



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:43 PM UTC

PDB ID : 6QX2 / pdb_00006qx2
Title : 3.4A structure of benzoisoxazole 3 with S.aureus DNA gyrase and DNA
Authors : Bax, B.D.
Deposited on : 2019-03-06
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

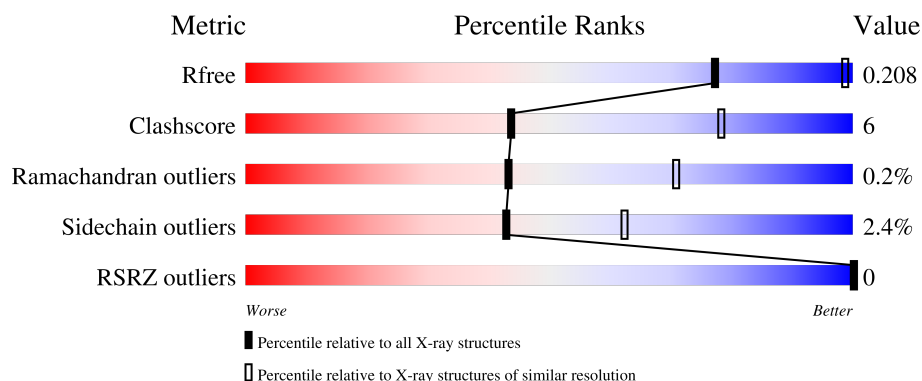
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



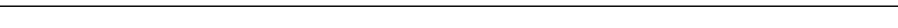
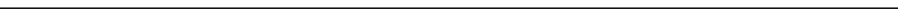
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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

Mol	Chain	Length	Quality of chain
1	B	186	
1	S	186	
1	b	186	
1	s	186	
2	A	490	

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Mol	Chain	Length	Quality of chain
2	C	490	 88% 10% .
2	L	490	 88% 10% .
2	R	490	 87% 11% ..
2	T	490	 87% 10% ..
2	a	490	 87% 11% .
2	c	490	 87% 10% .
2	j	490	 87% 11% ..
2	l	490	 88% 10% .
2	r	490	 86% 12% ..
2	t	490	 87% 11% .
3	D	188	 86% 13% .
3	U	188	 87% 12% .
3	m	188	 87% 12% .
4	E	20	 45% 50% 5%
4	F	20	 60% 35% 5%
4	N	20	 55% 40% 5%
4	O	20	 70% 30%
4	W	20	 35% 60% 5%
4	e	20	 50% 45% 5%
4	n	20	 40% 45% 15%
4	v	20	 75% 20% 5%
4	w	20	 50% 40% 10%
5	K	187	 85% 14% ..
6	J	480	 87% 12% .
7	M	189	 87% 13%

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Mol	Chain	Length	Quality of chain
8	V	19	 58%37%5%
8	o	19	 58%32%5%5%
9	d	181	 86%13%.
10	f	17	 71%24%6%
11	k	188	 88%11%.
12	u	187	 87%13%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 68236 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 DNA gyrase subunit B,DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	185	Total	C	N	O	S	0	5	0
			1441	900	252	278	11			
1	S	185	Total	C	N	O	S	0	5	0
			1439	898	249	281	11			
1	b	185	Total	C	N	O	S	0	5	0
			1430	893	246	280	11			
1	s	186	Total	C	N	O	S	0	4	0
			1434	896	249	278	11			

- Molecule 2 is a protein called DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	479	Total	C	N	O	S	0	13	0
			3846	2387	693	748	18			
2	C	482	Total	C	N	O	S	0	8	0
			3784	2354	678	735	17			
2	L	481	Total	C	N	O	S	0	6	0
			3785	2354	681	733	17			
2	R	482	Total	C	N	O	S	0	11	0
			3830	2382	685	746	17			
2	T	481	Total	C	N	O	S	0	8	0
			3793	2362	680	734	17			
2	a	481	Total	C	N	O	S	0	12	0
			3802	2365	678	742	17			
2	c	482	Total	C	N	O	S	0	8	0
			3784	2357	677	733	17			
2	j	482	Total	C	N	O	S	0	13	0
			3848	2392	691	747	18			
2	l	481	Total	C	N	O	S	0	6	0
			3784	2357	681	729	17			
2	r	484	Total	C	N	O	S	0	15	0
			3870	2403	697	752	18			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	t	481	Total	C	N	O	S	0	10	0
			3809	2371	685	736	17			

- Molecule 3 is a protein called DNA gyrase subunit B,DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	188	Total	C	N	O	S	0	2	0
			1447	906	247	285	9			
3	U	188	Total	C	N	O	S	0	3	0
			1463	917	248	289	9			
3	m	188	Total	C	N	O	S	0	1	0
			1442	906	246	281	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	544	THR	-	linker	UNP P0A0K8
D	545	GLY	-	linker	UNP P0A0K8
U	544	THR	-	linker	UNP P0A0K8
U	545	GLY	-	linker	UNP P0A0K8
m	544	THR	-	linker	UNP P0A0K8
m	545	GLY	-	linker	UNP P0A0K8

- Molecule 4 is a DNA chain called DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	20	Total	C	N	O	P	0	3	0
			455	215	89	130	21			
4	F	20	Total	C	N	O	P	0	0	0
			392	184	74	115	19			
4	N	20	Total	C	N	O	P	0	3	0
			455	215	89	130	21			
4	O	20	Total	C	N	O	P	0	0	0
			392	184	74	115	19			
4	W	20	Total	C	N	O	P	0	0	0
			408	194	76	119	19			
4	e	20	Total	C	N	O	P	0	0	0
			392	185	74	114	19			
4	n	20	Total	C	N	O	P	0	2	0
			418	196	76	125	21			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	v	19	Total	C	N	O	P	0	2	0
			399	186	71	121	21			
4	w	20	Total	C	N	O	P	0	0	0
			400	189	75	117	19			

- Molecule 5 is a protein called DNA gyrase subunit B,DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	187	Total	C	N	O	S	0	4	0
			1439	898	247	283	11			

- Molecule 6 is a protein called DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	480	Total	C	N	O	S	0	15	0
			3862	2399	694	751	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	?	-	ARG	deletion	UNP Q99XG5

- Molecule 7 is a protein called DNA gyrase subunit B,DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	M	189	Total	C	N	O	S	0	3	0
			1468	920	249	290	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	544	THR	-	linker	UNP P66937
M	545	GLY	-	linker	UNP P66937

- Molecule 8 is a DNA chain called DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	V	19	Total	C	N	O	P	0	0	0
			388	184	74	112	18			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	o	18	Total	C	N	O	P	0	0	0
			369	174	69	108	18			

- Molecule 9 is a protein called DNA gyrase subunit B,DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	d	181	Total	C	N	O	S	0	2	0
			1395	875	240	272	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	544	THR	-	linker	UNP P66937
d	545	GLY	-	linker	UNP P66937

- Molecule 10 is a DNA chain called DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	f	17	Total	C	N	O	P	0	0	0
			348	164	64	103	17			

- Molecule 11 is a protein called DNA gyrase subunit B,DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	k	188	Total	C	N	O	S	0	4	0
			1453	910	251	281	11			

- Molecule 12 is a protein called DNA gyrase subunit B,DNA gyrase subunit B.

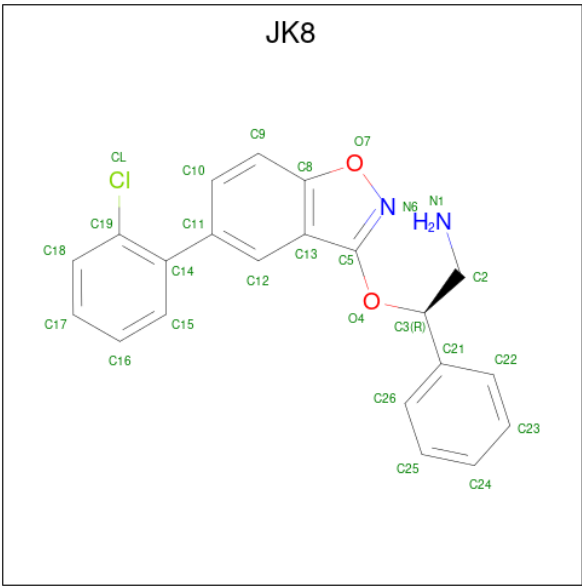
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	u	187	Total	C	N	O	S	0	3	0
			1460	915	248	288	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	544	THR	-	linker	UNP P66937
u	545	GLY	-	linker	UNP P66937

- Molecule 13 is (2 {R})-2-[[5-(2-chlorophenyl)-1,2-benzoxazol-3-yl]oxy]-2-phenyl-ethanamine

(CCD ID: JK8) (formula: C₂₁H₁₇ClN₂O₂).



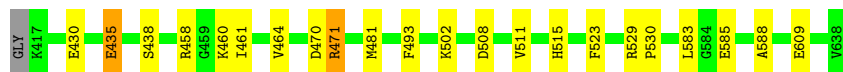
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Cl	N	O	0	0
			26	21	1	2	2		
13	C	1	Total	C	Cl	N	O	0	1
			26	21	1	2	2		
13	J	1	Total	C	Cl	N	O	0	0
			26	21	1	2	2		
13	L	1	Total	C	Cl	N	O	0	1
			26	21	1	2	2		
13	R	1	Total	C	Cl	N	O	0	0
			26	21	1	2	2		
13	U	1	Total	C	Cl	N	O	0	1
			26	21	1	2	2		
13	b	1	Total	C	Cl	N	O	0	0
			26	21	1	2	2		
13	d	1	Total	C	Cl	N	O	0	1
			26	21	1	2	2		
13	k	1	Total	C	Cl	N	O	0	0
			26	21	1	2	2		
13	l	1	Total	C	Cl	N	O	0	1
			26	21	1	2	2		
13	s	1	Total	C	Cl	N	O	0	0
			26	21	1	2	2		
13	t	1	Total	C	Cl	N	O	0	1
			26	21	1	2	2		

3 Residue-property plots [i](#)

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

- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B

Chain B: 



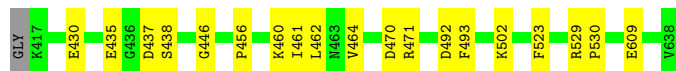
- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B

Chain S: 



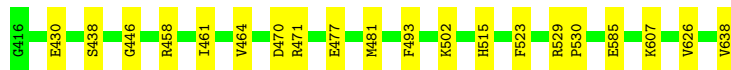
- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B

Chain b: 



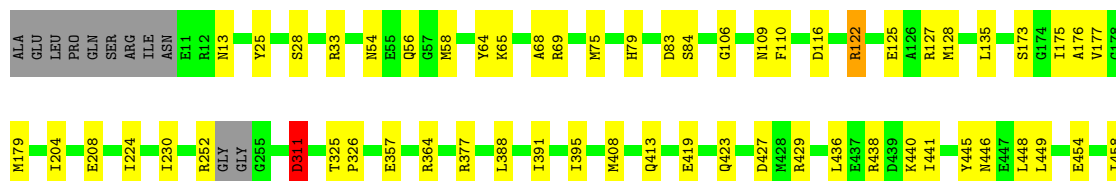
- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B

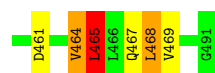
Chain s: 



- Molecule 2: DNA gyrase subunit A

Chain A: 





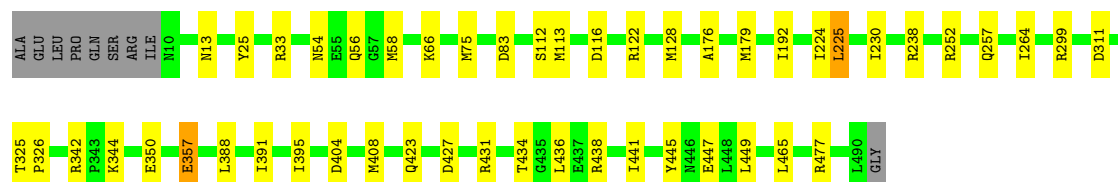
• Molecule 2: DNA gyrase subunit A

Chain C: 88% 10%



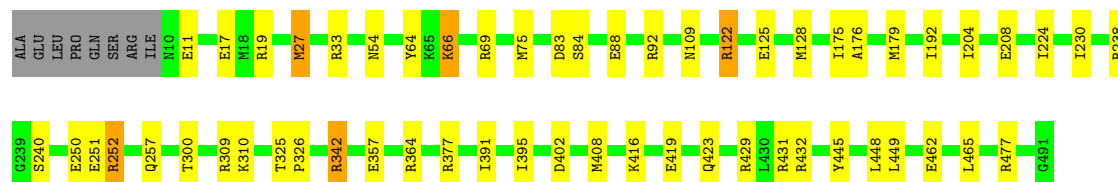
• Molecule 2: DNA gyrase subunit A

Chain L: 88% 10%



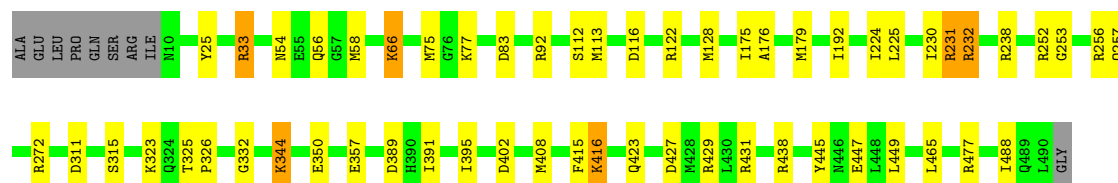
• Molecule 2: DNA gyrase subunit A

Chain R: 87% 11%



• Molecule 2: DNA gyrase subunit A

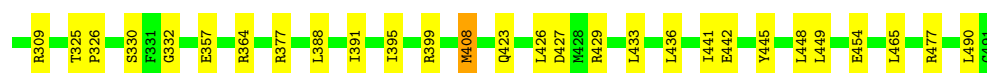
Chain T: 87% 10%



• Molecule 2: DNA gyrase subunit A

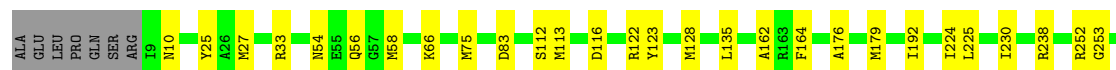
Chain a: 87% 11%





• Molecule 2: DNA gyrase subunit A

Chain c: 87% 10%



• Molecule 2: DNA gyrase subunit A

Chain j: 87% 11%



• Molecule 2: DNA gyrase subunit A

Chain l: 88% 10%



• Molecule 2: DNA gyrase subunit A

Chain r: 86% 12%



• Molecule 2: DNA gyrase subunit A

Chain t: 87% 11%





- Molecule 3: DNA gyrase subunit B,DNA gyrase subunit B

Chain D: 86% 13%



- Molecule 3: DNA gyrase subunit B,DNA gyrase subunit B

Chain U: 87% 12%



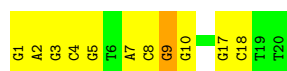
- Molecule 3: DNA gyrase subunit B,DNA gyrase subunit B

Chain m: 87% 12%



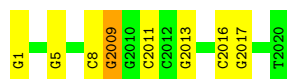
- Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain E: 45% 50% 5%



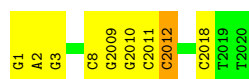
- Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain F: 60% 35% 5%



- Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain N: 55% 40% 5%



- Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain O:  70% 30%



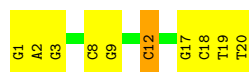
- Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain W:  35% 60% 5%

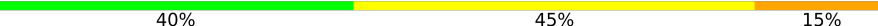


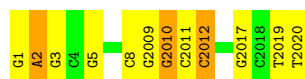
- Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain e:  50% 45% 5%



- Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain n:  40% 45% 15%



- Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain v:  75% 20% 5%



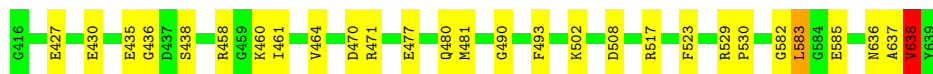
- Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain w:  50% 40% 10%



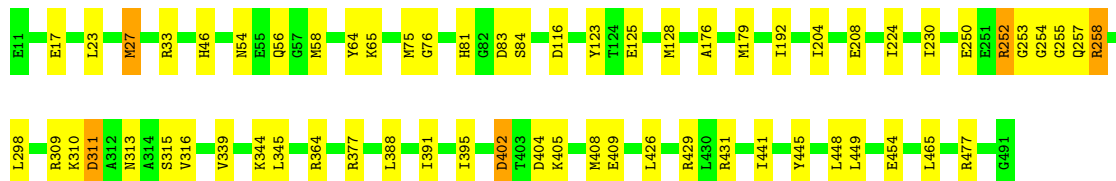
- Molecule 5: DNA gyrase subunit B,DNA gyrase subunit B

Chain K:  85% 14% ..



- Molecule 6: DNA gyrase subunit A

Chain J:  87% 12% .



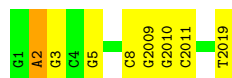
- Molecule 7: DNA gyrase subunit B,DNA gyrase subunit B

Chain M:  87% 13%



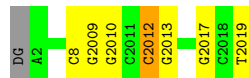
- Molecule 8: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain V:  58% 37% 5%



- Molecule 8: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain o:  58% 32% 5% 5%



- Molecule 9: DNA gyrase subunit B,DNA gyrase subunit B

Chain d:  86% 13% .



- Molecule 10: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain f:  71% 24% 6%



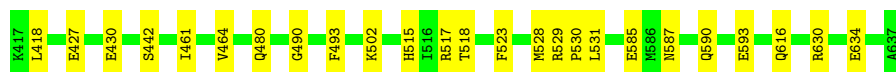
- Molecule 11: DNA gyrase subunit B,DNA gyrase subunit B

Chain k:  88% 11% .



- Molecule 12: DNA gyrase subunit B,DNA gyrase subunit B

Chain u:  87% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	187.64Å 410.12Å 93.94Å 90.00° 120.22° 90.00°	Depositor
Resolution (Å)	162.15 – 3.40 162.15 – 3.40	Depositor EDS
% Data completeness (in resolution range)	80.3 (162.15-3.40) 80.3 (162.15-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 3.41Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.176 , 0.208 0.179 , 0.208	Depositor DCC
R_{free} test set	6799 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 10.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.420 for -h-2*1,-k,l	Xtriage
Reported twinning fraction	0.525 for H, K, L 0.475 for -H-4/2L, -K, L	Depositor
Outliers	0 of 135780 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	68236	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.68% 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: JK8

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	B	1.08	1/1461 (0.1%)	1.54	1/1975 (0.1%)
1	S	1.09	0/1458	1.55	4/1971 (0.2%)
1	b	1.09	0/1450	1.54	2/1962 (0.1%)
1	s	1.08	0/1454	1.54	1/1966 (0.1%)
2	A	1.06	0/3896	1.49	4/5260 (0.1%)
2	C	1.03	0/3831	1.49	1/5179 (0.0%)
2	L	1.04	0/3833	1.50	2/5180 (0.0%)
2	R	1.06	0/3881	1.50	6/5241 (0.1%)
2	T	1.07	0/3844	1.51	3/5194 (0.1%)
2	a	1.04	0/3852	1.50	2/5206 (0.0%)
2	c	1.04	0/3835	1.49	1/5185 (0.0%)
2	j	1.06	1/3899 (0.0%)	1.51	5/5264 (0.1%)
2	l	1.03	0/3832	1.50	2/5177 (0.0%)
2	r	1.05	0/3921	1.50	7/5296 (0.1%)
2	t	1.05	1/3860 (0.0%)	1.48	0/5215
3	D	1.08	0/1469	1.53	0/1990
3	U	1.08	0/1486	1.54	3/2013 (0.1%)
3	m	1.07	0/1465	1.55	0/1985
4	E	0.50	0/511	0.86	2/789 (0.3%)
4	F	0.55	0/438	1.14	4/673 (0.6%)
4	N	0.52	0/510	0.95	4/785 (0.5%)
4	O	0.64	1/439 (0.2%)	0.96	2/677 (0.3%)
4	W	0.52	0/456	0.97	1/700 (0.1%)
4	e	0.57	0/439	1.06	3/677 (0.4%)
4	n	0.56	0/465	1.11	3/712 (0.4%)
4	v	0.46	0/443	0.95	2/677 (0.3%)
4	w	0.66	0/447	1.13	5/686 (0.7%)
5	K	1.10	0/1459	1.55	3/1974 (0.2%)
6	J	1.05	1/3912 (0.0%)	1.50	5/5278 (0.1%)
7	M	1.09	0/1491	1.54	1/2020 (0.0%)
8	V	0.54	0/434	1.10	2/666 (0.3%)
8	o	0.58	0/412	0.93	1/631 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	d	1.07	0/1416	1.55	1/1918 (0.1%)
10	f	0.57	1/389 (0.3%)	1.08	3/598 (0.5%)
11	k	1.09	0/1474	1.52	0/1994
12	u	1.09	0/1483	1.52	2/2007 (0.1%)
All	All	1.03	6/69345 (0.0%)	1.47	88/94721 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1
2	C	0	2
2	L	0	1
2	T	0	1
2	a	0	1
2	c	0	1
2	l	0	1
2	r	0	1
2	t	0	1
6	J	0	1
All	All	0	11

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	46	HIS	CE1-NE2	6.71	1.39	1.32
4	O	8	DC	O3'-P	6.48	1.70	1.61
1	B	471	ARG	CZ-NH2	6.15	1.41	1.33
2	t	46	HIS	CE1-NE2	5.75	1.38	1.32
2	j	11	GLU	C-O	5.57	1.31	1.24
10	f	8	DC	O3'-P	5.25	1.69	1.61

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	2	DA	C4'-C3'-O3'	10.93	126.40	110.00
10	f	8	DC	C4'-C3'-O3'	10.57	125.85	110.00
4	F	2011	DC	O5'-P-OP2	-10.30	77.08	108.00
6	J	258	ARG	CG-CD-NE	9.52	132.95	112.00
4	F	2009	DG	O5'-C5'-C4'	9.40	124.90	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	2009	DG	P-O5'-C5'	-8.69	106.96	120.00
2	a	442	GLU	CB-CG-CD	8.49	127.04	112.60
2	r	442	GLU	CB-CG-CD	8.07	126.33	112.60
8	V	2	DA	C2'-C3'-O3'	-7.68	99.98	111.50
4	n	2012	DC	C2'-C3'-O3'	7.64	122.96	111.50
2	j	69	ARG	CB-CG-CD	7.58	128.73	111.30
4	N	2009	DG	P-O5'-C5'	-7.50	108.75	120.00
9	d	630	ARG	CG-CD-NE	-7.49	95.52	112.00
3	U	638	VAL	CA-C-O	7.15	132.96	120.80
8	o	2012	DC	C2'-C3'-O3'	7.09	122.13	111.50
2	A	311	ASP	CA-CB-CG	7.05	119.65	112.60
2	T	256	ARG	CG-CD-NE	-7.04	96.51	112.00
1	s	638	VAL	CA-C-O	6.93	132.58	120.80
1	S	508	ASP	CA-CB-CG	6.86	119.46	112.60
4	n	2	DA	P-O5'-C5'	6.63	129.95	120.00
4	w	2009	DG	O5'-C5'-C4'	-6.61	100.88	110.80
10	f	18	DC	C4'-C3'-O3'	6.57	119.85	110.00
4	N	2012	DC	C2'-C3'-O3'	6.43	121.15	111.50
4	W	2009	DG	P-O5'-C5'	-6.43	110.35	120.00
1	B	471	ARG	NE-CZ-NH2	6.36	124.92	119.20
1	S	638	VAL	CA-C-O	6.36	131.60	120.80
2	A	469	VAL	CA-C-O	-6.24	114.78	121.27
4	E	18	DC	C4'-C3'-O3'	-6.17	100.75	110.00
4	w	2012	DC	C5'-C4'-C3'	-6.16	105.67	114.90
4	N	2018	DC	C4'-C3'-O3'	-6.15	100.78	110.00
2	l	253	GLY	CA-C-O	-6.09	118.03	122.23
6	J	311	ASP	CA-C-O	-6.08	113.13	120.12
4	O	12	DC	C2'-C3'-O3'	6.08	120.61	111.50
2	R	252	ARG	N-CA-CB	-6.05	98.50	110.48
2	R	250	GLU	CA-C-N	6.02	129.39	120.90
2	R	250	GLU	C-N-CA	6.02	129.39	120.90
4	w	2017	DG	O3'-P-O5'	-6.00	95.00	104.00
4	e	12	DC	C2'-C3'-O3'	5.94	120.41	111.50
4	F	2011	DC	O5'-P-OP1	5.89	126.67	109.00
2	l	252	ARG	N-CA-CB	-5.87	101.75	110.61
2	R	310	LYS	CA-C-O	-5.82	114.71	120.82
10	f	19	DT	N1-C1'-C2'	5.82	122.23	113.50
7	M	637	ALA	CA-C-O	-5.77	114.44	120.55
2	r	10	ASN	CA-C-N	5.73	132.48	121.54
2	r	10	ASN	C-N-CA	5.73	132.48	121.54
4	e	18	DC	C4'-C3'-O3'	-5.71	101.43	110.00
2	j	416	LYS	CA-CB-CG	5.70	125.49	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	116	ASP	CA-CB-CG	5.66	118.26	112.60
2	R	252	ARG	CB-CA-C	-5.50	102.14	110.83
2	T	232	ARG	CG-CD-NE	-5.50	99.91	112.00
2	a	116	ASP	CA-CB-CG	5.46	118.06	112.60
2	r	442	GLU	CA-CB-CG	-5.39	103.32	114.10
4	n	2010	DG	C5'-C4'-C3'	-5.38	106.83	114.90
4	e	9	DG	O5'-C5'-C4'	-5.36	102.76	110.80
4	O	5	DG	P-O5'-C5'	5.35	128.03	120.00
4	w	2011	DC	C4'-C3'-O3'	5.31	117.97	110.00
6	J	116	ASP	CA-CB-CG	5.28	117.88	112.60
2	j	450	ASN	N-CA-CB	5.27	117.65	110.01
2	c	256	ARG	CG-CD-NE	-5.26	100.43	112.00
5	K	582	GLY	CA-C-O	-5.22	115.15	122.51
4	w	2018	DC	C5'-C4'-C3'	-5.22	107.08	114.90
5	K	490	GLY	CA-C-N	5.18	125.69	120.00
5	K	490	GLY	C-N-CA	5.18	125.69	120.00
2	L	434	THR	CA-C-N	5.17	125.57	119.94
2	L	434	THR	C-N-CA	5.17	125.57	119.94
2	r	116	ASP	CA-CB-CG	5.14	117.74	112.60
12	u	490	GLY	CA-C-N	5.14	125.65	120.00
12	u	490	GLY	C-N-CA	5.14	125.65	120.00
4	v	2011	DC	C4'-C3'-O3'	5.13	117.70	110.00
2	r	434	THR	CA-C-N	5.12	125.63	119.94
2	r	434	THR	C-N-CA	5.12	125.63	119.94
2	A	465	LEU	CA-C-O	-5.10	115.44	120.90
1	b	456	PRO	N-CA-CB	5.10	107.59	103.36
4	N	2018	DC	O3'-P-O5'	-5.10	96.35	104.00
2	j	122	ARG	CB-CG-CD	5.08	122.99	111.30
6	J	81	HIS	CA-C-N	5.08	124.80	119.92
6	J	81	HIS	C-N-CA	5.08	124.80	119.92
2	R	300	THR	CA-CB-OG1	5.07	117.21	109.60
3	U	490	GLY	CA-C-N	5.07	125.58	120.00
3	U	490	GLY	C-N-CA	5.07	125.58	120.00
1	b	437	ASP	CA-CB-CG	5.05	117.65	112.60
2	T	253	GLY	CA-C-O	-5.04	118.75	122.23
2	A	116	ASP	CA-CB-CG	5.04	117.64	112.60
4	E	9	DG	O5'-C5'-C4'	5.04	118.36	110.80
4	v	2018	DC	C4'-C3'-O3'	-5.03	102.46	110.00
1	S	490	GLY	CA-C-N	5.01	125.40	119.94
1	S	490	GLY	C-N-CA	5.01	125.40	119.94
2	C	310	LYS	CA-C-O	-5.00	115.25	120.55

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	311	ASP	Peptide
2	C	311	ASP	Peptide
2	C	9	ILE	Peptide
6	J	311	ASP	Mainchain
2	L	311	ASP	Peptide
2	T	311	ASP	Peptide
2	a	490	LEU	Peptide
2	c	311	ASP	Peptide
2	l	311	ASP	Peptide
2	r	10	ASN	Peptide
2	t	311	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1441	0	1381	26	0
1	S	1439	0	1374	18	0
1	b	1430	0	1354	13	0
1	s	1434	0	1372	14	0
2	A	3846	0	3780	88	0
2	C	3784	0	3713	47	1
2	L	3785	0	3731	38	0
2	R	3830	0	3769	47	1
2	T	3793	0	3740	53	0
2	a	3802	0	3718	52	0
2	c	3784	0	3717	46	1
2	j	3848	0	3786	52	0
2	l	3784	0	3744	43	0
2	r	3870	0	3787	47	1
2	t	3809	0	3753	41	0
3	D	1447	0	1376	23	0
3	U	1463	0	1388	16	0
3	m	1442	0	1376	18	0
4	E	455	0	247	34	0
4	F	392	0	214	7	0
4	N	455	0	248	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	392	0	213	5	0
4	W	408	0	227	21	0
4	e	392	0	210	20	0
4	n	418	0	226	18	0
4	v	399	0	214	2	0
4	w	400	0	222	6	0
5	K	1439	0	1367	16	0
6	J	3862	0	3802	60	0
7	M	1468	0	1390	16	0
8	V	388	0	215	17	0
8	o	369	0	203	9	0
9	d	1395	0	1326	27	0
10	f	348	0	191	9	0
11	k	1453	0	1393	19	0
12	u	1460	0	1390	19	0
13	A	26	0	0	0	0
13	C	26	0	0	2	0
13	J	26	0	0	4	0
13	L	26	0	0	2	0
13	R	26	0	0	3	0
13	U	26	0	0	3	0
13	b	26	0	0	1	0
13	d	26	0	0	2	0
13	k	26	0	0	2	0
13	l	26	0	0	2	0
13	s	26	0	0	1	0
13	t	26	0	0	5	0
All	All	68236	0	64157	809	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (809) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:581:LYS:CB	7:M:585:GLU:OE1	1.82	1.27
9:d:629:ARG:NH2	4:e:17:DG:OP1	1.65	1.26
4:E:1[A]:DG:O5'	4:E:1[A]:DG:C8	1.80	1.23
4:E:1[A]:DG:O5'	4:E:1[A]:DG:H8	1.12	1.22
2:A:58[B]:MET:HE2	2:A:58[B]:MET:HA	1.22	1.20
4:E:1[B]:DG:C2'	4:E:2[B]:DA:H5'	1.73	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:58[B]:MET:HA	2:j:58[B]:MET:CE	1.76	1.15
6:J:431:ARG:NH1	2:L:404:ASP:OD2	1.84	1.11
2:A:58[B]:MET:HA	2:A:58[B]:MET:CE	1.78	1.10
2:j:272[B]:ARG:HG2	2:j:272[B]:ARG:HH11	0.98	1.10
9:d:629:ARG:NH2	4:e:17:DG:P	2.23	1.10
2:a:332:GLY:HA3	10:f:19:DT:H1'	1.34	1.08
1:B:458[B]:ARG:HD2	4:E:10:DG:H4'	1.34	1.07
2:A:454[B]:GLU:HA	2:A:454[B]:GLU:OE1	1.50	1.06
4:E:1[A]:DG:H2''	4:E:2[A]:DA:H5'	1.36	1.06
4:n:2019[B]:DT:H2''	4:n:2020[B]:DT:C5'	1.87	1.04
2:a:58[B]:MET:HE2	2:a:58[B]:MET:HA	1.41	1.02
2:A:106:GLY:HA3	2:A:110:PHE:CE2	1.94	1.02
2:j:58[B]:MET:HA	2:j:58[B]:MET:HE2	1.01	1.01
2:a:69[B]:ARG:HG3	2:a:69[B]:ARG:HH11	1.24	1.01
6:J:123:TYR:OH	4:O:9:DG:OP2	1.79	1.01
2:A:449:LEU:HD13	9:d:470:ASP:CG	1.86	1.00
2:a:332:GLY:CA	10:f:19:DT:H1'	1.91	1.00
2:A:208[B]:GLU:O	2:A:208[B]:GLU:OE1	1.80	0.99
6:J:58[B]:MET:HG2	6:J:65[B]:LYS:CG	1.93	0.99
1:B:458[B]:ARG:CD	4:E:10:DG:H4'	1.92	0.98
2:a:423:GLN:OE1	2:c:431:ARG:NH2	1.96	0.98
2:j:313:ASN:HD22	2:j:316:VAL:HG23	1.28	0.98
8:o:8:DC:O3'	8:o:2009:DG:OP1	1.80	0.97
6:J:313:ASN:HD22	6:J:316:VAL:HG23	1.27	0.97
2:A:69[B]:ARG:HG3	2:A:69[B]:ARG:HH11	1.27	0.97
2:T:66:LYS:NZ	2:T:122:ARG:O	1.97	0.97
3:D:603:LEU:O	2:C:10:ASN:HB3	1.65	0.96
2:a:65[A]:LYS:CG	2:a:69[A]:ARG:HD3	1.96	0.96
6:J:315:SER:OG	2:T:257:GLN:NE2	1.99	0.95
2:A:208[B]:GLU:OE1	2:A:208[B]:GLU:C	2.10	0.95
4:N:1[B]:DG:N2	4:N:2[B]:DA:N6	2.15	0.94
2:j:272[B]:ARG:HH11	2:j:272[B]:ARG:CG	1.79	0.94
2:A:461:ASP:HB3	2:A:464:VAL:CG2	1.97	0.93
4:W:8:DC:O3'	4:W:2009:DG:OP2	1.83	0.93
2:j:58[B]:MET:HE2	2:j:58[B]:MET:CA	1.97	0.93
2:R:429:ARG:NH1	2:T:427:ASP:O	2.02	0.93
2:a:69[B]:ARG:HH11	2:a:69[B]:ARG:CG	1.83	0.92
2:A:461:ASP:HB3	2:A:464:VAL:HG23	1.53	0.91
2:A:65[A]:LYS:CG	2:A:69[A]:ARG:HD3	2.03	0.89
2:A:69[B]:ARG:HH11	2:A:69[B]:ARG:CG	1.84	0.89
4:w:8:DC:O3'	4:w:2009:DG:OP2	1.91	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:272[B]:ARG:HG2	2:j:272[B]:ARG:NH1	1.79	0.89
4:n:8:DC:O3'	4:n:2009:DG:OP1	1.91	0.88
6:J:123:TYR:OH	4:O:9:DG:P	2.31	0.87
1:b:446:GLY:HA2	2:c:298[B]:LEU:HD11	1.55	0.87
4:N:1[A]:DG:H8	4:N:1[A]:DG:HO5'	1.04	0.87
4:N:1[A]:DG:H8	4:N:1[A]:DG:O5'	1.58	0.86
6:J:58[B]:MET:HE2	6:J:58[B]:MET:HA	1.57	0.86
2:A:454[B]:GLU:OE1	2:A:454[B]:GLU:CA	2.24	0.85
13:J:501:JK8:N6	13:J:501:JK8:C26	2.38	0.85
4:N:2[B]:DA:H2''	4:N:3[B]:DG:OP2	1.76	0.85
6:J:58[B]:MET:HA	6:J:58[B]:MET:CE	2.05	0.85
2:A:106:GLY:HA3	2:A:110:PHE:HE2	1.36	0.84
6:J:315:SER:HG	2:T:257:GLN:HE22	1.25	0.84
2:C:27:MET:HE1	13:C:501[A]:JK8:CL	2.15	0.84
2:T:408:MET:SD	2:T:423:GLN:NE2	2.50	0.83
4:E:1[B]:DG:H2''	4:E:2[B]:DA:H5'	1.61	0.83
3:m:480[B]:GLN:HA	3:m:480[B]:GLN:HE21	1.44	0.82
2:a:58[B]:MET:HA	2:a:58[B]:MET:CE	1.98	0.82
2:A:106:GLY:CA	2:A:110:PHE:HE2	1.92	0.82
13:U:701[A]:JK8:C22	13:U:701[A]:JK8:N6	2.43	0.82
2:r:58[B]:MET:HE2	2:r:58[B]:MET:HA	1.62	0.82
2:A:122:ARG:H	2:A:122:ARG:HD3	1.45	0.81
4:E:1[B]:DG:H2'	4:E:2[B]:DA:H5'	1.63	0.81
4:E:1[B]:DG:C3'	4:E:2[B]:DA:H5'	2.09	0.81
6:J:313:ASN:ND2	6:J:316:VAL:HG23	1.96	0.81
2:r:423:GLN:OE1	2:t:431:ARG:NH2	2.14	0.80
2:A:122:ARG:HB2	2:A:122:ARG:HH11	1.47	0.80
3:m:480[B]:GLN:HA	3:m:480[B]:GLN:NE2	1.96	0.80
1:s:446:GLY:HA2	2:t:298[B]:LEU:HD11	1.63	0.80
4:E:2[B]:DA:H2''	4:E:3[B]:DG:OP2	1.79	0.80
2:A:65[A]:LYS:CG	2:A:69[A]:ARG:CD	2.60	0.80
2:j:313:ASN:ND2	2:j:316:VAL:HG23	1.96	0.79
2:R:240:SER:HB2	4:W:2020:DT:OP1	1.83	0.79
2:j:75:MET:SD	2:l:66[A]:LYS:HE2	2.23	0.78
4:E:1[B]:DG:C2'	4:E:2[B]:DA:C5'	2.59	0.78
6:J:250:GLU:OE2	6:J:258:ARG:NH1	2.17	0.78
2:j:465[B]:LEU:HD23	2:j:465[B]:LEU:C	2.09	0.78
2:A:106:GLY:CA	2:A:110:PHE:CE2	2.67	0.78
11:k:541:GLN:OE1	11:k:604:LEU:HD13	1.84	0.78
2:a:454[B]:GLU:HA	2:a:454[B]:GLU:OE1	1.83	0.77
2:l:66[B]:LYS:HD3	2:l:66[B]:LYS:N	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:58[B]:MET:HA	2:r:58[B]:MET:CE	2.14	0.77
2:a:330:SER:HB3	4:e:1:DG:N7	2.00	0.77
4:E:2[A]:DA:C8	4:E:2[A]:DA:OP2	2.37	0.76
4:E:1[A]:DG:C2'	4:E:2[A]:DA:H5'	2.16	0.76
2:R:240:SER:CB	4:W:2020:DT:OP1	2.34	0.76
2:R:431:ARG:NH2	2:T:427:ASP:OD1	2.17	0.76
4:E:1[B]:DG:H2''	4:E:2[B]:DA:C5'	2.16	0.75
4:E:2[A]:DA:OP2	4:E:2[A]:DA:H2'	1.87	0.75
6:J:208[B]:GLU:O	6:J:208[B]:GLU:OE1	2.05	0.74
2:T:238:ARG:NH1	8:V:2019:DT:OP1	2.19	0.74
2:r:409[B]:GLU:OE1	2:r:409[B]:GLU:CA	2.34	0.74
1:B:458[B]:ARG:HD2	4:E:10:DG:C4'	2.13	0.74
13:U:701[A]:JK8:N6	13:U:701[A]:JK8:C21	2.49	0.74
2:l:63:SER:O	2:l:65:LYS:HD2	1.88	0.74
4:n:2010:DG:C2	8:o:2012:DC:O2	2.41	0.74
2:j:313:ASN:HD22	2:j:316:VAL:CG2	1.99	0.73
2:A:467:GLN:O	2:A:467:GLN:NE2	2.21	0.73
2:r:409[B]:GLU:OE1	2:r:409[B]:GLU:HA	1.87	0.73
6:J:313:ASN:HD22	6:J:316:VAL:CG2	1.99	0.73
2:j:75:MET:HG2	2:l:66[A]:LYS:CD	2.18	0.72
2:c:447[B]:GLU:OE1	2:c:447[B]:GLU:HA	1.88	0.72
6:J:405:LYS:O	6:J:409[B]:GLU:HG2	1.88	0.72
8:V:2010:DG:N2	4:W:2011:DC:O2	2.22	0.72
6:J:429:ARG:NH1	2:L:427:ASP:O	2.23	0.71
2:j:454[B]:GLU:OE1	2:j:454[B]:GLU:HA	1.90	0.71
2:A:58[B]:MET:HE2	2:A:58[B]:MET:CA	2.12	0.71
2:a:58[B]:MET:HE2	2:a:58[B]:MET:CA	2.20	0.71
4:N:1[B]:DG:N2	4:N:2[B]:DA:H61	1.86	0.70
2:R:342:ARG:HG2	13:R:501:JK8:C16	2.22	0.70
2:A:173:SER:OG	4:E:5:DG:H5'	1.90	0.70
1:S:617:THR:OG1	2:R:19:ARG:NH1	2.25	0.69
2:R:423:GLN:OE1	2:T:431:ARG:NH2	2.25	0.69
1:S:584:GLY:N	1:S:584:GLY:C	2.50	0.69
13:R:501:JK8:C10	13:R:501:JK8:CL	2.77	0.69
12:u:480[B]:GLN:OE1	12:u:480[B]:GLN:HA	1.92	0.69
2:C:298[A]:LEU:HD23	2:C:298[A]:LEU:O	1.93	0.69
4:e:1:DG:H1'	4:e:2:DA:OP2	1.93	0.69
4:e:19:DT:C2'	4:e:20:DT:OP2	2.40	0.69
2:r:454[B]:GLU:HA	2:r:454[B]:GLU:OE1	1.91	0.69
2:r:58[B]:MET:HE3	2:r:65[B]:LYS:CG	2.22	0.69
2:c:56:GLN:HB2	2:c:58:MET:HE2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:272[B]:ARG:HE	4:W:3:DG:H5''	1.58	0.68
4:N:1[B]:DG:H2''	4:N:2[B]:DA:H5'	1.73	0.68
9:d:629:ARG:CZ	4:e:17:DG:OP1	2.41	0.68
1:B:458[B]:ARG:HH11	1:B:458[B]:ARG:HB3	1.58	0.68
2:R:238:ARG:HH22	4:W:2019:DT:P	2.16	0.68
2:R:408[B]:MET:HE1	2:R:419:GLU:HG3	1.76	0.68
2:t:56:GLN:HB2	2:t:58:MET:HE2	1.76	0.68
1:B:515:HIS:HB2	2:A:25:TYR:CD1	2.29	0.67
2:t:75:MET:HE1	2:t:83:ASP:HB3	1.76	0.67
2:R:92:ARG:HD2	8:V:5:DG:OP1	1.94	0.67
4:N:2[B]:DA:H2''	4:N:3[B]:DG:C8	2.29	0.67
4:e:19:DT:H2''	4:e:20:DT:OP2	1.95	0.67
11:k:637:ALA:O	11:k:638:VAL:HG12	1.95	0.67
4:E:9:DG:H4'	4:E:9:DG:OP1	1.93	0.67
13:L:501[A]:JK8:CL	13:L:501[A]:JK8:C10	2.80	0.67
13:t:501[A]:JK8:C10	13:t:501[A]:JK8:CL	2.79	0.66
2:j:58[B]:MET:HG3	2:j:127:ARG:HA	1.77	0.66
4:N:1[B]:DG:C2	4:N:2[B]:DA:C6	2.83	0.66
1:s:458:ARG:HH12	4:w:2013:DG:H1'	1.60	0.66
12:u:587:ASN:O	12:u:590:GLN:HG2	1.96	0.66
6:J:465[B]:LEU:C	6:J:465[B]:LEU:HD23	2.21	0.66
8:V:2:DA:H4'	8:V:3:DG:OP1	1.95	0.66
9:d:587:ASN:O	9:d:590:GLN:HG2	1.96	0.66
2:R:342:ARG:HH11	2:R:342:ARG:CG	2.08	0.66
2:c:66[A]:LYS:HE3	2:c:122:ARG:O	1.95	0.65
6:J:27:MET:HE3	13:J:501:JK8:CL	2.33	0.65
7:M:587:ASN:O	7:M:590:GLN:HG2	1.96	0.65
2:L:56:GLN:HB2	2:L:58:MET:HE2	1.78	0.65
3:D:587:ASN:O	3:D:590:GLN:HG2	1.97	0.65
6:J:454[B]:GLU:OE1	6:J:454[B]:GLU:HA	1.96	0.65
4:e:12:DC:O2	10:f:10:DG:N2	2.29	0.65
2:T:56:GLN:HB2	2:T:58:MET:HE2	1.76	0.65
2:L:66[B]:LYS:HD3	2:L:66[B]:LYS:N	2.12	0.65
3:U:587:ASN:O	3:U:590:GLN:HG2	1.97	0.65
2:l:56:GLN:HB2	2:l:58:MET:HE2	1.77	0.65
6:J:208[B]:GLU:OE1	6:J:208[B]:GLU:C	2.39	0.65
3:m:587:ASN:O	3:m:590:GLN:HG2	1.97	0.64
4:n:8:DC:H2'	4:n:2009:DG:H5'	1.77	0.64
2:t:253:GLY:O	2:t:256:ARG:HG3	1.98	0.64
2:A:75:MET:HE1	2:A:83:ASP:HB3	1.79	0.64
2:T:175:ILE:N	2:T:175:ILE:HD12	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:75:MET:HE1	2:a:83:ASP:HB3	1.79	0.64
2:C:56:GLN:HB2	2:C:58:MET:HE2	1.79	0.63
2:R:240:SER:OG	4:W:2020:DT:OP1	2.16	0.63
2:C:66[A]:LYS:HE3	2:C:122:ARG:O	1.98	0.63
2:j:75:MET:HE1	2:j:83:ASP:HB3	1.80	0.63
2:l:75:MET:HE1	2:l:83:ASP:HB3	1.80	0.63
2:r:75:MET:HE1	2:r:83:ASP:HB3	1.80	0.63
2:C:75:MET:HE1	2:C:83:ASP:HB3	1.80	0.63
2:R:66:LYS:HE2	2:R:122:ARG:O	1.99	0.63
13:J:501:JK8:CL	13:J:501:JK8:C10	2.84	0.63
2:j:58[B]:MET:SD	2:j:58[B]:MET:C	2.81	0.63
2:t:66[A]:LYS:HE3	2:t:122:ARG:O	1.99	0.63
2:j:173:SER:OG	4:n:5:DG:H5'	1.99	0.63
2:T:75:MET:HE1	2:T:83:ASP:HB3	1.81	0.62
2:C:272[B]:ARG:HG2	2:C:272[B]:ARG:HH11	1.64	0.62
5:K:458:ARG:HH21	5:K:480:GLN:HE22	1.45	0.62
2:R:431:ARG:HH21	2:T:427:ASP:CG	2.06	0.62
4:N:1[B]:DG:H21	4:N:2[B]:DA:N6	1.97	0.62
2:R:224:ILE:HG21	2:R:230:ILE:HD11	1.81	0.62
2:A:461:ASP:O	2:A:464:VAL:HG23	2.00	0.62
2:j:315:SER:OG	2:t:257:GLN:NE2	2.22	0.62
2:c:75:MET:HE1	2:c:83:ASP:HB3	1.80	0.62
2:r:224:ILE:HG21	2:r:230:ILE:HD11	1.82	0.61
2:A:458:ILE:HG23	2:A:465:LEU:HD12	1.82	0.61
5:K:636:ASN:HD22	6:J:23:LEU:HD22	1.64	0.61
4:e:2:DA:H2''	4:e:3:DG:OP2	2.00	0.61
2:C:272[B]:ARG:HG2	2:C:272[B]:ARG:NH1	2.16	0.61
4:N:1[B]:DG:H2'	4:N:2[B]:DA:C8	2.36	0.61
2:L:75:MET:HE1	2:L:83:ASP:HB3	1.82	0.61
5:K:637:ALA:O	5:K:638:VAL:HG23	2.00	0.61
6:J:58[B]:MET:CG	6:J:65[B]:LYS:CG	2.73	0.61
10:f:19:DT:H2'	10:f:19:DT:O2	2.00	0.61
2:r:465[B]:LEU:C	2:r:465[B]:LEU:HD23	2.26	0.61
12:u:430:GLU:HB3	12:u:502:LYS:HB2	1.83	0.61
4:W:8:DC:C3'	4:W:2009:DG:OP2	2.49	0.60
2:L:344:LYS:NZ	2:L:350:GLU:OE1	2.34	0.60
8:V:8:DC:H2'	8:V:2009:DG:H5'	1.82	0.60
4:W:1:DG:H2''	4:W:2:DA:H5'	1.83	0.60
2:C:224:ILE:HG21	2:C:230:ILE:HD11	1.84	0.60
6:J:75:MET:HE1	6:J:83:ASP:HB3	1.84	0.60
1:b:462:LEU:HD13	10:f:14:DT:H5''	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:100:ARG:HG3	2:r:101:TYR:CE1	2.36	0.60
4:F:8:DC:O3'	4:F:2009:DG:OP2	2.19	0.60
2:j:405:LYS:O	2:j:409[B]:GLU:HG2	2.02	0.60
12:u:427[B]:GLU:H	12:u:427[B]:GLU:CD	2.10	0.60
2:t:389:ASP:OD1	2:t:438[B]:ARG:NH1	2.35	0.60
11:k:430:GLU:HB3	11:k:502:LYS:HB2	1.83	0.59
6:J:224:ILE:HG21	6:J:230:ILE:HD11	1.84	0.59
2:l:66[A]:LYS:HE3	2:l:122:ARG:O	2.02	0.59
3:D:541:GLN:NE2	3:D:604:LEU:HD13	2.18	0.59
2:L:224:ILE:HG21	2:L:230:ILE:HD11	1.84	0.59
2:A:224:ILE:HG21	2:A:230:ILE:HD11	1.84	0.58
2:T:224:ILE:HG21	2:T:230:ILE:HD11	1.85	0.58
2:c:113[B]:MET:SD	2:c:264:ILE:HD11	2.43	0.58
2:A:75:MET:HG2	2:C:66[A]:LYS:CD	2.33	0.58
5:K:435:GLU:HG2	5:K:436:GLY:N	2.19	0.58
2:a:58[B]:MET:HE3	2:a:65[B]:LYS:CG	2.33	0.58
2:A:68:ALA:HB1	2:C:75:MET:HE3	1.84	0.58
5:K:430:GLU:HB3	5:K:502:LYS:HB2	1.84	0.58
6:J:76:GLY:HA2	2:L:66[B]:LYS:HG3	1.85	0.58
2:a:224:ILE:HG21	2:a:230:ILE:HD11	1.83	0.58
6:J:345:LEU:H	13:J:501:JK8:C23	2.16	0.58
7:M:430:GLU:HB3	7:M:502:LYS:HB2	1.85	0.58
2:l:224:ILE:HG21	2:l:230:ILE:HD11	1.85	0.58
2:t:224:ILE:HG21	2:t:230:ILE:HD11	1.84	0.58
1:B:430:GLU:HB3	1:B:502:LYS:HB2	1.85	0.58
2:A:69[B]:ARG:CG	2:A:69[B]:ARG:NH1	2.55	0.58
4:E:2[A]:DA:OP2	4:E:2[A]:DA:H8	1.84	0.58
1:S:430:GLU:HB3	1:S:502:LYS:HB2	1.84	0.58
2:A:106:GLY:HA3	2:A:110:PHE:CD2	2.36	0.58
3:U:515:HIS:HB2	2:T:25:TYR:CD1	2.39	0.58
9:d:430:GLU:HB3	9:d:502:LYS:HB2	1.84	0.58
2:j:465[B]:LEU:C	2:j:465[B]:LEU:CD2	2.77	0.58
2:T:332:GLY:CA	8:V:2019:DT:H4'	2.34	0.58
1:b:430:GLU:HB3	1:b:502:LYS:HB2	1.86	0.58
2:j:465[B]:LEU:HD23	2:j:465[B]:LEU:O	2.03	0.58
2:a:69[B]:ARG:CG	2:a:69[B]:ARG:NH1	2.53	0.57
2:l:330:SER:OG	4:n:2020[B]:DT:OP1	2.21	0.57
2:a:332:GLY:HA3	10:f:19:DT:C1'	2.21	0.57
2:A:109:ASN:HB2	3:D:442:SER:OG	2.05	0.57
2:L:66[A]:LYS:HE3	2:L:122:ARG:O	2.05	0.57
2:j:224:ILE:HG21	2:j:230:ILE:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:s:430:GLU:HB3	1:s:502:LYS:HB2	1.85	0.57
2:t:112:SER:OG	2:t:116:ASP:OD2	2.15	0.57
2:A:175:ILE:HD11	4:E:4:DC:N3	2.20	0.57
2:c:224:ILE:HG21	2:c:230:ILE:HD11	1.86	0.57
2:a:408:MET:SD	2:a:423:GLN:NE2	2.77	0.57
3:m:430:GLU:HB3	3:m:502:LYS:HB2	1.85	0.57
1:S:460:LYS:HG2	8:V:8:DC:H1'	1.85	0.57
2:T:408:MET:CE	2:T:423:GLN:HE21	2.16	0.57
2:j:390:HIS:HB3	2:j:393:GLU:HG3	1.86	0.57
4:N:2[A]:DA:C2	4:O:19:DT:O2	2.57	0.57
3:D:430:GLU:HB3	3:D:502:LYS:HB2	1.85	0.56
5:K:461:ILE:HD11	5:K:481:MET:HE2	1.87	0.56
3:U:430:GLU:HB3	3:U:502:LYS:HB2	1.86	0.56
2:j:75:MET:HG2	2:l:66[A]:LYS:HD2	1.87	0.56
2:c:112:SER:OG	2:c:116:ASP:OD2	2.15	0.56
6:J:75:MET:HG2	2:L:66[A]:LYS:CE	2.36	0.56
4:W:2020:DT:H72	2:t:393:GLU:HG2	1.87	0.56
2:C:112:SER:OG	2:C:116:ASP:OD2	2.16	0.56
2:A:75:MET:CG	2:C:66[A]:LYS:HE2	2.36	0.56
1:S:620:MET:HE1	2:R:19:ARG:NH2	2.20	0.56
11:k:446:GLY:HA2	2:l:298[B]:LEU:HD11	1.87	0.56
2:a:426:LEU:O	2:c:431:ARG:HB3	2.06	0.56
2:r:122:ARG:CZ	2:r:123:TYR:HE1	2.19	0.56
13:k:701:JK8:C10	13:k:701:JK8:CL	2.92	0.55
1:b:609:GLU:HG2	2:a:13:ASN:HD22	1.71	0.55
3:D:541:GLN:HE22	3:D:604:LEU:HD13	1.69	0.55
2:T:332:GLY:HA3	8:V:2019:DT:H4'	1.89	0.55
2:r:409[B]:GLU:OE1	2:r:409[B]:GLU:N	2.40	0.55
2:R:238:ARG:NH2	4:W:2019:DT:OP1	2.38	0.55
2:T:415:PHE:O	2:T:416:LYS:HG3	2.07	0.55
2:T:112:SER:OG	2:T:116:ASP:OD2	2.15	0.55
9:d:629:ARG:HH22	4:e:17:DG:P	2.25	0.55
2:L:388:LEU:HD13	2:L:438:ARG:HG2	1.89	0.55
2:l:112:SER:OG	2:l:116:ASP:OD2	2.14	0.55
2:t:443:ALA:O	2:t:447[B]:GLU:OE2	2.24	0.55
1:B:515:HIS:HB2	2:A:25:TYR:CG	2.43	0.54
2:l:423:GLN:OE1	2:l:423:GLN:HA	2.07	0.54
2:A:179:MET:C	4:F:2017:DG:H4'	2.32	0.54
6:J:339:VAL:HB	6:J:344:LYS:HD3	1.90	0.54
11:k:626:VAL:HG11	8:o:2017:DG:H3'	1.88	0.54
2:a:454[B]:GLU:OE1	2:a:454[B]:GLU:CA	2.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:164:PHE:HB3	2:c:476:ILE:HG21	1.88	0.54
1:B:588:ALA:HB1	2:C:298[B]:LEU:HD11	1.88	0.54
5:K:508:ASP:OD1	5:K:583:LEU:HG	2.08	0.54
2:a:75:MET:HG2	2:c:66[A]:LYS:CD	2.38	0.54
2:A:468:LEU:O	2:A:468:LEU:HD12	2.08	0.54
4:N:1[B]:DG:C2	4:N:2[B]:DA:N6	2.76	0.54
2:C:423:GLN:OE1	2:C:423:GLN:HA	2.08	0.54
3:U:585:GLU:O	3:U:585:GLU:HG3	2.08	0.54
2:c:423:GLN:OE1	2:c:423:GLN:HA	2.07	0.54
2:t:272[B]:ARG:NH2	4:w:3:DG:H5'	2.23	0.54
5:K:517:ARG:NE	6:J:17:GLU:OE2	2.38	0.54
4:n:8:DC:H2'	4:n:2009:DG:C5'	2.38	0.54
2:A:58[B]:MET:SD	2:A:58[B]:MET:C	2.87	0.53
2:R:69:ARG:HE	2:T:77:LYS:HE3	1.73	0.53
2:a:65[A]:LYS:CG	2:a:69[A]:ARG:CD	2.81	0.53
12:u:480[B]:GLN:OE1	12:u:480[B]:GLN:CA	2.56	0.53
2:L:388:LEU:HD11	2:L:441:ILE:HD12	1.89	0.53
1:B:435:GLU:H	1:B:435:GLU:CD	2.17	0.53
2:A:75:MET:HG2	2:C:66[A]:LYS:HE2	1.89	0.53
12:u:517:ARG:NE	2:t:17:GLU:OE2	2.40	0.53
8:o:8:DC:O3'	8:o:2009:DG:P	2.66	0.53
1:s:461:ILE:HD11	1:s:481:MET:HE2	1.90	0.53
1:B:609:GLU:HG2	2:A:13:ASN:HD22	1.72	0.53
6:J:257:GLN:HE22	2:T:315:SER:HG	1.54	0.53
2:R:251:GLU:O	2:R:251:GLU:CD	2.52	0.53
2:T:92:ARG:NH1	4:W:5:DG:OP1	2.42	0.53
2:a:208[B]:GLU:OE1	2:a:208[B]:GLU:O	2.26	0.53
2:l:179:MET:CE	13:l:501[A]:JK8:C24	2.87	0.53
2:L:423:GLN:OE1	2:L:423:GLN:HA	2.08	0.53
2:c:447[B]:GLU:OE1	2:c:447[B]:GLU:CA	2.56	0.53
4:n:1:DG:H2''	4:n:2:DA:H5'	1.91	0.53
1:B:458[A]:ARG:O	1:B:458[A]:ARG:HG2	2.10	0.52
4:N:2[A]:DA:H2	4:O:19:DT:O2	1.91	0.52
11:k:522:THR:HA	11:k:618:PHE:CE2	2.44	0.52
2:A:56:GLN:CB	2:A:58[A]:MET:HE2	2.40	0.52
2:A:75:MET:HE3	2:C:68:ALA:HB1	1.90	0.52
9:d:458:ARG:HD2	9:d:477:GLU:OE2	2.09	0.52
2:t:423:GLN:OE1	2:t:423:GLN:HA	2.08	0.52
2:R:465[B]:LEU:HD23	2:R:465[B]:LEU:C	2.35	0.52
11:k:458:ARG:HH12	8:o:2013:DG:H1'	1.74	0.52
3:U:528:MET:HB3	3:U:531:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:65[A]:LYS:CG	2:A:69[A]:ARG:HD2	2.38	0.52
2:r:109:ASN:HB2	12:u:442:SER:OG	2.09	0.52
1:S:458:ARG:CG	8:V:2009:DG:H2''	2.40	0.52
3:U:493:PHE:CE1	3:U:530:PRO:HB2	2.45	0.52
1:b:493:PHE:CE1	1:b:530:PRO:HB2	2.45	0.52
2:r:388:LEU:HD13	2:r:438:ARG:HG2	1.90	0.52
1:S:470:ASP:OD1	1:S:471:ARG:N	2.43	0.52
1:B:493:PHE:CE1	1:B:530:PRO:HB2	2.45	0.51
3:m:493:PHE:CE1	3:m:530:PRO:HB2	2.46	0.51
2:A:458:ILE:CG2	2:A:465:LEU:HD12	2.39	0.51
6:J:56:GLN:CB	6:J:58[A]:MET:HE2	2.41	0.51
1:S:435:GLU:H	1:S:435:GLU:CD	2.17	0.51
6:J:315:SER:CB	2:T:257:GLN:HE22	2.19	0.51
2:T:344:LYS:NZ	2:T:350:GLU:OE1	2.42	0.51
13:d:701[A]:JK8:C10	13:d:701[A]:JK8:CL	2.95	0.51
11:k:437:ASP:N	4:n:2010:DG:OP1	2.43	0.51
1:B:458[B]:ARG:CZ	4:E:10:DG:H2''	2.40	0.51
1:b:470:ASP:OD1	1:b:471:ARG:N	2.43	0.51
9:d:458:ARG:HE	10:f:10:DG:H4'	1.75	0.51
2:j:56:GLN:CB	2:j:58[A]:MET:HE2	2.41	0.51
8:o:8:DC:C3'	8:o:2009:DG:OP1	2.58	0.51
12:u:493:PHE:CE1	12:u:530:PRO:HB2	2.45	0.51
2:A:461:ASP:CB	2:A:464:VAL:HG23	2.31	0.51
8:V:2:DA:C2	4:W:2019:DT:O2	2.63	0.51
4:e:12:DC:O2	10:f:10:DG:C2	2.63	0.51
7:M:493:PHE:CE1	7:M:530:PRO:HB2	2.45	0.51
11:k:446:GLY:HA2	2:l:298[B]:LEU:CD1	2.41	0.51
11:k:470:ASP:OD1	11:k:471:ARG:N	2.44	0.51
11:k:493:PHE:CE1	11:k:530:PRO:HB2	2.45	0.51
1:s:493:PHE:CE1	1:s:530:PRO:HB2	2.45	0.51
1:b:462:LEU:HA	10:f:14:DT:O3'	2.10	0.51
3:m:585:GLU:O	3:m:585:GLU:HG3	2.10	0.51
3:D:493:PHE:CE1	3:D:530:PRO:HB2	2.46	0.51
2:L:112:SER:OG	2:L:116:ASP:OD2	2.16	0.51
9:d:493:PHE:CE1	9:d:530:PRO:HB2	2.46	0.51
5:K:470:ASP:OD1	5:K:471:ARG:N	2.44	0.50
5:K:493:PHE:CE1	5:K:530:PRO:HB2	2.45	0.50
6:J:402:ASP:O	2:L:436:LEU:HD13	2.11	0.50
2:R:69:ARG:HH21	2:T:77:LYS:CE	2.23	0.50
2:r:56:GLN:CB	2:r:58[A]:MET:HE2	2.41	0.50
2:r:208[B]:GLU:OE1	2:r:208[B]:GLU:O	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ILE:HD11	1:B:481:MET:HE2	1.93	0.50
1:B:470:ASP:OD1	1:B:471:ARG:N	2.43	0.50
2:a:69[B]:ARG:HG3	2:a:69[B]:ARG:NH1	2.06	0.50
6:J:75:MET:HG2	2:L:66[A]:LYS:CD	2.41	0.50
4:N:3[B]:DG:OP2	4:N:3[B]:DG:H8	1.95	0.50
2:R:175:ILE:HD12	8:V:5:DG:C2	2.46	0.50
9:d:528:MET:HB3	9:d:531:LEU:HD12	1.93	0.50
1:S:493:PHE:CE1	1:S:530:PRO:HB2	2.46	0.50
1:b:435[B]:GLU:H	1:b:435[B]:GLU:CD	2.18	0.50
2:a:56:GLN:CB	2:a:58[A]:MET:HE2	2.41	0.50
9:d:605:GLN:HB3	2:c:10:ASN:O	2.11	0.50
2:A:56:GLN:HB2	2:A:58[A]:MET:HE2	1.92	0.50
2:a:76:GLY:HA2	2:c:66[B]:LYS:HG3	1.93	0.50
2:a:399:ARG:CZ	2:c:391:ILE:CG2	2.90	0.50
2:j:75:MET:HG2	2:l:66[A]:LYS:CE	2.41	0.50
3:m:437:ASP:OD2	8:o:2010:DG:H5''	2.11	0.50
3:m:528:MET:HB3	3:m:531:LEU:HD12	1.93	0.50
4:n:2:DA:H2	8:o:2019:DT:O2	1.95	0.50
1:s:626:VAL:HG11	4:w:2017:DG:H3'	1.94	0.50
12:u:528:MET:HB3	12:u:531:LEU:HD12	1.92	0.50
2:A:429:ARG:NH1	2:C:427:ASP:O	2.45	0.50
5:K:460:LYS:HG2	4:N:8:DC:H1'	1.93	0.50
6:J:298:LEU:HD11	7:M:588:ALA:HB3	1.93	0.50
2:c:253:GLY:O	2:c:256:ARG:HG3	2.11	0.50
2:j:423:GLN:OE1	2:l:431:ARG:NH2	2.45	0.49
2:r:75:MET:HG2	2:t:66[A]:LYS:HE2	1.93	0.49
2:A:377:ARG:HG3	2:A:448:LEU:HD11	1.93	0.49
9:d:515:HIS:HB2	2:c:25:TYR:CD1	2.47	0.49
2:a:119:ALA:HB2	9:d:438:SER:HA	1.94	0.49
3:D:528:MET:HB3	3:D:531:LEU:HD12	1.93	0.49
1:s:470:ASP:OD1	1:s:471:ARG:N	2.43	0.49
1:B:458[A]:ARG:NH1	4:F:2013:DG:H1'	2.27	0.49
9:d:629:ARG:NH2	4:e:17:DG:OP2	2.44	0.49
2:A:449:LEU:CD1	9:d:470:ASP:HB2	2.42	0.49
3:D:541:GLN:NE2	3:D:602:ALA:O	2.46	0.49
6:J:252:ARG:HB2	6:J:258:ARG:HE	1.76	0.49
3:D:517:ARG:NE	2:C:17:GLU:OE2	2.45	0.49
7:M:528:MET:HB3	7:M:531:LEU:HD12	1.94	0.49
1:S:634:GLU:OE1	13:R:501:JK8:N1	2.45	0.49
2:l:357:GLU:HA	2:l:357:GLU:OE1	2.13	0.49
2:A:79:HIS:CE1	4:E:7:DA:OP1	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:603:LEU:O	2:C:10:ASN:CB	2.49	0.49
6:J:192:ILE:HG21	6:J:477:ARG:HB2	1.95	0.49
2:R:88[B]:GLU:HA	2:R:88[B]:GLU:OE1	2.13	0.49
2:a:429:ARG:HA	2:c:429:ARG:HA	1.95	0.49
5:K:636:ASN:ND2	6:J:23:LEU:HD22	2.28	0.48
2:j:56:GLN:HB2	2:j:58[A]:MET:HE2	1.94	0.48
2:c:192:ILE:HG21	2:c:477:ARG:HB2	1.93	0.48
2:A:75:MET:HG2	2:C:66[A]:LYS:HD3	1.94	0.48
2:L:357:GLU:HA	2:L:357:GLU:OE1	2.13	0.48
3:U:493:PHE:CZ	3:U:531:LEU:HG	2.48	0.48
6:J:315:SER:CB	2:T:257:GLN:NE2	2.75	0.48
1:S:631:GLN:OE1	1:S:631:GLN:HA	2.12	0.48
2:R:192:ILE:HG21	2:R:477:ARG:HB2	1.96	0.48
2:c:389:ASP:OD1	2:c:438[B]:ARG:NH1	2.46	0.48
12:u:634:GLU:HA	13:t:501[A]:JK8:C10	2.44	0.48
13:t:501[A]:JK8:C21	13:t:501[A]:JK8:N6	2.76	0.48
3:D:603:LEU:O	2:C:10:ASN:ND2	2.45	0.48
9:d:493:PHE:CZ	9:d:531:LEU:HG	2.49	0.48
1:s:607:LYS:CB	2:r:11:GLU:OE2	2.62	0.48
12:u:493:PHE:CZ	12:u:531:LEU:HG	2.49	0.48
2:A:427:ASP:O	2:C:429:ARG:NH1	2.47	0.48
2:T:238:ARG:CZ	8:V:2019:DT:OP1	2.62	0.48
1:B:588:ALA:CB	2:C:298[B]:LEU:HD11	2.43	0.48
6:J:253:GLY:O	6:J:255:GLY:N	2.47	0.48
2:T:272[A]:ARG:HD3	4:W:3:DG:OP1	2.14	0.48
2:j:447:GLU:O	2:j:450:ASN:ND2	2.47	0.48
3:m:493:PHE:CZ	3:m:531:LEU:HG	2.49	0.48
2:t:393:GLU:OE1	2:t:393:GLU:N	2.46	0.48
2:R:75:MET:HE1	2:R:83:ASP:HB3	1.96	0.48
2:a:68:ALA:HB1	2:c:75:MET:HE3	1.95	0.47
2:c:357:GLU:OE1	2:c:357:GLU:HA	2.13	0.47
2:l:192:ILE:HG21	2:l:477:ARG:HB2	1.96	0.47
2:A:175:ILE:HB	4:E:5:DG:N2	2.29	0.47
2:a:192:ILE:HG21	2:a:477:ARG:HB2	1.96	0.47
2:A:445:TYR:CE2	2:A:449:LEU:HD11	2.50	0.47
6:J:377:ARG:HG3	6:J:448:LEU:HD11	1.95	0.47
7:M:493:PHE:CZ	7:M:531:LEU:HG	2.49	0.47
2:T:231:ARG:HE	2:T:231:ARG:HB2	1.34	0.47
2:C:272[B]:ARG:HH11	2:C:272[B]:ARG:CG	2.28	0.47
2:R:69:ARG:HH21	2:T:77:LYS:HE3	1.79	0.47
2:T:272[B]:ARG:NE	4:W:3:DG:H5"	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:389:ASP:OD1	2:T:438[B]:ARG:NH1	2.48	0.47
12:u:515:HIS:HB2	2:t:25:TYR:CD1	2.49	0.47
3:D:493:PHE:CZ	3:D:531:LEU:HG	2.49	0.47
4:E:1[B]:DG:H2''	4:E:2[B]:DA:H5''	1.93	0.47
2:T:192:ILE:HG21	2:T:477:ARG:HB2	1.96	0.47
11:k:637:ALA:O	11:k:638:VAL:CG1	2.61	0.47
3:m:515:HIS:HB2	2:l:25:TYR:CD1	2.49	0.47
2:A:106:GLY:HA2	2:A:110:PHE:HE2	1.77	0.47
2:C:192:ILE:HG21	2:C:477:ARG:HB2	1.97	0.47
2:L:192:ILE:HG21	2:L:477:ARG:HB2	1.97	0.47
2:j:192:ILE:HG21	2:j:477:ARG:HB2	1.96	0.47
1:s:515:HIS:HB2	2:r:25:TYR:CD1	2.49	0.47
2:r:56:GLN:HB2	2:r:58[A]:MET:HE2	1.96	0.47
2:A:58[B]:MET:HG3	2:A:127:ARG:HA	1.97	0.47
2:A:458:ILE:CG2	2:A:465:LEU:CD1	2.92	0.47
2:R:179:MET:C	4:W:2017:DG:H4'	2.39	0.47
2:a:56:GLN:HB2	2:a:58[A]:MET:HE2	1.96	0.47
9:d:593:GLU:OE1	9:d:593:GLU:HA	2.15	0.47
2:C:92:ARG:NH1	4:F:5:DG:OP1	2.48	0.47
6:J:56:GLN:HB2	6:J:58[A]:MET:HE2	1.96	0.47
2:R:377:ARG:HG3	2:R:448:LEU:HD11	1.97	0.47
2:T:445:TYR:CE2	2:T:449:LEU:HD11	2.50	0.47
2:a:445:TYR:CE2	2:a:449:LEU:HD11	2.50	0.47
2:j:75:MET:CG	2:l:66[A]:LYS:HE2	2.45	0.47
2:j:445:TYR:CE2	2:j:449:LEU:HD11	2.50	0.47
2:c:56:GLN:CB	2:c:58:MET:HE2	2.43	0.46
3:m:464:VAL:HG21	3:m:523:PHE:HA	1.97	0.46
2:L:445:TYR:CE2	2:L:449:LEU:HD11	2.49	0.46
1:S:469:LEU:HD23	2:t:446:ASN:CG	2.40	0.46
2:R:445:TYR:CE2	2:R:449:LEU:HD11	2.50	0.46
3:U:515:HIS:HB2	2:T:25:TYR:CG	2.50	0.46
3:m:480[B]:GLN:HE21	3:m:480[B]:GLN:CA	2.24	0.46
3:m:626:VAL:HG21	4:n:2017:DG:H3'	1.97	0.46
2:r:433:LEU:N	2:r:433:LEU:HD12	2.30	0.46
6:J:298:LEU:CD1	7:M:588:ALA:HB3	2.46	0.46
4:N:2[B]:DA:C2'	4:N:3[B]:DG:OP2	2.55	0.46
3:U:460:LYS:HG2	4:W:8:DC:H1'	1.97	0.46
2:T:175:ILE:HD12	2:T:175:ILE:H	1.79	0.46
2:c:445:TYR:CE2	2:c:449:LEU:HD11	2.50	0.46
4:e:2:DA:C2'	4:e:3:DG:OP2	2.63	0.46
2:l:445:TYR:CE2	2:l:449:LEU:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:177:VAL:HG22	4:w:2016:DC:H4'	1.97	0.46
3:D:593:GLU:OE1	3:D:593:GLU:HA	2.16	0.46
2:C:445:TYR:CE2	2:C:449:LEU:HD11	2.50	0.46
6:J:445:TYR:CE2	6:J:449:LEU:HD11	2.50	0.46
3:U:493:PHE:HZ	3:U:531:LEU:HG	1.81	0.46
2:l:56:GLN:CB	2:l:58:MET:HE2	2.45	0.46
2:r:388:LEU:HD11	2:r:441:ILE:HD12	1.97	0.46
2:t:56:GLN:CB	2:t:58:MET:HE2	2.44	0.46
1:B:529:ARG:N	1:B:530:PRO:CD	2.79	0.46
2:A:75:MET:HG2	2:C:66[A]:LYS:CE	2.46	0.46
9:d:637:ALA:HA	2:c:27:MET:HE3	1.96	0.46
3:m:493:PHE:HZ	3:m:531:LEU:HG	1.81	0.46
2:r:445:TYR:CE2	2:r:449:LEU:HD11	2.50	0.46
2:t:445:TYR:CE2	2:t:449:LEU:HD11	2.50	0.46
2:t:465:LEU:HD23	2:t:465:LEU:C	2.41	0.46
5:K:458:ARG:HD3	4:N:2010:DG:H4'	1.96	0.46
6:J:75:MET:HG2	2:L:66[A]:LYS:HE2	1.97	0.46
1:S:464:VAL:HG21	1:S:523:PHE:HA	1.97	0.46
3:U:593:GLU:OE1	3:U:593:GLU:HA	2.15	0.46
2:j:58[B]:MET:SD	2:j:127:ARG:HB3	2.56	0.46
3:D:493:PHE:HZ	3:D:531:LEU:HG	1.81	0.46
5:K:529:ARG:N	5:K:530:PRO:CD	2.79	0.46
2:L:54:ASN:HA	2:L:128:MET:CE	2.46	0.46
3:m:593:GLU:OE1	3:m:593:GLU:HA	2.15	0.46
2:r:75:MET:CG	2:t:66[A]:LYS:HE2	2.46	0.46
12:u:630:ARG:NH1	13:t:501[A]:JK8:N6	2.62	0.46
4:W:2011:DC:H2''	4:W:2012:DC:O5'	2.16	0.46
4:e:1:DG:H4'	4:e:2:DA:H5'	1.96	0.46
2:l:66[B]:LYS:N	2:l:66[B]:LYS:CD	2.68	0.46
12:u:529:ARG:N	12:u:530:PRO:CD	2.79	0.46
3:U:529:ARG:N	3:U:530:PRO:CD	2.79	0.46
1:b:460:LYS:HG2	4:e:8:DC:H1'	1.97	0.46
3:m:529:ARG:N	3:m:530:PRO:CD	2.79	0.46
4:n:2011:DC:H2'	4:n:2012:DC:C6	2.51	0.46
12:u:593:GLU:OE1	12:u:593:GLU:HA	2.16	0.46
2:L:113[B]:MET:HB2	2:L:113[B]:MET:HE3	1.62	0.45
9:d:529:ARG:N	9:d:530:PRO:CD	2.79	0.45
2:c:408:MET:HE1	2:c:419:GLU:HG2	1.97	0.45
2:t:192:ILE:HG21	2:t:477:ARG:HB2	1.97	0.45
2:A:438:ARG:O	2:A:438:ARG:NH1	2.48	0.45
2:C:54:ASN:HA	2:C:128:MET:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:113[B]:MET:SD	2:L:264:ILE:HD11	2.57	0.45
2:R:27:MET:HE2	2:R:27:MET:HB3	1.90	0.45
1:b:464:VAL:HG21	1:b:523:PHE:HA	1.99	0.45
11:k:464:VAL:HG21	11:k:523:PHE:HA	1.97	0.45
11:k:637:ALA:O	11:k:638:VAL:CB	2.63	0.45
1:s:515:HIS:HB2	2:r:25:TYR:CG	2.52	0.45
6:J:426:LEU:O	2:L:431:ARG:HB3	2.17	0.45
1:b:529:ARG:N	1:b:530:PRO:CD	2.79	0.45
2:j:391:ILE:HG21	2:l:399:ARG:HD3	1.98	0.45
2:t:54:ASN:HA	2:t:128:MET:CE	2.46	0.45
2:A:177:VAL:HG22	4:F:2016:DC:H4'	1.98	0.45
6:J:54:ASN:HA	6:J:128:MET:CE	2.46	0.45
6:J:75:MET:CG	2:L:66[A]:LYS:HE2	2.47	0.45
6:J:75:MET:SD	2:L:66[A]:LYS:HE2	2.56	0.45
2:j:54:ASN:HA	2:j:128:MET:CE	2.46	0.45
2:j:377:ARG:HG3	2:j:448:LEU:HD11	1.99	0.45
2:l:54:ASN:HA	2:l:128:MET:CE	2.45	0.45
3:D:529:ARG:N	3:D:530:PRO:CD	2.79	0.45
2:C:56:GLN:CB	2:C:58:MET:HE2	2.46	0.45
2:L:225:LEU:CD1	2:L:225:LEU:N	2.80	0.45
2:L:465:LEU:C	2:L:465:LEU:HD23	2.41	0.45
4:N:1[A]:DG:O5'	4:N:1[A]:DG:C8	2.43	0.45
1:S:529:ARG:N	1:S:530:PRO:CD	2.80	0.45
9:d:493:PHE:HZ	9:d:531:LEU:HG	1.82	0.45
11:k:529:ARG:N	11:k:530:PRO:CD	2.80	0.45
2:j:88[B]:GLU:OE1	2:j:88[B]:GLU:HA	2.16	0.45
2:l:225:LEU:N	2:l:225:LEU:CD1	2.80	0.45
3:D:602:ALA:HB1	2:C:10:ASN:HD21	1.81	0.45
2:a:208[B]:GLU:OE1	2:a:208[B]:GLU:C	2.58	0.45
2:a:377:ARG:HG3	2:a:448:LEU:HD11	1.98	0.45
2:A:54:ASN:HA	2:A:128:MET:CE	2.47	0.45
7:M:529:ARG:N	7:M:530:PRO:CD	2.79	0.45
7:M:593:GLU:HA	7:M:593:GLU:OE1	2.16	0.45
3:U:464:VAL:HG21	3:U:523:PHE:HA	1.99	0.45
7:M:515:HIS:HB2	2:L:25:TYR:CD1	2.52	0.45
2:l:408:MET:HE1	2:l:419:GLU:HG2	1.98	0.45
2:r:192:ILE:HG21	2:r:477:ARG:HB2	1.98	0.45
1:B:464:VAL:HG21	1:B:523:PHE:HA	1.98	0.45
3:D:508:ASP:OD1	3:D:583:LEU:HG	2.16	0.45
2:C:225:LEU:CD1	2:C:225:LEU:N	2.80	0.45
2:C:465:LEU:HD23	2:C:465:LEU:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:464:VAL:HG21	5:K:523:PHE:HA	1.98	0.45
7:M:493:PHE:HZ	7:M:531:LEU:HG	1.81	0.45
2:c:225:LEU:N	2:c:225:LEU:CD1	2.79	0.45
4:n:2:DA:C2	8:o:2019:DT:O2	2.69	0.45
1:s:529:ARG:N	1:s:530:PRO:CD	2.80	0.45
12:u:464:VAL:HG21	12:u:523:PHE:HA	1.99	0.45
13:U:701[A]:JK8:C22	13:U:701[A]:JK8:C5	2.95	0.45
2:r:75:MET:HG2	2:t:66[A]:LYS:CD	2.47	0.45
3:D:464:VAL:HG21	3:D:523:PHE:HA	1.99	0.44
2:C:173:SER:OG	4:F:5:DG:H5'	2.17	0.44
4:F:1:DG:N3	4:F:1:DG:O5'	2.48	0.44
4:n:2019[B]:DT:C2'	4:n:2020[B]:DT:C5'	2.77	0.44
2:A:69[B]:ARG:HG3	2:A:69[B]:ARG:NH1	2.07	0.44
2:R:408[A]:MET:CE	2:R:419:GLU:HG3	2.47	0.44
2:T:465:LEU:C	2:T:465:LEU:HD23	2.43	0.44
2:j:58[B]:MET:SD	2:j:127:ARG:CB	3.05	0.44
4:n:8:DC:C3'	4:n:2009:DG:OP1	2.66	0.44
13:s:701:JK8:O7	2:r:179:MET:HE1	2.17	0.44
2:r:54:ASN:HA	2:r:128:MET:CE	2.47	0.44
2:A:438:ARG:HH11	2:A:438:ARG:C	2.25	0.44
2:a:357[A]:GLU:OE1	2:a:357[A]:GLU:HA	2.18	0.44
1:s:464:VAL:HG21	1:s:523:PHE:HA	1.99	0.44
1:B:435:GLU:OE2	1:B:435:GLU:N	2.51	0.44
1:B:460:LYS:HG2	4:E:8:DC:H1'	1.99	0.44
2:A:413:GLN:HG2	2:c:324:GLN:HG2	2.00	0.44
7:M:464:VAL:HG21	7:M:523:PHE:HA	2.00	0.44
2:R:342:ARG:HG2	2:R:342:ARG:HH11	1.78	0.44
2:j:58[B]:MET:HE1	2:j:62:LYS:HB2	1.99	0.44
2:j:272[B]:ARG:CG	2:j:272[B]:ARG:NH1	2.50	0.44
2:L:56:GLN:CB	2:L:58:MET:HE2	2.45	0.44
2:c:54:ASN:HA	2:c:128:MET:CE	2.47	0.44
2:R:408[A]:MET:HE3	2:R:408[A]:MET:HB3	1.79	0.44
2:A:449:LEU:HD13	9:d:470:ASP:CB	2.48	0.44
6:J:404:ASP:CB	2:L:431:ARG:HH12	2.30	0.44
6:J:465[B]:LEU:C	6:J:465[B]:LEU:CD2	2.91	0.44
2:l:465:LEU:C	2:l:465:LEU:HD23	2.42	0.44
2:A:436:LEU:HD12	2:C:403:THR:HG22	2.00	0.44
2:R:429:ARG:NH2	2:T:429:ARG:NH2	2.66	0.44
2:c:465:LEU:HD23	2:c:465:LEU:C	2.42	0.44
2:j:408[B]:MET:HE1	2:j:419:GLU:HG3	2.00	0.44
1:s:458:ARG:HD2	4:v:2010:DG:H1'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:325:THR:HB	2:r:326:PRO:HD2	2.00	0.44
2:A:423:GLN:OE1	2:C:431:ARG:NH2	2.51	0.43
2:T:56:GLN:CB	2:T:58:MET:HE2	2.44	0.43
2:T:113[B]:MET:HE3	2:T:113[B]:MET:HB2	1.87	0.43
2:T:332:GLY:HA2	8:V:2019:DT:H4'	2.00	0.43
2:a:54:ASN:HA	2:a:128:MET:CE	2.48	0.43
2:r:309:ARG:HB3	2:r:309:ARG:NH1	2.33	0.43
2:A:204:ILE:HG13	2:A:208[A]:GLU:OE1	2.18	0.43
6:J:64:TYR:HB3	6:J:125:GLU:HB3	2.00	0.43
7:M:427[B]:GLU:CD	7:M:427[B]:GLU:H	2.25	0.43
2:T:54:ASN:HA	2:T:128:MET:CE	2.48	0.43
8:V:2011:DC:O2	4:W:2010:DG:N2	2.33	0.43
11:k:458:ARG:HD2	4:n:2010:DG:H1'	1.99	0.43
2:j:454[B]:GLU:OE1	2:j:454[B]:GLU:CA	2.62	0.43
2:r:408[A]:MET:HE3	2:r:408[A]:MET:HB3	1.95	0.43
4:w:1:DG:N3	4:w:1:DG:O5'	2.48	0.43
1:B:609:GLU:HG2	2:A:13:ASN:ND2	2.33	0.43
2:A:122:ARG:H	2:A:122:ARG:CD	2.21	0.43
1:S:517:ARG:NE	2:R:17:GLU:OE2	2.46	0.43
2:c:176:ALA:HB3	2:c:179:MET:O	2.19	0.43
2:l:179:MET:HE2	2:l:336:ILE:HD13	1.99	0.43
2:L:252:ARG:NH1	2:L:257:GLN:O	2.52	0.43
2:R:54:ASN:HA	2:R:128:MET:CE	2.48	0.43
2:C:231[A]:ARG:HE	2:C:231[A]:ARG:HB2	1.52	0.43
1:b:435[B]:GLU:OE2	1:b:435[B]:GLU:N	2.51	0.43
2:a:388:LEU:HD11	2:a:441:ILE:HD12	2.01	0.43
2:r:204:ILE:HG13	2:r:208[A]:GLU:OE1	2.19	0.43
12:u:493:PHE:HZ	12:u:531:LEU:HG	1.83	0.43
2:t:225:LEU:CD1	2:t:225:LEU:N	2.81	0.43
1:B:585:GLU:HG3	2:C:123:TYR:O	2.18	0.43
6:J:408[B]:MET:HE2	6:J:408[B]:MET:HB3	1.94	0.43
2:a:330:SER:CB	4:e:1:DG:O6	2.66	0.43
6:J:408[A]:MET:HE3	6:J:408[A]:MET:HB3	1.94	0.43
4:O:1:DG:N3	4:O:1:DG:O5'	2.48	0.43
1:S:458:ARG:HG2	8:V:2009:DG:H2''	1.99	0.43
2:R:252:ARG:HD3	2:R:257:GLN:O	2.18	0.43
2:r:357[A]:GLU:OE1	2:r:357[A]:GLU:HA	2.17	0.43
2:A:68:ALA:CB	2:C:75:MET:HE3	2.49	0.43
9:d:464:VAL:HG21	9:d:523:PHE:HA	2.00	0.43
2:t:325:THR:HB	2:t:326:PRO:HD2	2.01	0.43
2:A:64:TYR:HB3	2:A:125:GLU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:449:LEU:HD12	9:d:470:ASP:HB2	2.01	0.43
6:J:388:LEU:HD11	6:J:441:ILE:HD12	1.99	0.43
2:a:204:ILE:HG13	2:a:208[A]:GLU:OE1	2.18	0.43
2:l:330:SER:CB	4:n:2020[B]:DT:OP1	2.66	0.43
2:l:438:ARG:HH12	2:l:442:GLU:HB2	1.84	0.43
2:A:79:HIS:HE1	4:E:7:DA:OP1	2.02	0.43
2:L:325:THR:HB	2:L:326:PRO:HD2	2.00	0.43
2:L:408:MET:HE3	2:L:408:MET:HB3	1.95	0.43
1:S:435:GLU:OE2	1:S:435:GLU:N	2.51	0.43
2:R:204:ILE:HG13	2:R:208[A]:GLU:OE1	2.18	0.43
2:R:357[A]:GLU:HA	2:R:357[A]:GLU:OE1	2.18	0.43
1:b:438:SER:HB3	2:c:123:TYR:CD2	2.54	0.43
2:r:430:LEU:HB3	2:t:398:ILE:HD13	2.01	0.43
2:A:388:LEU:HD11	2:A:441:ILE:HD12	2.01	0.42
2:t:66[B]:LYS:N	2:t:66[B]:LYS:HD3	2.34	0.42
2:A:446:ASN:CG	9:d:469:LEU:HB3	2.44	0.42
2:T:225:LEU:N	2:T:225:LEU:CD1	2.82	0.42
4:E:1[A]:DG:H2''	4:E:2[A]:DA:C5'	2.27	0.42
2:T:408:MET:HE3	2:T:408:MET:HB3	1.91	0.42
2:j:204:ILE:HG13	2:j:208[A]:GLU:OE1	2.18	0.42
3:D:633:ILE:HG22	13:C:501[A]:JK8:C9	2.50	0.42
6:J:58[B]:MET:HE3	6:J:65[B]:LYS:CG	2.49	0.42
6:J:204:ILE:HG13	6:J:208[A]:GLU:OE1	2.18	0.42
2:R:342:ARG:HH11	2:R:342:ARG:HG3	1.81	0.42
2:c:408:MET:HE3	2:c:408:MET:HB3	1.96	0.42
2:r:426:LEU:HD22	2:t:431:ARG:HA	2.02	0.42
4:E:1[B]:DG:N3	4:E:1[B]:DG:O4'	2.52	0.42
2:R:391:ILE:O	2:R:395:ILE:HG12	2.20	0.42
2:j:357[A]:GLU:OE1	2:j:357[A]:GLU:HA	2.19	0.42
2:l:113[B]:MET:HE3	2:l:113[B]:MET:HB2	1.66	0.42
2:t:135:LEU:HD23	2:t:135:LEU:HA	1.92	0.42
2:t:405:LYS:O	2:t:409:GLU:HG3	2.20	0.42
2:A:176:ALA:HB3	2:A:179:MET:O	2.19	0.42
2:A:458:ILE:HG22	2:A:465:LEU:CD1	2.50	0.42
2:C:438:ARG:HH12	2:C:442:GLU:HB2	1.85	0.42
2:R:176:ALA:HB3	2:R:179:MET:O	2.19	0.42
2:a:465[B]:LEU:C	2:a:465[B]:LEU:HD23	2.45	0.42
2:j:75:MET:CG	2:l:66[A]:LYS:CE	2.98	0.42
1:B:511:VAL:HG21	2:A:28:SER:OG	2.19	0.42
2:A:79:HIS:HE2	4:E:7:DA:P	2.42	0.42
6:J:391:ILE:O	6:J:395:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:64:TYR:HB3	2:R:125:GLU:HB3	2.02	0.42
2:r:408[B]:MET:HE2	2:r:408[B]:MET:HB3	1.98	0.42
2:j:176:ALA:HB3	2:j:179:MET:O	2.20	0.42
2:t:176:ALA:HB3	2:t:179:MET:O	2.20	0.42
1:S:437:ASP:N	8:V:2010:DG:OP1	2.40	0.42
2:j:426:LEU:HB3	2:l:431:ARG:HB3	2.01	0.42
3:m:517:ARG:NE	2:l:17:GLU:OE2	2.53	0.42
2:A:325:THR:HB	2:A:326:PRO:HD2	2.02	0.41
2:A:391:ILE:O	2:A:395:ILE:HG12	2.20	0.41
2:a:433:LEU:N	2:a:433:LEU:HD12	2.35	0.41
2:c:113[B]:MET:SD	2:c:264:ILE:CD1	3.07	0.41
2:c:253:GLY:O	2:c:256:ARG:CG	2.68	0.41
12:u:518:THR:HB	2:t:18:MET:HE1	2.02	0.41
1:B:458[B]:ARG:NH2	4:E:10:DG:H2''	2.35	0.41
2:A:125:GLU:HG3	3:D:585:GLU:OE2	2.21	0.41
4:E:1[A]:DG:H2'	4:E:2[A]:DA:C5	2.56	0.41
2:T:272[B]:ARG:NH1	2:T:272[B]:ARG:HG2	2.34	0.41
3:D:427[B]:GLU:H	3:D:427[B]:GLU:CD	2.29	0.41
2:a:330:SER:HB3	4:e:1:DG:C5	2.54	0.41
2:a:427:ASP:OD1	2:c:431:ARG:NE	2.47	0.41
2:l:135:LEU:HD23	2:l:162:ALA:HA	2.02	0.41
2:t:342:ARG:HD3	13:t:501[A]:JK8:C16	2.50	0.41
2:A:458:ILE:HG22	2:A:465:LEU:HD11	2.02	0.41
2:T:325:THR:HB	2:T:326:PRO:HD2	2.02	0.41
9:d:629:ARG:CZ	4:e:17:DG:P	3.04	0.41
2:l:176:ALA:HB3	2:l:179:MET:O	2.20	0.41
2:r:175:ILE:HD12	4:v:5:DG:C2	2.55	0.41
4:E:1[A]:DG:H8	4:E:1[A]:DG:HO5'	0.46	0.41
2:R:109:ASN:HB2	3:U:442:SER:OG	2.19	0.41
13:b:701:JK8:CL	2:a:27:MET:HE1	2.58	0.41
2:a:176:ALA:HB3	2:a:179:MET:O	2.20	0.41
2:c:391:ILE:O	2:c:395:ILE:HG12	2.21	0.41
2:l:391:ILE:O	2:l:395:ILE:HG12	2.21	0.41
2:t:408:MET:HE3	2:t:408:MET:HB3	1.92	0.41
2:A:135:LEU:HD23	2:A:135:LEU:HA	1.92	0.41
3:D:528:MET:O	3:D:531:LEU:HB2	2.21	0.41
6:J:454[B]:GLU:OE1	6:J:454[B]:GLU:CA	2.65	0.41
4:N:1[A]:DG:H2''	4:N:2[A]:DA:H5'	2.02	0.41
2:a:325:THR:HB	2:a:326:PRO:HD2	2.01	0.41
13:d:701[A]:JK8:N6	13:d:701[A]:JK8:C26	2.84	0.41
2:j:433:LEU:HD12	2:j:433:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:528:MET:O	3:U:531:LEU:HB2	2.21	0.41
2:T:391:ILE:O	2:T:395:ILE:HG12	2.20	0.41
2:r:426:LEU:HB3	2:t:431:ARG:HB3	2.02	0.41
2:t:391:ILE:O	2:t:395:ILE:HG12	2.21	0.41
2:c:135:LEU:HD23	2:c:135:LEU:HA	1.91	0.41
1:s:438:SER:OG	2:t:123:TYR:CE2	2.58	0.41
2:A:377:ARG:CG	2:A:448:LEU:HD11	2.50	0.41
2:A:458:ILE:HG23	2:A:465:LEU:CD1	2.50	0.41
2:C:176:ALA:HB3	2:C:179:MET:O	2.21	0.41
2:C:391:ILE:O	2:C:395:ILE:HG12	2.20	0.41
2:L:391:ILE:O	2:L:395:ILE:HG12	2.20	0.41
2:T:33:ARG:CZ	4:W:7:DA:H4'	2.51	0.41
2:T:175:ILE:HB	4:W:5:DG:N2	2.35	0.41
2:T:176:ALA:HB3	2:T:179:MET:O	2.20	0.41
8:V:8:DC:C2'	8:V:2009:DG:H5'	2.48	0.41
2:a:64:TYR:HB3	2:a:125:GLU:HB3	2.03	0.41
9:d:528:MET:O	9:d:531:LEU:HB2	2.21	0.41
4:e:1:DG:H4'	4:e:2:DA:C5'	2.51	0.41
2:j:272[A]:ARG:HD3	4:n:3:DG:OP1	2.20	0.41
2:j:430:LEU:HD12	2:l:425:ILE:O	2.21	0.41
2:r:75:MET:HG2	2:t:66[A]:LYS:CE	2.50	0.41
2:r:232[A]:ARG:HB2	2:r:232[A]:ARG:NH2	2.36	0.41
12:u:427[B]:GLU:CD	12:u:427[B]:GLU:N	2.77	0.41
2:C:175:ILE:HG12	4:E:17:DG:C2	2.56	0.41
4:E:1[B]:DG:C3'	4:E:2[B]:DA:C5'	2.90	0.41
11:k:637:ALA:O	11:k:638:VAL:HB	2.21	0.41
2:r:64:TYR:HB3	2:r:125:GLU:HB3	2.02	0.41
2:A:408[B]:MET:HE1	2:A:419:GLU:HG2	2.03	0.40
2:L:176:ALA:HB3	2:L:179:MET:O	2.20	0.40
2:R:325:THR:HB	2:R:326:PRO:HD2	2.03	0.40
2:a:436:LEU:HD23	2:a:436:LEU:HA	1.94	0.40
2:c:323[A]:LYS:HB2	2:c:323[A]:LYS:HE3	1.89	0.40
2:C:135:LEU:HD23	2:C:162:ALA:HA	2.04	0.40
2:C:357:GLU:OE1	2:C:357:GLU:HA	2.21	0.40
5:K:637:ALA:O	5:K:638:VAL:CG2	2.69	0.40
6:J:176:ALA:HB3	6:J:179:MET:O	2.21	0.40
2:a:58[B]:MET:HG2	2:a:65[B]:LYS:CG	2.50	0.40
2:a:68:ALA:CB	2:c:75:MET:HE3	2.51	0.40
2:j:391:ILE:O	2:j:395:ILE:HG12	2.21	0.40
2:r:135:LEU:HD23	2:r:135:LEU:HA	1.91	0.40
2:C:325:THR:HB	2:C:326:PRO:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:512:ASP:OD2	2:T:33:ARG:NH2	2.35	0.40
2:c:135:LEU:HD23	2:c:162:ALA:HA	2.04	0.40
2:c:364:ARG:HB2	2:c:465:LEU:HD11	2.02	0.40
11:k:443:THR:HG22	11:k:454:ILE:CD1	2.52	0.40
13:k:701:JK8:CL	2:j:27:MET:SD	3.16	0.40
2:l:179:MET:HE1	13:l:501[A]:JK8:C24	2.51	0.40
2:l:325:THR:HB	2:l:326:PRO:HD2	2.03	0.40
2:l:408:MET:HE3	2:l:408:MET:HB3	1.93	0.40
1:B:508:ASP:OD1	1:B:583:LEU:HG	2.22	0.40
7:M:528:MET:O	7:M:531:LEU:HB2	2.21	0.40
2:L:342:ARG:HD3	13:L:501[A]:JK8:C15	2.51	0.40
4:N:2011:DC:H2'	4:N:2012:DC:C6	2.57	0.40
2:R:342:ARG:CG	2:R:342:ARG:NH1	2.75	0.40
2:c:179:MET:C	4:e:17:DG:H4'	2.47	0.40
11:k:541:GLN:OE1	11:k:604:LEU:CD1	2.63	0.40
3:m:528:MET:O	3:m:531:LEU:HB2	2.21	0.40
2:r:391:ILE:O	2:r:395:ILE:HG12	2.20	0.40
6:J:377:ARG:CG	6:J:448:LEU:HD11	2.52	0.40
7:M:609:GLU:HG3	2:L:13:ASN:HD22	1.85	0.40
2:R:251:GLU:O	2:R:251:GLU:OE2	2.40	0.40
2:T:408:MET:HE1	2:T:423:GLN:HG2	2.03	0.40
2:a:391:ILE:O	2:a:395:ILE:HG12	2.21	0.40
2:c:325:THR:HB	2:c:326:PRO:HD2	2.02	0.40
2:r:176:ALA:HB3	2:r:179:MET:O	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:489:GLN:NE2	2:R:251:GLU:OE2[2_546]	1.63	0.57
2:c:315:SER:OG	2:r:257:GLN:NE2[2_444]	2.03	0.17

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	B	186/186 (100%)	176 (95%)	10 (5%)	0	100	100
1	S	185/186 (100%)	177 (96%)	8 (4%)	0	100	100
1	b	186/186 (100%)	177 (95%)	9 (5%)	0	100	100
1	s	186/186 (100%)	177 (95%)	9 (5%)	0	100	100
2	A	488/490 (100%)	471 (96%)	16 (3%)	1 (0%)	43	71
2	C	488/490 (100%)	470 (96%)	17 (4%)	1 (0%)	43	71
2	L	485/490 (99%)	467 (96%)	17 (4%)	1 (0%)	43	71
2	R	491/490 (100%)	473 (96%)	17 (4%)	1 (0%)	43	71
2	T	487/490 (99%)	470 (96%)	16 (3%)	1 (0%)	43	71
2	a	491/490 (100%)	472 (96%)	18 (4%)	1 (0%)	43	71
2	c	488/490 (100%)	470 (96%)	17 (4%)	1 (0%)	43	71
2	j	493/490 (101%)	475 (96%)	17 (3%)	1 (0%)	43	71
2	l	485/490 (99%)	467 (96%)	17 (4%)	1 (0%)	43	71
2	r	497/490 (101%)	476 (96%)	19 (4%)	2 (0%)	30	59
2	t	489/490 (100%)	472 (96%)	16 (3%)	1 (0%)	43	71
3	D	188/188 (100%)	180 (96%)	8 (4%)	0	100	100
3	U	189/188 (100%)	180 (95%)	9 (5%)	0	100	100
3	m	187/188 (100%)	178 (95%)	9 (5%)	0	100	100
5	K	187/187 (100%)	176 (94%)	10 (5%)	1 (0%)	24	54
6	J	491/480 (102%)	472 (96%)	17 (4%)	2 (0%)	30	59
7	M	190/189 (100%)	182 (96%)	8 (4%)	0	100	100
9	d	179/181 (99%)	170 (95%)	9 (5%)	0	100	100
11	k	188/188 (100%)	177 (94%)	9 (5%)	2 (1%)	11	38
12	u	188/187 (100%)	180 (96%)	8 (4%)	0	100	100
All	All	8112/8110 (100%)	7785 (96%)	310 (4%)	17 (0%)	43	71

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	K	638	VAL
6	J	254	GLY
11	k	638	VAL

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Mol	Chain	Res	Type
2	r	11	GLU
11	k	417	LYS
2	A	33	ARG
2	C	33	ARG
6	J	33	ARG
2	L	33	ARG
2	R	33	ARG
2	T	33	ARG
2	a	33	ARG
2	c	33	ARG
2	j	33	ARG
2	l	33	ARG
2	r	33	ARG
2	t	33	ARG

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	B	147/155 (95%)	145 (99%)	2 (1%)	59	70
1	S	148/155 (96%)	142 (96%)	6 (4%)	27	52
1	b	145/155 (94%)	143 (99%)	2 (1%)	59	70
1	s	146/155 (94%)	144 (99%)	2 (1%)	59	70
2	A	405/423 (96%)	394 (97%)	11 (3%)	39	60
2	C	394/423 (93%)	389 (99%)	5 (1%)	61	71
2	L	397/423 (94%)	391 (98%)	6 (2%)	57	69
2	R	402/423 (95%)	390 (97%)	12 (3%)	36	59
2	T	397/423 (94%)	384 (97%)	13 (3%)	33	57
2	a	395/423 (93%)	388 (98%)	7 (2%)	51	67
2	c	394/423 (93%)	388 (98%)	6 (2%)	57	69
2	j	403/423 (95%)	392 (97%)	11 (3%)	39	60
2	l	397/423 (94%)	388 (98%)	9 (2%)	44	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	r	403/423 (95%)	392 (97%)	11 (3%)	39	60
2	t	398/423 (94%)	392 (98%)	6 (2%)	57	69
3	D	147/157 (94%)	140 (95%)	7 (5%)	23	50
3	U	149/157 (95%)	143 (96%)	6 (4%)	28	53
3	m	146/157 (93%)	139 (95%)	7 (5%)	23	50
5	K	147/156 (94%)	141 (96%)	6 (4%)	27	52
6	J	406/414 (98%)	399 (98%)	7 (2%)	53	67
7	M	149/158 (94%)	143 (96%)	6 (4%)	28	53
9	d	141/152 (93%)	134 (95%)	7 (5%)	22	49
11	k	148/156 (95%)	146 (99%)	2 (1%)	59	70
12	u	149/156 (96%)	145 (97%)	4 (3%)	39	60
All	All	6553/6936 (94%)	6392 (98%)	161 (2%)	43	62

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	435	GLU
1	B	438	SER
2	A	84	SER
2	A	122	ARG
2	A	252	ARG
2	A	311	ASP
2	A	357[A]	GLU
2	A	357[B]	GLU
2	A	364	ARG
2	A	440	LYS
2	A	464	VAL
2	A	465	LEU
2	A	468	LEU
3	D	418	LEU
3	D	461	ILE
3	D	477	GLU
3	D	541	GLN
3	D	583	LEU
3	D	604	LEU
3	D	616	GLN
2	C	225	LEU
2	C	231[A]	ARG

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Mol	Chain	Res	Type
2	C	231[B]	ARG
2	C	252	ARG
2	C	275	GLU
5	K	427	GLU
5	K	438	SER
5	K	477	GLU
5	K	583	LEU
5	K	585	GLU
5	K	638	VAL
6	J	27	MET
6	J	84	SER
6	J	252	ARG
6	J	309	ARG
6	J	310	LYS
6	J	364	ARG
6	J	402	ASP
7	M	418	LEU
7	M	438	SER
7	M	461	ILE
7	M	469	LEU
7	M	477	GLU
7	M	616	GLN
2	L	225	LEU
2	L	238	ARG
2	L	299	ARG
2	L	357	GLU
2	L	447[A]	GLU
2	L	447[B]	GLU
1	S	435	GLU
1	S	438	SER
1	S	461	ILE
1	S	477	GLU
1	S	508	ASP
1	S	638	VAL
2	R	11	GLU
2	R	27	MET
2	R	66	LYS
2	R	84	SER
2	R	122	ARG
2	R	309	ARG
2	R	342	ARG
2	R	364	ARG

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Mol	Chain	Res	Type
2	R	402	ASP
2	R	416	LYS
2	R	432	ARG
2	R	462	GLU
3	U	418	LEU
3	U	438	SER
3	U	461	ILE
3	U	477	GLU
3	U	585	GLU
3	U	616	GLN
2	T	66	LYS
2	T	231	ARG
2	T	232	ARG
2	T	252	ARG
2	T	323[A]	LYS
2	T	323[B]	LYS
2	T	344	LYS
2	T	357	GLU
2	T	402	ASP
2	T	416	LYS
2	T	447[A]	GLU
2	T	447[B]	GLU
2	T	488	ILE
1	b	461	ILE
1	b	492	ASP
2	a	27	MET
2	a	84	SER
2	a	238	ARG
2	a	252	ARG
2	a	309	ARG
2	a	364	ARG
2	a	408	MET
9	d	418	LEU
9	d	438	SER
9	d	461	ILE
9	d	477	GLU
9	d	492	ASP
9	d	616	GLN
9	d	630	ARG
2	c	238	ARG
2	c	252	ARG
2	c	256	ARG

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Mol	Chain	Res	Type
2	c	298[A]	LEU
2	c	298[B]	LEU
2	c	357	GLU
11	k	477	GLU
11	k	604	LEU
2	j	73	ASP
2	j	84	SER
2	j	122	ARG
2	j	179	MET
2	j	252	ARG
2	j	256	ARG
2	j	309	ARG
2	j	310	LYS
2	j	364	ARG
2	j	393	GLU
2	j	450	ASN
3	m	418	LEU
3	m	438	SER
3	m	461	ILE
3	m	477	GLU
3	m	492	ASP
3	m	585	GLU
3	m	616	GLN
2	l	65	LYS
2	l	238	ARG
2	l	256	ARG
2	l	323[A]	LYS
2	l	323[B]	LYS
2	l	357	GLU
2	l	436	LEU
2	l	447[A]	GLU
2	l	447[B]	GLU
1	s	477	GLU
1	s	585	GLU
2	r	84	SER
2	r	228	SER
2	r	232[A]	ARG
2	r	232[B]	ARG
2	r	252	ARG
2	r	256	ARG
2	r	309	ARG
2	r	364	ARG

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Mol	Chain	Res	Type
2	r	402	ASP
2	r	436	LEU
2	r	440	LYS
12	u	418	LEU
12	u	461	ILE
12	u	585	GLU
12	u	616	GLN
2	t	231[A]	ARG
2	t	231[B]	ARG
2	t	238	ARG
2	t	252	ARG
2	t	256	ARG
2	t	357	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	46	HIS
2	A	182	ASN
2	A	267	GLN
2	A	467	GLN
3	D	501	HIS
3	D	597	ASN
2	C	10	ASN
2	C	182	ASN
2	C	267	GLN
2	C	390	HIS
2	C	450	ASN
5	K	476	ASN
5	K	480	GLN
5	K	541	GLN
5	K	587	ASN
5	K	636	ASN
6	J	107	GLN
6	J	257	GLN
6	J	267	GLN
6	J	313	ASN
6	J	324	GLN
6	J	467	GLN
7	M	597	ASN
2	L	10	ASN
2	L	257	GLN

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Mol	Chain	Res	Type
2	L	267	GLN
2	L	324	GLN
2	L	390	HIS
2	L	450	ASN
1	S	541	GLN
2	R	267	GLN
2	R	324	GLN
2	R	467	GLN
3	U	597	ASN
2	T	10	ASN
2	T	182	ASN
2	T	257	GLN
2	T	267	GLN
2	T	390	HIS
2	T	423	GLN
2	T	450	ASN
2	T	467	GLN
1	b	541	GLN
2	a	267	GLN
9	d	597	ASN
2	c	182	ASN
2	c	267	GLN
2	c	390	HIS
2	j	56	GLN
2	j	257	GLN
2	j	267	GLN
2	j	313	ASN
2	j	450	ASN
2	j	467	GLN
3	m	597	ASN
2	l	10	ASN
2	l	267	GLN
2	l	390	HIS
2	l	450	ASN
2	l	467	GLN
2	r	107	GLN
2	r	267	GLN
2	r	324	GLN
2	r	467	GLN
12	u	597	ASN
2	t	10	ASN
2	t	182	ASN

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Mol	Chain	Res	Type
2	t	257	GLN
2	t	267	GLN
2	t	390	HIS
2	t	450	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
13	JK8	b	701	-	29,29,29	1.36	5 (17%)	38,40,40	3.27	18 (47%)
13	JK8	J	501	-	29,29,29	1.39	4 (13%)	38,40,40	2.78	17 (44%)
13	JK8	L	501[A]	-	29,29,29	1.28	4 (13%)	38,40,40	2.42	12 (31%)
13	JK8	A	501	-	29,29,29	1.21	4 (13%)	38,40,40	1.70	6 (15%)
13	JK8	d	701[A]	-	29,29,29	1.23	4 (13%)	38,40,40	2.05	8 (21%)
13	JK8	s	701	-	29,29,29	1.53	4 (13%)	38,40,40	3.09	18 (47%)
13	JK8	k	701	-	29,29,29	1.42	5 (17%)	38,40,40	1.62	8 (21%)
13	JK8	t	501[A]	-	29,29,29	1.48	3 (10%)	38,40,40	2.28	13 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	JK8	C	501[A]	-	29,29,29	1.26	4 (13%)	38,40,40	2.14	13 (34%)
13	JK8	U	701[A]	-	29,29,29	1.23	4 (13%)	38,40,40	2.18	8 (21%)
13	JK8	l	501[A]	-	29,29,29	1.51	5 (17%)	38,40,40	1.66	12 (31%)
13	JK8	R	501	-	29,29,29	1.21	3 (10%)	38,40,40	2.01	11 (28%)

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
13	JK8	b	701	-	-	1/14/14/14	0/4/4/4
13	JK8	J	501	-	-	5/14/14/14	0/4/4/4
13	JK8	L	501[A]	-	-	4/14/14/14	0/4/4/4
13	JK8	A	501	-	-	3/14/14/14	0/4/4/4
13	JK8	d	701[A]	-	-	5/14/14/14	0/4/4/4
13	JK8	s	701	-	-	3/14/14/14	0/4/4/4
13	JK8	k	701	-	-	2/14/14/14	0/4/4/4
13	JK8	t	501[A]	-	-	3/14/14/14	0/4/4/4
13	JK8	C	501[A]	-	-	5/14/14/14	0/4/4/4
13	JK8	U	701[A]	-	-	3/14/14/14	0/4/4/4
13	JK8	l	501[A]	-	-	3/14/14/14	0/4/4/4
13	JK8	R	501	-	-	4/14/14/14	0/4/4/4

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	s	701	JK8	C14-C11	-4.31	1.41	1.49
13	t	501[A]	JK8	C14-C11	-4.24	1.41	1.49
13	b	701	JK8	O7-N6	-4.09	1.39	1.43
13	C	501[A]	JK8	O7-N6	-3.86	1.39	1.43
13	t	501[A]	JK8	O7-N6	-3.82	1.39	1.43
13	L	501[A]	JK8	O7-N6	-3.61	1.39	1.43
13	J	501	JK8	C21-C3	3.52	1.57	1.51
13	l	501[A]	JK8	C14-C11	-3.50	1.43	1.49
13	d	701[A]	JK8	O7-N6	-3.46	1.39	1.43
13	J	501	JK8	O7-N6	-3.40	1.39	1.43
13	U	701[A]	JK8	O7-N6	-3.35	1.40	1.43
13	l	501[A]	JK8	C13-C5	-3.28	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	701	JK8	C14-C11	-3.21	1.43	1.49
13	s	701	JK8	C13-C5	-3.15	1.40	1.48
13	R	501	JK8	O7-N6	-3.11	1.40	1.43
13	l	501[A]	JK8	O7-N6	-3.10	1.40	1.43
13	U	701[A]	JK8	C14-C11	-3.00	1.44	1.49
13	k	701	JK8	C13-C5	-2.97	1.41	1.48
13	C	501[A]	JK8	C5-N6	2.94	1.36	1.29
13	k	701	JK8	C14-C11	-2.92	1.44	1.49
13	k	701	JK8	O4-C3	-2.92	1.42	1.46
13	A	501	JK8	O7-N6	-2.92	1.40	1.43
13	L	501[A]	JK8	C14-C11	-2.88	1.44	1.49
13	R	501	JK8	C13-C5	-2.87	1.41	1.48
13	s	701	JK8	C5-N6	2.79	1.35	1.29
13	d	701[A]	JK8	C14-C11	-2.74	1.44	1.49
13	s	701	JK8	O7-N6	-2.73	1.40	1.43
13	k	701	JK8	C5-N6	2.70	1.35	1.29
13	A	501	JK8	C5-N6	2.69	1.35	1.29
13	A	501	JK8	C14-C11	-2.62	1.44	1.49
13	R	501	JK8	C5-N6	2.60	1.35	1.29
13	l	501[A]	JK8	C5-N6	2.56	1.35	1.29
13	L	501[A]	JK8	C13-C5	-2.56	1.42	1.48
13	k	701	JK8	O7-N6	-2.52	1.40	1.43
13	d	701[A]	JK8	C13-C5	-2.51	1.42	1.48
13	C	501[A]	JK8	C13-C5	-2.46	1.42	1.48
13	A	501	JK8	C13-C5	-2.46	1.42	1.48
13	t	501[A]	JK8	C13-C5	-2.38	1.42	1.48
13	J	501	JK8	C5-N6	2.37	1.34	1.29
13	J	501	JK8	C13-C5	-2.37	1.42	1.48
13	U	701[A]	JK8	C13-C5	-2.35	1.42	1.48
13	L	501[A]	JK8	C5-N6	2.25	1.34	1.29
13	d	701[A]	JK8	C5-N6	2.23	1.34	1.29
13	l	501[A]	JK8	C12-C13	-2.20	1.36	1.39
13	b	701	JK8	C5-N6	2.15	1.34	1.29
13	C	501[A]	JK8	C19-CL	-2.13	1.68	1.73
13	b	701	JK8	C13-C5	-2.12	1.43	1.48
13	U	701[A]	JK8	C5-N6	2.02	1.33	1.29
13	b	701	JK8	C14-C19	-2.01	1.36	1.39

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	s	701	JK8	O4-C3-C2	9.48	118.11	106.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	701	JK8	O4-C5-C13	8.23	133.41	118.20
13	b	701	JK8	C3-O4-C5	-7.47	105.45	116.64
13	J	501	JK8	O4-C5-C13	7.29	131.67	118.20
13	b	701	JK8	C10-C11-C14	-7.00	109.31	120.91
13	d	701[A]	JK8	O4-C3-C2	6.64	114.50	106.02
13	L	501[A]	JK8	O4-C5-C13	6.45	130.12	118.20
13	J	501	JK8	O4-C3-C21	6.30	119.55	109.71
13	t	501[A]	JK8	O4-C5-C13	6.21	129.69	118.20
13	A	501	JK8	O4-C3-C21	6.14	119.31	109.71
13	s	701	JK8	C3-O4-C5	-5.97	107.70	116.64
13	U	701[A]	JK8	O4-C5-C13	5.95	129.19	118.20
13	s	701	JK8	O7-N6-C5	5.80	108.73	104.57
13	b	701	JK8	C14-C19-CL	-5.64	112.93	120.67
13	L	501[A]	JK8	O4-C3-C21	5.61	118.47	109.71
13	b	701	JK8	C12-C13-C5	5.59	139.63	129.44
13	J	501	JK8	C2-C3-C21	5.57	120.21	111.36
13	d	701[A]	JK8	O4-C5-C13	5.52	128.41	118.20
13	J	501	JK8	O7-N6-C5	5.47	108.48	104.57
13	b	701	JK8	C11-C14-C19	-5.30	115.04	123.48
13	U	701[A]	JK8	O4-C3-C21	5.23	117.87	109.71
13	s	701	JK8	C14-C19-CL	-5.19	113.55	120.67
13	R	501	JK8	O7-N6-C5	5.19	108.28	104.57
13	U	701[A]	JK8	C8-O7-N6	5.15	110.11	107.48
13	L	501[A]	JK8	O7-N6-C5	4.91	108.09	104.57
13	R	501	JK8	O4-C5-C13	4.62	126.75	118.20
13	s	701	JK8	C11-C14-C19	-4.62	116.13	123.48
13	t	501[A]	JK8	O4-C3-C2	4.62	111.91	106.02
13	U	701[A]	JK8	C12-C13-C5	4.58	137.80	129.44
13	L	501[A]	JK8	C12-C13-C5	4.55	137.74	129.44
13	C	501[A]	JK8	C15-C14-C19	-4.51	112.52	117.60
13	s	701	JK8	O4-C5-C13	4.41	126.36	118.20
13	t	501[A]	JK8	C8-O7-N6	4.38	109.72	107.48
13	t	501[A]	JK8	C12-C13-C5	4.31	137.30	129.44
13	C	501[A]	JK8	O4-C3-C21	4.31	116.44	109.71
13	s	701	JK8	C8-O7-N6	-4.23	105.31	107.48
13	C	501[A]	JK8	C11-C14-C19	4.14	130.07	123.48
13	C	501[A]	JK8	C12-C13-C5	4.12	136.95	129.44
13	d	701[A]	JK8	C12-C13-C5	4.10	136.92	129.44
13	L	501[A]	JK8	O7-C8-C9	-4.09	121.84	125.99
13	R	501	JK8	O4-C3-C21	3.96	115.89	109.71
13	s	701	JK8	C10-C11-C12	3.90	123.60	118.23
13	b	701	JK8	C12-C11-C14	3.88	127.11	120.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J	501	JK8	C10-C9-C8	-3.87	112.73	120.06
13	b	701	JK8	C10-C11-C12	3.84	123.51	118.23
13	J	501	JK8	C12-C13-C5	3.81	136.38	129.44
13	b	701	JK8	O7-C8-C9	-3.80	122.13	125.99
13	C	501[A]	JK8	C18-C19-CL	-3.69	111.16	118.42
13	k	701	JK8	C12-C13-C8	3.65	122.86	119.28
13	C	501[A]	JK8	C18-C19-C14	3.65	125.65	121.36
13	s	701	JK8	C10-C9-C8	-3.65	113.14	120.06
13	b	701	JK8	C10-C9-C8	-3.64	113.17	120.06
13	L	501[A]	JK8	C10-C9-C8	-3.63	113.18	120.06
13	L	501[A]	JK8	C10-C11-C12	3.62	123.21	118.23
13	l	501[A]	JK8	C10-C11-C12	3.62	123.21	118.23
13	U	701[A]	JK8	O4-C3-C2	3.58	110.59	106.02
13	s	701	JK8	C13-C12-C11	-3.58	114.17	120.82
13	A	501	JK8	C12-C13-C5	3.56	135.94	129.44
13	A	501	JK8	C8-O7-N6	3.41	109.22	107.48
13	J	501	JK8	C3-O4-C5	-3.40	111.55	116.64
13	s	701	JK8	C18-C19-CL	3.35	125.03	118.42
13	d	701[A]	JK8	C10-C9-C8	-3.34	113.74	120.06
13	t	501[A]	JK8	C10-C11-C12	3.32	122.80	118.23
13	t	501[A]	JK8	O4-C3-C21	3.32	114.90	109.71
13	J	501	JK8	C26-C21-C22	-3.32	114.19	118.30
13	b	701	JK8	C15-C14-C11	3.32	125.29	118.70
13	R	501	JK8	C10-C9-C8	-3.29	113.83	120.06
13	R	501	JK8	C12-C13-C5	3.27	135.40	129.44
13	J	501	JK8	C9-C8-C13	3.26	127.34	123.58
13	J	501	JK8	C10-C11-C12	3.25	122.71	118.23
13	d	701[A]	JK8	O7-N6-C5	3.24	106.89	104.57
13	C	501[A]	JK8	C8-C13-C5	-3.21	101.35	105.47
13	b	701	JK8	O4-C3-C2	3.20	110.11	106.02
13	k	701	JK8	C12-C13-C5	3.20	135.28	129.44
13	t	501[A]	JK8	C11-C14-C19	-3.19	118.41	123.48
13	t	501[A]	JK8	C15-C14-C19	3.17	121.18	117.60
13	J	501	JK8	C25-C26-C21	3.15	124.41	120.65
13	s	701	JK8	C15-C14-C19	3.13	121.13	117.60
13	b	701	JK8	C9-C8-C13	3.12	127.18	123.58
13	U	701[A]	JK8	C10-C11-C12	3.11	122.51	118.23
13	k	701	JK8	C13-C12-C11	-3.11	115.04	120.82
13	l	501[A]	JK8	C13-C12-C11	-3.09	115.08	120.82
13	l	501[A]	JK8	C10-C9-C8	-3.06	114.27	120.06
13	A	501	JK8	C3-O4-C5	3.06	121.22	116.64
13	L	501[A]	JK8	C10-C11-C14	-3.05	115.86	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J	501	JK8	O7-C8-C9	-3.04	122.91	125.99
13	l	501[A]	JK8	O4-C3-C2	3.03	109.89	106.02
13	t	501[A]	JK8	C12-C11-C14	-3.02	115.54	120.61
13	t	501[A]	JK8	C10-C9-C8	-2.99	114.39	120.06
13	b	701	JK8	C18-C19-CL	2.98	124.29	118.42
13	J	501	JK8	C12-C11-C14	-2.98	115.61	120.61
13	b	701	JK8	C8-O7-N6	2.97	109.00	107.48
13	s	701	JK8	C10-C11-C14	-2.91	116.09	120.91
13	C	501[A]	JK8	C9-C10-C11	2.89	124.83	121.12
13	L	501[A]	JK8	C9-C8-C13	2.87	126.88	123.58
13	L	501[A]	JK8	C13-C12-C11	-2.84	115.54	120.82
13	k	701	JK8	C10-C9-C8	-2.84	114.69	120.06
13	k	701	JK8	O4-C3-C2	-2.83	102.41	106.02
13	k	701	JK8	C8-C13-C5	-2.81	101.86	105.47
13	A	501	JK8	O4-C3-C2	2.79	109.58	106.02
13	J	501	JK8	C13-C5-N6	-2.79	108.81	115.80
13	U	701[A]	JK8	C2-C3-C21	-2.77	106.96	111.36
13	R	501	JK8	C3-O4-C5	-2.75	112.52	116.64
13	b	701	JK8	C13-C12-C11	-2.74	115.73	120.82
13	l	501[A]	JK8	C8-O7-N6	2.70	108.86	107.48
13	d	701[A]	JK8	C3-O4-C5	-2.70	112.60	116.64
13	b	701	JK8	C8-C13-C5	-2.60	102.12	105.47
13	l	501[A]	JK8	C12-C13-C5	2.60	134.18	129.44
13	U	701[A]	JK8	C10-C9-C8	-2.59	115.16	120.06
13	s	701	JK8	C12-C13-C5	2.58	134.15	129.44
13	k	701	JK8	O4-C3-C21	2.58	113.74	109.71
13	l	501[A]	JK8	O4-C3-C21	2.57	113.73	109.71
13	t	501[A]	JK8	C9-C8-C13	2.54	126.51	123.58
13	C	501[A]	JK8	C8-O7-N6	2.50	108.76	107.48
13	k	701	JK8	C10-C11-C12	2.49	121.65	118.23
13	s	701	JK8	C12-C13-C8	2.47	121.70	119.28
13	R	501	JK8	C8-O7-N6	-2.47	106.21	107.48
13	R	501	JK8	C13-C12-C11	-2.43	116.31	120.82
13	C	501[A]	JK8	C12-C13-C8	2.42	121.66	119.28
13	s	701	JK8	C13-C5-N6	-2.40	109.79	115.80
13	J	501	JK8	C13-C12-C11	-2.38	116.39	120.82
13	s	701	JK8	O7-C8-C9	-2.38	123.58	125.99
13	l	501[A]	JK8	O4-C5-C13	2.30	122.44	118.20
13	b	701	JK8	O4-C3-C21	2.28	113.27	109.71
13	R	501	JK8	O4-C3-C2	2.25	108.90	106.02
13	C	501[A]	JK8	C10-C9-C8	-2.25	115.80	120.06
13	L	501[A]	JK8	C13-C5-N6	-2.22	110.24	115.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	501[A]	JK8	C16-C17-C18	-2.20	117.52	120.24
13	J	501	JK8	O4-C3-C2	2.20	108.83	106.02
13	R	501	JK8	C13-C5-N6	-2.19	110.33	115.80
13	R	501	JK8	C9-C10-C11	2.17	123.91	121.12
13	t	501[A]	JK8	O7-N6-C5	2.17	106.12	104.57
13	t	501[A]	JK8	C13-C5-N6	-2.17	110.37	115.80
13	d	701[A]	JK8	C10-C11-C12	2.13	121.16	118.23
13	l	501[A]	JK8	C15-C14-C11	-2.11	114.50	118.70
13	L	501[A]	JK8	O4-C3-C2	2.11	108.72	106.02
13	l	501[A]	JK8	C12-C11-C14	-2.11	117.07	120.61
13	A	501	JK8	C10-C9-C8	-2.09	116.11	120.06
13	C	501[A]	JK8	O4-C5-C13	2.08	122.04	118.20
13	l	501[A]	JK8	C3-O4-C5	-2.07	113.54	116.64
13	d	701[A]	JK8	C13-C12-C11	-2.04	117.03	120.82
13	s	701	JK8	C15-C14-C11	2.02	122.72	118.70
13	J	501	JK8	C24-C23-C22	2.01	122.71	120.24
13	l	501[A]	JK8	C12-C13-C8	2.00	121.24	119.28

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	501	JK8	N1-C2-C3-C21
13	A	501	JK8	N1-C2-C3-O4
13	A	501	JK8	C21-C3-O4-C5
13	C	501[A]	JK8	C22-C21-C3-C2
13	C	501[A]	JK8	C26-C21-C3-C2
13	C	501[A]	JK8	N1-C2-C3-C21
13	J	501	JK8	C22-C21-C3-C2
13	J	501	JK8	C26-C21-C3-C2
13	J	501	JK8	N1-C2-C3-C21
13	J	501	JK8	N1-C2-C3-O4
13	R	501	JK8	C10-C11-C14-C19
13	R	501	JK8	C12-C11-C14-C19
13	U	701[A]	JK8	C21-C3-O4-C5
13	d	701[A]	JK8	N1-C2-C3-C21
13	d	701[A]	JK8	N1-C2-C3-O4
13	k	701	JK8	N1-C2-C3-C21
13	k	701	JK8	N1-C2-C3-O4
13	l	501[A]	JK8	N1-C2-C3-C21
13	l	501[A]	JK8	N1-C2-C3-O4
13	t	501[A]	JK8	N1-C2-C3-C21

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Mol	Chain	Res	Type	Atoms
13	t	501[A]	JK8	N1-C2-C3-O4
13	U	701[A]	JK8	N1-C2-C3-C21
13	s	701	JK8	N1-C2-C3-C21
13	s	701	JK8	C22-C21-C3-C2
13	s	701	JK8	C26-C21-C3-C2
13	J	501	JK8	C21-C3-O4-C5
13	d	701[A]	JK8	C22-C21-C3-O4
13	L	501[A]	JK8	C22-C21-C3-O4
13	d	701[A]	JK8	C26-C21-C3-O4
13	L	501[A]	JK8	N1-C2-C3-C21
13	b	701	JK8	N1-C2-C3-C21
13	C	501[A]	JK8	C2-C3-O4-C5
13	R	501	JK8	C12-C11-C14-C15
13	l	501[A]	JK8	C21-C3-O4-C5
13	t	501[A]	JK8	C21-C3-O4-C5
13	R	501	JK8	C10-C11-C14-C15
13	L	501[A]	JK8	N1-C2-C3-O4
13	U	701[A]	JK8	N1-C2-C3-O4
13	L	501[A]	JK8	C26-C21-C3-O4
13	C	501[A]	JK8	C26-C21-C3-O4
13	d	701[A]	JK8	C22-C21-C3-C2

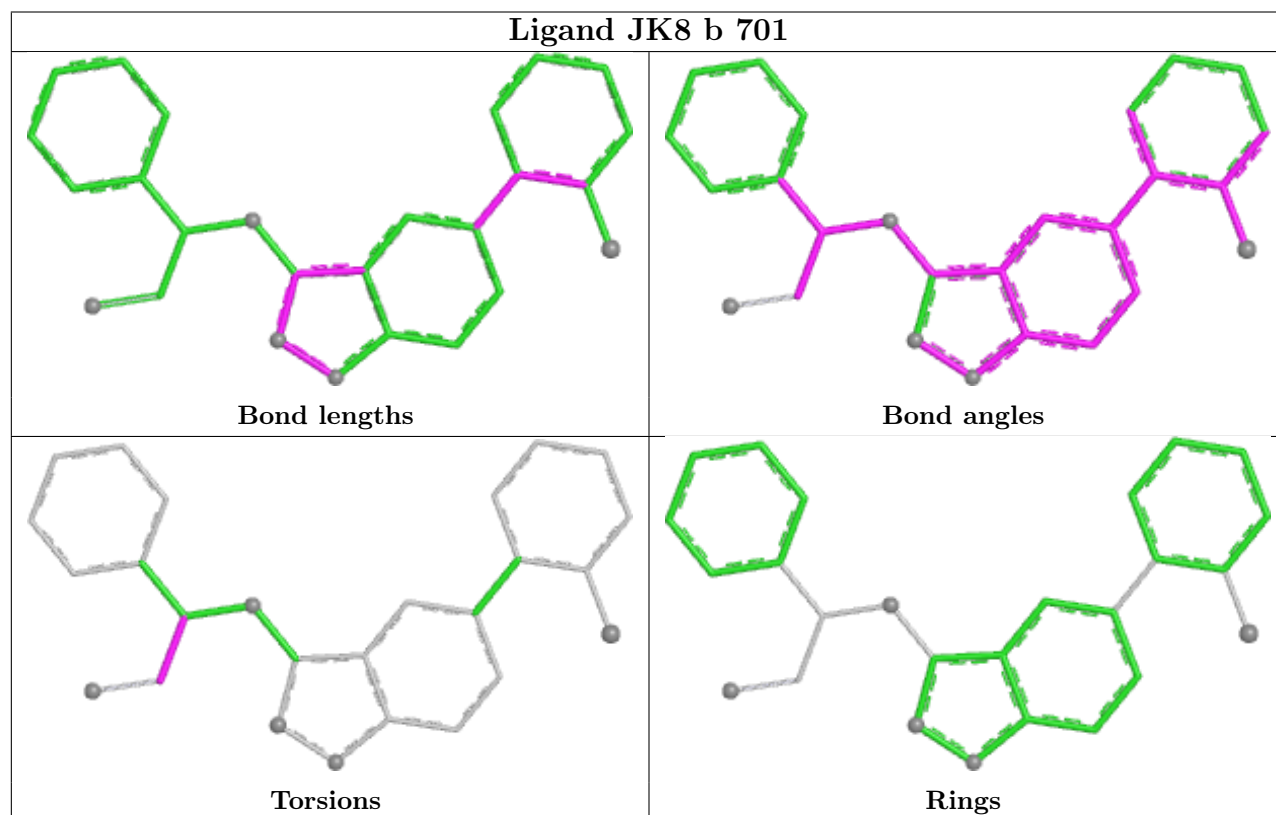
There are no ring outliers.

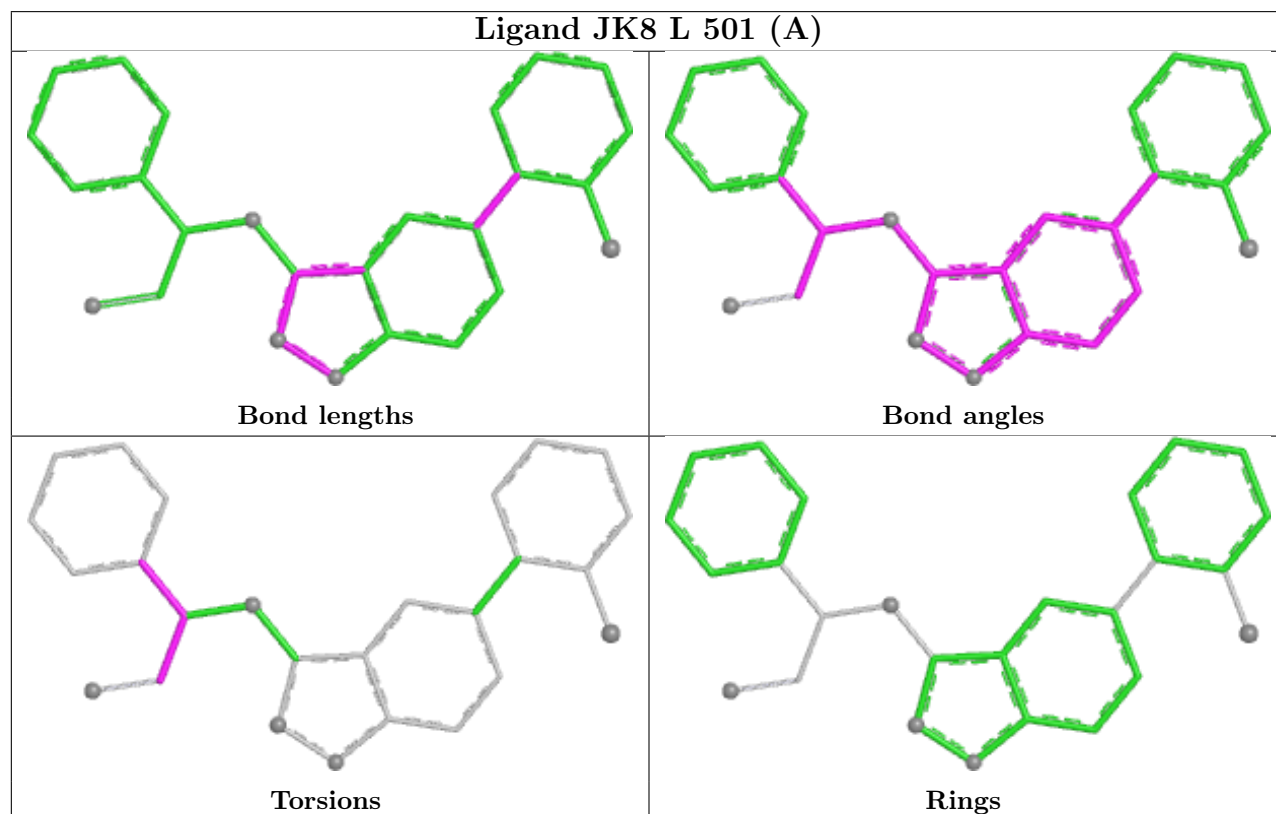
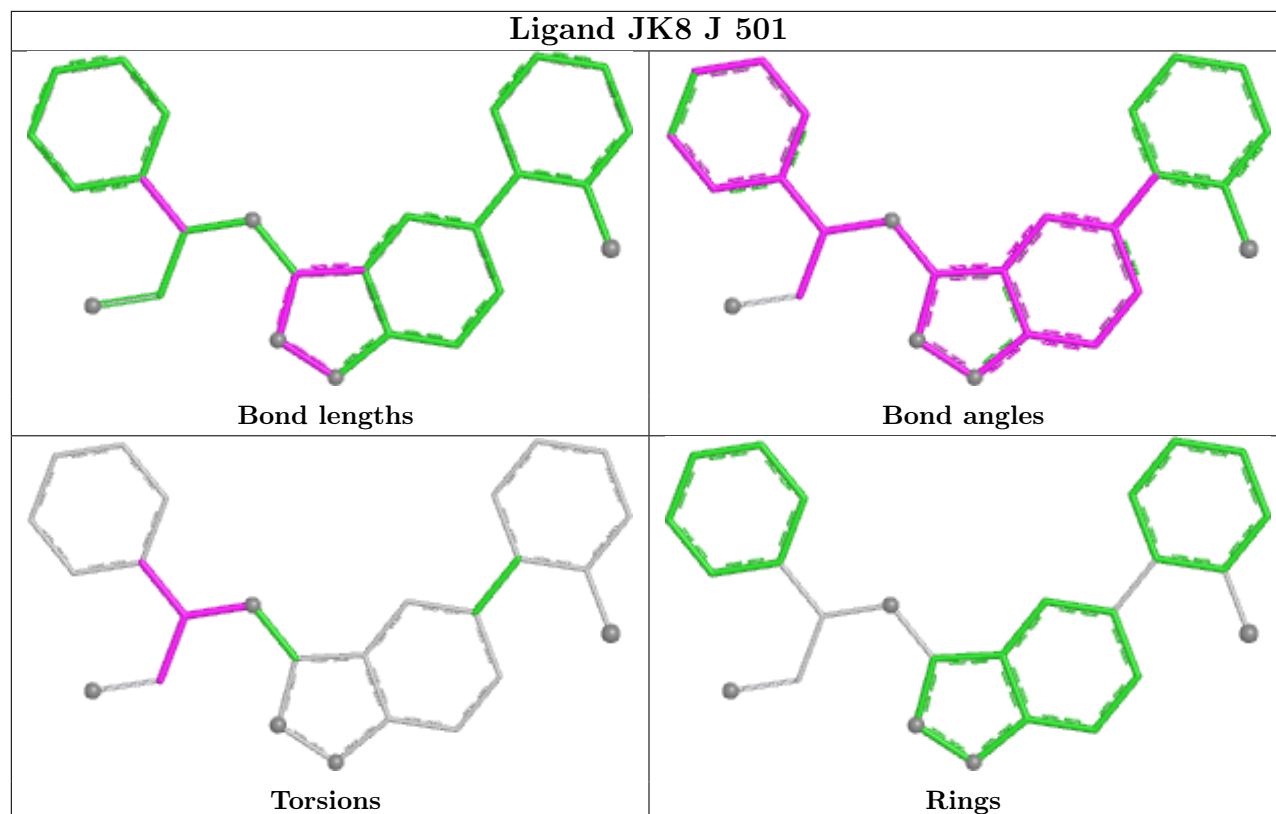
11 monomers are involved in 27 short contacts:

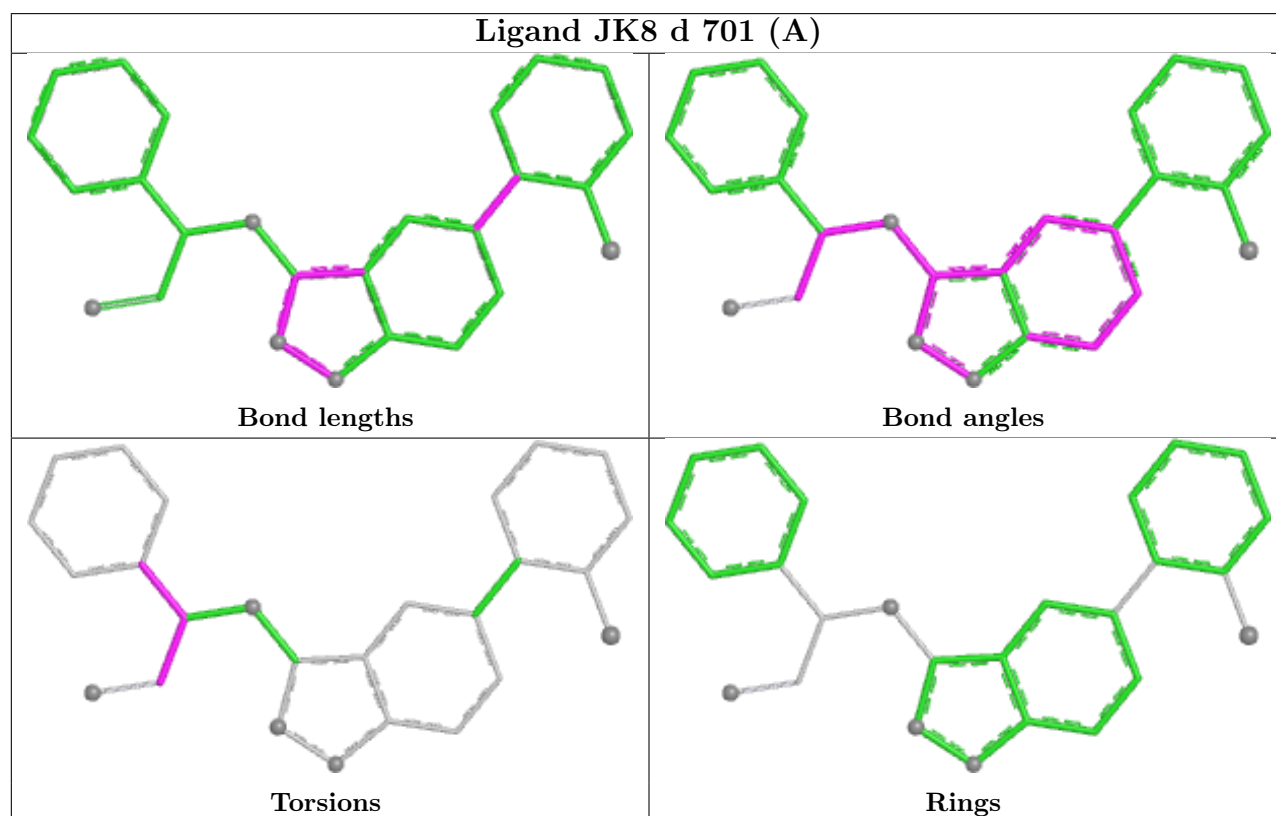
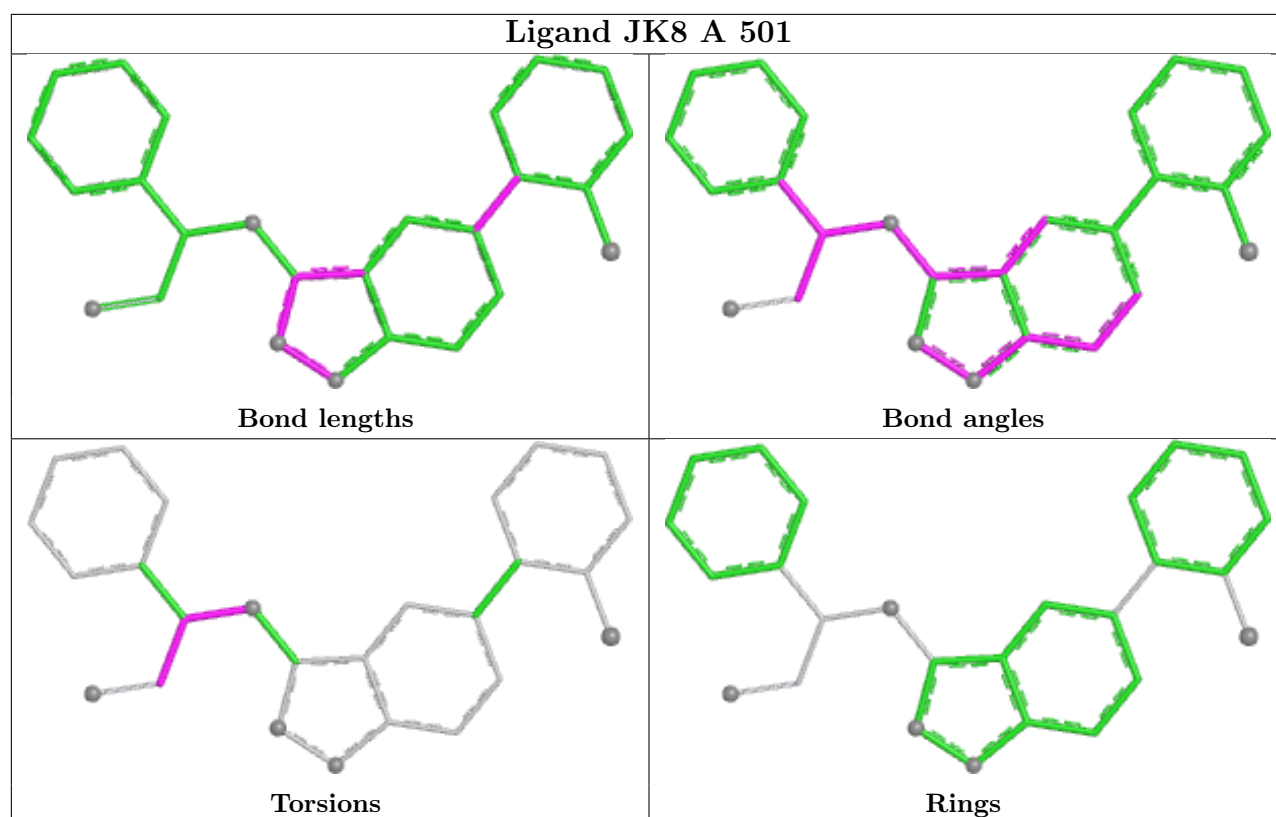
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	b	701	JK8	1	0
13	J	501	JK8	4	0
13	L	501[A]	JK8	2	0
13	d	701[A]	JK8	2	0
13	s	701	JK8	1	0
13	k	701	JK8	2	0
13	t	501[A]	JK8	5	0
13	C	501[A]	JK8	2	0
13	U	701[A]	JK8	3	0
13	l	501[A]	JK8	2	0
13	R	501	JK8	3	0

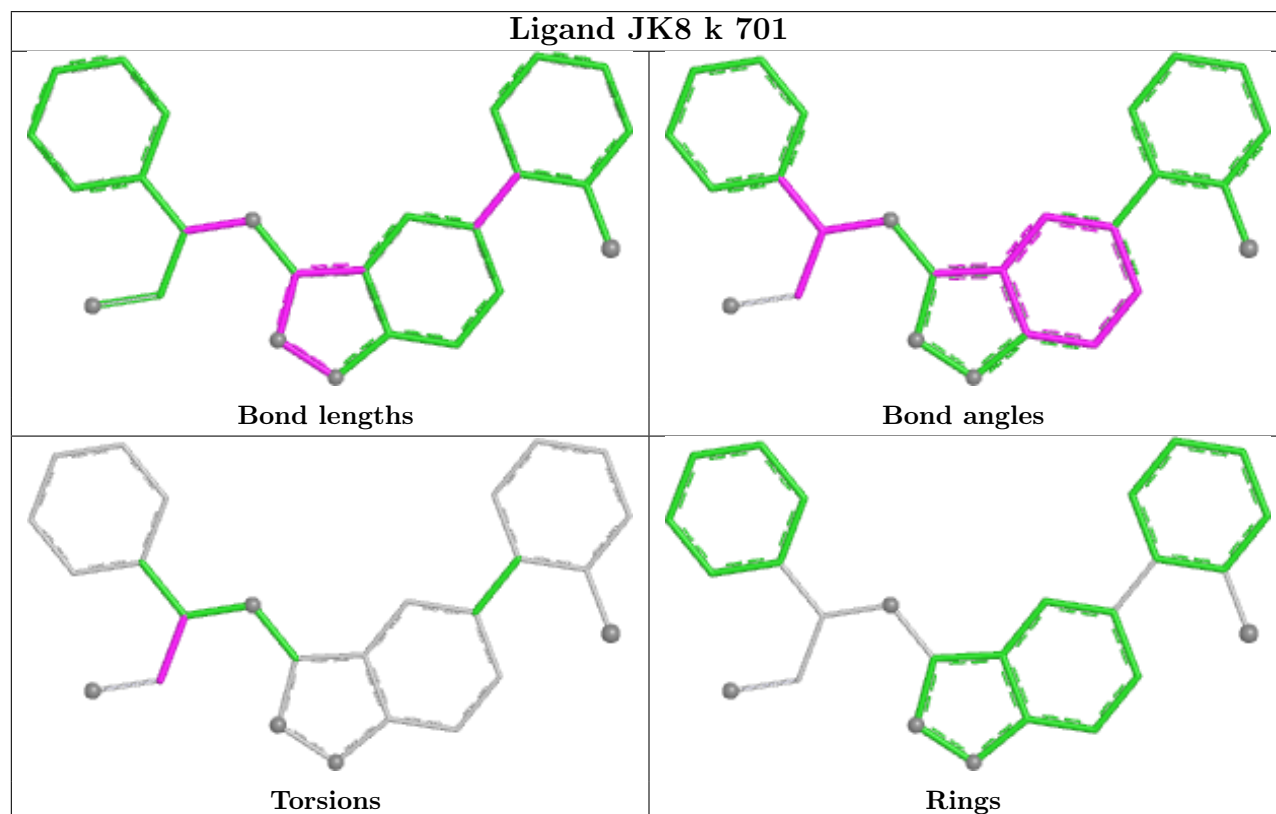
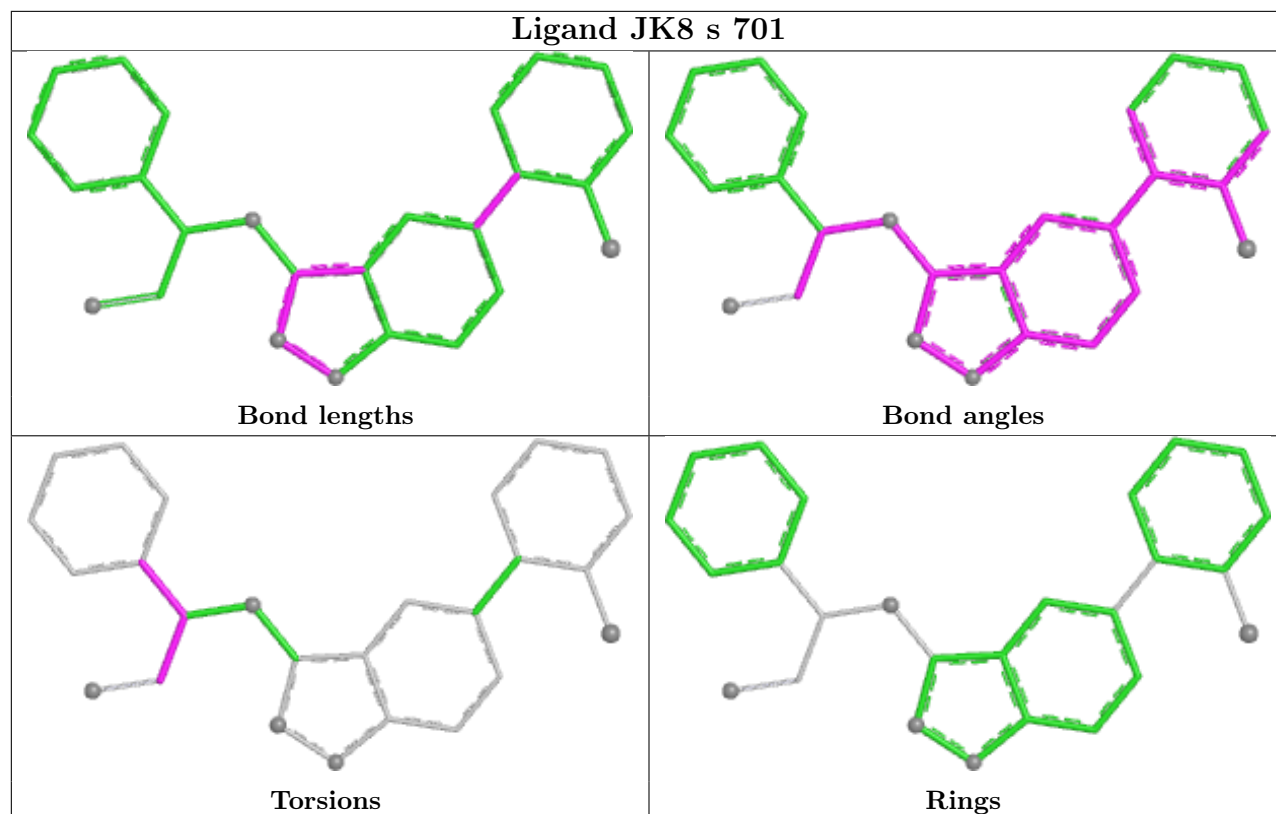
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

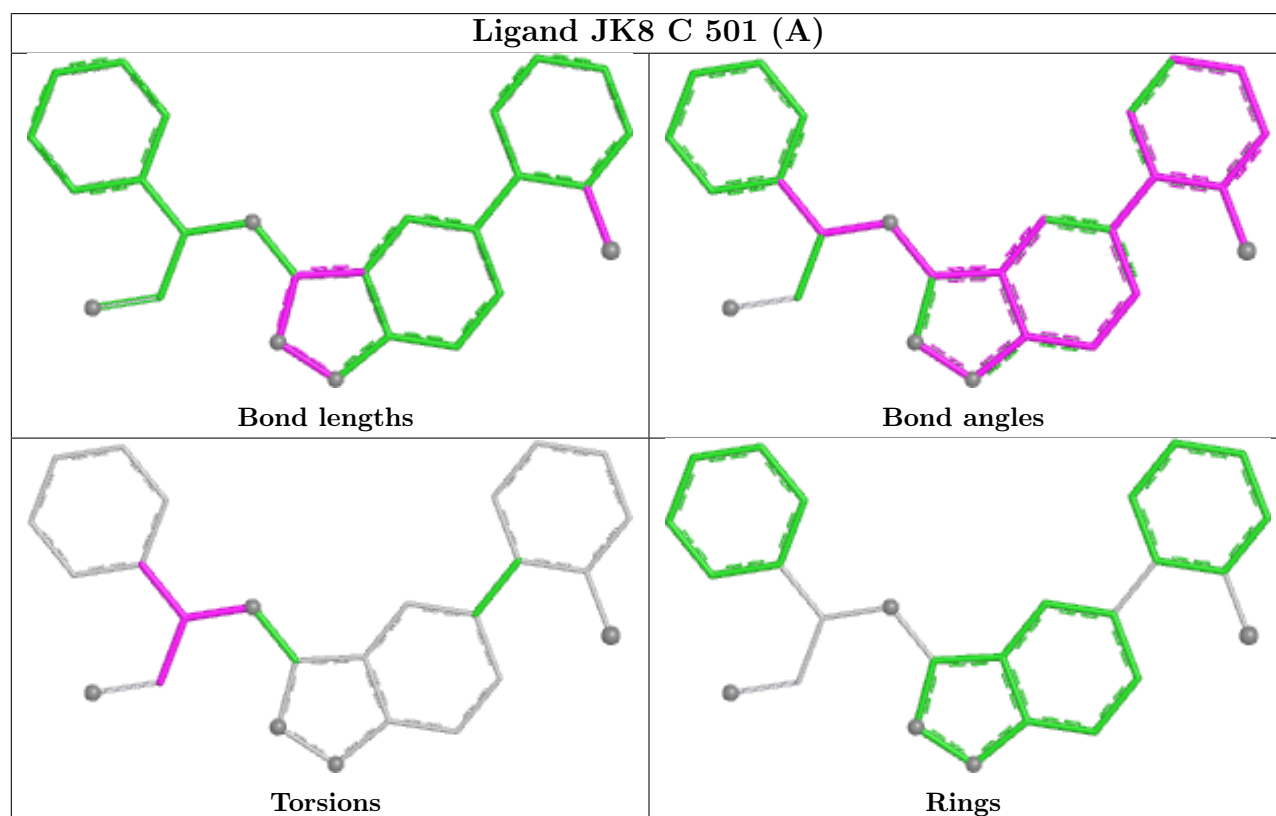
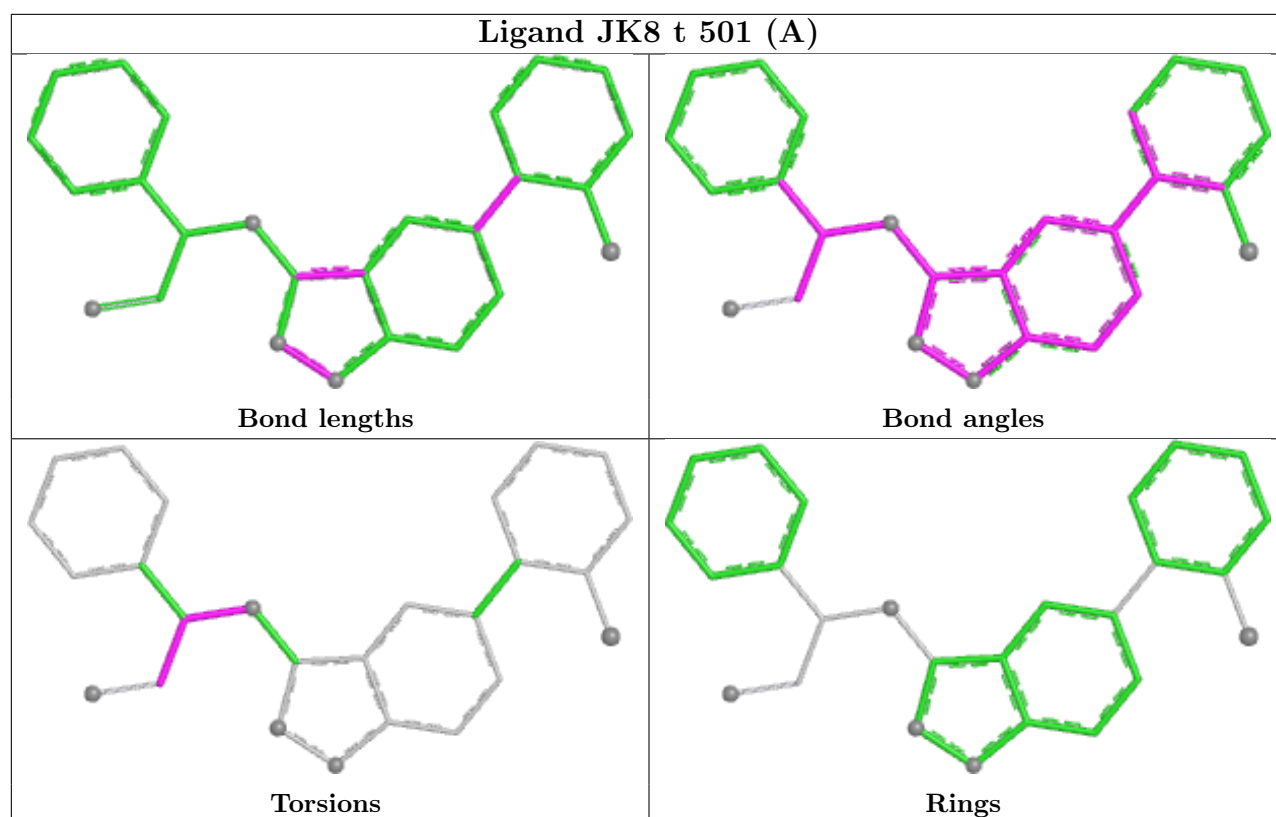
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question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



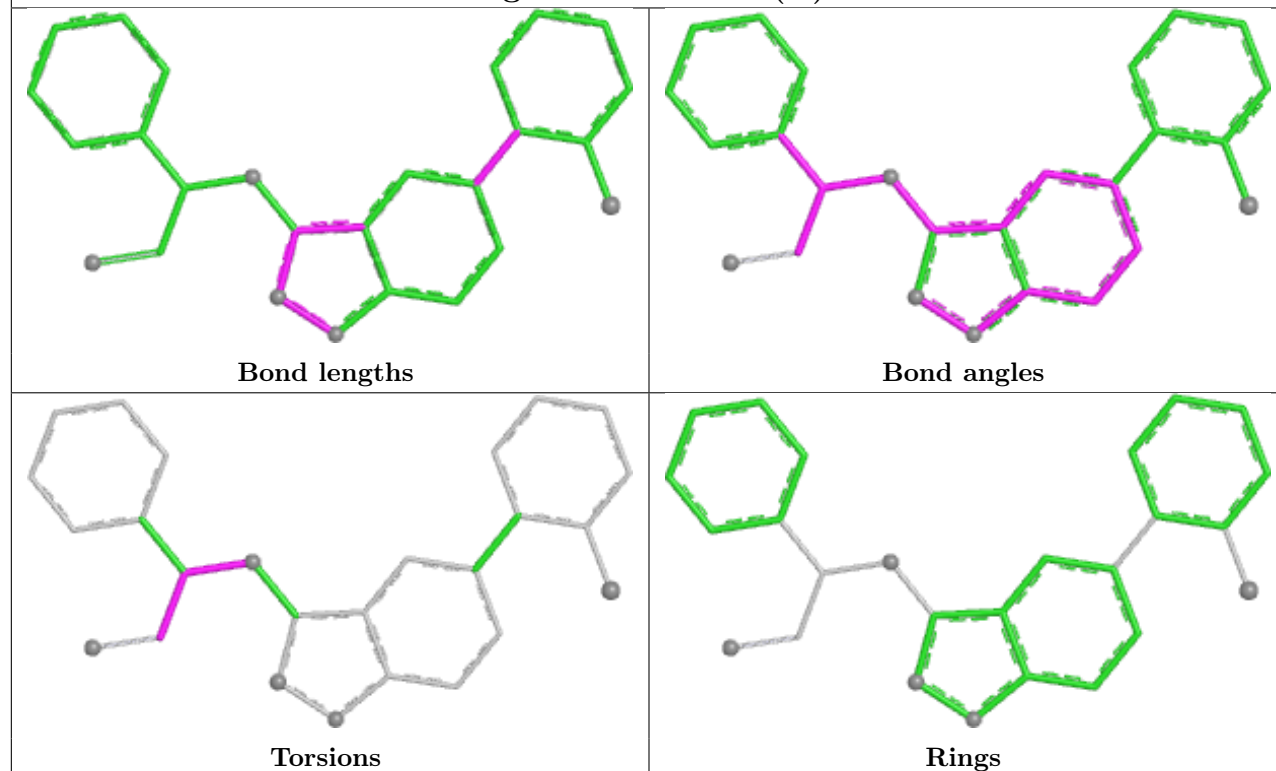




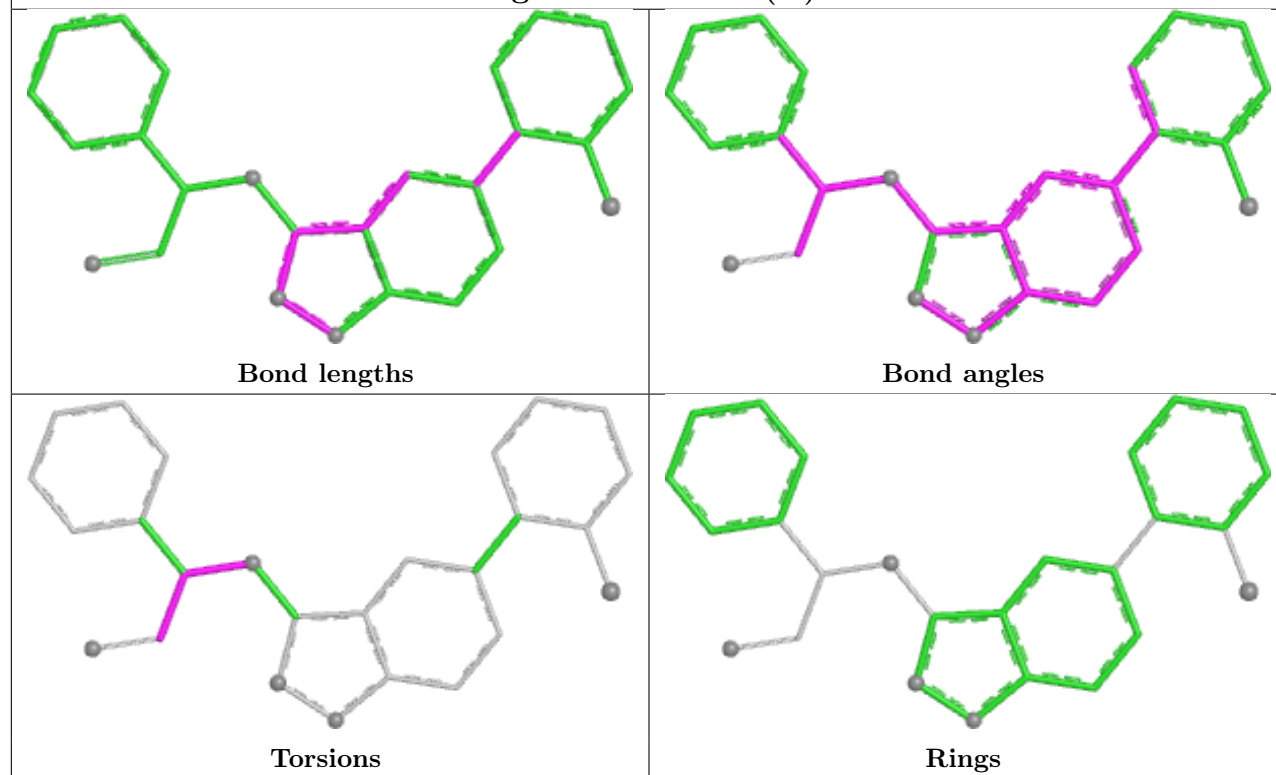


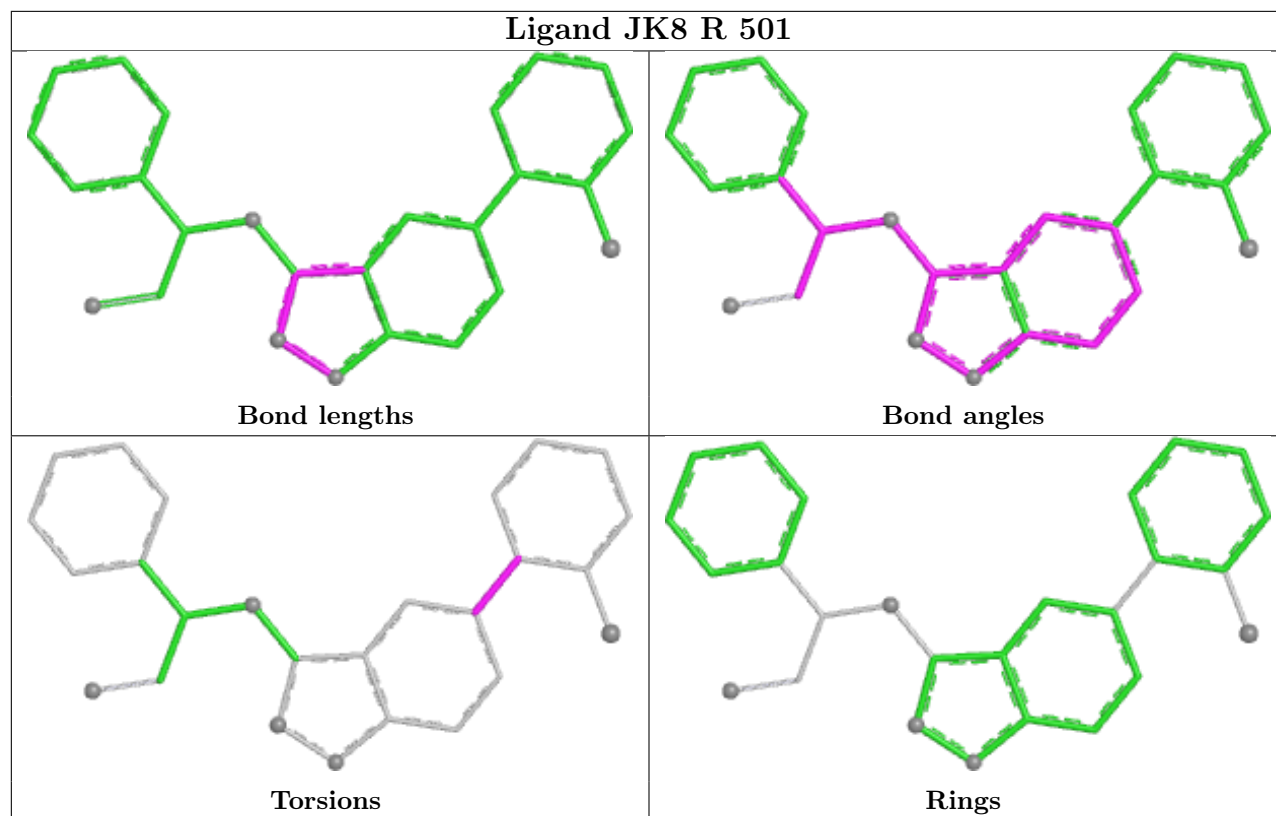


Ligand JK8 U 701 (A)



Ligand JK8 I 501 (A)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
9	d	1
1	S	1
1	s	1
1	b	1
11	k	1
5	K	1
6	J	1
8	V	1
4	W	1
4	N	1
4	n	1
4	v	1

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Mol	Chain	Number of breaks
4	F	1
4	w	1
8	o	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	543:PRO	C	581:LYS	N	8.39
1	d	545:GLY	C	586:MET	N	8.19
1	S	543:PRO	C	581:LYS	N	7.73
1	s	543:PRO	C	581:LYS	N	7.36
1	b	543:PRO	C	581:LYS	N	7.01
1	k	543:PRO	C	581:LYS	N	6.78
1	K	543:PRO	C	581:LYS	N	6.66
1	J	255:GLY	C	257:GLN	N	4.17
1	V	8:DC	O3'	2009:DG	P	3.75
1	W	8:DC	O3'	2009:DG	P	3.18
1	N	8:DC	O3'	2009:DG	P	3.10
1	n	8:DC	O3'	2009:DG	P	3.10
1	v	8:DC	O3'	2009:DG	P	3.10
1	F	8:DC	O3'	2009:DG	P	3.08
1	w	8:DC	O3'	2009:DG	P	3.02
1	o	8:DC	O3'	2009:DG	P	2.66

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	B	185/186 (99%)	-1.23	0 100 100	39, 91, 124, 173	5 (2%)
1	S	185/186 (99%)	-1.45	0 100 100	26, 60, 84, 112	5 (2%)
1	b	185/186 (99%)	-1.34	0 100 100	36, 79, 114, 134	5 (2%)
1	s	186/186 (100%)	-1.41	0 100 100	30, 62, 95, 112	4 (2%)
2	A	479/490 (97%)	-1.36	0 100 100	25, 74, 105, 175	13 (2%)
2	C	482/490 (98%)	-1.44	0 100 100	24, 61, 90, 123	8 (1%)
2	L	481/490 (98%)	-1.53	0 100 100	16, 45, 73, 110	6 (1%)
2	R	482/490 (98%)	-1.56	0 100 100	16, 45, 70, 92	11 (2%)
2	T	481/490 (98%)	-1.54	0 100 100	13, 43, 67, 97	8 (1%)
2	a	481/490 (98%)	-1.42	0 100 100	25, 62, 89, 113	12 (2%)
2	c	482/490 (98%)	-1.43	0 100 100	24, 63, 100, 143	8 (1%)
2	j	482/490 (98%)	-1.51	0 100 100	16, 46, 73, 122	13 (2%)
2	l	481/490 (98%)	-1.52	0 100 100	21, 46, 78, 132	6 (1%)
2	r	484/490 (98%)	-1.52	0 100 100	14, 44, 74, 105	15 (3%)
2	t	481/490 (98%)	-1.53	0 100 100	14, 44, 77, 125	10 (2%)
3	D	188/188 (100%)	-1.35	0 100 100	33, 83, 117, 148	2 (1%)
3	U	188/188 (100%)	-1.35	0 100 100	34, 67, 94, 138	3 (1%)
3	m	188/188 (100%)	-1.32	0 100 100	34, 68, 109, 154	1 (0%)
4	E	20/20 (100%)	-1.44	0 100 100	34, 59, 112, 130	3 (15%)
4	F	20/20 (100%)	-1.56	0 100 100	32, 70, 103, 148	0
4	N	20/20 (100%)	-1.70	0 100 100	25, 39, 59, 61	3 (15%)
4	O	20/20 (100%)	-1.73	0 100 100	31, 49, 78, 88	0
4	W	20/20 (100%)	-1.73	0 100 100	29, 48, 88, 116	0
4	e	20/20 (100%)	-1.51	0 100 100	47, 81, 112, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9	
4	n	20/20 (100%)	-1.52	0	100 100	24, 48, 96, 143	2 (10%)
4	v	19/20 (95%)	-1.63	0	100 100	21, 38, 77, 95	2 (10%)
4	w	20/20 (100%)	-1.77	0	100 100	36, 42, 67, 81	0
5	K	187/187 (100%)	-1.45	0	100 100	22, 53, 88, 113	4 (2%)
6	J	480/480 (100%)	-1.49	0	100 100	17, 47, 76, 105	15 (3%)
7	M	189/189 (100%)	-1.42	0	100 100	30, 68, 96, 112	3 (1%)
8	V	19/19 (100%)	-1.53	0	100 100	27, 50, 95, 123	0
8	o	18/19 (94%)	-1.61	0	100 100	31, 43, 91, 98	0
9	d	181/181 (100%)	-1.22	0	100 100	38, 95, 125, 150	2 (1%)
10	f	17/17 (100%)	-1.53	0	100 100	63, 79, 110, 113	0
11	k	188/188 (100%)	-1.36	0	100 100	27, 60, 98, 136	4 (2%)
12	u	187/187 (100%)	-1.43	0	100 100	27, 60, 88, 151	3 (1%)
All	All	8246/8345 (98%)	-1.46	0	100 100	13, 56, 99, 175	176 (2%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	JK8	A	501	26/26	0.99	0.05	26,33,47,52	26
13	JK8	C	501[A]	26/26	0.99	0.03	42,63,68,68	0
13	JK8	J	501	26/26	0.99	0.04	33,46,54,57	0

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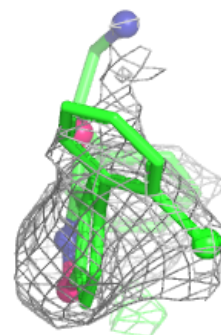
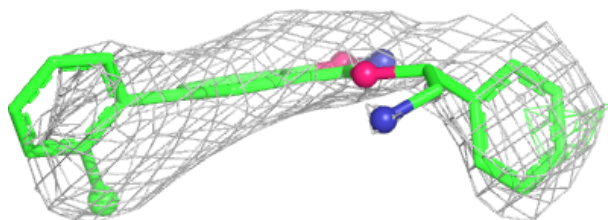
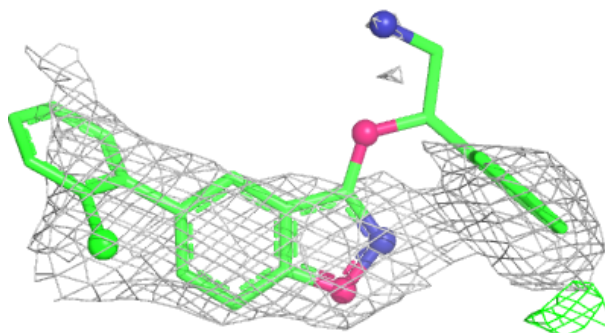
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	JK8	L	501[A]	26/26	0.99	0.04	20,21,29,30	26
13	JK8	R	501	26/26	0.99	0.05	16,17,18,22	26
13	JK8	U	701[A]	26/26	0.99	0.08	7,9,11,11	26
13	JK8	b	701	26/26	0.99	0.10	7,9,9,10	26
13	JK8	d	701[A]	26/26	0.99	0.05	34,42,60,61	26
13	JK8	k	701	26/26	0.99	0.04	36,47,69,71	0
13	JK8	l	501[A]	26/26	0.99	0.03	45,58,69,72	0
13	JK8	s	701	26/26	0.99	0.05	11,13,18,19	26
13	JK8	t	501[A]	26/26	1.00	0.04	26,31,33,43	26

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.

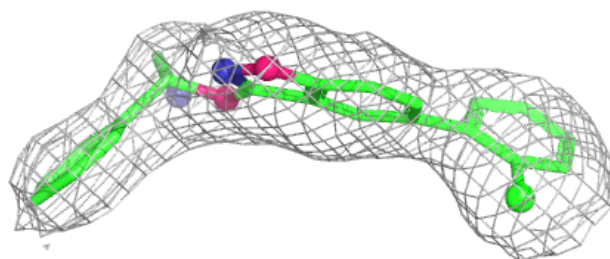
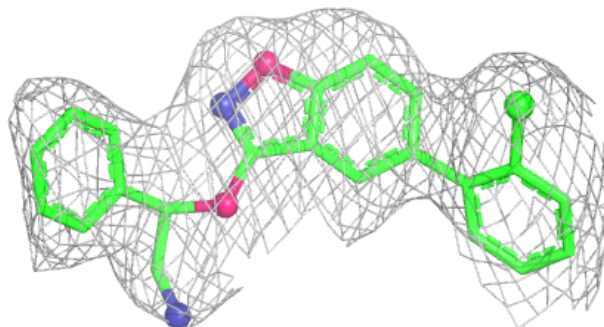
Electron density around JK8 A 501:

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

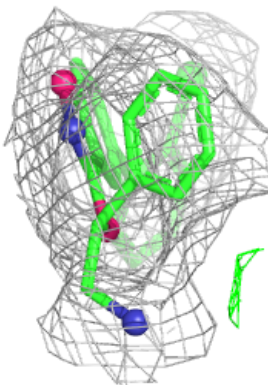
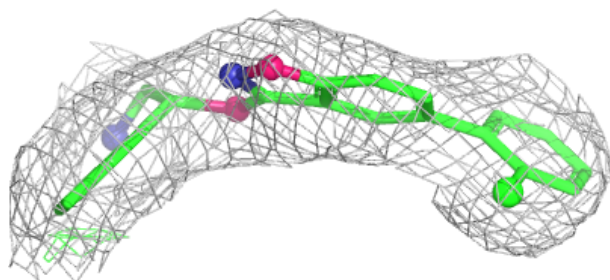
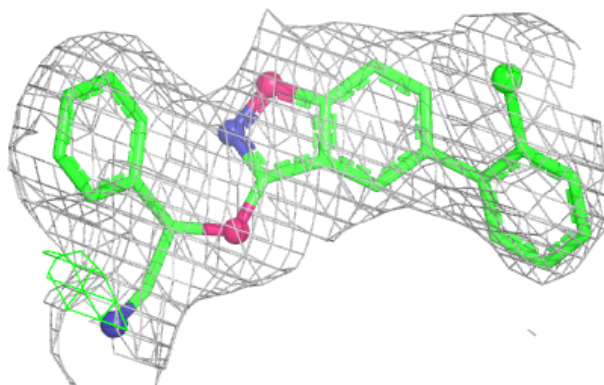


Electron density around JK8 C 501 (A):

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

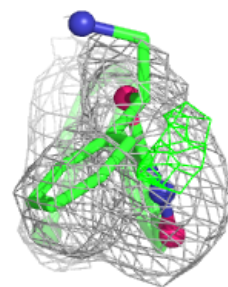
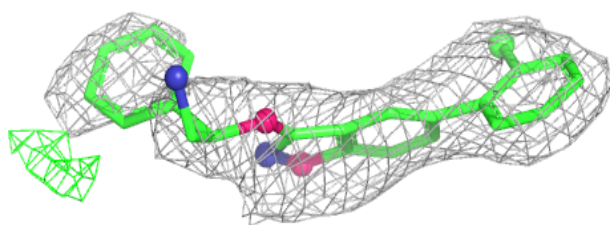
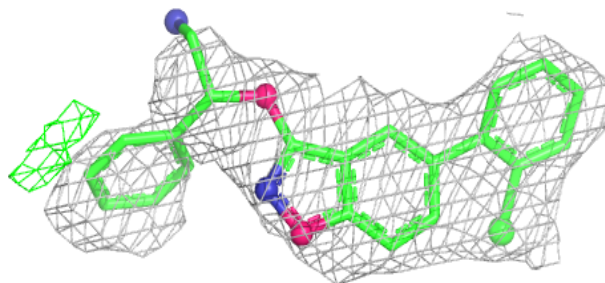
**Electron density around JK8 J 501:**

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

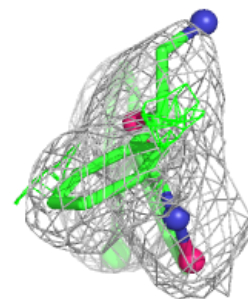
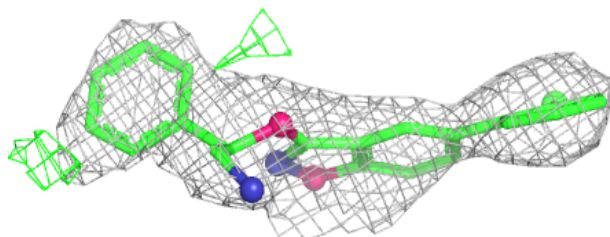
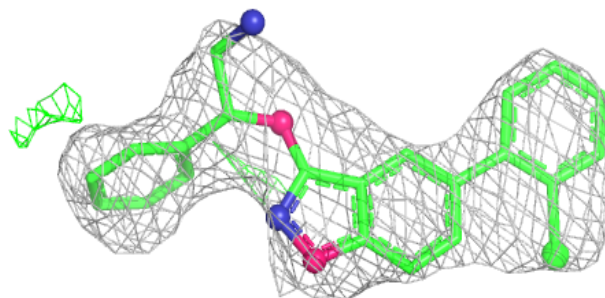


Electron density around JK8 L 501 (A):

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and green (positive)

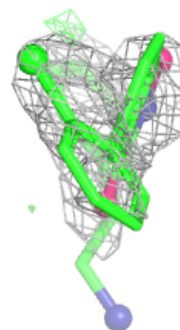
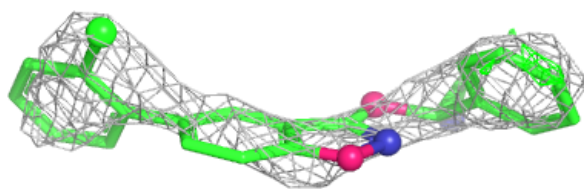
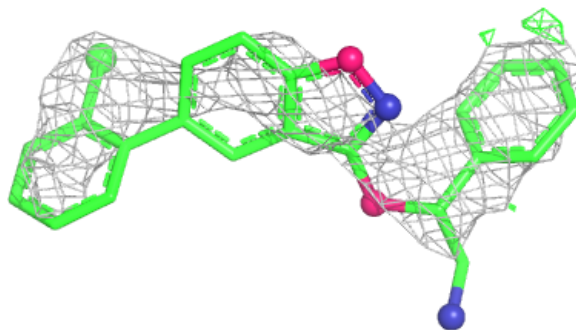
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and green (positive)

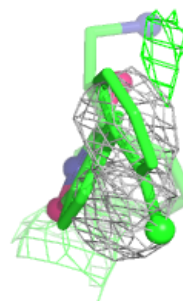
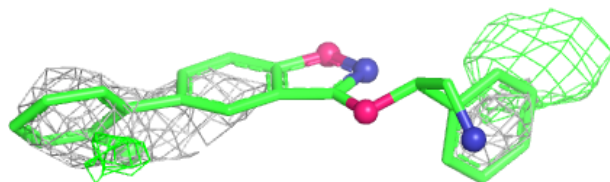


Electron density around JK8 U 701 (A):

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

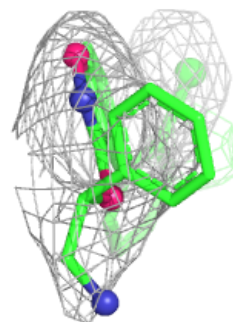
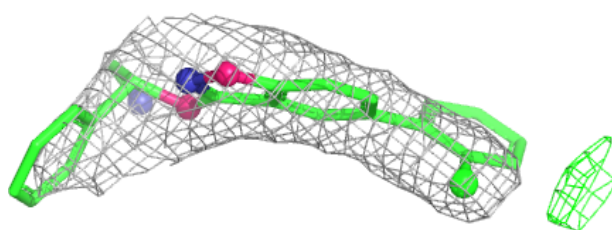
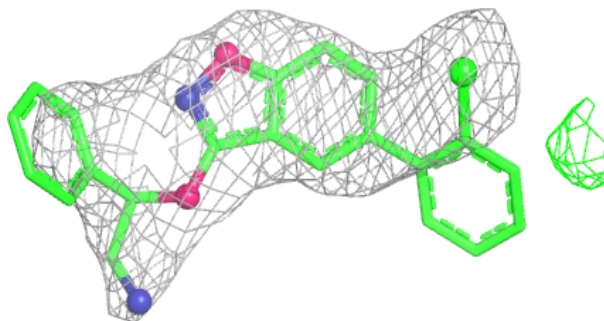
**Electron density around JK8 b 701:**

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

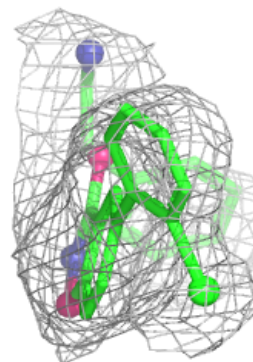
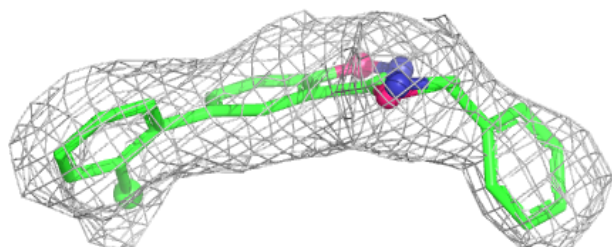
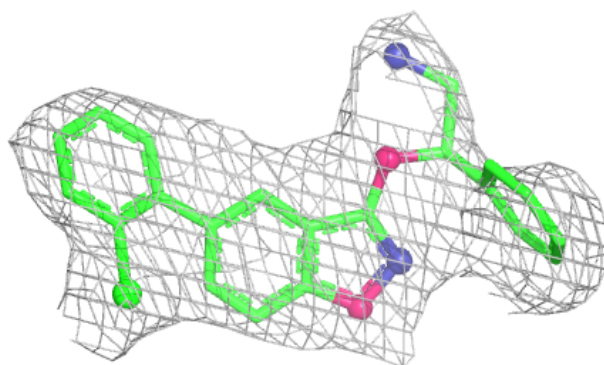


Electron density around JK8 d 701 (A):

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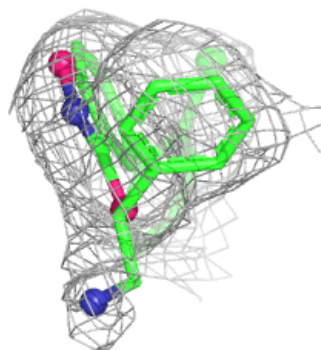
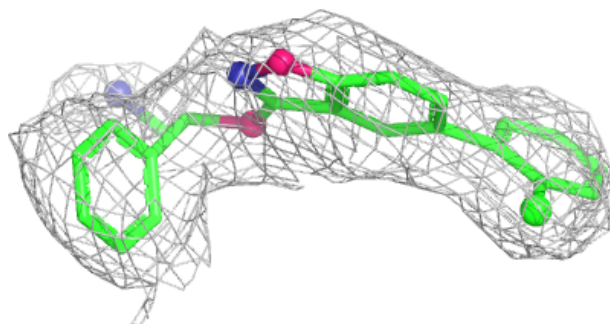
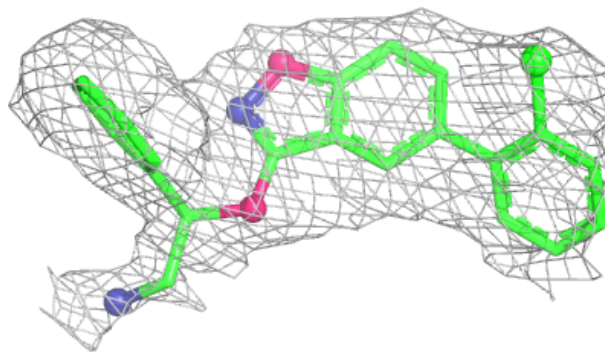
**Electron density around JK8 k 701:**

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

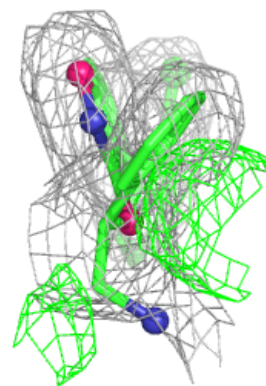
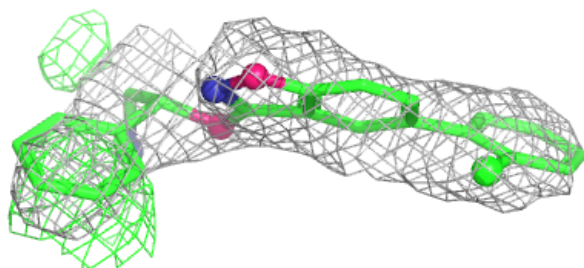
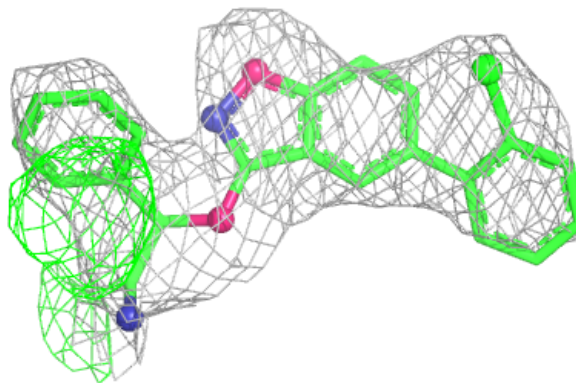


Electron density around JK8 I 501 (A):

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

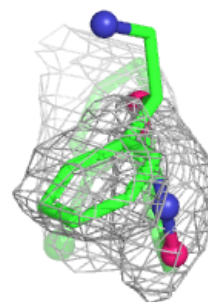
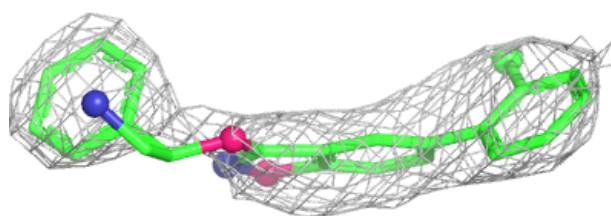
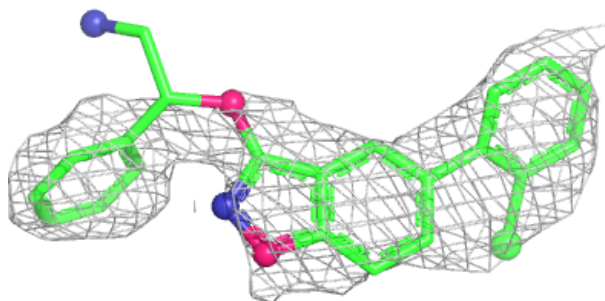
**Electron density around JK8 s 701:**

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and green (positive)



Electron density around JK8 t 501 (A):

$2mF_o-DF_c$ (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.