	1.26	1.39
1	A	50	ASP	CB-CG	6.21	1.64	1.51
1	A	20	GLU	CD-OE2	6.19	1.32	1.25
1	A	169	LYS	CE-NZ	6.12	1.64	1.49
1	B	274	PHE	CE1-CZ	-6.07	1.25	1.37
1	B	76	VAL	CB-CG1	-6.02	1.40	1.52
1	B	113	TYR	CD1-CE1	6.01	1.48	1.39
1	B	46	TRP	CZ3-CH2	5.94	1.49	1.40
2	E	10	DT	C3'-O3'	-5.92	1.36	1.44
1	A	340	GLU	CB-CG	-5.91	1.41	1.52
1	A	76	VAL	CB-CG1	5.91	1.65	1.52
1	D	340	GLU	CG-CD	5.89	1.60	1.51
1	B	14	ASP	CB-CG	-5.88	1.39	1.51
1	B	18	VAL	CB-CG2	5.88	1.65	1.52
1	A	263	TYR	CD1-CE1	-5.84	1.30	1.39
1	A	338	GLN	CB-CG	-5.81	1.36	1.52
1	B	190	TYR	CG-CD2	-5.80	1.31	1.39
1	B	11	TYR	CB-CG	-5.79	1.43	1.51
1	B	149	PHE	CG-CD2	5.77	1.47	1.38
1	C	330	ILE	CB-CG2	5.74	1.70	1.52
1	A	210	SER	CB-OG	5.73	1.49	1.42
1	A	318	SER	CB-OG	5.71	1.49	1.42
1	B	340	GLU	CG-CD	5.71	1.60	1.51
1	A	338	GLN	CD-OE1	5.68	1.36	1.24
1	A	344	LYS	CD-CE	5.67	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	340	GLU	CD-OE1	5.67	1.31	1.25
1	A	301	TYR	CZ-OH	5.65	1.47	1.37
1	A	334	GLU	CD-OE2	5.65	1.31	1.25
1	A	221	GLU	CB-CG	-5.64	1.41	1.52
1	A	183	PHE	CE1-CZ	5.63	1.48	1.37
1	A	257	VAL	CB-CG1	-5.63	1.41	1.52
1	C	257	VAL	CB-CG2	-5.61	1.41	1.52
1	A	107	LYS	CB-CG	-5.58	1.37	1.52
1	C	322	GLU	CD-OE2	5.48	1.31	1.25
1	A	53	VAL	CB-CG2	5.46	1.64	1.52
1	A	96	GLU	CD-OE2	5.46	1.31	1.25
1	B	170	THR	CB-CG2	-5.46	1.34	1.52
1	A	335	GLU	CD-OE1	5.43	1.31	1.25
1	B	25	VAL	CB-CG2	5.40	1.64	1.52
1	A	20	GLU	CG-CD	5.40	1.60	1.51
1	A	346	LYS	CE-NZ	5.40	1.62	1.49
1	A	60	PHE	CE1-CZ	5.37	1.47	1.37
1	A	287	GLU	CD-OE2	5.32	1.31	1.25
1	B	133	TRP	CB-CG	-5.29	1.40	1.50
1	B	320	TYR	CE1-CZ	-5.26	1.31	1.38
1	A	228	VAL	CB-CG2	-5.25	1.41	1.52
1	B	137	GLU	CG-CD	5.23	1.59	1.51
1	B	135	GLU	CD-OE2	5.18	1.31	1.25
1	A	287	GLU	CB-CG	-5.17	1.42	1.52
2	E	12	DT	C1'-N1	5.16	1.55	1.49
1	B	255	PHE	CE2-CZ	5.10	1.47	1.37
1	B	327	VAL	CB-CG2	-5.07	1.42	1.52
1	B	233	SER	CB-OG	5.07	1.48	1.42
1	C	17	GLN	CG-CD	5.06	1.62	1.51
1	B	140	ARG	CZ-NH1	5.03	1.39	1.33
1	A	195	GLU	CB-CG	5.00	1.61	1.52

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	345	ASP	CB-CG-OD1	-14.75	105.03	118.30
1	B	28	ARG	NE-CZ-NH2	-12.38	114.11	120.30
1	A	50	ASP	CB-CG-OD1	11.53	128.68	118.30
1	B	345	ASP	CB-CG-OD1	-10.92	108.47	118.30
1	B	37	ASP	CB-CG-OD1	-10.59	108.77	118.30
1	A	50	ASP	CB-CG-OD2	-10.55	108.80	118.30
1	A	345	ASP	CB-CG-OD2	10.37	127.63	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	397	ASP	CB-CG-OD2	9.83	127.14	118.30
1	A	196	ARG	NE-CZ-NH2	-9.81	115.39	120.30
1	D	81	ARG	NE-CZ-NH1	-9.55	115.52	120.30
1	A	396	ARG	NE-CZ-NH1	-9.41	115.59	120.30
1	B	28	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	B	279	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	B	282	ASP	CB-CG-OD1	9.02	126.42	118.30
1	A	246	LEU	CB-CG-CD1	-8.83	96.00	111.00
1	A	321	ARG	NE-CZ-NH1	-8.83	115.89	120.30
1	B	230	ASP	CB-CG-OD1	8.66	126.10	118.30
1	A	281	LYS	CD-CE-NZ	-8.46	92.25	111.70
1	A	196	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	D	81	ARG	NE-CZ-NH2	8.36	124.48	120.30
1	A	23	ASP	CB-CG-OD1	-8.21	110.91	118.30
1	C	50	ASP	CB-CG-OD2	-7.94	111.15	118.30
1	C	50	ASP	CB-CG-OD1	7.75	125.27	118.30
1	D	28	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	C	148	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	C	148	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	A	65	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	B	217	ASP	CB-CG-OD1	-7.49	111.56	118.30
1	A	54	ASP	CB-CG-OD2	7.47	125.03	118.30
1	B	54	ASP	CB-CG-OD1	7.47	125.02	118.30
1	A	396	ARG	NE-CZ-NH2	7.23	123.92	120.30
1	B	213	ASP	CB-CG-OD1	7.21	124.79	118.30
1	A	28	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	C	345	ASP	CB-CG-OD2	7.11	124.70	118.30
1	B	57	LEU	CA-CB-CG	7.01	131.42	115.30
1	A	78	ASP	CB-CG-OD1	6.94	124.55	118.30
1	B	362	ASP	CB-CG-OD1	-6.87	112.11	118.30
1	B	217	ASP	CB-CG-OD2	6.85	124.46	118.30
1	B	37	ASP	CB-CG-OD2	6.78	124.40	118.30
1	B	352	ALA	C-N-CA	-6.74	104.84	121.70
1	A	232	VAL	CA-CB-CG1	-6.69	100.86	110.90
1	A	203	LEU	CB-CG-CD1	-6.65	99.69	111.00
1	A	215	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	140	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	B	345	ASP	CB-CG-OD2	6.42	124.08	118.30
1	D	28	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	B	136	VAL	CG1-CB-CG2	6.31	121.00	110.90
1	B	213	ASP	CB-CG-OD2	-6.28	112.65	118.30
2	F	5	DA	O4'-C4'-C3'	-6.26	101.99	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	97	VAL	CA-CB-CG1	-6.25	101.53	110.90
1	A	389	ARG	NE-CZ-NH1	-6.25	117.18	120.30
1	A	330	ILE	CB-CG1-CD1	-6.23	96.45	113.90
1	D	347	LEU	CB-CG-CD1	-6.16	100.52	111.00
1	B	140	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	D	347	LEU	CB-CG-CD2	6.00	121.20	111.00
1	C	328	LEU	CB-CG-CD1	-5.97	100.85	111.00
1	A	134	LEU	CB-CG-CD1	5.96	121.13	111.00
1	A	197	LEU	CB-CG-CD1	-5.94	100.91	111.00
1	A	387	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	351	LEU	CA-CB-CG	-5.90	101.73	115.30
1	B	368	LEU	CA-CB-CG	-5.89	101.76	115.30
1	B	393	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	B	179	ASP	CB-CG-OD1	5.86	123.58	118.30
1	A	189	LYS	CD-CE-NZ	5.82	125.09	111.70
1	B	14	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	B	282	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	308	LEU	CA-CB-CG	5.76	128.56	115.30
1	A	308	LEU	CB-CG-CD1	5.76	120.80	111.00
1	B	63	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	154	LYS	CB-CG-CD	5.71	126.44	111.60
1	A	282	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	290	LEU	CB-CG-CD2	5.66	120.62	111.00
1	D	282	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	B	216	THR	CA-CB-CG2	-5.64	104.51	112.40
2	F	3	DA	O4'-C1'-N9	5.63	111.94	108.00
1	C	26	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	C	203	LEU	CA-CB-CG	-5.59	102.44	115.30
1	C	209	LEU	CA-CB-CG	5.55	128.08	115.30
1	B	230	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	A	246	LEU	CA-CB-CG	5.54	128.05	115.30
1	B	386	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	F	4	DT	C5-C4-O4	-5.53	121.03	124.90
1	A	272	LEU	CB-CG-CD2	-5.52	101.62	111.00
1	A	319	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	298	MET	CG-SD-CE	-5.47	91.45	100.20
1	B	281	LYS	CG-CD-CE	-5.44	95.58	111.90
1	B	279	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	B	330	ILE	CG1-CB-CG2	-5.41	99.51	111.40
1	B	87	MET	CG-SD-CE	5.39	108.82	100.20
1	B	400	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	327	VAL	CA-CB-CG1	-5.35	102.88	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	136	VAL	CG1-CB-CG2	5.34	119.44	110.90
1	C	364	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	B	362	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	148	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	E	10	DT	N3-C4-O4	5.30	123.08	119.90
1	C	81	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	312	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	A	134	LEU	CB-CG-CD2	-5.20	102.17	111.00
1	A	355	VAL	C-N-CA	-5.19	108.72	121.70
1	A	122	VAL	CG1-CB-CG2	5.17	119.17	110.90
1	B	102	LEU	CB-CG-CD2	-5.17	102.22	111.00
1	A	351	LEU	C-N-CA	-5.16	108.81	121.70
1	C	272	LEU	CB-CG-CD1	5.16	119.77	111.00
2	F	4	DT	N3-C4-O4	5.15	122.99	119.90
1	B	187	ASP	CB-CG-OD2	5.14	122.93	118.30
2	E	10	DT	C5-C4-O4	-5.12	121.32	124.90
1	C	345	ASP	CB-CG-OD1	-5.12	113.70	118.30
2	F	8	DT	N3-C4-O4	5.11	122.96	119.90
1	B	8	ILE	CG1-CB-CG2	-5.10	100.17	111.40
1	B	41	LEU	CB-CG-CD2	5.08	119.64	111.00
1	A	309	LYS	CD-CE-NZ	5.06	123.34	111.70
1	B	272	LEU	CB-CG-CD2	-5.05	102.42	111.00
1	C	357	ASP	CB-CG-OD1	-5.03	113.77	118.30
1	B	115	THR	CA-CB-CG2	-5.01	105.38	112.40
1	B	14	ASP	N-CA-CB	-5.00	101.60	110.60

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 (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	3016	0	2919	142	0
1	B	2930	0	2759	144	0
1	C	2847	0	2625	166	0
1	D	2643	0	2225	170	0
2	E	284	0	161	34	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	4	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	653	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 28.

All (653) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:179:ASP:OD1	1:D:181:THR:OG1	2.03	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:D:73:SER:HB3	1:D:177:MET:HE3	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:341:GLY:C	1:D:343:THR:H	1.91	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:83:MET:HE1	1:C:98:ILE:HG21	1.71	0.72
2:E:3:DA:H2"	2:E:4:DT:H71	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:A:134:LEU:HD23	1:A:134:LEU:C	2.11	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
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:A:256[A]:GLN:CD	1:A:331:LEU:HD22	2.12	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:179:ASP:CG	1:A:181:THR:HG22	2.14	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:72:GLY:C	1:D:177:MET:HE1	2.17	0.65
1:B:220:ILE:HG12	1:B:221:GLU:H	1.62	0.65
1:C:148:ARG:O	1:C:156:VAL:HG22	1.97	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
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:134:LEU:HD23	1:C:134:LEU:C	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ASP:C	1:A:362:ASP:OD1	2.37	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:C:83:MET:HE2	1:C:98:ILE:HG21	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: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
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:C:271:ILE:C	1:C:272:LEU:HD23	2.21	0.60
1:A:146:LYS:HG3	1:A:147:GLN:N	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:D:352:ALA:O	1:D:355:VAL:N	2.35	0.58
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: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: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:C:184:SER:C	1:C:185:THR:HG22	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:83:MET:HE1	1:C:98:ILE:CG2	2.37	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:204:LEU:C	1:B:206:ASN:H	2.11	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:D:271:ILE:C	1:D:271:ILE:HD13	2.29	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:C:290:LEU:HD22	1:C:328:LEU:HD13	1.91	0.52
1:B:190:TYR:CD1	1:B:190:TYR:C	2.82	0.52
1:C:243:THR:OG1	1:C:374:LEU:HD21	2.09	0.52
1:D:89:ALA:C	1:D:91:GLY:H	2.12	0.52
1:D:341:GLY:C	1:D:343:THR:N	2.56	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: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:B:364:LEU:O	1:B:365:THR:C	2.47	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:134:LEU:C	1:B:134:LEU:HD23	2.31	0.51
1:D:204:LEU:C	1:D:206:ASN:H	2.14	0.50
1:A:137:GLU:C	1:A:138:ILE:HD13	2.31	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:C:197:LEU:HD22	1:C:209:LEU:HD23	1.93	0.50
1:D:73:SER:CB	1:D:177:MET:HE3	2.39	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: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:146:LYS:C	1:C:159:LEU:HD12	2.31	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:35:SER:OG	1:A:37:ASP:OD1	2.30	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
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: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:C:81:ARG:NH1	1:C:113:TYR:CE2	2.80	0.49
1:D:150:GLU:CD	1:D:156:VAL:HG11	2.32	0.49
1:C:243:THR:HG22	1:C:263:TYR:H	1.76	0.49
1:C:245:VAL:C	1:C:246:LEU:HD23	2.32	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: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:D:45:VAL:CG2	1:D:74:LEU:HD13	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:102:LEU:O	1:A:103:HIS:HB2	2.13	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: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:D:41:LEU:HD11	1:D:178:PRO:HG2	1.95	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: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:B:119:LEU:HD21	1:B:120:HIS:NE2	2.29	0.48
1:C:368:LEU:C	1:C:370:GLU:H	2.17	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:C:259:VAL:HG22	1:C:260:ALA:N	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:PHE:CD1	1:A:279:ARG:HA	2.49	0.47
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:21:GLY:O	1:D:22:LEU:C	2.51	0.47
1:D:130:LEU:O	1:D:179:ASP:HB2	2.15	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:B:341:GLY:O	1:B:342:GLN:C	2.51	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:72:GLY:O	1:D:177:MET:HE1	2.15	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:B:237:GLU:C	1:B:239:LYS:H	2.16	0.46
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:D:206:ASN:C	1:D:207:VAL:HG23	2.35	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:B:393:ARG:O	1:B:394:LYS:C	2.54	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:204:LEU:C	1:B:206:ASN:N	2.69	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: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:B:357:ASP:OD2	1:B:357:ASP:C	2.55	0.45
1:D:304:LYS:C	1:D:306:GLY:H	2.20	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:B:332:VAL:CG2	1:B:332:VAL:O	2.64	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:172:THR:CG2	1:C:173:LYS:N	2.79	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:D:21:GLY:C	1:D:23:ASP:N	2.69	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:VAL:O	1:B:233:SER:C	2.55	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: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:252:ASP:C	1:D:254:GLY:N	2.70	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: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:C:140:ARG:O	1:C:141:ASP:C	2.55	0.44
1:D:301:TYR:CE1	1:D:375:ALA:HB1	2.52	0.44
1:D:383:ILE:HG13	1:D:384:LYS:N	2.32	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:93:PRO:O	1:D:94:THR:C	2.56	0.44
1:D:179:ASP:C	1:D:181:THR:H	2.21	0.44
1:D:271:ILE:HD13	1:D:271:ILE:O	2.18	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:C:303:ARG:O	1:C:304:LYS:C	2.56	0.44
1:D:273:SER:HB3	1:D:287[B]:GLU:CG	2.47	0.44
1:B:294:ILE:O	1:B:295:THR:C	2.55	0.44
1:C:184:SER:C	1:C:185:THR:CG2	2.86	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
1:C:75:THR:HA	1:C:174:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ASN:O	1:D:207:VAL:HG23	2.17	0.44
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:D:122:VAL:O	1:D:123:GLY:C	2.55	0.43
1:A:295:THR:OG1	1:A:317:GLY:HA2	2.17	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:87:MET:HE3	1:C:87:MET:HB2	1.71	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:B:74:LEU:C	1:B:74:LEU:HD23	2.39	0.43
1:C:172:THR:HG22	1:C:173:LYS:N	2.31	0.43
1:C:259:VAL:CG2	1:C:260:ALA:N	2.82	0.43
1:D:352:ALA:O	1:D:353:ARG:C	2.57	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:D:21:GLY:CA	1:D:102:LEU:HD12	2.49	0.42
1:D:134:LEU:C	1:D:134:LEU:HD23	2.39	0.42
1:A:92:ILE:O	1:A:93:PRO:C	2.57	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:C:64:ILE:O	1:C:209:LEU:HA	2.19	0.42
1:C:201:ALA:O	1:C:202:PHE:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:ARG:HA	1:D:383:ILE:HG12	2.02	0.42
1:A:242:LEU:O	1:A:243:THR:HB	2.19	0.42
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: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:C:368:LEU:C	1:C:370:GLU:N	2.73	0.42
1:D:33:ILE:O	1:D:35:SER:N	2.51	0.42
1:D:73:SER:CA	1:D:177:MET:HE3	2.50	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:204:LEU:CD2	1:C:277:ASN:OD1	2.67	0.42
1:D:374:LEU:O	1:D:375:ALA:C	2.58	0.42
1:A:201:ALA:O	1:A:202:PHE:C	2.55	0.41
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:B:298:MET:HB3	1:B:298:MET:HE3	1.90	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
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:B:87:MET:HE2	1:B:87:MET:HA	2.01	0.41
1:C:229:GLN:NE2	1:C:247:TYR:HB2	2.36	0.41
1:C:343:THR:O	1:C:344:LYS:C	2.59	0.41
1:D:46:TRP:HA	1:D:46:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:198:ASN:ND2	1:C:234:TYR:CZ	2.88	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:B:107:LYS:HD3	1:B:116:SER:OG	2.20	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
1:A:68:ILE:HG21	1:A:215:ARG:CZ	2.50	0.41
1:C:256:GLN:HB3	1:C:331:LEU:HB2	2.02	0.41
1:C:301:TYR:CE1	1:C:375:ALA:CB	3.02	0.41
1:D:72:GLY:C	1:D:177:MET:CE	2.88	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:A:275:VAL:O	1:A:278:VAL:HB	2.21	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: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
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:B:360:VAL:O	1:B:361:ALA:C	2.58	0.40
1:C:30:GLY:O	1:C:34:GLY:HA2	2.21	0.40
1:C:78:ASP:OD1	1:C:78:ASP:C	2.59	0.40
1:D:72:GLY:O	1:D:177:MET:CE	2.69	0.40
1:D:288:THR:O	1:D:289:GLY:C	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ILE:HG21	1:A:262:GLN:CD	2.41	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:A:368:LEU:C	1:A:370:GLU:H	2.25	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:B:204:LEU:O	1:B:205:LYS:C	2.60	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:A:293:ALA:O	1:A:294:ILE:C	2.60	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: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%)	8 19
1	B	396/409 (97%)	341 (86%)	37 (9%)	18 (4%)	2 4
1	C	395/409 (97%)	348 (88%)	38 (10%)	9 (2%)	6 13
1	D	394/409 (96%)	315 (80%)	60 (15%)	19 (5%)	2 4
All	All	1583/1636 (97%)	1358 (86%)	172 (11%)	53 (3%)	3 8

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
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

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Mol	Chain	Res	Type
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 (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	314/340 (92%)	275 (88%)	39 (12%)	4 9
1	B	292/340 (86%)	258 (88%)	34 (12%)	5 11
1	C	270/340 (79%)	232 (86%)	38 (14%)	3 6
1	D	208/340 (61%)	189 (91%)	19 (9%)	9 19
All	All	1084/1360 (80%)	954 (88%)	130 (12%)	5 10

All (130) residues with a non-rotameric sidechain are listed below:

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

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Mol	Chain	Res	Type
1	A	164	THR
1	A	185	THR
1	A	189	LYS
1	A	200	SER
1	A	209	LEU
1	A	210	SER
1	A	231	PHE
1	A	234	TYR
1	A	235	LEU
1	A	242	LEU
1	A	246	LEU
1	A	249	GLU
1	A	261	LEU
1	A	280	THR
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	337	LEU
1	A	346	LYS
1	A	362	ASP
1	A	369	MET
1	A	377	ASN
1	A	378	LEU
1	B	8	ILE
1	B	25	VAL
1	B	31	MET
1	B	63	ARG
1	B	92	ILE
1	B	95	VAL
1	B	115	THR
1	B	116	SER
1	B	119	LEU
1	B	124	SER
1	B	136	VAL
1	B	138	ILE
1	B	140	ARG
1	B	164	THR

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Mol	Chain	Res	Type
1	B	169	LYS
1	B	172	THR
1	B	173	LYS
1	B	189	LYS
1	B	195	GLU
1	B	196	ARG
1	B	210	SER
1	B	220	ILE
1	B	231	PHE
1	B	256	GLN
1	B	257	VAL
1	B	268	SER
1	B	271	ILE
1	B	286	HIS
1	B	318	SER
1	B	331	LEU
1	B	335	GLU
1	B	353	ARG
1	B	371	ASN
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	119	LEU
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	231	PHE
1	C	249	GLU

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Mol	Chain	Res	Type
1	C	261	LEU
1	C	262	GLN
1	C	268	SER
1	C	269	ASP
1	C	277	ASN
1	C	281	LYS
1	C	285	THR
1	C	286	HIS
1	C	303	ARG
1	C	312	ASP
1	C	318	SER
1	C	332	VAL
1	C	337	LEU
1	C	357	ASP
1	C	378	LEU
1	C	383	ILE
1	D	8	ILE
1	D	22	LEU
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	172	THR
1	D	177	MET
1	D	203	LEU
1	D	215	ARG
1	D	232	VAL
1	D	261	LEU
1	D	267	PHE
1	D	271	ILE
1	D	330	ILE
1	D	345	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	256	GLN
1	D	120	HIS

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)

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	D	501	4	29,33,33	2.43	6 (20%)	31,52,52	3.10	7 (22%)
3	ANP	B	501	4	29,33,33	2.69	7 (24%)	31,52,52	2.42	9 (29%)
3	ANP	C	501	4	29,33,33	2.42	5 (17%)	31,52,52	2.06	6 (19%)
3	ANP	A	501	4	29,33,33	1.64	3 (10%)	31,52,52	3.19	8 (25%)
3	ANP	F	101	-	22,25,33	0.99	2 (9%)	25,38,52	1.44	4 (16%)

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	D	501	4	-	7/14/38/38	0/3/3/3
3	ANP	B	501	4	-	8/14/38/38	0/3/3/3
3	ANP	C	501	4	-	4/14/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	501	4	-	5/14/38/38	0/3/3/3
3	ANP	F	101	-	-	6/6/26/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	ANP	PB-O1B	11.07	1.63	1.46
3	D	501	ANP	PB-O1B	8.88	1.60	1.46
3	B	501	ANP	PB-O1B	8.08	1.59	1.46
3	B	501	ANP	PB-O2B	-7.29	1.37	1.56
3	D	501	ANP	PG-O1G	6.58	1.56	1.46
3	B	501	ANP	PB-O3A	-6.35	1.51	1.59
3	A	501	ANP	PB-O1B	5.39	1.54	1.46
3	B	501	ANP	PG-O1G	4.43	1.53	1.46
3	A	501	ANP	PG-O1G	4.17	1.52	1.46
3	D	501	ANP	PG-N3B	3.64	1.72	1.63
3	C	501	ANP	PB-O3A	-3.61	1.54	1.59
3	C	501	ANP	PB-O2B	-3.49	1.47	1.56
3	D	501	ANP	PB-O3A	-3.31	1.54	1.59
3	D	501	ANP	PB-O2B	-3.02	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	2.34	1.63	1.56
3	B	501	ANP	PG-O2G	2.20	1.62	1.56
3	C	501	ANP	C8-N7	-2.14	1.30	1.34
3	F	101	ANP	O5'-C5'	2.07	1.52	1.44
3	F	101	ANP	PA-O5'	2.06	1.66	1.60
3	A	501	ANP	PB-N3B	2.05	1.68	1.63
3	D	501	ANP	PG-O2G	-2.04	1.51	1.56

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	-8.33	92.51	113.45
3	D	501	ANP	O1B-PB-N3B	-8.29	99.56	111.77
3	B	501	ANP	O3G-PG-O1G	-6.48	97.15	113.45
3	A	501	ANP	O2G-PG-O3G	-6.45	90.47	107.64
3	A	501	ANP	O3G-PG-O1G	6.26	129.18	113.45
3	B	501	ANP	O2B-PB-O3A	5.50	122.99	104.64
3	A	501	ANP	O1B-PB-N3B	-4.81	104.68	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	ANP	PB-O3A-PA	-4.67	116.18	132.62
3	D	501	ANP	O2G-PG-O1G	4.36	124.41	113.45
3	A	501	ANP	O2B-PB-O1B	4.28	118.89	109.92
3	B	501	ANP	O2B-PB-O1B	-4.26	100.99	109.92
3	B	501	ANP	O1G-PG-N3B	4.23	118.00	111.77
3	F	101	ANP	PA-O5'-C5'	4.16	129.76	118.30
3	C	501	ANP	O2B-PB-O1B	-3.96	101.61	109.92
3	A	501	ANP	O2A-PA-O5'	3.82	125.48	107.75
3	A	501	ANP	O2G-PG-O1G	-3.64	104.29	113.45
3	D	501	ANP	O2B-PB-O1B	3.49	117.23	109.92
3	B	501	ANP	O2G-PG-O1G	3.22	121.54	113.45
3	F	101	ANP	O2A-PA-O5'	3.12	115.02	106.73
3	B	501	ANP	O2G-PG-O3G	3.04	115.72	107.64
3	D	501	ANP	C5-C6-N6	2.94	124.83	120.35
3	C	501	ANP	O2B-PB-O3A	2.92	114.40	104.64
3	B	501	ANP	C5-C6-N6	2.83	124.66	120.35
3	C	501	ANP	PB-O3A-PA	-2.65	123.28	132.62
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	C	501	ANP	C5-C6-N6	2.46	124.10	120.35
3	F	101	ANP	C3'-C2'-C1'	2.45	104.67	100.98
3	F	101	ANP	C5-C6-N6	2.24	123.76	120.35
3	D	501	ANP	C1'-N9-C4	-2.03	123.08	126.64
3	A	501	ANP	O5'-PA-O1A	-2.02	101.19	109.07
3	C	501	ANP	O1B-PB-N3B	-2.02	108.80	111.77

There are no chirality outliers.

All (30) 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-O1B
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	C	501	ANP	PA-O3A-PB-O1B
3	D	501	ANP	PB-N3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
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
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	B	501	ANP	C3'-C4'-C5'-O5'
3	D	501	ANP	O4'-C4'-C5'-O5'
3	F	101	ANP	C4'-C5'-O5'-PA
3	D	501	ANP	PB-O3A-PA-O5'
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	B	501	ANP	C5'-O5'-PA-O3A
3	B	501	ANP	C5'-O5'-PA-O2A

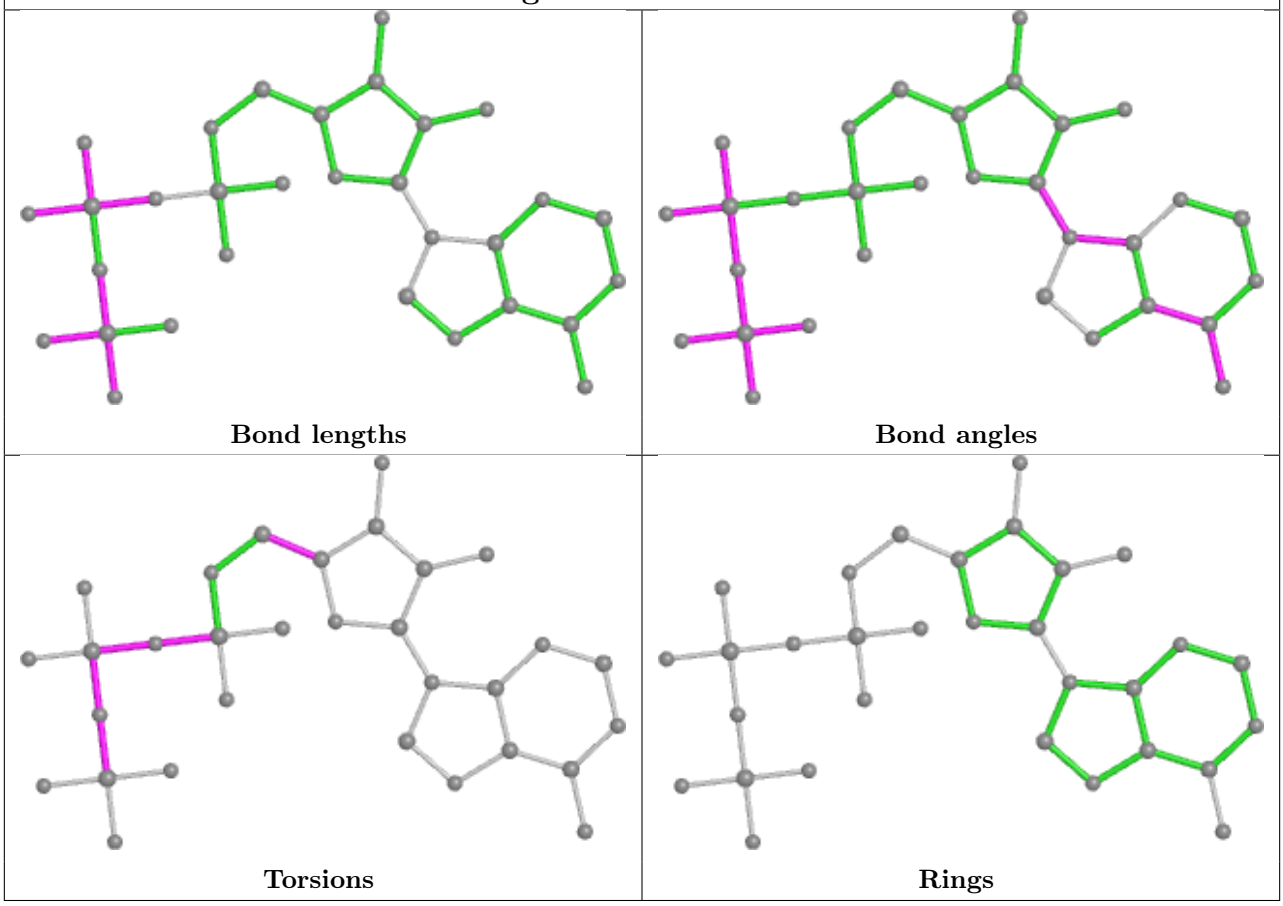
There are no ring outliers.

4 monomers are involved in 13 short contacts:

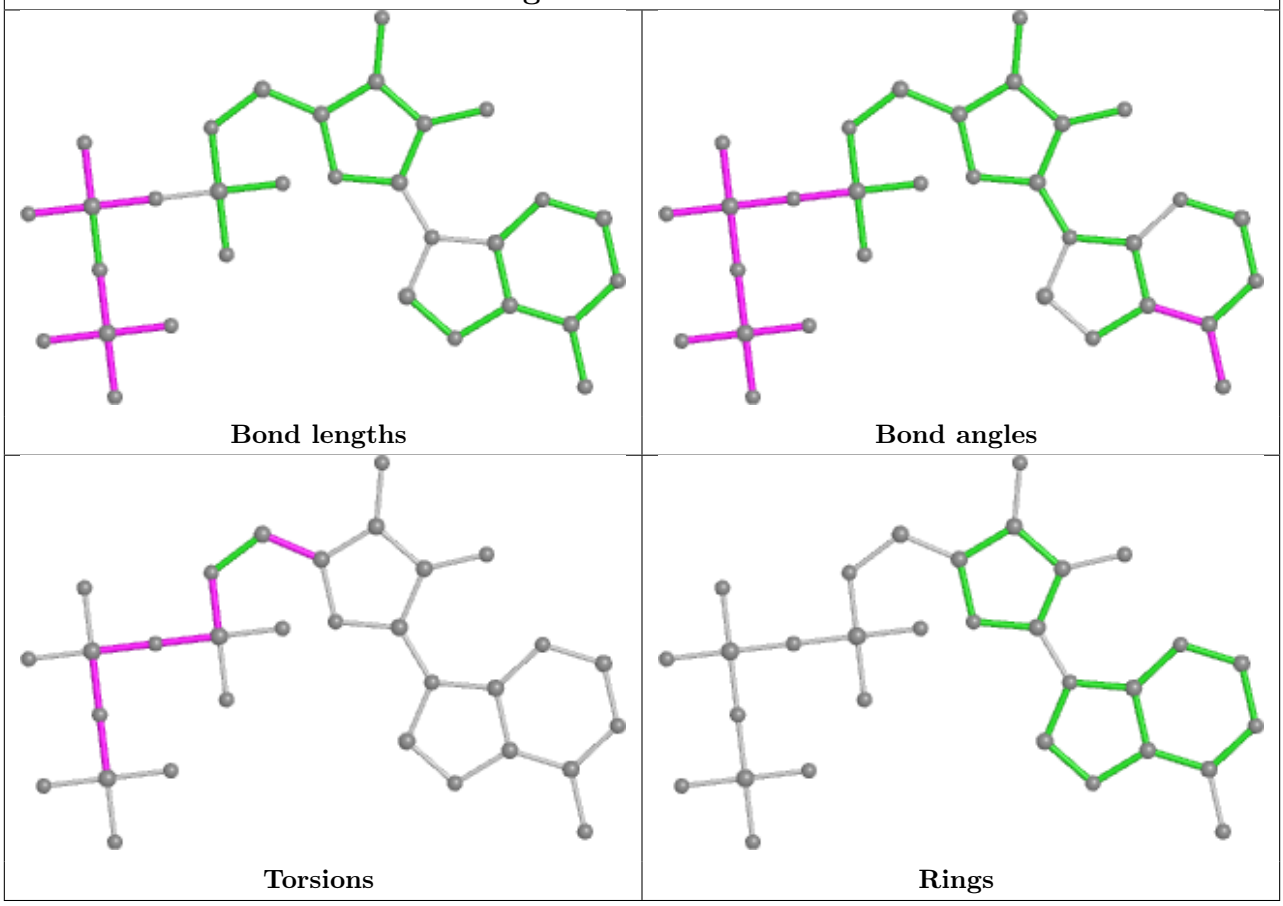
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	ANP	5	0
3	C	501	ANP	4	0
3	A	501	ANP	2	0
3	F	101	ANP	2	0

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.

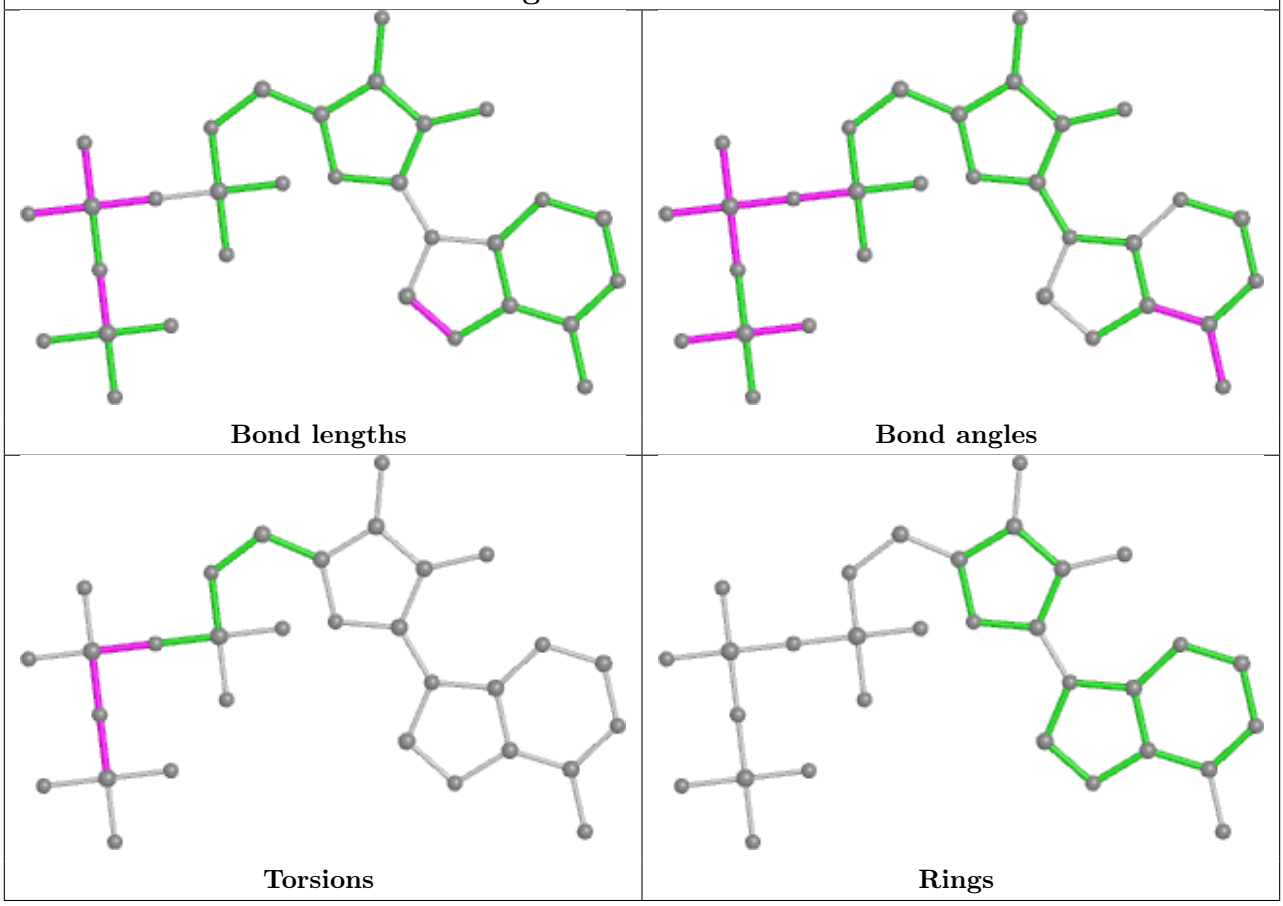
Ligand ANP D 501



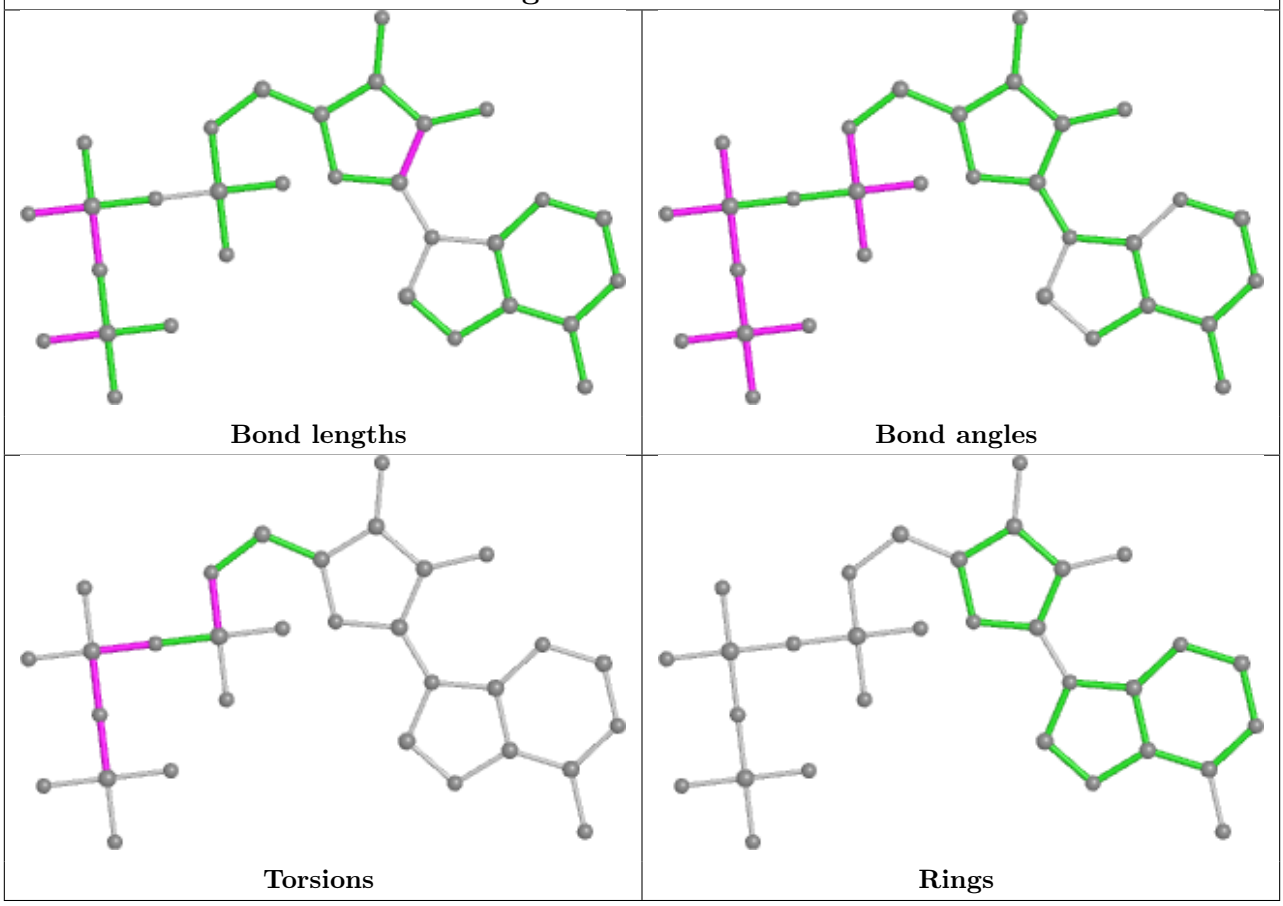
Ligand ANP B 501



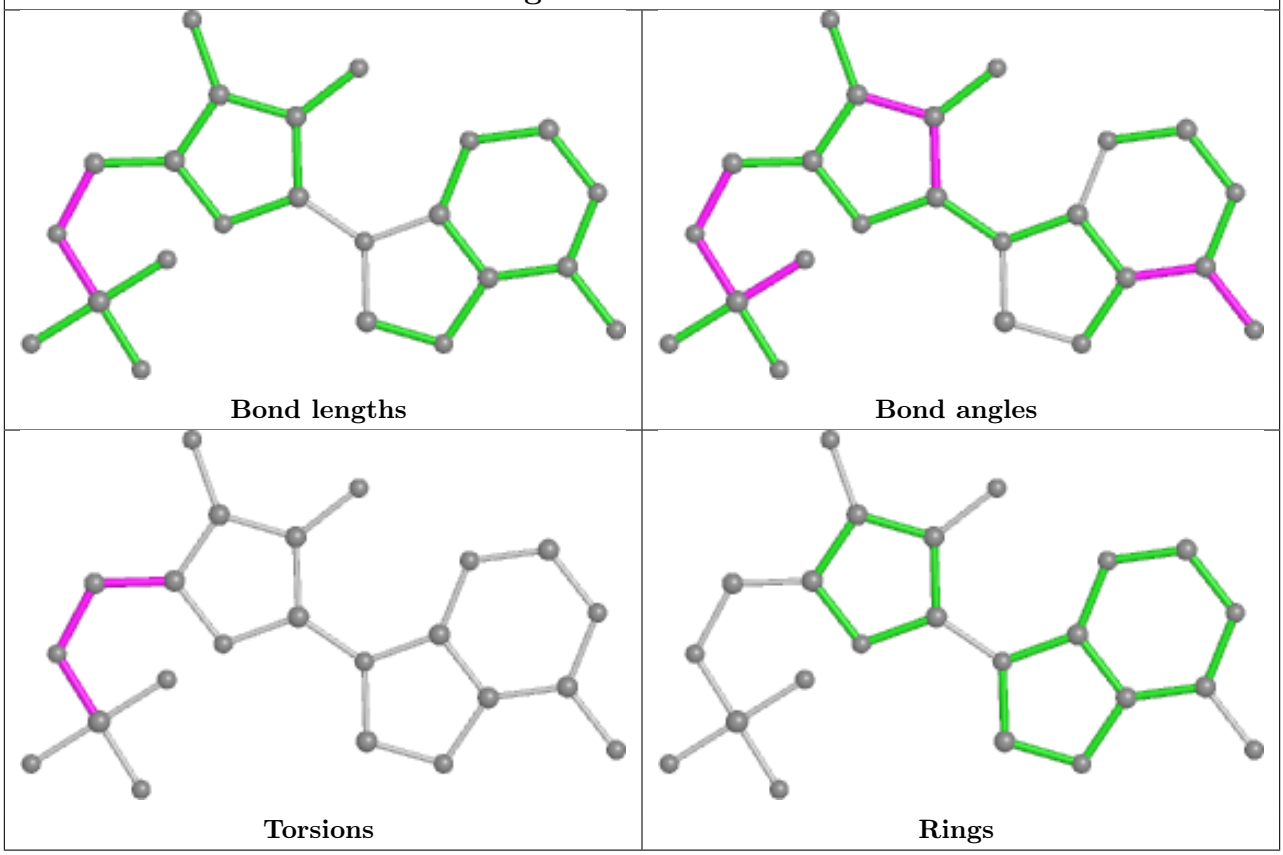
Ligand ANP C 501



Ligand ANP A 501



Ligand ANP F 101



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%)	-0.48	0	100	100	32, 56, 85, 116	0
1	B	396/409 (96%)	-0.61	0	100	100	32, 61, 102, 142	0
1	C	394/409 (96%)	-0.47	5 (1%)	77	74	47, 85, 132, 206	0
1	D	395/409 (96%)	-0.39	6 (1%)	73	70	57, 105, 156, 203	0
2	E	14/14 (100%)	0.90	2 (14%)	2	1	164, 203, 345, 351	0
2	F	14/14 (100%)	0.62	2 (14%)	2	1	182, 202, 257, 261	0
All	All	1609/1664 (96%)	-0.47	15 (0%)	84	83	32, 75, 140, 351	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	1	DG	4.8
1	C	6	ILE	3.7
1	D	15	ALA	3.0
1	D	379	ILE	3.0
1	C	396	ARG	2.9
1	D	315	LEU	2.6
1	D	372	GLY	2.6
1	C	14[A]	ASP	2.5
2	E	7	DA	2.4
1	C	330	ILE	2.4
1	D	111	GLY	2.2
1	D	226	ASN	2.2
2	F	3	DA	2.0
2	F	1	DG	2.0
1	C	11	TYR	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)

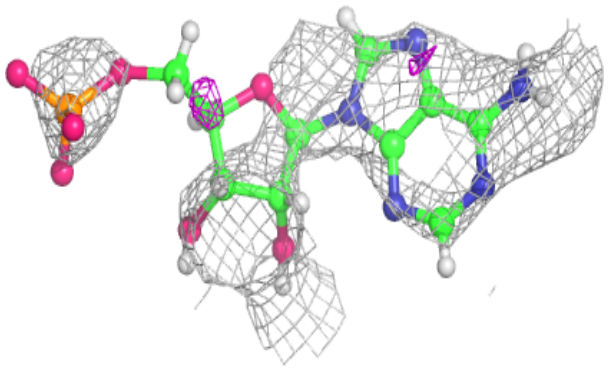
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

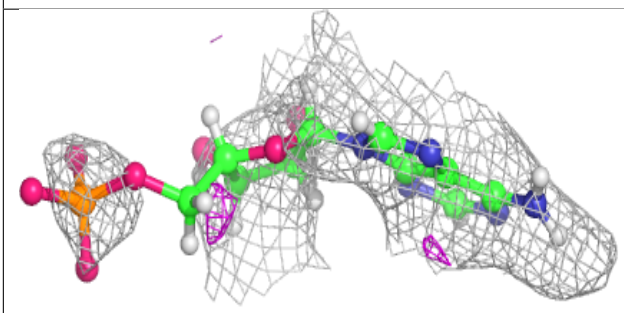
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ANP	F	101	23/31	0.59	0.29	9,200,209,211	0
4	MG	B	502	1/1	0.83	0.20	49,49,49,49	0
4	MG	D	502	1/1	0.94	0.17	71,71,71,71	0
3	ANP	D	501	31/31	0.96	0.14	76,92,115,128	0
4	MG	C	502	1/1	0.96	0.18	64,64,64,64	0
4	MG	A	502	1/1	0.96	0.19	36,36,36,36	0
3	ANP	C	501	31/31	0.97	0.16	61,78,115,128	0
3	ANP	B	501	31/31	0.98	0.14	39,50,69,95	0
3	ANP	A	501	31/31	0.98	0.18	32,42,54,63	0

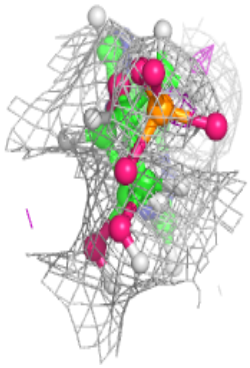
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP F 101:

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

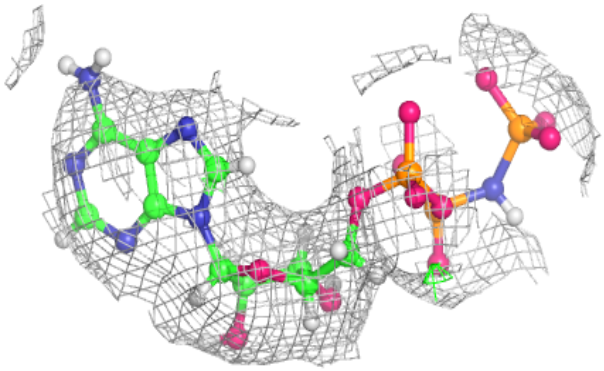


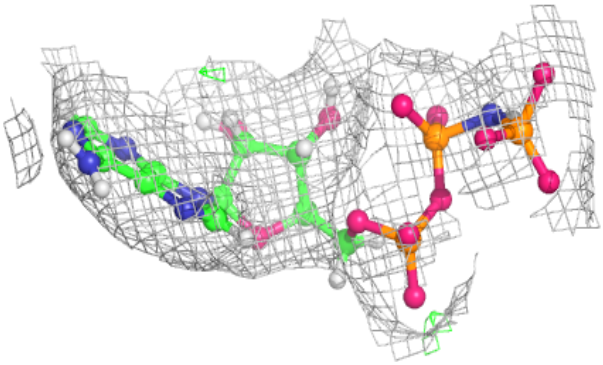


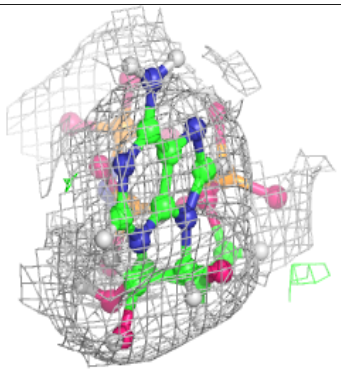


Electron density around ANP D 501:

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

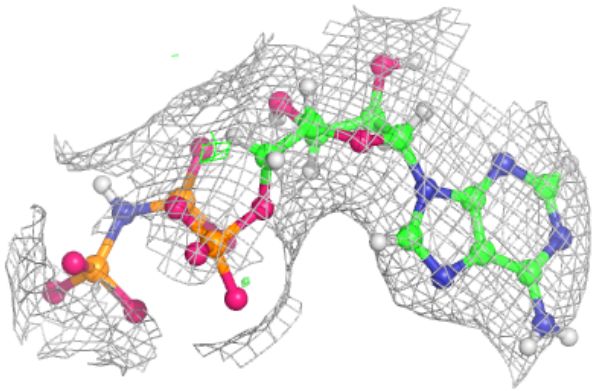


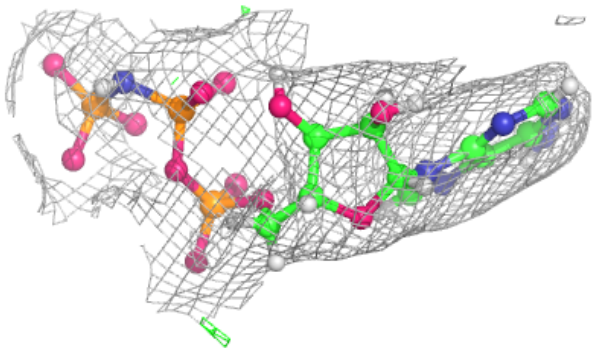


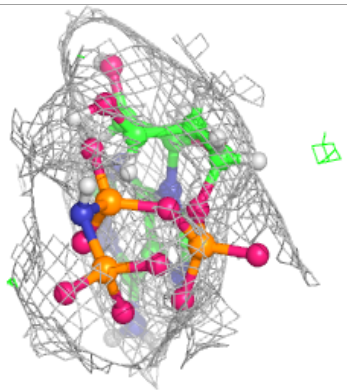


Electron density around ANP C 501:

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

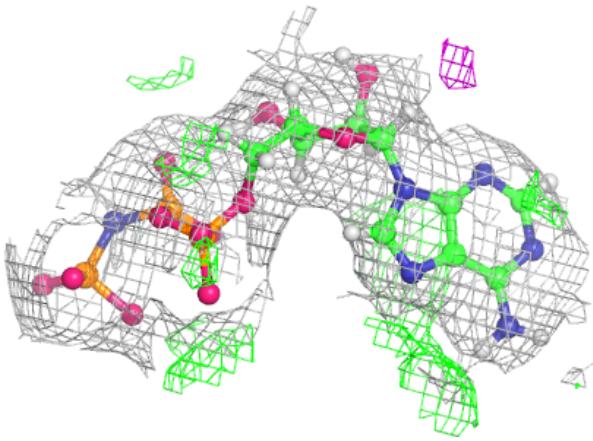


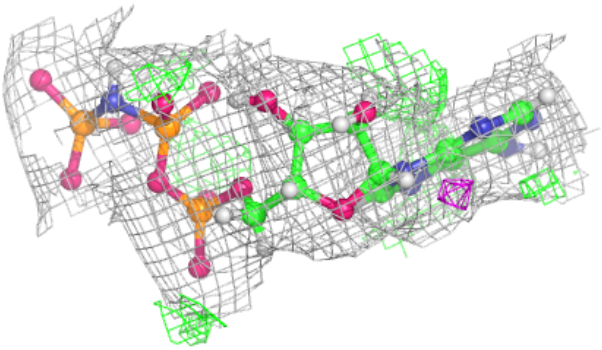


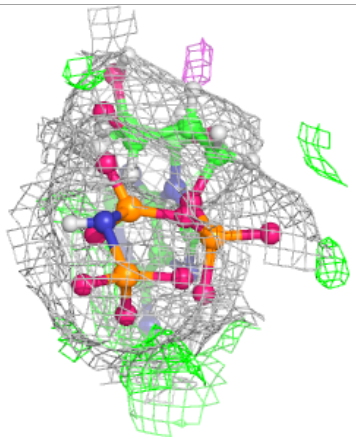


Electron density around ANP B 501:

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

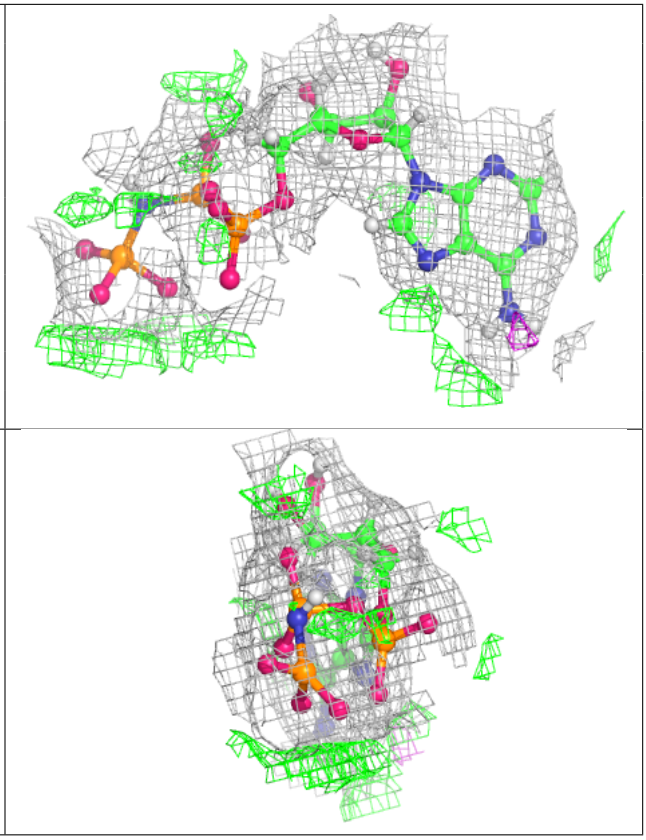






Electron density around ANP A 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.