



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2020 – 03:08 PM BST

PDB ID : 4V4O
Title : Crystal Structure of the Chaperonin Complex Cpn60/Cpn10/(ADP)7 from Thermus Thermophilus
Authors : Shimamura, T.; Koike-Takeshita, A.; Yokoyama, K.; Masui, R.; Murai, N.; Yoshida, M.; Taguchi, H.; Iwata, S.
Deposited on : 2004-05-23
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

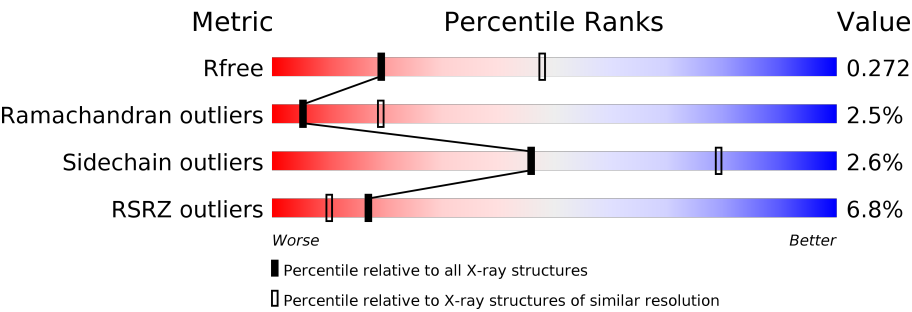
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	543	<div><div>%</div><div><div></div><div>93%</div><div></div></div><div><div></div><div></div><div></div></div></div>
1	B	543	<div><div>%</div><div><div></div><div>93%</div><div></div></div><div><div></div><div></div><div></div></div></div>
1	C	543	<div><div></div><div><div></div><div>92%</div><div></div></div><div><div></div><div></div><div>5%</div><div></div></div></div>
1	D	543	<div><div>2%</div><div><div></div><div>92%</div><div></div></div><div><div></div><div></div><div></div></div></div>
1	E	543	<div><div>2%</div><div><div></div><div>90%</div><div></div></div><div><div></div><div></div><div>6%</div><div></div></div></div>
1	F	543	<div><div>2%</div><div><div></div><div>93%</div><div></div></div><div><div></div><div></div><div></div></div></div>
1	G	543	<div><div>%</div><div><div></div><div>93%</div><div></div></div><div><div></div><div></div><div></div></div></div>

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Mol	Chain	Length	Quality of chain
1	H	543	
1	I	543	
1	J	543	
1	K	543	
1	L	543	
1	M	543	
1	N	543	
1	a	543	
1	b	543	
1	c	543	
1	d	543	
1	e	543	
1	f	543	
1	g	543	
1	h	543	
1	i	543	
1	j	543	
1	k	543	
1	l	543	
1	m	543	
1	n	543	
2	O	100	
2	P	100	
2	Q	100	
2	R	100	

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Mol	Chain	Length	Quality of chain
2	S	100	<div> <div>14%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
2	T	100	<div> <div>11%</div> <div>86%</div> <div>9%</div> <div>.</div> </div>
2	U	100	<div> <div>10%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>
2	o	100	<div> <div>28%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
2	p	100	<div> <div>14%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>
2	q	100	<div> <div>5%</div> <div>79%</div> <div>16%</div> <div>.</div> </div>
2	r	100	<div> <div>10%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
2	s	100	<div> <div>14%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
2	t	100	<div> <div>16%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
2	u	100	<div> <div>17%</div> <div>84%</div> <div>11%</div> <div>.</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121267 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 cpn60(GroEL).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	B	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	C	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	D	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	E	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	F	529	Total	C	N	O	S	0	0	0
			3974	2495	689	785	5			
1	G	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	H	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	I	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	J	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	K	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	L	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	M	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	N	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	a	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	b	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	c	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	d	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	e	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	f	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	g	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	h	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	i	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	j	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	k	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	l	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	m	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	n	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			

- Molecule 2 is a protein called cpn10(GroES).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	96	Total	C	N	O		0	0	0
			739	470	126	143				
2	P	94	Total	C	N	O		0	0	0
			723	460	123	140				
2	Q	96	Total	C	N	O		0	0	0
			739	470	126	143				
2	R	96	Total	C	N	O		0	0	0
			739	470	126	143				
2	S	96	Total	C	N	O		0	0	0
			739	470	126	143				
2	T	96	Total	C	N	O		0	0	0
			739	470	126	143				
2	U	96	Total	C	N	O		0	0	0
			739	470	126	143				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	o	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	p	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	q	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	r	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	s	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	t	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	u	96	Total	C	N	O	0	0	0
			739	470	126	143			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

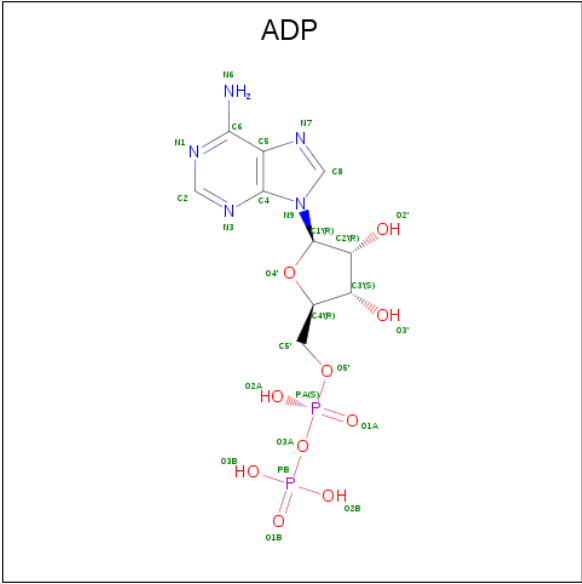
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	g	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	e	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	a	1	Total	Mg	0	0
			1	1		
3	c	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	f	1	Total	Mg	0	0
			1	1		
3	d	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	b	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

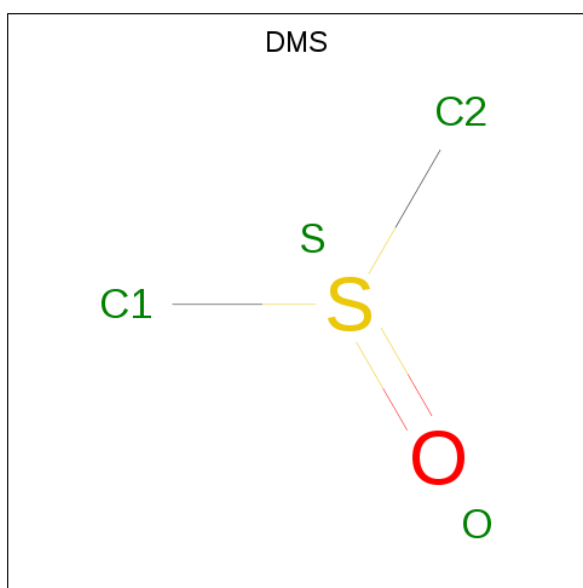
- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	c	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	d	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	e	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	f	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	g	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	O	S	0	0
			4	2	1	1		
5	I	1	Total	C	O	S	0	0
			4	2	1	1		
5	J	1	Total	C	O	S	0	0
			4	2	1	1		
5	K	1	Total	C	O	S	0	0
			4	2	1	1		
5	L	1	Total	C	O	S	0	0
			4	2	1	1		
5	M	1	Total	C	O	S	0	0
			4	2	1	1		

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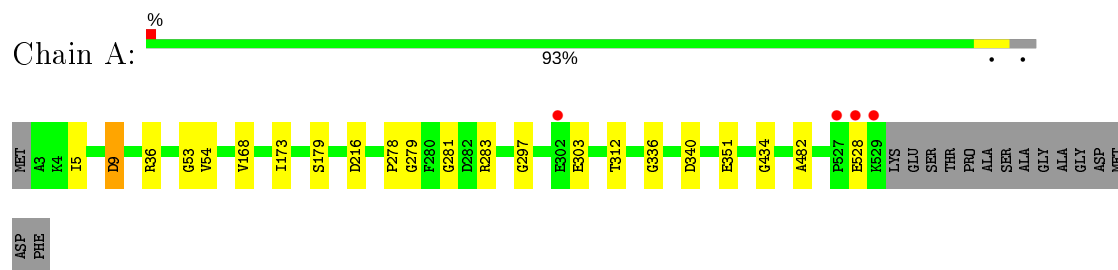
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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5	h	1	Total 4	C 2	O 1	S 1	0	0
5	i	1	Total 4	C 2	O 1	S 1	0	0
5	j	1	Total 4	C 2	O 1	S 1	0	0
5	k	1	Total 4	C 2	O 1	S 1	0	0
5	l	1	Total 4	C 2	O 1	S 1	0	0
5	m	1	Total 4	C 2	O 1	S 1	0	0
5	n	1	Total 4	C 2	O 1	S 1	0	0

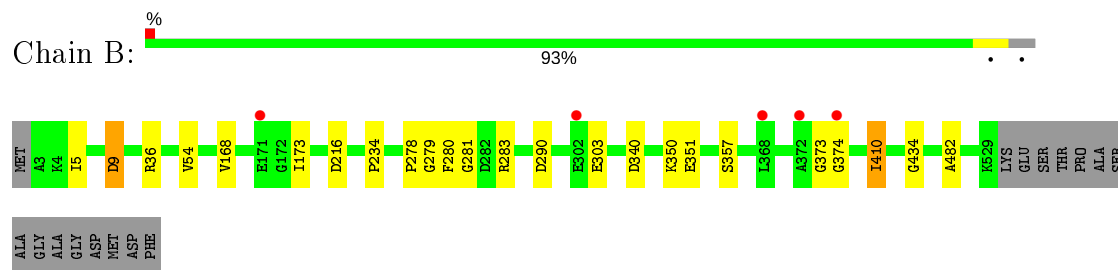
3 Residue-property plots [i](#)

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

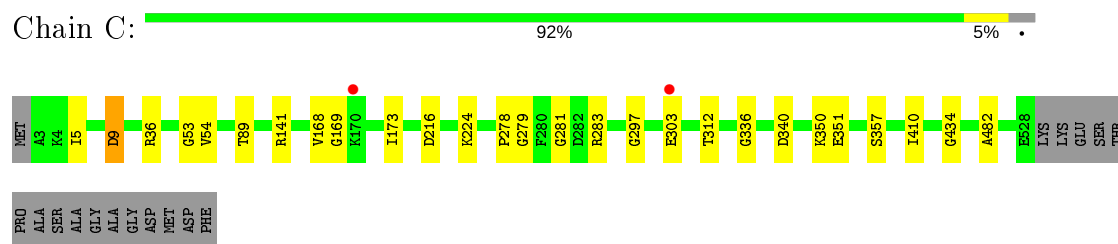
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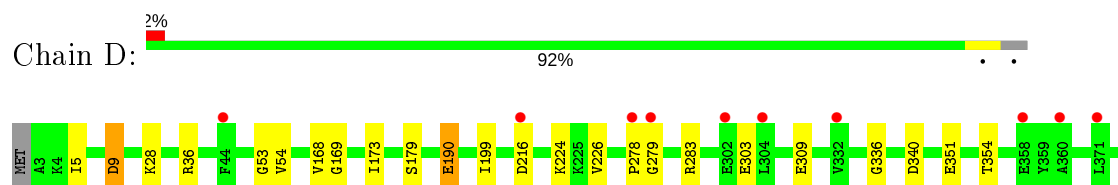
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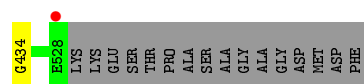


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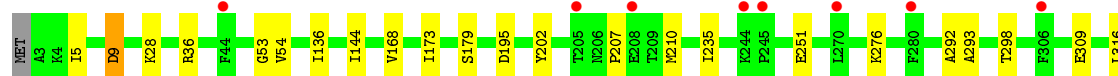
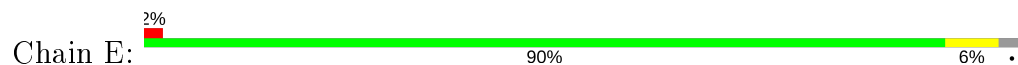


- Molecule 1: cpn60(GroEL)

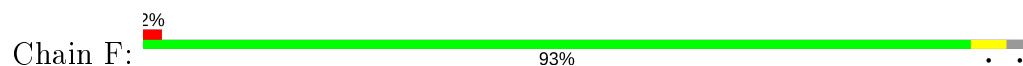




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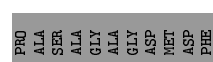
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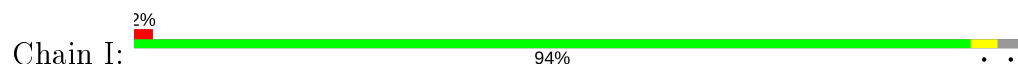
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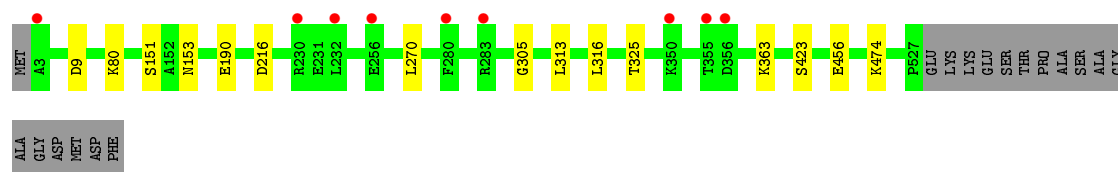


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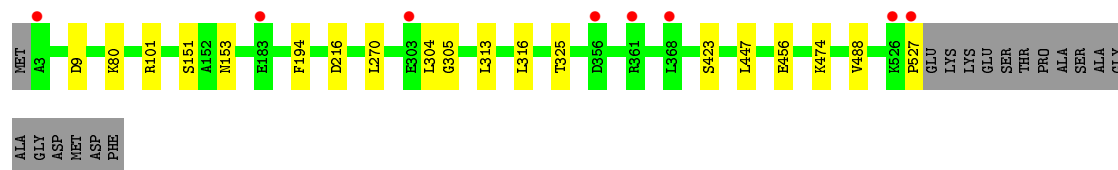


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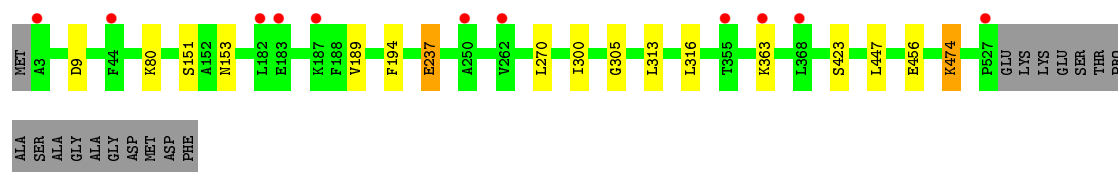




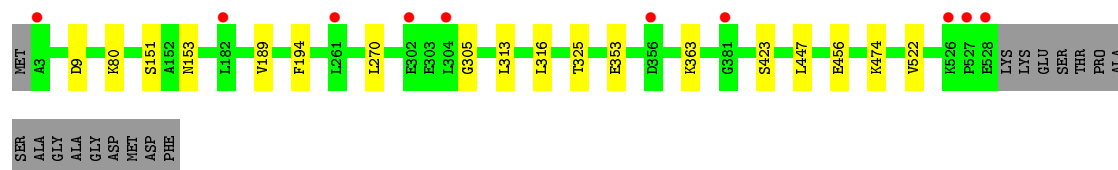
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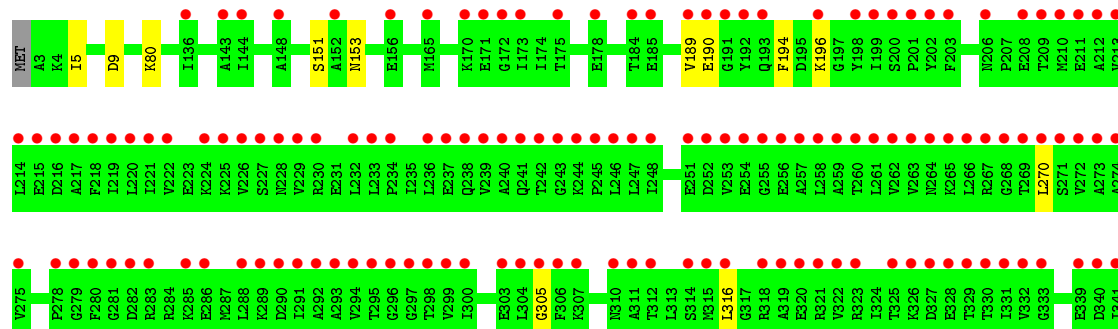
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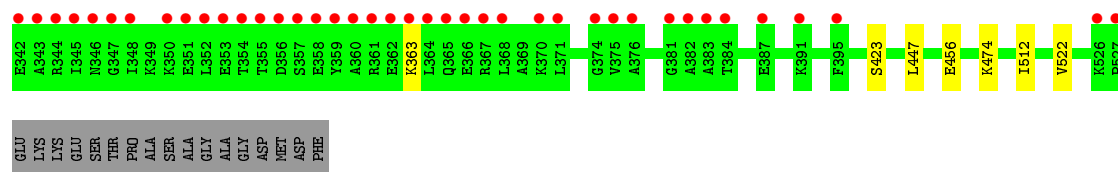


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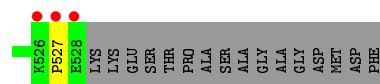
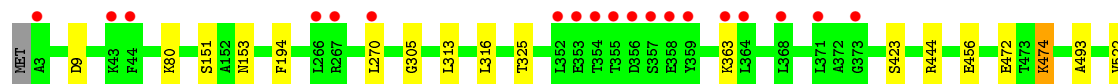


- Molecule 1: cpn60(GroEL)

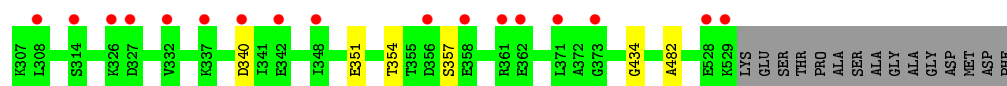




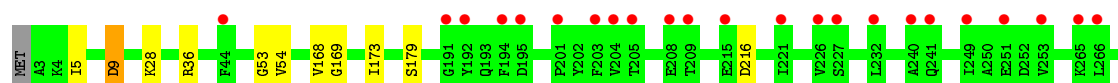
- Molecule 1: cpn60(GroEL)



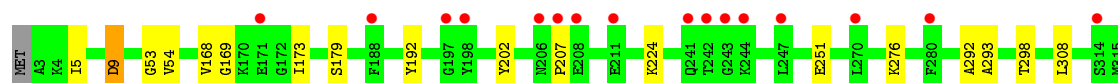
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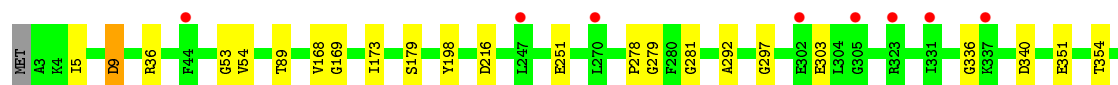


- Molecule 1: cpn60(GroEL)

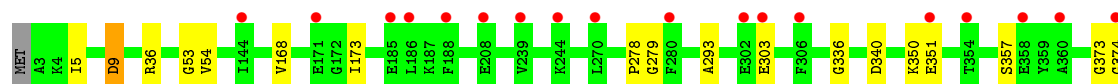




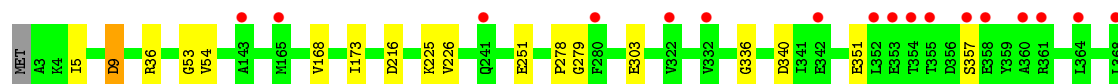
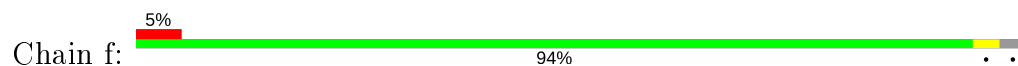
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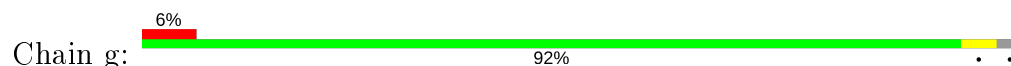
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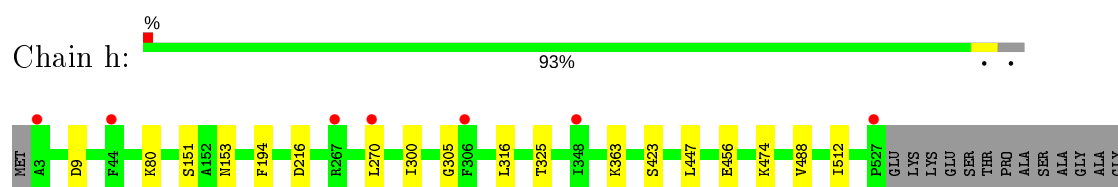


- Molecule 1: cpn60(GroEL)

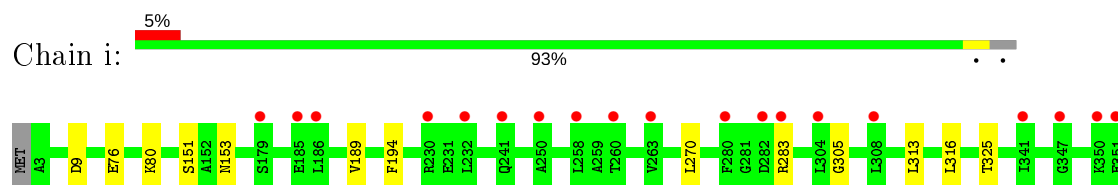


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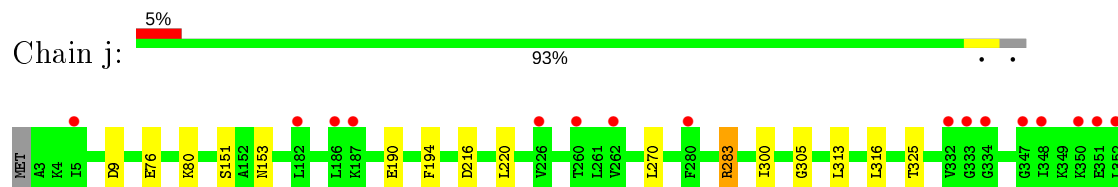




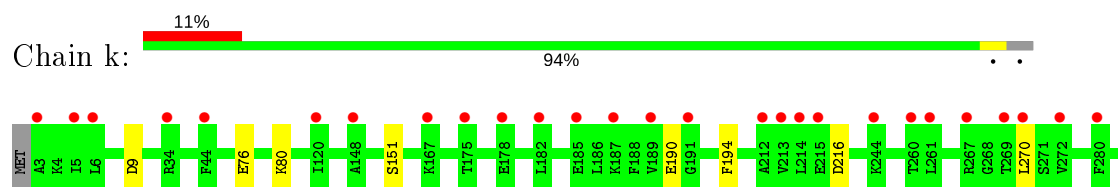
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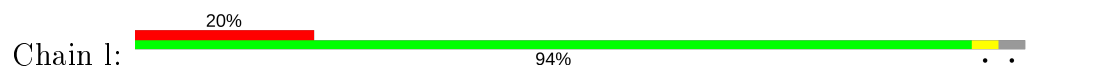
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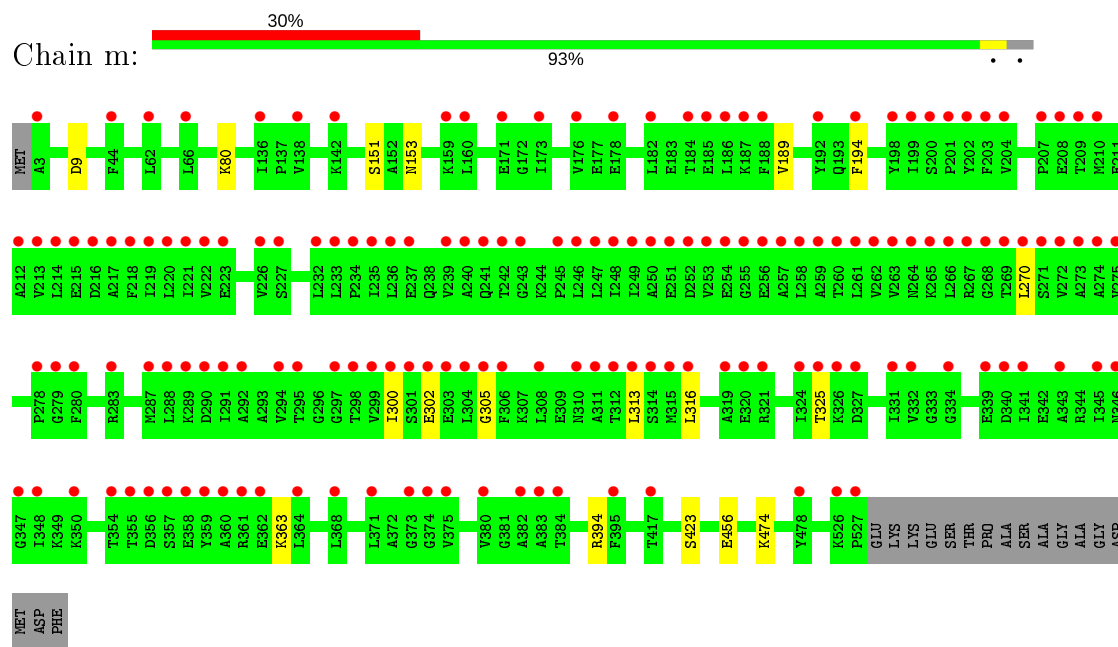
- Molecule 1: cpn60(GroEL)



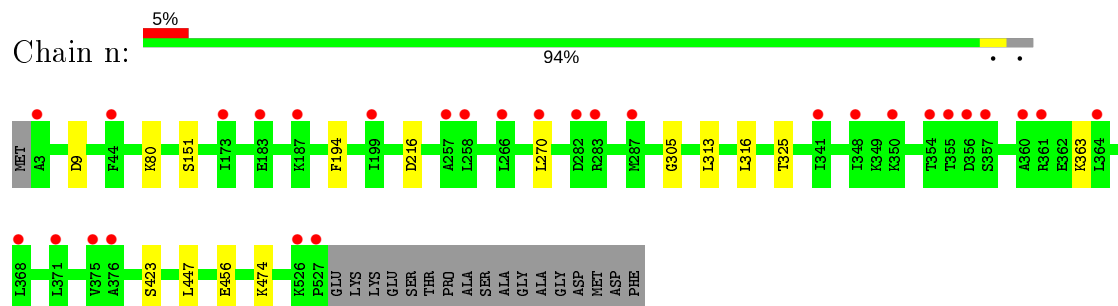
- Molecule 1: cpn60(GroEL)



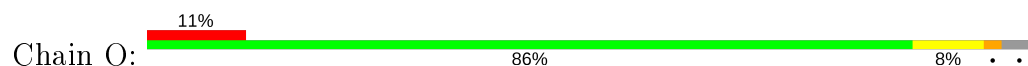
- Molecule 1: cpn60(GroEL)



- Molecule 1: cpn60(GroEL)

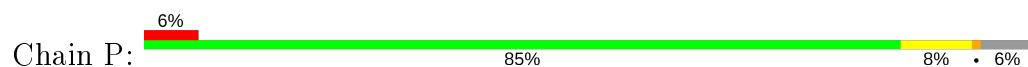


- Molecule 2: cpn10(GroES)

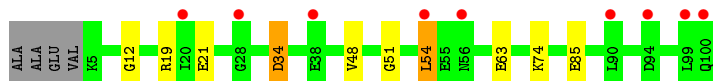
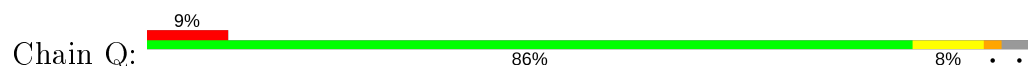




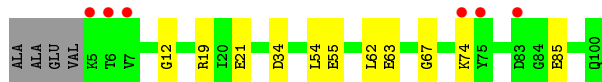
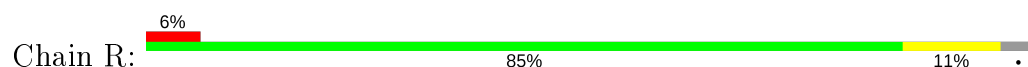
- Molecule 2: cpn10(GroES)



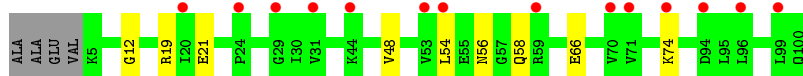
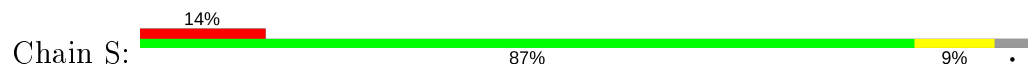
- Molecule 2: cpn10(GroES)



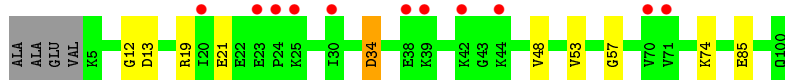
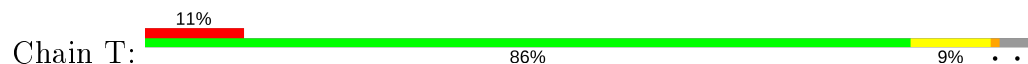
- Molecule 2: cpn10(GroES)



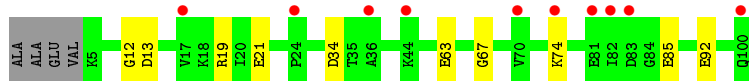
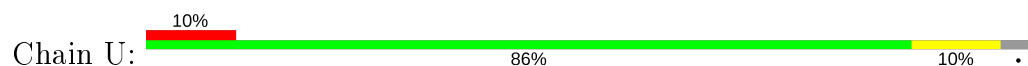
- Molecule 2: cpn10(GroES)



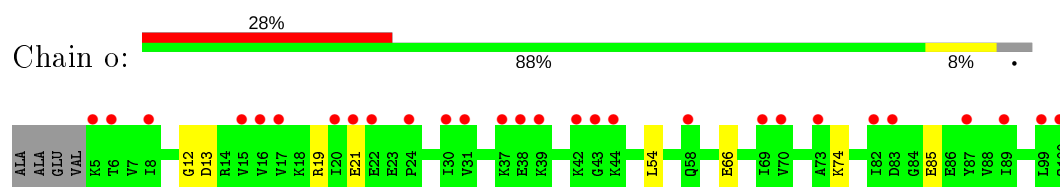
- Molecule 2: cpn10(GroES)



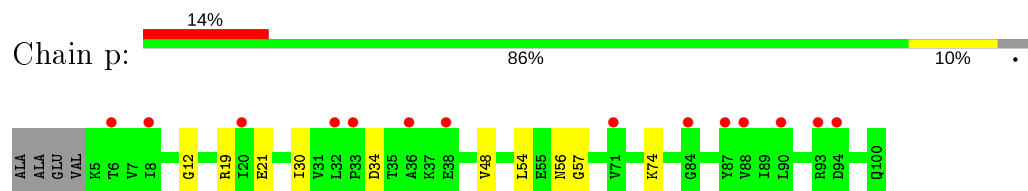
- Molecule 2: cpn10(GroES)



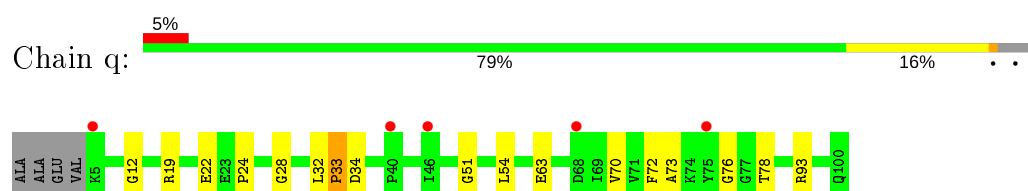
- Molecule 2: cpn10(GroES)



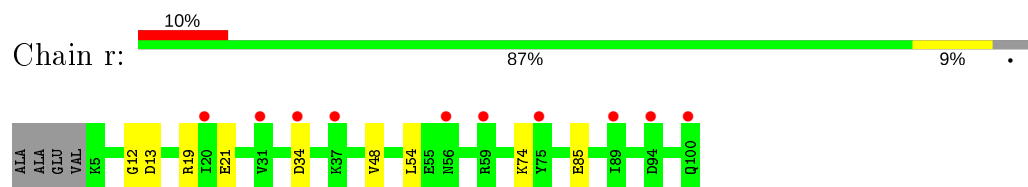
• Molecule 2: cpn10(GroES)



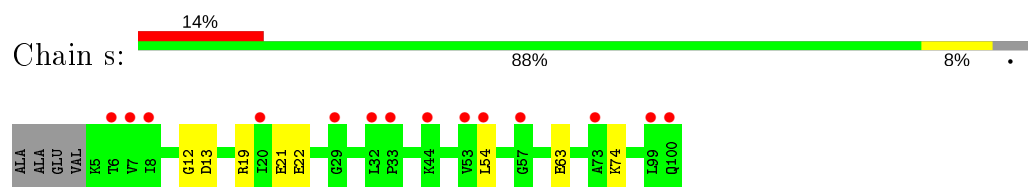
• Molecule 2: cpn10(GroES)



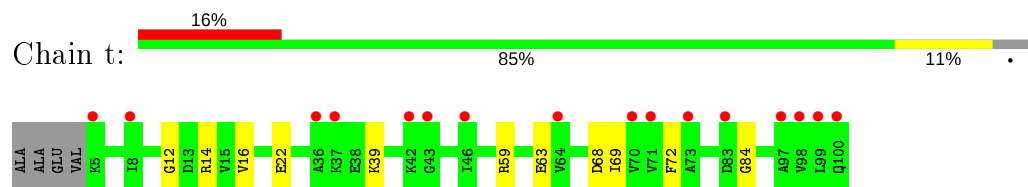
• Molecule 2: cpn10(GroES)



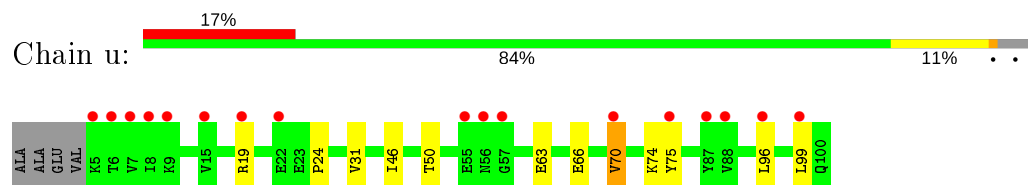
• Molecule 2: cpn10(GroES)



• Molecule 2: cpn10(GroES)



• Molecule 2: cpn10(GroES)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	140.38Å 156.42Å 273.15Å 82.88° 85.35° 68.52°	Depositor
Resolution (Å)	39.98 – 2.80 39.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	81.3 (39.98-2.80) 81.4 (39.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.279 0.233 , 0.272	Depositor DCC
R_{free} test set	12690 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 73.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	121267	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: MG, DMS, 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	0.44	0/3989	0.65	0/5383
1	B	0.43	1/3989 (0.0%)	0.65	1/5383 (0.0%)
1	C	0.45	0/3980	0.67	0/5372
1	D	0.42	0/3980	0.65	1/5372 (0.0%)
1	E	0.43	0/3980	0.64	0/5372
1	F	0.39	0/4007	0.63	0/5406
1	G	0.41	0/3971	0.64	0/5360
1	H	0.36	0/3980	0.60	0/5372
1	I	0.37	0/3971	0.60	0/5360
1	J	0.40	0/3971	0.62	0/5360
1	K	0.39	1/3971 (0.0%)	0.62	0/5360
1	L	0.38	0/3980	0.60	0/5372
1	M	0.39	1/3971 (0.0%)	0.62	1/5360 (0.0%)
1	N	0.38	0/3980	0.63	1/5372 (0.0%)
1	a	0.41	0/3989	0.64	0/5383
1	b	0.40	0/3980	0.63	0/5372
1	c	0.39	0/3989	0.64	0/5383
1	d	0.39	0/3989	0.62	0/5383
1	e	0.37	0/3980	0.62	0/5372
1	f	0.34	0/3989	0.59	0/5383
1	g	0.41	1/3980 (0.0%)	0.62	1/5372 (0.0%)
1	h	0.40	0/3971	0.62	1/5360 (0.0%)
1	i	0.36	1/3971 (0.0%)	0.60	0/5360
1	j	0.35	0/3971	0.61	1/5360 (0.0%)
1	k	0.34	0/3971	0.59	0/5360
1	l	0.33	0/3971	0.59	0/5360
1	m	0.36	1/3971 (0.0%)	0.59	0/5360
1	n	0.34	0/3971	0.58	0/5360
2	O	0.40	0/746	0.68	0/1003
2	P	0.54	0/730	0.77	0/982
2	Q	0.39	0/746	0.70	2/1003 (0.2%)
2	R	0.42	0/746	0.69	0/1003

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	S	0.42	0/746	0.72	1/1003 (0.1%)
2	T	0.39	0/746	0.67	0/1003
2	U	0.46	0/746	0.72	0/1003
2	o	0.52	0/746	0.71	0/1003
2	p	0.40	0/746	0.68	0/1003
2	q	0.38	0/746	0.72	0/1003
2	r	0.41	0/746	0.67	0/1003
2	s	0.53	0/746	0.76	0/1003
2	t	0.31	0/746	0.64	0/1003
2	u	0.30	0/746	0.62	0/1003
All	All	0.39	6/121841 (0.0%)	0.63	10/164393 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	133	ALA	CA-CB	-13.30	1.24	1.52
1	m	394	ARG	CZ-NH2	-8.93	1.21	1.33
1	K	237	GLU	CD-OE1	-5.26	1.19	1.25
1	M	512	ILE	CB-CG2	5.16	1.68	1.52
1	B	410	ILE	CB-CG2	5.08	1.68	1.52
1	i	352	LEU	CG-CD2	-5.03	1.33	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	444	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	g	133	ALA	CB-CA-C	-7.31	99.13	110.10
1	j	283	ARG	CG-CD-NE	5.69	123.75	111.80
2	Q	51	GLY	N-CA-C	-5.32	99.81	113.10
1	M	512	ILE	CG1-CB-CG2	5.29	123.03	111.40
1	h	512	ILE	CG1-CB-CG2	5.25	122.96	111.40
2	Q	54	LEU	CA-CB-CG	5.18	127.20	115.30
2	S	58	GLN	CA-CB-CG	5.13	124.69	113.40
1	D	190	GLU	N-CA-C	5.08	124.71	111.00
1	B	410	ILE	CG1-CB-CG2	5.05	122.51	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	525/543 (97%)	456 (87%)	56 (11%)	13 (2%)	5	19
1	B	525/543 (97%)	458 (87%)	55 (10%)	12 (2%)	6	21
1	C	524/543 (96%)	451 (86%)	58 (11%)	15 (3%)	4	15
1	D	524/543 (96%)	441 (84%)	67 (13%)	16 (3%)	4	14
1	E	524/543 (96%)	440 (84%)	65 (12%)	19 (4%)	3	11
1	F	527/543 (97%)	453 (86%)	60 (11%)	14 (3%)	5	17
1	G	523/543 (96%)	447 (86%)	65 (12%)	11 (2%)	7	23
1	H	524/543 (96%)	457 (87%)	60 (12%)	7 (1%)	12	36
1	I	523/543 (96%)	457 (87%)	61 (12%)	5 (1%)	15	44
1	J	523/543 (96%)	456 (87%)	58 (11%)	9 (2%)	9	29
1	K	523/543 (96%)	458 (88%)	57 (11%)	8 (2%)	10	33
1	L	524/543 (96%)	454 (87%)	63 (12%)	7 (1%)	12	36
1	M	523/543 (96%)	455 (87%)	61 (12%)	7 (1%)	12	36
1	N	524/543 (96%)	457 (87%)	61 (12%)	6 (1%)	14	41
1	a	525/543 (97%)	453 (86%)	57 (11%)	15 (3%)	4	15
1	b	524/543 (96%)	452 (86%)	61 (12%)	11 (2%)	7	23
1	c	525/543 (97%)	446 (85%)	61 (12%)	18 (3%)	3	13
1	d	525/543 (97%)	451 (86%)	56 (11%)	18 (3%)	3	13
1	e	524/543 (96%)	455 (87%)	57 (11%)	12 (2%)	6	21
1	f	525/543 (97%)	458 (87%)	55 (10%)	12 (2%)	6	21
1	g	524/543 (96%)	450 (86%)	60 (12%)	14 (3%)	5	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	h	523/543 (96%)	459 (88%)	57 (11%)	7 (1%)	12	36
1	i	523/543 (96%)	456 (87%)	58 (11%)	9 (2%)	9	29
1	j	523/543 (96%)	454 (87%)	60 (12%)	9 (2%)	9	29
1	k	523/543 (96%)	456 (87%)	61 (12%)	6 (1%)	14	41
1	l	523/543 (96%)	457 (87%)	59 (11%)	7 (1%)	12	36
1	m	523/543 (96%)	465 (89%)	51 (10%)	7 (1%)	12	36
1	n	523/543 (96%)	459 (88%)	58 (11%)	6 (1%)	14	41
2	O	94/100 (94%)	74 (79%)	13 (14%)	7 (7%)	1	2
2	P	92/100 (92%)	72 (78%)	13 (14%)	7 (8%)	1	2
2	Q	94/100 (94%)	75 (80%)	12 (13%)	7 (7%)	1	2
2	R	94/100 (94%)	75 (80%)	11 (12%)	8 (8%)	1	1
2	S	94/100 (94%)	72 (77%)	17 (18%)	5 (5%)	2	6
2	T	94/100 (94%)	72 (77%)	15 (16%)	7 (7%)	1	2
2	U	94/100 (94%)	77 (82%)	10 (11%)	7 (7%)	1	2
2	o	94/100 (94%)	75 (80%)	13 (14%)	6 (6%)	1	3
2	p	94/100 (94%)	72 (77%)	15 (16%)	7 (7%)	1	2
2	q	94/100 (94%)	58 (62%)	21 (22%)	15 (16%)	0	0
2	r	94/100 (94%)	71 (76%)	17 (18%)	6 (6%)	1	3
2	s	94/100 (94%)	76 (81%)	13 (14%)	5 (5%)	2	6
2	t	94/100 (94%)	69 (73%)	17 (18%)	8 (8%)	1	1
2	u	94/100 (94%)	66 (70%)	18 (19%)	10 (11%)	0	1
All	All	15983/16604 (96%)	13715 (86%)	1863 (12%)	405 (2%)	5	19

All (405) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	278	PRO
1	B	9	ASP
1	B	278	PRO
1	C	9	ASP
1	C	278	PRO
1	C	279	GLY
1	D	9	ASP
1	D	190	GLU

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Mol	Chain	Res	Type
1	D	278	PRO
1	E	9	ASP
1	E	292	ALA
1	E	293	ALA
1	F	9	ASP
1	F	278	PRO
1	G	9	ASP
1	G	278	PRO
1	H	9	ASP
1	I	9	ASP
1	J	9	ASP
1	K	9	ASP
1	L	9	ASP
1	M	9	ASP
1	N	9	ASP
2	O	74	LYS
2	P	22	GLU
2	P	74	LYS
2	Q	19	ARG
2	Q	54	LEU
2	Q	74	LYS
2	R	74	LYS
2	S	12	GLY
2	S	74	LYS
2	T	12	GLY
2	T	19	ARG
2	T	74	LYS
2	U	74	LYS
1	a	9	ASP
1	a	278	PRO
1	b	9	ASP
1	b	278	PRO
1	c	9	ASP
1	c	202	TYR
1	c	292	ALA
1	c	293	ALA
1	c	338	LYS
1	d	9	ASP
1	d	278	PRO
1	e	9	ASP
1	e	278	PRO
1	e	373	GLY

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Mol	Chain	Res	Type
1	f	9	ASP
1	f	278	PRO
1	f	279	GLY
1	g	9	ASP
1	h	9	ASP
1	i	9	ASP
1	j	9	ASP
1	k	9	ASP
1	l	9	ASP
1	m	9	ASP
1	n	9	ASP
2	o	12	GLY
2	o	19	ARG
2	o	74	LYS
2	p	12	GLY
2	p	74	LYS
2	q	22	GLU
2	q	51	GLY
2	q	54	LEU
2	q	63	GLU
2	r	12	GLY
2	r	19	ARG
2	r	54	LEU
2	r	74	LYS
2	s	12	GLY
2	s	74	LYS
2	t	63	GLU
2	u	50	THR
2	u	66	GLU
2	u	96	LEU
1	A	168	VAL
1	A	279	GLY
1	A	336	GLY
1	A	528	GLU
1	B	168	VAL
1	B	216	ASP
1	B	279	GLY
1	B	350	LYS
1	B	374	GLY
1	B	434	GLY
1	C	168	VAL
1	C	169	GLY

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Mol	Chain	Res	Type
1	C	281	GLY
1	C	336	GLY
1	C	434	GLY
1	D	168	VAL
1	D	336	GLY
1	E	28	LYS
1	E	179	SER
1	E	336	GLY
1	G	373	GLY
1	G	374	GLY
1	H	305	GLY
1	I	305	GLY
1	J	305	GLY
1	K	305	GLY
1	L	305	GLY
1	M	305	GLY
1	N	305	GLY
2	O	54	LEU
2	Q	12	GLY
2	Q	34	ASP
2	R	19	ARG
2	S	19	ARG
2	S	54	LEU
2	T	57	GLY
2	U	12	GLY
2	U	34	ASP
2	U	63	GLU
1	a	28	LYS
1	a	168	VAL
1	a	434	GLY
1	b	168	VAL
1	b	179	SER
1	c	168	VAL
1	c	276	LYS
1	c	336	GLY
1	c	527	PRO
1	d	279	GLY
1	d	434	GLY
1	e	168	VAL
1	e	374	GLY
1	f	168	VAL
1	g	168	VAL

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Mol	Chain	Res	Type
1	h	305	GLY
1	i	305	GLY
1	j	305	GLY
1	k	305	GLY
1	l	305	GLY
1	m	305	GLY
1	n	305	GLY
2	o	54	LEU
2	o	66	GLU
2	q	12	GLY
2	q	34	ASP
2	q	78	THR
2	s	54	LEU
2	u	19	ARG
2	u	63	GLU
1	A	482	ALA
1	C	216	ASP
1	C	350	LYS
1	D	199	ILE
1	D	216	ASP
1	E	168	VAL
1	E	276	LYS
1	E	342	GLU
1	F	169	GLY
1	F	190	GLU
1	F	216	ASP
1	F	350	LYS
1	G	168	VAL
1	G	216	ASP
1	G	434	GLY
1	H	80	LYS
1	J	313	LEU
1	K	80	LYS
1	L	80	LYS
1	L	313	LEU
1	L	447	LEU
1	N	80	LYS
1	N	527	PRO
2	O	12	GLY
2	O	19	ARG
2	O	34	ASP
2	P	12	GLY

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Mol	Chain	Res	Type
2	P	19	ARG
2	P	21	GLU
2	R	34	ASP
2	R	54	LEU
2	S	66	GLU
2	T	34	ASP
2	U	19	ARG
1	a	53	GLY
1	a	179	SER
1	b	53	GLY
1	b	434	GLY
1	c	53	GLY
1	c	169	GLY
1	c	434	GLY
1	d	168	VAL
1	d	251	GLU
1	d	281	GLY
1	e	350	LYS
1	f	216	ASP
1	f	336	GLY
1	f	434	GLY
1	g	292	ALA
1	g	434	GLY
1	h	80	LYS
1	h	447	LEU
1	i	80	LYS
1	j	80	LYS
1	j	313	LEU
1	l	474	LYS
1	m	474	LYS
1	n	80	LYS
2	q	32	LEU
2	q	33	PRO
2	q	73	ALA
2	r	34	ASP
2	s	63	GLU
2	t	12	GLY
2	t	59	ARG
2	u	75	TYR
2	u	99	LEU
1	A	216	ASP
1	A	297	GLY

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Mol	Chain	Res	Type
1	A	434	GLY
1	B	281	GLY
1	B	357	SER
1	B	373	GLY
1	C	357	SER
1	C	482	ALA
1	D	53	GLY
1	D	179	SER
1	D	224	LYS
1	E	207	PRO
1	E	482	ALA
1	E	527	PRO
1	F	230	ARG
1	F	279	GLY
1	G	224	LYS
1	H	313	LEU
1	H	474	LYS
1	I	313	LEU
1	J	80	LYS
1	J	447	LEU
1	J	474	LYS
1	K	313	LEU
1	K	447	LEU
1	K	474	LYS
1	M	80	LYS
1	M	189	VAL
1	N	313	LEU
1	N	474	LYS
2	P	85	GLU
2	Q	85	GLU
2	R	12	GLY
2	R	63	GLU
1	a	216	ASP
1	a	251	GLU
1	a	357	SER
1	b	169	GLY
1	b	357	SER
1	c	482	ALA
1	d	179	SER
1	d	216	ASP
1	e	293	ALA
1	e	336	GLY

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Mol	Chain	Res	Type
1	e	434	GLY
1	f	225	LYS
1	f	226	VAL
1	g	28	LYS
1	g	207	PRO
1	g	336	GLY
1	g	371	LEU
1	h	474	LYS
1	i	76	GLU
1	i	447	LEU
1	i	474	LYS
1	j	474	LYS
1	k	80	LYS
1	k	313	LEU
1	k	474	LYS
1	l	80	LYS
1	m	80	LYS
1	n	313	LEU
1	n	447	LEU
1	n	474	LYS
2	o	85	GLU
2	p	19	ARG
2	p	54	LEU
2	q	19	ARG
2	q	28	GLY
2	s	19	ARG
2	u	24	PRO
1	A	179	SER
1	C	224	LYS
1	D	28	LYS
1	D	279	GLY
1	D	354	THR
1	D	434	GLY
1	E	195	ASP
1	E	202	TYR
1	E	371	LEU
1	E	374	GLY
1	F	168	VAL
1	F	353	GLU
1	G	292	ALA
1	G	350	LYS
1	H	300	ILE

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Mol	Chain	Res	Type
1	I	80	LYS
1	I	474	LYS
1	J	101	ARG
1	L	474	LYS
1	M	474	LYS
2	O	50	THR
2	O	85	GLU
2	Q	63	GLU
2	R	85	GLU
2	T	85	GLU
1	a	230	ARG
1	a	482	ALA
1	b	28	LYS
1	c	179	SER
1	c	207	PRO
1	c	308	LEU
1	c	342	GLU
1	c	371	LEU
1	d	354	THR
1	d	357	SER
1	d	364	LEU
1	d	482	ALA
1	f	251	GLU
1	f	357	SER
1	g	179	SER
1	g	267	ARG
1	g	293	ALA
1	i	313	LEU
1	j	76	GLU
1	k	76	GLU
1	l	313	LEU
1	m	313	LEU
2	p	34	ASP
2	q	76	GLY
2	r	85	GLU
2	t	22	GLU
1	B	482	ALA
1	D	169	GLY
1	E	53	GLY
1	F	346	ASN
1	F	357	SER
1	F	434	GLY

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Mol	Chain	Res	Type
1	J	304	LEU
1	M	447	LEU
2	U	85	GLU
1	a	354	THR
1	b	281	GLY
1	d	169	GLY
1	d	292	ALA
1	d	336	GLY
1	e	357	SER
1	f	53	GLY
1	g	53	GLY
1	g	190	GLU
1	j	220	LEU
2	q	24	PRO
2	t	39	LYS
2	t	68	ASP
2	t	84	GLY
1	a	279	GLY
1	b	336	GLY
1	e	279	GLY
2	u	46	ILE
2	u	70	VAL
1	A	281	GLY
1	C	53	GLY
1	E	322	VAL
1	F	527	PRO
1	K	300	ILE
1	M	5	ILE
2	P	30	ILE
1	d	297	GLY
1	e	53	GLY
1	m	189	VAL
2	p	57	GLY
2	t	16	VAL
1	A	53	GLY
1	E	434	GLY
1	G	53	GLY
2	T	53	VAL
1	d	53	GLY
1	g	169	GLY
1	h	300	ILE
1	i	189	VAL

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Mol	Chain	Res	Type
1	C	297	GLY
1	D	226	VAL
1	J	488	VAL
1	L	189	VAL
2	R	67	GLY
1	h	488	VAL
1	i	488	VAL
1	l	189	VAL
1	l	300	ILE
1	m	300	ILE
2	q	70	VAL
1	H	488	VAL
1	K	189	VAL
2	U	67	GLY
1	a	281	GLY
1	j	300	ILE
1	j	488	VAL
2	p	30	ILE

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	412/423 (97%)	402 (98%)	10 (2%)	49	81
1	B	412/423 (97%)	399 (97%)	13 (3%)	39	73
1	C	411/423 (97%)	399 (97%)	12 (3%)	42	76
1	D	411/423 (97%)	401 (98%)	10 (2%)	49	81
1	E	411/423 (97%)	395 (96%)	16 (4%)	32	66
1	F	414/423 (98%)	405 (98%)	9 (2%)	52	83
1	G	410/423 (97%)	400 (98%)	10 (2%)	49	81
1	H	411/423 (97%)	403 (98%)	8 (2%)	57	85
1	I	410/423 (97%)	400 (98%)	10 (2%)	49	81
1	J	410/423 (97%)	400 (98%)	10 (2%)	49	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	410/423 (97%)	401 (98%)	9 (2%)	52	83
1	L	411/423 (97%)	401 (98%)	10 (2%)	49	81
1	M	410/423 (97%)	399 (97%)	11 (3%)	44	78
1	N	411/423 (97%)	401 (98%)	10 (2%)	49	81
1	a	412/423 (97%)	404 (98%)	8 (2%)	57	85
1	b	411/423 (97%)	401 (98%)	10 (2%)	49	81
1	c	412/423 (97%)	400 (97%)	12 (3%)	42	76
1	d	412/423 (97%)	401 (97%)	11 (3%)	44	78
1	e	411/423 (97%)	403 (98%)	8 (2%)	57	85
1	f	412/423 (97%)	404 (98%)	8 (2%)	57	85
1	g	411/423 (97%)	401 (98%)	10 (2%)	49	81
1	h	410/423 (97%)	400 (98%)	10 (2%)	49	81
1	i	410/423 (97%)	399 (97%)	11 (3%)	44	78
1	j	410/423 (97%)	398 (97%)	12 (3%)	42	76
1	k	410/423 (97%)	399 (97%)	11 (3%)	44	78
1	l	410/423 (97%)	400 (98%)	10 (2%)	49	81
1	m	410/423 (97%)	400 (98%)	10 (2%)	49	81
1	n	410/423 (97%)	401 (98%)	9 (2%)	52	83
2	O	81/83 (98%)	76 (94%)	5 (6%)	18	47
2	P	79/83 (95%)	76 (96%)	3 (4%)	33	67
2	Q	81/83 (98%)	78 (96%)	3 (4%)	34	68
2	R	81/83 (98%)	78 (96%)	3 (4%)	34	68
2	S	81/83 (98%)	78 (96%)	3 (4%)	34	68
2	T	81/83 (98%)	77 (95%)	4 (5%)	25	57
2	U	81/83 (98%)	78 (96%)	3 (4%)	34	68
2	o	81/83 (98%)	79 (98%)	2 (2%)	47	80
2	p	81/83 (98%)	78 (96%)	3 (4%)	34	68
2	q	81/83 (98%)	78 (96%)	3 (4%)	34	68
2	r	81/83 (98%)	78 (96%)	3 (4%)	34	68
2	s	81/83 (98%)	78 (96%)	3 (4%)	34	68
2	t	81/83 (98%)	78 (96%)	3 (4%)	34	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	u	81/83 (98%)	78 (96%)	3 (4%)	34	68
All	All	12637/13006 (97%)	12305 (97%)	332 (3%)	46	79

All (332) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	9	ASP
1	A	36	ARG
1	A	54	VAL
1	A	173	ILE
1	A	283	ARG
1	A	303	GLU
1	A	312	THR
1	A	340	ASP
1	A	351	GLU
1	B	5	ILE
1	B	9	ASP
1	B	36	ARG
1	B	54	VAL
1	B	173	ILE
1	B	234	PRO
1	B	280	PHE
1	B	283	ARG
1	B	290	ASP
1	B	303	GLU
1	B	340	ASP
1	B	351	GLU
1	B	410	ILE
1	C	5	ILE
1	C	9	ASP
1	C	36	ARG
1	C	54	VAL
1	C	89	THR
1	C	173	ILE
1	C	283	ARG
1	C	303	GLU
1	C	312	THR
1	C	340	ASP
1	C	351	GLU
1	C	410	ILE
1	D	5	ILE

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Mol	Chain	Res	Type
1	D	9	ASP
1	D	36	ARG
1	D	54	VAL
1	D	173	ILE
1	D	283	ARG
1	D	303	GLU
1	D	309	GLU
1	D	340	ASP
1	D	351	GLU
1	E	5	ILE
1	E	9	ASP
1	E	36	ARG
1	E	54	VAL
1	E	136	ILE
1	E	144	ILE
1	E	173	ILE
1	E	210	MET
1	E	235	ILE
1	E	251	GLU
1	E	298	THR
1	E	309	GLU
1	E	316	LEU
1	E	342	GLU
1	E	349	LYS
1	E	368	LEU
1	F	5	ILE
1	F	9	ASP
1	F	36	ARG
1	F	54	VAL
1	F	173	ILE
1	F	198	TYR
1	F	283	ARG
1	F	340	ASP
1	F	351	GLU
1	G	5	ILE
1	G	9	ASP
1	G	36	ARG
1	G	54	VAL
1	G	198	TYR
1	G	283	ARG
1	G	303	GLU
1	G	312	THR

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Mol	Chain	Res	Type
1	G	340	ASP
1	G	351	GLU
1	H	151	SER
1	H	153	ASN
1	H	190	GLU
1	H	270	LEU
1	H	316	LEU
1	H	325	THR
1	H	423	SER
1	H	456	GLU
1	I	151	SER
1	I	153	ASN
1	I	190	GLU
1	I	216	ASP
1	I	270	LEU
1	I	316	LEU
1	I	325	THR
1	I	363	LYS
1	I	423	SER
1	I	456	GLU
1	J	151	SER
1	J	153	ASN
1	J	194	PHE
1	J	216	ASP
1	J	270	LEU
1	J	316	LEU
1	J	325	THR
1	J	423	SER
1	J	456	GLU
1	J	527	PRO
1	K	151	SER
1	K	153	ASN
1	K	194	PHE
1	K	237	GLU
1	K	270	LEU
1	K	316	LEU
1	K	363	LYS
1	K	423	SER
1	K	456	GLU
1	L	151	SER
1	L	153	ASN
1	L	194	PHE

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Mol	Chain	Res	Type
1	L	270	LEU
1	L	316	LEU
1	L	325	THR
1	L	363	LYS
1	L	423	SER
1	L	456	GLU
1	L	522	VAL
1	M	151	SER
1	M	153	ASN
1	M	190	GLU
1	M	194	PHE
1	M	196	LYS
1	M	270	LEU
1	M	316	LEU
1	M	363	LYS
1	M	423	SER
1	M	456	GLU
1	M	522	VAL
1	N	151	SER
1	N	153	ASN
1	N	194	PHE
1	N	270	LEU
1	N	316	LEU
1	N	325	THR
1	N	363	LYS
1	N	423	SER
1	N	456	GLU
1	N	522	VAL
2	O	15	VAL
2	O	21	GLU
2	O	34	ASP
2	O	50	THR
2	O	55	GLU
2	P	15	VAL
2	P	21	GLU
2	P	56	ASN
2	Q	21	GLU
2	Q	34	ASP
2	Q	48	VAL
2	R	21	GLU
2	R	55	GLU
2	R	62	LEU

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Mol	Chain	Res	Type
2	S	21	GLU
2	S	48	VAL
2	S	56	ASN
2	T	13	ASP
2	T	21	GLU
2	T	34	ASP
2	T	48	VAL
2	U	13	ASP
2	U	21	GLU
2	U	92	GLU
1	a	5	ILE
1	a	9	ASP
1	a	36	ARG
1	a	54	VAL
1	a	173	ILE
1	a	303	GLU
1	a	340	ASP
1	a	351	GLU
1	b	5	ILE
1	b	9	ASP
1	b	36	ARG
1	b	54	VAL
1	b	173	ILE
1	b	216	ASP
1	b	303	GLU
1	b	312	THR
1	b	340	ASP
1	b	351	GLU
1	c	5	ILE
1	c	9	ASP
1	c	54	VAL
1	c	173	ILE
1	c	192	TYR
1	c	224	LYS
1	c	251	GLU
1	c	298	THR
1	c	316	LEU
1	c	342	GLU
1	c	368	LEU
1	c	410	ILE
1	d	5	ILE
1	d	9	ASP

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Mol	Chain	Res	Type
1	d	36	ARG
1	d	54	VAL
1	d	89	THR
1	d	173	ILE
1	d	198	TYR
1	d	303	GLU
1	d	340	ASP
1	d	351	GLU
1	d	365	GLN
1	e	5	ILE
1	e	9	ASP
1	e	36	ARG
1	e	54	VAL
1	e	173	ILE
1	e	303	GLU
1	e	340	ASP
1	e	351	GLU
1	f	5	ILE
1	f	9	ASP
1	f	36	ARG
1	f	54	VAL
1	f	173	ILE
1	f	303	GLU
1	f	340	ASP
1	f	351	GLU
1	g	5	ILE
1	g	9	ASP
1	g	36	ARG
1	g	54	VAL
1	g	173	ILE
1	g	204	VAL
1	g	251	GLU
1	g	298	THR
1	g	316	LEU
1	g	342	GLU
1	h	151	SER
1	h	153	ASN
1	h	194	PHE
1	h	216	ASP
1	h	270	LEU
1	h	316	LEU
1	h	325	THR

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Mol	Chain	Res	Type
1	h	363	LYS
1	h	423	SER
1	h	456	GLU
1	i	151	SER
1	i	153	ASN
1	i	194	PHE
1	i	270	LEU
1	i	283	ARG
1	i	316	LEU
1	i	325	THR
1	i	352	LEU
1	i	363	LYS
1	i	423	SER
1	i	456	GLU
1	j	151	SER
1	j	153	ASN
1	j	190	GLU
1	j	194	PHE
1	j	216	ASP
1	j	270	LEU
1	j	283	ARG
1	j	316	LEU
1	j	325	THR
1	j	363	LYS
1	j	423	SER
1	j	456	GLU
1	k	151	SER
1	k	190	GLU
1	k	194	PHE
1	k	216	ASP
1	k	270	LEU
1	k	283	ARG
1	k	316	LEU
1	k	325	THR
1	k	363	LYS
1	k	423	SER
1	k	456	GLU
1	l	151	SER
1	l	153	ASN
1	l	190	GLU
1	l	194	PHE
1	l	196	LYS

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Mol	Chain	Res	Type
1	l	270	LEU
1	l	316	LEU
1	l	363	LYS
1	l	423	SER
1	l	456	GLU
1	m	151	SER
1	m	153	ASN
1	m	194	PHE
1	m	270	LEU
1	m	302	GLU
1	m	316	LEU
1	m	325	THR
1	m	363	LYS
1	m	423	SER
1	m	456	GLU
1	n	151	SER
1	n	194	PHE
1	n	216	ASP
1	n	270	LEU
1	n	316	LEU
1	n	325	THR
1	n	363	LYS
1	n	423	SER
1	n	456	GLU
2	o	13	ASP
2	o	21	GLU
2	p	21	GLU
2	p	48	VAL
2	p	56	ASN
2	q	33	PRO
2	q	72	PHE
2	q	93	ARG
2	r	13	ASP
2	r	21	GLU
2	r	48	VAL
2	s	13	ASP
2	s	21	GLU
2	s	22	GLU
2	t	14	ARG
2	t	69	ILE
2	t	72	PHE
2	u	31	VAL

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Mol	Chain	Res	Type
2	u	70	VAL
2	u	74	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (271) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	106	ASN
1	A	228	ASN
1	A	310	ASN
1	A	400	ASN
1	A	457	ASN
1	B	72	GLN
1	B	228	ASN
1	B	310	ASN
1	B	400	ASN
1	B	457	ASN
1	C	72	GLN
1	C	106	ASN
1	C	241	GLN
1	C	310	ASN
1	C	400	ASN
1	C	457	ASN
1	D	72	GLN
1	D	106	ASN
1	D	310	ASN
1	D	400	ASN
1	D	457	ASN
1	E	72	GLN
1	E	193	GLN
1	E	310	ASN
1	E	346	ASN
1	E	400	ASN
1	E	457	ASN
1	F	72	GLN
1	F	310	ASN
1	F	400	ASN
1	F	457	ASN
1	G	72	GLN
1	G	310	ASN
1	G	400	ASN
1	G	457	ASN

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Mol	Chain	Res	Type
1	H	37	ASN
1	H	97	GLN
1	H	106	ASN
1	H	153	ASN
1	H	193	GLN
1	H	228	ASN
1	H	310	ASN
1	H	346	ASN
1	H	365	GLN
1	H	400	ASN
1	H	468	GLN
1	H	481	ASN
1	H	507	GLN
1	H	508	ASN
1	I	37	ASN
1	I	97	GLN
1	I	153	ASN
1	I	193	GLN
1	I	228	ASN
1	I	264	ASN
1	I	310	ASN
1	I	346	ASN
1	I	365	GLN
1	I	400	ASN
1	I	468	GLN
1	I	481	ASN
1	I	507	GLN
1	I	508	ASN
1	J	37	ASN
1	J	97	GLN
1	J	153	ASN
1	J	193	GLN
1	J	228	ASN
1	J	310	ASN
1	J	346	ASN
1	J	365	GLN
1	J	400	ASN
1	J	468	GLN
1	J	481	ASN
1	J	507	GLN
1	J	508	ASN
1	K	37	ASN

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Mol	Chain	Res	Type
1	K	97	GLN
1	K	106	ASN
1	K	112	ASN
1	K	153	ASN
1	K	193	GLN
1	K	228	ASN
1	K	264	ASN
1	K	310	ASN
1	K	346	ASN
1	K	365	GLN
1	K	400	ASN
1	K	468	GLN
1	K	481	ASN
1	K	507	GLN
1	K	508	ASN
1	L	37	ASN
1	L	97	GLN
1	L	153	ASN
1	L	193	GLN
1	L	228	ASN
1	L	310	ASN
1	L	365	GLN
1	L	400	ASN
1	L	468	GLN
1	L	481	ASN
1	L	507	GLN
1	L	508	ASN
1	M	37	ASN
1	M	97	GLN
1	M	153	ASN
1	M	193	GLN
1	M	228	ASN
1	M	310	ASN
1	M	346	ASN
1	M	365	GLN
1	M	400	ASN
1	M	468	GLN
1	M	481	ASN
1	M	507	GLN
1	M	508	ASN
1	N	37	ASN
1	N	97	GLN

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Mol	Chain	Res	Type
1	N	153	ASN
1	N	228	ASN
1	N	310	ASN
1	N	346	ASN
1	N	365	GLN
1	N	400	ASN
1	N	468	GLN
1	N	481	ASN
1	N	507	GLN
1	N	508	ASN
2	O	56	ASN
2	Q	41	GLN
1	a	72	GLN
1	a	106	ASN
1	a	228	ASN
1	a	310	ASN
1	a	400	ASN
1	a	457	ASN
1	b	72	GLN
1	b	106	ASN
1	b	228	ASN
1	b	310	ASN
1	b	400	ASN
1	b	457	ASN
1	c	72	GLN
1	c	106	ASN
1	c	310	ASN
1	c	346	ASN
1	c	400	ASN
1	c	457	ASN
1	d	72	GLN
1	d	310	ASN
1	d	400	ASN
1	d	457	ASN
1	e	72	GLN
1	e	106	ASN
1	e	228	ASN
1	e	310	ASN
1	e	400	ASN
1	e	457	ASN
1	f	72	GLN
1	f	106	ASN

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Mol	Chain	Res	Type
1	f	228	ASN
1	f	310	ASN
1	f	400	ASN
1	f	457	ASN
1	g	72	GLN
1	g	106	ASN
1	g	310	ASN
1	g	346	ASN
1	g	365	GLN
1	g	400	ASN
1	g	457	ASN
1	h	37	ASN
1	h	65	HIS
1	h	97	GLN
1	h	153	ASN
1	h	193	GLN
1	h	228	ASN
1	h	310	ASN
1	h	346	ASN
1	h	365	GLN
1	h	400	ASN
1	h	468	GLN
1	h	481	ASN
1	h	507	GLN
1	h	508	ASN
1	i	37	ASN
1	i	97	GLN
1	i	153	ASN
1	i	228	ASN
1	i	310	ASN
1	i	346	ASN
1	i	365	GLN
1	i	400	ASN
1	i	468	GLN
1	i	481	ASN
1	i	507	GLN
1	i	508	ASN
1	j	37	ASN
1	j	65	HIS
1	j	97	GLN
1	j	153	ASN
1	j	193	GLN

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Mol	Chain	Res	Type
1	j	228	ASN
1	j	264	ASN
1	j	310	ASN
1	j	365	GLN
1	j	400	ASN
1	j	468	GLN
1	j	481	ASN
1	j	507	GLN
1	j	508	ASN
1	k	37	ASN
1	k	97	GLN
1	k	153	ASN
1	k	193	GLN
1	k	228	ASN
1	k	310	ASN
1	k	346	ASN
1	k	365	GLN
1	k	400	ASN
1	k	468	GLN
1	k	481	ASN
1	k	507	GLN
1	k	508	ASN
1	l	37	ASN
1	l	97	GLN
1	l	153	ASN
1	l	193	GLN
1	l	228	ASN
1	l	310	ASN
1	l	346	ASN
1	l	365	GLN
1	l	400	ASN
1	l	468	GLN
1	l	481	ASN
1	l	507	GLN
1	l	508	ASN
1	m	37	ASN
1	m	97	GLN
1	m	153	ASN
1	m	193	GLN
1	m	228	ASN
1	m	310	ASN
1	m	346	ASN

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Mol	Chain	Res	Type
1	m	365	GLN
1	m	400	ASN
1	m	468	GLN
1	m	481	ASN
1	m	507	GLN
1	m	508	ASN
1	n	37	ASN
1	n	97	GLN
1	n	153	ASN
1	n	193	GLN
1	n	228	ASN
1	n	310	ASN
1	n	346	ASN
1	n	365	GLN
1	n	400	ASN
1	n	468	GLN
1	n	481	ASN
1	n	507	GLN
1	n	508	ASN
2	q	41	GLN
2	r	41	GLN
2	t	41	GLN
2	t	100	GLN
2	u	41	GLN
2	u	56	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 42 ligands modelled in this entry, 14 are monoatomic - leaving 28 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$
5	DMS	K	601	-	3,3,3	0.29	0	3,3,3	0.69	0
5	DMS	i	601	-	3,3,3	0.33	0	3,3,3	0.71	0
5	DMS	j	601	-	3,3,3	0.29	0	3,3,3	0.66	0
4	ADP	g	602	3	24,29,29	1.51	5 (20%)	29,45,45	1.57	3 (10%)
5	DMS	k	601	-	3,3,3	0.30	0	3,3,3	0.67	0
5	DMS	H	601	-	3,3,3	0.22	0	3,3,3	0.67	0
5	DMS	N	701	-	3,3,3	0.25	0	3,3,3	0.66	0
4	ADP	B	602	3	24,29,29	1.48	4 (16%)	29,45,45	1.56	3 (10%)
4	ADP	D	602	3	24,29,29	1.65	6 (25%)	29,45,45	1.56	2 (6%)
5	DMS	L	601	-	3,3,3	0.31	0	3,3,3	0.69	0
5	DMS	M	601	-	3,3,3	0.28	0	3,3,3	0.64	0
5	DMS	h	601	-	3,3,3	0.35	0	3,3,3	0.71	0
4	ADP	A	602	3	24,29,29	1.41	4 (16%)	29,45,45	1.57	3 (10%)
5	DMS	n	701	-	3,3,3	0.25	0	3,3,3	0.62	0
4	ADP	C	602	3	24,29,29	1.54	3 (12%)	29,45,45	1.61	3 (10%)
4	ADP	E	602	3	24,29,29	1.40	5 (20%)	29,45,45	1.65	4 (13%)
4	ADP	b	602	3	24,29,29	1.71	5 (20%)	29,45,45	1.63	2 (6%)
4	ADP	d	602	3	24,29,29	1.65	6 (25%)	29,45,45	1.63	4 (13%)
4	ADP	F	602	3	24,29,29	1.53	4 (16%)	29,45,45	1.58	3 (10%)
5	DMS	l	601	-	3,3,3	0.33	0	3,3,3	0.68	0
5	DMS	m	601	-	3,3,3	0.26	0	3,3,3	0.62	0
4	ADP	a	602	3	24,29,29	1.60	4 (16%)	29,45,45	1.57	3 (10%)
5	DMS	J	601	-	3,3,3	0.37	0	3,3,3	0.75	0
4	ADP	f	602	3	24,29,29	1.56	5 (20%)	29,45,45	1.60	3 (10%)
4	ADP	c	602	3	24,29,29	1.61	4 (16%)	29,45,45	1.74	3 (10%)
4	ADP	e	602	3	24,29,29	1.68	5 (20%)	29,45,45	1.64	3 (10%)
4	ADP	G	602	3	24,29,29	1.49	6 (25%)	29,45,45	1.61	3 (10%)
5	DMS	I	601	-	3,3,3	0.26	0	3,3,3	0.68	0

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
4	ADP	B	602	3	-	7/12/32/32	0/3/3/3
4	ADP	D	602	3	-	8/12/32/32	0/3/3/3
4	ADP	A	602	3	-	6/12/32/32	0/3/3/3
4	ADP	C	602	3	-	7/12/32/32	0/3/3/3
4	ADP	g	602	3	-	8/12/32/32	0/3/3/3
4	ADP	F	602	3	-	7/12/32/32	0/3/3/3
4	ADP	E	602	3	-	8/12/32/32	0/3/3/3
4	ADP	c	602	3	-	8/12/32/32	0/3/3/3
4	ADP	b	602	3	-	8/12/32/32	0/3/3/3
4	ADP	e	602	3	-	7/12/32/32	0/3/3/3
4	ADP	a	602	3	-	7/12/32/32	0/3/3/3
4	ADP	G	602	3	-	7/12/32/32	0/3/3/3
4	ADP	d	602	3	-	6/12/32/32	0/3/3/3
4	ADP	f	602	3	-	8/12/32/32	0/3/3/3

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	602	ADP	C2'-C1'	-4.59	1.46	1.53
4	C	602	ADP	C2'-C1'	-4.32	1.47	1.53
4	F	602	ADP	C2'-C1'	-4.26	1.47	1.53
4	a	602	ADP	C2'-C1'	-4.22	1.47	1.53
4	D	602	ADP	C2-N3	4.20	1.38	1.32
4	B	602	ADP	C2-N3	3.90	1.38	1.32
4	a	602	ADP	C2-N3	3.80	1.38	1.32
4	d	602	ADP	C2'-C1'	-3.75	1.48	1.53
4	c	602	ADP	C2-N3	3.75	1.38	1.32
4	e	602	ADP	C2'-C1'	-3.69	1.48	1.53
4	e	602	ADP	C2-N3	3.41	1.37	1.32
4	F	602	ADP	C2-N3	3.35	1.37	1.32
4	d	602	ADP	C4-N3	3.31	1.40	1.35
4	g	602	ADP	C2-N3	3.29	1.37	1.32
4	f	602	ADP	C2-N3	3.27	1.37	1.32
4	B	602	ADP	C2'-C1'	-3.24	1.48	1.53
4	G	602	ADP	C2'-C1'	-3.19	1.48	1.53
4	D	602	ADP	C2'-C1'	-3.13	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	ADP	C2'-C1'	-3.10	1.49	1.53
4	f	602	ADP	O4'-C1'	3.03	1.45	1.41
4	C	602	ADP	C2-N3	3.02	1.37	1.32
4	b	602	ADP	C2-N3	3.02	1.37	1.32
4	A	602	ADP	C2-N3	2.99	1.36	1.32
4	b	602	ADP	C4-N3	2.96	1.39	1.35
4	A	602	ADP	O4'-C1'	2.93	1.45	1.41
4	G	602	ADP	O4'-C1'	2.93	1.45	1.41
4	d	602	ADP	C2-N3	2.93	1.36	1.32
4	c	602	ADP	C2'-C1'	-2.82	1.49	1.53
4	b	602	ADP	O4'-C1'	2.81	1.45	1.41
4	g	602	ADP	C2'-C1'	-2.67	1.49	1.53
4	E	602	ADP	C2-N3	2.65	1.36	1.32
4	G	602	ADP	C4-N3	2.65	1.39	1.35
4	c	602	ADP	O4'-C1'	2.64	1.44	1.41
4	e	602	ADP	C4-N3	2.63	1.39	1.35
4	f	602	ADP	C4-N3	2.63	1.39	1.35
4	D	602	ADP	O4'-C1'	2.62	1.44	1.41
4	e	602	ADP	O4'-C1'	2.61	1.44	1.41
4	g	602	ADP	O4'-C1'	2.60	1.44	1.41
4	D	602	ADP	PB-O2B	2.55	1.64	1.54
4	c	602	ADP	C2-N1	2.53	1.38	1.33
4	d	602	ADP	O4'-C1'	2.52	1.44	1.41
4	E	602	ADP	C4-N3	2.51	1.39	1.35
4	C	602	ADP	C4-N3	2.43	1.39	1.35
4	E	602	ADP	C2'-C1'	-2.41	1.50	1.53
4	F	602	ADP	C5-N7	-2.36	1.31	1.39
4	e	602	ADP	C2-N1	2.30	1.38	1.33
4	g	602	ADP	C4-N3	2.28	1.38	1.35
4	a	602	ADP	C4-N3	2.27	1.38	1.35
4	b	602	ADP	C2-N1	2.26	1.38	1.33
4	f	602	ADP	C2'-C1'	-2.23	1.50	1.53
4	g	602	ADP	C5-N7	-2.23	1.31	1.39
4	G	602	ADP	C2-N1	2.22	1.38	1.33
4	D	602	ADP	C4-N3	2.18	1.38	1.35
4	f	602	ADP	C2-N1	2.15	1.37	1.33
4	G	602	ADP	PA-O2A	-2.15	1.45	1.55
4	E	602	ADP	PA-O2A	-2.12	1.45	1.55
4	F	602	ADP	C4-N3	2.11	1.38	1.35
4	G	602	ADP	C5'-C4'	2.09	1.58	1.51
4	d	602	ADP	C2-N1	2.09	1.37	1.33
4	D	602	ADP	PA-O2A	-2.08	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	602	ADP	C5-N7	-2.06	1.32	1.39
4	E	602	ADP	C5'-C4'	2.03	1.57	1.51
4	B	602	ADP	C5-N7	-2.03	1.32	1.39
4	B	602	ADP	PA-O2A	-2.03	1.45	1.55
4	a	602	ADP	PA-O2A	-2.02	1.45	1.55
4	A	602	ADP	C5'-C4'	2.00	1.57	1.51

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	c	602	ADP	N3-C2-N1	-7.15	117.50	128.68
4	f	602	ADP	N3-C2-N1	-7.01	117.72	128.68
4	b	602	ADP	N3-C2-N1	-6.98	117.77	128.68
4	d	602	ADP	N3-C2-N1	-6.97	117.78	128.68
4	C	602	ADP	N3-C2-N1	-6.92	117.86	128.68
4	G	602	ADP	N3-C2-N1	-6.89	117.91	128.68
4	E	602	ADP	N3-C2-N1	-6.79	118.06	128.68
4	g	602	ADP	N3-C2-N1	-6.78	118.08	128.68
4	e	602	ADP	N3-C2-N1	-6.71	118.19	128.68
4	D	602	ADP	N3-C2-N1	-6.67	118.25	128.68
4	a	602	ADP	N3-C2-N1	-6.66	118.27	128.68
4	A	602	ADP	N3-C2-N1	-6.63	118.32	128.68
4	F	602	ADP	N3-C2-N1	-6.61	118.35	128.68
4	B	602	ADP	N3-C2-N1	-6.56	118.42	128.68
4	c	602	ADP	C4-C5-N7	-4.10	105.13	109.40
4	e	602	ADP	C4-C5-N7	-3.52	105.73	109.40
4	F	602	ADP	O4'-C4'-C5'	2.83	118.70	109.37
4	c	602	ADP	O4'-C4'-C5'	2.63	118.01	109.37
4	B	602	ADP	C4-C5-N7	-2.62	106.67	109.40
4	B	602	ADP	O4'-C4'-C5'	2.58	117.88	109.37
4	E	602	ADP	C4-C5-N7	-2.53	106.76	109.40
4	F	602	ADP	C4-C5-N7	-2.53	106.76	109.40
4	D	602	ADP	O4'-C4'-C5'	2.52	117.66	109.37
4	a	602	ADP	C4-C5-N7	-2.46	106.83	109.40
4	a	602	ADP	O4'-C4'-C5'	2.45	117.44	109.37
4	G	602	ADP	O4'-C4'-C5'	2.44	117.41	109.37
4	E	602	ADP	C3'-C2'-C1'	-2.44	97.31	100.98
4	b	602	ADP	O4'-C4'-C5'	2.42	117.34	109.37
4	C	602	ADP	O4'-C4'-C5'	2.39	117.23	109.37
4	g	602	ADP	C4-C5-N7	-2.37	106.93	109.40
4	d	602	ADP	C4-C5-N7	-2.37	106.93	109.40
4	g	602	ADP	O4'-C4'-C5'	2.33	117.04	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	602	ADP	C4-C5-N7	-2.32	106.98	109.40
4	e	602	ADP	O4'-C4'-C5'	2.28	116.89	109.37
4	f	602	ADP	O4'-C4'-C5'	2.28	116.86	109.37
4	f	602	ADP	C4-C5-N7	-2.28	107.03	109.40
4	E	602	ADP	O4'-C4'-C5'	2.27	116.83	109.37
4	d	602	ADP	O4'-C4'-C5'	2.27	116.83	109.37
4	A	602	ADP	O4'-C4'-C5'	2.25	116.79	109.37
4	A	602	ADP	C2-N1-C6	2.22	122.55	118.75
4	d	602	ADP	C2-N1-C6	2.12	122.37	118.75
4	C	602	ADP	C2-N1-C6	2.05	122.26	118.75

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	ADP	C5'-O5'-PA-O1A
4	A	602	ADP	C5'-O5'-PA-O2A
4	A	602	ADP	C5'-O5'-PA-O3A
4	A	602	ADP	O4'-C4'-C5'-O5'
4	g	602	ADP	C5'-O5'-PA-O1A
4	g	602	ADP	C5'-O5'-PA-O2A
4	g	602	ADP	C5'-O5'-PA-O3A
4	g	602	ADP	O4'-C4'-C5'-O5'
4	B	602	ADP	C5'-O5'-PA-O1A
4	B	602	ADP	C5'-O5'-PA-O2A
4	B	602	ADP	C5'-O5'-PA-O3A
4	B	602	ADP	O4'-C4'-C5'-O5'
4	D	602	ADP	C5'-O5'-PA-O1A
4	D	602	ADP	C5'-O5'-PA-O2A
4	D	602	ADP	C5'-O5'-PA-O3A
4	D	602	ADP	O4'-C4'-C5'-O5'
4	D	602	ADP	C3'-C4'-C5'-O5'
4	C	602	ADP	C5'-O5'-PA-O1A
4	C	602	ADP	C5'-O5'-PA-O2A
4	C	602	ADP	C5'-O5'-PA-O3A
4	C	602	ADP	O4'-C4'-C5'-O5'
4	E	602	ADP	C5'-O5'-PA-O1A
4	E	602	ADP	C5'-O5'-PA-O2A
4	E	602	ADP	C5'-O5'-PA-O3A
4	E	602	ADP	O4'-C4'-C5'-O5'
4	E	602	ADP	C3'-C4'-C5'-O5'
4	b	602	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	b	602	ADP	C5'-O5'-PA-O2A
4	b	602	ADP	C5'-O5'-PA-O3A
4	b	602	ADP	O4'-C4'-C5'-O5'
4	b	602	ADP	C3'-C4'-C5'-O5'
4	d	602	ADP	C5'-O5'-PA-O1A
4	d	602	ADP	C5'-O5'-PA-O2A
4	d	602	ADP	C5'-O5'-PA-O3A
4	d	602	ADP	O4'-C4'-C5'-O5'
4	F	602	ADP	C5'-O5'-PA-O1A
4	F	602	ADP	C5'-O5'-PA-O2A
4	F	602	ADP	C5'-O5'-PA-O3A
4	F	602	ADP	O4'-C4'-C5'-O5'
4	F	602	ADP	C3'-C4'-C5'-O5'
4	a	602	ADP	C5'-O5'-PA-O1A
4	a	602	ADP	C5'-O5'-PA-O2A
4	a	602	ADP	C5'-O5'-PA-O3A
4	a	602	ADP	O4'-C4'-C5'-O5'
4	c	602	ADP	C5'-O5'-PA-O1A
4	c	602	ADP	C5'-O5'-PA-O2A
4	c	602	ADP	C5'-O5'-PA-O3A
4	c	602	ADP	O4'-C4'-C5'-O5'
4	e	602	ADP	C5'-O5'-PA-O1A
4	e	602	ADP	C5'-O5'-PA-O2A
4	e	602	ADP	C5'-O5'-PA-O3A
4	G	602	ADP	C5'-O5'-PA-O1A
4	G	602	ADP	C5'-O5'-PA-O2A
4	G	602	ADP	C5'-O5'-PA-O3A
4	G	602	ADP	O4'-C4'-C5'-O5'
4	f	602	ADP	C5'-O5'-PA-O1A
4	f	602	ADP	C5'-O5'-PA-O2A
4	f	602	ADP	C5'-O5'-PA-O3A
4	f	602	ADP	O4'-C4'-C5'-O5'
4	A	602	ADP	C3'-C4'-C5'-O5'
4	g	602	ADP	C3'-C4'-C5'-O5'
4	B	602	ADP	C3'-C4'-C5'-O5'
4	C	602	ADP	C3'-C4'-C5'-O5'
4	d	602	ADP	C3'-C4'-C5'-O5'
4	a	602	ADP	C3'-C4'-C5'-O5'
4	c	602	ADP	C3'-C4'-C5'-O5'
4	e	602	ADP	O4'-C4'-C5'-O5'
4	e	602	ADP	C3'-C4'-C5'-O5'
4	G	602	ADP	C3'-C4'-C5'-O5'

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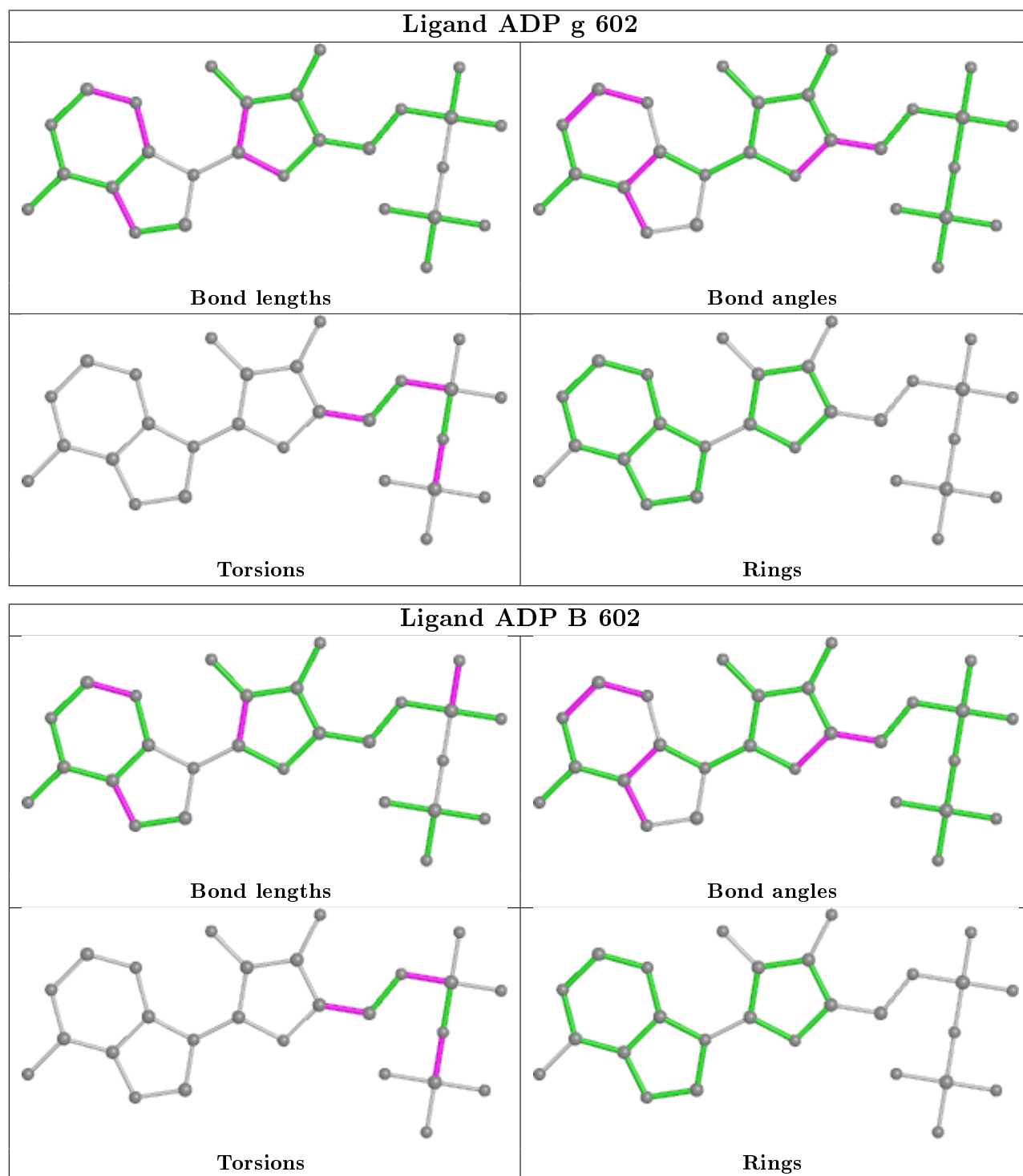
Mol	Chain	Res	Type	Atoms
4	f	602	ADP	C3'-C4'-C5'-O5'
4	g	602	ADP	PA-O3A-PB-O1B
4	E	602	ADP	PA-O3A-PB-O1B
4	b	602	ADP	PA-O3A-PB-O1B
4	c	602	ADP	PA-O3A-PB-O1B
4	A	602	ADP	PA-O3A-PB-O2B
4	F	602	ADP	PA-O3A-PB-O2B
4	G	602	ADP	PB-O3A-PA-O1A
4	C	602	ADP	PB-O3A-PA-O1A
4	f	602	ADP	PA-O3A-PB-O1B
4	C	602	ADP	PB-O3A-PA-O2A
4	D	602	ADP	PA-O3A-PB-O1B
4	e	602	ADP	PA-O3A-PB-O1B
4	g	602	ADP	PA-O3A-PB-O2B
4	g	602	ADP	PA-O3A-PB-O3B
4	B	602	ADP	PA-O3A-PB-O2B
4	B	602	ADP	PA-O3A-PB-O3B
4	D	602	ADP	PA-O3A-PB-O2B
4	D	602	ADP	PA-O3A-PB-O3B
4	E	602	ADP	PA-O3A-PB-O2B
4	E	602	ADP	PA-O3A-PB-O3B
4	b	602	ADP	PA-O3A-PB-O2B
4	b	602	ADP	PA-O3A-PB-O3B
4	d	602	ADP	PA-O3A-PB-O2B
4	F	602	ADP	PA-O3A-PB-O3B
4	a	602	ADP	PA-O3A-PB-O2B
4	a	602	ADP	PA-O3A-PB-O3B
4	c	602	ADP	PA-O3A-PB-O2B
4	c	602	ADP	PA-O3A-PB-O3B
4	e	602	ADP	PA-O3A-PB-O3B
4	f	602	ADP	PA-O3A-PB-O2B
4	f	602	ADP	PA-O3A-PB-O3B
4	G	602	ADP	PB-O3A-PA-O2A

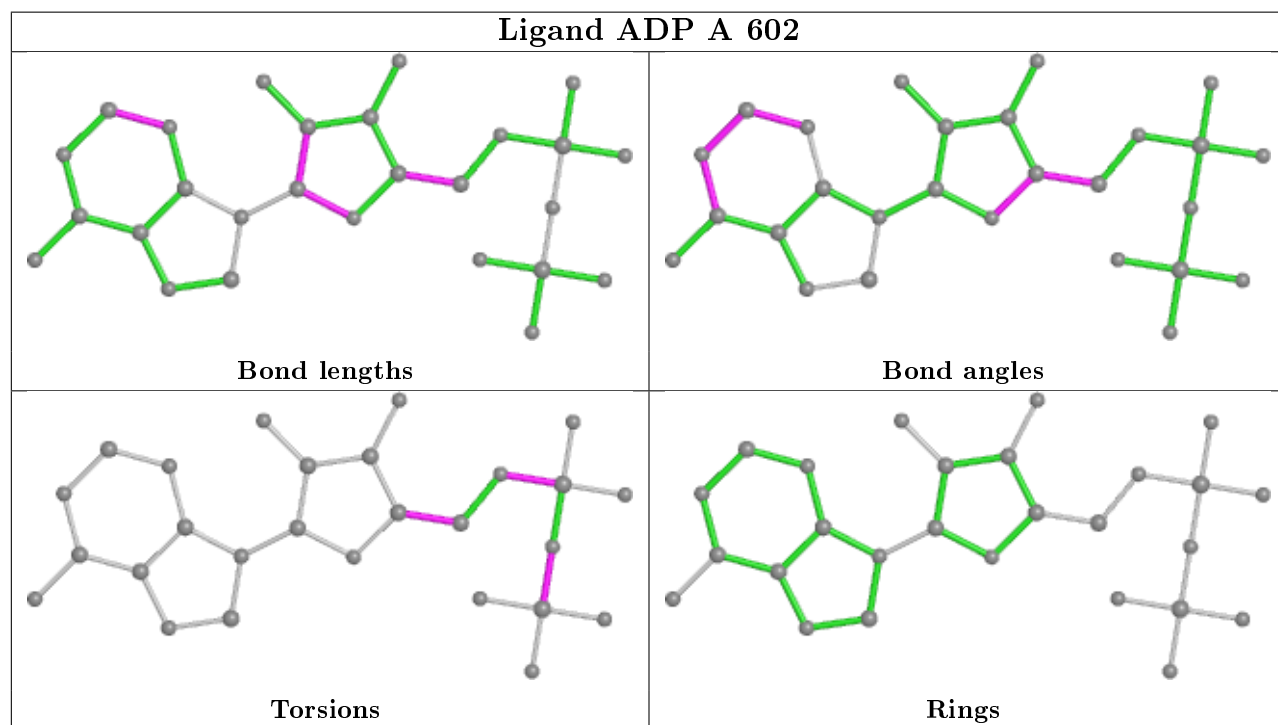
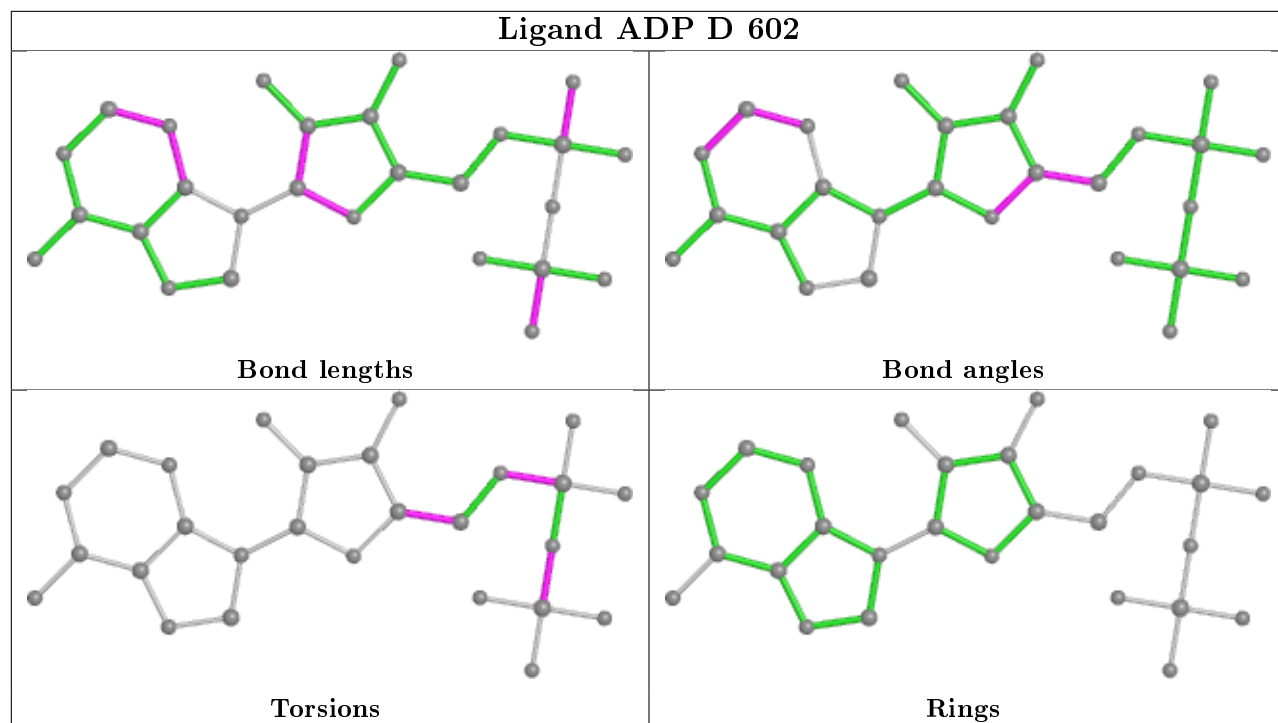
There are no ring outliers.

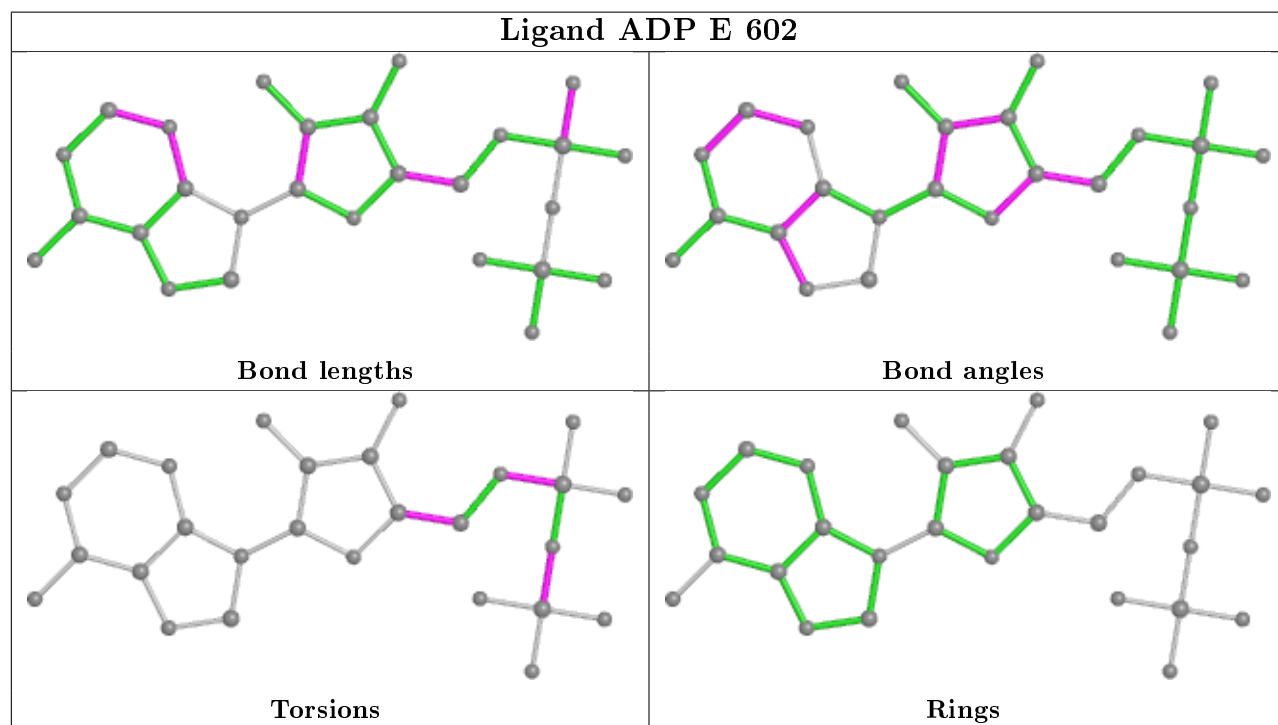
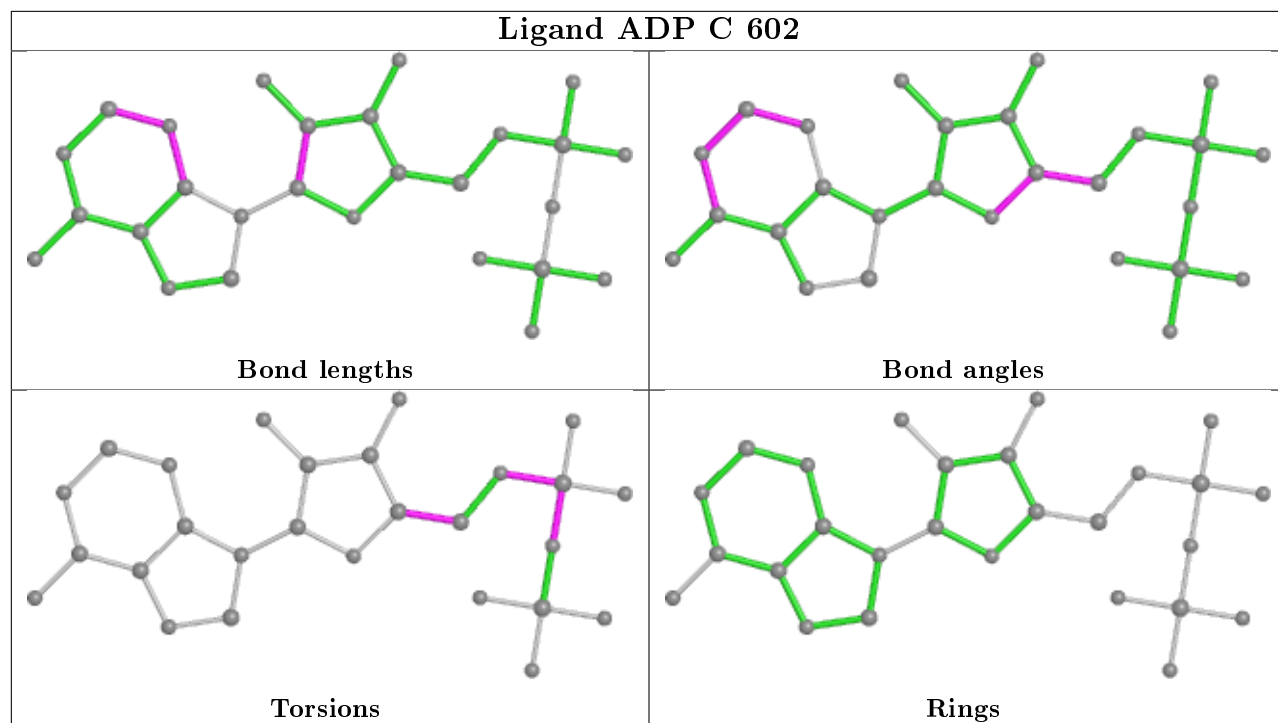
No monomer is involved in short contacts.

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

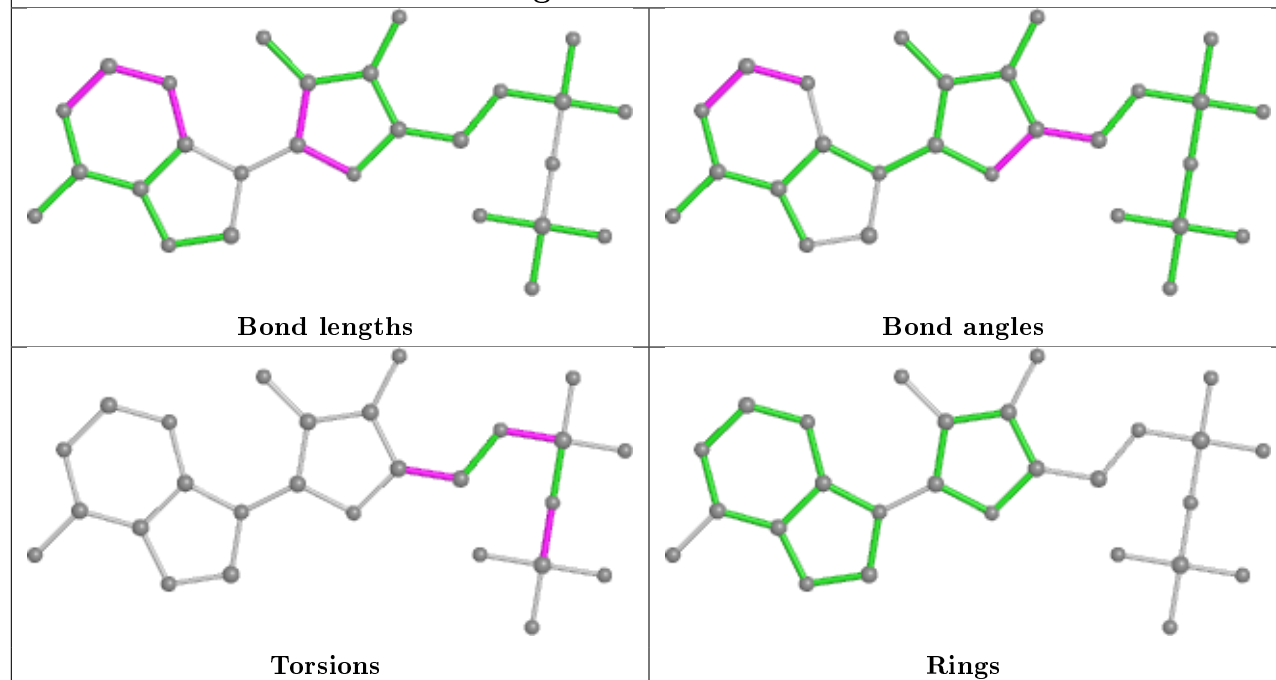
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



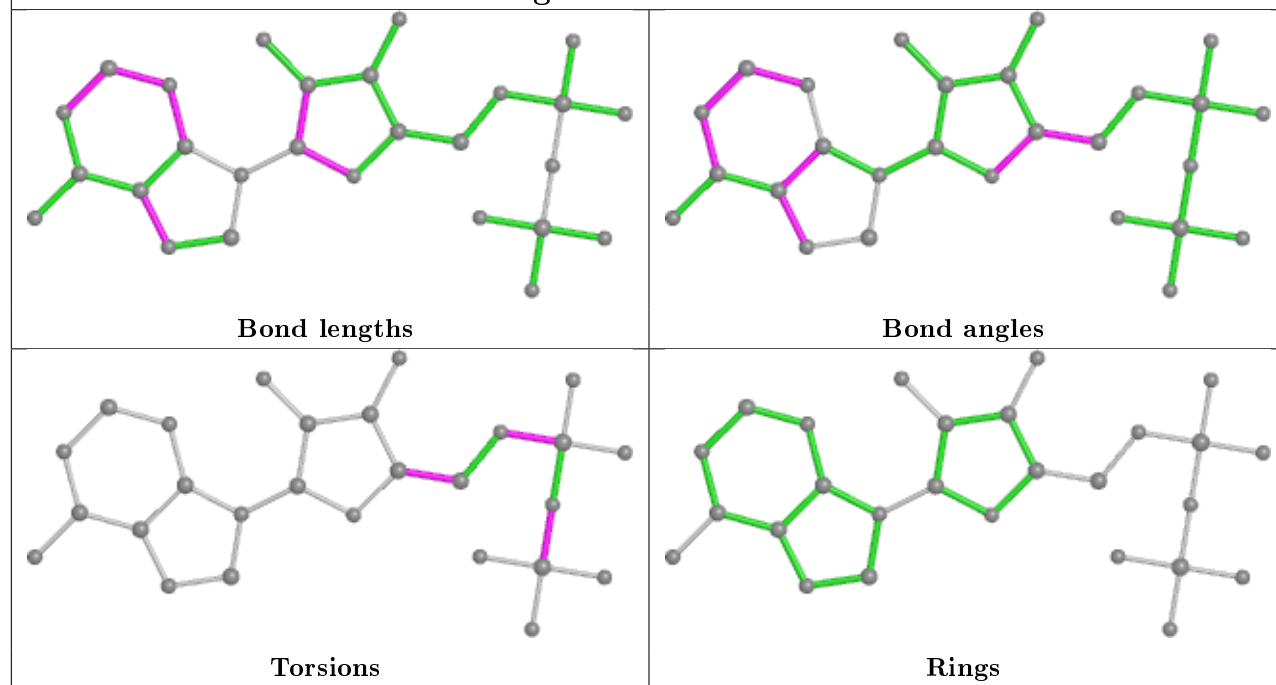


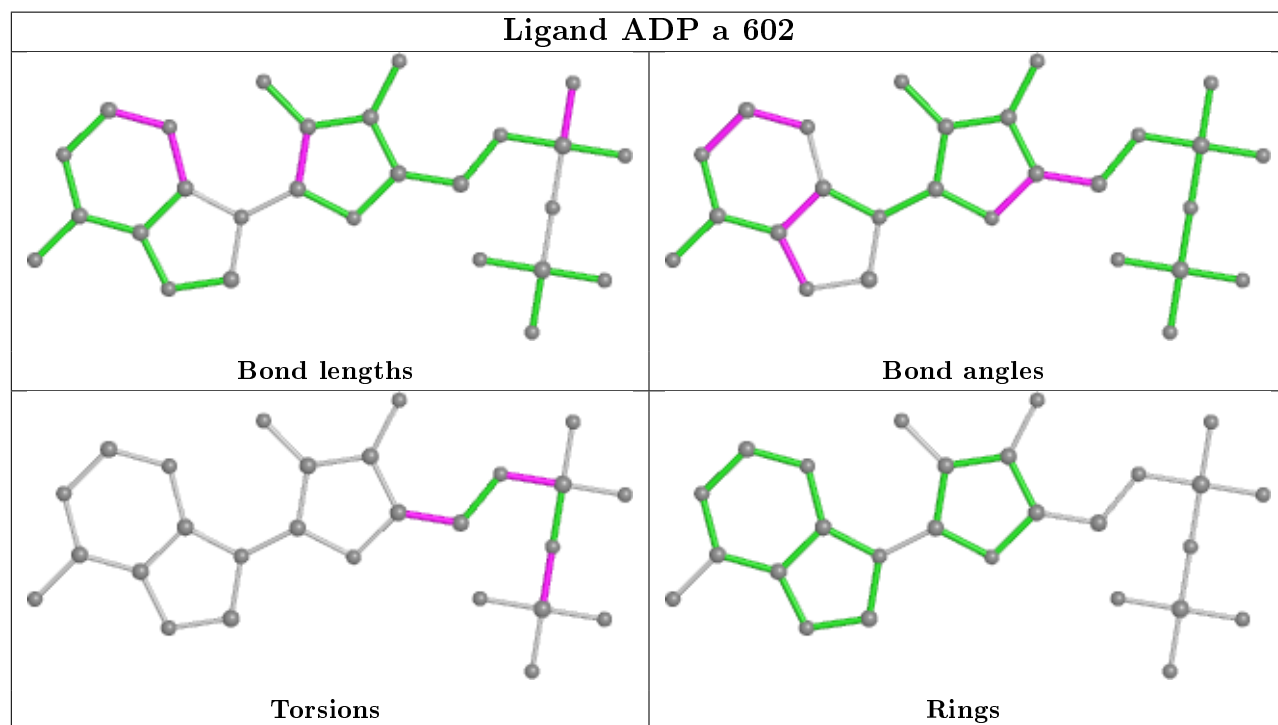
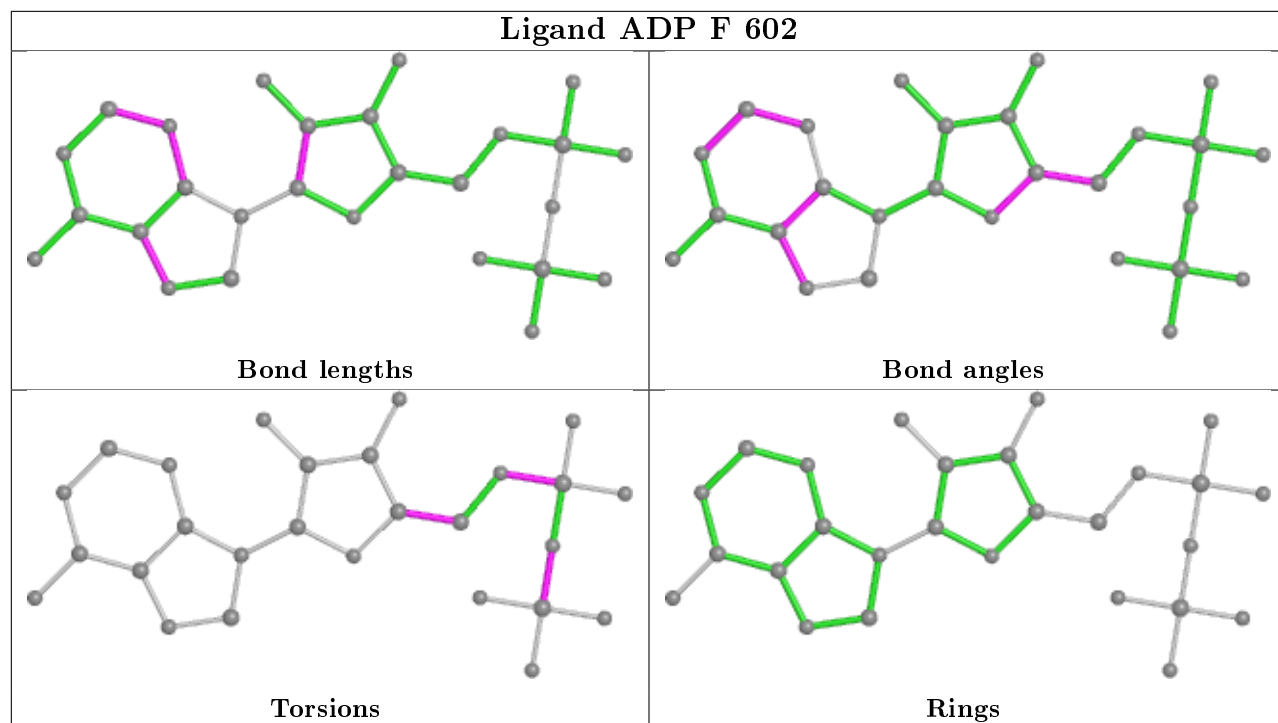


Ligand ADP b 602

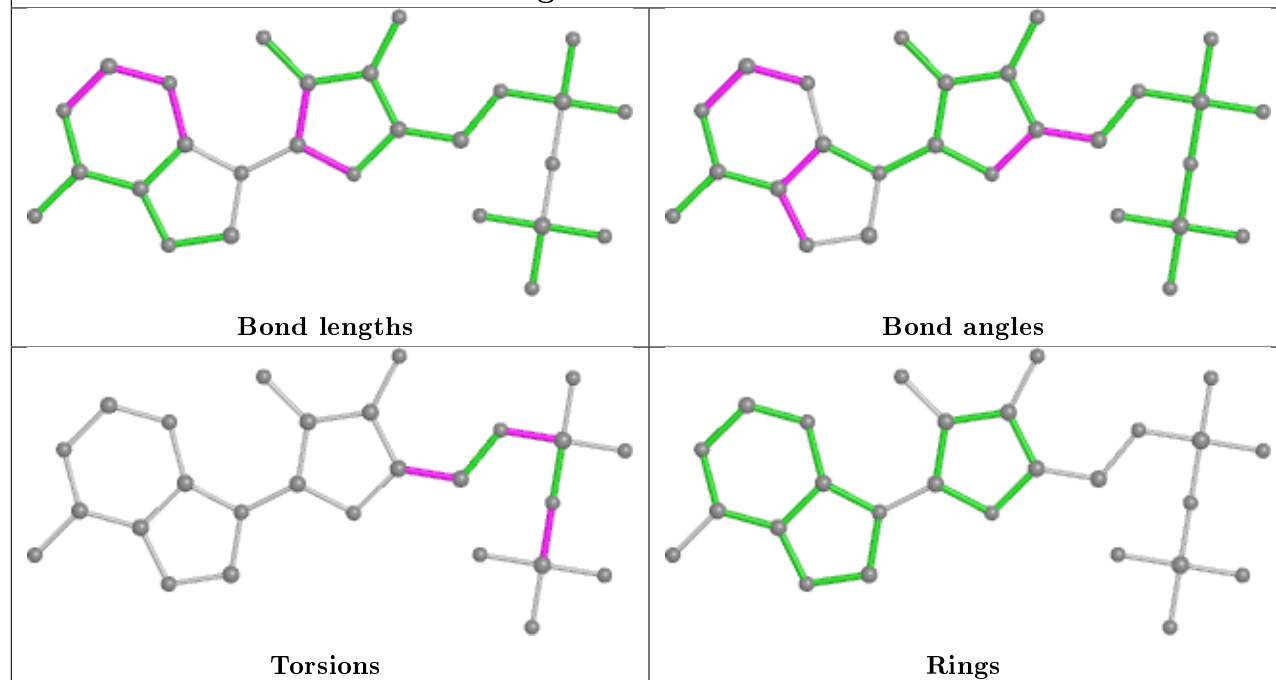


Ligand ADP d 602

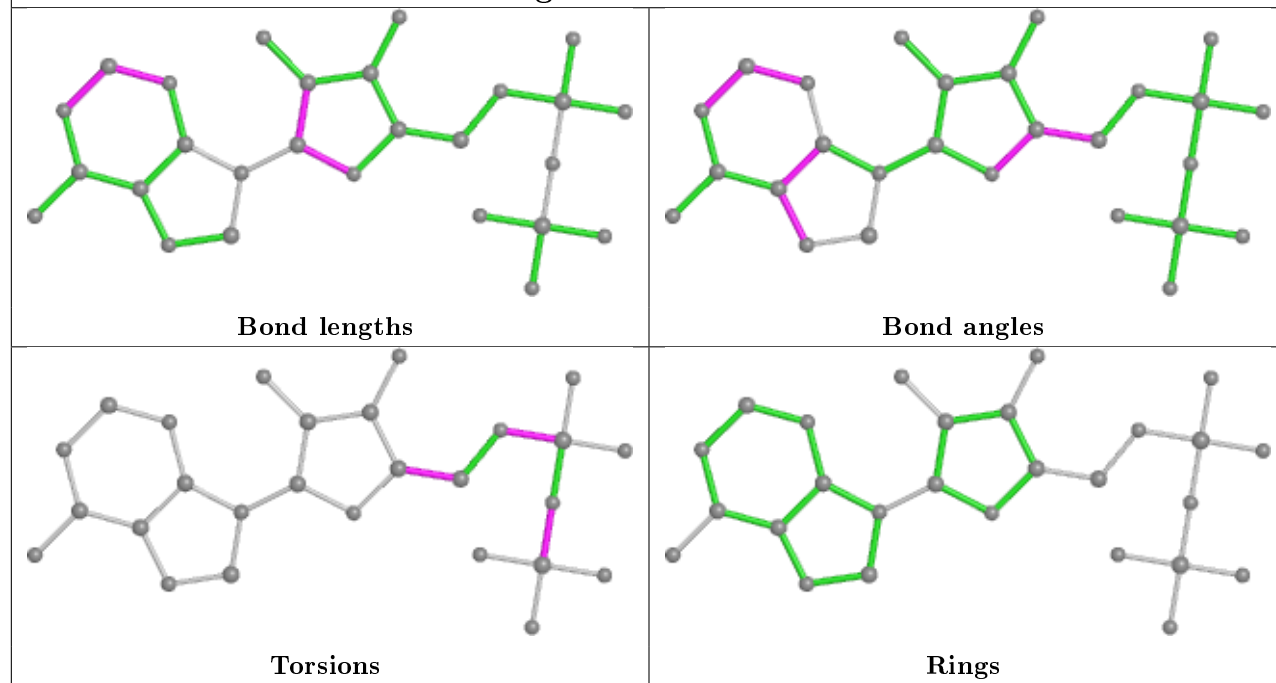


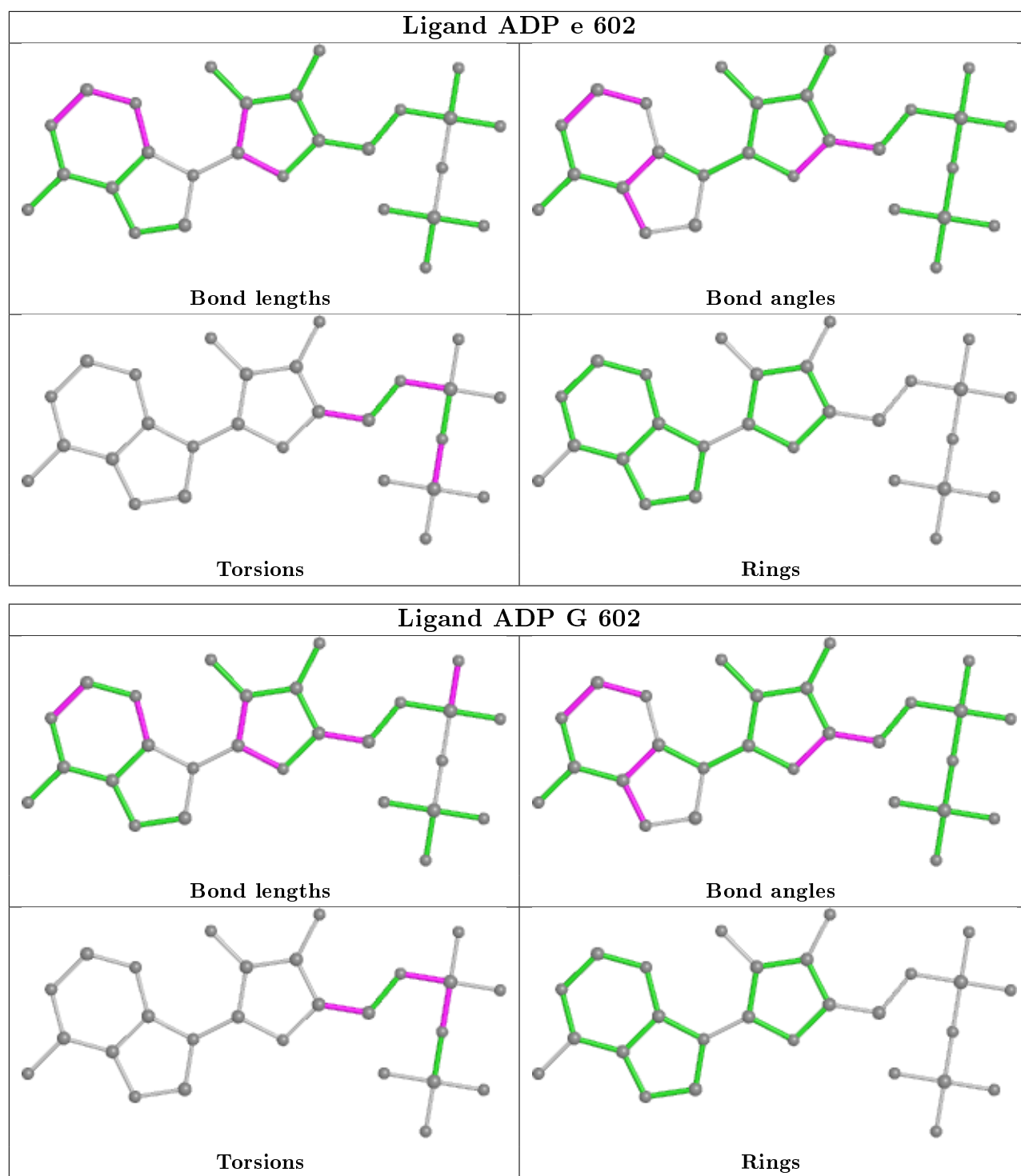


Ligand ADP f 602



Ligand ADP c 602





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	527/543 (97%)	-0.22	4 (0%)	86 81	16, 51, 95, 147	0
1	B	527/543 (97%)	-0.17	5 (0%)	84 80	15, 52, 101, 146	0
1	C	526/543 (96%)	-0.24	2 (0%)	92 91	14, 50, 101, 140	0
1	D	526/543 (96%)	-0.09	11 (2%)	63 54	14, 55, 120, 154	0
1	E	526/543 (96%)	-0.03	12 (2%)	60 51	9, 51, 127, 164	0
1	F	529/543 (97%)	-0.08	9 (1%)	70 63	17, 58, 108, 159	0
1	G	525/543 (96%)	-0.14	4 (0%)	86 81	19, 57, 106, 140	0
1	H	526/543 (96%)	-0.03	14 (2%)	54 44	26, 70, 120, 163	0
1	I	525/543 (96%)	-0.10	9 (1%)	70 63	24, 67, 121, 151	0
1	J	525/543 (96%)	-0.13	8 (1%)	73 68	14, 55, 110, 163	0
1	K	525/543 (96%)	-0.08	11 (2%)	63 54	16, 63, 120, 157	0
1	L	526/543 (96%)	-0.09	10 (1%)	66 59	23, 62, 115, 154	0
1	M	525/543 (96%)	1.90	181 (34%)	0 0	25, 95, 150, 167	0
1	N	526/543 (96%)	0.07	22 (4%)	36 26	25, 70, 124, 167	0
1	a	527/543 (97%)	0.26	37 (7%)	16 9	18, 71, 128, 157	0
1	b	526/543 (96%)	0.21	47 (8%)	9 5	18, 66, 121, 163	0
1	c	527/543 (97%)	0.14	28 (5%)	26 17	23, 72, 134, 166	0
1	d	527/543 (97%)	0.03	12 (2%)	60 51	29, 77, 118, 146	0
1	e	526/543 (96%)	0.16	20 (3%)	40 30	42, 81, 116, 155	0
1	f	527/543 (97%)	0.30	25 (4%)	31 22	45, 88, 123, 149	0
1	g	526/543 (96%)	0.21	31 (5%)	22 14	27, 88, 136, 163	0
1	h	525/543 (96%)	-0.08	7 (1%)	77 72	24, 61, 112, 150	0
1	i	525/543 (96%)	0.09	25 (4%)	30 21	28, 76, 125, 160	0
1	j	525/543 (96%)	0.22	29 (5%)	25 16	32, 79, 125, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	k	525/543 (96%)	0.49	60 (11%) 5 3	37, 94, 135, 158	0
1	l	525/543 (96%)	1.00	110 (20%) 1 0	48, 106, 143, 162	0
1	m	525/543 (96%)	1.52	161 (30%) 0 0	56, 104, 146, 174	0
1	n	525/543 (96%)	0.10	29 (5%) 25 16	37, 79, 130, 158	0
2	O	96/100 (96%)	0.62	11 (11%) 4 2	59, 109, 142, 146	0
2	P	94/100 (94%)	0.52	6 (6%) 19 12	69, 108, 142, 146	0
2	Q	96/100 (96%)	0.61	9 (9%) 8 4	60, 108, 142, 149	0
2	R	96/100 (96%)	0.41	6 (6%) 20 12	60, 99, 134, 151	0
2	S	96/100 (96%)	0.75	14 (14%) 2 1	61, 107, 140, 150	0
2	T	96/100 (96%)	0.74	11 (11%) 4 2	65, 106, 141, 154	0
2	U	96/100 (96%)	0.71	10 (10%) 6 3	55, 107, 142, 148	0
2	o	96/100 (96%)	1.39	28 (29%) 0 0	86, 116, 152, 164	0
2	p	96/100 (96%)	0.82	14 (14%) 2 1	80, 112, 146, 150	0
2	q	96/100 (96%)	0.49	5 (5%) 27 18	45, 101, 141, 157	0
2	r	96/100 (96%)	0.66	10 (10%) 6 3	60, 109, 141, 150	0
2	s	96/100 (96%)	0.82	14 (14%) 2 1	73, 114, 143, 150	0
2	t	96/100 (96%)	0.68	16 (16%) 1 1	82, 118, 147, 159	0
2	u	96/100 (96%)	0.89	17 (17%) 1 1	83, 122, 153, 167	0
All	All	16067/16604 (96%)	0.23	1094 (6%) 17 10	9, 76, 133, 174	0

All (1094) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	294	VAL	17.1
1	M	291	ILE	16.7
1	M	273	ALA	16.4
1	M	247	LEU	15.1
1	M	246	LEU	13.3
1	M	290	ASP	12.8
1	m	271	SER	12.7
1	M	219	ILE	12.6
1	m	356	ASP	12.4
1	M	332	VAL	11.7
1	M	199	ILE	11.5
1	m	355	THR	10.7
1	M	229	VAL	10.6

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Mol	Chain	Res	Type	RSRZ
1	M	295	THR	10.4
1	M	260	THR	10.1
1	M	200	SER	9.9
1	m	261	LEU	9.8
1	M	279	GLY	9.7
1	m	236	LEU	9.5
1	M	375	VAL	9.4
1	M	315	MET	9.3
1	M	217	ALA	9.2
1	M	371	LEU	9.2
1	M	245	PRO	9.2
1	M	368	LEU	9.0
1	M	283	ARG	9.0
1	M	264	ASN	8.9
1	M	222	VAL	8.8
1	M	299	VAL	8.8
1	M	306	PHE	8.5
1	M	330	THR	8.5
1	M	262	VAL	8.5
1	m	319	ALA	8.3
1	m	315	MET	8.3
1	m	217	ALA	8.3
1	m	257	ALA	8.3
1	m	298	THR	8.2
1	M	192	TYR	8.2
1	M	234	PRO	8.2
1	m	214	LEU	8.1
1	M	209	THR	8.1
1	m	234	PRO	8.0
1	M	354	THR	7.9
1	M	215	GLU	7.9
1	M	208	GLU	7.9
1	M	259	ALA	7.9
1	M	356	ASP	7.9
1	M	189	VAL	7.8
1	M	171	GLU	7.8
1	M	266	LEU	7.7
1	l	357	SER	7.5
1	M	193	GLN	7.5
1	M	357	SER	7.5
1	m	291	ILE	7.5
1	m	273	ALA	7.4

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Mol	Chain	Res	Type	RSRZ
1	m	210	MET	7.4
1	M	280	PHE	7.4
1	M	343	ALA	7.3
1	M	367	ARG	7.3
1	M	233	LEU	7.2
1	m	316	LEU	7.2
1	l	304	LEU	7.2
1	M	270	LEU	7.2
1	H	527	PRO	7.2
1	M	263	VAL	7.2
1	m	371	LEU	7.1
1	m	264	ASN	7.1
1	k	527	PRO	7.1
1	m	209	THR	7.0
1	M	298	THR	6.9
1	m	235	ILE	6.8
1	M	202	TYR	6.8
1	M	218	PHE	6.8
1	m	280	PHE	6.8
1	l	359	TYR	6.8
1	m	266	LEU	6.8
1	m	245	PRO	6.6
1	m	233	LEU	6.6
1	L	527	PRO	6.6
1	m	357	SER	6.6
1	M	213	VAL	6.6
1	m	279	GLY	6.6
1	L	528	GLU	6.6
1	m	260	THR	6.5
1	M	327	ASP	6.5
1	M	257	ALA	6.5
1	m	265	LYS	6.5
1	M	227	SER	6.5
1	m	288	LEU	6.5
1	m	262	VAL	6.4
1	M	232	LEU	6.4
1	M	251	GLU	6.4
1	M	268	GLY	6.4
1	m	263	VAL	6.3
1	k	358	GLU	6.3
1	k	214	LEU	6.3
1	m	253	VAL	6.3

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Mol	Chain	Res	Type	RSRZ
1	m	215	GLU	6.3
1	M	274	ALA	6.3
1	m	299	VAL	6.2
1	m	382	ALA	6.2
1	N	527	PRO	6.2
1	m	270	LEU	6.2
1	m	201	PRO	6.2
1	N	528	GLU	6.2
1	l	191	GLY	6.2
1	m	232	LEU	6.2
1	M	255	GLY	6.1
1	m	267	ARG	6.1
1	M	201	PRO	6.1
1	M	314	SER	6.0
1	a	332	VAL	6.0
1	M	350	LYS	6.0
1	j	368	LEU	6.0
1	m	192	TYR	6.0
1	b	362	GLU	5.9
2	o	44	LYS	5.9
2	T	24	PRO	5.9
1	m	237	GLU	5.9
1	M	214	LEU	5.9
2	u	6	THR	5.9
1	M	253	VAL	5.9
1	M	322	VAL	5.9
1	l	375	VAL	5.9
1	M	318	ARG	5.9
1	M	282	ASP	5.9
1	m	294	VAL	5.9
1	m	255	GLY	5.8
1	M	382	ALA	5.8
1	M	258	LEU	5.8
2	o	24	PRO	5.8
1	M	267	ARG	5.8
1	A	529	LYS	5.7
1	k	371	LEU	5.7
1	m	360	ALA	5.6
1	M	239	VAL	5.6
1	M	300	ILE	5.6
1	M	173	ILE	5.6
1	i	356	ASP	5.6

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Mol	Chain	Res	Type	RSRZ
2	s	100	GLN	5.6
1	k	357	SER	5.6
1	l	168	VAL	5.5
1	M	252	ASP	5.5
1	k	355	THR	5.5
1	M	230	ARG	5.5
1	m	200	SER	5.5
1	M	265	LYS	5.4
1	a	529	LYS	5.4
1	m	247	LEU	5.4
1	m	348	ILE	5.4
1	M	244	LYS	5.4
1	m	292	ALA	5.4
1	M	311	ALA	5.4
1	n	527	PRO	5.3
1	m	203	PHE	5.3
1	M	359	TYR	5.2
1	M	254	GLU	5.2
1	M	355	THR	5.2
1	m	325	THR	5.2
1	l	395	PHE	5.2
1	m	306	PHE	5.2
1	m	222	VAL	5.2
2	s	57	GLY	5.1
1	m	246	LEU	5.1
1	c	529	LYS	5.1
1	c	270	LEU	5.1
1	c	208	GLU	5.1
1	l	370	LYS	5.1
1	M	236	LEU	5.1
1	m	311	ALA	5.1
1	F	530	LYS	5.1
2	o	99	LEU	5.0
1	a	279	GLY	5.0
1	m	202	TYR	5.0
1	N	266	LEU	5.0
1	b	226	VAL	5.0
1	l	348	ILE	5.0
1	a	277	ALA	5.0
1	M	271	SER	4.9
1	m	258	LEU	4.9
1	a	278	PRO	4.9

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Mol	Chain	Res	Type	RSRZ
2	U	24	PRO	4.9
1	M	289	LYS	4.9
1	m	241	GLN	4.9
1	M	320	GLU	4.9
1	g	339	GLU	4.9
1	m	313	LEU	4.9
2	Q	28	GLY	4.9
1	m	354	THR	4.9
1	c	528	GLU	4.9
1	M	331	ILE	4.9
1	m	256	GLU	4.9
1	M	341	ILE	4.9
1	m	208	GLU	4.8
1	m	374	GLY	4.8
1	f	529	LYS	4.8
1	M	328	GLU	4.8
1	L	304	LEU	4.8
1	a	300	ILE	4.8
1	M	269	THR	4.8
1	h	527	PRO	4.8
1	l	345	ILE	4.8
1	M	292	ALA	4.8
1	m	219	ILE	4.8
1	m	295	THR	4.8
1	M	346	ASN	4.8
1	k	368	LEU	4.7
1	m	297	GLY	4.7
1	M	305	GLY	4.7
1	N	359	TYR	4.7
2	R	5	LYS	4.7
2	o	69	ILE	4.7
1	b	303	GLU	4.6
1	N	526	LYS	4.6
1	m	305	GLY	4.6
1	f	527	PRO	4.6
1	i	355	THR	4.6
2	o	39	LYS	4.6
1	m	268	GLY	4.6
1	M	206	ASN	4.6
1	m	283	ARG	4.6
1	K	527	PRO	4.6
1	M	365	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
1	m	350	LYS	4.6
1	k	304	LEU	4.5
1	m	375	VAL	4.5
1	l	223	GLU	4.5
1	M	242	THR	4.5
1	M	261	LEU	4.5
1	D	528	GLU	4.5
1	m	243	GLY	4.5
1	M	228	ASN	4.5
1	c	351	GLU	4.5
1	M	361	ARG	4.5
1	j	182	LEU	4.5
1	l	173	ILE	4.4
1	M	216	ASP	4.4
1	b	528	GLU	4.4
1	h	3	ALA	4.4
1	N	44	PHE	4.4
1	c	280	PHE	4.4
1	m	340	ASP	4.4
1	M	210	MET	4.4
1	N	368	LEU	4.4
1	m	239	VAL	4.4
1	m	212	ALA	4.4
1	M	256	GLU	4.4
1	l	257	ALA	4.4
1	g	280	PHE	4.4
1	n	354	THR	4.4
1	J	527	PRO	4.3
1	M	363	LYS	4.3
1	E	270	LEU	4.3
2	T	39	LYS	4.3
1	b	368	LEU	4.3
1	m	334	GLY	4.3
2	o	31	VAL	4.3
1	e	374	GLY	4.3
2	o	43	GLY	4.3
1	M	304	LEU	4.3
1	m	216	ASP	4.3
1	m	300	ILE	4.3
1	m	290	ASP	4.3
1	b	329	THR	4.3
1	f	364	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	l	366	GLU	4.3
2	u	5	LYS	4.3
1	M	339	GLU	4.2
1	M	226	VAL	4.2
1	m	308	LEU	4.2
1	m	314	SER	4.2
1	m	364	LEU	4.2
2	p	94	ASP	4.2
1	m	346	ASN	4.2
1	m	312	THR	4.2
2	p	88	VAL	4.2
1	M	347	GLY	4.2
1	m	278	PRO	4.2
1	b	352	LEU	4.1
1	m	368	LEU	4.1
1	D	358	GLU	4.1
1	M	156	GLU	4.1
1	M	342	GLU	4.1
1	M	353	GLU	4.1
1	l	350	LYS	4.1
1	M	297	GLY	4.1
1	m	373	GLY	4.1
1	F	531	GLU	4.1
1	M	293	ALA	4.1
1	M	360	ALA	4.1
1	M	376	ALA	4.1
2	t	73	ALA	4.1
1	B	374	GLY	4.1
1	m	345	ILE	4.1
1	m	171	GLU	4.1
1	m	303	GLU	4.1
1	l	264	ASN	4.1
1	m	274	ALA	4.1
1	j	355	THR	4.1
1	b	275	VAL	4.1
1	b	227	SER	4.1
2	T	38	GLU	4.1
1	l	230	ARG	4.0
1	G	374	GLY	4.0
1	k	187	LYS	4.0
1	m	249	ILE	4.0
1	F	529	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	M	172	GLY	4.0
1	l	142	LYS	3.9
1	k	356	ASP	3.9
1	E	244	LYS	3.9
1	l	181	SER	3.9
1	M	240	ALA	3.9
1	k	270	LEU	3.9
1	m	178	GLU	3.9
1	m	347	GLY	3.9
2	p	90	LEU	3.9
1	n	3	ALA	3.9
1	l	371	LEU	3.9
2	r	56	ASN	3.9
2	r	37	LYS	3.9
1	M	366	GLU	3.9
1	l	226	VAL	3.9
2	S	44	LYS	3.9
1	M	225	LYS	3.9
1	N	373	GLY	3.9
1	K	183	GLU	3.8
1	m	254	GLU	3.8
1	M	384	THR	3.8
1	l	248	ILE	3.8
1	n	357	SER	3.8
1	l	527	PRO	3.8
1	m	250	ALA	3.8
1	f	322	VAL	3.8
1	k	352	LEU	3.8
1	l	360	ALA	3.8
1	m	3	ALA	3.8
1	f	354	THR	3.8
1	m	160	LEU	3.8
2	o	87	TYR	3.8
1	M	395	PHE	3.8
1	f	353	GLU	3.8
1	l	267	ARG	3.8
1	l	227	SER	3.8
1	M	326	LYS	3.7
1	m	287	MET	3.7
1	H	44	PHE	3.7
1	c	365	GLN	3.7
1	n	355	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	M	272	VAL	3.7
1	l	189	VAL	3.7
1	M	358	GLU	3.7
1	l	138	VAL	3.7
1	E	356	ASP	3.6
1	l	169	GLY	3.6
1	M	352	LEU	3.6
1	M	281	GLY	3.6
1	m	213	VAL	3.6
1	c	359	TYR	3.6
1	l	182	LEU	3.6
1	l	183	GLU	3.6
1	n	283	ARG	3.6
1	j	348	ILE	3.6
1	M	526	LYS	3.6
1	M	178	GLU	3.6
2	u	9	LYS	3.6
1	k	381	GLY	3.6
1	n	371	LEU	3.6
1	M	329	THR	3.6
1	k	383	ALA	3.6
1	l	167	LYS	3.6
1	M	351	GLU	3.6
1	k	185	GLU	3.6
1	k	213	VAL	3.6
2	p	20	ILE	3.5
1	m	44	PHE	3.5
1	f	352	LEU	3.5
1	h	270	LEU	3.5
1	N	363	LYS	3.5
1	F	356	ASP	3.5
1	B	302	GLU	3.5
1	a	337	LYS	3.5
1	j	186	LEU	3.5
1	m	341	ILE	3.5
1	M	278	PRO	3.5
1	l	139	GLU	3.5
1	l	266	LEU	3.5
1	l	221	ILE	3.5
1	N	354	THR	3.5
1	g	190	GLU	3.5
2	O	34	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	b	371	LEU	3.5
2	S	20	ILE	3.5
1	H	528	GLU	3.5
1	L	526	LYS	3.5
1	N	356	ASP	3.5
1	m	361	ARG	3.5
1	M	381	GLY	3.5
1	I	3	ALA	3.5
1	M	221	ILE	3.5
1	M	307	LYS	3.5
1	N	371	LEU	3.5
1	f	371	LEU	3.5
1	l	299	VAL	3.5
1	m	199	ILE	3.5
2	o	100	GLN	3.5
1	M	340	ASP	3.5
2	U	83	ASP	3.5
1	b	339	GLU	3.4
1	l	256	GLU	3.4
1	N	3	ALA	3.4
1	b	204	VAL	3.4
1	l	362	GLU	3.4
1	F	364	LEU	3.4
1	l	352	LEU	3.4
1	b	205	THR	3.4
1	l	330	THR	3.4
2	U	100	GLN	3.4
2	t	36	ALA	3.4
1	D	278	PRO	3.4
1	M	310	ASN	3.4
2	S	29	GLY	3.4
1	l	367	ARG	3.4
1	m	302	GLU	3.4
1	n	257	ALA	3.4
1	k	178	GLU	3.4
1	n	356	ASP	3.4
1	l	355	THR	3.4
1	H	382	ALA	3.4
1	n	266	LEU	3.3
2	u	15	VAL	3.3
1	E	349	LYS	3.3
1	c	358	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	l	308	LEU	3.3
1	l	192	TYR	3.3
1	l	526	LYS	3.3
2	T	23	GLU	3.3
2	u	55	GLU	3.3
1	M	364	LEU	3.3
1	b	313	LEU	3.3
1	m	186	LEU	3.3
1	l	373	GLY	3.3
1	I	280	PHE	3.3
1	M	387	GLU	3.3
1	f	241	GLN	3.3
1	i	354	THR	3.3
2	S	31	VAL	3.3
2	q	75	TYR	3.3
1	k	167	LYS	3.3
2	S	59	ARG	3.3
2	S	74	LYS	3.3
1	g	187	LYS	3.3
1	m	227	SER	3.3
1	b	208	GLU	3.3
1	l	213	VAL	3.3
1	j	474	LYS	3.3
1	L	182	LEU	3.3
1	m	526	LYS	3.2
1	M	248	ILE	3.2
1	E	280	PHE	3.2
1	j	350	LYS	3.2
1	M	243	GLY	3.2
1	k	321	ARG	3.2
2	u	19	ARG	3.2
1	m	242	THR	3.2
1	a	241	GLN	3.2
1	i	283	ARG	3.2
1	l	361	ARG	3.2
1	D	304	LEU	3.2
1	J	526	LYS	3.2
1	b	300	ILE	3.2
1	c	345	ILE	3.2
1	c	348	ILE	3.2
1	l	272	VAL	3.2
1	m	182	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	u	96	LEU	3.2
1	f	361	ARG	3.2
1	k	322	VAL	3.2
1	n	282	ASP	3.2
2	r	75	TYR	3.1
1	g	364	LEU	3.1
1	m	204	VAL	3.1
2	s	7	VAL	3.1
1	k	305	GLY	3.1
1	l	280	PHE	3.1
1	m	252	ASP	3.1
1	l	3	ALA	3.1
2	t	100	GLN	3.1
1	a	361	ARG	3.1
2	p	33	PRO	3.1
1	k	348	ILE	3.1
1	m	259	ALA	3.1
2	T	70	VAL	3.1
2	o	17	VAL	3.1
1	e	280	PHE	3.1
1	k	269	THR	3.1
1	l	356	ASP	3.1
2	P	29	GLY	3.1
1	M	237	GLU	3.1
1	j	371	LEU	3.1
1	g	359	TYR	3.1
1	b	277	ALA	3.1
1	d	472	GLU	3.1
1	H	270	LEU	3.1
1	l	188	PHE	3.1
1	E	205	THR	3.1
1	I	350	LYS	3.1
2	S	94	ASP	3.1
1	M	362	GLU	3.1
1	j	358	GLU	3.1
1	m	223	GLU	3.1
2	S	54	LEU	3.1
1	k	361	ARG	3.1
1	a	528	GLU	3.1
1	m	362	GLU	3.1
1	j	379	ARG	3.0
1	l	145	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	M	370	LYS	3.0
1	e	171	GLU	3.0
2	O	76	GLY	3.0
1	k	359	TYR	3.0
1	l	244	LYS	3.0
2	o	37	LYS	3.0
1	l	382	ALA	3.0
1	N	353	GLU	3.0
1	k	526	LYS	3.0
1	l	285	LYS	3.0
2	R	83	ASP	3.0
1	M	152	ALA	3.0
1	c	360	ALA	3.0
1	M	345	ILE	3.0
1	b	337	LYS	3.0
1	b	358	GLU	3.0
1	l	242	THR	3.0
2	o	21	GLU	3.0
1	l	268	GLY	3.0
2	O	84	GLY	3.0
2	t	46	ILE	3.0
1	l	229	VAL	3.0
1	M	224	LYS	3.0
1	m	142	LYS	3.0
1	a	314	SER	3.0
1	M	323	ARG	3.0
1	B	171	GLU	3.0
1	n	368	LEU	3.0
1	k	330	THR	3.0
1	m	176	VAL	3.0
2	u	22	GLU	3.0
1	I	230	ARG	3.0
1	b	194	PHE	2.9
1	j	187	LYS	2.9
2	O	28	GLY	2.9
2	u	75	TYR	2.9
1	M	175	THR	2.9
1	N	355	THR	2.9
1	a	348	ILE	2.9
1	m	395	PHE	2.9
1	m	304	LEU	2.9
1	E	358	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	e	351	GLU	2.9
1	j	347	GLY	2.9
1	e	303	GLU	2.9
1	l	289	LYS	2.9
2	o	89	ILE	2.9
1	i	260	THR	2.9
1	g	188	PHE	2.9
1	l	245	PRO	2.9
1	a	226	VAL	2.9
1	M	348	ILE	2.9
1	f	528	GLU	2.9
1	g	165	MET	2.9
2	O	99	LEU	2.9
2	o	42	LYS	2.9
2	u	56	ASN	2.9
1	K	355	THR	2.9
1	l	155	PRO	2.9
1	m	207	PRO	2.9
1	l	474	LYS	2.9
1	j	351	GLU	2.9
1	l	353	GLU	2.9
1	k	191	GLY	2.9
1	l	222	VAL	2.9
1	M	220	LEU	2.9
1	l	233	LEU	2.9
1	m	269	THR	2.8
1	f	332	VAL	2.8
1	k	380	VAL	2.8
1	m	138	VAL	2.8
1	m	188	PHE	2.8
1	G	372	ALA	2.8
1	m	220	LEU	2.8
2	R	74	LYS	2.8
1	l	260	THR	2.8
1	k	331	ILE	2.8
1	K	368	LEU	2.8
1	l	236	LEU	2.8
1	m	301	SER	2.8
1	a	358	GLU	2.8
1	m	136	ILE	2.8
2	P	46	ILE	2.8
1	i	250	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	a	362	GLU	2.8
1	M	344	ARG	2.8
1	j	357	SER	2.8
1	j	226	VAL	2.8
1	a	247	LEU	2.8
1	D	360	ALA	2.8
1	D	302	GLU	2.8
2	q	40	PRO	2.8
1	I	356	ASP	2.8
1	f	143	ALA	2.8
1	l	228	ASN	2.8
1	l	179	SER	2.8
1	a	306	PHE	2.8
1	M	198	TYR	2.8
1	M	288	LEU	2.8
1	l	214	LEU	2.8
1	M	374	GLY	2.8
1	g	161	ILE	2.8
2	p	8	ILE	2.8
1	M	275	VAL	2.8
1	e	208	GLU	2.8
1	m	251	GLU	2.8
1	a	192	TYR	2.8
2	t	5	LYS	2.8
1	H	3	ALA	2.8
1	l	363	LYS	2.8
1	N	352	LEU	2.8
1	b	253	VAL	2.8
2	R	7	VAL	2.8
2	o	70	VAL	2.8
1	M	319	ALA	2.8
1	g	305	GLY	2.7
1	a	303	GLU	2.7
2	O	100	GLN	2.7
1	M	312	THR	2.7
1	e	354	THR	2.7
1	k	354	THR	2.7
1	k	382	ALA	2.7
1	b	324	ILE	2.7
1	b	340	ASP	2.7
1	j	428	LEU	2.7
1	k	261	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	k	332	VAL	2.7
1	b	209	THR	2.7
1	b	251	GLU	2.7
2	U	82	ILE	2.7
1	a	236	LEU	2.7
1	i	241	GLN	2.7
2	t	70	VAL	2.7
1	n	350	LYS	2.7
1	M	190	GLU	2.7
1	g	341	ILE	2.7
2	o	20	ILE	2.7
2	o	82	ILE	2.7
2	R	6	THR	2.7
1	g	228	ASN	2.7
1	l	318	ARG	2.7
1	j	262	VAL	2.7
2	s	33	PRO	2.7
1	C	303	GLU	2.7
1	n	376	ALA	2.7
1	m	248	ILE	2.7
1	m	185	GLU	2.7
2	o	83	ASP	2.7
1	m	159	LYS	2.7
1	H	280	PHE	2.7
2	t	8	ILE	2.7
1	a	342	GLU	2.7
1	c	198	TYR	2.6
2	u	87	TYR	2.6
1	H	371	LEU	2.6
2	q	68	ASP	2.6
1	c	243	GLY	2.6
1	e	188	PHE	2.6
1	A	302	GLU	2.6
1	M	196	LYS	2.6
1	m	339	GLU	2.6
1	m	321	ARG	2.6
1	M	391	LYS	2.6
1	h	306	PHE	2.6
2	t	99	LEU	2.6
2	p	6	THR	2.6
1	F	474	LYS	2.6
1	m	358	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	a	308	LEU	2.6
2	u	7	VAL	2.6
2	q	5	LYS	2.6
1	e	185	GLU	2.6
1	j	260	THR	2.6
1	k	5	ILE	2.6
1	l	283	ARG	2.6
1	g	313	LEU	2.6
1	l	364	LEU	2.6
1	e	244	LYS	2.6
1	k	474	LYS	2.6
1	H	355	THR	2.6
2	o	8	ILE	2.6
1	D	371	LEU	2.6
1	N	364	LEU	2.6
1	a	305	GLY	2.6
1	i	368	LEU	2.6
1	k	272	VAL	2.6
1	b	221	ILE	2.6
1	l	224	LYS	2.6
1	n	287	MET	2.6
1	l	136	ILE	2.6
1	g	347	GLY	2.6
1	g	138	VAL	2.6
1	g	356	ASP	2.6
1	j	332	VAL	2.6
1	M	321	ARG	2.6
1	e	360	ALA	2.6
1	m	527	PRO	2.6
2	o	30	ILE	2.5
2	s	8	ILE	2.5
1	D	279	GLY	2.5
1	M	333	GLY	2.5
2	U	81	GLU	2.5
1	d	323	ARG	2.5
1	m	289	LYS	2.5
1	L	3	ALA	2.5
1	b	191	GLY	2.5
1	i	347	GLY	2.5
2	s	29	GLY	2.5
1	J	368	LEU	2.5
2	s	99	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	t	37	LYS	2.5
1	D	216	ASP	2.5
1	M	241	GLN	2.5
1	M	527	PRO	2.5
1	n	526	LYS	2.5
1	a	371	LEU	2.5
1	m	66	LEU	2.5
1	l	354	THR	2.5
2	s	6	THR	2.5
1	d	527	PRO	2.5
1	g	185	GLU	2.5
1	j	527	PRO	2.5
1	g	230	ARG	2.5
1	l	334	GLY	2.5
1	a	298	THR	2.5
1	m	184	THR	2.5
2	T	44	LYS	2.5
1	l	336	GLY	2.5
1	a	242	THR	2.5
1	l	358	GLU	2.5
1	l	387	GLU	2.5
1	M	144	ILE	2.5
2	S	24	PRO	2.5
1	N	270	LEU	2.5
1	g	362	GLU	2.5
1	g	366	GLU	2.5
2	r	94	ASP	2.5
1	c	242	THR	2.5
1	k	267	ARG	2.5
1	M	191	GLY	2.5
1	m	173	ILE	2.5
1	n	348	ILE	2.5
1	m	310	ASN	2.5
1	e	528	GLU	2.5
1	k	375	VAL	2.5
2	o	16	VAL	2.5
2	u	88	VAL	2.5
1	i	230	ARG	2.5
1	n	44	PHE	2.5
1	M	212	ALA	2.5
1	k	148	ALA	2.5
1	i	304	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	S	99	LEU	2.5
1	K	262	VAL	2.5
1	c	211	GLU	2.5
1	e	302	GLU	2.5
1	k	215	GLU	2.5
1	M	203	PHE	2.5
2	t	83	ASP	2.5
1	m	324	ILE	2.5
1	k	34	ARG	2.4
1	b	265	LYS	2.4
1	M	143	ALA	2.4
1	m	343	ALA	2.4
1	k	182	LEU	2.4
1	l	249	ILE	2.4
1	m	417	THR	2.4
1	A	528	GLU	2.4
1	E	208	GLU	2.4
1	N	267	ARG	2.4
1	i	179	SER	2.4
1	g	44	PHE	2.4
2	Q	56	ASN	2.4
2	u	70	VAL	2.4
1	M	148	ALA	2.4
1	l	250	ALA	2.4
2	T	30	ILE	2.4
2	o	6	THR	2.4
1	b	338	LYS	2.4
1	c	188	PHE	2.4
1	l	296	GLY	2.4
2	P	36	ALA	2.4
2	r	20	ILE	2.4
1	g	325	THR	2.4
1	E	44	PHE	2.4
1	l	380	VAL	2.4
1	M	165	MET	2.4
1	d	305	GLY	2.4
1	J	3	ALA	2.4
1	m	221	ILE	2.4
1	M	325	THR	2.4
1	g	315	MET	2.4
1	j	373	GLY	2.4
1	l	381	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	a	326	LYS	2.4
2	o	5	LYS	2.4
1	M	383	ALA	2.4
1	k	280	PHE	2.4
1	k	334	GLY	2.4
1	M	238	GLN	2.4
1	m	320	GLU	2.4
1	f	368	LEU	2.4
2	Q	99	LEU	2.4
1	l	306	PHE	2.4
1	L	381	GLY	2.4
1	N	358	GLU	2.4
1	i	185	GLU	2.4
2	T	71	VAL	2.4
2	s	53	VAL	2.4
1	j	354	THR	2.4
1	H	358	GLU	2.4
1	d	302	GLU	2.4
2	p	38	GLU	2.4
1	m	198	TYR	2.4
1	m	383	ALA	2.4
2	O	8	ILE	2.4
1	f	373	GLY	2.3
1	n	361	ARG	2.3
2	O	27	LYS	2.3
2	t	97	ALA	2.3
1	k	120	ILE	2.3
1	i	350	LYS	2.3
2	p	87	TYR	2.3
1	K	3	ALA	2.3
1	l	482	ALA	2.3
2	u	99	LEU	2.3
1	F	358	GLU	2.3
1	I	256	GLU	2.3
1	a	251	GLU	2.3
1	D	44	PHE	2.3
1	e	306	PHE	2.3
1	h	44	PHE	2.3
1	b	201	PRO	2.3
1	m	478	TYR	2.3
1	H	303	GLU	2.3
1	b	351	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	m	62	LEU	2.3
2	S	96	LEU	2.3
1	N	357	SER	2.3
1	d	529	LYS	2.3
1	m	380	VAL	2.3
1	g	527	PRO	2.3
1	c	362	GLU	2.3
1	j	376	ALA	2.3
1	L	261	LEU	2.3
1	M	316	LEU	2.3
1	e	270	LEU	2.3
1	k	364	LEU	2.3
1	n	364	LEU	2.3
1	b	363	LYS	2.3
1	b	44	PHE	2.3
1	i	357	SER	2.3
1	i	395	PHE	2.3
1	j	334	GLY	2.3
1	A	527	PRO	2.3
1	J	303	GLU	2.3
1	M	303	GLU	2.3
1	b	266	LEU	2.3
1	i	280	PHE	2.3
1	k	44	PHE	2.3
1	l	384	THR	2.3
1	l	263	VAL	2.3
1	b	215	GLU	2.3
1	i	351	GLU	2.3
1	n	183	GLU	2.3
2	r	34	ASP	2.3
1	b	359	TYR	2.3
1	i	232	LEU	2.3
1	m	240	ALA	2.3
1	a	218	PHE	2.3
1	a	373	GLY	2.3
2	p	84	GLY	2.3
2	t	98	VAL	2.3
1	j	352	LEU	2.3
1	k	6	LEU	2.3
1	l	148	ALA	2.3
2	s	54	LEU	2.3
1	l	144	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	f	280	PHE	2.3
1	c	244	LYS	2.3
2	Q	100	GLN	2.3
1	J	356	ASP	2.3
1	b	240	ALA	2.3
1	l	85	ALA	2.3
1	a	221	ILE	2.3
1	e	144	ILE	2.3
1	K	44	PHE	2.3
1	a	203	PHE	2.3
1	M	211	GLU	2.3
2	O	60	VAL	2.2
1	G	373	GLY	2.2
1	K	250	ALA	2.2
1	e	186	LEU	2.2
1	f	474	LYS	2.2
1	c	241	GLN	2.2
2	o	38	GLU	2.2
1	m	272	VAL	2.2
2	p	93	ARG	2.2
1	k	260	THR	2.2
1	H	348	ILE	2.2
1	n	173	ILE	2.2
1	I	283	ARG	2.2
2	t	71	VAL	2.2
1	g	374	GLY	2.2
2	u	57	GLY	2.2
1	i	341	ILE	2.2
1	n	341	ILE	2.2
2	s	20	ILE	2.2
1	c	363	LYS	2.2
1	c	356	ASP	2.2
1	i	282	ASP	2.2
1	k	3	ALA	2.2
2	S	71	VAL	2.2
1	M	285	LYS	2.2
1	e	527	PRO	2.2
1	l	161	ILE	2.2
2	p	36	ALA	2.2
1	l	391	LYS	2.2
1	j	460	TYR	2.2
1	a	204	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	t	64	VAL	2.2
1	M	296	GLY	2.2
1	c	197	GLY	2.2
2	o	22	GLU	2.2
1	M	170	LYS	2.2
2	P	99	LEU	2.2
1	l	193	GLN	2.2
1	m	275	VAL	2.2
1	E	326	LYS	2.2
1	b	232	LEU	2.2
1	l	232	LEU	2.2
1	b	249	ILE	2.2
2	P	69	ILE	2.2
2	U	36	ALA	2.2
1	f	357	SER	2.2
2	r	31	VAL	2.2
1	J	361	ARG	2.2
1	b	282	ASP	2.2
1	h	348	ILE	2.2
1	n	199	ILE	2.2
1	E	245	PRO	2.2
1	f	165	MET	2.2
1	K	187	LYS	2.2
1	h	267	ARG	2.2
2	o	15	VAL	2.2
1	g	308	LEU	2.1
1	d	331	ILE	2.1
2	Q	20	ILE	2.1
1	k	244	LYS	2.1
1	b	353	GLU	2.1
1	k	339	GLU	2.1
1	k	175	THR	2.1
1	b	192	TYR	2.1
1	d	247	LEU	2.1
1	j	280	PHE	2.1
1	n	270	LEU	2.1
1	l	274	ALA	2.1
2	O	69	ILE	2.1
1	d	358	GLU	2.1
1	f	358	GLU	2.1
1	f	355	THR	2.1
1	g	485	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	t	43	GLY	2.1
1	B	368	LEU	2.1
1	a	356	ASP	2.1
1	d	270	LEU	2.1
2	Q	54	LEU	2.1
2	Q	90	LEU	2.1
2	s	44	LYS	2.1
1	F	348	ILE	2.1
1	k	366	GLU	2.1
1	D	332	VAL	2.1
2	p	71	VAL	2.1
1	I	355	THR	2.1
2	U	44	LYS	2.1
2	U	74	LYS	2.1
1	L	356	ASP	2.1
1	M	286	GLU	2.1
1	b	195	ASP	2.1
1	l	131	ILE	2.1
1	g	363	LYS	2.1
2	O	64	VAL	2.1
2	U	70	VAL	2.1
1	a	327	ASP	2.1
1	a	340	ASP	2.1
1	e	358	GLU	2.1
1	m	218	PHE	2.1
2	s	32	LEU	2.1
1	n	360	ALA	2.1
2	o	73	ALA	2.1
1	a	245	PRO	2.1
1	H	236	LEU	2.1
1	L	302	GLU	2.1
1	b	203	PHE	2.1
1	g	358	GLU	2.1
1	i	308	LEU	2.1
1	m	384	THR	2.1
2	Q	94	ASP	2.1
2	o	58	GLN	2.1
1	m	331	ILE	2.1
1	n	375	VAL	2.1
1	i	186	LEU	2.1
1	l	487	PHE	2.1
1	n	258	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	l	298	THR	2.1
1	l	500	LYS	2.1
1	m	187	LYS	2.1
2	r	100	GLN	2.1
1	k	212	ALA	2.1
1	c	207	PRO	2.1
1	k	189	VAL	2.1
1	l	178	GLU	2.1
1	l	278	PRO	2.1
1	m	332	VAL	2.1
1	E	306	PHE	2.1
1	H	261	LEU	2.1
1	j	5	ILE	2.1
2	P	75	TYR	2.1
1	M	185	GLU	2.1
1	C	170	LYS	2.1
2	T	25	LYS	2.1
2	U	17	VAL	2.1
1	I	232	LEU	2.0
2	p	32	LEU	2.0
1	m	327	ASP	2.0
1	f	360	ALA	2.0
1	f	473	THR	2.0
2	s	73	ALA	2.0
1	F	208	GLU	2.0
1	c	171	GLU	2.0
2	T	42	LYS	2.0
1	e	239	VAL	2.0
1	g	332	VAL	2.0
1	i	263	VAL	2.0
1	G	280	PHE	2.0
1	d	44	PHE	2.0
1	i	258	LEU	2.0
1	k	399	LEU	2.0
1	l	261	LEU	2.0
1	l	65	HIS	2.0
1	c	314	SER	2.0
1	b	343	ALA	2.0
2	T	20	ILE	2.0
1	N	43	LYS	2.0
1	m	359	TYR	2.0
1	b	241	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	l	316	LEU	2.0
2	r	59	ARG	2.0
1	K	363	LYS	2.0
1	M	136	ILE	2.0
1	d	337	LYS	2.0
1	m	326	LYS	2.0
2	t	42	LYS	2.0
2	u	8	ILE	2.0
1	J	183	GLU	2.0
2	R	75	TYR	2.0
2	S	53	VAL	2.0
2	S	70	VAL	2.0
1	k	379	ARG	2.0
1	k	428	LEU	2.0
1	b	342	GLU	2.0
1	f	342	GLU	2.0
1	g	331	ILE	2.0
1	B	372	ALA	2.0
1	j	333	GLY	2.0
2	Q	38	GLU	2.0
2	q	46	ILE	2.0
2	r	89	ILE	2.0
1	M	184	THR	2.0
1	m	226	VAL	2.0
1	f	487	PHE	2.0
1	m	194	PHE	2.0
1	K	182	LEU	2.0
1	c	247	LEU	2.0
1	l	247	LEU	2.0
1	n	187	LYS	2.0
1	c	206	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	d	601	1/1	0.72	0.39	68,68,68,68	0
5	DMS	j	601	4/4	0.78	0.28	82,83,101,117	0
3	MG	e	601	1/1	0.83	0.31	62,62,62,62	0
5	DMS	J	601	4/4	0.84	0.24	39,53,65,90	0
5	DMS	n	701	4/4	0.87	0.27	69,85,87,99	0
5	DMS	l	601	4/4	0.88	0.24	63,95,106,125	0
5	DMS	k	601	4/4	0.88	0.25	89,96,103,115	0
3	MG	c	601	1/1	0.88	0.33	51,51,51,51	0
3	MG	b	601	1/1	0.89	0.27	53,53,53,53	0
5	DMS	K	601	4/4	0.90	0.18	43,44,76,91	0
5	DMS	L	601	4/4	0.90	0.24	39,58,61,94	0
5	DMS	H	601	4/4	0.91	0.24	24,28,74,96	0
4	ADP	f	602	27/27	0.91	0.28	47,93,109,116	0
4	ADP	g	602	27/27	0.92	0.26	56,84,98,103	0
3	MG	C	601	1/1	0.92	0.21	28,28,28,28	0
3	MG	f	601	1/1	0.92	0.49	70,70,70,70	0
5	DMS	h	601	4/4	0.93	0.22	52,58,85,96	0
3	MG	A	601	1/1	0.93	0.25	27,27,27,27	0
3	MG	g	601	1/1	0.93	0.53	66,66,66,66	0
4	ADP	d	602	27/27	0.93	0.23	45,72,87,93	0
5	DMS	M	601	4/4	0.93	0.20	26,29,60,79	0
5	DMS	m	601	4/4	0.93	0.23	82,92,95,105	0
3	MG	D	601	1/1	0.94	0.23	29,29,29,29	0
5	DMS	i	601	4/4	0.94	0.22	27,32,40,87	0
4	ADP	c	602	27/27	0.94	0.23	24,67,80,102	0
4	ADP	e	602	27/27	0.94	0.23	48,78,103,108	0
4	ADP	a	602	27/27	0.94	0.24	21,70,81,90	0
3	MG	E	601	1/1	0.95	0.22	20,20,20,20	0
3	MG	B	601	1/1	0.95	0.32	44,44,44,44	0
3	MG	a	601	1/1	0.95	0.34	54,54,54,54	0
4	ADP	D	602	27/27	0.95	0.20	1,38,64,69	0
5	DMS	I	601	4/4	0.95	0.20	37,58,66,93	0
4	ADP	C	602	27/27	0.96	0.19	1,34,70,78	0
4	ADP	E	602	27/27	0.96	0.20	12,44,74,80	0
4	ADP	b	602	27/27	0.96	0.20	13,58,79,85	0
4	ADP	B	602	27/27	0.96	0.23	18,54,75,80	0
4	ADP	G	602	27/27	0.96	0.21	1,61,76,85	0

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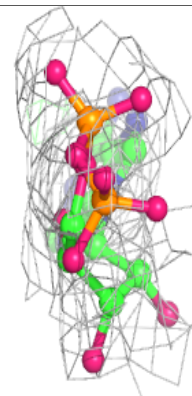
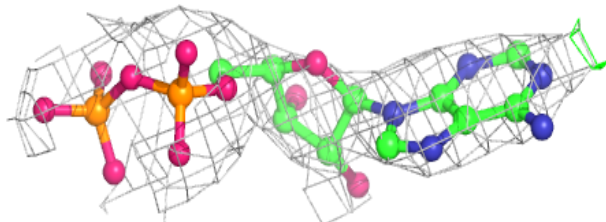
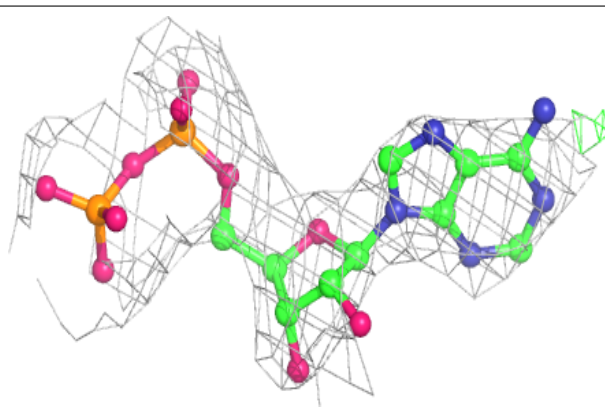
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	F	601	1/1	0.96	0.27	25,25,25,25	0
4	ADP	A	602	27/27	0.97	0.21	1,47,68,77	0
3	MG	G	601	1/1	0.97	0.21	29,29,29,29	0
4	ADP	F	602	27/27	0.97	0.21	23,51,75,88	0
5	DMS	N	701	4/4	0.98	0.16	53,57,64,90	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.

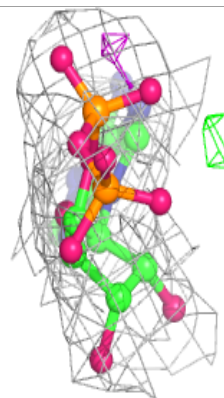
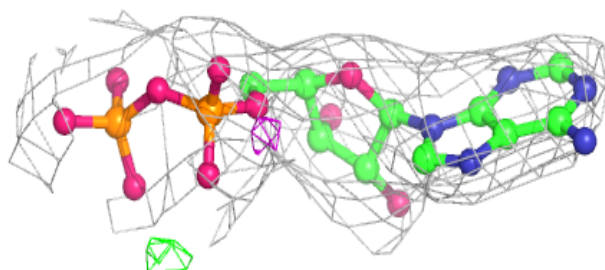
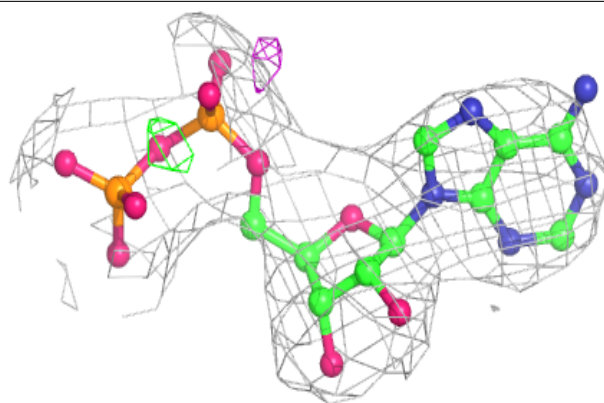
Electron density around ADP f 602:

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

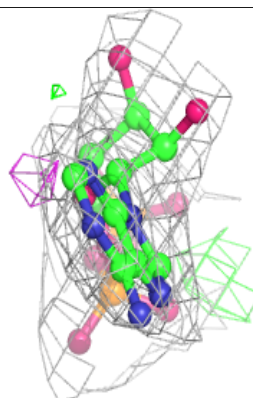
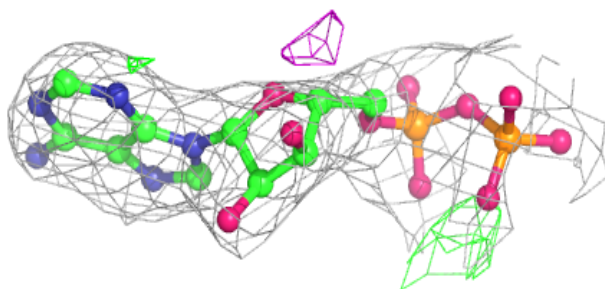
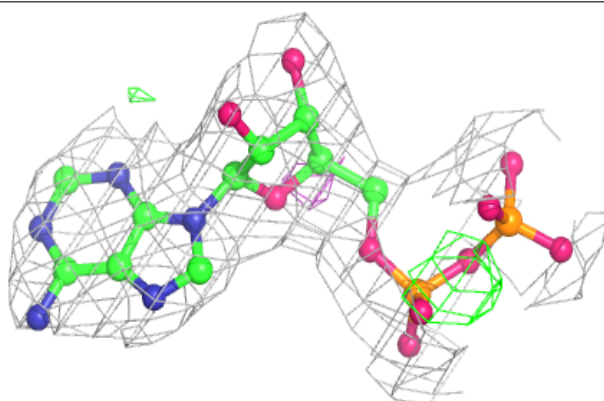


Electron density around ADP g 602:

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

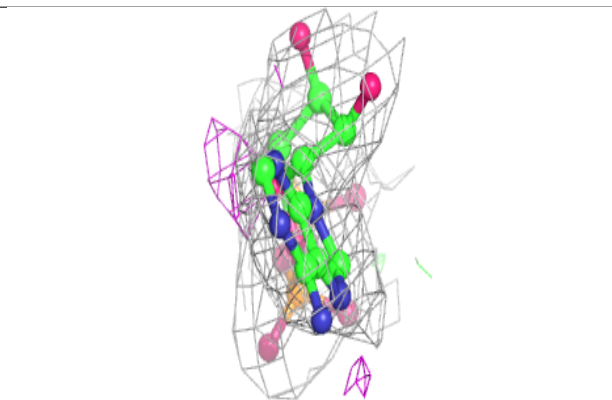
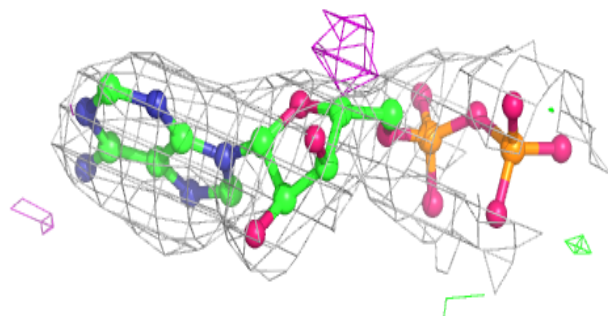
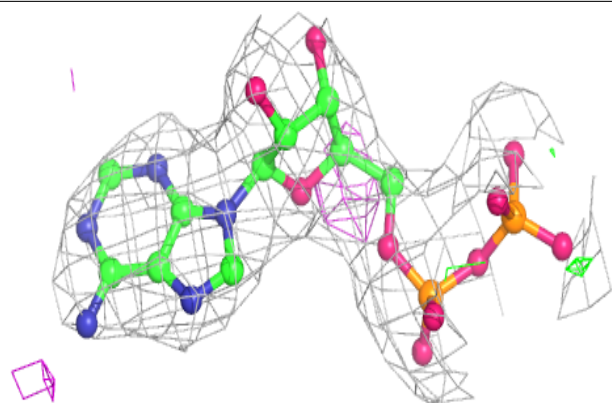
**Electron density around ADP d 602:**

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

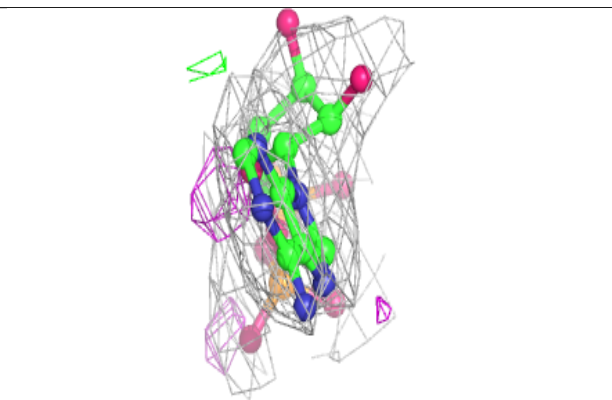
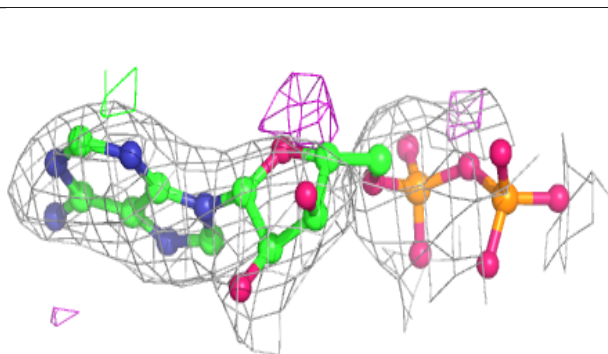
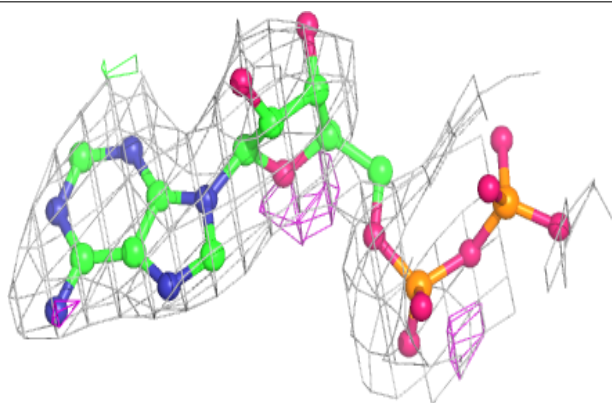


Electron density around ADP c 602:

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

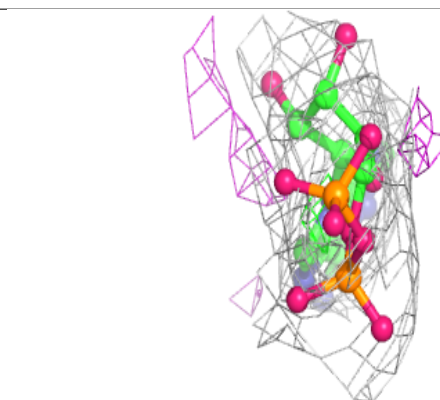
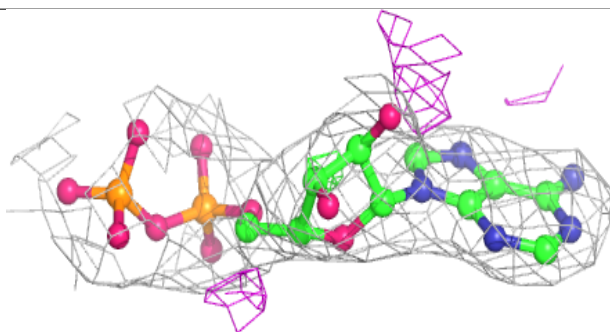
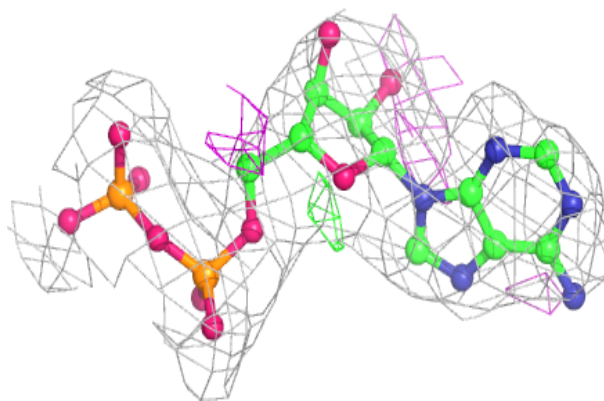
**Electron density around ADP e 602:**

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

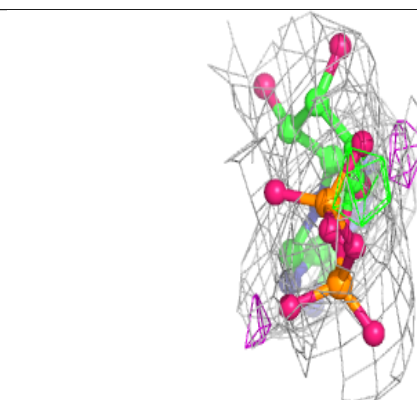
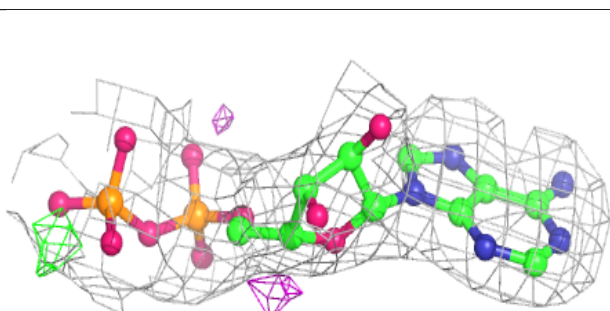
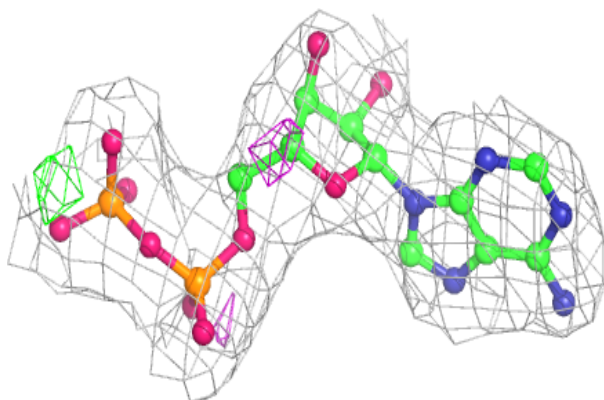


Electron density around ADP a 602:

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

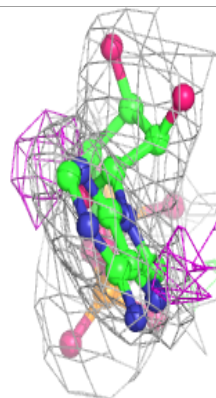
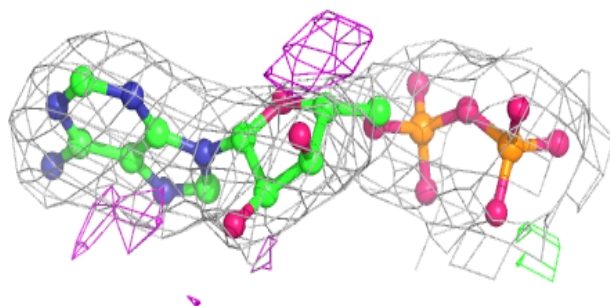
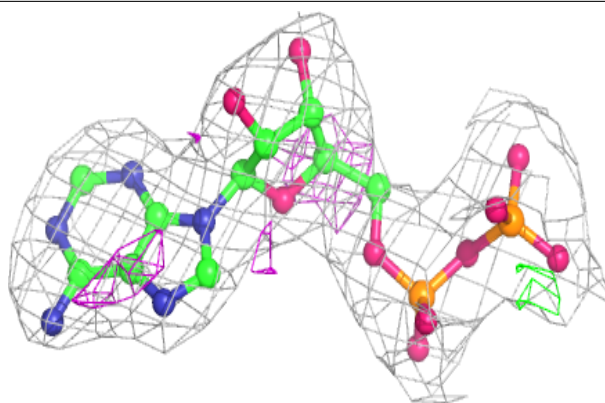
**Electron density around ADP D 602:**

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

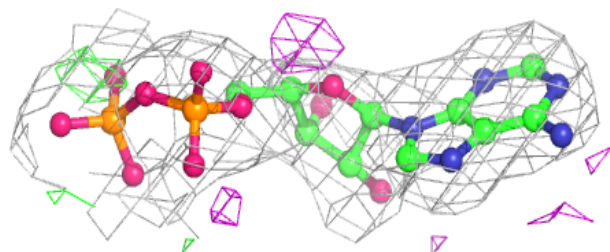
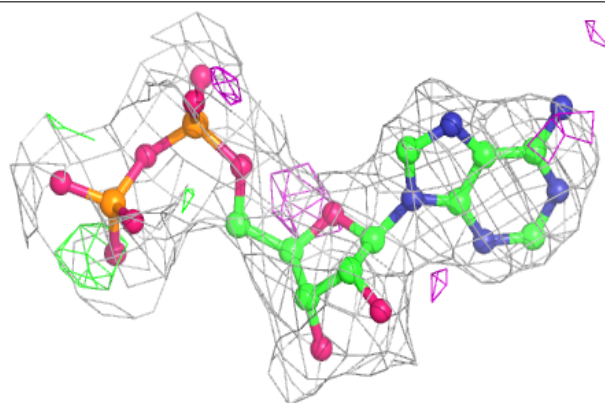


Electron density around ADP C 602:

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

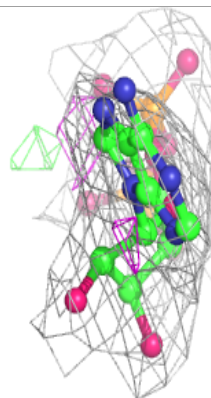
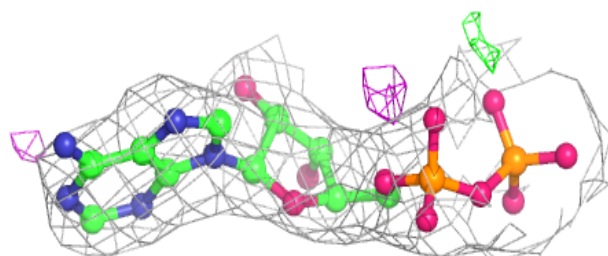
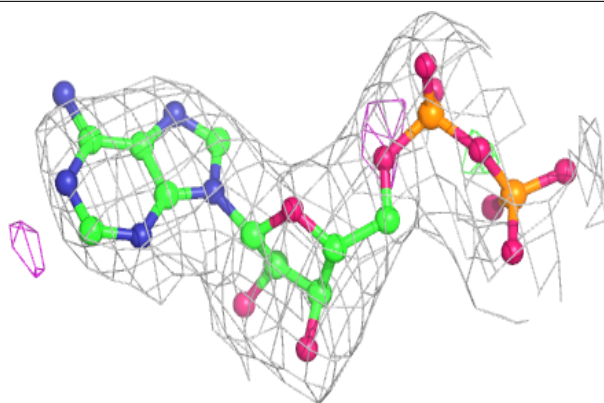
**Electron density around ADP E 602:**

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and green (positive)

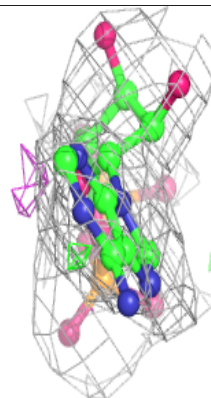
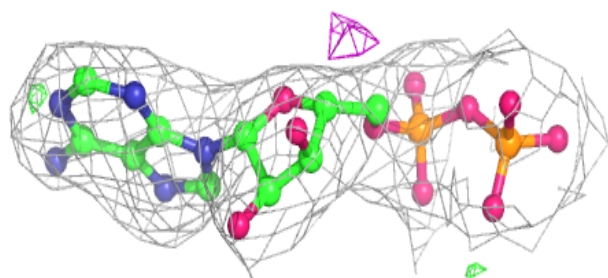
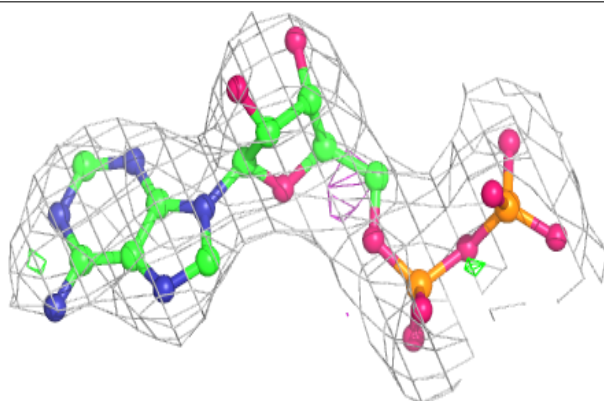


Electron density around ADP b 602:

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

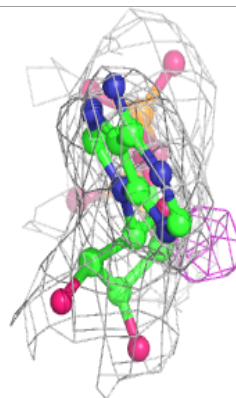
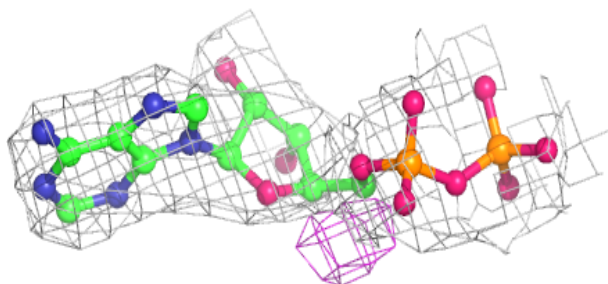
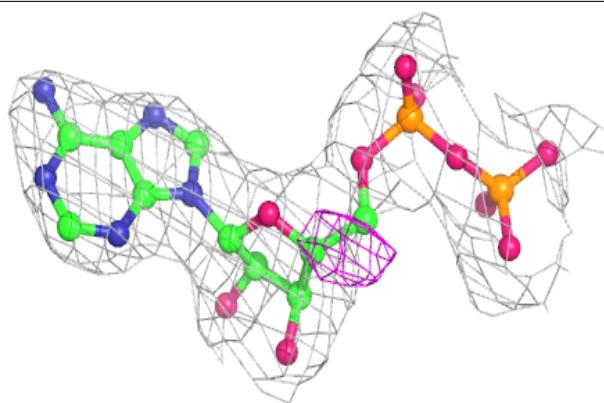
**Electron density around ADP B 602:**

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

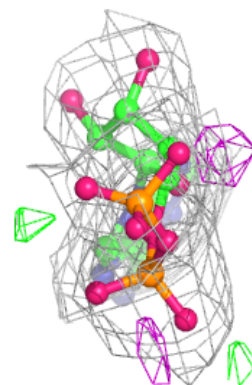
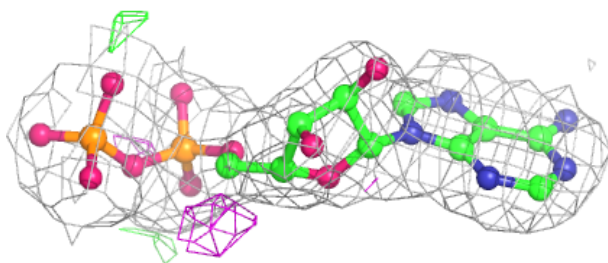
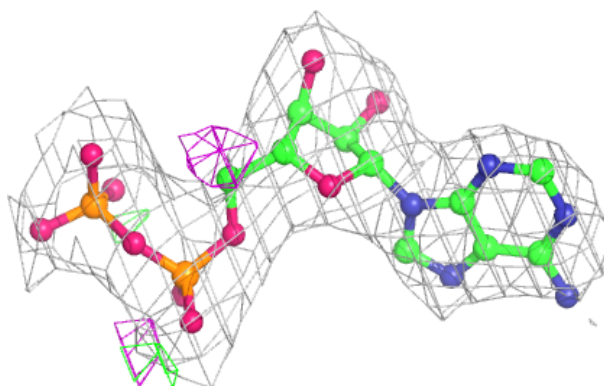


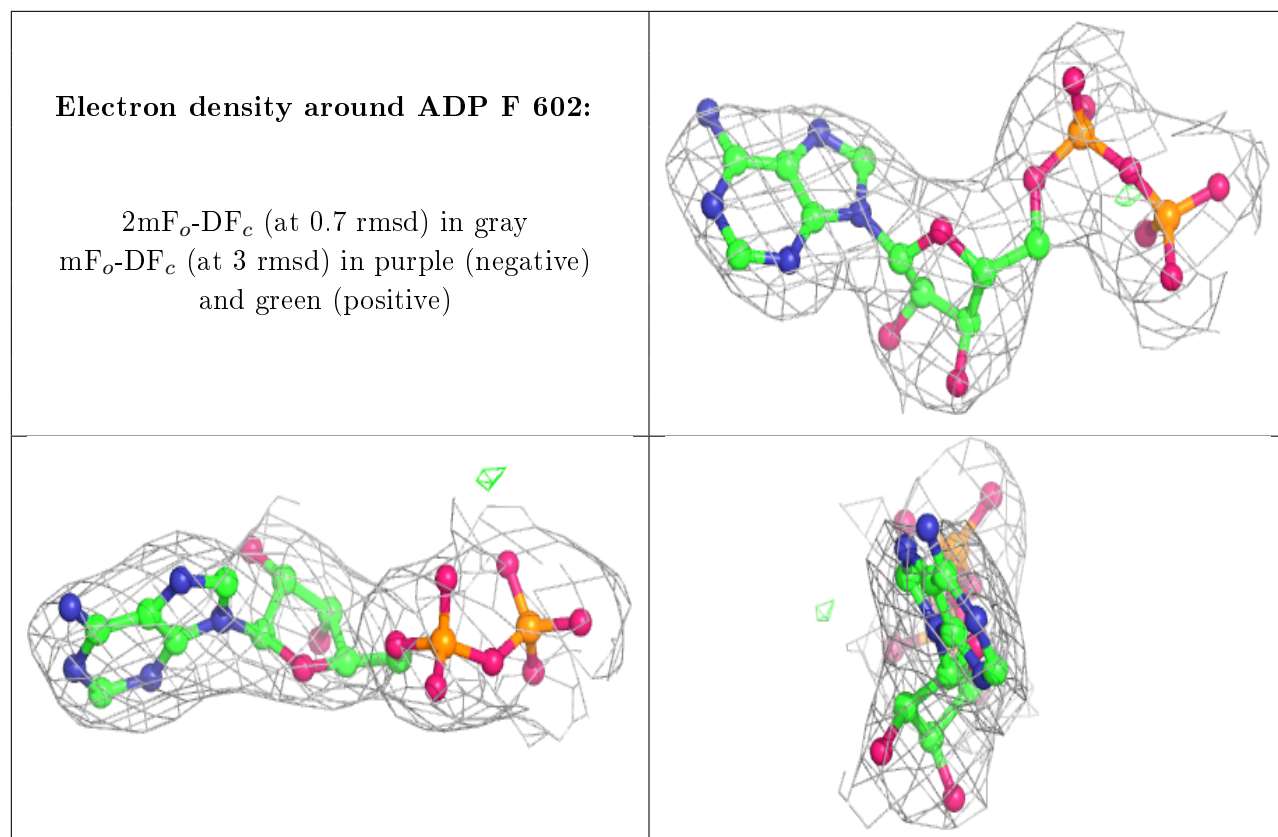
Electron density around ADP G 602:

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

**Electron density around ADP A 602:**

$2mF_o - DF_c$ (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.