



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:46 AM UTC

PDB ID : 3LA6 / pdb_00003la6
Title : Octameric kinase domain of the E. coli tyrosine kinase Wzc with bound ADP
Authors : Gruszczyk, J.; Nessler, S.; Gueguen-Chaignon, V.; Vigouroux, A.; Bechet, E.; Grangeasse, C.
Deposited on : 2010-01-06
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

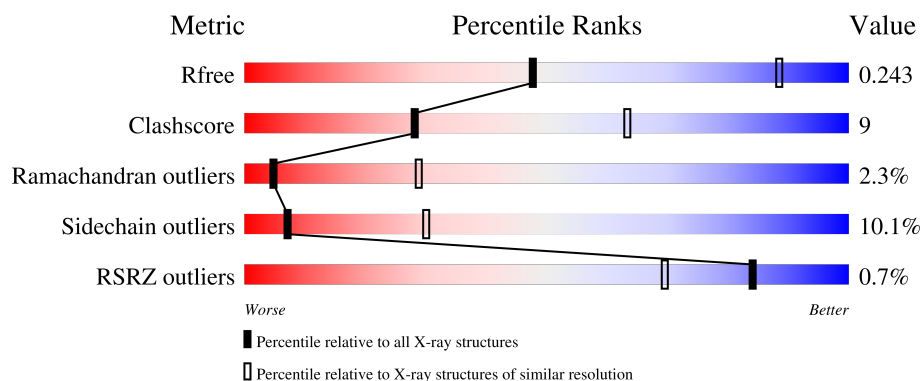
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	286	% 60% 24% • • 9%
1	B	286	% 64% 21% 5% • 9%
1	C	286	% 66% 21% • 9%
1	D	286	60% 23% 6% • 10%
1	E	286	% 66% 19% 5% • 9%

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Mol	Chain	Length	Quality of chain
1	F	286	
1	G	286	
1	H	286	
1	I	286	
1	J	286	
1	K	286	
1	L	286	
1	M	286	
1	N	286	
1	O	286	
1	P	286	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32420 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tyrosine-protein kinase wzc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			1998	1262	343	383	10			
1	B	260	Total	C	N	O	S	0	0	0
			2004	1265	344	385	10			
1	C	260	Total	C	N	O	S	0	0	0
			2006	1266	345	385	10			
1	D	258	Total	C	N	O	S	0	0	0
			1993	1259	343	381	10			
1	E	260	Total	C	N	O	S	0	0	0
			2013	1272	345	386	10			
1	F	257	Total	C	N	O	S	0	0	0
			1982	1252	340	380	10			
1	G	259	Total	C	N	O	S	0	0	0
			2003	1266	343	384	10			
1	H	260	Total	C	N	O	S	0	0	0
			2004	1265	344	385	10			
1	I	260	Total	C	N	O	S	0	0	0
			2008	1268	345	385	10			
1	J	259	Total	C	N	O	S	0	0	0
			2000	1264	344	382	10			
1	K	258	Total	C	N	O	S	0	0	0
			1993	1259	343	381	10			
1	L	259	Total	C	N	O	S	0	0	0
			1999	1265	343	381	10			
1	M	256	Total	C	N	O	S	0	0	0
			1977	1249	339	379	10			
1	N	260	Total	C	N	O	S	0	0	0
			2008	1268	345	385	10			
1	O	260	Total	C	N	O	S	0	0	0
			2008	1269	344	385	10			
1	P	256	Total	C	N	O	S	0	0	0
			1976	1250	338	378	10			

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	435	MET	-	expression tag	UNP P76387
A	436	ARG	-	expression tag	UNP P76387
A	437	GLY	-	expression tag	UNP P76387
A	438	SER	-	expression tag	UNP P76387
A	439	HIS	-	expression tag	UNP P76387
A	440	HIS	-	expression tag	UNP P76387
A	441	HIS	-	expression tag	UNP P76387
A	442	HIS	-	expression tag	UNP P76387
A	443	HIS	-	expression tag	UNP P76387
A	444	HIS	-	expression tag	UNP P76387
A	445	GLY	-	expression tag	UNP P76387
A	446	SER	-	expression tag	UNP P76387
A	540	MET	LYS	SEE REMARK 999	UNP P76387
B	435	MET	-	expression tag	UNP P76387
B	436	ARG	-	expression tag	UNP P76387
B	437	GLY	-	expression tag	UNP P76387
B	438	SER	-	expression tag	UNP P76387
B	439	HIS	-	expression tag	UNP P76387
B	440	HIS	-	expression tag	UNP P76387
B	441	HIS	-	expression tag	UNP P76387
B	442	HIS	-	expression tag	UNP P76387
B	443	HIS	-	expression tag	UNP P76387
B	444	HIS	-	expression tag	UNP P76387
B	445	GLY	-	expression tag	UNP P76387
B	446	SER	-	expression tag	UNP P76387
B	540	MET	LYS	SEE REMARK 999	UNP P76387
C	435	MET	-	expression tag	UNP P76387
C	436	ARG	-	expression tag	UNP P76387
C	437	GLY	-	expression tag	UNP P76387
C	438	SER	-	expression tag	UNP P76387
C	439	HIS	-	expression tag	UNP P76387
C	440	HIS	-	expression tag	UNP P76387
C	441	HIS	-	expression tag	UNP P76387
C	442	HIS	-	expression tag	UNP P76387
C	443	HIS	-	expression tag	UNP P76387
C	444	HIS	-	expression tag	UNP P76387
C	445	GLY	-	expression tag	UNP P76387
C	446	SER	-	expression tag	UNP P76387
C	540	MET	LYS	SEE REMARK 999	UNP P76387
D	435	MET	-	expression tag	UNP P76387
D	436	ARG	-	expression tag	UNP P76387
D	437	GLY	-	expression tag	UNP P76387

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Chain	Residue	Modelled	Actual	Comment	Reference
D	438	SER	-	expression tag	UNP P76387
D	439	HIS	-	expression tag	UNP P76387
D	440	HIS	-	expression tag	UNP P76387
D	441	HIS	-	expression tag	UNP P76387
D	442	HIS	-	expression tag	UNP P76387
D	443	HIS	-	expression tag	UNP P76387
D	444	HIS	-	expression tag	UNP P76387
D	445	GLY	-	expression tag	UNP P76387
D	446	SER	-	expression tag	UNP P76387
D	540	MET	LYS	SEE REMARK 999	UNP P76387
E	435	MET	-	expression tag	UNP P76387
E	436	ARG	-	expression tag	UNP P76387
E	437	GLY	-	expression tag	UNP P76387
E	438	SER	-	expression tag	UNP P76387
E	439	HIS	-	expression tag	UNP P76387
E	440	HIS	-	expression tag	UNP P76387
E	441	HIS	-	expression tag	UNP P76387
E	442	HIS	-	expression tag	UNP P76387
E	443	HIS	-	expression tag	UNP P76387
E	444	HIS	-	expression tag	UNP P76387
E	445	GLY	-	expression tag	UNP P76387
E	446	SER	-	expression tag	UNP P76387
E	540	MET	LYS	SEE REMARK 999	UNP P76387
F	435	MET	-	expression tag	UNP P76387
F	436	ARG	-	expression tag	UNP P76387
F	437	GLY	-	expression tag	UNP P76387
F	438	SER	-	expression tag	UNP P76387
F	439	HIS	-	expression tag	UNP P76387
F	440	HIS	-	expression tag	UNP P76387
F	441	HIS	-	expression tag	UNP P76387
F	442	HIS	-	expression tag	UNP P76387
F	443	HIS	-	expression tag	UNP P76387
F	444	HIS	-	expression tag	UNP P76387
F	445	GLY	-	expression tag	UNP P76387
F	446	SER	-	expression tag	UNP P76387
F	540	MET	LYS	SEE REMARK 999	UNP P76387
G	435	MET	-	expression tag	UNP P76387
G	436	ARG	-	expression tag	UNP P76387
G	437	GLY	-	expression tag	UNP P76387
G	438	SER	-	expression tag	UNP P76387
G	439	HIS	-	expression tag	UNP P76387
G	440	HIS	-	expression tag	UNP P76387

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Chain	Residue	Modelled	Actual	Comment	Reference
G	441	HIS	-	expression tag	UNP P76387
G	442	HIS	-	expression tag	UNP P76387
G	443	HIS	-	expression tag	UNP P76387
G	444	HIS	-	expression tag	UNP P76387
G	445	GLY	-	expression tag	UNP P76387
G	446	SER	-	expression tag	UNP P76387
G	540	MET	LYS	SEE REMARK 999	UNP P76387
H	435	MET	-	expression tag	UNP P76387
H	436	ARG	-	expression tag	UNP P76387
H	437	GLY	-	expression tag	UNP P76387
H	438	SER	-	expression tag	UNP P76387
H	439	HIS	-	expression tag	UNP P76387
H	440	HIS	-	expression tag	UNP P76387
H	441	HIS	-	expression tag	UNP P76387
H	442	HIS	-	expression tag	UNP P76387
H	443	HIS	-	expression tag	UNP P76387
H	444	HIS	-	expression tag	UNP P76387
H	445	GLY	-	expression tag	UNP P76387
H	446	SER	-	expression tag	UNP P76387
H	540	MET	LYS	SEE REMARK 999	UNP P76387
I	435	MET	-	expression tag	UNP P76387
I	436	ARG	-	expression tag	UNP P76387
I	437	GLY	-	expression tag	UNP P76387
I	438	SER	-	expression tag	UNP P76387
I	439	HIS	-	expression tag	UNP P76387
I	440	HIS	-	expression tag	UNP P76387
I	441	HIS	-	expression tag	UNP P76387
I	442	HIS	-	expression tag	UNP P76387
I	443	HIS	-	expression tag	UNP P76387
I	444	HIS	-	expression tag	UNP P76387
I	445	GLY	-	expression tag	UNP P76387
I	446	SER	-	expression tag	UNP P76387
I	540	MET	LYS	SEE REMARK 999	UNP P76387
J	435	MET	-	expression tag	UNP P76387
J	436	ARG	-	expression tag	UNP P76387
J	437	GLY	-	expression tag	UNP P76387
J	438	SER	-	expression tag	UNP P76387
J	439	HIS	-	expression tag	UNP P76387
J	440	HIS	-	expression tag	UNP P76387
J	441	HIS	-	expression tag	UNP P76387
J	442	HIS	-	expression tag	UNP P76387
J	443	HIS	-	expression tag	UNP P76387

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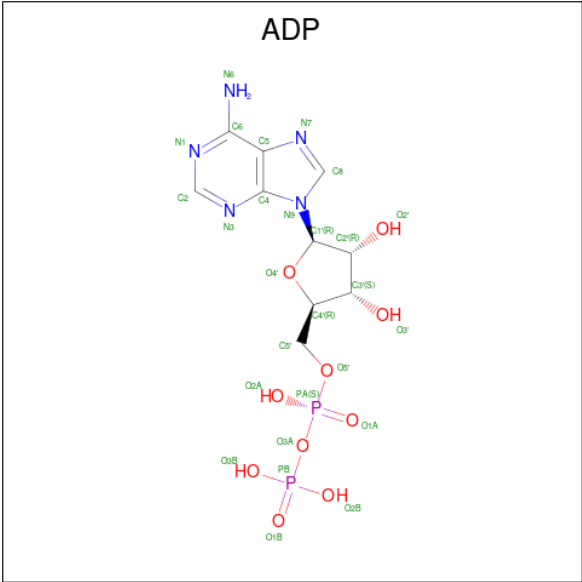
Chain	Residue	Modelled	Actual	Comment	Reference
J	444	HIS	-	expression tag	UNP P76387
J	445	GLY	-	expression tag	UNP P76387
J	446	SER	-	expression tag	UNP P76387
J	540	MET	LYS	SEE REMARK 999	UNP P76387
K	435	MET	-	expression tag	UNP P76387
K	436	ARG	-	expression tag	UNP P76387
K	437	GLY	-	expression tag	UNP P76387
K	438	SER	-	expression tag	UNP P76387
K	439	HIS	-	expression tag	UNP P76387
K	440	HIS	-	expression tag	UNP P76387
K	441	HIS	-	expression tag	UNP P76387
K	442	HIS	-	expression tag	UNP P76387
K	443	HIS	-	expression tag	UNP P76387
K	444	HIS	-	expression tag	UNP P76387
K	445	GLY	-	expression tag	UNP P76387
K	446	SER	-	expression tag	UNP P76387
K	540	MET	LYS	SEE REMARK 999	UNP P76387
L	435	MET	-	expression tag	UNP P76387
L	436	ARG	-	expression tag	UNP P76387
L	437	GLY	-	expression tag	UNP P76387
L	438	SER	-	expression tag	UNP P76387
L	439	HIS	-	expression tag	UNP P76387
L	440	HIS	-	expression tag	UNP P76387
L	441	HIS	-	expression tag	UNP P76387
L	442	HIS	-	expression tag	UNP P76387
L	443	HIS	-	expression tag	UNP P76387
L	444	HIS	-	expression tag	UNP P76387
L	445	GLY	-	expression tag	UNP P76387
L	446	SER	-	expression tag	UNP P76387
L	540	MET	LYS	SEE REMARK 999	UNP P76387
M	435	MET	-	expression tag	UNP P76387
M	436	ARG	-	expression tag	UNP P76387
M	437	GLY	-	expression tag	UNP P76387
M	438	SER	-	expression tag	UNP P76387
M	439	HIS	-	expression tag	UNP P76387
M	440	HIS	-	expression tag	UNP P76387
M	441	HIS	-	expression tag	UNP P76387
M	442	HIS	-	expression tag	UNP P76387
M	443	HIS	-	expression tag	UNP P76387
M	444	HIS	-	expression tag	UNP P76387
M	445	GLY	-	expression tag	UNP P76387
M	446	SER	-	expression tag	UNP P76387

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Chain	Residue	Modelled	Actual	Comment	Reference
M	540	MET	LYS	SEE REMARK 999	UNP P76387
N	435	MET	-	expression tag	UNP P76387
N	436	ARG	-	expression tag	UNP P76387
N	437	GLY	-	expression tag	UNP P76387
N	438	SER	-	expression tag	UNP P76387
N	439	HIS	-	expression tag	UNP P76387
N	440	HIS	-	expression tag	UNP P76387
N	441	HIS	-	expression tag	UNP P76387
N	442	HIS	-	expression tag	UNP P76387
N	443	HIS	-	expression tag	UNP P76387
N	444	HIS	-	expression tag	UNP P76387
N	445	GLY	-	expression tag	UNP P76387
N	446	SER	-	expression tag	UNP P76387
N	540	MET	LYS	SEE REMARK 999	UNP P76387
O	435	MET	-	expression tag	UNP P76387
O	436	ARG	-	expression tag	UNP P76387
O	437	GLY	-	expression tag	UNP P76387
O	438	SER	-	expression tag	UNP P76387
O	439	HIS	-	expression tag	UNP P76387
O	440	HIS	-	expression tag	UNP P76387
O	441	HIS	-	expression tag	UNP P76387
O	442	HIS	-	expression tag	UNP P76387
O	443	HIS	-	expression tag	UNP P76387
O	444	HIS	-	expression tag	UNP P76387
O	445	GLY	-	expression tag	UNP P76387
O	446	SER	-	expression tag	UNP P76387
O	540	MET	LYS	SEE REMARK 999	UNP P76387
P	435	MET	-	expression tag	UNP P76387
P	436	ARG	-	expression tag	UNP P76387
P	437	GLY	-	expression tag	UNP P76387
P	438	SER	-	expression tag	UNP P76387
P	439	HIS	-	expression tag	UNP P76387
P	440	HIS	-	expression tag	UNP P76387
P	441	HIS	-	expression tag	UNP P76387
P	442	HIS	-	expression tag	UNP P76387
P	443	HIS	-	expression tag	UNP P76387
P	444	HIS	-	expression tag	UNP P76387
P	445	GLY	-	expression tag	UNP P76387
P	446	SER	-	expression tag	UNP P76387
P	540	MET	LYS	SEE REMARK 999	UNP P76387

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	P	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

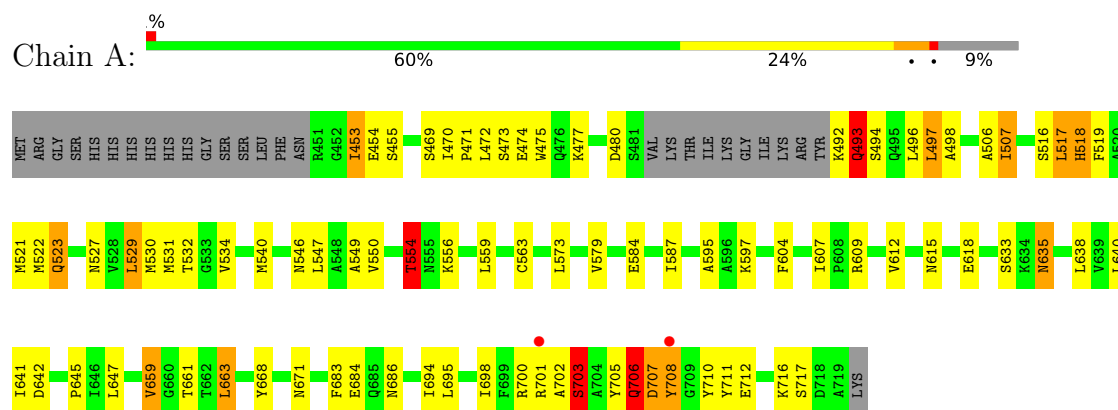
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	F	1	Total	Ca	0	0
			1	1		
3	G	1	Total	Ca	0	0
			1	1		
3	H	1	Total	Ca	0	0
			1	1		
3	I	1	Total	Ca	0	0
			1	1		
3	J	1	Total	Ca	0	0
			1	1		
3	K	1	Total	Ca	0	0
			1	1		
3	L	1	Total	Ca	0	0
			1	1		
3	M	1	Total	Ca	0	0
			1	1		
3	N	1	Total	Ca	0	0
			1	1		
3	O	1	Total	Ca	0	0
			1	1		
3	P	1	Total	Ca	0	0
			1	1		

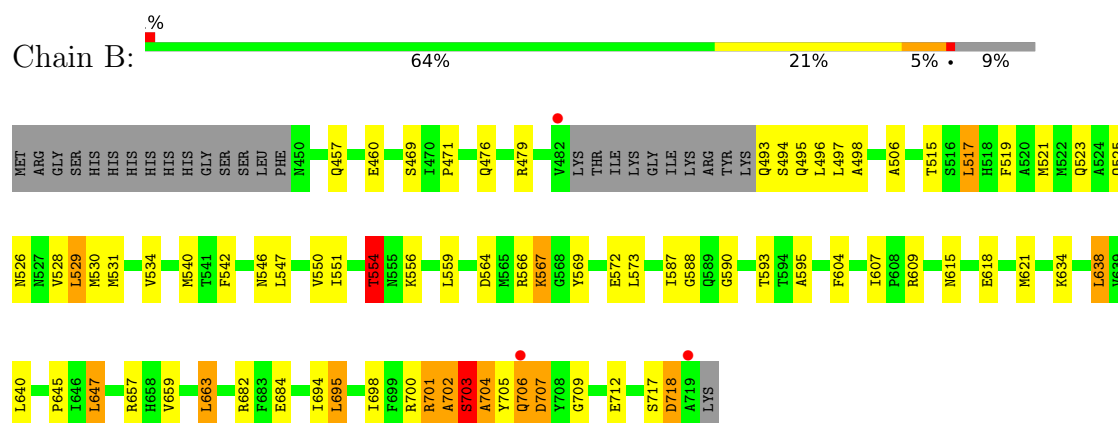
3 Residue-property plots [i](#)

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.

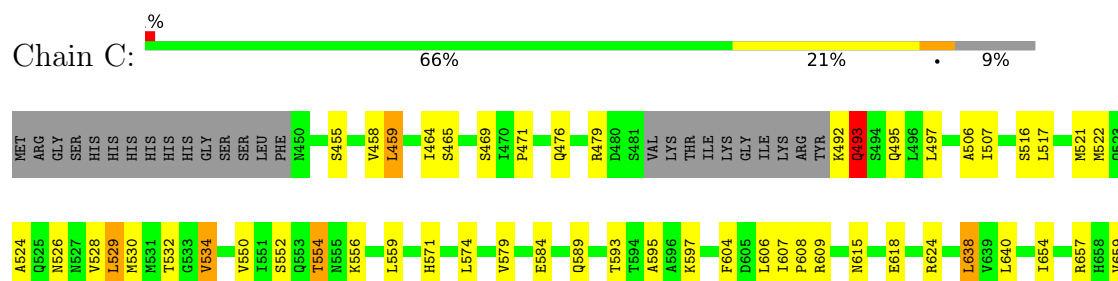
• Molecule 1: Tyrosine-protein kinase wzc



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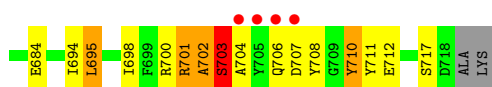




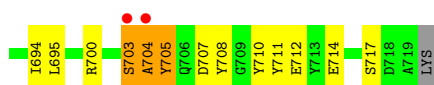
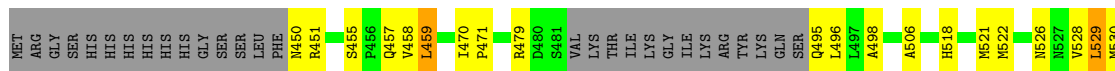
- Molecule 1: Tyrosine-protein kinase wzc



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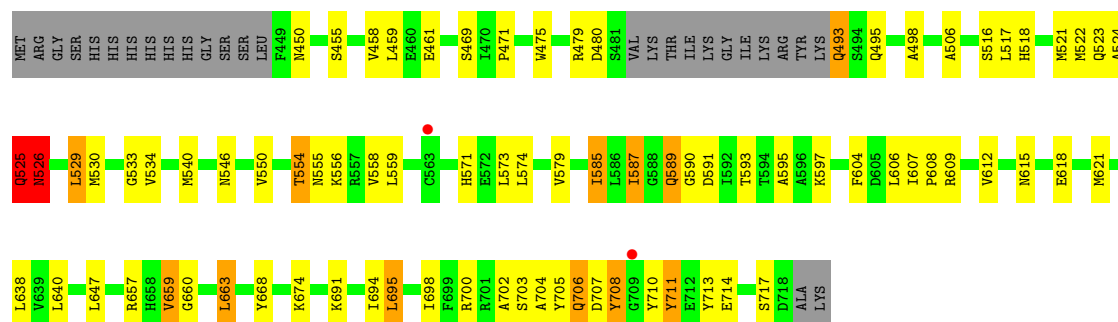


- Molecule 1: Tyrosine-protein kinase wzc



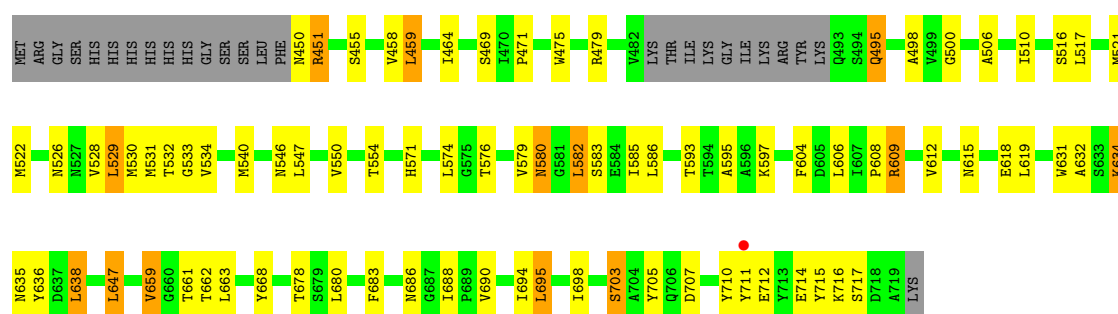
- Molecule 1: Tyrosine-protein kinase wzc





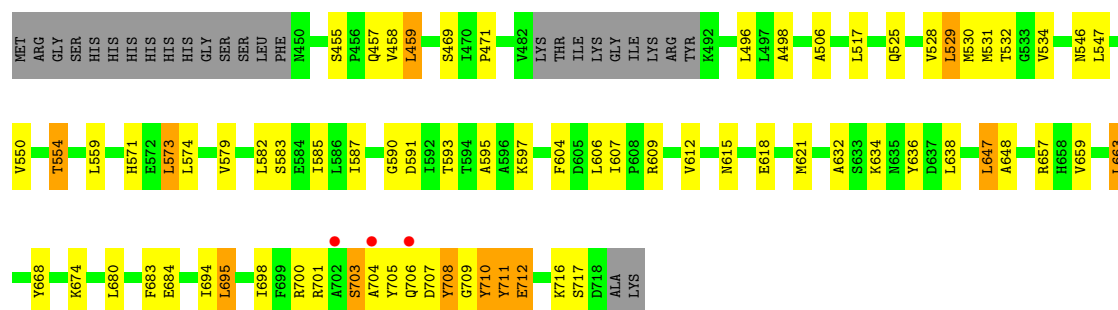
• Molecule 1: Tyrosine-protein kinase wzc

Chain H: 62% 24% 5% 9%



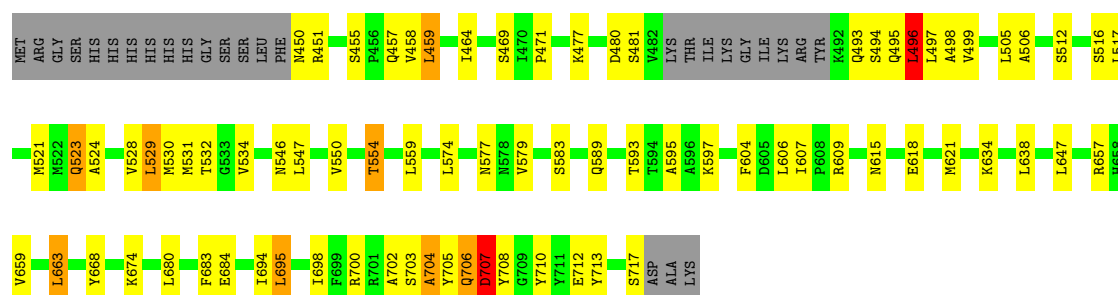
• Molecule 1: Tyrosine-protein kinase wzc

Chain I: 65% 22% 9%

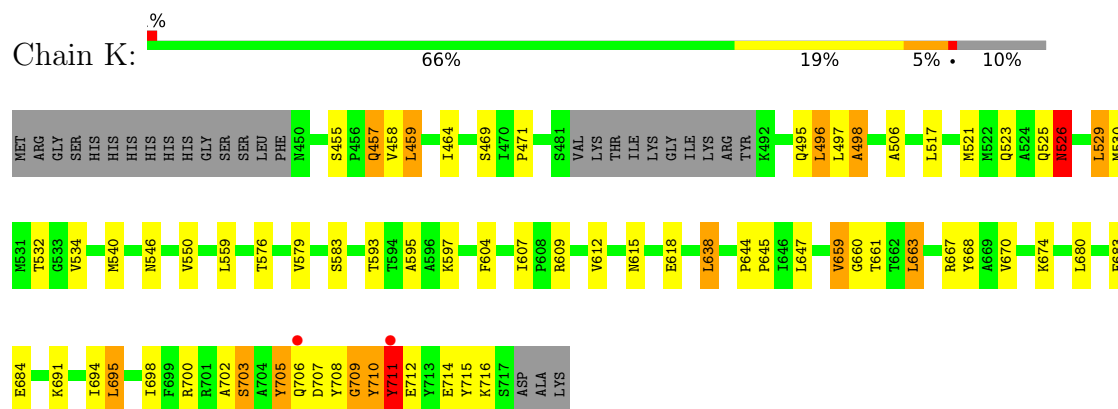


• Molecule 1: Tyrosine-protein kinase wzc

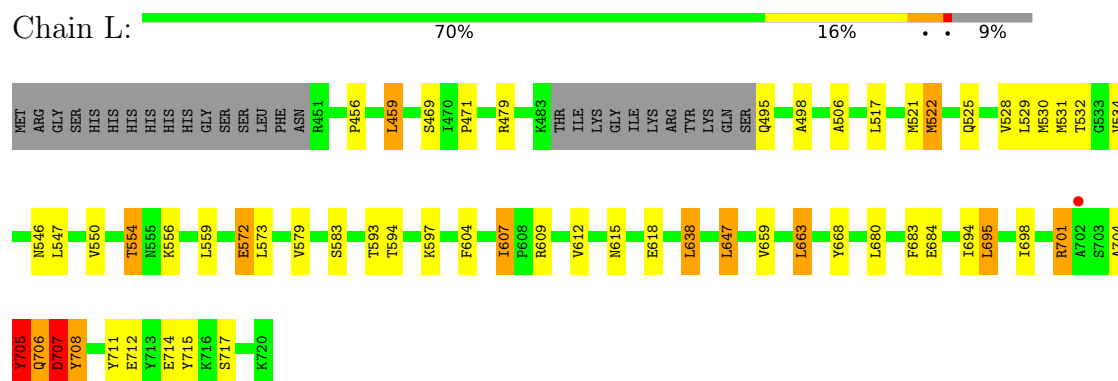
Chain J: 63% 24% 9%



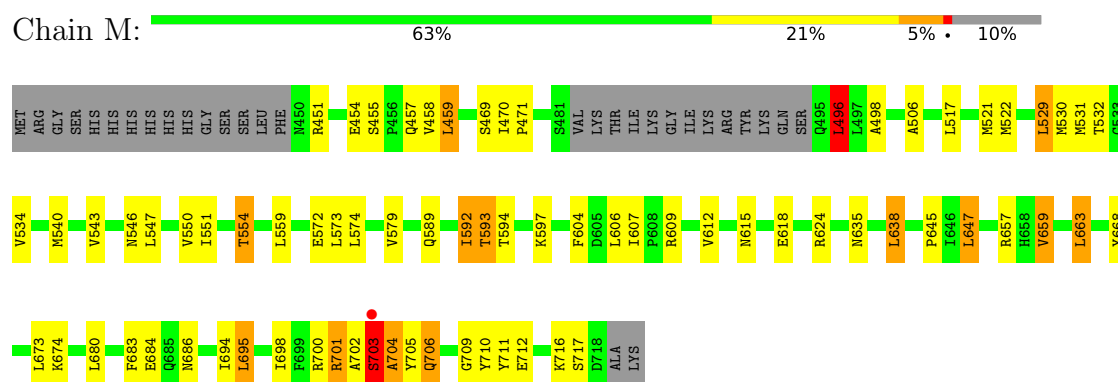
- Molecule 1: Tyrosine-protein kinase wzc



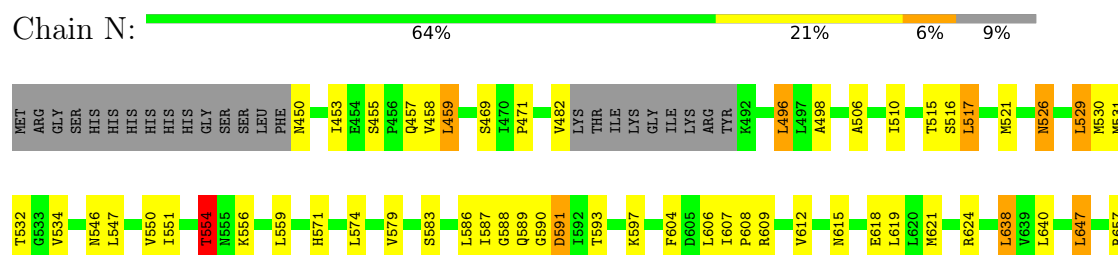
- Molecule 1: Tyrosine-protein kinase wzc



- Molecule 1: Tyrosine-protein kinase wzc

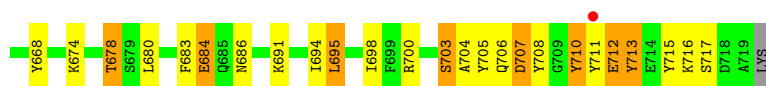


- Molecule 1: Tyrosine-protein kinase wzc

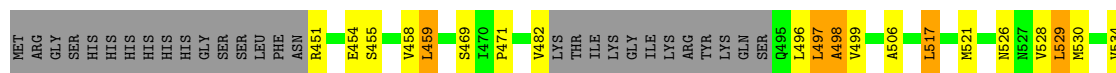




- Molecule 1: Tyrosine-protein kinase wzc



- Molecule 1: Tyrosine-protein kinase wzc



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	245.16Å 137.78Å 158.96Å 90.00° 92.99° 90.00°	Depositor
Resolution (Å)	49.74 – 3.20 49.74 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.74-3.20) 96.3 (49.74-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.19Å)	Xtriage
Refinement program	TNT, BUSTER 2.8.0	Depositor
R, R_{free}	0.186 , 0.223 0.202 , 0.243	Depositor DCC
R_{free} test set	833 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	85.0	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 77.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.003 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.004 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.006 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.006 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.012 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32420	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.89	1/2032 (0.0%)	1.46	19/2759 (0.7%)
1	B	0.90	2/2038 (0.1%)	1.46	18/2769 (0.7%)
1	C	0.90	0/2040	1.44	9/2770 (0.3%)
1	D	0.89	2/2027 (0.1%)	1.49	28/2752 (1.0%)
1	E	0.90	1/2048 (0.0%)	1.50	24/2781 (0.9%)
1	F	0.87	0/2016	1.46	13/2739 (0.5%)
1	G	0.84	0/2038	1.40	10/2768 (0.4%)
1	H	0.91	0/2038	1.52	27/2769 (1.0%)
1	I	0.87	0/2042	1.44	16/2773 (0.6%)
1	J	0.88	1/2034 (0.0%)	1.47	19/2762 (0.7%)
1	K	0.93	0/2027	1.48	17/2752 (0.6%)
1	L	0.88	0/2033	1.44	15/2760 (0.5%)
1	M	0.88	0/2011	1.47	17/2732 (0.6%)
1	N	0.90	0/2042	1.47	21/2773 (0.8%)
1	O	0.91	1/2043 (0.0%)	1.52	21/2775 (0.8%)
1	P	0.89	3/2010 (0.1%)	1.48	13/2731 (0.5%)
All	All	0.89	11/32519 (0.0%)	1.47	287/44165 (0.6%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	507	ILE	CG1-CD1	-8.56	1.18	1.51
1	D	507	ILE	CG1-CD1	-6.62	1.25	1.51
1	B	703	SER	CA-C	5.53	1.60	1.52
1	A	493	GLN	CA-C	5.52	1.60	1.52
1	O	707	ASP	C-N	5.50	1.41	1.33
1	D	707	ASP	CA-C	5.24	1.59	1.52
1	P	703	SER	CA-C	5.16	1.58	1.52
1	B	521	MET	SD-CE	-5.14	1.66	1.79
1	P	713	TYR	CA-C	5.10	1.59	1.52
1	J	707	ASP	CA-C	5.04	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	521	MET	SD-CE	-5.03	1.67	1.79

All (287) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	706	GLN	CA-C-N	9.11	133.70	120.95
1	N	706	GLN	C-N-CA	9.11	133.70	120.95
1	H	710	TYR	CA-C-N	8.75	133.84	121.24
1	H	710	TYR	C-N-CA	8.75	133.84	121.24
1	I	590	GLY	N-CA-C	8.72	121.09	111.85
1	L	604	PHE	CA-CB-CG	8.58	122.38	113.80
1	M	704	ALA	N-CA-C	8.38	120.33	111.03
1	J	523	GLN	N-CA-C	-8.29	101.17	113.61
1	F	604	PHE	CA-CB-CG	8.12	121.92	113.80
1	M	705	TYR	N-CA-C	-8.11	100.94	113.02
1	O	712	GLU	CA-C-N	8.06	136.22	121.70
1	O	712	GLU	C-N-CA	8.06	136.22	121.70
1	O	713	TYR	CA-C-N	7.99	131.31	120.44
1	O	713	TYR	C-N-CA	7.99	131.31	120.44
1	J	604	PHE	CA-CB-CG	7.76	121.56	113.80
1	M	705	TYR	CA-C-N	7.63	136.11	121.54
1	M	705	TYR	C-N-CA	7.63	136.11	121.54
1	O	494	SER	N-CA-C	7.46	119.20	111.14
1	J	480	ASP	CA-CB-CG	7.44	120.04	112.60
1	B	705	TYR	CA-C-N	7.39	135.65	121.54
1	B	705	TYR	C-N-CA	7.39	135.65	121.54
1	L	522	MET	N-CA-C	-7.37	103.18	111.14
1	A	705	TYR	CA-C-N	7.30	135.48	121.54
1	A	705	TYR	C-N-CA	7.30	135.48	121.54
1	A	473	SER	CA-C-N	7.20	130.65	120.28
1	A	473	SER	C-N-CA	7.20	130.65	120.28
1	K	702	ALA	CA-C-N	7.11	135.12	121.54
1	K	702	ALA	C-N-CA	7.11	135.12	121.54
1	H	707	ASP	N-CA-C	7.05	117.97	108.23
1	J	554	THR	N-CA-C	-7.05	99.30	109.31
1	B	705	TYR	N-CA-C	-7.00	104.62	113.72
1	P	704	ALA	CA-C-N	6.98	134.88	121.54
1	P	704	ALA	C-N-CA	6.98	134.88	121.54
1	D	703	SER	CA-C-N	6.97	134.85	121.54
1	D	703	SER	C-N-CA	6.97	134.85	121.54
1	D	704	ALA	CA-C-N	6.91	132.83	122.47
1	D	704	ALA	C-N-CA	6.91	132.83	122.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	684	GLU	CB-CG-CD	6.85	124.25	112.60
1	K	604	PHE	CA-CB-CG	6.85	120.65	113.80
1	M	684	GLU	CB-CG-CD	6.84	124.22	112.60
1	G	480	ASP	N-CA-C	-6.78	105.57	114.31
1	J	684	GLU	CB-CG-CD	6.73	124.04	112.60
1	E	480	ASP	CA-C-N	6.65	133.66	121.70
1	E	480	ASP	C-N-CA	6.65	133.66	121.70
1	A	684	GLU	CB-CG-CD	6.63	123.87	112.60
1	P	712	GLU	CA-C-N	6.62	131.58	122.77
1	P	712	GLU	C-N-CA	6.62	131.58	122.77
1	L	572	GLU	N-CA-C	-6.60	101.24	110.35
1	D	706	GLN	CA-C-N	6.58	134.11	121.54
1	D	706	GLN	C-N-CA	6.58	134.11	121.54
1	E	703	SER	CA-C-N	6.55	129.89	120.79
1	E	703	SER	C-N-CA	6.55	129.89	120.79
1	E	684	GLU	CB-CG-CD	6.52	123.69	112.60
1	M	604	PHE	CA-CB-CG	6.51	120.31	113.80
1	B	706	GLN	CA-C-N	6.50	133.96	121.54
1	B	706	GLN	C-N-CA	6.50	133.96	121.54
1	P	707	ASP	N-CA-C	6.50	119.49	108.90
1	M	703	SER	CA-C-N	6.49	129.45	120.63
1	M	703	SER	C-N-CA	6.49	129.45	120.63
1	D	604	PHE	CA-CB-CG	6.44	120.24	113.80
1	O	526	ASN	CA-CB-CG	6.43	119.03	112.60
1	O	707	ASP	CA-CB-CG	6.43	119.03	112.60
1	B	684	GLU	CB-CG-CD	6.42	123.52	112.60
1	N	684	GLU	CB-CG-CD	6.36	123.42	112.60
1	I	705	TYR	CA-C-N	6.35	133.67	121.54
1	I	705	TYR	C-N-CA	6.35	133.67	121.54
1	N	604	PHE	CA-CB-CG	6.34	120.14	113.80
1	F	704	ALA	CA-C-N	6.33	131.22	121.53
1	F	704	ALA	C-N-CA	6.33	131.22	121.53
1	A	518	HIS	N-CA-C	-6.32	101.59	110.50
1	L	607	ILE	N-CA-C	-6.32	101.89	108.15
1	D	684	GLU	CB-CG-CD	6.30	123.32	112.60
1	D	712	GLU	CA-C-N	6.30	131.87	122.99
1	D	712	GLU	C-N-CA	6.30	131.87	122.99
1	O	525	GLN	CA-C-N	6.26	131.62	121.74
1	O	525	GLN	C-N-CA	6.26	131.62	121.74
1	C	604	PHE	CA-CB-CG	6.24	120.03	113.80
1	C	712	GLU	CB-CG-CD	6.23	123.19	112.60
1	D	496	LEU	CA-C-N	6.23	129.13	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	496	LEU	C-N-CA	6.23	129.13	120.29
1	B	604	PHE	CA-CB-CG	6.22	120.03	113.80
1	C	684	GLU	CA-C-N	6.13	133.25	121.54
1	C	684	GLU	C-N-CA	6.13	133.25	121.54
1	H	609	ARG	N-CA-C	6.13	117.96	111.28
1	E	604	PHE	CA-CB-CG	6.11	119.91	113.80
1	I	604	PHE	CA-CB-CG	6.11	119.91	113.80
1	H	604	PHE	CA-CB-CG	6.09	119.89	113.80
1	A	474	GLU	CB-CG-CD	6.08	122.94	112.60
1	E	707	ASP	CA-C-N	6.06	133.12	121.54
1	E	707	ASP	C-N-CA	6.06	133.12	121.54
1	I	529	LEU	CD1-CG-CD2	6.05	124.12	110.80
1	A	604	PHE	CA-CB-CG	6.00	119.80	113.80
1	L	705	TYR	CA-C-N	5.98	132.46	121.70
1	L	705	TYR	C-N-CA	5.98	132.46	121.70
1	F	714	GLU	CB-CG-CD	5.95	122.72	112.60
1	J	705	TYR	CA-C-N	5.90	132.81	121.54
1	J	705	TYR	C-N-CA	5.90	132.81	121.54
1	N	583	SER	CA-C-N	5.90	128.47	120.44
1	N	583	SER	C-N-CA	5.90	128.47	120.44
1	G	705	TYR	CA-C-N	5.89	132.80	121.54
1	G	705	TYR	C-N-CA	5.89	132.80	121.54
1	H	634	LYS	N-CA-C	-5.88	100.62	109.79
1	I	684	GLU	CA-C-N	5.87	128.73	120.28
1	I	684	GLU	C-N-CA	5.87	128.73	120.28
1	D	705	TYR	CA-C-N	5.85	132.72	121.54
1	D	705	TYR	C-N-CA	5.85	132.72	121.54
1	N	712	GLU	CB-CG-CD	5.84	122.53	112.60
1	O	604	PHE	CA-CB-CG	5.83	119.63	113.80
1	N	703	SER	N-CA-C	5.80	118.07	108.49
1	K	583	SER	CA-C-N	5.79	127.96	120.44
1	K	583	SER	C-N-CA	5.79	127.96	120.44
1	E	474	GLU	CA-C-N	5.78	128.30	120.44
1	E	474	GLU	C-N-CA	5.78	128.30	120.44
1	M	704	ALA	CA-C-N	5.78	131.27	122.08
1	M	704	ALA	C-N-CA	5.78	131.27	122.08
1	K	716	LYS	CA-C-N	5.77	132.08	121.70
1	K	716	LYS	C-N-CA	5.77	132.08	121.70
1	E	704	ALA	CA-C-N	5.75	129.83	120.23
1	E	704	ALA	C-N-CA	5.75	129.83	120.23
1	P	604	PHE	CA-CB-CG	5.75	119.55	113.80
1	H	583	SER	CA-C-N	5.74	127.97	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	583	SER	C-N-CA	5.74	127.97	120.28
1	F	586	LEU	N-CA-C	5.72	117.52	111.28
1	L	456	PRO	CA-C-N	5.71	127.92	120.28
1	L	456	PRO	C-N-CA	5.71	127.92	120.28
1	H	582	LEU	CA-C-N	5.70	128.72	120.79
1	H	582	LEU	C-N-CA	5.70	128.72	120.79
1	L	701	ARG	N-CA-C	-5.70	106.87	113.88
1	D	497	LEU	N-CA-C	5.68	117.55	111.36
1	O	460	GLU	CA-C-N	5.68	128.16	120.38
1	O	460	GLU	C-N-CA	5.68	128.16	120.38
1	P	705	TYR	CA-C-N	5.65	131.46	122.93
1	P	705	TYR	C-N-CA	5.65	131.46	122.93
1	N	704	ALA	N-CA-C	-5.64	105.03	111.07
1	D	706	GLN	N-CA-C	5.64	122.82	110.80
1	B	703	SER	CA-C-N	5.63	132.29	121.54
1	B	703	SER	C-N-CA	5.63	132.29	121.54
1	L	583	SER	CA-C-N	5.63	127.76	120.44
1	L	583	SER	C-N-CA	5.63	127.76	120.44
1	P	707	ASP	CA-C-N	5.63	132.29	121.54
1	P	707	ASP	C-N-CA	5.63	132.29	121.54
1	F	705	TYR	CA-C-N	5.62	132.28	121.54
1	F	705	TYR	C-N-CA	5.62	132.28	121.54
1	N	704	ALA	CA-C-N	5.61	130.28	121.08
1	N	704	ALA	C-N-CA	5.61	130.28	121.08
1	O	684	GLU	CB-CG-CD	5.61	122.14	112.60
1	K	684	GLU	CB-CG-CD	5.60	122.12	112.60
1	N	707	ASP	N-CA-C	5.59	118.35	109.96
1	H	631	TRP	CA-C-N	5.59	127.78	120.28
1	H	631	TRP	C-N-CA	5.59	127.78	120.28
1	D	522	MET	CA-C-N	5.56	128.05	120.54
1	D	522	MET	C-N-CA	5.56	128.05	120.54
1	H	516	SER	CA-C-N	5.56	128.00	120.44
1	H	516	SER	C-N-CA	5.56	128.00	120.44
1	H	712	GLU	N-CA-C	5.53	117.42	108.41
1	L	707	ASP	N-CA-C	5.52	118.19	108.75
1	G	604	PHE	CA-CB-CG	5.51	119.31	113.80
1	B	572	GLU	CA-C-N	5.50	127.65	120.28
1	B	572	GLU	C-N-CA	5.50	127.65	120.28
1	I	705	TYR	N-CA-C	-5.50	106.60	113.15
1	K	457	GLN	CA-C-N	5.50	128.29	120.53
1	K	457	GLN	C-N-CA	5.50	128.29	120.53
1	G	516	SER	CA-C-N	5.49	127.58	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	516	SER	C-N-CA	5.49	127.58	120.44
1	J	496	LEU	N-CA-C	5.49	118.44	111.69
1	O	707	ASP	CA-C-N	5.49	131.58	121.70
1	O	707	ASP	C-N-CA	5.49	131.58	121.70
1	F	703	SER	N-CA-C	5.48	119.59	113.01
1	K	705	TYR	CA-C-N	5.47	131.55	121.70
1	K	705	TYR	C-N-CA	5.47	131.55	121.70
1	A	642	ASP	CA-CB-CG	5.46	118.06	112.60
1	F	529	LEU	CD1-CG-CD2	5.45	122.79	110.80
1	O	712	GLU	CB-CG-CD	5.43	121.83	112.60
1	D	607	ILE	N-CA-CB	5.43	118.81	111.21
1	E	473	SER	CA-C-N	5.40	128.27	120.38
1	E	473	SER	C-N-CA	5.40	128.27	120.38
1	H	580	ASN	CA-CB-CG	5.40	118.00	112.60
1	D	583	SER	CA-C-N	5.39	127.77	120.65
1	D	583	SER	C-N-CA	5.39	127.77	120.65
1	B	495	GLN	CA-C-N	5.37	131.80	121.54
1	B	495	GLN	C-N-CA	5.37	131.80	121.54
1	H	450	ASN	CA-CB-CG	5.36	117.96	112.60
1	M	451	ARG	CA-C-N	5.36	125.06	119.92
1	M	451	ARG	C-N-CA	5.36	125.06	119.92
1	G	591	ASP	CA-C-N	5.35	127.78	120.46
1	G	591	ASP	C-N-CA	5.35	127.78	120.46
1	B	707	ASP	CA-C-N	5.34	131.31	121.70
1	B	707	ASP	C-N-CA	5.34	131.31	121.70
1	O	678	THR	CA-C-N	5.33	127.69	120.65
1	O	678	THR	C-N-CA	5.33	127.69	120.65
1	O	715	TYR	N-CA-C	5.32	118.73	111.39
1	I	583	SER	CA-C-N	5.32	127.35	120.44
1	I	583	SER	C-N-CA	5.32	127.35	120.44
1	M	529	LEU	CD1-CG-CD2	5.31	122.48	110.80
1	D	458	VAL	CA-C-N	5.29	127.32	120.44
1	D	458	VAL	C-N-CA	5.29	127.32	120.44
1	A	703	SER	N-CA-C	5.28	116.90	111.03
1	B	497	LEU	N-CA-C	5.28	117.03	111.28
1	M	635	ASN	N-CA-C	5.28	119.70	113.16
1	J	554	THR	CA-C-N	-5.27	115.73	122.79
1	J	554	THR	C-N-CA	-5.27	115.73	122.79
1	A	706	GLN	CA-C-N	5.26	131.58	121.54
1	A	706	GLN	C-N-CA	5.26	131.58	121.54
1	H	678	THR	CA-C-N	5.24	127.61	120.54
1	H	678	THR	C-N-CA	5.24	127.61	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	571	HIS	CA-C-N	5.23	127.72	120.29
1	I	571	HIS	C-N-CA	5.23	127.72	120.29
1	K	523	GLN	N-CA-C	-5.23	106.48	112.92
1	F	554	THR	CB-CA-C	5.23	119.40	110.56
1	J	516	SER	CA-C-N	5.23	127.24	120.44
1	J	516	SER	C-N-CA	5.23	127.24	120.44
1	H	707	ASP	CA-C-N	5.23	130.79	122.74
1	H	707	ASP	C-N-CA	5.23	130.79	122.74
1	B	718	ASP	N-CA-C	5.23	121.39	114.12
1	O	595	ALA	N-CA-C	5.23	117.40	111.02
1	N	516	SER	CA-C-N	5.22	127.23	120.44
1	N	516	SER	C-N-CA	5.22	127.23	120.44
1	M	572	GLU	CA-C-N	5.21	127.22	120.44
1	M	572	GLU	C-N-CA	5.21	127.22	120.44
1	E	706	GLN	CA-C-N	5.20	131.47	121.54
1	E	706	GLN	C-N-CA	5.20	131.47	121.54
1	I	554	THR	CB-CA-C	5.20	119.34	110.56
1	D	492	LYS	CA-C-N	5.19	128.14	120.82
1	D	492	LYS	C-N-CA	5.19	128.14	120.82
1	N	716	LYS	CA-C-N	5.19	128.44	120.82
1	N	716	LYS	C-N-CA	5.19	128.44	120.82
1	P	684	GLU	CA-C-N	5.18	127.73	120.28
1	P	684	GLU	C-N-CA	5.18	127.73	120.28
1	H	632	ALA	CA-C-N	5.17	127.64	120.29
1	H	632	ALA	C-N-CA	5.17	127.64	120.29
1	K	498	ALA	CA-C-N	5.17	128.30	123.08
1	K	498	ALA	C-N-CA	5.17	128.30	123.08
1	E	516	SER	CA-C-N	5.17	127.16	120.44
1	E	516	SER	C-N-CA	5.17	127.16	120.44
1	E	554	THR	CB-CA-C	5.17	119.30	110.56
1	J	529	LEU	CD1-CG-CD2	5.17	122.16	110.80
1	J	707	ASP	CA-C-N	5.16	130.99	121.70
1	J	707	ASP	C-N-CA	5.16	130.99	121.70
1	I	573	LEU	N-CA-C	5.16	119.42	113.18
1	D	595	ALA	CA-C-N	5.14	128.41	121.05
1	D	595	ALA	C-N-CA	5.14	128.41	121.05
1	E	474	GLU	CB-CG-CD	5.13	121.32	112.60
1	I	707	ASP	CA-C-N	5.12	131.32	121.54
1	I	707	ASP	C-N-CA	5.12	131.32	121.54
1	H	522	MET	CA-C-N	5.12	127.40	120.44
1	H	522	MET	C-N-CA	5.12	127.40	120.44
1	J	583	SER	CA-C-N	5.12	127.09	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	583	SER	C-N-CA	5.12	127.09	120.44
1	O	526	ASN	N-CA-C	5.11	117.42	109.60
1	L	522	MET	CA-C-N	5.11	127.54	120.29
1	L	522	MET	C-N-CA	5.11	127.54	120.29
1	G	525	GLN	CA-C-N	5.10	131.28	121.54
1	G	525	GLN	C-N-CA	5.10	131.28	121.54
1	A	497	LEU	CA-C-N	5.09	127.61	120.28
1	A	497	LEU	C-N-CA	5.09	127.61	120.28
1	D	671	ASN	N-CA-C	5.09	121.65	110.80
1	P	707	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	474	GLU	CA-C-N	5.08	127.35	120.44
1	A	474	GLU	C-N-CA	5.08	127.35	120.44
1	M	554	THR	CB-CA-C	5.08	119.14	110.56
1	H	705	TYR	CA-C-N	5.08	131.24	121.54
1	H	705	TYR	C-N-CA	5.08	131.24	121.54
1	N	707	ASP	CA-CB-CG	5.08	117.68	112.60
1	C	703	SER	N-CA-C	5.07	121.60	110.80
1	N	554	THR	CB-CA-C	5.07	119.12	110.56
1	A	554	THR	CB-CA-C	5.05	119.10	110.56
1	N	496	LEU	N-CA-C	5.05	118.60	112.23
1	E	562	ASP	CA-CB-CG	5.05	117.65	112.60
1	K	529	LEU	CD1-CG-CD2	5.05	121.91	110.80
1	B	554	THR	CB-CA-C	5.04	119.08	110.56
1	F	703	SER	CA-C-N	5.04	131.16	121.54
1	F	703	SER	C-N-CA	5.04	131.16	121.54
1	K	526	ASN	CA-CB-CG	5.03	117.63	112.60
1	E	702	ALA	CA-C-N	5.03	131.14	121.54
1	E	702	ALA	C-N-CA	5.03	131.14	121.54
1	E	602	ALA	N-CA-C	5.03	121.50	110.80
1	C	706	GLN	CA-C-N	5.02	130.74	121.70
1	C	706	GLN	C-N-CA	5.02	130.74	121.70
1	F	707	ASP	N-CA-C	5.02	114.77	108.45
1	N	591	ASP	CA-C-N	5.01	127.33	120.46
1	N	591	ASP	C-N-CA	5.01	127.33	120.46
1	A	522	MET	CA-C-N	5.01	131.11	121.54
1	A	522	MET	C-N-CA	5.01	131.11	121.54
1	C	516	SER	CA-C-N	5.01	126.95	120.44
1	C	516	SER	C-N-CA	5.01	126.95	120.44
1	J	704	ALA	CA-C-N	5.00	129.40	121.44
1	J	704	ALA	C-N-CA	5.00	129.40	121.44

There are no chirality outliers.

There are no planarity outliers.

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	1998	0	2015	64	0
1	B	2004	0	2017	38	0
1	C	2006	0	2021	30	0
1	D	1993	0	2012	55	0
1	E	2013	0	2025	30	0
1	F	1982	0	1995	28	0
1	G	2003	0	2012	43	0
1	H	2004	0	2017	34	0
1	I	2008	0	2025	31	0
1	J	2000	0	2021	39	0
1	K	1993	0	2012	36	0
1	L	1999	0	2024	24	0
1	M	1977	0	1990	44	0
1	N	2008	0	2025	54	0
1	O	2008	0	2017	52	0
1	P	1976	0	1993	35	0
2	A	27	0	12	0	0
2	B	27	0	12	1	0
2	C	27	0	12	2	0
2	D	27	0	12	1	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
2	G	27	0	12	1	0
2	H	27	0	12	0	0
2	I	27	0	12	0	0
2	J	27	0	12	1	0
2	K	27	0	12	0	0
2	L	27	0	12	0	0
2	M	27	0	12	0	0
2	N	27	0	12	1	0
2	O	27	0	12	1	0
2	P	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
All	All	32420	0	32413	576	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 9.

All (576) 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:454:GLU:CG	1:A:701:ARG:HH22	1.00	1.58
1:A:454:GLU:HG2	1:A:701:ARG:NH2	0.91	1.23
1:N:587:ILE:CG2	1:N:619:LEU:HD22	1.71	1.20
1:N:587:ILE:CG2	1:N:619:LEU:CD2	2.22	1.17
1:A:497:LEU:HG	1:A:507:ILE:HD11	1.26	1.15
1:N:587:ILE:HG21	1:N:619:LEU:HD21	1.32	1.10
1:J:577:ASN:ND2	1:J:579:VAL:HG22	1.69	1.08
1:N:588:GLY:O	1:N:589:GLN:HG2	1.49	1.07
1:E:497:LEU:HG	1:E:507:ILE:HD11	1.37	1.06
1:O:525:GLN:HG3	1:O:526:ASN:H	1.17	1.04
1:A:454:GLU:CB	1:A:701:ARG:HH22	1.70	1.04
1:A:454:GLU:HG2	1:A:701:ARG:CZ	1.92	1.00
1:D:706:GLN:HE22	1:D:711:TYR:CB	1.73	1.00
1:A:706:GLN:HB3	1:A:711:TYR:HD1	1.27	0.99
1:D:497:LEU:HG	1:D:507:ILE:HD11	1.44	0.99
1:N:587:ILE:HG21	1:N:619:LEU:CD2	1.89	0.98
1:K:700:ARG:HG2	1:K:710:TYR:HE1	1.29	0.98
1:N:587:ILE:HD12	1:N:587:ILE:O	1.66	0.96
1:N:587:ILE:HG22	1:N:619:LEU:HD22	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:706:GLN:HE22	1:D:711:TYR:HB3	1.31	0.95
1:A:701:ARG:NH1	1:O:451:ARG:NH2	2.15	0.94
1:N:588:GLY:C	1:N:589:GLN:HG2	1.89	0.93
1:A:454:GLU:CG	1:A:701:ARG:NH2	1.78	0.91
1:A:497:LEU:HG	1:A:507:ILE:CD1	2.02	0.89
1:A:493:GLN:HB2	1:A:494:SER:HA	1.55	0.88
1:O:525:GLN:HG3	1:O:526:ASN:N	1.93	0.84
1:C:702:ALA:HA	1:N:704:ALA:HA	1.60	0.83
1:H:528:VAL:HG12	1:H:659:VAL:HG23	1.61	0.82
1:K:700:ARG:HG2	1:K:710:TYR:CE1	2.14	0.82
1:A:706:GLN:HB3	1:A:711:TYR:CD1	2.15	0.81
1:N:587:ILE:HG22	1:N:619:LEU:CD2	2.04	0.80
1:N:587:ILE:CG2	1:N:619:LEU:HD21	1.98	0.80
1:L:705:TYR:H	1:L:706:GLN:HA	1.46	0.80
1:N:587:ILE:O	1:N:587:ILE:CG1	2.30	0.80
1:N:587:ILE:O	1:N:587:ILE:CD1	2.29	0.80
1:E:504:ASP:HB3	1:E:507:ILE:HD12	1.64	0.79
1:J:577:ASN:HD22	1:J:579:VAL:HG22	1.45	0.79
1:L:612:VAL:HG11	1:M:717:SER:HB3	1.63	0.79
1:M:612:VAL:HG11	1:N:717:SER:HB3	1.65	0.78
1:D:706:GLN:HE22	1:D:711:TYR:HB2	1.48	0.77
1:A:612:VAL:HG11	1:B:717:SER:HB3	1.67	0.77
1:D:706:GLN:NE2	1:D:711:TYR:CB	2.47	0.76
1:D:704:ALA:HB1	1:M:702:ALA:HB1	1.68	0.76
1:N:588:GLY:O	1:N:589:GLN:CG	2.30	0.76
1:J:707:ASP:HB3	1:J:708:TYR:HA	1.67	0.76
1:A:703:SER:H	1:P:704:ALA:HB3	1.51	0.76
1:A:527:ASN:HD21	1:A:633:SER:HA	1.51	0.76
1:O:707:ASP:HB2	1:O:708:TYR:HA	1.68	0.76
1:N:587:ILE:HG23	1:N:619:LEU:HD22	1.68	0.75
1:K:700:ARG:HH21	1:K:712:GLU:HB3	1.51	0.74
1:C:455:SER:OG	1:C:458:VAL:HG23	1.87	0.74
1:G:707:ASP:H	1:G:711:TYR:HD2	1.35	0.73
1:N:530:MET:HB2	1:N:659:VAL:HG11	1.70	0.73
1:M:592:ILE:C	1:M:594:THR:H	1.97	0.72
1:D:703:SER:H	1:M:704:ALA:HA	1.54	0.72
1:I:717:SER:HB3	1:P:612:VAL:HG11	1.70	0.72
1:O:525:GLN:CG	1:O:526:ASN:H	2.00	0.72
1:F:612:VAL:HG11	1:G:717:SER:HB3	1.71	0.71
1:A:701:ARG:HH11	1:O:451:ARG:HH21	1.38	0.71
1:D:706:GLN:NE2	1:D:711:TYR:HB3	2.02	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:706:GLN:HG3	1:C:711:TYR:HB3	1.71	0.71
1:D:504:ASP:HB3	1:D:507:ILE:HD12	1.73	0.70
1:P:700:ARG:HG3	1:P:710:TYR:HE1	1.57	0.70
1:M:469:SER:HB3	1:M:698:ILE:HD12	1.73	0.69
1:I:469:SER:HB3	1:I:698:ILE:HD12	1.76	0.68
1:L:469:SER:HB3	1:L:698:ILE:HD12	1.75	0.68
1:N:469:SER:HB3	1:N:698:ILE:HD12	1.75	0.68
1:A:701:ARG:NH1	1:O:451:ARG:HH22	1.89	0.68
1:C:469:SER:HB3	1:C:698:ILE:HD12	1.76	0.68
1:A:469:SER:HB3	1:A:698:ILE:HD12	1.74	0.67
1:D:670:VAL:HG12	1:D:671:ASN:H	1.58	0.67
1:P:528:VAL:HG12	1:P:659:VAL:HG23	1.77	0.67
1:A:497:LEU:CG	1:A:507:ILE:HD11	2.16	0.67
1:B:704:ALA:HA	1:O:703:SER:H	1.60	0.66
1:D:706:GLN:NE2	1:D:711:TYR:HB2	2.08	0.66
1:C:704:ALA:HB3	1:N:703:SER:N	2.10	0.66
1:E:528:VAL:HG12	1:E:659:VAL:HG23	1.78	0.66
1:G:469:SER:HB3	1:G:698:ILE:HD12	1.77	0.66
1:E:475:TRP:O	1:E:479:ARG:HG2	1.96	0.66
1:K:469:SER:HB3	1:K:698:ILE:HD12	1.79	0.65
1:A:518:HIS:O	1:A:519:PHE:HB3	1.96	0.65
1:K:455:SER:HB3	1:K:458:VAL:HG23	1.79	0.65
1:B:469:SER:HB3	1:B:698:ILE:HD12	1.78	0.64
1:O:469:SER:HB3	1:O:698:ILE:HD12	1.78	0.64
1:D:671:ASN:O	1:D:675:GLU:HB2	1.98	0.64
1:G:498:ALA:H	1:G:546:ASN:ND2	1.96	0.64
1:K:663:LEU:HD23	1:K:694:ILE:HD11	1.80	0.64
1:A:706:GLN:CB	1:A:711:TYR:HD1	2.08	0.64
1:J:469:SER:HB3	1:J:698:ILE:HD12	1.78	0.63
1:G:663:LEU:HD23	1:G:694:ILE:HD11	1.80	0.63
1:G:554:THR:HG22	1:G:556:LYS:HG3	1.81	0.63
1:H:469:SER:HB3	1:H:698:ILE:HD12	1.80	0.63
1:D:469:SER:HB3	1:D:698:ILE:HD12	1.79	0.63
1:O:663:LEU:HD23	1:O:694:ILE:HD11	1.81	0.63
1:A:516:SER:HA	1:H:686:ASN:ND2	2.15	0.62
1:M:663:LEU:HD23	1:M:694:ILE:HD11	1.81	0.62
1:L:663:LEU:HD23	1:L:694:ILE:HD11	1.79	0.62
1:E:469:SER:HB3	1:E:698:ILE:HD12	1.80	0.62
1:J:528:VAL:HG12	1:J:659:VAL:HG23	1.81	0.62
1:D:528:VAL:HG12	1:D:659:VAL:HG23	1.81	0.62
1:P:459:LEU:HD23	1:P:459:LEU:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:469:SER:HB3	1:P:698:ILE:HD12	1.80	0.62
1:C:530:MET:HB2	1:C:659:VAL:HG11	1.82	0.62
1:F:459:LEU:HD23	1:F:459:LEU:H	1.65	0.62
1:H:663:LEU:HD23	1:H:694:ILE:HD11	1.82	0.61
1:M:457:GLN:NE2	1:M:709:GLY:HA2	2.15	0.61
1:D:612:VAL:HG11	1:E:717:SER:HB3	1.82	0.61
1:I:528:VAL:HG12	1:I:659:VAL:HG23	1.81	0.61
1:D:539:GLY:HA2	2:D:1000:ADP:H5'1	1.83	0.61
1:F:521:MET:HE1	1:F:638:LEU:HD21	1.83	0.61
1:F:615:ASN:HB2	1:F:618:GLU:HB2	1.83	0.61
1:B:566:ARG:O	1:B:567:LYS:HB2	2.01	0.61
1:G:615:ASN:HB2	1:G:618:GLU:HB2	1.82	0.61
1:F:518:HIS:O	1:F:522:MET:HG2	2.00	0.61
1:F:528:VAL:HG12	1:F:659:VAL:HG23	1.81	0.61
1:B:528:VAL:HG12	1:B:659:VAL:HG23	1.82	0.60
1:D:663:LEU:HD23	1:D:694:ILE:HD11	1.83	0.60
1:F:538:ILE:HD12	1:F:665:VAL:HG12	1.82	0.60
1:A:663:LEU:HD23	1:A:694:ILE:HD11	1.82	0.60
1:P:497:LEU:HG	1:P:498:ALA:H	1.65	0.60
1:P:574:LEU:HD12	1:P:606:LEU:HD22	1.84	0.60
1:H:459:LEU:HD23	1:H:459:LEU:H	1.67	0.60
1:N:615:ASN:HB2	1:N:618:GLU:HB2	1.84	0.60
1:D:705:TYR:HD1	1:M:701:ARG:O	1.85	0.60
1:J:577:ASN:HD21	1:J:579:VAL:HG22	1.64	0.60
1:K:612:VAL:HG11	1:L:717:SER:HB3	1.84	0.60
1:G:571:HIS:HB3	1:G:608:PRO:HB3	1.84	0.59
1:L:528:VAL:HG12	1:L:659:VAL:HG23	1.83	0.59
1:E:454:GLU:HG2	1:E:701:ARG:HH21	1.67	0.59
1:I:574:LEU:HD12	1:I:606:LEU:HD22	1.85	0.59
1:J:521:MET:HA	1:J:524:ALA:HB2	1.84	0.59
1:P:497:LEU:C	1:P:499:VAL:H	2.11	0.59
1:A:454:GLU:CB	1:A:701:ARG:NH2	2.47	0.59
1:C:663:LEU:HD23	1:C:694:ILE:HD11	1.85	0.59
1:H:615:ASN:HB2	1:H:618:GLU:HB2	1.84	0.59
1:P:663:LEU:HD23	1:P:694:ILE:HD11	1.84	0.59
1:E:663:LEU:HD23	1:E:694:ILE:HD11	1.84	0.59
1:K:700:ARG:NH2	1:K:712:GLU:HB3	2.18	0.58
1:O:498:ALA:H	1:O:546:ASN:ND2	2.01	0.58
1:O:657:ARG:HH21	1:O:686:ASN:HB3	1.69	0.58
1:N:459:LEU:HD23	1:N:459:LEU:H	1.69	0.58
1:N:517:LEU:O	1:N:521:MET:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:615:ASN:HB2	1:P:618:GLU:HB2	1.85	0.58
1:E:615:ASN:HB2	1:E:618:GLU:HB2	1.85	0.58
1:O:615:ASN:HB2	1:O:618:GLU:HB2	1.85	0.58
1:I:663:LEU:HD23	1:I:694:ILE:HD11	1.86	0.58
1:O:524:ALA:O	1:O:525:GLN:HG2	2.04	0.58
1:A:615:ASN:HB2	1:A:618:GLU:HB2	1.86	0.58
1:C:654:ILE:O	1:C:657:ARG:HG2	2.03	0.58
1:C:521:MET:HE1	1:C:638:LEU:HD21	1.85	0.57
1:N:695:LEU:HB3	1:N:698:ILE:HD11	1.86	0.57
1:I:615:ASN:HB2	1:I:618:GLU:HB2	1.86	0.57
1:J:496:LEU:HB3	1:J:499:VAL:HG22	1.86	0.57
1:N:498:ALA:HB2	1:N:546:ASN:HD22	1.68	0.57
1:F:526:ASN:HD21	1:F:528:VAL:HB	1.68	0.57
1:A:717:SER:HB3	1:H:612:VAL:HG11	1.86	0.57
1:D:559:LEU:HD11	1:D:607:ILE:HG23	1.87	0.57
1:K:615:ASN:HB2	1:K:618:GLU:HB2	1.85	0.57
1:B:534:VAL:O	1:B:647:LEU:HB2	2.04	0.57
1:O:707:ASP:HB2	1:O:708:TYR:CA	2.35	0.57
1:C:615:ASN:HB2	1:C:618:GLU:HB2	1.86	0.57
1:F:663:LEU:HD23	1:F:694:ILE:HD11	1.87	0.57
1:P:695:LEU:HB3	1:P:698:ILE:HD11	1.87	0.57
1:B:663:LEU:HD23	1:B:694:ILE:HD11	1.85	0.57
1:J:615:ASN:HB2	1:J:618:GLU:HB2	1.85	0.57
1:M:521:MET:HE1	1:M:638:LEU:HD21	1.86	0.57
1:M:534:VAL:O	1:M:647:LEU:HB2	2.05	0.57
1:H:695:LEU:HB3	1:H:698:ILE:HD11	1.87	0.57
1:M:498:ALA:HB2	1:M:546:ASN:HD22	1.68	0.57
1:M:700:ARG:HG3	1:M:710:TYR:HE2	1.70	0.57
1:D:615:ASN:HB2	1:D:618:GLU:HB2	1.85	0.56
1:I:695:LEU:HB3	1:I:698:ILE:HD11	1.87	0.56
1:B:615:ASN:HB2	1:B:618:GLU:HB2	1.86	0.56
1:M:615:ASN:HB2	1:M:618:GLU:HB2	1.86	0.56
1:J:663:LEU:HD23	1:J:694:ILE:HD11	1.87	0.56
1:K:705:TYR:H	1:K:706:GLN:HA	1.69	0.56
1:L:559:LEU:HD11	1:L:607:ILE:HG13	1.87	0.56
1:P:526:ASN:HD21	1:P:528:VAL:HB	1.70	0.56
1:J:498:ALA:HB2	1:J:546:ASN:HD22	1.71	0.56
1:F:703:SER:OG	1:K:703:SER:O	2.21	0.56
1:A:530:MET:HB2	1:A:659:VAL:HG11	1.86	0.56
1:D:707:ASP:CB	1:D:708:TYR:HA	2.35	0.56
1:G:518:HIS:O	1:G:522:MET:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:521:MET:HE1	1:D:638:LEU:HD21	1.87	0.56
1:A:703:SER:H	1:P:704:ALA:CB	2.18	0.56
1:O:521:MET:HE1	1:O:638:LEU:HD21	1.87	0.56
1:K:534:VAL:O	1:K:647:LEU:HB2	2.06	0.55
1:N:663:LEU:HD23	1:N:694:ILE:HD11	1.88	0.55
1:J:534:VAL:O	1:J:647:LEU:HB2	2.06	0.55
1:A:517:LEU:HD21	1:A:529:LEU:HD22	1.88	0.55
1:D:498:ALA:H	1:D:546:ASN:ND2	2.04	0.55
1:E:534:VAL:O	1:E:647:LEU:HB2	2.06	0.55
1:J:695:LEU:HB3	1:J:698:ILE:HD11	1.88	0.55
1:H:534:VAL:O	1:H:647:LEU:HB2	2.07	0.55
1:I:534:VAL:O	1:I:647:LEU:HB2	2.07	0.55
1:A:534:VAL:O	1:A:647:LEU:HB2	2.07	0.55
1:L:615:ASN:HB2	1:L:618:GLU:HB2	1.88	0.55
1:O:612:VAL:HG11	1:P:717:SER:HB3	1.88	0.55
1:E:454:GLU:HG2	1:E:701:ARG:NH2	2.22	0.55
1:L:534:VAL:O	1:L:647:LEU:HB2	2.06	0.55
1:A:703:SER:OG	1:P:703:SER:HB2	2.07	0.55
1:B:695:LEU:HB3	1:B:698:ILE:HD11	1.89	0.55
1:D:534:VAL:O	1:D:647:LEU:HB2	2.07	0.55
1:D:704:ALA:HB2	1:M:704:ALA:HB2	1.88	0.55
1:H:586:LEU:HD23	1:H:619:LEU:HB3	1.88	0.55
1:G:704:ALA:HB3	1:J:703:SER:H	1.72	0.54
1:D:695:LEU:HB3	1:D:698:ILE:HD11	1.89	0.54
1:A:701:ARG:HH11	1:O:451:ARG:NH2	1.90	0.54
1:C:526:ASN:HD21	1:C:528:VAL:HB	1.73	0.54
1:H:521:MET:HE1	1:H:638:LEU:HD21	1.89	0.54
1:G:695:LEU:HB3	1:G:698:ILE:HD11	1.90	0.54
1:P:534:VAL:O	1:P:647:LEU:HB2	2.07	0.54
1:D:526:ASN:HB3	1:D:660:GLY:HA3	1.88	0.54
1:L:695:LEU:HB3	1:L:698:ILE:HD11	1.90	0.54
1:M:592:ILE:C	1:M:594:THR:N	2.65	0.54
1:O:695:LEU:HB3	1:O:698:ILE:HD11	1.88	0.54
1:A:453:ILE:HG13	1:A:671:ASN:O	2.08	0.53
1:F:534:VAL:O	1:F:647:LEU:HB2	2.07	0.53
1:G:612:VAL:HG11	1:H:717:SER:HB3	1.90	0.53
1:H:634:LYS:O	1:H:636:TYR:N	2.38	0.53
1:O:534:VAL:O	1:O:647:LEU:HB2	2.08	0.53
1:C:695:LEU:HB3	1:C:698:ILE:HD11	1.89	0.53
1:G:706:GLN:O	1:G:711:TYR:HB3	2.09	0.53
1:J:577:ASN:HD22	1:J:579:VAL:CG2	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:517:LEU:HB3	1:D:521:MET:HE2	1.91	0.53
1:D:479:ARG:CZ	1:D:495:GLN:HB2	2.39	0.53
1:M:530:MET:HB2	1:M:659:VAL:HG11	1.91	0.53
1:N:534:VAL:O	1:N:647:LEU:HB2	2.09	0.52
1:F:498:ALA:H	1:F:546:ASN:ND2	2.07	0.52
1:M:695:LEU:HB3	1:M:698:ILE:HD11	1.90	0.52
1:M:612:VAL:CG1	1:N:717:SER:HB3	2.39	0.52
1:N:559:LEU:HD11	1:N:607:ILE:HG13	1.92	0.52
1:H:529:LEU:HD12	1:H:661:THR:HB	1.92	0.52
1:M:706:GLN:HB2	1:M:711:TYR:HD1	1.74	0.52
1:O:450:ASN:HD21	1:O:674:LYS:HB2	1.74	0.52
1:G:533:GLY:HA3	1:G:540:MET:SD	2.50	0.52
1:N:587:ILE:O	1:N:587:ILE:HG13	2.07	0.52
1:D:707:ASP:HB3	1:D:708:TYR:HA	1.92	0.52
1:G:534:VAL:O	1:G:647:LEU:HB2	2.10	0.52
1:A:516:SER:HA	1:H:686:ASN:HD22	1.75	0.52
1:B:701:ARG:HD3	1:O:705:TYR:HE2	1.74	0.52
1:F:471:PRO:HD2	1:F:506:ALA:HA	1.92	0.52
1:J:471:PRO:HD2	1:J:506:ALA:HA	1.92	0.52
1:K:661:THR:HG23	1:K:691:LYS:HG3	1.90	0.52
1:E:551:ILE:HG21	1:E:638:LEU:HD11	1.92	0.51
1:N:612:VAL:HG11	1:O:717:SER:HB3	1.93	0.51
1:G:455:SER:HB3	1:G:458:VAL:HG23	1.93	0.51
1:L:705:TYR:H	1:L:706:GLN:CA	2.19	0.51
1:M:471:PRO:HD2	1:M:506:ALA:HA	1.92	0.51
1:P:498:ALA:HB2	1:P:546:ASN:HD22	1.75	0.51
1:G:530:MET:HB2	1:G:659:VAL:HG11	1.91	0.51
1:M:455:SER:OG	1:M:457:GLN:HG2	2.11	0.51
1:M:559:LEU:HD11	1:M:607:ILE:HG13	1.92	0.51
1:D:455:SER:OG	1:D:458:VAL:HG23	2.11	0.51
1:E:455:SER:OG	1:E:457:GLN:HG2	2.10	0.51
1:C:459:LEU:HB2	1:C:464:ILE:HB	1.92	0.51
1:G:700:ARG:HD3	1:G:707:ASP:OD1	2.11	0.51
1:G:621:MET:HE3	1:G:657:ARG:HH12	1.76	0.50
1:K:695:LEU:HB3	1:K:698:ILE:HD11	1.91	0.50
1:H:498:ALA:H	1:H:546:ASN:ND2	2.08	0.50
1:G:498:ALA:H	1:G:546:ASN:HD21	1.57	0.50
1:I:559:LEU:HD11	1:I:607:ILE:HG13	1.94	0.50
1:J:577:ASN:ND2	1:J:579:VAL:CG2	2.58	0.50
1:L:459:LEU:H	1:L:459:LEU:HD23	1.76	0.50
1:M:457:GLN:HE21	1:M:709:GLY:HA2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:700:ARG:HG3	1:M:710:TYR:CE2	2.46	0.50
1:E:559:LEU:HD11	1:E:607:ILE:HG13	1.94	0.50
1:I:471:PRO:HD2	1:I:506:ALA:HA	1.93	0.50
1:N:471:PRO:HD2	1:N:506:ALA:HA	1.92	0.50
1:A:498:ALA:HB2	1:A:546:ASN:HD22	1.77	0.50
1:A:563:CYS:SG	1:A:641:ILE:CG2	3.00	0.50
1:A:635:ASN:N	1:A:635:ASN:HD22	2.10	0.50
1:J:559:LEU:HD11	1:J:607:ILE:HG13	1.93	0.50
1:K:559:LEU:HD11	1:K:607:ILE:HG13	1.94	0.50
1:N:506:ALA:O	1:N:510:ILE:HG13	2.12	0.50
1:E:695:LEU:HB3	1:E:698:ILE:HD11	1.93	0.50
1:A:703:SER:N	1:P:704:ALA:HB3	2.22	0.50
1:G:704:ALA:HB3	1:J:702:ALA:HA	1.94	0.50
1:I:498:ALA:H	1:I:546:ASN:ND2	2.09	0.50
1:I:612:VAL:HG11	1:J:717:SER:HB3	1.94	0.49
1:J:700:ARG:HG3	1:J:710:TYR:HE1	1.77	0.49
1:G:521:MET:HA	1:G:524:ALA:HB3	1.94	0.49
1:G:526:ASN:HB3	1:G:660:GLY:HA3	1.93	0.49
1:N:621:MET:HE3	1:N:657:ARG:HH12	1.77	0.49
1:A:695:LEU:HB3	1:A:698:ILE:HD11	1.94	0.49
1:B:498:ALA:H	1:B:546:ASN:ND2	2.10	0.49
1:D:707:ASP:HA	1:D:711:TYR:HD1	1.78	0.49
1:O:559:LEU:HD11	1:O:607:ILE:HG13	1.94	0.49
1:B:471:PRO:HD2	1:B:506:ALA:HA	1.94	0.49
1:B:519:PHE:O	1:B:523:GLN:HB2	2.12	0.49
1:B:559:LEU:HD11	1:B:607:ILE:HG13	1.94	0.49
1:G:471:PRO:HD2	1:G:506:ALA:HA	1.94	0.49
1:H:703:SER:HB2	1:I:703:SER:OG	2.11	0.49
1:H:455:SER:HB3	1:H:458:VAL:HG23	1.94	0.49
1:L:471:PRO:HD2	1:L:506:ALA:HA	1.94	0.49
2:N:1000:ADP:H5'1	2:N:1000:ADP:H8	1.77	0.49
1:B:621:MET:HE3	1:B:657:ARG:HH12	1.78	0.49
1:F:559:LEU:HD11	1:F:607:ILE:HG13	1.94	0.49
1:G:585:ILE:HG22	1:G:590:GLY:HA3	1.94	0.49
1:B:702:ALA:CB	1:O:704:ALA:HA	2.43	0.49
1:E:471:PRO:HD2	1:E:506:ALA:HA	1.94	0.49
1:H:532:THR:HG21	1:H:683:PHE:CZ	2.47	0.49
1:K:579:VAL:O	1:K:597:LYS:NZ	2.45	0.49
1:A:531:MET:HE1	1:A:547:LEU:HD23	1.95	0.48
1:G:525:GLN:O	1:G:526:ASN:HB2	2.11	0.48
1:O:532:THR:HG21	1:O:683:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:700:ARG:NH2	1:M:712:GLU:HB3	2.28	0.48
1:D:471:PRO:HD2	1:D:506:ALA:HA	1.95	0.48
1:E:574:LEU:HD12	1:E:606:LEU:HD22	1.95	0.48
1:F:498:ALA:HB2	1:F:546:ASN:HD22	1.78	0.48
1:M:459:LEU:HD12	1:M:673:LEU:HD13	1.95	0.48
1:C:471:PRO:HD2	1:C:506:ALA:HA	1.93	0.48
1:I:457:GLN:NE2	1:I:709:GLY:HA2	2.28	0.48
1:O:528:VAL:HG12	1:O:659:VAL:HG23	1.95	0.48
1:K:667:ARG:HB3	1:K:670:VAL:HB	1.95	0.48
1:A:471:PRO:HD2	1:A:506:ALA:HA	1.96	0.48
1:H:530:MET:HE2	1:H:662:THR:HG23	1.95	0.48
1:N:517:LEU:HD21	1:N:529:LEU:HD22	1.95	0.48
1:J:459:LEU:HB2	1:J:464:ILE:HB	1.93	0.48
1:A:559:LEU:HD11	1:A:607:ILE:HG13	1.95	0.48
1:A:584:GLU:O	1:A:587:ILE:HG22	2.13	0.48
1:K:530:MET:HB2	1:K:659:VAL:HG11	1.94	0.48
1:J:455:SER:OG	1:J:457:GLN:HG2	2.14	0.48
1:K:526:ASN:ND2	1:K:660:GLY:HA3	2.28	0.48
1:L:498:ALA:H	1:L:546:ASN:ND2	2.12	0.48
1:G:493:GLN:HG3	2:G:1000:ADP:C2'	2.43	0.48
1:A:493:GLN:CB	1:A:494:SER:HA	2.37	0.47
1:B:517:LEU:HD21	1:B:529:LEU:HD22	1.95	0.47
1:K:455:SER:OG	1:K:457:GLN:HG2	2.14	0.47
1:O:498:ALA:H	1:O:546:ASN:HD21	1.61	0.47
1:B:530:MET:N	1:B:659:VAL:HG21	2.29	0.47
1:C:554:THR:HG22	1:C:556:LYS:HG3	1.96	0.47
1:G:498:ALA:HB2	1:G:546:ASN:HD22	1.78	0.47
1:I:701:ARG:NH1	1:I:708:TYR:OH	2.47	0.47
1:K:471:PRO:HD2	1:K:506:ALA:HA	1.96	0.47
1:N:703:SER:HB2	1:N:706:GLN:HA	1.97	0.47
1:A:579:VAL:O	1:A:597:LYS:NZ	2.48	0.47
1:B:476:GLN:HG3	1:B:542:PHE:HE1	1.79	0.47
1:E:455:SER:HB3	1:E:458:VAL:HG23	1.97	0.47
1:E:700:ARG:HG3	1:E:710:TYR:HE1	1.79	0.47
1:N:571:HIS:HB3	1:N:608:PRO:HB3	1.97	0.47
1:O:471:PRO:HD2	1:O:506:ALA:HA	1.97	0.47
1:J:505:LEU:HD22	1:J:712:GLU:HG2	1.96	0.47
1:B:564:ASP:OD1	1:B:566:ARG:O	2.32	0.47
1:O:554:THR:HG22	1:O:556:LYS:HG3	1.97	0.47
1:A:554:THR:HG22	1:A:556:LYS:HG3	1.97	0.47
1:C:493:GLN:HG3	2:C:1000:ADP:O2'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:703:SER:C	1:J:703:SER:HB2	2.40	0.47
1:O:528:VAL:HG12	1:O:659:VAL:CG2	2.45	0.47
1:F:455:SER:HB3	1:F:458:VAL:HG23	1.96	0.46
1:K:667:ARG:HG2	1:K:667:ARG:HH11	1.80	0.46
1:P:579:VAL:O	1:P:597:LYS:NZ	2.48	0.46
1:C:559:LEU:HD11	1:C:607:ILE:HG13	1.97	0.46
1:E:579:VAL:O	1:E:597:LYS:NZ	2.48	0.46
1:G:704:ALA:CB	1:J:703:SER:H	2.28	0.46
1:I:459:LEU:HD23	1:I:459:LEU:H	1.80	0.46
1:P:471:PRO:HD2	1:P:506:ALA:HA	1.96	0.46
1:B:566:ARG:HD2	1:C:715:TYR:HD2	1.81	0.46
1:E:587:ILE:HD11	1:E:589:GLN:HE21	1.81	0.46
1:E:612:VAL:HG11	1:F:717:SER:HB3	1.97	0.46
1:F:455:SER:OG	1:F:457:GLN:HG2	2.16	0.46
1:G:579:VAL:O	1:G:597:LYS:NZ	2.48	0.46
1:O:449:PHE:HE2	1:O:674:LYS:HG3	1.80	0.46
1:F:700:ARG:HG3	1:F:710:TYR:CE1	2.50	0.46
1:H:574:LEU:HD12	1:H:606:LEU:HD22	1.96	0.46
1:N:579:VAL:O	1:N:597:LYS:NZ	2.49	0.46
1:A:707:ASP:CG	1:A:708:TYR:H	2.24	0.46
1:B:704:ALA:HA	1:O:703:SER:N	2.28	0.46
1:H:531:MET:HE1	1:H:547:LEU:HD23	1.98	0.46
1:O:455:SER:OG	1:O:457:GLN:HG2	2.16	0.46
1:D:498:ALA:HB2	1:D:546:ASN:HD22	1.81	0.46
1:I:531:MET:HE1	1:I:547:LEU:HD23	1.97	0.46
1:A:563:CYS:SG	1:A:641:ILE:HG23	2.56	0.46
1:D:700:ARG:NH2	1:D:703:SER:HA	2.31	0.46
1:A:493:GLN:HB2	1:A:494:SER:CA	2.34	0.46
1:N:710:TYR:CD1	1:N:710:TYR:C	2.94	0.46
1:O:529:LEU:HD23	1:O:640:LEU:HG	1.97	0.46
1:I:621:MET:HE3	1:I:657:ARG:HH12	1.80	0.46
1:M:674:LYS:HE3	1:N:707:ASP:HB3	1.98	0.46
1:J:455:SER:HB3	1:J:458:VAL:HG23	1.98	0.45
1:N:455:SER:OG	1:N:457:GLN:HG2	2.16	0.45
1:C:529:LEU:HD23	1:C:640:LEU:HG	1.98	0.45
1:D:621:MET:HE3	1:D:657:ARG:HH12	1.80	0.45
1:P:455:SER:HB3	1:P:458:VAL:HG23	1.99	0.45
1:P:529:LEU:HD23	1:P:640:LEU:HG	1.98	0.45
1:D:607:ILE:O	1:D:607:ILE:HG13	2.16	0.45
1:L:498:ALA:HB2	1:L:546:ASN:HD22	1.81	0.45
1:M:686:ASN:ND2	1:N:515:THR:HG22	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:531:MET:HE1	1:N:547:LEU:HD23	1.98	0.45
1:G:459:LEU:H	1:G:459:LEU:HD23	1.82	0.45
1:I:498:ALA:HB2	1:I:546:ASN:HD22	1.81	0.45
1:J:579:VAL:O	1:J:597:LYS:NZ	2.49	0.45
1:M:706:GLN:NE2	1:M:712:GLU:O	2.50	0.45
1:D:586:LEU:HD13	1:D:619:LEU:HB3	1.97	0.45
1:B:702:ALA:HB1	1:O:704:ALA:HA	1.98	0.45
1:H:579:VAL:O	1:H:597:LYS:NZ	2.50	0.45
1:A:702:ALA:HA	1:P:704:ALA:HB3	1.99	0.45
1:B:479:ARG:HE	1:B:494:SER:HB2	1.82	0.45
1:H:471:PRO:HD2	1:H:506:ALA:HA	1.98	0.45
1:M:455:SER:HB3	1:M:458:VAL:HG23	1.99	0.45
1:N:551:ILE:HD13	1:N:638:LEU:HD22	1.99	0.45
1:E:517:LEU:HD21	1:E:529:LEU:HD22	1.99	0.45
1:J:493:GLN:HB3	2:J:1000:ADP:O2'	2.16	0.45
1:L:530:MET:N	1:L:659:VAL:HG21	2.31	0.45
1:I:455:SER:HB3	1:I:458:VAL:HG23	1.99	0.44
1:J:530:MET:N	1:J:659:VAL:HG21	2.32	0.44
1:J:531:MET:HE1	1:J:547:LEU:HD23	1.98	0.44
1:M:579:VAL:O	1:M:597:LYS:NZ	2.50	0.44
1:O:493:GLN:HB2	2:O:1000:ADP:H3'	1.99	0.44
1:J:621:MET:HE3	1:J:657:ARG:HH12	1.82	0.44
1:L:579:VAL:O	1:L:597:LYS:NZ	2.50	0.44
1:O:710:TYR:CE1	1:O:712:GLU:HG2	2.52	0.44
1:P:517:LEU:HD21	1:P:529:LEU:HD22	2.00	0.44
1:D:668:TYR:C	1:D:670:VAL:H	2.25	0.44
1:H:533:GLY:N	1:H:540:MET:SD	2.90	0.44
1:H:662:THR:HB	1:H:690:VAL:HA	1.99	0.44
1:H:686:ASN:HB2	1:H:688:ILE:HD12	2.00	0.44
1:I:532:THR:HG21	1:I:683:PHE:CZ	2.53	0.44
1:N:455:SER:HB3	1:N:458:VAL:HG23	1.98	0.44
1:D:498:ALA:H	1:D:546:ASN:HD21	1.65	0.44
1:G:587:ILE:HD11	1:G:589:GLN:HB2	2.00	0.44
1:H:475:TRP:CH2	1:H:500:GLY:HA3	2.52	0.44
1:A:519:PHE:O	1:A:523:GLN:HB3	2.18	0.44
1:F:621:MET:HE3	1:F:657:ARG:HH12	1.82	0.44
1:A:703:SER:CB	1:P:703:SER:HB2	2.47	0.44
1:E:496:LEU:HD23	1:E:496:LEU:HA	1.89	0.44
1:I:530:MET:N	1:I:659:VAL:HG21	2.32	0.44
1:I:700:ARG:NH2	1:I:712:GLU:HB3	2.33	0.44
1:K:521:MET:HE1	1:K:638:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:574:LEU:HD12	1:C:606:LEU:HD22	2.00	0.44
1:F:498:ALA:H	1:F:546:ASN:HD21	1.65	0.44
1:I:579:VAL:O	1:I:597:LYS:NZ	2.51	0.44
1:D:584:GLU:OE1	1:D:610:GLY:HA3	2.18	0.44
1:H:571:HIS:HB3	1:H:608:PRO:HB3	2.00	0.44
1:J:706:GLN:NE2	1:J:712:GLU:O	2.51	0.44
1:K:496:LEU:HD13	1:K:546:ASN:ND2	2.32	0.44
1:B:498:ALA:HB2	1:B:546:ASN:HD22	1.83	0.44
1:O:517:LEU:HD21	1:O:529:LEU:HD22	2.00	0.44
1:A:498:ALA:H	1:A:546:ASN:ND2	2.16	0.43
1:H:498:ALA:HB2	1:H:546:ASN:HD22	1.82	0.43
1:B:531:MET:HE1	1:B:547:LEU:HD23	2.01	0.43
1:E:551:ILE:HD13	1:E:638:LEU:HD11	1.99	0.43
1:B:554:THR:HG22	1:B:556:LYS:HG3	2.01	0.43
1:D:704:ALA:HA	1:M:703:SER:C	2.44	0.43
1:G:574:LEU:HD12	1:G:606:LEU:HD22	2.00	0.43
1:L:521:MET:HE1	1:L:638:LEU:HD21	2.00	0.43
1:N:532:THR:HG21	1:N:683:PHE:CZ	2.54	0.43
1:D:530:MET:N	1:D:659:VAL:HG21	2.33	0.43
1:F:531:MET:HE1	1:F:547:LEU:HD23	2.00	0.43
1:G:521:MET:HE2	1:G:521:MET:HB3	1.95	0.43
1:H:533:GLY:HA3	1:H:540:MET:SD	2.59	0.43
1:I:706:GLN:HB3	1:I:711:TYR:HB3	2.00	0.43
1:K:705:TYR:N	1:K:706:GLN:HA	2.33	0.43
1:O:455:SER:HB3	1:O:458:VAL:HG23	1.99	0.43
1:E:530:MET:N	1:E:659:VAL:HG21	2.33	0.43
1:F:530:MET:N	1:F:659:VAL:HG21	2.33	0.43
1:F:554:THR:HG22	1:F:556:LYS:HG3	2.00	0.43
1:G:702:ALA:HA	1:J:704:ALA:HA	2.01	0.43
1:H:582:LEU:HA	1:H:585:ILE:HD12	2.00	0.43
1:K:674:LYS:HD2	1:L:707:ASP:OD2	2.18	0.43
1:O:530:MET:HE2	1:O:662:THR:HG23	2.00	0.43
1:A:496:LEU:HD21	1:A:549:ALA:HB2	2.00	0.43
1:M:551:ILE:HD13	1:M:638:LEU:HD22	2.01	0.43
1:M:574:LEU:HD12	1:M:606:LEU:HD22	2.00	0.43
1:C:534:VAL:HG11	1:C:675:GLU:HB3	2.01	0.43
1:D:579:VAL:O	1:D:597:LYS:NZ	2.51	0.43
1:G:706:GLN:HB2	1:G:713:TYR:CE1	2.53	0.43
1:O:450:ASN:ND2	1:O:674:LYS:HB2	2.34	0.43
1:C:492:LYS:O	2:C:1000:ADP:H3'	2.19	0.43
1:F:551:ILE:HD13	1:F:638:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:579:VAL:O	1:C:597:LYS:NZ	2.51	0.43
1:E:593:THR:HG23	1:E:631:TRP:HE1	1.83	0.43
1:I:648:ALA:HB2	1:J:713:TYR:HB2	2.01	0.43
1:M:532:THR:HG21	1:M:683:PHE:CZ	2.54	0.43
1:N:574:LEU:HD12	1:N:606:LEU:HD22	2.01	0.43
1:A:521:MET:HG2	1:A:661:THR:HG21	1.99	0.43
1:D:529:LEU:HD23	1:D:640:LEU:HG	2.00	0.43
1:G:529:LEU:HD23	1:G:640:LEU:HG	2.00	0.43
1:I:455:SER:OG	1:I:457:GLN:HG2	2.19	0.43
1:J:574:LEU:HD12	1:J:606:LEU:HD22	2.00	0.43
1:B:702:ALA:CB	1:O:705:TYR:H	2.31	0.42
1:A:686:ASN:HD22	1:B:515:THR:HG22	1.84	0.42
1:B:493:GLN:HG2	2:B:1000:ADP:O2'	2.18	0.42
1:F:653:ALA:HB1	1:F:686:ASN:HD22	1.84	0.42
1:I:700:ARG:HG3	1:I:710:TYR:HE2	1.84	0.42
1:G:559:LEU:HD11	1:G:607:ILE:HG13	2.01	0.42
1:M:498:ALA:H	1:M:546:ASN:ND2	2.17	0.42
1:O:530:MET:HB2	1:O:659:VAL:HG21	2.00	0.42
1:B:457:GLN:HE22	1:B:709:GLY:HA2	1.84	0.42
1:C:675:GLU:OE2	1:D:706:GLN:HB3	2.19	0.42
1:A:532:THR:HG21	1:A:683:PHE:CZ	2.54	0.42
1:C:532:THR:HG21	1:C:683:PHE:CZ	2.55	0.42
1:D:470:ILE:HA	1:D:471:PRO:HD3	1.97	0.42
1:H:459:LEU:HB2	1:H:464:ILE:HB	2.02	0.42
1:I:674:LYS:HD3	1:I:674:LYS:HA	1.90	0.42
1:N:529:LEU:HD23	1:N:640:LEU:HG	2.01	0.42
1:O:579:VAL:O	1:O:597:LYS:NZ	2.53	0.42
1:B:540:MET:HE1	1:B:645:PRO:HB3	2.01	0.42
1:E:702:ALA:HA	1:L:704:ALA:HA	2.02	0.42
1:P:530:MET:N	1:P:659:VAL:HG21	2.34	0.42
1:F:450:ASN:HD22	1:F:674:LYS:HB2	1.84	0.42
1:B:551:ILE:HD13	1:B:638:LEU:HD22	2.00	0.42
1:E:529:LEU:HD23	1:E:640:LEU:HG	2.02	0.42
1:G:475:TRP:CE2	1:G:479:ARG:HD2	2.55	0.42
1:G:533:GLY:N	1:G:540:MET:SD	2.93	0.42
1:K:540:MET:HE1	1:K:645:PRO:HB3	2.02	0.42
1:N:554:THR:HG22	1:N:556:LYS:HG3	2.01	0.42
1:P:497:LEU:O	1:P:499:VAL:N	2.40	0.42
1:A:475:TRP:CE3	1:A:497:LEU:HD13	2.55	0.42
1:B:526:ASN:ND2	1:B:528:VAL:H	2.17	0.42
1:D:531:MET:HE1	1:D:547:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:706:GLN:O	1:K:711:TYR:HD1	2.02	0.42
1:L:532:THR:HG21	1:L:683:PHE:CZ	2.54	0.42
1:P:621:MET:HE3	1:P:657:ARG:HH12	1.85	0.42
1:A:540:MET:HE1	1:A:645:PRO:HB3	2.02	0.42
1:C:476:GLN:HE21	1:C:497:LEU:HB2	1.84	0.42
1:D:540:MET:HE1	1:D:645:PRO:HB3	2.02	0.42
1:K:459:LEU:HB2	1:K:464:ILE:HB	2.02	0.42
1:M:531:MET:HE1	1:M:547:LEU:HD23	2.02	0.41
1:M:540:MET:HE1	1:M:645:PRO:HB3	2.02	0.41
1:N:586:LEU:O	1:N:588:GLY:HA2	2.20	0.41
1:D:475:TRP:CE3	1:D:497:LEU:HD13	2.55	0.41
1:D:609:ARG:NH2	1:D:612:VAL:HG23	2.36	0.41
1:H:479:ARG:NH1	1:H:495:GLN:HB3	2.35	0.41
1:A:703:SER:HB2	1:P:703:SER:CB	2.50	0.41
1:C:700:ARG:CG	1:C:710:TYR:HE2	2.34	0.41
1:D:532:THR:HG21	1:D:683:PHE:CZ	2.55	0.41
1:O:700:ARG:HH22	1:O:703:SER:HB3	1.85	0.41
1:E:557:ARG:NH1	1:E:635:ASN:O	2.54	0.41
1:K:532:THR:HG21	1:K:683:PHE:CZ	2.56	0.41
1:A:529:LEU:HD23	1:A:640:LEU:HG	2.02	0.41
1:I:582:LEU:HA	1:I:585:ILE:HD12	2.03	0.41
1:P:700:ARG:HG3	1:P:710:TYR:CE1	2.46	0.41
1:M:686:ASN:HD22	1:N:515:THR:HG22	1.85	0.41
1:N:498:ALA:H	1:N:546:ASN:ND2	2.18	0.41
1:N:586:LEU:C	1:N:588:GLY:HA2	2.46	0.41
1:B:566:ARG:O	1:B:567:LYS:CB	2.68	0.41
1:L:531:MET:HE1	1:L:547:LEU:HD23	2.03	0.41
1:M:470:ILE:HD13	1:M:543:VAL:HG22	2.03	0.41
1:P:699:PHE:HE2	1:P:701:ARG:HE	1.68	0.41
1:B:701:ARG:HD3	1:O:705:TYR:CE2	2.55	0.41
1:F:470:ILE:HA	1:F:471:PRO:HD3	1.96	0.41
1:K:644:PRO:HB3	1:L:715:TYR:CE2	2.55	0.41
1:N:526:ASN:ND2	1:N:660:GLY:HA3	2.35	0.41
1:O:531:MET:HE1	1:O:547:LEU:HD23	2.03	0.41
1:C:700:ARG:HG2	1:C:710:TYR:CE2	2.56	0.41
1:C:710:TYR:CE1	1:C:712:GLU:HG2	2.56	0.41
1:K:526:ASN:HD22	1:K:660:GLY:HA3	1.86	0.41
1:L:554:THR:HG22	1:L:556:LYS:HG3	2.01	0.41
1:M:592:ILE:HG22	1:M:593:THR:H	1.85	0.41
1:O:574:LEU:HD12	1:O:606:LEU:HD22	2.02	0.41
1:D:505:LEU:HD23	1:D:712:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:703:SER:O	1:J:703:SER:HB2	2.20	0.41
1:J:532:THR:HG21	1:J:683:PHE:CZ	2.56	0.41
1:M:496:LEU:HD23	1:M:496:LEU:HA	1.89	0.41
1:M:498:ALA:H	1:M:546:ASN:HD21	1.69	0.41
1:O:525:GLN:HE21	1:O:526:ASN:HB3	1.86	0.41
1:D:571:HIS:HB3	1:D:608:PRO:HB3	2.03	0.40
1:K:708:TYR:O	1:K:709:GLY:C	2.63	0.40
1:N:526:ASN:ND2	1:N:526:ASN:C	2.79	0.40
1:O:533:GLY:HA3	1:O:540:MET:SD	2.61	0.40
1:P:559:LEU:HD11	1:P:607:ILE:HG13	2.03	0.40
1:A:612:VAL:CG1	1:B:717:SER:HB3	2.45	0.40
1:A:703:SER:HB2	1:P:703:SER:HB2	2.02	0.40
1:A:703:SER:HB2	1:P:703:SER:OG	2.21	0.40
1:C:571:HIS:HB3	1:C:608:PRO:HB3	2.03	0.40
1:K:498:ALA:H	1:K:546:ASN:ND2	2.19	0.40
1:O:498:ALA:HB2	1:O:546:ASN:HD22	1.85	0.40
1:A:470:ILE:HD12	1:A:694:ILE:CG2	2.51	0.40
1:D:634:LYS:HD3	1:D:635:ASN:ND2	2.36	0.40
1:I:632:ALA:O	1:I:636:TYR:HB2	2.22	0.40
1:B:529:LEU:HD23	1:B:640:LEU:HG	2.03	0.40
1:G:458:VAL:O	1:G:461:GLU:HG2	2.22	0.40
1:K:667:ARG:HD3	1:K:670:VAL:HG21	2.03	0.40
1:J:477:LYS:O	1:J:481:SER:HB2	2.22	0.40
1:K:668:TYR:HB2	1:K:698:ILE:HG12	2.04	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	255/286 (89%)	235 (92%)	14 (6%)	6 (2%)	4 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	256/286 (90%)	233 (91%)	14 (6%)	9 (4%)	3	20
1	C	256/286 (90%)	231 (90%)	20 (8%)	5 (2%)	6	31
1	D	254/286 (89%)	237 (93%)	11 (4%)	6 (2%)	4	28
1	E	256/286 (90%)	234 (91%)	16 (6%)	6 (2%)	5	29
1	F	253/286 (88%)	234 (92%)	13 (5%)	6 (2%)	4	28
1	G	255/286 (89%)	233 (91%)	15 (6%)	7 (3%)	4	25
1	H	256/286 (90%)	231 (90%)	19 (7%)	6 (2%)	5	29
1	I	256/286 (90%)	237 (93%)	14 (6%)	5 (2%)	6	31
1	J	255/286 (89%)	232 (91%)	19 (8%)	4 (2%)	7	36
1	K	254/286 (89%)	232 (91%)	13 (5%)	9 (4%)	3	20
1	L	255/286 (89%)	238 (93%)	15 (6%)	2 (1%)	16	50
1	M	252/286 (88%)	228 (90%)	18 (7%)	6 (2%)	4	28
1	N	256/286 (90%)	236 (92%)	16 (6%)	4 (2%)	7	36
1	O	256/286 (90%)	234 (91%)	16 (6%)	6 (2%)	5	29
1	P	252/286 (88%)	231 (92%)	14 (6%)	7 (3%)	4	25
All	All	4077/4576 (89%)	3736 (92%)	247 (6%)	94 (2%)	5	29

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	668	TYR
1	A	708	TYR
1	B	496	LEU
1	B	703	SER
1	B	704	ALA
1	C	493	GLN
1	D	704	ALA
1	D	706	GLN
1	D	707	ASP
1	E	589	GLN
1	E	602	ALA
1	E	668	TYR
1	E	703	SER
1	E	708	TYR
1	F	668	TYR
1	F	704	ALA
1	F	711	TYR

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Mol	Chain	Res	Type
1	G	526	ASN
1	G	668	TYR
1	H	495	GLN
1	H	668	TYR
1	I	668	TYR
1	I	704	ALA
1	I	708	TYR
1	J	668	TYR
1	K	495	GLN
1	K	595	ALA
1	K	703	SER
1	K	709	GLY
1	K	711	TYR
1	K	715	TYR
1	L	668	TYR
1	L	708	TYR
1	M	592	ILE
1	M	668	TYR
1	M	703	SER
1	M	706	GLN
1	N	591	ASP
1	N	668	TYR
1	N	708	TYR
1	O	525	GLN
1	O	593	THR
1	O	668	TYR
1	P	668	TYR
1	P	708	TYR
1	A	706	GLN
1	A	707	ASP
1	B	567	LYS
1	B	706	GLN
1	C	524	ALA
1	F	589	GLN
1	I	703	SER
1	J	706	GLN
1	K	497	LEU
1	K	714	GLU
1	M	496	LEU
1	M	589	GLN
1	P	497	LEU
1	P	715	TYR

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Mol	Chain	Res	Type
1	B	590	GLY
1	C	707	ASP
1	D	453	ILE
1	D	671	ASN
1	D	672	THR
1	F	595	ALA
1	G	706	GLN
1	H	451	ARG
1	H	595	ALA
1	H	715	TYR
1	I	595	ALA
1	K	710	TYR
1	P	704	ALA
1	B	595	ALA
1	C	595	ALA
1	C	704	ALA
1	E	595	ALA
1	G	525	GLN
1	J	595	ALA
1	O	591	ASP
1	O	706	GLN
1	P	498	ALA
1	P	595	ALA
1	F	708	TYR
1	G	708	TYR
1	H	526	ASN
1	A	453	ILE
1	A	595	ALA
1	B	702	ALA
1	G	495	GLN
1	G	595	ALA
1	J	497	LEU
1	N	590	GLY
1	O	713	TYR
1	B	588	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	220/244 (90%)	197 (90%)	23 (10%)	6	28
1	B	221/244 (91%)	198 (90%)	23 (10%)	7	28
1	C	221/244 (91%)	195 (88%)	26 (12%)	5	23
1	D	220/244 (90%)	197 (90%)	23 (10%)	6	28
1	E	222/244 (91%)	201 (90%)	21 (10%)	8	32
1	F	218/244 (89%)	201 (92%)	17 (8%)	11	41
1	G	221/244 (91%)	195 (88%)	26 (12%)	5	23
1	H	221/244 (91%)	200 (90%)	21 (10%)	8	32
1	I	222/244 (91%)	200 (90%)	22 (10%)	7	31
1	J	221/244 (91%)	199 (90%)	22 (10%)	7	30
1	K	220/244 (90%)	203 (92%)	17 (8%)	12	41
1	L	220/244 (90%)	193 (88%)	27 (12%)	4	22
1	M	218/244 (89%)	197 (90%)	21 (10%)	8	32
1	N	222/244 (91%)	200 (90%)	22 (10%)	7	31
1	O	221/244 (91%)	197 (89%)	24 (11%)	6	26
1	P	218/244 (89%)	196 (90%)	22 (10%)	7	30
All	All	3526/3904 (90%)	3169 (90%)	357 (10%)	7	30

All (357) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	455	SER
1	A	472	LEU
1	A	477	LYS
1	A	480	ASP
1	A	492	LYS
1	A	493	GLN
1	A	507	ILE
1	A	517	LEU
1	A	523	GLN
1	A	529	LEU
1	A	550	VAL
1	A	554	THR
1	A	573	LEU
1	A	609	ARG
1	A	635	ASN

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Mol	Chain	Res	Type
1	A	638	LEU
1	A	659	VAL
1	A	663	LEU
1	A	700	ARG
1	A	703	SER
1	A	710	TYR
1	A	712	GLU
1	A	716	LYS
1	B	460	GLU
1	B	517	LEU
1	B	525	GLN
1	B	529	LEU
1	B	550	VAL
1	B	554	THR
1	B	569	TYR
1	B	573	LEU
1	B	587	ILE
1	B	593	THR
1	B	609	ARG
1	B	634	LYS
1	B	638	LEU
1	B	647	LEU
1	B	663	LEU
1	B	682	ARG
1	B	695	LEU
1	B	700	ARG
1	B	701	ARG
1	B	703	SER
1	B	707	ASP
1	B	712	GLU
1	B	718	ASP
1	C	459	LEU
1	C	465	SER
1	C	479	ARG
1	C	493	GLN
1	C	495	GLN
1	C	507	ILE
1	C	517	LEU
1	C	522	MET
1	C	529	LEU
1	C	534	VAL
1	C	550	VAL

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Mol	Chain	Res	Type
1	C	552	SER
1	C	554	THR
1	C	584	GLU
1	C	589	GLN
1	C	593	THR
1	C	609	ARG
1	C	624	ARG
1	C	638	LEU
1	C	663	LEU
1	C	679	SER
1	C	695	LEU
1	C	705	TYR
1	C	710	TYR
1	C	711	TYR
1	C	714	GLU
1	D	454	GLU
1	D	460	GLU
1	D	479	ARG
1	D	495	GLN
1	D	496	LEU
1	D	529	LEU
1	D	550	VAL
1	D	554	THR
1	D	573	LEU
1	D	583	SER
1	D	593	THR
1	D	607	ILE
1	D	609	ARG
1	D	624	ARG
1	D	638	LEU
1	D	663	LEU
1	D	672	THR
1	D	677	GLU
1	D	695	LEU
1	D	705	TYR
1	D	707	ASP
1	D	710	TYR
1	D	711	TYR
1	E	474	GLU
1	E	479	ARG
1	E	491	TYR
1	E	496	LEU

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Mol	Chain	Res	Type
1	E	517	LEU
1	E	521	MET
1	E	522	MET
1	E	529	LEU
1	E	550	VAL
1	E	554	THR
1	E	589	GLN
1	E	593	THR
1	E	609	ARG
1	E	638	LEU
1	E	663	LEU
1	E	695	LEU
1	E	701	ARG
1	E	703	SER
1	E	710	TYR
1	E	711	TYR
1	E	712	GLU
1	F	451	ARG
1	F	459	LEU
1	F	479	ARG
1	F	495	GLN
1	F	496	LEU
1	F	529	LEU
1	F	550	VAL
1	F	554	THR
1	F	587	ILE
1	F	593	THR
1	F	609	ARG
1	F	638	LEU
1	F	647	LEU
1	F	663	LEU
1	F	695	LEU
1	F	705	TYR
1	F	712	GLU
1	G	450	ASN
1	G	493	GLN
1	G	517	LEU
1	G	523	GLN
1	G	526	ASN
1	G	529	LEU
1	G	550	VAL
1	G	554	THR

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Mol	Chain	Res	Type
1	G	555	ASN
1	G	558	VAL
1	G	573	LEU
1	G	585	ILE
1	G	587	ILE
1	G	589	GLN
1	G	593	THR
1	G	609	ARG
1	G	638	LEU
1	G	659	VAL
1	G	663	LEU
1	G	674	LYS
1	G	691	LYS
1	G	695	LEU
1	G	708	TYR
1	G	710	TYR
1	G	711	TYR
1	G	714	GLU
1	H	451	ARG
1	H	459	LEU
1	H	510	ILE
1	H	517	LEU
1	H	529	LEU
1	H	550	VAL
1	H	554	THR
1	H	576	THR
1	H	580	ASN
1	H	593	THR
1	H	609	ARG
1	H	635	ASN
1	H	638	LEU
1	H	647	LEU
1	H	659	VAL
1	H	680	LEU
1	H	695	LEU
1	H	703	SER
1	H	711	TYR
1	H	714	GLU
1	H	716	LYS
1	I	459	LEU
1	I	496	LEU
1	I	517	LEU

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Mol	Chain	Res	Type
1	I	525	GLN
1	I	529	LEU
1	I	550	VAL
1	I	554	THR
1	I	573	LEU
1	I	587	ILE
1	I	591	ASP
1	I	593	THR
1	I	609	ARG
1	I	634	LYS
1	I	638	LEU
1	I	647	LEU
1	I	663	LEU
1	I	680	LEU
1	I	695	LEU
1	I	710	TYR
1	I	711	TYR
1	I	712	GLU
1	I	716	LYS
1	J	450	ASN
1	J	451	ARG
1	J	459	LEU
1	J	494	SER
1	J	495	GLN
1	J	496	LEU
1	J	512	SER
1	J	517	LEU
1	J	523	GLN
1	J	529	LEU
1	J	550	VAL
1	J	554	THR
1	J	589	GLN
1	J	593	THR
1	J	609	ARG
1	J	634	LYS
1	J	638	LEU
1	J	663	LEU
1	J	674	LYS
1	J	680	LEU
1	J	695	LEU
1	J	707	ASP
1	K	459	LEU

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Mol	Chain	Res	Type
1	K	496	LEU
1	K	517	LEU
1	K	525	GLN
1	K	526	ASN
1	K	529	LEU
1	K	550	VAL
1	K	576	THR
1	K	593	THR
1	K	609	ARG
1	K	638	LEU
1	K	659	VAL
1	K	663	LEU
1	K	680	LEU
1	K	695	LEU
1	K	707	ASP
1	K	711	TYR
1	L	459	LEU
1	L	479	ARG
1	L	495	GLN
1	L	517	LEU
1	L	522	MET
1	L	525	GLN
1	L	529	LEU
1	L	550	VAL
1	L	554	THR
1	L	572	GLU
1	L	573	LEU
1	L	593	THR
1	L	594	THR
1	L	609	ARG
1	L	638	LEU
1	L	647	LEU
1	L	663	LEU
1	L	680	LEU
1	L	695	LEU
1	L	701	ARG
1	L	705	TYR
1	L	706	GLN
1	L	707	ASP
1	L	708	TYR
1	L	711	TYR
1	L	712	GLU

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Mol	Chain	Res	Type
1	L	714	GLU
1	M	454	GLU
1	M	459	LEU
1	M	496	LEU
1	M	517	LEU
1	M	522	MET
1	M	529	LEU
1	M	550	VAL
1	M	554	THR
1	M	573	LEU
1	M	593	THR
1	M	609	ARG
1	M	624	ARG
1	M	638	LEU
1	M	647	LEU
1	M	657	ARG
1	M	659	VAL
1	M	663	LEU
1	M	680	LEU
1	M	695	LEU
1	M	701	ARG
1	M	716	LYS
1	N	450	ASN
1	N	453	ILE
1	N	459	LEU
1	N	482	VAL
1	N	496	LEU
1	N	517	LEU
1	N	526	ASN
1	N	529	LEU
1	N	550	VAL
1	N	554	THR
1	N	593	THR
1	N	609	ARG
1	N	624	ARG
1	N	638	LEU
1	N	647	LEU
1	N	659	VAL
1	N	663	LEU
1	N	680	LEU
1	N	695	LEU
1	N	710	TYR

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Mol	Chain	Res	Type
1	N	711	TYR
1	N	714	GLU
1	O	451	ARG
1	O	479	ARG
1	O	481	SER
1	O	495	GLN
1	O	496	LEU
1	O	517	LEU
1	O	526	ASN
1	O	529	LEU
1	O	550	VAL
1	O	554	THR
1	O	609	ARG
1	O	624	ARG
1	O	638	LEU
1	O	659	VAL
1	O	663	LEU
1	O	678	THR
1	O	680	LEU
1	O	684	GLU
1	O	691	LYS
1	O	695	LEU
1	O	703	SER
1	O	710	TYR
1	O	711	TYR
1	O	716	LYS
1	P	451	ARG
1	P	454	GLU
1	P	459	LEU
1	P	482	VAL
1	P	496	LEU
1	P	517	LEU
1	P	529	LEU
1	P	550	VAL
1	P	558	VAL
1	P	593	THR
1	P	609	ARG
1	P	624	ARG
1	P	638	LEU
1	P	647	LEU
1	P	663	LEU
1	P	680	LEU

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Mol	Chain	Res	Type
1	P	684	GLU
1	P	695	LEU
1	P	703	SER
1	P	710	TYR
1	P	711	TYR
1	P	714	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	476	GLN
1	A	523	GLN
1	A	527	ASN
1	A	546	ASN
1	A	658	HIS
1	A	686	ASN
1	B	462	HIS
1	B	476	GLN
1	B	525	GLN
1	B	526	ASN
1	B	546	ASN
1	B	580	ASN
1	B	589	GLN
1	B	658	HIS
1	C	476	GLN
1	C	495	GLN
1	C	526	ASN
1	C	658	HIS
1	D	457	GLN
1	D	476	GLN
1	D	523	GLN
1	D	546	ASN
1	D	635	ASN
1	D	658	HIS
1	D	706	GLN
1	E	457	GLN
1	E	476	GLN
1	E	495	GLN
1	E	553	GLN
1	E	589	GLN
1	E	658	HIS
1	E	685	GLN

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Mol	Chain	Res	Type
1	E	686	ASN
1	F	450	ASN
1	F	457	GLN
1	F	476	GLN
1	F	518	HIS
1	F	523	GLN
1	F	526	ASN
1	F	546	ASN
1	F	580	ASN
1	F	589	GLN
1	F	658	HIS
1	F	706	GLN
1	G	518	HIS
1	G	526	ASN
1	G	546	ASN
1	G	580	ASN
1	G	589	GLN
1	G	658	HIS
1	G	685	GLN
1	H	476	GLN
1	H	495	GLN
1	H	518	HIS
1	H	523	GLN
1	H	546	ASN
1	H	555	ASN
1	H	630	ASN
1	H	658	HIS
1	H	686	ASN
1	I	457	GLN
1	I	525	GLN
1	I	546	ASN
1	I	580	ASN
1	I	635	ASN
1	I	658	HIS
1	J	523	GLN
1	J	546	ASN
1	J	553	GLN
1	J	555	ASN
1	J	630	ASN
1	J	658	HIS
1	K	457	GLN
1	K	476	GLN

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Mol	Chain	Res	Type
1	K	493	GLN
1	K	495	GLN
1	K	525	GLN
1	K	526	ASN
1	K	546	ASN
1	K	553	GLN
1	K	658	HIS
1	K	706	GLN
1	L	476	GLN
1	L	523	GLN
1	L	546	ASN
1	L	580	ASN
1	L	589	GLN
1	L	658	HIS
1	M	457	GLN
1	M	476	GLN
1	M	546	ASN
1	M	658	HIS
1	M	685	GLN
1	M	686	ASN
1	N	457	GLN
1	N	476	GLN
1	N	526	ASN
1	N	546	ASN
1	O	450	ASN
1	O	457	GLN
1	O	476	GLN
1	O	493	GLN
1	O	525	GLN
1	O	546	ASN
1	O	580	ASN
1	O	658	HIS
1	O	706	GLN
1	P	518	HIS
1	P	526	ASN
1	P	546	ASN
1	P	658	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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$
2	ADP	B	1000	3	28,29,29	1.38	5 (17%)	43,45,45	0.94	2 (4%)
2	ADP	A	1000	3	28,29,29	1.25	3 (10%)	43,45,45	1.16	5 (11%)
2	ADP	D	1000	3	28,29,29	1.38	5 (17%)	43,45,45	1.14	4 (9%)
2	ADP	O	1000	3	28,29,29	1.72	5 (17%)	43,45,45	1.09	4 (9%)
2	ADP	E	1000	3	28,29,29	1.09	3 (10%)	43,45,45	1.07	2 (4%)
2	ADP	C	1000	3	28,29,29	1.31	3 (10%)	43,45,45	1.13	4 (9%)
2	ADP	H	1000	3	28,29,29	1.42	4 (14%)	43,45,45	1.12	4 (9%)
2	ADP	G	1000	3	28,29,29	1.57	3 (10%)	43,45,45	1.59	8 (18%)
2	ADP	K	1000	3	28,29,29	1.16	2 (7%)	43,45,45	1.06	4 (9%)
2	ADP	L	1000	3	28,29,29	1.41	5 (17%)	43,45,45	1.03	4 (9%)
2	ADP	M	1000	3	28,29,29	1.21	3 (10%)	43,45,45	1.11	3 (6%)
2	ADP	N	1000	3	28,29,29	1.15	2 (7%)	43,45,45	1.18	3 (6%)
2	ADP	I	1000	3	28,29,29	1.22	2 (7%)	43,45,45	1.04	3 (6%)
2	ADP	P	1000	3	28,29,29	1.24	4 (14%)	43,45,45	1.06	3 (6%)
2	ADP	J	1000	3	28,29,29	1.20	4 (14%)	43,45,45	1.30	6 (13%)
2	ADP	F	1000	3	28,29,29	1.33	3 (10%)	43,45,45	1.15	4 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	1000	3	-	0/16/32/32	0/3/3/3
2	ADP	A	1000	3	-	0/16/32/32	0/3/3/3
2	ADP	D	1000	3	-	5/16/32/32	0/3/3/3
2	ADP	O	1000	3	-	2/16/32/32	0/3/3/3
2	ADP	E	1000	3	-	2/16/32/32	0/3/3/3
2	ADP	C	1000	3	-	0/16/32/32	0/3/3/3
2	ADP	H	1000	3	-	2/16/32/32	0/3/3/3
2	ADP	G	1000	3	-	5/16/32/32	0/3/3/3
2	ADP	K	1000	3	-	0/16/32/32	0/3/3/3
2	ADP	L	1000	3	-	2/16/32/32	0/3/3/3
2	ADP	M	1000	3	-	2/16/32/32	0/3/3/3
2	ADP	N	1000	3	-	0/16/32/32	0/3/3/3
2	ADP	I	1000	3	-	0/16/32/32	0/3/3/3
2	ADP	P	1000	3	-	0/16/32/32	0/3/3/3
2	ADP	J	1000	3	-	0/16/32/32	0/3/3/3
2	ADP	F	1000	3	-	0/16/32/32	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1000	ADP	C2-N1	4.93	1.42	1.33
2	H	1000	ADP	PA-O3A	-4.44	1.54	1.59
2	G	1000	ADP	PA-O3A	-4.25	1.54	1.59
2	L	1000	ADP	C2-N1	3.87	1.40	1.33
2	A	1000	ADP	C2-N1	3.86	1.40	1.33
2	O	1000	ADP	PA-O3A	-3.49	1.55	1.59
2	G	1000	ADP	C4-N3	3.40	1.40	1.34
2	C	1000	ADP	C2-N1	3.30	1.39	1.33
2	F	1000	ADP	C2-N1	3.28	1.39	1.33
2	B	1000	ADP	C2-N1	3.26	1.39	1.33
2	C	1000	ADP	PA-O3A	-3.22	1.56	1.59
2	G	1000	ADP	C2-N1	3.14	1.39	1.33
2	B	1000	ADP	C4-N3	3.13	1.40	1.34
2	O	1000	ADP	C5-C4	3.12	1.44	1.39
2	K	1000	ADP	C2-N1	3.05	1.39	1.33
2	O	1000	ADP	C4-N3	3.04	1.40	1.34
2	I	1000	ADP	C2-N1	3.02	1.39	1.33
2	J	1000	ADP	C2-N1	2.98	1.39	1.33
2	L	1000	ADP	C4-N3	2.97	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1000	ADP	C2-N1	2.96	1.39	1.33
2	K	1000	ADP	C2-N3	2.93	1.39	1.33
2	O	1000	ADP	C2-N3	2.89	1.39	1.33
2	N	1000	ADP	C2-N1	2.86	1.39	1.33
2	P	1000	ADP	C2-N1	2.84	1.39	1.33
2	B	1000	ADP	C2-N3	2.77	1.38	1.33
2	H	1000	ADP	C2-N3	2.75	1.38	1.33
2	C	1000	ADP	C4-N3	2.73	1.39	1.34
2	A	1000	ADP	C5-C4	2.70	1.43	1.39
2	F	1000	ADP	C4-N3	2.68	1.39	1.34
2	D	1000	ADP	C4-N3	2.68	1.39	1.34
2	E	1000	ADP	C2-N3	2.65	1.38	1.33
2	H	1000	ADP	C4-N3	2.64	1.39	1.34
2	M	1000	ADP	C4-N3	2.61	1.39	1.34
2	F	1000	ADP	C2-N3	2.60	1.38	1.33
2	P	1000	ADP	C2-N3	2.59	1.38	1.33
2	P	1000	ADP	C4-N3	2.57	1.39	1.34
2	H	1000	ADP	C2-N1	2.55	1.38	1.33
2	J	1000	ADP	C5-C4	2.52	1.43	1.39
2	A	1000	ADP	C2-N3	2.51	1.38	1.33
2	L	1000	ADP	C2-N3	2.47	1.38	1.33
2	E	1000	ADP	C2-N1	2.46	1.38	1.33
2	I	1000	ADP	C2-N3	2.38	1.38	1.33
2	P	1000	ADP	C5-C4	2.33	1.43	1.39
2	D	1000	ADP	PA-O3A	-2.32	1.57	1.59
2	J	1000	ADP	C4-N3	2.31	1.38	1.34
2	L	1000	ADP	C5-C4	2.29	1.43	1.39
2	B	1000	ADP	C5-C4	2.28	1.43	1.39
2	D	1000	ADP	C6-N6	2.28	1.40	1.34
2	M	1000	ADP	C2-N1	2.24	1.37	1.33
2	D	1000	ADP	O4'-C1'	2.19	1.47	1.42
2	M	1000	ADP	C5-C4	2.19	1.43	1.39
2	N	1000	ADP	O4'-C1'	2.15	1.47	1.42
2	E	1000	ADP	C6-N6	2.14	1.39	1.34
2	J	1000	ADP	O4'-C1'	2.06	1.46	1.42
2	L	1000	ADP	C6-N6	2.06	1.39	1.34
2	B	1000	ADP	PA-O3A	-2.06	1.57	1.59

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1000	ADP	O3B-PB-O3A	4.13	118.49	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1000	ADP	O3B-PB-O3A	3.89	117.69	104.64
2	O	1000	ADP	O3B-PB-O3A	3.77	117.28	104.64
2	J	1000	ADP	C4-N9-C8	3.68	109.61	105.74
2	E	1000	ADP	O3B-PB-O3A	3.67	116.94	104.64
2	G	1000	ADP	C5-C4-N9	-3.60	101.88	105.81
2	M	1000	ADP	O3B-PB-O3A	3.59	116.68	104.64
2	F	1000	ADP	O2A-PA-O3A	3.55	116.88	107.27
2	G	1000	ADP	C4-N9-C8	3.43	109.34	105.74
2	J	1000	ADP	O2A-PA-O3A	3.30	116.18	107.27
2	F	1000	ADP	O3B-PB-O3A	3.20	115.36	104.64
2	P	1000	ADP	O3B-PB-O3A	3.10	115.04	104.64
2	P	1000	ADP	O2A-PA-O3A	3.10	115.65	107.27
2	K	1000	ADP	O2A-PA-O3A	3.07	115.56	107.27
2	H	1000	ADP	O2A-PA-O3A	3.04	115.48	107.27
2	C	1000	ADP	O3B-PB-O3A	3.00	114.70	104.64
2	D	1000	ADP	C4-N9-C8	2.90	108.78	105.74
2	C	1000	ADP	C4-N9-C8	2.85	108.73	105.74
2	J	1000	ADP	C5-C4-N9	-2.84	102.71	105.81
2	L	1000	ADP	C4-N9-C8	2.83	108.71	105.74
2	C	1000	ADP	O2A-PA-O3A	2.82	114.89	107.27
2	L	1000	ADP	O3B-PB-O3A	2.81	114.06	104.64
2	G	1000	ADP	O3B-PB-O1B	-2.73	100.21	110.83
2	M	1000	ADP	C4-N9-C8	2.72	108.59	105.74
2	A	1000	ADP	O2A-PA-O3A	2.71	114.58	107.27
2	I	1000	ADP	C4-N9-C8	2.70	108.57	105.74
2	E	1000	ADP	O2A-PA-O3A	2.66	114.47	107.27
2	B	1000	ADP	O2A-PA-O3A	2.65	114.43	107.27
2	K	1000	ADP	O3B-PB-O3A	2.65	113.51	104.64
2	G	1000	ADP	C2'-C3'-C4'	-2.62	97.54	102.61
2	A	1000	ADP	O3B-PB-O3A	2.54	113.16	104.64
2	M	1000	ADP	O2A-PA-O3A	2.50	114.04	107.27
2	I	1000	ADP	O2A-PA-O3A	2.50	114.03	107.27
2	K	1000	ADP	C4-N9-C8	2.49	108.35	105.74
2	G	1000	ADP	N3-C2-N1	-2.46	124.85	128.58
2	O	1000	ADP	C4-N9-C8	2.46	108.32	105.74
2	A	1000	ADP	O2B-PB-O3A	2.37	112.59	104.64
2	L	1000	ADP	C5-C4-N9	-2.36	103.24	105.81
2	F	1000	ADP	O2B-PB-O3A	2.33	112.45	104.64
2	I	1000	ADP	O3B-PB-O3A	2.33	112.44	104.64
2	J	1000	ADP	O3B-PB-O3A	2.31	112.39	104.64
2	C	1000	ADP	C5-C4-N9	-2.29	103.32	105.81
2	A	1000	ADP	C5-N7-C8	2.28	107.04	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	ADP	C4-N9-C8	2.26	108.11	105.74
2	H	1000	ADP	C4-N9-C8	2.26	108.11	105.74
2	N	1000	ADP	O3B-PB-O3A	2.25	112.20	104.64
2	L	1000	ADP	O2A-PA-O3A	2.24	113.34	107.27
2	D	1000	ADP	O2'-C2'-C1'	-2.24	102.39	110.10
2	G	1000	ADP	N3-C4-N9	2.23	130.96	127.17
2	O	1000	ADP	C5-C4-N9	-2.23	103.38	105.81
2	N	1000	ADP	C4-N9-C8	2.22	108.07	105.74
2	K	1000	ADP	O2B-PB-O3A	2.22	112.09	104.64
2	J	1000	ADP	O2B-PB-O3A	2.22	112.07	104.64
2	P	1000	ADP	C4-N9-C8	2.19	108.04	105.74
2	B	1000	ADP	O4'-C4'-C3'	2.16	109.45	105.15
2	J	1000	ADP	N9-C8-N7	-2.15	110.89	113.94
2	D	1000	ADP	C5-C4-N9	-2.11	103.51	105.81
2	O	1000	ADP	O2A-PA-O3A	2.07	112.86	107.27
2	N	1000	ADP	O4'-C4'-C3'	-2.06	101.05	105.15
2	G	1000	ADP	O2A-PA-O3A	2.05	112.82	107.27
2	H	1000	ADP	O3B-PB-O1B	-2.04	102.87	110.83
2	F	1000	ADP	C5-N7-C8	2.04	106.66	103.45
2	D	1000	ADP	C5-N7-C8	2.00	106.59	103.45

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1000	ADP	PA-O3A-PB-O3B
2	D	1000	ADP	C5'-O5'-PA-O3A
2	E	1000	ADP	PA-O3A-PB-O2B
2	E	1000	ADP	PA-O3A-PB-O3B
2	G	1000	ADP	PA-O3A-PB-O2B
2	G	1000	ADP	PA-O3A-PB-O3B
2	H	1000	ADP	PA-O3A-PB-O2B
2	H	1000	ADP	PA-O3A-PB-O3B
2	L	1000	ADP	PA-O3A-PB-O3B
2	M	1000	ADP	PA-O3A-PB-O2B
2	M	1000	ADP	PA-O3A-PB-O3B
2	O	1000	ADP	PA-O3A-PB-O3B
2	D	1000	ADP	PB-O3A-PA-O5'
2	L	1000	ADP	PA-O3A-PB-O2B
2	O	1000	ADP	PA-O3A-PB-O2B
2	D	1000	ADP	C5'-O5'-PA-O1A
2	G	1000	ADP	C3'-C4'-C5'-O5'

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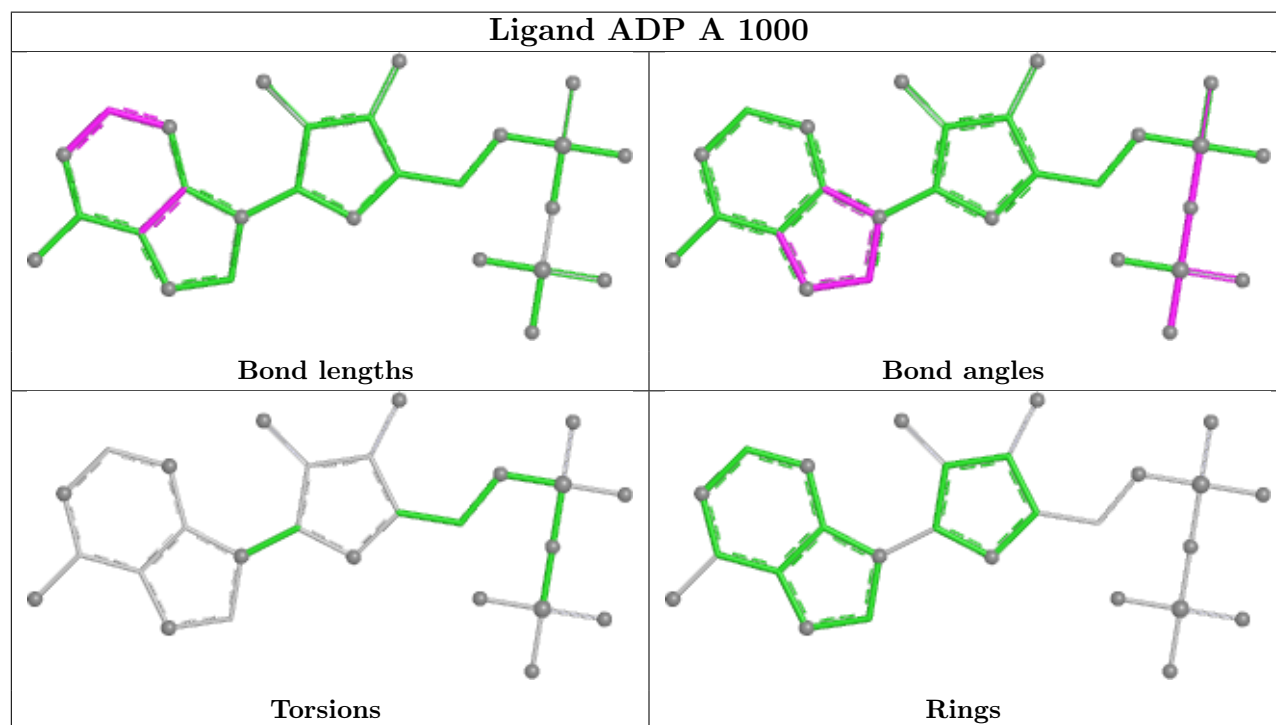
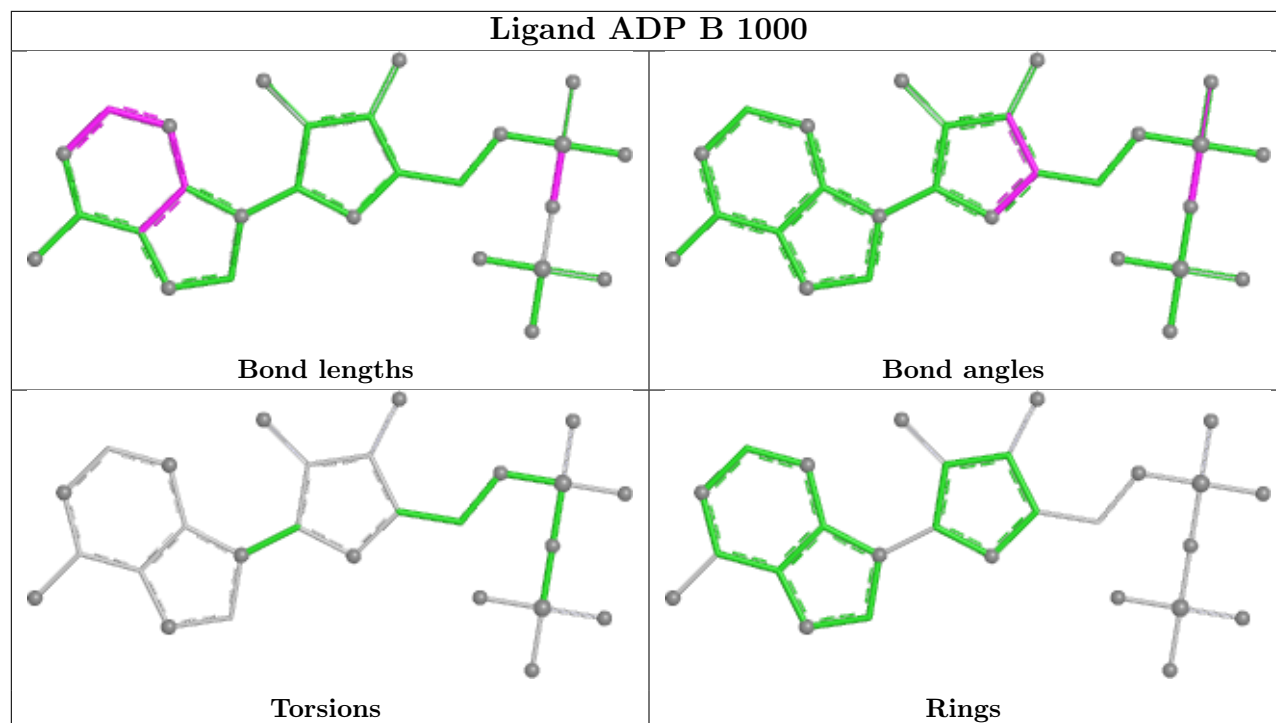
Mol	Chain	Res	Type	Atoms
2	G	1000	ADP	O4'-C4'-C5'-O5'
2	D	1000	ADP	C4'-C5'-O5'-PA
2	G	1000	ADP	PA-O3A-PB-O1B

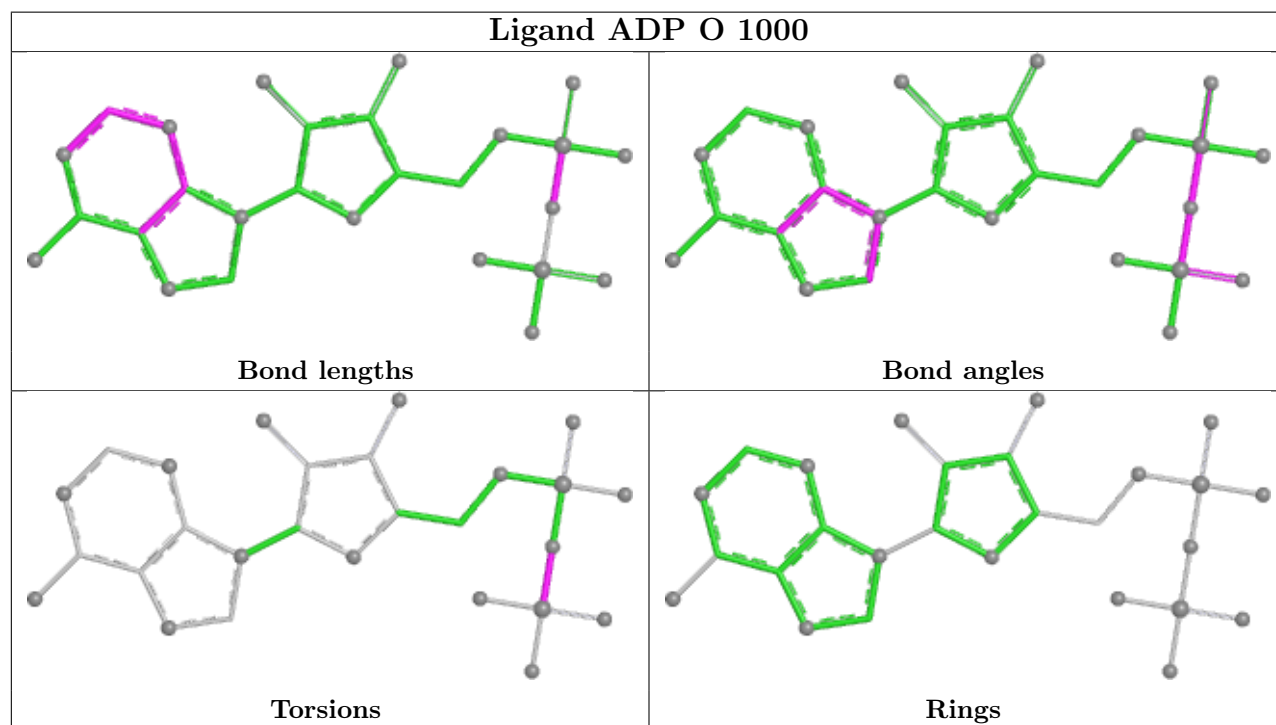
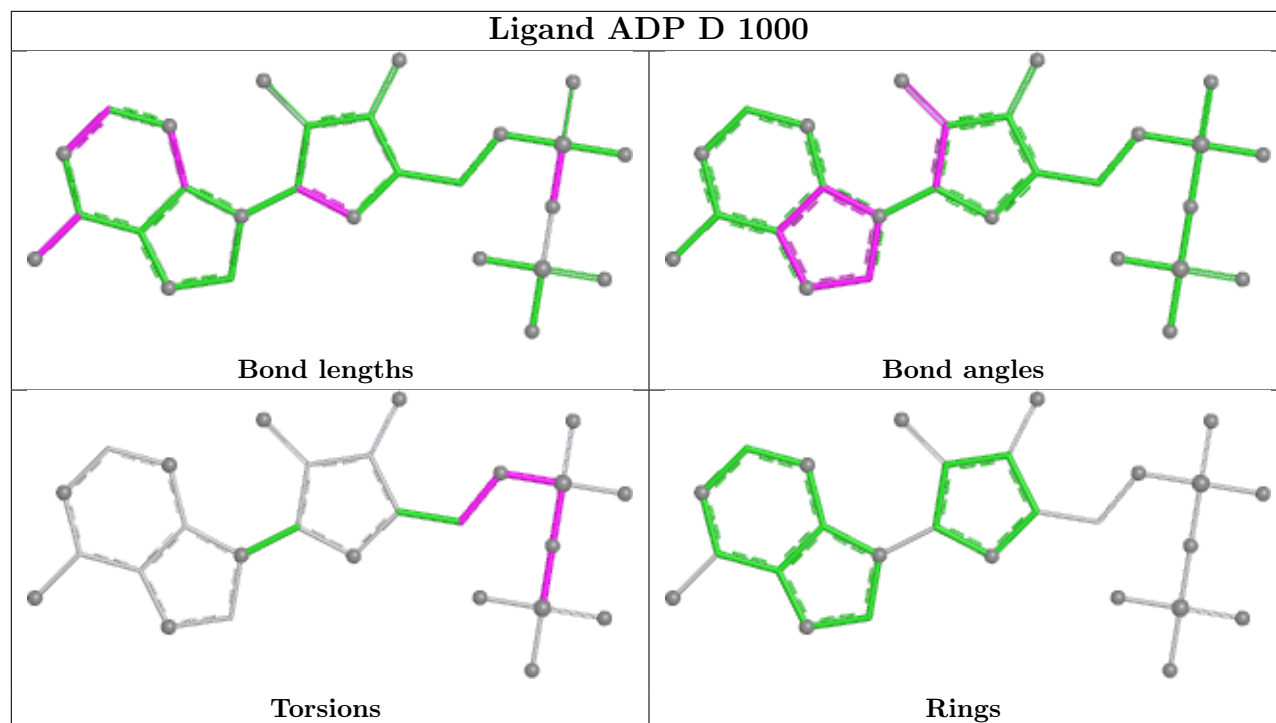
There are no ring outliers.

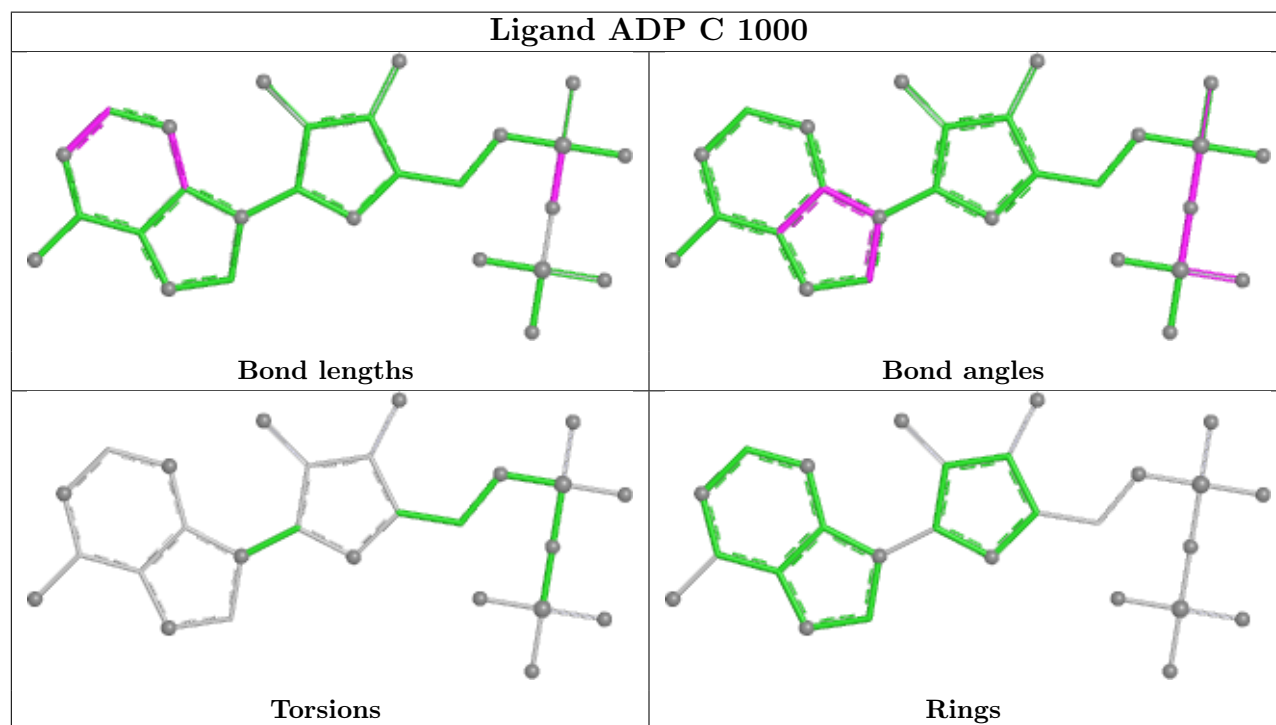
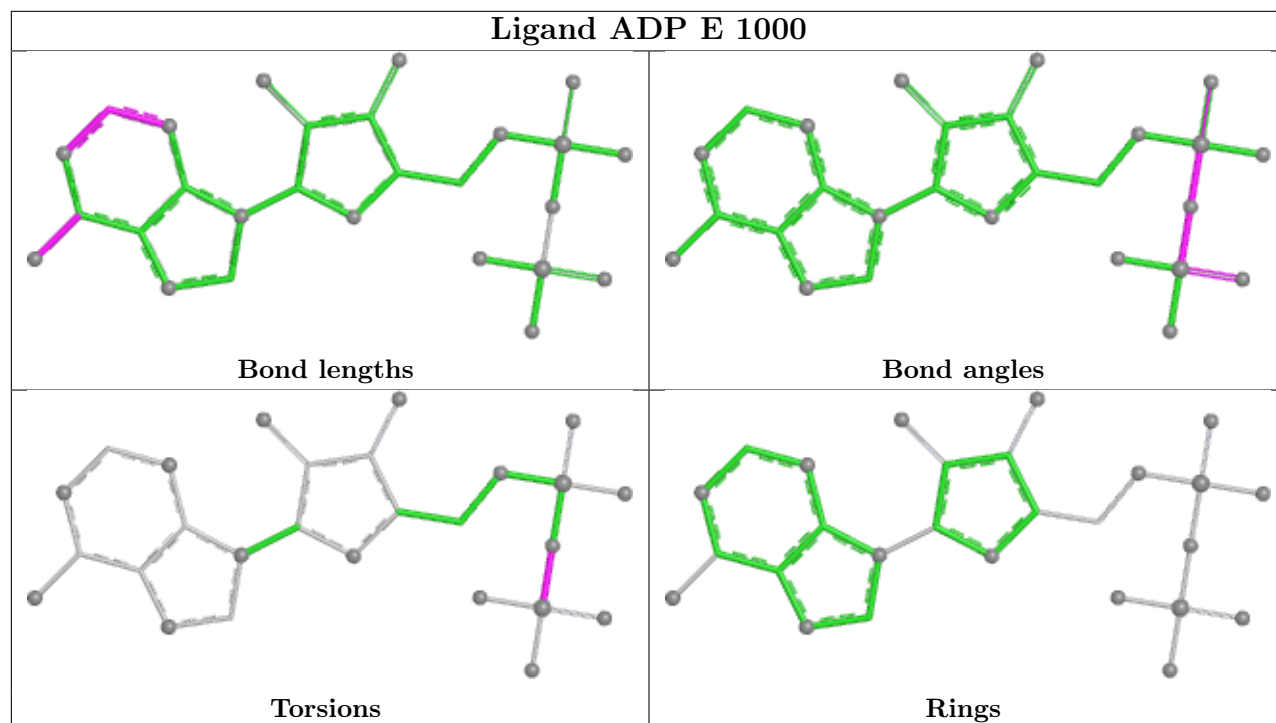
7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1000	ADP	1	0
2	D	1000	ADP	1	0
2	O	1000	ADP	1	0
2	C	1000	ADP	2	0
2	G	1000	ADP	1	0
2	N	1000	ADP	1	0
2	J	1000	ADP	1	0

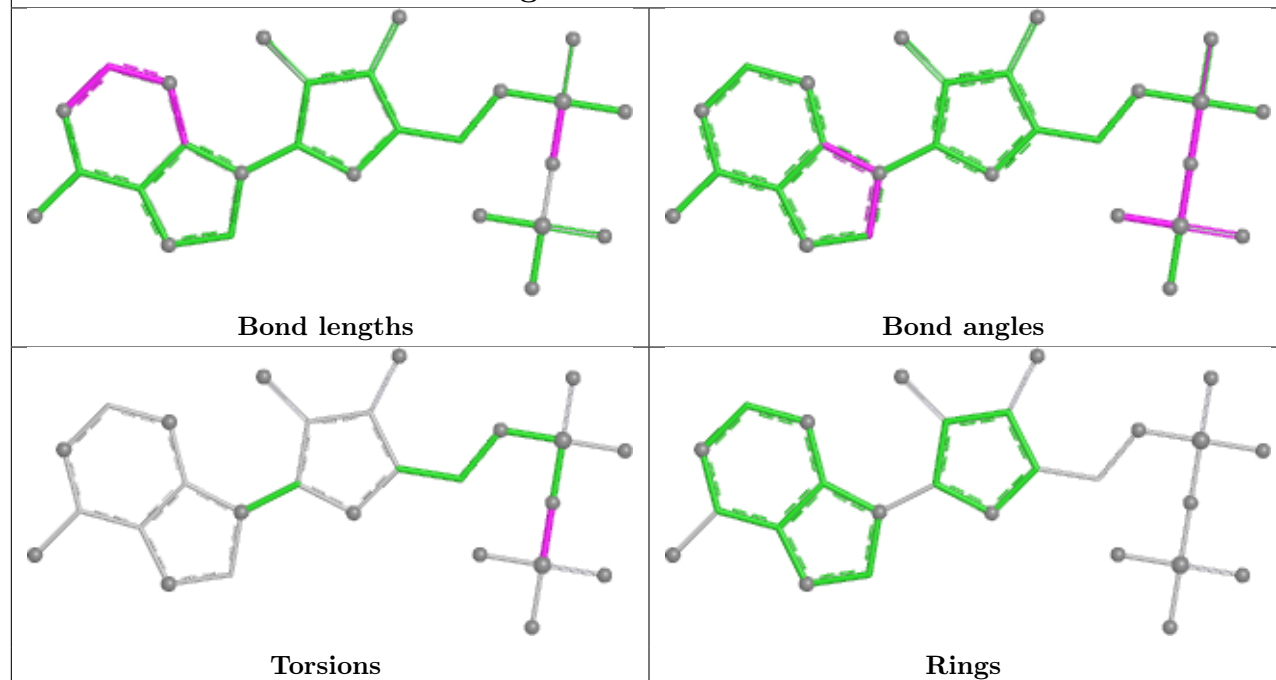
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



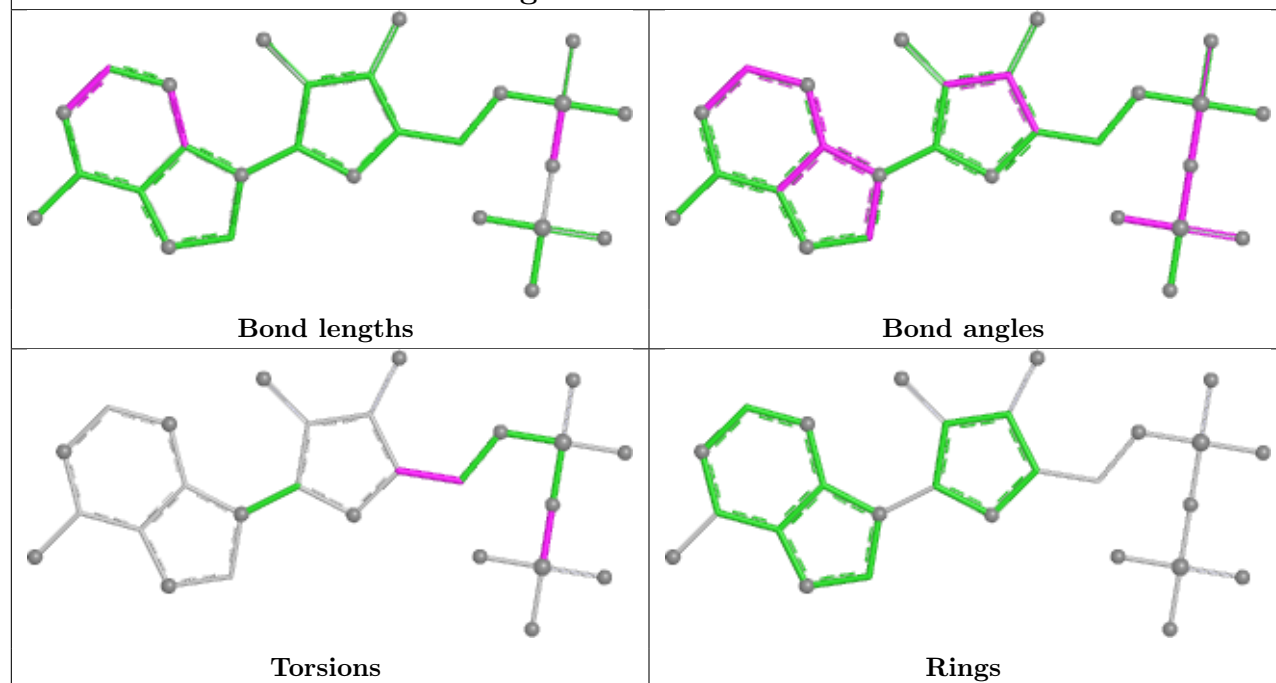


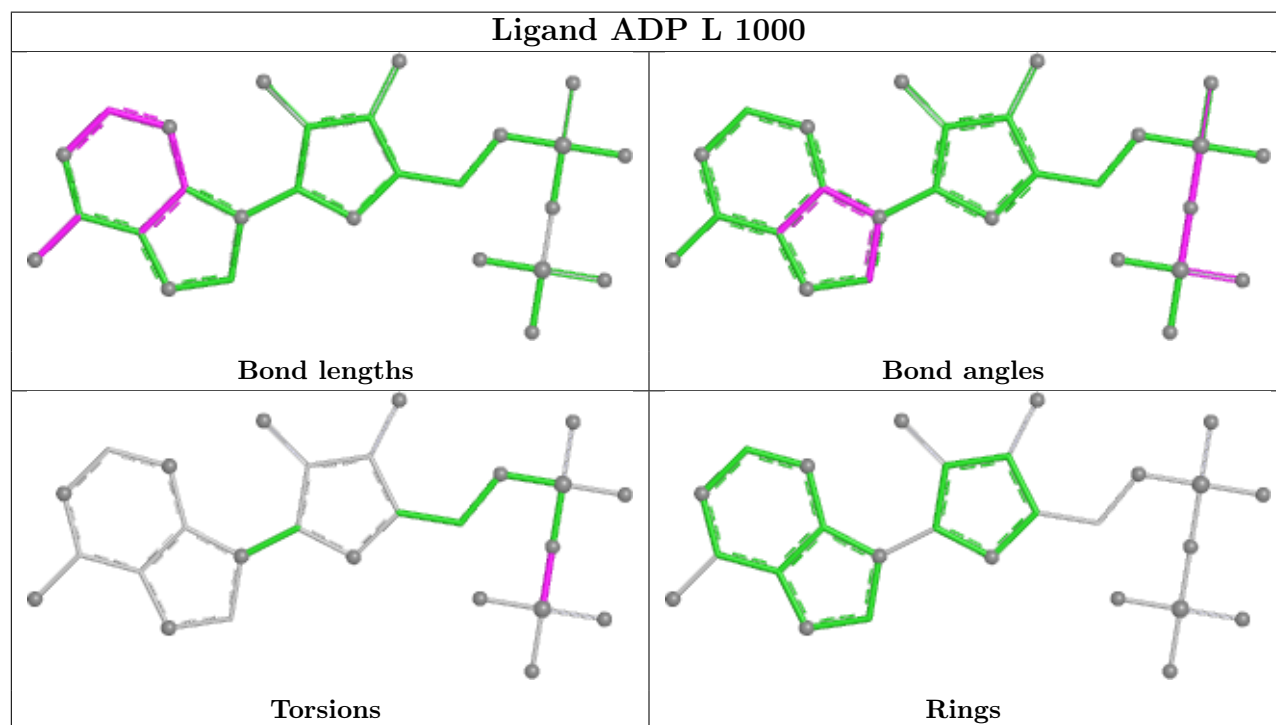
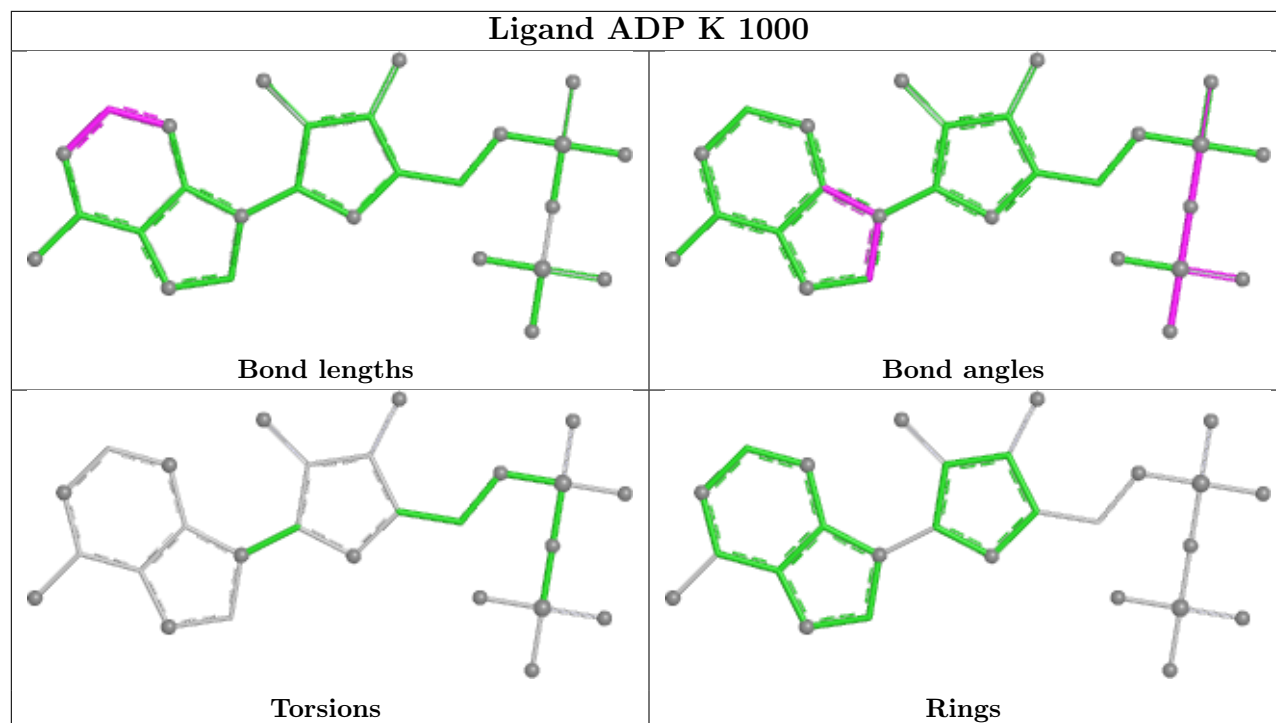


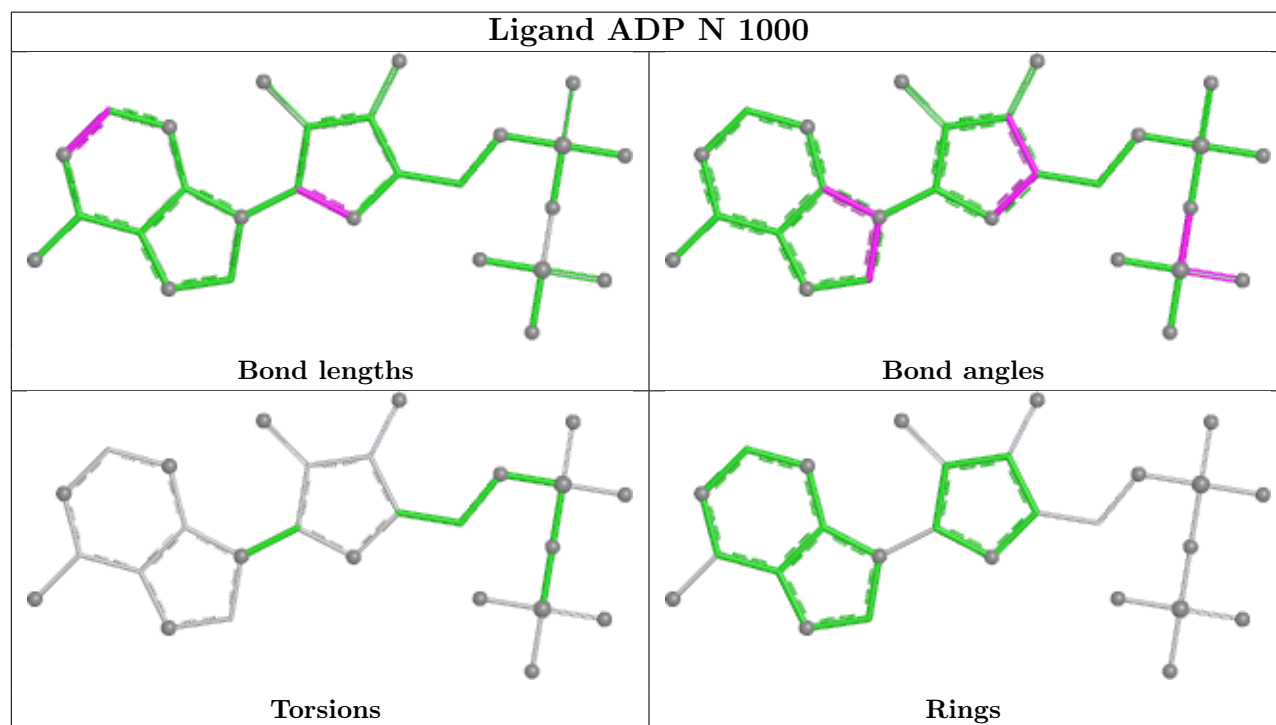
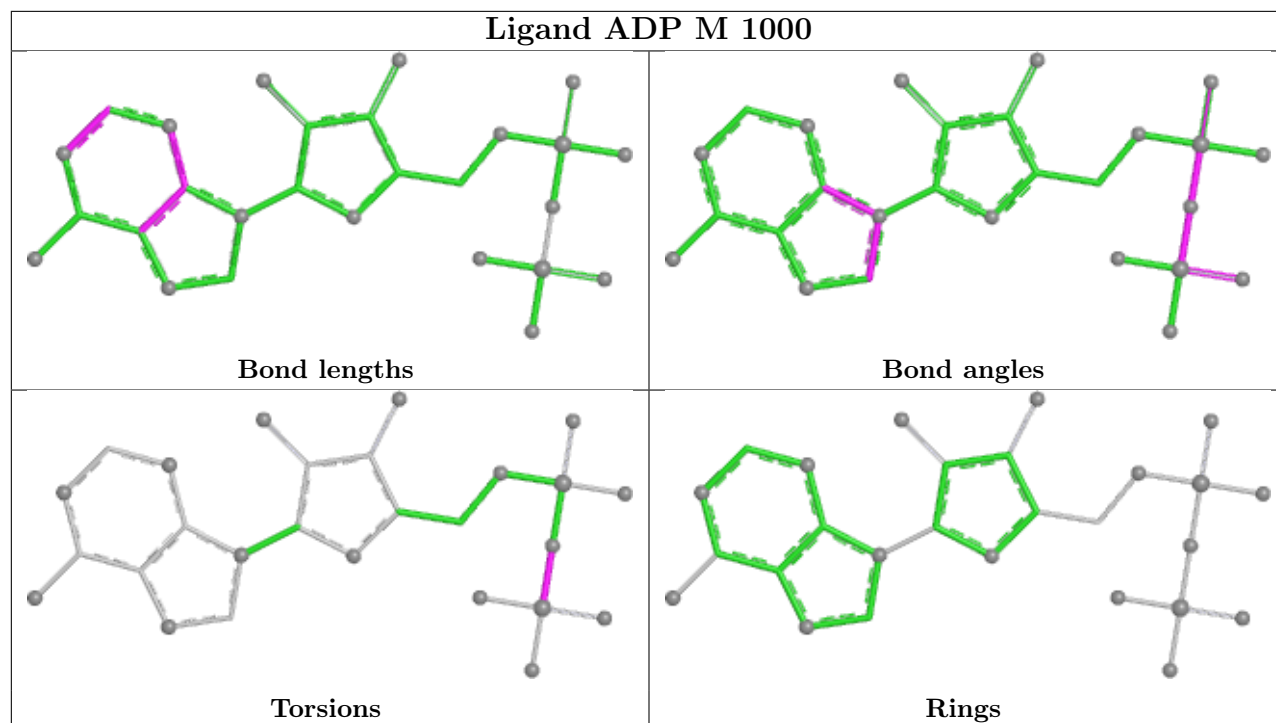
Ligand ADP H 1000

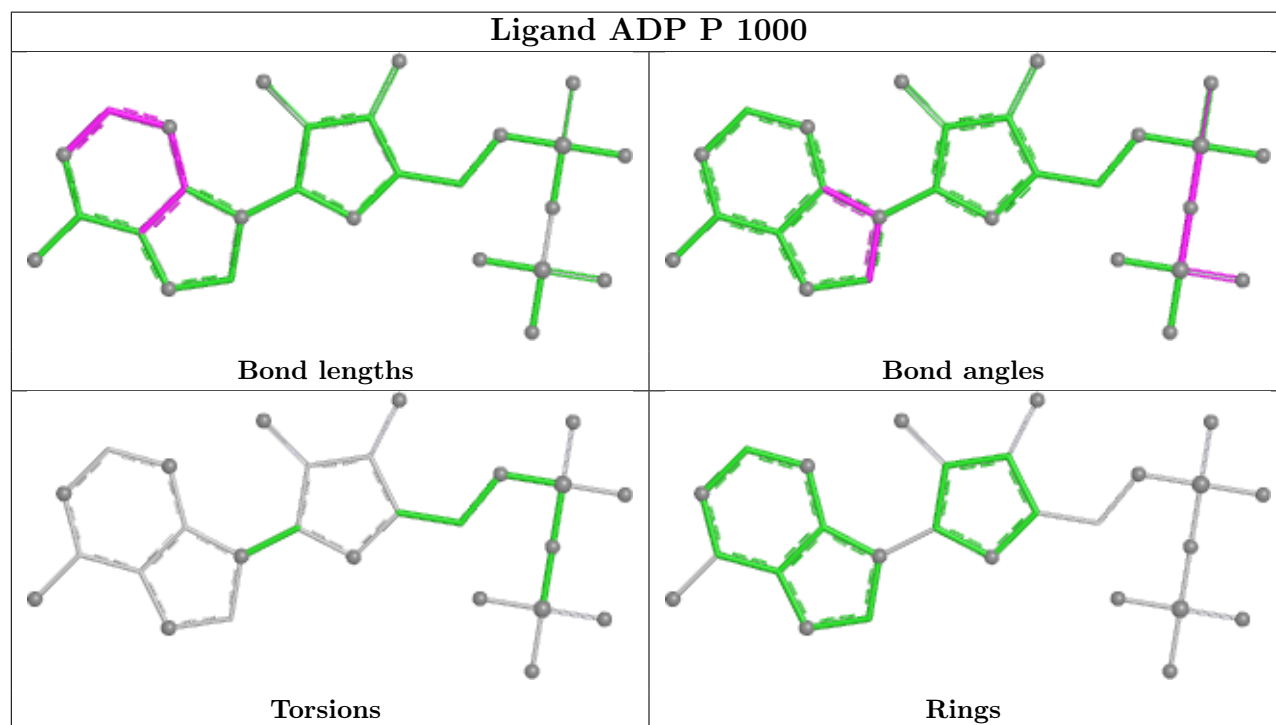
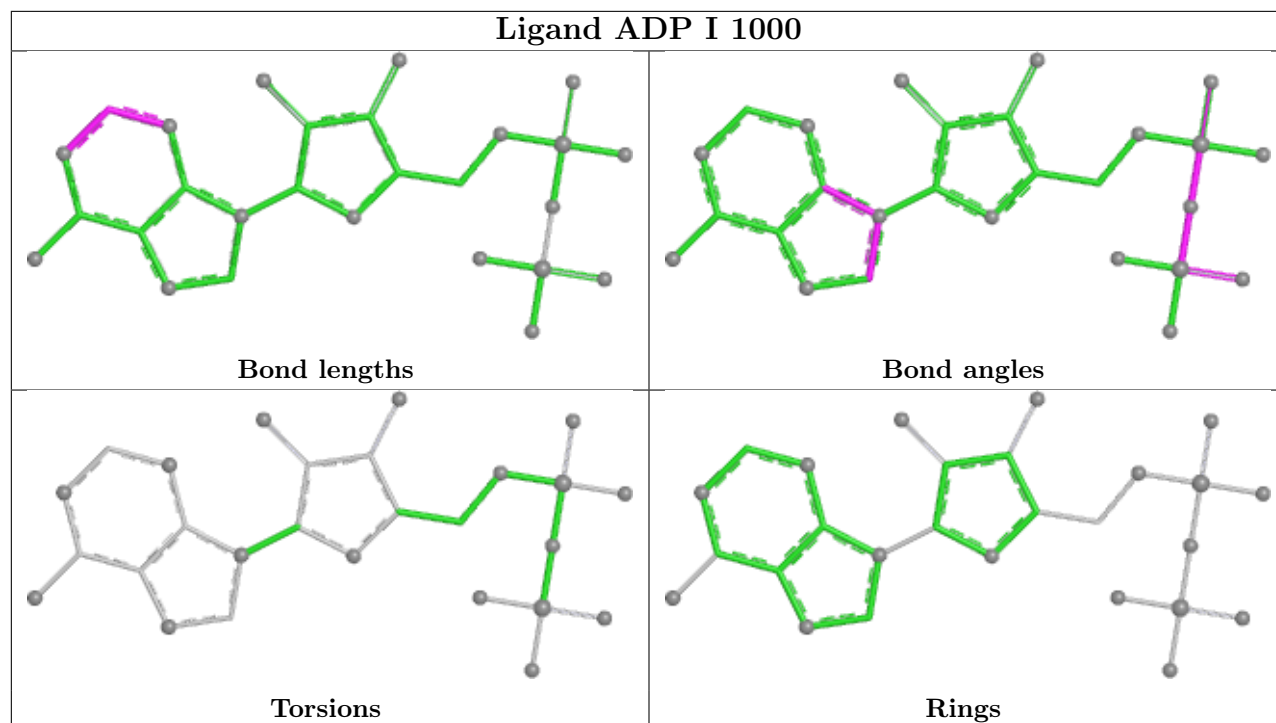


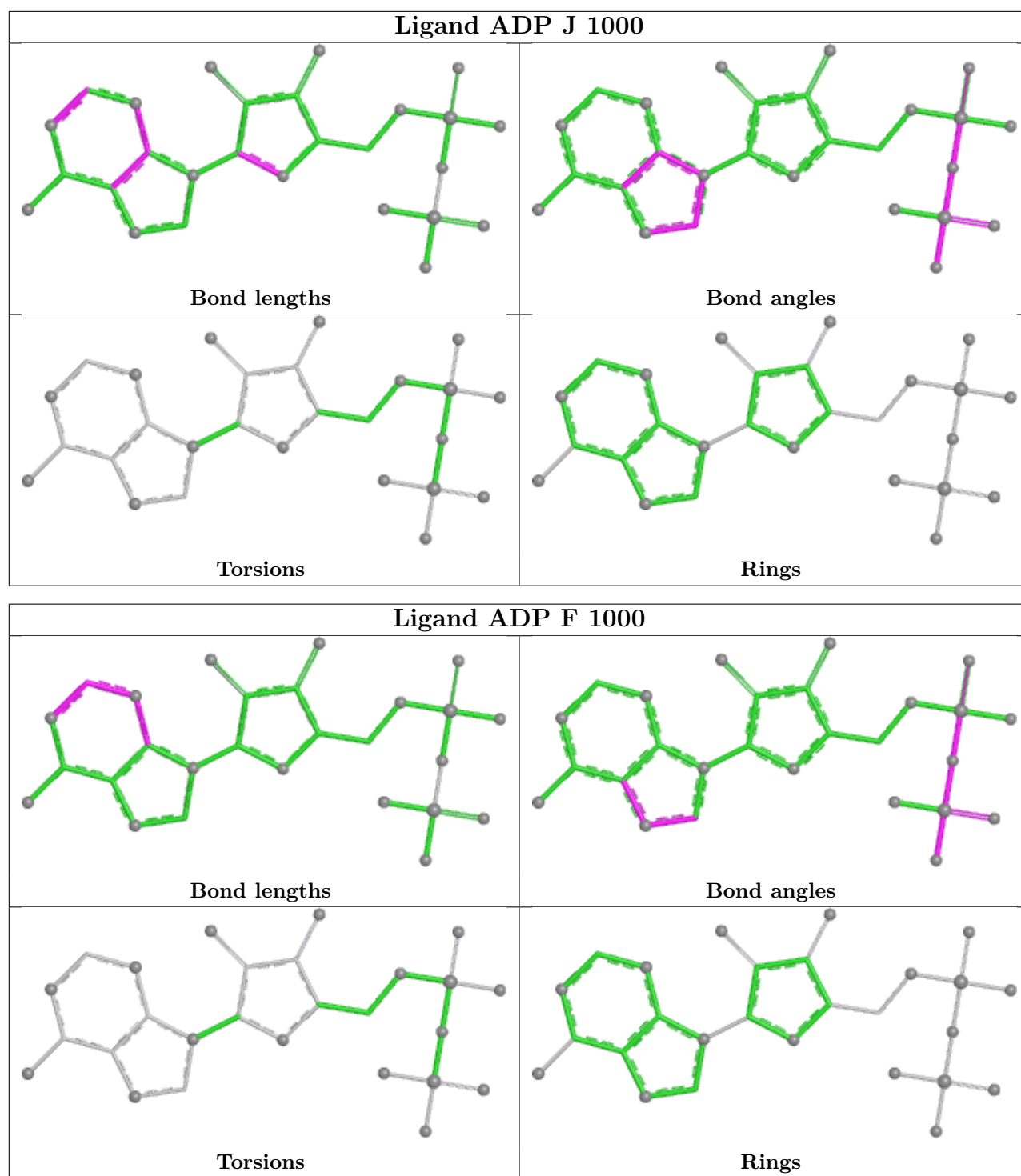
Ligand ADP G 1000











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	259/286 (90%)	-0.28	2 (0%) 82 67	48, 72, 112, 127	0
1	B	260/286 (90%)	-0.15	3 (1%) 76 58	57, 83, 119, 129	0
1	C	260/286 (90%)	-0.18	3 (1%) 76 58	51, 79, 112, 141	0
1	D	258/286 (90%)	-0.09	1 (0%) 88 79	62, 90, 120, 148	0
1	E	260/286 (90%)	-0.18	4 (1%) 72 52	60, 85, 117, 139	0
1	F	257/286 (89%)	-0.24	2 (0%) 82 67	58, 80, 110, 139	0
1	G	259/286 (90%)	-0.07	2 (0%) 82 67	67, 91, 120, 143	0
1	H	260/286 (90%)	-0.02	1 (0%) 88 79	64, 88, 124, 144	0
1	I	260/286 (90%)	-0.20	3 (1%) 76 58	57, 83, 117, 136	0
1	J	259/286 (90%)	-0.19	0 100 100	57, 80, 115, 133	0
1	K	258/286 (90%)	-0.28	2 (0%) 82 67	54, 73, 112, 147	0
1	L	259/286 (90%)	-0.33	1 (0%) 88 79	51, 72, 112, 140	0
1	M	256/286 (89%)	-0.29	1 (0%) 88 79	48, 74, 106, 128	0
1	N	260/286 (90%)	-0.31	1 (0%) 88 79	50, 70, 111, 131	0
1	O	260/286 (90%)	-0.23	1 (0%) 88 79	51, 74, 113, 133	0
1	P	256/286 (89%)	-0.29	1 (0%) 88 79	53, 76, 108, 136	0
All	All	4141/4576 (90%)	-0.21	28 (0%) 84 69	48, 80, 116, 148	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	701	ARG	3.5
1	P	704	ALA	3.1
1	D	707	ASP	2.9
1	K	711	TYR	2.8
1	B	719	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	706	GLN	2.7
1	M	703	SER	2.7
1	C	710	TYR	2.6
1	F	703	SER	2.6
1	E	705	TYR	2.6
1	B	706	GLN	2.5
1	I	702	ALA	2.4
1	C	706	GLN	2.4
1	N	707	ASP	2.4
1	F	704	ALA	2.4
1	E	707	ASP	2.3
1	H	711	TYR	2.3
1	G	709	GLY	2.3
1	K	706	GLN	2.3
1	L	702	ALA	2.2
1	B	482	VAL	2.1
1	O	711	TYR	2.1
1	C	707	ASP	2.1
1	E	706	GLN	2.1
1	G	563	CYS	2.1
1	A	708	TYR	2.1
1	I	704	ALA	2.1
1	E	704	ALA	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 [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.

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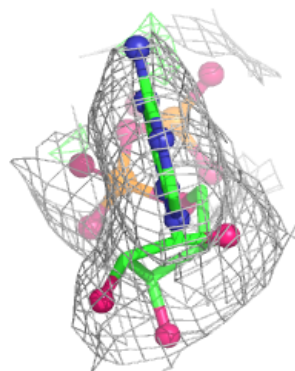
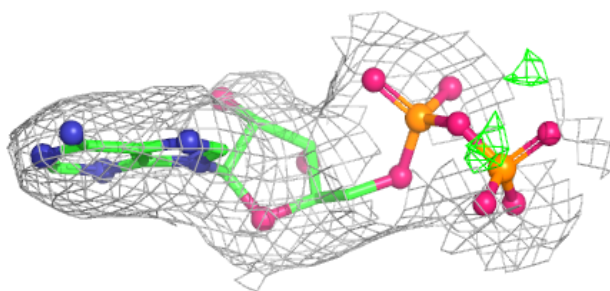
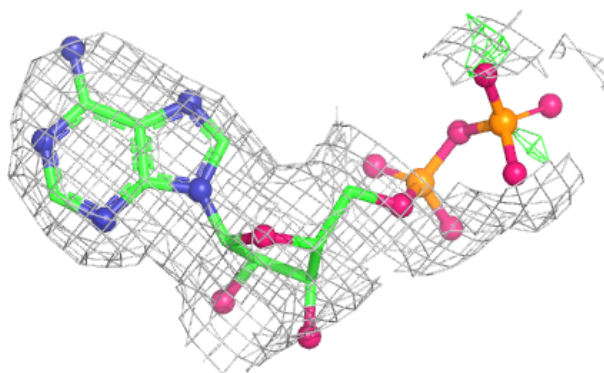
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	C	1001	1/1	0.88	0.17	80,80,80,80	0
3	CA	B	1001	1/1	0.89	0.11	73,73,73,73	0
3	CA	N	1001	1/1	0.91	0.14	70,70,70,70	0
3	CA	G	1001	1/1	0.92	0.14	89,89,89,89	0
3	CA	F	1001	1/1	0.92	0.18	83,83,83,83	0
3	CA	E	1001	1/1	0.94	0.11	86,86,86,86	0
3	CA	H	1001	1/1	0.94	0.11	79,79,79,79	0
3	CA	L	1001	1/1	0.94	0.09	71,71,71,71	0
3	CA	D	1001	1/1	0.94	0.12	94,94,94,94	0
3	CA	O	1001	1/1	0.94	0.12	64,64,64,64	0
3	CA	A	1001	1/1	0.95	0.17	79,79,79,79	0
2	ADP	D	1000	27/27	0.96	0.06	79,83,85,87	0
2	ADP	E	1000	27/27	0.96	0.07	74,76,78,79	0
2	ADP	F	1000	27/27	0.96	0.07	72,74,76,77	0
2	ADP	H	1000	27/27	0.96	0.08	81,83,85,88	0
2	ADP	I	1000	27/27	0.96	0.07	84,85,87,89	0
2	ADP	J	1000	27/27	0.96	0.07	74,77,80,82	0
3	CA	I	1001	1/1	0.96	0.12	82,82,82,82	0
3	CA	J	1001	1/1	0.96	0.13	81,81,81,81	0
3	CA	K	1001	1/1	0.96	0.09	69,69,69,69	0
2	ADP	K	1000	27/27	0.96	0.07	67,69,72,72	0
2	ADP	A	1000	27/27	0.96	0.06	53,57,63,64	0
2	ADP	C	1000	27/27	0.96	0.07	72,75,77,79	0
3	CA	P	1001	1/1	0.96	0.14	76,76,76,76	0
2	ADP	M	1000	27/27	0.97	0.07	72,74,76,78	0
2	ADP	O	1000	27/27	0.97	0.06	55,58,61,62	0
2	ADP	P	1000	27/27	0.97	0.06	66,69,71,72	0
3	CA	M	1001	1/1	0.97	0.13	74,74,74,74	0
2	ADP	B	1000	27/27	0.97	0.06	82,83,85,86	0
2	ADP	G	1000	27/27	0.97	0.07	83,86,88,90	0
2	ADP	L	1000	27/27	0.97	0.07	75,76,78,80	0
2	ADP	N	1000	27/27	0.98	0.05	58,60,62,64	0

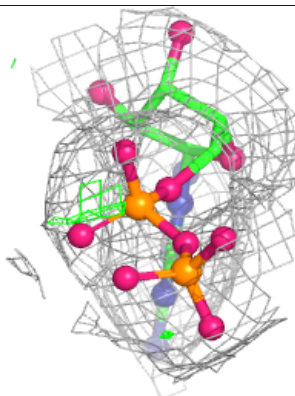
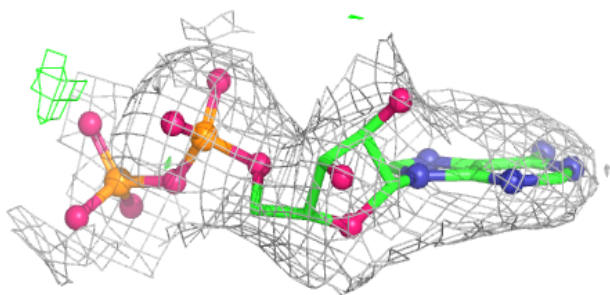
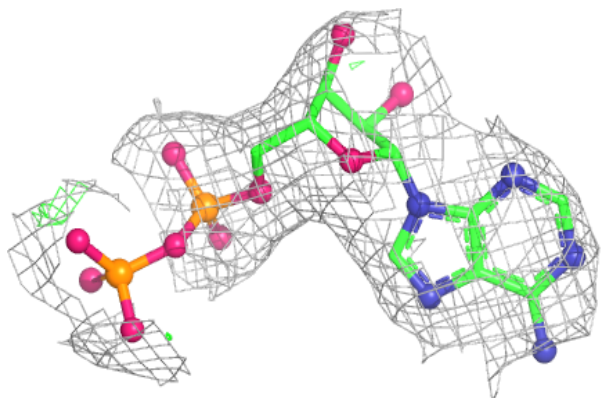
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP D 1000:

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

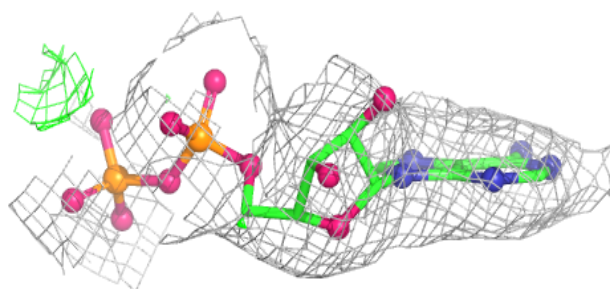
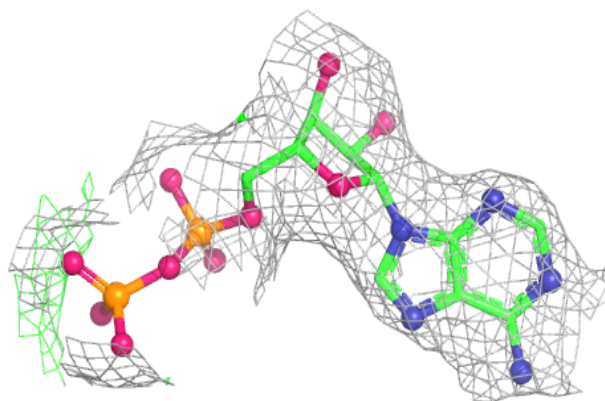
**Electron density around ADP E 1000:**

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

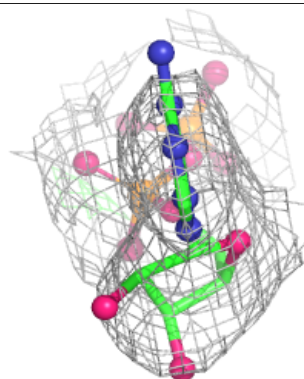
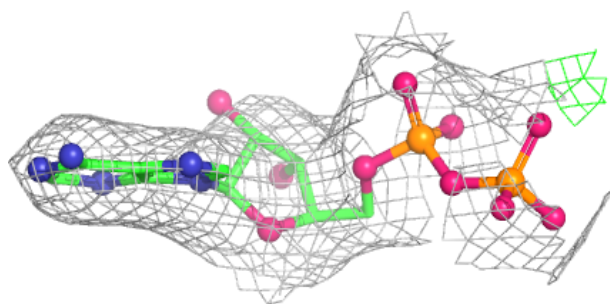
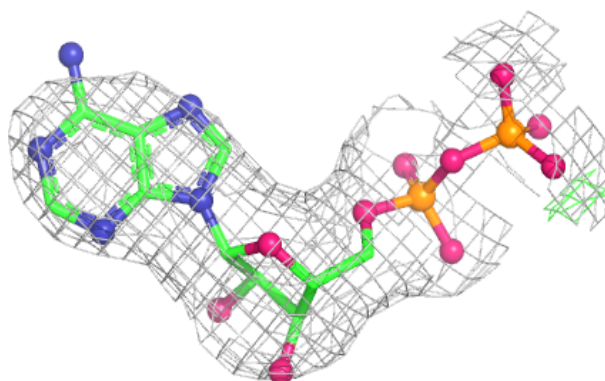


Electron density around ADP F 1000:

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

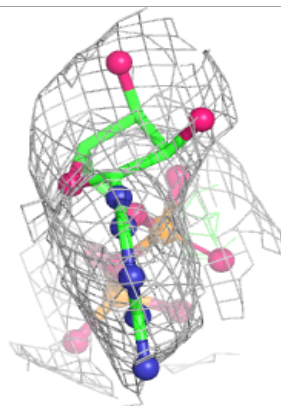
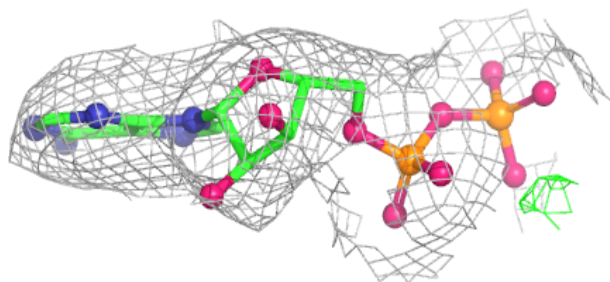
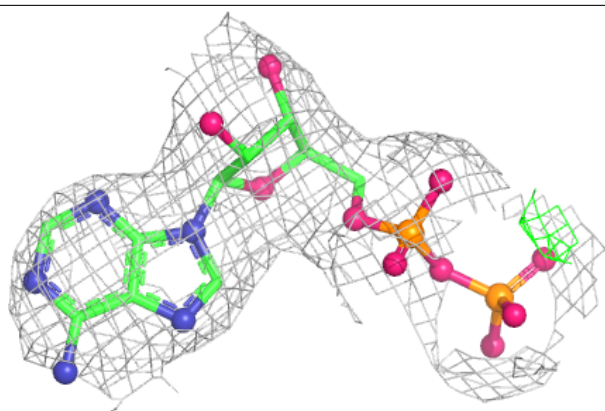
**Electron density around ADP H 1000:**

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

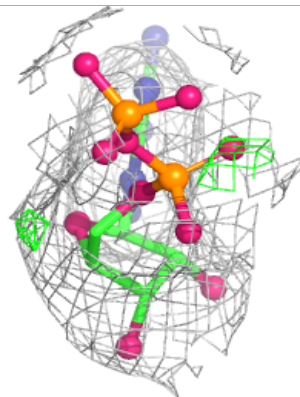
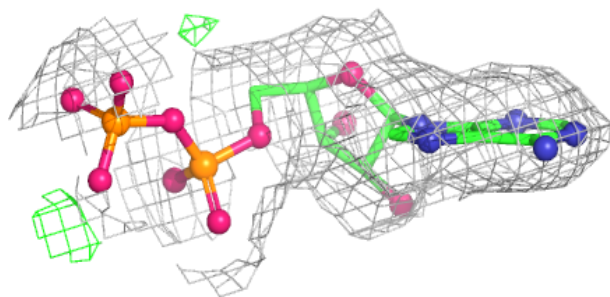
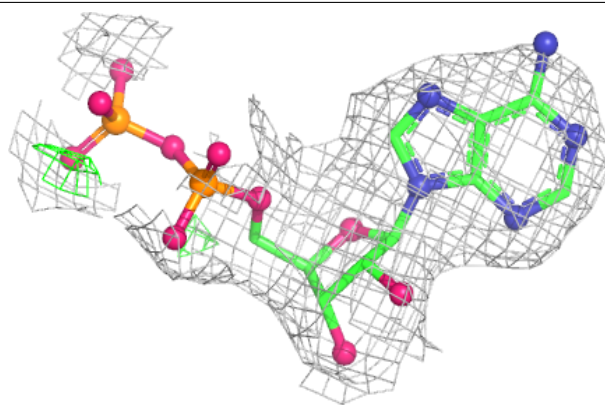


Electron density around ADP I 1000:

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

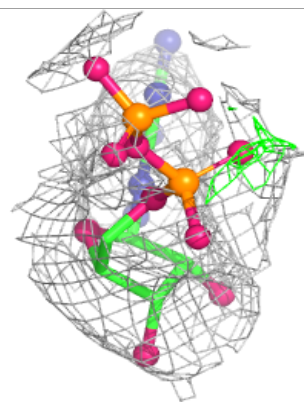
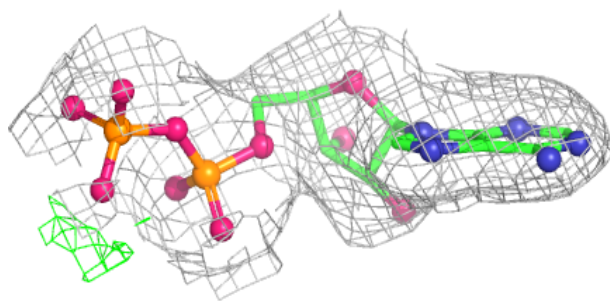
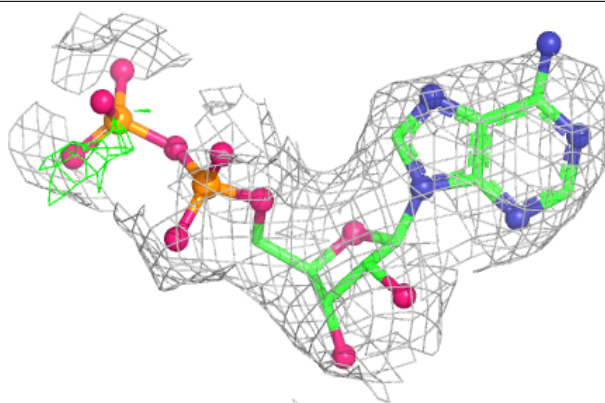
**Electron density around ADP J 1000:**

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

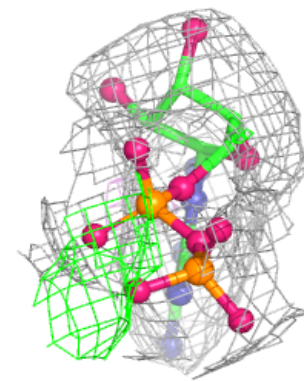
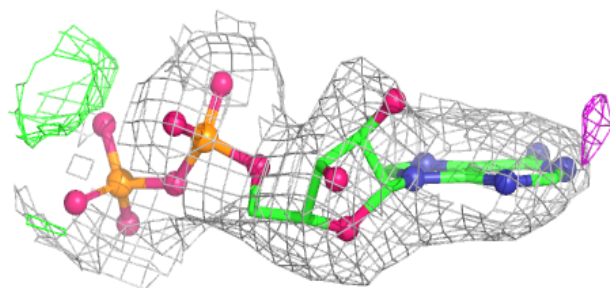
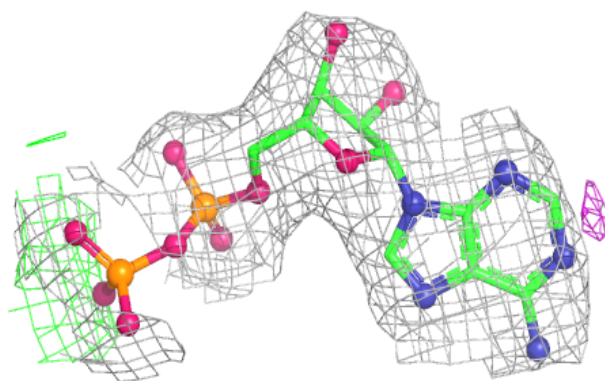


Electron density around ADP K 1000:

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

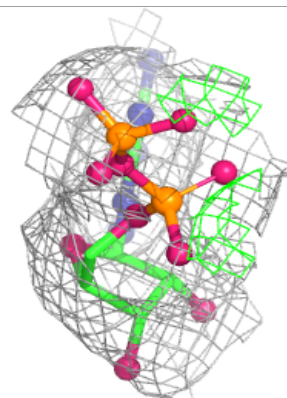
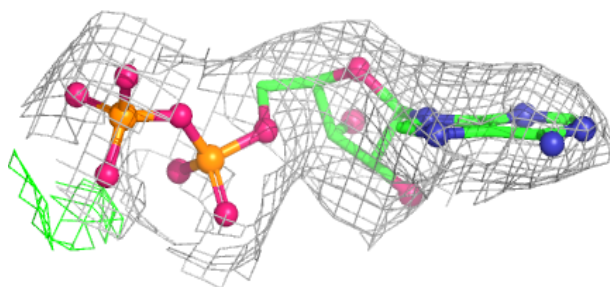
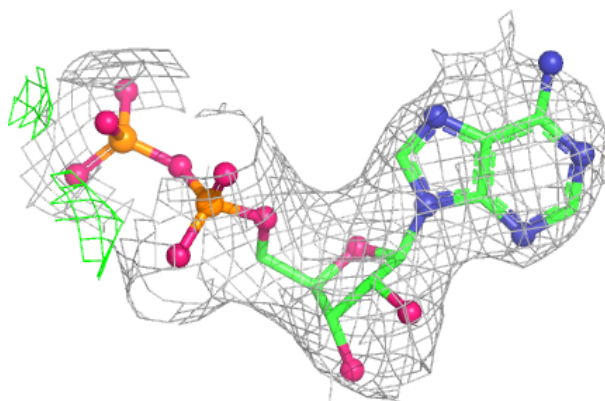
**Electron density around ADP A 1000:**

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

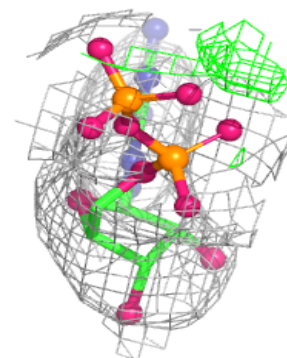
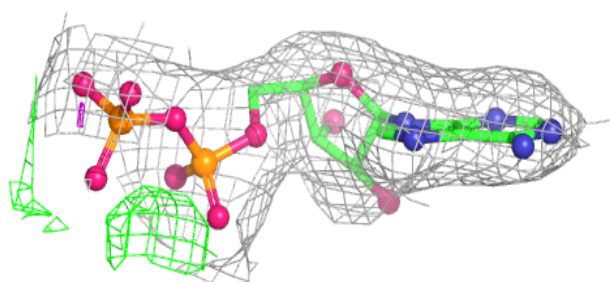
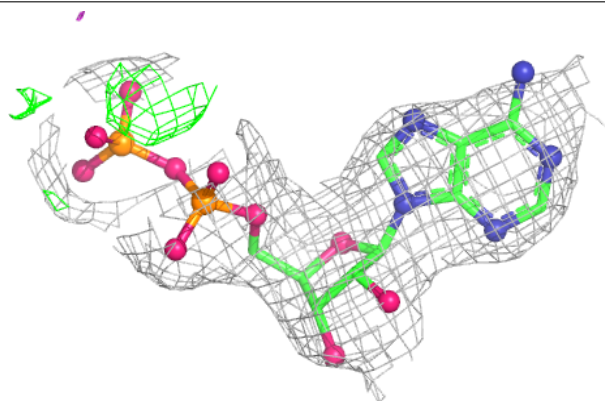


Electron density around ADP C 1000:

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

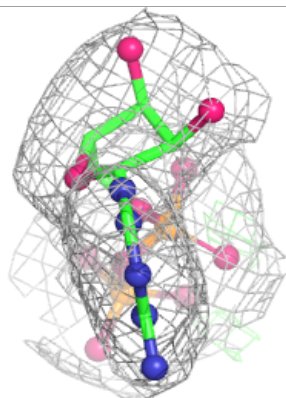
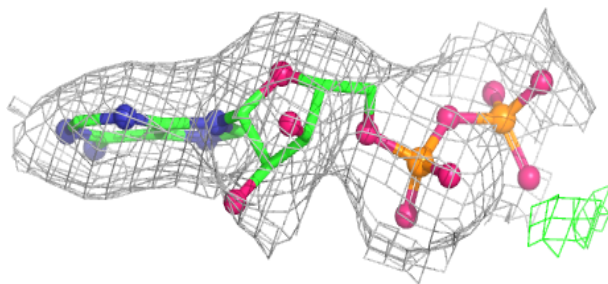
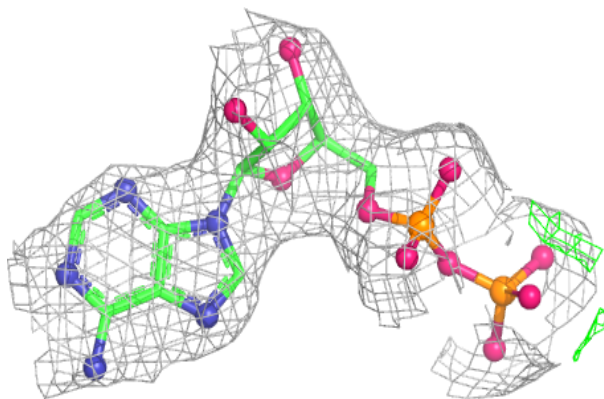
**Electron density around ADP M 1000:**

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

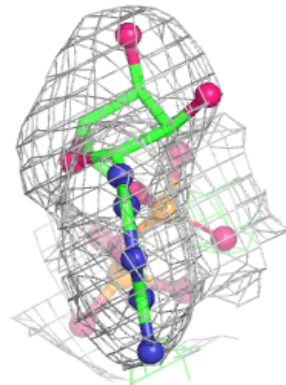
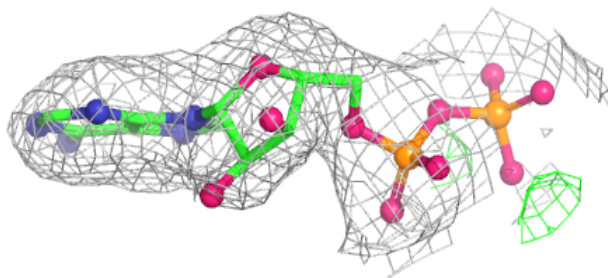
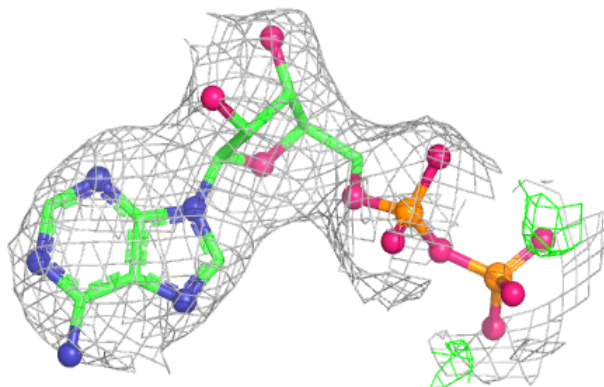


Electron density around ADP O 1000:

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

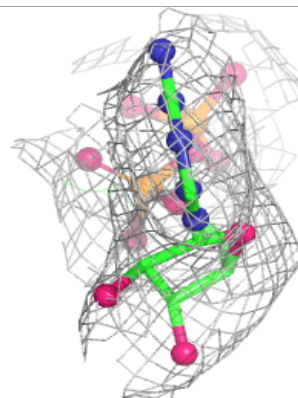
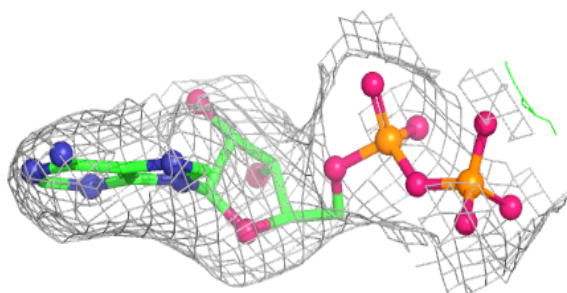
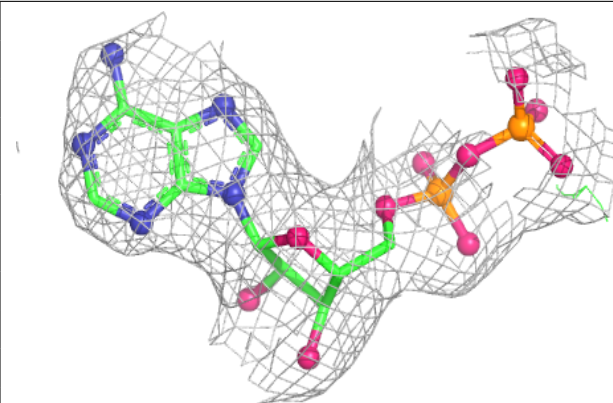
**Electron density around ADP P 1000:**

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

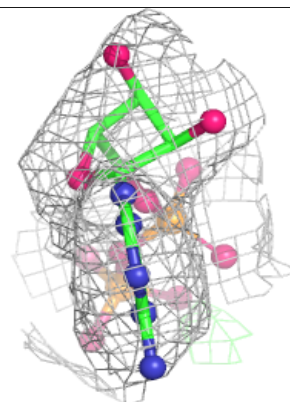
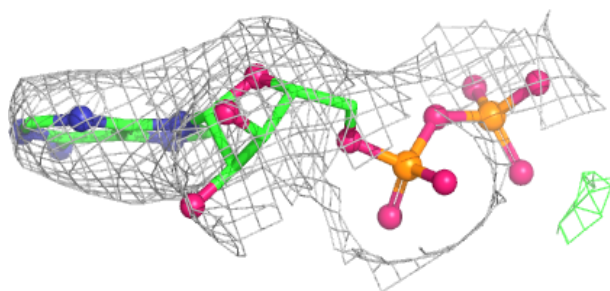
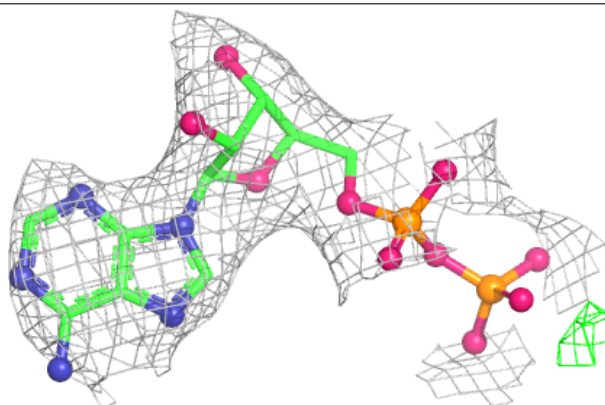


Electron density around ADP B 1000:

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

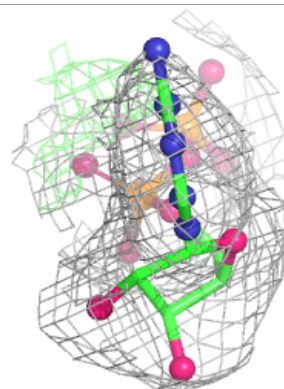
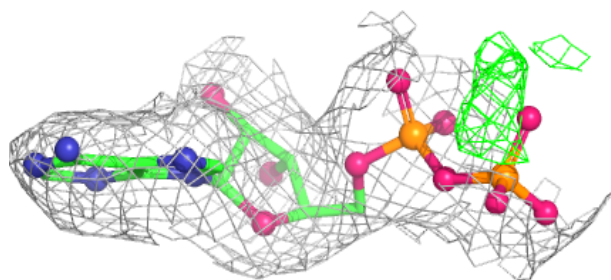
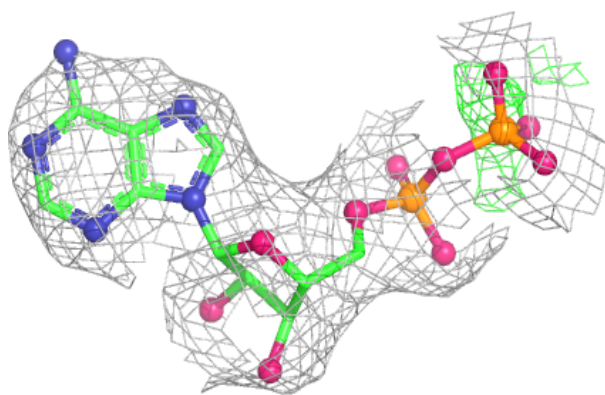
**Electron density around ADP G 1000:**

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

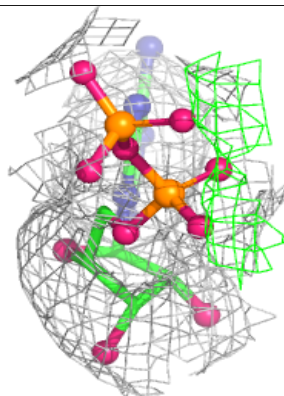
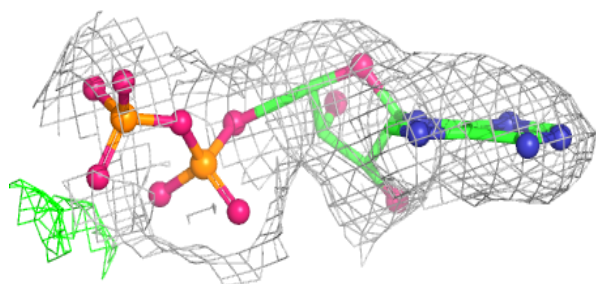
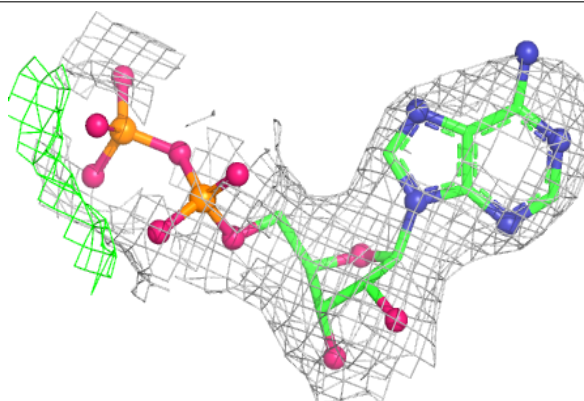


Electron density around ADP L 1000:

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

**Electron density around ADP N 1000:**

$2mF_o-DF_c$ (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.