



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:33 PM UTC

PDB ID : 4YLH / pdb_00004ylh
Title : Crystal structure of DpgC with bound substrate analog and Xe on oxygen diffusion pathway
Authors : Li, K.; Di Russo, N.V.; Condurso, H.L.; Roitberg, A.E.; Bruner, S.D.
Deposited on : 2015-03-05
Resolution : 2.58 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

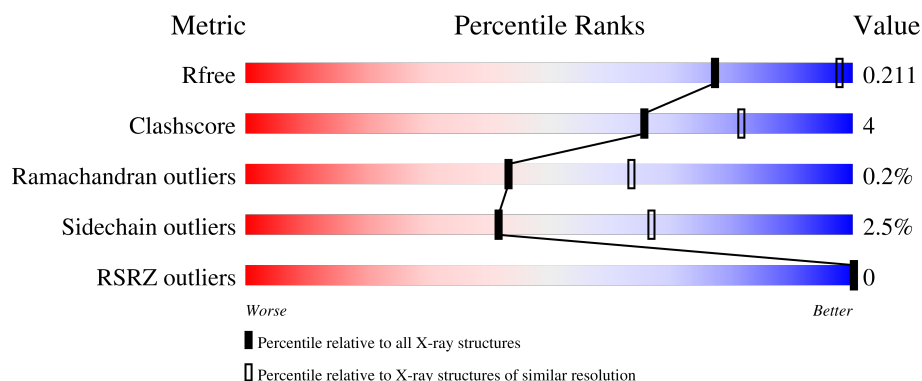
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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

Mol	Chain	Length	Quality of chain
1	A	440	 87% 8% . .
1	B	440	 86% 10% .
1	C	440	 86% 8% . .
1	D	440	 86% 10% . .
1	E	440	 85% 10% .

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Mol	Chain	Length	Quality of chain
1	F	440	 83% 12% . .
1	G	440	 85% 9% . .
1	H	440	 85% 10% . .
1	I	440	 85% 10% . .
1	J	440	 87% 8% . .
1	K	440	 87% 9% .
1	L	440	 86% 9% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	XE	A	501[A]	-	-	X	-
2	XE	B	501[A]	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 40478 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 DpgC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	1	0
			3216	2031	595	580	10			
1	B	422	Total	C	N	O	S	0	1	0
			3268	2057	605	596	10			
1	C	421	Total	C	N	O	S	0	1	0
			3265	2054	607	594	10			
1	D	423	Total	C	N	O	S	0	1	0
			3258	2051	604	593	10			
1	E	421	Total	C	N	O	S	0	1	0
			3256	2049	604	593	10			
1	F	421	Total	C	N	O	S	0	1	0
			3258	2051	607	590	10			
1	G	422	Total	C	N	O	S	0	1	0
			3251	2048	602	591	10			
1	H	422	Total	C	N	O	S	0	1	0
			3256	2051	603	592	10			
1	I	421	Total	C	N	O	S	0	1	0
			3261	2052	607	592	10			
1	J	422	Total	C	N	O	S	0	1	0
			3240	2042	602	586	10			
1	K	422	Total	C	N	O	S	0	1	0
			3265	2055	604	596	10			
1	L	421	Total	C	N	O	S	0	1	0
			3258	2049	606	593	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP Q8KLK7
A	0	MET	-	expression tag	UNP Q8KLK7
A	1	GLY	-	expression tag	UNP Q8KLK7
B	-1	ALA	-	expression tag	UNP Q8KLK7
B	0	MET	-	expression tag	UNP Q8KLK7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	expression tag	UNP Q8KLLK7
C	-1	ALA	-	expression tag	UNP Q8KLLK7
C	0	MET	-	expression tag	UNP Q8KLLK7
C	1	GLY	-	expression tag	UNP Q8KLLK7
D	-1	ALA	-	expression tag	UNP Q8KLLK7
D	0	MET	-	expression tag	UNP Q8KLLK7
D	1	GLY	-	expression tag	UNP Q8KLLK7
E	-1	ALA	-	expression tag	UNP Q8KLLK7
E	0	MET	-	expression tag	UNP Q8KLLK7
E	1	GLY	-	expression tag	UNP Q8KLLK7
F	-1	ALA	-	expression tag	UNP Q8KLLK7
F	0	MET	-	expression tag	UNP Q8KLLK7
F	1	GLY	-	expression tag	UNP Q8KLLK7
G	-1	ALA	-	expression tag	UNP Q8KLLK7
G	0	MET	-	expression tag	UNP Q8KLLK7
G	1	GLY	-	expression tag	UNP Q8KLLK7
H	-1	ALA	-	expression tag	UNP Q8KLLK7
H	0	MET	-	expression tag	UNP Q8KLLK7
H	1	GLY	-	expression tag	UNP Q8KLLK7
I	-1	ALA	-	expression tag	UNP Q8KLLK7
I	0	MET	-	expression tag	UNP Q8KLLK7
I	1	GLY	-	expression tag	UNP Q8KLLK7
J	-1	ALA	-	expression tag	UNP Q8KLLK7
J	0	MET	-	expression tag	UNP Q8KLLK7
J	1	GLY	-	expression tag	UNP Q8KLLK7
K	-1	ALA	-	expression tag	UNP Q8KLLK7
K	0	MET	-	expression tag	UNP Q8KLLK7
K	1	GLY	-	expression tag	UNP Q8KLLK7
L	-1	ALA	-	expression tag	UNP Q8KLLK7
L	0	MET	-	expression tag	UNP Q8KLLK7
L	1	GLY	-	expression tag	UNP Q8KLLK7

- Molecule 2 is XENON (CCD ID: XE) (formula: Xe).

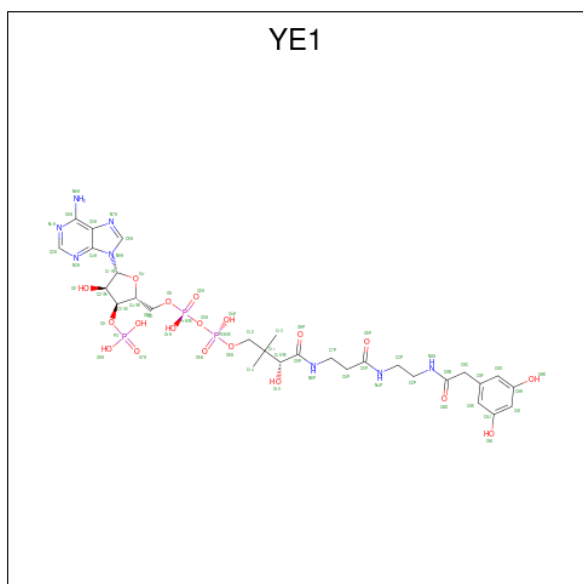
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Xe 2 2	0	1
2	B	1	Total Xe 2 2	0	1
2	C	1	Total Xe 1 1	0	1
2	D	1	Total Xe 1 1	0	1

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Xe	0	1
			1	1		
2	F	1	Total	Xe	0	1
			1	1		
2	G	1	Total	Xe	0	1
			1	1		
2	H	1	Total	Xe	0	1
			1	1		
2	I	1	Total	Xe	0	1
			1	1		
2	J	1	Total	Xe	0	1
			1	1		
2	K	1	Total	Xe	0	1
			1	1		
2	L	1	Total	Xe	0	1
			1	1		

- Molecule 3 is [(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-4-HYDROXY-3-(PHOSPHONOXY)TETRAHYDROFURAN-2-YL]METHYL (3R)-4-({3-[(2-{[(3,5-DIHYDROXYPHENYL)ACETYL]AMINO}ETHYL)AMINO]-3-OXOPROPYL}AMINO)-3-HYDROXY-2,2-DIMETHYL-4-OXOBUTYL DIHYDROGEN DIPHOSPHATE (CCD ID: YE1) (formula: $C_{29}H_{43}N_8O_{19}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			59	29	8	19	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			59	29	8	19	3		
3	C	1	Total	C	N	O	P	0	0
			59	29	8	19	3		
3	D	1	Total	C	N	O	P	0	0
			59	29	8	19	3		
3	E	1	Total	C	N	O	P	0	0
			59	29	8	19	3		
3	F	1	Total	C	N	O	P	0	0
			59	29	8	19	3		
3	G	1	Total	C	N	O	P	0	0
			59	29	8	19	3		
3	H	1	Total	C	N	O	P	0	0
			59	29	8	19	3		
3	I	1	Total	C	N	O	P	0	0
			59	29	8	19	3		
3	J	1	Total	C	N	O	P	0	0
			59	29	8	19	3		
3	K	1	Total	C	N	O	P	0	0
			59	29	8	19	3		
3	L	1	Total	C	N	O	P	0	0
			59	29	8	19	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	B	62	Total	O	0	0
			62	62		
4	C	42	Total	O	0	0
			42	42		
4	D	56	Total	O	0	0
			56	56		
4	E	74	Total	O	0	0
			74	74		
4	F	74	Total	O	0	0
			74	74		
4	G	54	Total	O	0	0
			54	54		
4	H	59	Total	O	0	0
			59	59		

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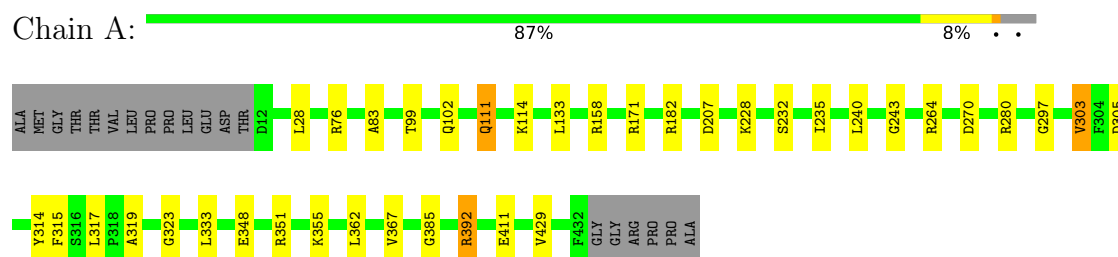
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	65	Total 65	O 65	0	0
4	J	37	Total 37	O 37	0	0
4	K	76	Total 76	O 76	0	0
4	L	57	Total 57	O 57	0	0

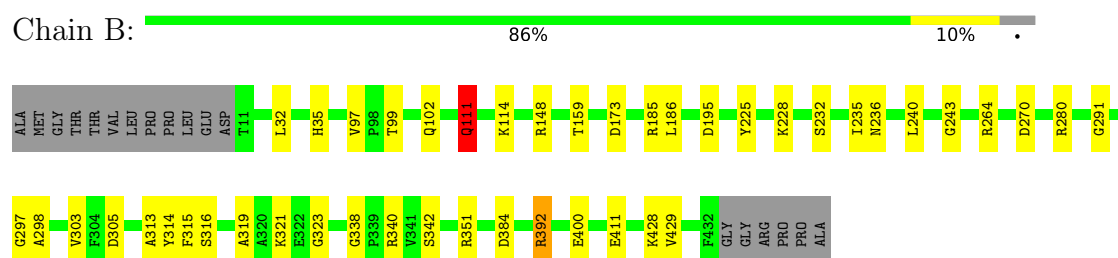
3 Residue-property plots

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

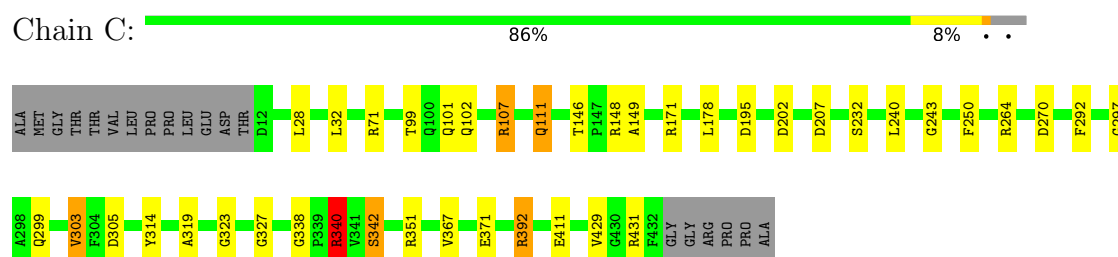
• Molecule 1: DpgC



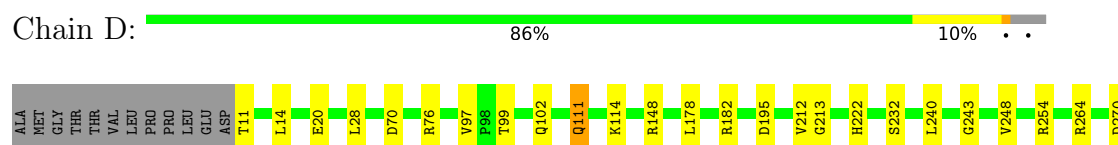
• Molecule 1: DpgC



• Molecule 1: DpgC

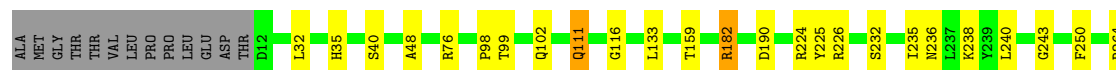
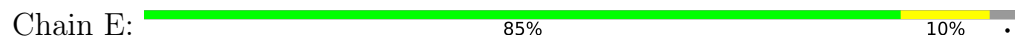


• Molecule 1: DpgC

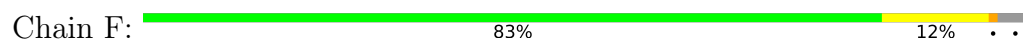




• Molecule 1: DpgC



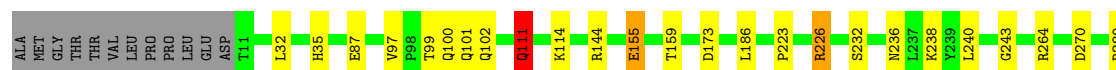
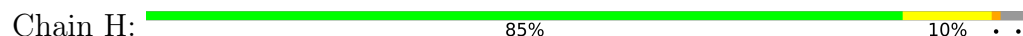
• Molecule 1: DpgC



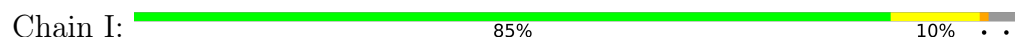
• Molecule 1: DpgC

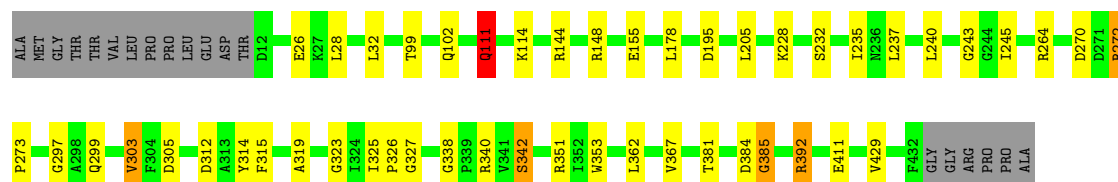


• Molecule 1: DpgC



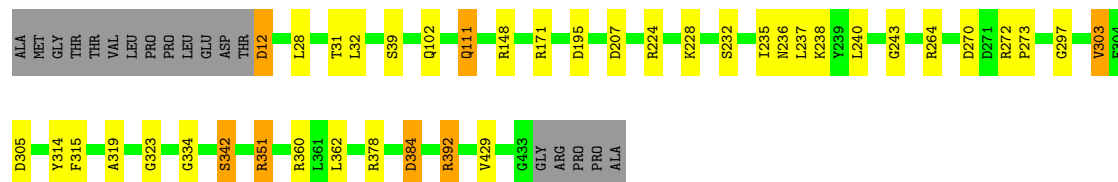
• Molecule 1: DpgC





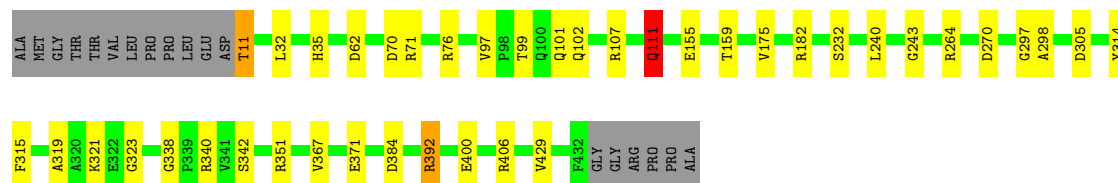
• Molecule 1: DpgC

Chain J: 87% 8% . .



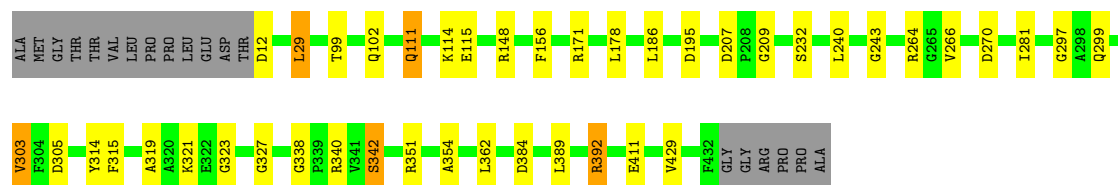
• Molecule 1: DpgC

Chain K: 87% 9% .



• Molecule 1: DpgC

Chain L: 86% 9% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	139.13Å 170.94Å 156.00Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	39.52 – 2.58 39.52 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.52-2.58) 98.7 (39.52-2.58)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.171 , 0.208 0.176 , 0.211	Depositor DCC
R_{free} test set	11219 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.648	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 9.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.447 for h,-k,-l	Xtriage
Reported twinning fraction	0.515 for H, K, L 0.485 for -h,-k,l	Depositor
Outliers	1 of 225931 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	40478	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3374e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: XE, YE1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.14	4/3277 (0.1%)	1.09	7/4449 (0.2%)
1	B	1.17	5/3330 (0.2%)	1.11	9/4516 (0.2%)
1	C	1.17	2/3327 (0.1%)	1.09	5/4511 (0.1%)
1	D	1.24	4/3319 (0.1%)	1.12	11/4502 (0.2%)
1	E	1.17	2/3317 (0.1%)	1.08	9/4498 (0.2%)
1	F	1.19	3/3320 (0.1%)	1.11	10/4502 (0.2%)
1	G	1.20	5/3312 (0.2%)	1.10	7/4494 (0.2%)
1	H	1.13	5/3317 (0.2%)	1.09	9/4499 (0.2%)
1	I	1.22	5/3323 (0.2%)	1.09	12/4506 (0.3%)
1	J	1.07	4/3301 (0.1%)	1.07	6/4478 (0.1%)
1	K	1.26	6/3327 (0.2%)	1.12	14/4513 (0.3%)
1	L	1.16	5/3320 (0.2%)	1.08	4/4502 (0.1%)
All	All	1.18	50/39790 (0.1%)	1.10	103/53970 (0.2%)

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	340	ARG	CD-NE	-6.76	1.36	1.46
1	E	400	GLU	CA-C	-6.65	1.46	1.53
1	B	97	VAL	C-O	-6.64	1.19	1.24
1	I	325	ILE	CA-C	6.57	1.58	1.52
1	K	400	GLU	CA-C	-6.38	1.46	1.53
1	H	97	VAL	C-O	-6.26	1.19	1.24
1	H	173	ASP	CA-CB	6.25	1.63	1.53
1	G	282	GLU	CA-C	-6.19	1.45	1.52
1	L	281	ILE	N-CA	-6.12	1.38	1.46
1	I	272	ARG	CD-NE	6.11	1.54	1.46
1	A	333	LEU	N-CA	-6.06	1.39	1.46
1	H	280	ARG	CA-C	-5.95	1.45	1.52
1	C	250	PHE	CA-C	5.95	1.57	1.52
1	B	173	ASP	CA-CB	5.94	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	264	ARG	CD-NE	5.89	1.54	1.46
1	C	101	GLN	CA-CB	5.85	1.62	1.53
1	E	250	PHE	N-CA	-5.82	1.41	1.46
1	F	97	VAL	C-O	-5.77	1.20	1.24
1	D	97	VAL	C-O	-5.74	1.19	1.24
1	B	400	GLU	CA-C	-5.62	1.47	1.53
1	I	326	PRO	CA-C	-5.61	1.47	1.52
1	K	101	GLN	CA-CB	5.51	1.61	1.53
1	A	280	ARG	CA-C	-5.46	1.46	1.52
1	H	101	GLN	CA-CB	5.42	1.61	1.53
1	D	348	GLU	N-CA	5.41	1.53	1.45
1	J	224	ARG	CA-C	5.33	1.60	1.52
1	A	385	GLY	N-CA	5.32	1.52	1.44
1	L	389	LEU	N-CA	5.30	1.52	1.46
1	B	428	LYS	N-CA	5.29	1.52	1.46
1	F	317	LEU	C-O	-5.28	1.18	1.24
1	I	303	VAL	C-O	-5.28	1.16	1.23
1	J	12	ASP	N-CA	5.25	1.56	1.46
1	G	280	ARG	CA-C	-5.22	1.46	1.52
1	J	351	ARG	C-O	-5.21	1.17	1.23
1	A	348	GLU	C-O	-5.20	1.17	1.24
1	B	280	ARG	CA-C	-5.16	1.46	1.52
1	D	348	GLU	C-O	-5.14	1.17	1.24
1	K	97	VAL	C-O	-5.14	1.20	1.24
1	K	175	VAL	N-CA	-5.13	1.40	1.46
1	D	309	ALA	CA-C	-5.13	1.46	1.52
1	L	354	ALA	CA-C	-5.12	1.45	1.52
1	F	306	ARG	C-O	-5.11	1.17	1.23
1	I	245	ILE	N-CA	5.09	1.52	1.46
1	L	156	PHE	N-CA	-5.08	1.40	1.46
1	G	385	GLY	N-CA	5.05	1.51	1.45
1	G	97	VAL	C-O	-5.05	1.20	1.24
1	G	147	PRO	N-CA	5.05	1.54	1.47
1	K	62	ASP	CB-CG	5.04	1.64	1.52
1	J	102	GLN	CG-CD	5.02	1.64	1.52
1	L	209	GLY	N-CA	5.01	1.53	1.45

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	ARG	CB-CA-C	-12.66	87.82	110.35
1	B	185	ARG	CG-CD-NE	-9.37	91.38	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	303	VAL	CB-CA-C	8.71	119.32	110.70
1	A	182	ARG	CG-CD-NE	8.69	131.11	112.00
1	K	406	ARG	NE-CZ-NH1	8.57	130.07	121.50
1	L	303	VAL	CB-CA-C	8.23	118.85	110.70
1	I	303	VAL	CB-CA-C	8.04	118.66	110.70
1	A	303	VAL	CB-CA-C	7.88	118.51	110.70
1	C	303	VAL	CB-CA-C	7.48	118.11	110.70
1	I	26	GLU	CB-CA-C	-7.25	98.75	110.79
1	F	406	ARG	CD-NE-CZ	7.13	134.38	124.40
1	C	340	ARG	CD-NE-CZ	-6.98	114.63	124.40
1	G	303	VAL	CB-CA-C	6.93	117.56	110.70
1	D	182	ARG	CA-CB-CG	-6.88	100.35	114.10
1	D	303	VAL	N-CA-CB	-6.87	102.16	112.67
1	C	340	ARG	CB-CG-CD	6.75	126.82	111.30
1	J	342	SER	CA-CB-OG	6.71	124.52	111.10
1	D	342	SER	CA-CB-OG	6.69	124.48	111.10
1	G	367	VAL	CA-CB-CG1	-6.68	99.05	110.40
1	H	264	ARG	CB-CG-CD	6.65	126.59	111.30
1	H	35	HIS	N-CA-C	6.60	122.25	111.37
1	F	98	PRO	N-CA-C	6.52	121.57	111.21
1	F	303	VAL	CB-CA-C	6.49	117.13	110.70
1	K	182	ARG	CG-CD-NE	6.46	126.22	112.00
1	F	384	ASP	N-CA-C	6.42	118.36	111.36
1	G	384	ASP	CA-C-N	-6.37	113.17	121.96
1	G	384	ASP	C-N-CA	-6.37	113.17	121.96
1	I	303	VAL	N-CA-CB	-6.28	103.07	112.67
1	K	406	ARG	NE-CZ-NH2	-6.20	113.62	119.20
1	D	384	ASP	CA-C-N	-6.19	113.42	121.96
1	D	384	ASP	C-N-CA	-6.19	113.42	121.96
1	K	406	ARG	CD-NE-CZ	6.14	132.99	124.40
1	A	367	VAL	CA-CB-CG1	-6.12	99.99	110.40
1	J	342	SER	CB-CA-C	-6.06	101.36	110.88
1	B	185	ARG	N-CA-C	6.03	122.72	113.19
1	A	303	VAL	N-CA-CB	-6.02	103.45	112.67
1	E	35	HIS	N-CA-C	5.94	121.17	111.37
1	E	303	VAL	CB-CA-C	5.94	116.58	110.70
1	C	303	VAL	N-CA-CB	-5.93	103.60	112.67
1	K	35	HIS	N-CA-C	5.93	121.15	111.37
1	I	385	GLY	N-CA-C	5.90	121.69	112.31
1	G	303	VAL	N-CA-CB	-5.87	103.69	112.67
1	E	98	PRO	N-CA-C	5.84	120.66	111.38
1	K	71	ARG	CD-NE-CZ	5.83	132.56	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	384	ASP	CA-C-N	-5.77	114.00	121.96
1	I	384	ASP	C-N-CA	-5.77	114.00	121.96
1	K	384	ASP	CA-C-N	-5.77	114.00	121.96
1	K	384	ASP	C-N-CA	-5.77	114.00	121.96
1	D	20	GLU	CB-CG-CD	5.76	122.40	112.60
1	B	111	GLN	CB-CA-C	-5.67	101.73	110.81
1	L	303	VAL	N-CA-CB	-5.67	103.99	112.67
1	E	226	ARG	CG-CD-NE	5.67	124.47	112.00
1	H	303	VAL	CB-CA-C	5.65	116.29	110.70
1	F	392	ARG	CD-NE-CZ	5.64	132.30	124.40
1	D	392	ARG	CG-CD-NE	5.63	124.39	112.00
1	F	303	VAL	N-CA-CB	-5.62	104.08	112.67
1	I	28	LEU	CB-CG-CD2	5.58	127.43	110.70
1	D	342	SER	CB-CA-C	-5.54	102.19	110.88
1	I	384	ASP	N-CA-C	5.52	118.48	111.69
1	D	248	VAL	CB-CA-C	-5.52	104.81	112.04
1	I	111	GLN	CB-CA-C	-5.52	101.58	110.74
1	F	385	GLY	N-CA-C	5.51	120.97	111.98
1	J	303	VAL	N-CA-CB	-5.51	102.13	111.23
1	A	28	LEU	CB-CG-CD2	5.50	127.21	110.70
1	A	392	ARG	CG-CD-NE	5.50	124.09	112.00
1	H	159	THR	N-CA-CB	5.50	118.58	110.33
1	G	392	ARG	CD-NE-CZ	5.46	132.05	124.40
1	F	111	GLN	CB-CA-C	-5.44	101.70	110.74
1	J	378	ARG	CG-CD-NE	-5.44	100.04	112.00
1	E	182	ARG	CG-CD-NE	5.42	123.93	112.00
1	C	28	LEU	CB-CG-CD2	5.37	126.81	110.70
1	B	384	ASP	CA-C-N	-5.35	114.58	121.96
1	B	384	ASP	C-N-CA	-5.35	114.58	121.96
1	H	226	ARG	CB-CA-C	-5.35	102.63	110.06
1	B	35	HIS	N-CA-C	5.34	120.19	111.37
1	K	182	ARG	CB-CG-CD	-5.33	99.04	111.30
1	A	385	GLY	N-CA-C	5.33	120.66	111.98
1	B	303	VAL	CB-CA-C	5.33	115.97	110.70
1	J	384	ASP	CA-C-N	-5.32	114.62	121.96
1	J	384	ASP	C-N-CA	-5.32	114.62	121.96
1	K	384	ASP	N-CA-C	5.27	117.11	111.36
1	I	367	VAL	CA-CB-CG1	5.27	119.36	110.40
1	L	384	ASP	N-CA-C	5.26	117.09	111.36
1	D	28	LEU	CB-CG-CD2	5.25	126.46	110.70
1	F	384	ASP	CB-CA-C	-5.24	101.94	110.85
1	E	384	ASP	CA-C-N	-5.24	114.73	121.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	384	ASP	C-N-CA	-5.24	114.73	121.96
1	H	111	GLN	CB-CA-C	-5.24	102.04	110.74
1	E	159	THR	N-CA-CB	5.22	118.16	110.33
1	G	392	ARG	NE-CZ-NH2	-5.21	114.51	119.20
1	K	159	THR	N-CA-CB	5.21	118.14	110.33
1	F	177	ARG	CB-CG-CD	-5.20	99.34	111.30
1	K	340	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	B	159	THR	N-CA-CB	5.19	118.11	110.33
1	I	205	LEU	N-CA-C	5.11	116.92	111.36
1	I	367	VAL	CA-CB-CG2	-5.10	101.72	110.40
1	H	384	ASP	CA-C-N	-5.07	114.96	121.96
1	H	384	ASP	C-N-CA	-5.07	114.96	121.96
1	E	392	ARG	CG-CD-NE	-5.05	100.89	112.00
1	H	264	ARG	N-CA-C	5.05	119.59	113.38
1	L	266	VAL	N-CA-CB	5.04	116.22	110.72
1	K	11	THR	CA-CB-CG2	5.02	119.03	110.50
1	K	111	GLN	CB-CA-C	-5.01	102.42	110.74

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3216	0	3201	23	0
1	B	3268	0	3266	22	0
1	C	3265	0	3266	26	0
1	D	3258	0	3254	20	0
1	E	3256	0	3255	31	0
1	F	3258	0	3260	29	0
1	G	3251	0	3241	22	0
1	H	3256	0	3255	28	0
1	I	3261	0	3262	33	0
1	J	3240	0	3235	27	0
1	K	3265	0	3257	16	0
1	L	3258	0	3251	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	2	0
2	B	2	0	0	3	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	59	0	38	1	0
3	B	59	0	39	4	0
3	C	59	0	38	2	0
3	D	59	0	38	2	0
3	E	59	0	39	5	0
3	F	59	0	36	2	0
3	G	59	0	38	2	0
3	H	59	0	38	4	0
3	I	59	0	38	4	0
3	J	59	0	39	9	0
3	K	59	0	38	0	0
3	L	59	0	38	1	0
4	A	48	0	0	2	0
4	B	62	0	0	0	0
4	C	42	0	0	1	0
4	D	56	0	0	1	0
4	E	74	0	0	2	0
4	F	74	0	0	3	0
4	G	54	0	0	1	0
4	H	59	0	0	4	0
4	I	65	0	0	1	0
4	J	37	0	0	0	0
4	K	76	0	0	0	0
4	L	57	0	0	1	0
All	All	40478	0	39460	298	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (298) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:HH12	1:A:133:LEU:HD22	1.31	0.95
1:L:29:LEU:HD21	1:L:115:GLU:HG3	1.49	0.94
1:E:76:ARG:HH12	1:E:133:LEU:HD22	1.34	0.93
1:A:317:LEU:HD11	2:A:501[A]:XE:XE	2.56	0.84
1:K:70:ASP:OD1	1:K:76:ARG:NH1	2.11	0.83
1:D:70:ASP:OD1	1:D:76:ARG:NH1	2.12	0.81
1:I:272:ARG:HG2	1:I:273:PRO:HD2	1.66	0.78
1:J:272:ARG:CG	1:J:273:PRO:HD2	2.14	0.77
1:J:272:ARG:HG2	1:J:273:PRO:HD2	1.67	0.77
1:I:272:ARG:CG	1:I:273:PRO:HD2	2.15	0.76
1:A:76:ARG:NH1	1:A:133:LEU:HB3	2.00	0.75
1:E:182:ARG:NH1	1:E:190:ASP:OD2	2.20	0.75
1:J:314:TYR:CD2	1:J:351:ARG:HD2	2.21	0.75
1:E:76:ARG:NH1	1:E:133:LEU:HB3	2.02	0.74
1:H:360:ARG:NH2	1:H:364:ASP:O	2.25	0.70
1:C:431:ARG:HD3	4:C:613:HOH:O	1.90	0.70
1:C:107:ARG:HG3	1:C:107:ARG:HH11	1.56	0.70
1:D:335:ARG:HG3	4:D:649:HOH:O	1.92	0.70
1:E:76:ARG:NH1	1:E:133:LEU:HD22	2.08	0.69
1:B:315[A]:PHE:C	2:B:501[A]:XE:XE	3.16	0.67
1:A:76:ARG:NH1	1:A:133:LEU:HD22	2.06	0.66
3:H:502:YE1:OAD	3:H:502:YE1:HAE	1.95	0.66
1:F:353:TRP:CH2	1:I:312:ASP:HB3	2.31	0.66
1:A:171:ARG:NH1	1:A:207:ASP:OD2	2.32	0.63
1:H:144:ARG:HG2	1:H:144:ARG:HH11	1.63	0.63
1:C:171:ARG:NH1	1:C:207:ASP:OD2	2.31	0.62
1:E:408:TYR:CE1	1:F:394:MET:HE3	2.35	0.62
1:F:312:ASP:HB3	1:I:353:TRP:CH2	2.34	0.62
1:J:171:ARG:NH1	1:J:207:ASP:OD2	2.31	0.62
1:C:146:THR:HG22	1:C:202:ASP:OD2	2.00	0.62
1:G:165:GLU:HG2	1:G:182:ARG:HH12	1.63	0.62
1:L:171:ARG:NH1	1:L:207:ASP:OD2	2.30	0.61
1:L:315[B]:PHE:CD2	1:L:362:LEU:HD13	2.35	0.61
1:D:298:ALA:HB1	1:D:315[B]:PHE:CE2	2.36	0.61
1:L:319:ALA:HB1	1:L:323:GLY:HA3	1.82	0.60
4:H:606:HOH:O	1:I:385:GLY:HA3	2.01	0.60
1:J:272:ARG:HG3	1:J:273:PRO:HD2	1.84	0.60
3:J:502:YE1:HN62	3:J:502:YE1:HC71	1.64	0.60
1:G:12:ASP:OD2	1:G:14:LEU:HD22	2.02	0.59
1:C:305:ASP:OD2	1:C:392:ARG:HD2	2.02	0.59
1:E:76:ARG:HH11	1:E:133:LEU:HB3	1.68	0.59
1:L:305:ASP:OD2	1:L:392:ARG:HD2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ALA:HB1	1:B:315[B]:PHE:CE2	2.38	0.58
1:E:238:LYS:NZ	3:E:502:YE1:O9A	2.36	0.58
1:I:305:ASP:OD2	1:I:392:ARG:HD2	2.04	0.57
1:B:316:SER:HA	2:B:501[A]:XE:XE	2.83	0.57
1:B:236:ASN:HA	3:B:502:YE1:N1A	2.20	0.57
1:H:319:ALA:HB1	1:H:323:GLY:HA3	1.87	0.57
1:D:319:ALA:HB1	1:D:323:GLY:HA3	1.87	0.56
1:E:99:THR:H	1:E:102:GLN:HE21	1.54	0.56
1:E:305:ASP:OD2	1:E:392:ARG:HD2	2.04	0.56
1:I:319:ALA:HB1	1:I:323:GLY:HA3	1.86	0.56
1:I:272:ARG:HG3	1:I:273:PRO:HD2	1.88	0.56
1:J:272:ARG:HG2	1:J:273:PRO:CD	2.37	0.55
1:B:305:ASP:OD2	1:B:392:ARG:HD2	2.07	0.55
1:F:319:ALA:HB1	1:F:323:GLY:HA3	1.88	0.55
1:J:319:ALA:HB1	1:J:323:GLY:HA3	1.88	0.55
1:C:319:ALA:HB1	1:C:323:GLY:HA3	1.88	0.55
1:G:319:ALA:HB1	1:G:323:GLY:HA3	1.89	0.55
1:J:384:ASP:HB2	1:L:321:LYS:NZ	2.21	0.55
1:H:111:GLN:HE21	1:H:243:GLY:HA2	1.72	0.55
1:I:99:THR:H	1:I:102:GLN:HE21	1.54	0.54
1:K:305:ASP:OD2	1:K:392:ARG:HD2	2.06	0.54
1:H:305:ASP:OD2	1:H:392:ARG:HD2	2.07	0.54
1:G:264:ARG:HG2	1:G:264:ARG:HH11	1.73	0.54
1:L:315[B]:PHE:CD1	1:L:315[B]:PHE:C	2.85	0.54
1:J:237:LEU:HD11	3:J:502:YE1:O5P	2.07	0.54
1:K:264:ARG:HG2	1:K:264:ARG:HH11	1.73	0.54
1:K:319:ALA:HB1	1:K:323:GLY:HA3	1.89	0.54
1:B:264:ARG:HH11	1:B:264:ARG:HG2	1.72	0.54
3:E:502:YE1:HAI	4:E:615:HOH:O	2.06	0.54
1:L:12:ASP:HA	4:L:656:HOH:O	2.08	0.54
1:I:272:ARG:HG2	1:I:273:PRO:CD	2.36	0.54
1:E:319:ALA:HB1	1:E:323:GLY:HA3	1.89	0.54
1:L:111:GLN:HE21	1:L:243:GLY:HA2	1.73	0.53
1:H:238:LYS:NZ	3:H:502:YE1:O9A	2.41	0.53
1:I:111:GLN:HE21	1:I:243:GLY:HA2	1.73	0.53
1:A:315[B]:PHE:CD1	1:A:315[B]:PHE:C	2.86	0.53
1:A:76:ARG:HH11	1:A:133:LEU:HB3	1.71	0.53
1:C:99:THR:H	1:C:102:GLN:HE21	1.55	0.53
1:I:305:ASP:OD1	1:I:392:ARG:NH1	2.42	0.53
1:L:305:ASP:OD1	1:L:392:ARG:NH1	2.41	0.53
1:H:321:LYS:NZ	1:I:381:THR:O	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:ALA:HB1	1:B:323:GLY:HA3	1.91	0.53
1:C:232:SER:HB3	1:C:297:GLY:HA3	1.90	0.53
1:F:99:THR:H	1:F:102:GLN:HE21	1.57	0.53
1:J:305:ASP:OD2	1:J:392:ARG:HD2	2.08	0.53
1:E:111:GLN:HE21	1:E:243:GLY:HA2	1.73	0.52
1:K:315[B]:PHE:CD1	1:K:315[B]:PHE:C	2.87	0.52
1:A:111:GLN:HE21	1:A:243:GLY:HA2	1.73	0.52
1:B:111:GLN:HE21	1:B:243:GLY:HA2	1.74	0.52
1:F:111:GLN:HE21	1:F:243:GLY:HA2	1.75	0.52
1:G:111:GLN:HE21	1:G:243:GLY:HA2	1.74	0.52
1:J:111:GLN:HE21	1:J:243:GLY:HA2	1.73	0.52
1:H:99:THR:H	1:H:102:GLN:HE21	1.57	0.52
1:A:314:TYR:CD1	1:A:351:ARG:HD2	2.45	0.52
1:C:111:GLN:HE21	1:C:243:GLY:HA2	1.74	0.52
1:G:305:ASP:OD1	1:G:392:ARG:NH1	2.42	0.52
1:D:111:GLN:HE21	1:D:243:GLY:HA2	1.73	0.51
1:A:99:THR:H	1:A:102:GLN:HE21	1.59	0.51
1:C:305:ASP:OD1	1:C:392:ARG:NH1	2.43	0.51
1:D:314:TYR:CD1	1:D:351:ARG:HD2	2.45	0.51
1:D:264:ARG:HH11	1:D:264:ARG:HG2	1.76	0.51
1:G:314:TYR:CD1	1:G:351:ARG:HD2	2.46	0.51
1:K:305:ASP:OD1	1:K:392:ARG:NH1	2.44	0.51
1:A:158:ARG:HB2	1:E:48:ALA:HB1	1.93	0.51
1:F:357:PRO:HA	1:F:360:ARG:NH1	2.25	0.51
1:F:236:ASN:HA	3:F:502:YE1:N1A	2.26	0.51
1:A:319:ALA:HB1	1:A:323:GLY:HA3	1.93	0.51
1:H:305:ASP:OD1	1:H:392:ARG:NH1	2.44	0.51
1:K:111:GLN:HE21	1:K:243:GLY:HA2	1.74	0.51
1:E:111:GLN:NE2	4:E:605:HOH:O	2.43	0.50
1:I:111:GLN:NE2	1:I:114:LYS:HE3	2.26	0.50
1:J:305:ASP:OD1	1:J:392:ARG:NH1	2.44	0.50
1:E:314:TYR:CD1	1:E:351:ARG:HD2	2.46	0.50
1:L:99:THR:H	1:L:102:GLN:HE21	1.60	0.50
1:J:236:ASN:HA	3:J:502:YE1:N1A	2.27	0.50
1:A:232:SER:HB3	1:A:297:GLY:HA3	1.94	0.50
1:F:264:ARG:HG2	1:F:264:ARG:HH11	1.76	0.50
1:L:111:GLN:HG2	1:L:240:LEU:O	2.12	0.49
1:G:39:SER:O	1:G:43:ARG:HG3	2.11	0.49
1:L:232:SER:HB3	1:L:297:GLY:HA3	1.94	0.49
1:G:305:ASP:CG	1:G:392:ARG:HH11	2.20	0.49
1:H:360:ARG:CZ	1:H:364:ASP:O	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:334:GLY:HA2	1:J:342:SER:OG	2.13	0.49
1:D:254:ARG:CZ	3:D:502:YE1:OAL	2.60	0.49
1:K:232:SER:HB3	1:K:297:GLY:HA3	1.93	0.49
1:C:264:ARG:HG2	1:C:264:ARG:HH11	1.78	0.49
1:G:279:PRO:HD2	4:G:645:HOH:O	2.12	0.49
1:F:117:HIS:HD2	4:F:609:HOH:O	1.95	0.49
1:A:264:ARG:HG2	1:A:264:ARG:HH11	1.78	0.49
1:D:222:HIS:NE2	3:D:502:YE1:O8A	2.40	0.49
1:E:298:ALA:HB1	1:E:315[B]:PHE:CE2	2.48	0.49
1:I:272:ARG:CG	1:I:273:PRO:CD	2.88	0.49
1:K:298:ALA:HB1	1:K:315[B]:PHE:CE2	2.48	0.49
1:A:111:GLN:HG2	1:A:240:LEU:O	2.12	0.49
3:J:502:YE1:HC71	3:J:502:YE1:N6A	2.27	0.49
1:D:334:GLY:HA2	1:D:342:SER:OG	2.13	0.49
1:E:305:ASP:OD1	1:E:392:ARG:NH1	2.46	0.49
1:K:314:TYR:CD1	1:K:351:ARG:HD2	2.48	0.49
1:A:317:LEU:CD1	2:A:501[A]:XE:XE	3.37	0.48
1:G:99:THR:H	1:G:102:GLN:HE21	1.61	0.48
1:J:272:ARG:CG	1:J:273:PRO:CD	2.87	0.48
1:C:111:GLN:HG2	1:C:240:LEU:O	2.12	0.48
1:E:116:GLY:HA2	1:E:421:TYR:CE2	2.48	0.48
1:F:338:GLY:O	1:F:342:SER:HB3	2.12	0.48
1:F:82:LEU:HB2	4:F:645:HOH:O	2.11	0.48
1:F:298:ALA:HB1	1:F:315[B]:PHE:CE2	2.47	0.48
1:G:232:SER:HB3	1:G:297:GLY:HA3	1.95	0.48
1:H:355:LYS:HE2	4:H:601:HOH:O	2.12	0.48
1:I:237:LEU:HD11	3:I:502:YE1:O5P	2.12	0.48
1:J:305:ASP:CG	1:J:392:ARG:HH11	2.22	0.48
1:A:305:ASP:C	1:C:340:ARG:NH2	2.71	0.48
1:H:155:GLU:CD	1:H:155:GLU:H	2.21	0.48
1:D:111:GLN:HG2	1:D:240:LEU:O	2.13	0.48
1:F:111:GLN:HG2	1:F:240:LEU:O	2.13	0.48
1:B:235:ILE:HB	3:B:502:YE1:HAE	1.93	0.48
1:G:178:LEU:N	1:G:178:LEU:HD12	2.29	0.48
1:H:236:ASN:HA	3:H:502:YE1:N1A	2.28	0.48
1:J:232:SER:HB3	1:J:297:GLY:HA3	1.94	0.48
1:I:338:GLY:O	1:I:342:SER:HB3	2.13	0.48
1:B:99:THR:H	1:B:102:GLN:HE21	1.62	0.48
1:B:232:SER:HB3	1:B:297:GLY:HA3	1.96	0.48
1:B:305:ASP:OD1	1:B:392:ARG:NH1	2.44	0.47
1:J:111:GLN:HG2	1:J:240:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:ARG:NH1	1:C:195:ASP:OD2	2.45	0.47
1:L:186:LEU:HD12	3:L:502:YE1:HC8	1.95	0.47
1:C:338:GLY:O	1:C:342:SER:HB3	2.14	0.47
1:C:367:VAL:CG1	1:C:371:GLU:HB2	2.44	0.47
1:E:367:VAL:CG1	1:E:371:GLU:HB2	2.44	0.47
3:G:502:YE1:OAD	3:G:502:YE1:HAE	2.15	0.47
1:J:235:ILE:HB	3:J:502:YE1:HAE	1.97	0.47
1:I:305:ASP:CG	1:I:392:ARG:HH11	2.23	0.47
1:B:111:GLN:HG2	1:B:240:LEU:O	2.15	0.47
1:E:340:ARG:HD3	1:F:364:ASP:OD1	2.15	0.47
1:F:312:ASP:HB3	1:I:353:TRP:HH2	1.79	0.47
1:H:360:ARG:HH12	1:H:365:GLU:HA	1.80	0.47
1:J:238:LYS:HE3	3:J:502:YE1:O2'	2.14	0.47
1:I:264:ARG:HH11	1:I:264:ARG:HG2	1.80	0.47
1:J:264:ARG:HG2	1:J:264:ARG:HH11	1.80	0.47
1:C:71:ARG:O	1:C:71:ARG:HG3	2.15	0.47
1:D:178:LEU:N	1:D:178:LEU:HD12	2.29	0.47
1:E:264:ARG:HG2	1:E:264:ARG:HH11	1.79	0.47
1:G:28:LEU:HD22	1:G:32:LEU:HD11	1.97	0.47
1:H:111:GLN:HG2	1:H:240:LEU:O	2.15	0.47
1:B:314:TYR:CD1	1:B:351:ARG:HD2	2.50	0.47
1:G:236:ASN:HA	3:G:502:YE1:N1A	2.30	0.47
1:F:111:GLN:NE2	1:F:114:LYS:HE3	2.29	0.47
1:C:107:ARG:HG3	1:C:107:ARG:NH1	2.25	0.47
1:C:314:TYR:CD1	1:C:351:ARG:HD2	2.50	0.47
1:D:148:ARG:NH1	1:D:195:ASP:OD2	2.46	0.47
1:E:232:SER:HB3	1:E:297:GLY:HA3	1.96	0.47
3:F:502:YE1:OAD	3:F:502:YE1:HAE	2.15	0.47
1:D:394:MET:HE3	1:F:408:TYR:CE2	2.50	0.46
1:H:232:SER:HB3	1:H:297:GLY:HA3	1.97	0.46
1:G:370:ASP:OD1	1:G:370:ASP:N	2.42	0.46
1:I:235:ILE:HB	3:I:502:YE1:CAE	2.45	0.46
1:D:99:THR:H	1:D:102:GLN:HE21	1.63	0.46
1:G:111:GLN:HG2	1:G:240:LEU:O	2.14	0.46
1:H:360:ARG:NH1	1:H:364:ASP:O	2.49	0.46
1:K:111:GLN:HG2	1:K:240:LEU:O	2.15	0.46
1:L:305:ASP:CG	1:L:392:ARG:HH11	2.23	0.46
1:C:292:PHE:CZ	3:C:502:YE1:H132	2.51	0.46
1:C:146:THR:HG23	1:C:149:ALA:H	1.81	0.46
1:C:305:ASP:CG	1:C:392:ARG:HH11	2.24	0.46
1:H:305:ASP:CG	1:H:392:ARG:HH11	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:GLN:HG2	1:E:240:LEU:O	2.16	0.46
1:I:111:GLN:HG2	1:I:240:LEU:O	2.15	0.46
1:L:338:GLY:O	1:L:342:SER:HB3	2.15	0.46
1:A:355:LYS:NZ	4:A:605:HOH:O	2.47	0.46
1:I:232:SER:HB3	1:I:297:GLY:HA3	1.98	0.46
1:K:305:ASP:CG	1:K:392:ARG:HH11	2.24	0.46
1:B:305:ASP:CG	1:B:392:ARG:HH11	2.23	0.46
1:I:148:ARG:NH1	1:I:195:ASP:OD2	2.46	0.46
1:H:111:GLN:NE2	1:H:114:LYS:HE3	2.31	0.46
1:H:144:ARG:HG2	1:H:144:ARG:NH1	2.29	0.46
1:F:314:TYR:CD1	1:F:351:ARG:HD2	2.50	0.45
1:H:314:TYR:CD1	1:H:351:ARG:HD2	2.51	0.45
1:A:305:ASP:CG	1:A:392:ARG:HE	2.24	0.45
1:F:28:LEU:HD22	1:F:32:LEU:HD11	1.99	0.45
1:J:148:ARG:NH1	1:J:195:ASP:OD2	2.47	0.45
1:A:235:ILE:HB	3:A:502:YE1:HAE	1.99	0.45
1:E:305:ASP:CG	1:E:392:ARG:HH11	2.25	0.45
1:F:232:SER:HB3	1:F:297:GLY:HA3	1.99	0.45
1:L:264:ARG:HG2	1:L:264:ARG:HH11	1.80	0.45
1:E:235:ILE:HB	3:E:502:YE1:HAE	1.99	0.45
1:L:314:TYR:CD1	1:L:351:ARG:HD2	2.51	0.45
1:B:148:ARG:NH1	1:B:195:ASP:OD2	2.48	0.45
1:D:305:ASP:CG	1:D:392:ARG:HE	2.25	0.45
1:G:148:ARG:NH1	1:G:195:ASP:OD2	2.50	0.45
1:D:232:SER:HB3	1:D:297:GLY:HA3	1.98	0.45
1:E:225:TYR:OH	3:E:502:YE1:O5A	2.32	0.45
1:F:355:LYS:HG3	1:I:353:TRP:CD1	2.52	0.45
1:K:367:VAL:CG1	1:K:371:GLU:HB2	2.47	0.44
1:B:338:GLY:O	1:B:342:SER:HB3	2.17	0.44
1:C:340:ARG:HH11	1:C:340:ARG:HD2	1.52	0.44
1:E:236:ASN:HA	3:E:502:YE1:N1A	2.32	0.44
1:E:338:GLY:O	1:E:342:SER:HB3	2.18	0.44
3:J:502:YE1:HAE	3:J:502:YE1:OAD	2.17	0.44
1:K:99:THR:H	1:K:102:GLN:HE21	1.64	0.44
1:H:338:GLY:O	1:H:342:SER:HB3	2.18	0.44
1:I:314:TYR:CD1	1:I:351:ARG:HD2	2.53	0.44
1:H:325:ILE:O	3:H:502:YE1:HAG	2.18	0.44
1:L:148:ARG:NH1	1:L:195:ASP:OD2	2.51	0.44
1:I:155:GLU:HA	4:I:638:HOH:O	2.17	0.44
1:L:178:LEU:N	1:L:178:LEU:HD12	2.33	0.44
1:B:315[A]:PHE:O	2:B:501[A]:XE:XE	3.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:502:YE1:OAD	3:C:502:YE1:HAE	2.18	0.44
1:J:28:LEU:HD22	1:J:32:LEU:HD11	2.00	0.44
1:H:223:PRO:HA	1:H:226:ARG:HG3	2.01	0.43
1:J:235:ILE:HB	3:J:502:YE1:CAE	2.48	0.43
1:B:235:ILE:HB	3:B:502:YE1:CAE	2.49	0.43
1:E:367:VAL:HG12	1:E:371:GLU:HB2	2.01	0.43
1:C:299:GLN:NE2	1:C:327:GLY:HA3	2.34	0.43
1:E:182:ARG:HH12	1:E:190:ASP:CG	2.20	0.43
1:G:315[B]:PHE:CD1	1:G:315[B]:PHE:C	2.97	0.43
1:G:111:GLN:NE2	1:G:114:LYS:HE3	2.34	0.43
1:H:87:GLU:HG3	1:H:100:GLN:HE21	1.83	0.43
3:J:502:YE1:H4'	3:J:502:YE1:O7A	2.18	0.43
1:A:315[B]:PHE:CD2	1:A:362:LEU:HD13	2.54	0.43
1:I:319:ALA:CB	1:I:323:GLY:HA3	2.49	0.43
1:B:225:TYR:OH	3:B:502:YE1:O5A	2.35	0.42
4:H:606:HOH:O	1:I:385:GLY:CA	2.65	0.42
1:I:235:ILE:HB	3:I:502:YE1:HAE	2.01	0.42
1:G:87:GLU:HG3	1:G:100:GLN:HE21	1.85	0.42
1:A:83:ALA:HA	4:A:626:HOH:O	2.20	0.42
1:K:338:GLY:O	1:K:342:SER:HB3	2.20	0.42
1:E:408:TYR:CE1	1:F:394:MET:CE	3.03	0.42
1:J:315[B]:PHE:CE2	1:J:362:LEU:HD13	2.54	0.42
1:L:319:ALA:CB	1:L:323:GLY:HA3	2.49	0.42
1:I:299:GLN:NE2	1:I:327:GLY:HA3	2.35	0.42
1:F:291:GLY:O	1:F:313:ALA:HA	2.20	0.42
1:G:264:ARG:HG2	1:G:264:ARG:NH1	2.35	0.42
1:C:178:LEU:HD12	1:C:178:LEU:N	2.36	0.41
1:A:111:GLN:NE2	1:A:114:LYS:HE3	2.35	0.41
1:D:319:ALA:CB	1:D:323:GLY:HA3	2.50	0.41
1:F:299:GLN:NE2	1:F:327:GLY:HA3	2.35	0.41
1:D:111:GLN:NE2	1:D:114:LYS:HE3	2.35	0.41
1:F:87:GLU:HG3	1:F:100:GLN:HE21	1.86	0.41
1:F:114:LYS:NZ	4:F:606:HOH:O	2.46	0.41
1:C:367:VAL:HG12	1:C:371:GLU:HB2	2.03	0.41
1:E:321:LYS:NZ	1:F:381:THR:O	2.48	0.41
1:I:178:LEU:HD12	1:I:178:LEU:N	2.36	0.41
1:B:111:GLN:NE2	1:B:114:LYS:HE3	2.36	0.41
1:I:315[B]:PHE:CD2	1:I:362:LEU:HD13	2.56	0.41
1:B:291:GLY:O	1:B:313:ALA:HA	2.20	0.41
1:H:315[B]:PHE:CD2	1:H:362:LEU:HD13	2.56	0.41
1:L:111:GLN:NE2	1:L:114:LYS:HE3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:315[B]:PHE:HD1	1:L:315[B]:PHE:O	2.04	0.41
1:D:212:VAL:HG12	1:D:213:GLY:N	2.36	0.41
1:L:299:GLN:NE2	1:L:327:GLY:HA3	2.36	0.41
1:H:355:LYS:CE	4:H:601:HOH:O	2.69	0.40
1:J:315[B]:PHE:CD2	1:J:362:LEU:HD13	2.56	0.40
1:K:367:VAL:HG12	1:K:371:GLU:HB2	2.04	0.40
1:H:298:ALA:HB1	1:H:315[B]:PHE:CE2	2.56	0.40
3:I:502:YE1:HAE	3:I:502:YE1:OAD	2.22	0.40
1:F:148:ARG:NH1	1:F:195:ASP:OD2	2.50	0.40
1:J:315[B]:PHE:CD1	1:J:315[B]:PHE:C	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	420/440 (96%)	411 (98%)	8 (2%)	1 (0%)	43	63
1	B	421/440 (96%)	413 (98%)	7 (2%)	1 (0%)	43	63
1	C	420/440 (96%)	411 (98%)	8 (2%)	1 (0%)	43	63
1	D	422/440 (96%)	414 (98%)	7 (2%)	1 (0%)	43	63
1	E	420/440 (96%)	411 (98%)	8 (2%)	1 (0%)	43	63
1	F	420/440 (96%)	410 (98%)	9 (2%)	1 (0%)	43	63
1	G	421/440 (96%)	412 (98%)	8 (2%)	1 (0%)	43	63
1	H	421/440 (96%)	413 (98%)	7 (2%)	1 (0%)	43	63
1	I	420/440 (96%)	411 (98%)	8 (2%)	1 (0%)	43	63
1	J	421/440 (96%)	413 (98%)	7 (2%)	1 (0%)	43	63
1	K	421/440 (96%)	411 (98%)	9 (2%)	1 (0%)	43	63
1	L	420/440 (96%)	411 (98%)	8 (2%)	1 (0%)	43	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5047/5280 (96%)	4941 (98%)	94 (2%)	12 (0%)	43 63

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	270	ASP
1	A	270	ASP
1	B	270	ASP
1	D	270	ASP
1	E	270	ASP
1	F	270	ASP
1	G	270	ASP
1	H	270	ASP
1	I	270	ASP
1	J	270	ASP
1	K	270	ASP
1	L	270	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	316/345 (92%)	311 (98%)	5 (2%)	55 77
1	B	328/345 (95%)	319 (97%)	9 (3%)	39 65
1	C	328/345 (95%)	319 (97%)	9 (3%)	39 65
1	D	325/345 (94%)	317 (98%)	8 (2%)	42 67
1	E	326/345 (94%)	320 (98%)	6 (2%)	51 74
1	F	326/345 (94%)	316 (97%)	10 (3%)	35 60
1	G	323/345 (94%)	313 (97%)	10 (3%)	35 60
1	H	325/345 (94%)	318 (98%)	7 (2%)	45 70
1	I	327/345 (95%)	317 (97%)	10 (3%)	35 60
1	J	321/345 (93%)	312 (97%)	9 (3%)	38 64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	327/345 (95%)	319 (98%)	8 (2%)	43	68
1	L	326/345 (94%)	318 (98%)	8 (2%)	42	67
All	All	3898/4140 (94%)	3799 (98%)	99 (2%)	42	67

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	228	LYS
1	A	303	VAL
1	A	411	GLU
1	A	429	VAL
1	B	32	LEU
1	B	111	GLN
1	B	186	LEU
1	B	228	LYS
1	B	321	LYS
1	B	340	ARG
1	B	392	ARG
1	B	411	GLU
1	B	429	VAL
1	C	32	LEU
1	C	107	ARG
1	C	111	GLN
1	C	303	VAL
1	C	340	ARG
1	C	342	SER
1	C	392	ARG
1	C	411	GLU
1	C	429	VAL
1	D	11	THR
1	D	14	LEU
1	D	111	GLN
1	D	303	VAL
1	D	321	LYS
1	D	360	ARG
1	D	411	GLU
1	D	429	VAL
1	E	32	LEU
1	E	40	SER
1	E	111	GLN

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Mol	Chain	Res	Type
1	E	224	ARG
1	E	392	ARG
1	E	429	VAL
1	F	31	THR
1	F	111	GLN
1	F	144	ARG
1	F	155	GLU
1	F	228	LYS
1	F	303	VAL
1	F	321	LYS
1	F	342	SER
1	F	392	ARG
1	F	429	VAL
1	G	14	LEU
1	G	111	GLN
1	G	155	GLU
1	G	228	LYS
1	G	303	VAL
1	G	321	LYS
1	G	360	ARG
1	G	370	ASP
1	G	392	ARG
1	G	429	VAL
1	H	32	LEU
1	H	111	GLN
1	H	155	GLU
1	H	186	LEU
1	H	340	ARG
1	H	392	ARG
1	H	429	VAL
1	I	32	LEU
1	I	111	GLN
1	I	144	ARG
1	I	228	LYS
1	I	303	VAL
1	I	340	ARG
1	I	342	SER
1	I	392	ARG
1	I	411	GLU
1	I	429	VAL
1	J	12	ASP
1	J	31	THR

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Mol	Chain	Res	Type
1	J	39	SER
1	J	111	GLN
1	J	228	LYS
1	J	303	VAL
1	J	360	ARG
1	J	392	ARG
1	J	429	VAL
1	K	11	THR
1	K	32	LEU
1	K	107	ARG
1	K	111	GLN
1	K	155	GLU
1	K	321	LYS
1	K	392	ARG
1	K	429	VAL
1	L	29	LEU
1	L	111	GLN
1	L	303	VAL
1	L	340	ARG
1	L	342	SER
1	L	392	ARG
1	L	411	GLU
1	L	429	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	111	GLN
1	A	168	HIS
1	B	35	HIS
1	B	102	GLN
1	B	111	GLN
1	C	102	GLN
1	C	111	GLN
1	C	168	HIS
1	C	299	GLN
1	D	102	GLN
1	D	111	GLN
1	E	102	GLN
1	E	111	GLN
1	E	222	HIS

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Mol	Chain	Res	Type
1	E	423	HIS
1	F	75	HIS
1	F	79	HIS
1	F	100	GLN
1	F	102	GLN
1	F	111	GLN
1	F	117	HIS
1	F	192	GLN
1	F	299	GLN
1	G	100	GLN
1	G	102	GLN
1	G	111	GLN
1	H	100	GLN
1	H	102	GLN
1	H	111	GLN
1	H	222	HIS
1	I	79	HIS
1	I	102	GLN
1	I	111	GLN
1	I	117	HIS
1	I	299	GLN
1	J	50	HIS
1	J	79	HIS
1	J	100	GLN
1	J	111	GLN
1	K	35	HIS
1	K	102	GLN
1	K	111	GLN
1	K	193	GLN
1	L	64	HIS
1	L	75	HIS
1	L	102	GLN
1	L	111	GLN
1	L	193	GLN
1	L	222	HIS
1	L	299	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 14 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	YE1	C	502	-	60,62,62	3.32	32 (53%)	87,92,92	1.54	14 (16%)
3	YE1	A	502	-	60,62,62	2.71	21 (35%)	87,92,92	1.54	19 (21%)
3	YE1	E	502	-	60,62,62	2.43	20 (33%)	87,92,92	1.51	13 (14%)
3	YE1	F	502	-	60,62,62	2.65	25 (41%)	87,92,92	2.02	25 (28%)
3	YE1	B	502	-	60,62,62	2.64	24 (40%)	87,92,92	1.57	18 (20%)
3	YE1	G	502	-	60,62,62	2.87	23 (38%)	87,92,92	1.55	18 (20%)
3	YE1	I	502	-	60,62,62	2.49	17 (28%)	87,92,92	1.56	12 (13%)
3	YE1	D	502	-	60,62,62	2.51	25 (41%)	87,92,92	1.61	16 (18%)
3	YE1	H	502	-	60,62,62	2.65	24 (40%)	87,92,92	1.67	20 (22%)
3	YE1	J	502	-	60,62,62	2.96	24 (40%)	87,92,92	1.47	14 (16%)
3	YE1	K	502	-	60,62,62	2.48	17 (28%)	87,92,92	1.56	12 (13%)
3	YE1	L	502	-	60,62,62	2.80	22 (36%)	87,92,92	1.74	20 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	YE1	C	502	-	-	5/55/71/71	0/4/4/4
3	YE1	A	502	-	-	10/55/71/71	0/4/4/4
3	YE1	E	502	-	-	8/55/71/71	0/4/4/4
3	YE1	F	502	-	-	7/55/71/71	0/4/4/4
3	YE1	B	502	-	-	11/55/71/71	0/4/4/4
3	YE1	G	502	-	-	8/55/71/71	0/4/4/4
3	YE1	I	502	-	-	3/55/71/71	0/4/4/4
3	YE1	D	502	-	-	12/55/71/71	0/4/4/4
3	YE1	H	502	-	-	11/55/71/71	0/4/4/4
3	YE1	J	502	-	-	17/55/71/71	0/4/4/4
3	YE1	K	502	-	-	3/55/71/71	0/4/4/4
3	YE1	L	502	-	-	10/55/71/71	0/4/4/4

All (274) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	502	YE1	P3'-O3'	15.33	1.86	1.59
3	C	502	YE1	P3'-O3'	15.16	1.86	1.59
3	A	502	YE1	P3'-O3'	14.05	1.84	1.59
3	L	502	YE1	P3'-O3'	11.22	1.79	1.59
3	G	502	YE1	P3'-O3'	10.89	1.78	1.59
3	I	502	YE1	P3'-O3'	10.83	1.78	1.59
3	K	502	YE1	P3'-O3'	10.83	1.78	1.59
3	D	502	YE1	P3'-O3'	9.76	1.76	1.59
3	H	502	YE1	P3'-O3'	9.53	1.76	1.59
3	G	502	YE1	OAK-CAH	9.45	1.58	1.37
3	E	502	YE1	P3'-O3'	9.28	1.75	1.59
3	F	502	YE1	P3'-O3'	7.69	1.73	1.59
3	H	502	YE1	P2A-O6A	7.35	1.88	1.59
3	B	502	YE1	P3'-O3'	7.24	1.72	1.59
3	B	502	YE1	P2A-O6A	7.04	1.87	1.59
3	B	502	YE1	P1A-O3A	7.03	1.67	1.59
3	L	502	YE1	O10-C10	-6.87	1.30	1.42
3	E	502	YE1	P2A-O6A	6.51	1.84	1.59
3	F	502	YE1	P2A-O3A	6.35	1.66	1.59
3	K	502	YE1	OAL-CAJ	6.23	1.51	1.37
3	I	502	YE1	OAL-CAJ	6.21	1.50	1.37
3	C	502	YE1	P2A-O6A	6.21	1.83	1.59
3	C	502	YE1	CAG-CAF	6.17	1.49	1.39
3	J	502	YE1	C12-C11	5.79	1.62	1.52
3	B	502	YE1	C2'-C3'	5.75	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	502	YE1	C14-C11	5.54	1.65	1.53
3	E	502	YE1	C5P-N4P	5.49	1.46	1.33
3	C	502	YE1	C7P-C6P	5.44	1.69	1.51
3	C	502	YE1	C6P-C5P	5.26	1.61	1.51
3	F	502	YE1	C2A-N1A	5.14	1.43	1.33
3	J	502	YE1	P2A-O6A	5.10	1.79	1.59
3	H	502	YE1	CAE-CAJ	-5.02	1.31	1.39
3	F	502	YE1	P2A-O6A	4.94	1.78	1.59
3	F	502	YE1	C8A-N9A	4.90	1.45	1.37
3	C	502	YE1	OAK-CAH	4.77	1.47	1.37
3	C	502	YE1	O10-C10	-4.75	1.33	1.42
3	C	502	YE1	OAD-CAB	4.69	1.32	1.23
3	G	502	YE1	C2P-NAA	4.68	1.56	1.46
3	G	502	YE1	CAG-CAH	4.68	1.46	1.39
3	D	502	YE1	C8A-N7A	4.65	1.40	1.31
3	B	502	YE1	C5A-C4A	4.64	1.47	1.39
3	I	502	YE1	CAI-CAH	4.64	1.46	1.39
3	K	502	YE1	CAI-CAH	4.64	1.46	1.39
3	L	502	YE1	C13-C11	-4.62	1.44	1.53
3	G	502	YE1	C8A-N7A	4.57	1.40	1.31
3	E	502	YE1	OAL-CAJ	4.56	1.47	1.37
3	J	502	YE1	C6P-C5P	-4.52	1.42	1.51
3	J	502	YE1	P1A-O3A	-4.51	1.54	1.59
3	G	502	YE1	P1A-O3A	-4.51	1.54	1.59
3	L	502	YE1	CAC-CAB	4.46	1.61	1.52
3	G	502	YE1	O10-C10	-4.43	1.34	1.42
3	G	502	YE1	C12-C11	4.42	1.59	1.52
3	L	502	YE1	C8A-N9A	4.39	1.45	1.37
3	L	502	YE1	C2'-C3'	4.37	1.62	1.53
3	H	502	YE1	C5P-N4P	4.37	1.43	1.33
3	A	502	YE1	CAG-CAF	4.34	1.46	1.39
3	A	502	YE1	C14-C11	4.28	1.62	1.53
3	L	502	YE1	C2P-NAA	-4.28	1.36	1.46
3	D	502	YE1	OAL-CAJ	4.27	1.46	1.37
3	J	502	YE1	C14-C11	4.22	1.62	1.53
3	D	502	YE1	P2A-O6A	4.21	1.75	1.59
3	D	502	YE1	C12-C11	4.16	1.59	1.52
3	A	502	YE1	C5A-C4A	4.15	1.46	1.39
3	C	502	YE1	C2P-NAA	-4.13	1.36	1.46
3	A	502	YE1	C8A-N7A	4.09	1.39	1.31
3	F	502	YE1	C6A-N6A	4.05	1.44	1.34
3	F	502	YE1	C5A-N7A	4.04	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	YE1	P2A-O6A	4.00	1.75	1.59
3	H	502	YE1	C4A-N3A	3.97	1.41	1.34
3	L	502	YE1	P1A-O5'	3.95	1.74	1.59
3	F	502	YE1	CAI-CAH	-3.93	1.33	1.39
3	B	502	YE1	OAL-CAJ	3.91	1.45	1.37
3	G	502	YE1	P2A-O6A	3.89	1.74	1.59
3	H	502	YE1	O4'-C4'	-3.89	1.36	1.45
3	F	502	YE1	C6P-C5P	-3.87	1.43	1.51
3	A	502	YE1	O2'-C2'	-3.86	1.33	1.43
3	H	502	YE1	O3'-C3'	-3.83	1.31	1.44
3	I	502	YE1	CAE-CAJ	3.81	1.44	1.39
3	K	502	YE1	CAE-CAJ	3.78	1.44	1.39
3	B	502	YE1	CAG-CAF	3.78	1.45	1.39
3	C	502	YE1	CAI-CAJ	3.75	1.44	1.39
3	J	502	YE1	C3'-C4'	3.75	1.62	1.52
3	H	502	YE1	CAB-NAA	3.74	1.42	1.33
3	J	502	YE1	CAI-CAJ	3.74	1.44	1.39
3	L	502	YE1	CAG-CAF	3.74	1.45	1.39
3	L	502	YE1	C5A-C4A	3.73	1.45	1.39
3	I	502	YE1	CAG-CAF	3.73	1.45	1.39
3	C	502	YE1	CAC-CAF	3.73	1.57	1.51
3	K	502	YE1	CAG-CAF	3.72	1.45	1.39
3	D	502	YE1	CAE-CAJ	3.71	1.44	1.39
3	F	502	YE1	C3'-C4'	3.71	1.62	1.52
3	E	502	YE1	C12-C11	3.67	1.58	1.52
3	C	502	YE1	C8A-N9A	3.64	1.43	1.37
3	H	502	YE1	CAG-CAF	3.64	1.45	1.39
3	G	502	YE1	CAI-CAJ	-3.64	1.33	1.39
3	A	502	YE1	C12-C11	3.63	1.58	1.52
3	A	502	YE1	C2P-NAA	3.63	1.54	1.46
3	I	502	YE1	C1'-N9A	3.63	1.56	1.46
3	F	502	YE1	C7P-N8P	3.62	1.54	1.46
3	F	502	YE1	CAI-CAJ	-3.61	1.33	1.39
3	K	502	YE1	C1'-N9A	3.61	1.56	1.46
3	B	502	YE1	C3'-C4'	3.59	1.62	1.52
3	D	502	YE1	C2'-C1'	3.52	1.64	1.53
3	F	502	YE1	CAE-CAJ	3.51	1.44	1.39
3	H	502	YE1	C8A-N9A	3.50	1.43	1.37
3	I	502	YE1	C2'-C3'	3.45	1.60	1.53
3	B	502	YE1	P1A-O5'	3.44	1.72	1.59
3	K	502	YE1	C2'-C3'	3.44	1.60	1.53
3	B	502	YE1	C14-C11	3.42	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	YE1	C6A-N6A	3.41	1.42	1.34
3	D	502	YE1	C7P-C6P	3.40	1.62	1.51
3	E	502	YE1	O4'-C4'	3.35	1.52	1.45
3	D	502	YE1	C5A-C4A	3.35	1.45	1.39
3	H	502	YE1	CAC-CAB	3.34	1.58	1.52
3	I	502	YE1	CAG-CAH	-3.32	1.34	1.39
3	D	502	YE1	C6P-C5P	-3.32	1.44	1.51
3	J	502	YE1	OAD-CAB	3.31	1.29	1.23
3	F	502	YE1	C2'-C1'	3.30	1.63	1.53
3	K	502	YE1	CAG-CAH	-3.28	1.34	1.39
3	F	502	YE1	C14-C11	3.28	1.60	1.53
3	H	502	YE1	C5A-C4A	3.26	1.44	1.39
3	J	502	YE1	C1'-N9A	3.24	1.55	1.46
3	F	502	YE1	O2'-C2'	-3.24	1.34	1.43
3	B	502	YE1	O4'-C1'	3.24	1.49	1.42
3	I	502	YE1	C2A-N1A	3.23	1.39	1.33
3	B	502	YE1	O3'-C3'	-3.23	1.33	1.44
3	C	502	YE1	CAB-NAA	3.22	1.41	1.33
3	G	502	YE1	C5A-N7A	3.22	1.45	1.39
3	K	502	YE1	C2A-N1A	3.22	1.39	1.33
3	A	502	YE1	C6P-C5P	-3.20	1.45	1.51
3	B	502	YE1	C2A-N1A	3.19	1.39	1.33
3	D	502	YE1	O3'-C3'	-3.19	1.33	1.44
3	J	502	YE1	C2P-C3P	3.15	1.64	1.51
3	C	502	YE1	C3'-C4'	3.13	1.61	1.52
3	A	502	YE1	CAI-CAH	3.13	1.43	1.39
3	I	502	YE1	CAB-NAA	3.13	1.40	1.33
3	K	502	YE1	CAB-NAA	3.12	1.40	1.33
3	G	502	YE1	OAD-CAB	3.11	1.29	1.23
3	I	502	YE1	C4A-N3A	3.09	1.40	1.34
3	K	502	YE1	C4A-N3A	3.09	1.40	1.34
3	E	502	YE1	C4A-N9A	-3.04	1.31	1.37
3	C	502	YE1	C3P-N4P	-3.04	1.39	1.46
3	H	502	YE1	C2P-C3P	3.03	1.64	1.51
3	C	502	YE1	P1A-O5'	3.01	1.71	1.59
3	I	502	YE1	O4'-C4'	3.01	1.51	1.45
3	H	502	YE1	C2A-N1A	3.00	1.39	1.33
3	D	502	YE1	O10-C10	3.00	1.47	1.42
3	C	502	YE1	C2A-N1A	3.00	1.39	1.33
3	L	502	YE1	O3'-C3'	-2.99	1.33	1.44
3	K	502	YE1	O4'-C4'	2.99	1.51	1.45
3	E	502	YE1	OAD-CAB	2.99	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	YE1	O6A-C12	-2.98	1.34	1.43
3	D	502	YE1	C3P-N4P	2.98	1.52	1.46
3	C	502	YE1	C14-C11	2.98	1.59	1.53
3	G	502	YE1	C5A-C4A	2.97	1.44	1.39
3	G	502	YE1	C5P-N4P	2.97	1.40	1.33
3	L	502	YE1	CAE-CAF	2.97	1.44	1.39
3	I	502	YE1	P2A-O6A	2.91	1.70	1.59
3	J	502	YE1	C8A-N7A	2.90	1.37	1.31
3	E	502	YE1	C5A-C4A	2.90	1.44	1.39
3	H	502	YE1	C7P-C6P	2.90	1.61	1.51
3	K	502	YE1	P2A-O6A	2.90	1.70	1.59
3	L	502	YE1	P2A-O6A	2.89	1.70	1.59
3	D	502	YE1	O2'-C2'	-2.88	1.35	1.43
3	K	502	YE1	C5A-C4A	2.87	1.44	1.39
3	I	502	YE1	C5A-C4A	2.87	1.44	1.39
3	L	502	YE1	C5P-N4P	2.85	1.40	1.33
3	G	502	YE1	CAG-CAF	2.84	1.44	1.39
3	E	502	YE1	C14-C11	2.84	1.59	1.53
3	E	502	YE1	C3P-N4P	-2.83	1.39	1.46
3	C	502	YE1	C2'-C1'	2.82	1.62	1.53
3	L	502	YE1	C6A-N6A	2.81	1.41	1.34
3	H	502	YE1	C13-C11	2.79	1.59	1.53
3	C	502	YE1	C6A-N6A	2.77	1.41	1.34
3	L	502	YE1	CAB-NAA	2.77	1.39	1.33
3	A	502	YE1	O3'-C3'	-2.76	1.34	1.44
3	B	502	YE1	C4A-N9A	-2.75	1.32	1.37
3	D	502	YE1	P1A-O5'	2.73	1.70	1.59
3	B	502	YE1	P2A-O3A	2.72	1.62	1.59
3	J	502	YE1	OAK-CAH	2.72	1.43	1.37
3	F	502	YE1	C5A-C4A	2.71	1.43	1.39
3	C	502	YE1	C2'-C3'	2.69	1.58	1.53
3	H	502	YE1	C6A-N6A	2.68	1.41	1.34
3	B	502	YE1	CAI-CAH	-2.68	1.35	1.39
3	K	502	YE1	C5'-C4'	2.66	1.59	1.51
3	H	502	YE1	O4'-C1'	-2.65	1.35	1.42
3	J	502	YE1	C5P-N4P	2.64	1.39	1.33
3	I	502	YE1	C5'-C4'	2.64	1.59	1.51
3	B	502	YE1	O6A-C12	-2.62	1.35	1.43
3	D	502	YE1	OAD-CAB	2.61	1.28	1.23
3	A	502	YE1	CAB-NAA	2.61	1.39	1.33
3	J	502	YE1	P1A-O5'	2.60	1.69	1.59
3	C	502	YE1	C5P-N4P	2.60	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	YE1	CAE-CAF	2.58	1.43	1.39
3	D	502	YE1	C7P-N8P	2.58	1.52	1.46
3	F	502	YE1	C5P-N4P	2.56	1.39	1.33
3	A	502	YE1	C2A-N1A	2.55	1.38	1.33
3	B	502	YE1	O2'-C2'	2.52	1.49	1.43
3	A	502	YE1	C13-C11	2.50	1.58	1.53
3	F	502	YE1	P1A-O1A	-2.50	1.43	1.55
3	G	502	YE1	C7P-N8P	2.48	1.51	1.46
3	D	502	YE1	C8A-N9A	2.48	1.41	1.37
3	E	502	YE1	O5'-C5'	-2.48	1.35	1.44
3	E	502	YE1	CAI-CAJ	-2.47	1.35	1.39
3	I	502	YE1	OAD-CAB	2.46	1.28	1.23
3	K	502	YE1	OAD-CAB	2.45	1.28	1.23
3	H	502	YE1	C6A-N1A	2.45	1.42	1.35
3	J	502	YE1	CAG-CAF	2.44	1.43	1.39
3	H	502	YE1	C2'-C3'	2.44	1.58	1.53
3	G	502	YE1	C6P-C5P	2.43	1.56	1.51
3	E	502	YE1	C3'-C4'	2.42	1.59	1.52
3	J	502	YE1	O5P-C5P	-2.41	1.18	1.23
3	J	502	YE1	O4'-C1'	-2.41	1.36	1.42
3	C	502	YE1	O2'-C2'	-2.40	1.37	1.43
3	B	502	YE1	O4'-C4'	2.40	1.50	1.45
3	D	502	YE1	OAK-CAH	2.38	1.42	1.37
3	J	502	YE1	O2'-C2'	-2.38	1.37	1.43
3	L	502	YE1	CAG-CAH	2.35	1.42	1.39
3	F	502	YE1	C12-C11	2.34	1.56	1.52
3	F	502	YE1	C5A-C6A	-2.33	1.34	1.41
3	A	502	YE1	CAI-CAJ	2.33	1.42	1.39
3	G	502	YE1	O3'-C3'	-2.32	1.36	1.44
3	B	502	YE1	C7P-N8P	2.31	1.51	1.46
3	L	502	YE1	C4A-N3A	2.31	1.38	1.34
3	E	502	YE1	O3'-C3'	-2.30	1.36	1.44
3	G	502	YE1	O4'-C4'	2.29	1.50	1.45
3	F	502	YE1	C4A-N9A	-2.29	1.32	1.37
3	F	502	YE1	CAE-CAF	2.28	1.43	1.39
3	D	502	YE1	C5A-C6A	-2.28	1.34	1.41
3	G	502	YE1	P1A-O5'	2.26	1.68	1.59
3	C	502	YE1	P3'-O7A	2.25	1.57	1.50
3	F	502	YE1	P2A-O4A	-2.24	1.45	1.55
3	G	502	YE1	CAB-NAA	2.23	1.38	1.33
3	D	502	YE1	CAB-NAA	2.22	1.38	1.33
3	B	502	YE1	C2P-C3P	2.22	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	YE1	P2A-O4A	-2.21	1.45	1.55
3	H	502	YE1	C14-C11	2.21	1.58	1.53
3	C	502	YE1	OAL-CAJ	2.20	1.41	1.37
3	L	502	YE1	C5'-C4'	-2.20	1.45	1.51
3	J	502	YE1	C8A-N9A	2.18	1.41	1.37
3	J	502	YE1	CAC-CAB	2.18	1.56	1.52
3	J	502	YE1	C2'-C1'	2.18	1.60	1.53
3	E	502	YE1	CAG-CAF	2.17	1.43	1.39
3	A	502	YE1	CAC-CAB	2.17	1.56	1.52
3	A	502	YE1	C1'-N9A	-2.17	1.40	1.46
3	C	502	YE1	C5A-C6A	-2.16	1.35	1.41
3	G	502	YE1	CAI-CAH	-2.14	1.36	1.39
3	D	502	YE1	C3'-C4'	2.13	1.58	1.52
3	E	502	YE1	C6A-N6A	2.13	1.39	1.34
3	D	502	YE1	C14-C11	2.13	1.58	1.53
3	L	502	YE1	OAD-CAB	2.13	1.27	1.23
3	C	502	YE1	P2A-O3A	-2.12	1.57	1.59
3	B	502	YE1	C1'-N9A	-2.11	1.40	1.46
3	G	502	YE1	O5P-C5P	2.11	1.27	1.23
3	I	502	YE1	C14-C11	2.11	1.58	1.53
3	A	502	YE1	P1A-O3A	2.11	1.61	1.59
3	C	502	YE1	C2P-C3P	2.10	1.60	1.51
3	B	502	YE1	C6P-C5P	-2.08	1.47	1.51
3	L	502	YE1	C2'-C1'	2.07	1.60	1.53
3	H	502	YE1	C9P-N8P	2.07	1.38	1.33
3	E	502	YE1	C2'-C1'	2.07	1.60	1.53
3	J	502	YE1	C13-C11	2.07	1.58	1.53
3	C	502	YE1	C13-C11	-2.07	1.49	1.53
3	H	502	YE1	O5'-C5'	-2.07	1.36	1.44
3	K	502	YE1	C14-C11	2.06	1.58	1.53
3	C	502	YE1	CAE-CAJ	2.06	1.42	1.39
3	F	502	YE1	P1A-O3A	2.05	1.61	1.59
3	A	502	YE1	P3'-O7A	2.04	1.56	1.50
3	C	502	YE1	C5'-C4'	-2.04	1.45	1.51
3	H	502	YE1	P3'-O7A	2.03	1.56	1.50
3	J	502	YE1	CAI-CAH	2.02	1.42	1.39
3	E	502	YE1	P2A-O3A	2.02	1.61	1.59
3	C	502	YE1	C7P-N8P	2.01	1.50	1.46
3	E	502	YE1	C2P-NAA	-2.00	1.41	1.46

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	502	YE1	O6A-C12-C11	-7.59	98.35	110.55
3	F	502	YE1	P3'-O3'-C3'	7.33	143.00	123.43
3	E	502	YE1	O3'-P3'-O7A	-5.86	88.43	109.33
3	B	502	YE1	O3'-P3'-O7A	-5.63	89.26	109.33
3	F	502	YE1	O4'-C1'-N9A	-5.57	97.39	108.09
3	F	502	YE1	CAJ-CAE-CAF	-5.11	116.62	120.35
3	G	502	YE1	CAH-CAG-CAF	-4.74	116.89	120.35
3	C	502	YE1	CAC-CAB-NAA	-4.72	109.51	116.06
3	E	502	YE1	C7P-C6P-C5P	-4.50	104.89	112.39
3	F	502	YE1	O3'-C3'-C2'	4.50	127.83	111.68
3	K	502	YE1	O3'-P3'-O7A	-4.37	93.75	109.33
3	I	502	YE1	O3'-P3'-O7A	-4.37	93.76	109.33
3	D	502	YE1	O6A-C12-C11	-4.32	103.60	110.55
3	G	502	YE1	CAC-CAB-NAA	-4.27	110.14	116.06
3	H	502	YE1	CAH-CAG-CAF	-4.26	117.25	120.35
3	H	502	YE1	C7P-C6P-C5P	-4.22	105.36	112.39
3	I	502	YE1	C7P-C6P-C5P	-4.16	105.46	112.39
3	K	502	YE1	C7P-C6P-C5P	-4.16	105.46	112.39
3	F	502	YE1	C4A-N9A-C8A	4.12	110.07	105.74
3	D	502	YE1	CAC-CAB-NAA	-4.12	110.33	116.06
3	F	502	YE1	O6A-C12-C11	-4.12	103.92	110.55
3	D	502	YE1	O3'-P3'-O7A	-4.09	94.76	109.33
3	L	502	YE1	O3'-P3'-O7A	-4.07	94.83	109.33
3	K	502	YE1	CAC-CAB-NAA	-4.01	110.50	116.06
3	I	502	YE1	CAC-CAB-NAA	-3.98	110.53	116.06
3	J	502	YE1	O6A-C12-C11	-3.97	104.17	110.55
3	C	502	YE1	O5P-C5P-C6P	3.93	129.13	122.02
3	B	502	YE1	CAH-CAG-CAF	-3.82	117.56	120.35
3	G	502	YE1	O3'-P3'-O7A	-3.78	95.87	109.33
3	H	502	YE1	P3'-O3'-C3'	3.78	133.51	123.43
3	E	502	YE1	CAC-CAB-NAA	-3.75	110.85	116.06
3	L	502	YE1	CAC-CAB-NAA	-3.65	110.99	116.06
3	I	502	YE1	O6A-C12-C11	-3.62	104.73	110.55
3	K	502	YE1	O6A-C12-C11	-3.62	104.73	110.55
3	K	502	YE1	CAC-CAF-CAG	-3.59	114.93	120.38
3	C	502	YE1	O1A-P1A-O3A	3.59	116.97	107.27
3	H	502	YE1	O8A-P3'-O3'	-3.59	91.88	105.85
3	J	502	YE1	CAC-CAB-NAA	-3.58	111.09	116.06
3	I	502	YE1	CAC-CAF-CAG	-3.58	114.96	120.38
3	J	502	YE1	C7P-C6P-C5P	-3.57	106.44	112.39
3	J	502	YE1	O4A-P2A-O5A	3.55	128.95	112.44
3	L	502	YE1	CAH-CAG-CAF	-3.48	117.81	120.35
3	L	502	YE1	O4A-P2A-O5A	3.47	128.58	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	YE1	O4A-P2A-O5A	3.44	128.44	112.44
3	B	502	YE1	CAF-CAC-CAB	3.42	122.54	112.33
3	A	502	YE1	CAF-CAC-CAB	3.40	122.46	112.33
3	D	502	YE1	C7P-C6P-C5P	-3.38	106.77	112.39
3	A	502	YE1	CAC-CAB-NAA	-3.33	111.44	116.06
3	K	502	YE1	O4A-P2A-O5A	3.29	127.76	112.44
3	H	502	YE1	C4A-N9A-C8A	3.29	109.19	105.74
3	I	502	YE1	O4A-P2A-O5A	3.28	127.72	112.44
3	L	502	YE1	O5P-C5P-C6P	3.25	127.91	122.02
3	C	502	YE1	O4A-P2A-O5A	3.25	127.57	112.44
3	A	502	YE1	O4A-P2A-O5A	3.24	127.52	112.44
3	C	502	YE1	CAJ-CAE-CAF	-3.24	117.99	120.35
3	I	502	YE1	P3'-O3'-C3'	-3.24	114.79	123.43
3	K	502	YE1	P3'-O3'-C3'	-3.23	114.81	123.43
3	B	502	YE1	O4A-P2A-O3A	3.21	115.96	107.27
3	D	502	YE1	O1A-P1A-O2A	3.18	127.25	112.44
3	A	502	YE1	O6A-C12-C11	-3.17	105.44	110.55
3	C	502	YE1	O8A-P3'-O3'	-3.15	93.59	105.85
3	C	502	YE1	O6A-P2A-O5A	-3.12	96.58	108.94
3	F	502	YE1	O4A-P2A-O5A	3.08	126.79	112.44
3	B	502	YE1	O4A-P2A-O5A	3.07	126.73	112.44
3	F	502	YE1	OAL-CAJ-CAI	-3.06	111.84	119.85
3	E	502	YE1	O4A-P2A-O3A	3.04	115.49	107.27
3	C	502	YE1	C6P-C5P-N4P	-3.04	110.80	116.34
3	H	502	YE1	C4A-N9A-C1'	-3.03	119.55	126.63
3	G	502	YE1	O6A-C12-C11	-3.02	105.69	110.55
3	H	502	YE1	O3'-C3'-C2'	3.01	122.48	111.68
3	H	502	YE1	O4'-C1'-C2'	2.99	113.01	106.62
3	D	502	YE1	C13-C11-C10	2.98	113.86	108.77
3	E	502	YE1	C6P-C5P-N4P	-2.91	111.03	116.34
3	F	502	YE1	C13-C11-C12	2.89	113.00	108.22
3	A	502	YE1	O3'-P3'-O7A	-2.86	99.13	109.33
3	G	502	YE1	CAI-CAJ-CAE	2.85	124.39	120.47
3	F	502	YE1	CAC-CAF-CAE	2.84	124.70	120.38
3	J	502	YE1	C2'-C1'-N9A	-2.84	106.26	113.30
3	G	502	YE1	O4A-P2A-O5A	2.84	125.64	112.44
3	A	502	YE1	C4A-N9A-C1'	-2.81	120.06	126.63
3	H	502	YE1	O4A-P2A-O5A	2.80	125.49	112.44
3	B	502	YE1	C3'-C2'-C1'	-2.79	93.76	99.89
3	H	502	YE1	O2'-C2'-C3'	2.77	118.95	111.19
3	L	502	YE1	C10-C9P-N8P	2.71	121.62	116.48
3	E	502	YE1	CAH-CAG-CAF	-2.71	118.38	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	502	YE1	O1A-P1A-O2A	2.70	125.03	112.44
3	L	502	YE1	O4A-P2A-O6A	-2.70	95.32	107.57
3	L	502	YE1	C6P-C5P-N4P	-2.70	111.43	116.34
3	G	502	YE1	C7P-C6P-C5P	-2.69	107.90	112.39
3	B	502	YE1	C4A-N9A-C8A	2.69	108.56	105.74
3	J	502	YE1	O1A-P1A-O2A	2.68	124.90	112.44
3	F	502	YE1	CAI-CAH-CAG	2.67	124.14	120.47
3	D	502	YE1	CAI-CAH-CAG	2.66	124.12	120.47
3	C	502	YE1	O9A-P3'-O8A	2.65	117.75	107.80
3	B	502	YE1	C7P-C6P-C5P	-2.63	108.01	112.39
3	D	502	YE1	O9A-P3'-O7A	2.63	121.08	110.83
3	A	502	YE1	P3'-O3'-C3'	2.62	130.43	123.43
3	E	502	YE1	O9A-P3'-O8A	2.62	117.62	107.80
3	G	502	YE1	O1A-P1A-O2A	2.61	124.61	112.44
3	H	502	YE1	CAC-CAB-NAA	-2.61	112.43	116.06
3	J	502	YE1	O4'-C1'-C2'	2.61	112.21	106.62
3	K	502	YE1	CAC-CAF-CAE	2.60	124.33	120.38
3	E	502	YE1	O4A-P2A-O5A	2.57	124.39	112.44
3	I	502	YE1	CAC-CAF-CAE	2.57	124.28	120.38
3	B	502	YE1	O9A-P3'-O7A	2.56	120.83	110.83
3	H	502	YE1	O4'-C1'-N9A	-2.55	103.19	108.09
3	C	502	YE1	C2'-C3'-C4'	-2.54	98.78	103.24
3	G	502	YE1	O5P-C5P-C6P	2.53	126.60	122.02
3	H	502	YE1	C6P-C5P-N4P	-2.52	111.75	116.34
3	G	502	YE1	OAD-CAB-CAC	2.51	127.44	121.99
3	A	502	YE1	O4'-C1'-C2'	2.51	112.00	106.62
3	F	502	YE1	O3'-C3'-C4'	-2.51	101.19	110.03
3	D	502	YE1	O3A-P1A-O2A	-2.50	103.17	110.70
3	A	502	YE1	C2'-C1'-N9A	-2.50	107.09	113.30
3	G	502	YE1	CAF-CAC-CAB	2.50	119.78	112.33
3	A	502	YE1	O2'-C2'-C1'	-2.50	101.51	110.10
3	F	502	YE1	O4'-C4'-C3'	2.49	110.18	104.92
3	B	502	YE1	O2'-C2'-C3'	2.48	118.14	111.19
3	D	502	YE1	C2P-NAA-CAB	2.48	127.45	122.82
3	I	502	YE1	O4'-C4'-C5'	2.48	117.28	109.33
3	K	502	YE1	O4'-C4'-C5'	2.48	117.28	109.33
3	F	502	YE1	OAK-CAH-CAI	-2.47	113.38	119.85
3	A	502	YE1	CAH-CAG-CAF	-2.46	118.56	120.35
3	L	502	YE1	O2'-C2'-C3'	2.45	118.04	111.19
3	D	502	YE1	CAC-CAF-CAE	2.45	124.10	120.38
3	G	502	YE1	OAK-CAH-CAI	-2.44	113.47	119.85
3	F	502	YE1	O1A-P1A-O2A	2.44	123.78	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	502	YE1	O4A-P2A-O3A	2.42	113.82	107.27
3	F	502	YE1	O4'-C1'-C2'	2.42	111.80	106.62
3	F	502	YE1	C14-C11-C10	2.42	112.89	108.77
3	A	502	YE1	C4A-N9A-C8A	2.42	108.27	105.74
3	K	502	YE1	C6P-C5P-N4P	-2.40	111.96	116.34
3	I	502	YE1	C6P-C5P-N4P	-2.40	111.98	116.34
3	J	502	YE1	C1'-N9A-C8A	2.39	132.41	127.09
3	L	502	YE1	O8A-P3'-O7A	2.38	120.10	110.83
3	D	502	YE1	C13-C11-C12	-2.37	104.31	108.22
3	F	502	YE1	C2A-N1A-C6A	-2.36	114.85	118.73
3	L	502	YE1	CAF-CAC-CAB	2.34	119.31	112.33
3	L	502	YE1	O6A-P2A-O5A	-2.34	99.66	108.94
3	A	502	YE1	O3'-C3'-C2'	2.32	119.98	111.68
3	A	502	YE1	CAC-CAF-CAG	-2.30	116.89	120.38
3	D	502	YE1	CAJ-CAE-CAF	-2.30	118.67	120.35
3	F	502	YE1	CAC-CAF-CAG	-2.30	116.89	120.38
3	H	502	YE1	O9A-P3'-O7A	2.30	119.79	110.83
3	A	502	YE1	O4A-P2A-O6A	-2.30	97.16	107.57
3	H	502	YE1	O4A-P2A-O3A	2.29	113.47	107.27
3	L	502	YE1	O3A-P1A-O2A	-2.27	103.88	110.70
3	B	502	YE1	O4'-C4'-C5'	2.25	116.55	109.33
3	B	502	YE1	O1A-P1A-O2A	2.24	122.85	112.44
3	H	502	YE1	CAI-CAJ-CAE	2.23	123.53	120.47
3	E	502	YE1	CAC-CAF-CAG	-2.23	117.01	120.38
3	C	502	YE1	C3P-C2P-NAA	-2.22	104.62	111.54
3	L	502	YE1	C7P-C6P-C5P	-2.22	108.69	112.39
3	G	502	YE1	C2A-N1A-C6A	-2.22	115.08	118.73
3	C	502	YE1	C7P-C6P-C5P	-2.22	108.69	112.39
3	J	502	YE1	O9A-P3'-O8A	2.21	116.11	107.80
3	E	502	YE1	O1A-P1A-O2A	2.21	122.73	112.44
3	G	502	YE1	C4A-N9A-C8A	2.21	108.06	105.74
3	F	502	YE1	O9A-P3'-O3'	-2.20	97.27	105.85
3	L	502	YE1	P3'-O3'-C3'	-2.20	117.55	123.43
3	F	502	YE1	C5'-C4'-C3'	-2.20	107.05	114.38
3	F	502	YE1	CAH-CAG-CAF	-2.19	118.75	120.35
3	G	502	YE1	O9A-P3'-O8A	2.19	116.02	107.80
3	B	502	YE1	C2P-NAA-CAB	-2.18	118.76	122.82
3	J	502	YE1	C4A-N9A-C1'	-2.18	121.53	126.63
3	K	502	YE1	O8A-P3'-O7A	2.18	119.32	110.83
3	I	502	YE1	O8A-P3'-O7A	2.18	119.32	110.83
3	G	502	YE1	O9A-P3'-O7A	2.15	119.22	110.83
3	C	502	YE1	OAD-CAB-NAA	2.14	127.23	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	YE1	OAK-CAH-CAI	-2.13	114.29	119.85
3	C	502	YE1	N9A-C8A-N7A	-2.12	110.93	113.94
3	H	502	YE1	O3'-C3'-C4'	-2.11	102.58	110.03
3	L	502	YE1	O4'-C1'-N9A	-2.11	104.03	108.09
3	A	502	YE1	O9A-P3'-O8A	2.11	115.72	107.80
3	B	502	YE1	O8A-P3'-O7A	2.11	119.06	110.83
3	A	502	YE1	O1A-P1A-O2A	2.11	122.27	112.44
3	E	502	YE1	O9A-P3'-O7A	2.11	119.05	110.83
3	B	502	YE1	O4'-C1'-C2'	2.10	111.11	106.62
3	A	502	YE1	O1A-P1A-O3A	2.10	112.95	107.27
3	J	502	YE1	C14-C11-C10	2.10	112.35	108.77
3	F	502	YE1	C6P-C5P-N4P	-2.10	112.52	116.34
3	L	502	YE1	O9P-C9P-C10	-2.10	115.04	120.89
3	J	502	YE1	CAC-CAF-CAG	-2.09	117.21	120.38
3	G	502	YE1	CAJ-CAE-CAF	-2.09	118.83	120.35
3	J	502	YE1	CAJ-CAE-CAF	-2.09	118.83	120.35
3	E	502	YE1	CAJ-CAE-CAF	-2.08	118.84	120.35
3	I	502	YE1	O5P-C5P-C6P	2.08	125.78	122.02
3	K	502	YE1	O5P-C5P-C6P	2.07	125.77	122.02
3	B	502	YE1	O4'-C1'-N9A	-2.07	104.12	108.09
3	H	502	YE1	N9A-C8A-N7A	-2.06	111.01	113.94
3	A	502	YE1	C1'-N9A-C8A	2.05	131.65	127.09
3	H	502	YE1	O1A-P1A-O2A	2.05	121.98	112.44
3	H	502	YE1	O9A-P3'-O8A	2.05	115.48	107.80
3	D	502	YE1	CAC-CAF-CAG	-2.05	117.28	120.38
3	G	502	YE1	O3A-P1A-O2A	-2.04	104.57	110.70
3	D	502	YE1	O5P-C5P-N4P	-2.02	119.06	123.03
3	F	502	YE1	OAL-CAJ-CAE	2.02	125.14	119.85
3	F	502	YE1	N9A-C8A-N7A	-2.01	111.08	113.94
3	B	502	YE1	C6P-C5P-N4P	-2.01	112.68	116.34
3	E	502	YE1	CAF-CAC-CAB	2.01	118.33	112.33
3	L	502	YE1	C13-C11-C10	2.00	112.18	108.77

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	YE1	C2'-C3'-O3'-P3'
3	A	502	YE1	C5'-O5'-P1A-O2A
3	A	502	YE1	C5'-O5'-P1A-O3A
3	B	502	YE1	P1A-O3A-P2A-O6A
3	B	502	YE1	C14-C11-C12-O6A

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Mol	Chain	Res	Type	Atoms
3	B	502	YE1	C13-C11-C12-O6A
3	B	502	YE1	C10-C11-C12-O6A
3	D	502	YE1	C5'-O5'-P1A-O2A
3	D	502	YE1	C5'-O5'-P1A-O3A
3	E	502	YE1	C5'-O5'-P1A-O2A
3	E	502	YE1	C5'-O5'-P1A-O3A
3	F	502	YE1	C2'-C3'-O3'-P3'
3	F	502	YE1	C5'-O5'-P1A-O2A
3	F	502	YE1	C5'-O5'-P1A-O3A
3	G	502	YE1	C5'-O5'-P1A-O2A
3	H	502	YE1	C2'-C3'-O3'-P3'
3	H	502	YE1	C5'-O5'-P1A-O1A
3	H	502	YE1	C5'-O5'-P1A-O3A
3	I	502	YE1	C5'-O5'-P1A-O2A
3	J	502	YE1	C5'-O5'-P1A-O2A
3	J	502	YE1	C5'-O5'-P1A-O3A
3	J	502	YE1	C12-O6A-P2A-O5A
3	J	502	YE1	C14-C11-C12-O6A
3	J	502	YE1	C13-C11-C12-O6A
3	K	502	YE1	C5'-O5'-P1A-O2A
3	L	502	YE1	C5'-O5'-P1A-O2A
3	L	502	YE1	O10-C10-C9P-N8P
3	J	502	YE1	C6P-C7P-N8P-C9P
3	J	502	YE1	C4'-C3'-O3'-P3'
3	H	502	YE1	C6P-C7P-N8P-C9P
3	J	502	YE1	C2'-C3'-O3'-P3'
3	H	502	YE1	CAB-CAC-CAF-CAE
3	L	502	YE1	O10-C10-C9P-O9P
3	H	502	YE1	CAB-CAC-CAF-CAG
3	B	502	YE1	C2P-C3P-N4P-C5P
3	B	502	YE1	P2A-O3A-P1A-O2A
3	G	502	YE1	P1A-O3A-P2A-O5A
3	D	502	YE1	CAB-CAC-CAF-CAE
3	F	502	YE1	CAB-CAC-CAF-CAE
3	J	502	YE1	CAB-CAC-CAF-CAE
3	L	502	YE1	CAB-CAC-CAF-CAG
3	L	502	YE1	CAB-CAC-CAF-CAE
3	G	502	YE1	CAB-CAC-CAF-CAG
3	G	502	YE1	CAB-CAC-CAF-CAE
3	J	502	YE1	CAB-CAC-CAF-CAG
3	D	502	YE1	CAB-CAC-CAF-CAG
3	F	502	YE1	CAB-CAC-CAF-CAG

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Mol	Chain	Res	Type	Atoms
3	I	502	YE1	CAB-CAC-CAF-CAG
3	K	502	YE1	CAB-CAC-CAF-CAG
3	I	502	YE1	CAB-CAC-CAF-CAE
3	K	502	YE1	CAB-CAC-CAF-CAE
3	D	502	YE1	P1A-O3A-P2A-O6A
3	J	502	YE1	C3P-C2P-NAA-CAB
3	L	502	YE1	C2'-C3'-O3'-P3'
3	A	502	YE1	CAB-CAC-CAF-CAG
3	A	502	YE1	CAB-CAC-CAF-CAE
3	C	502	YE1	CAB-CAC-CAF-CAE
3	B	502	YE1	P2A-O3A-P1A-O1A
3	C	502	YE1	P1A-O3A-P2A-O4A
3	G	502	YE1	P1A-O3A-P2A-O4A
3	C	502	YE1	O10-C10-C9P-O9P
3	D	502	YE1	C14-C11-C12-O6A
3	D	502	YE1	C13-C11-C12-O6A
3	J	502	YE1	C4'-C5'-O5'-P1A
3	C	502	YE1	CAB-CAC-CAF-CAG
3	D	502	YE1	C10-C11-C12-O6A
3	J	502	YE1	C10-C11-C12-O6A
3	A	502	YE1	C5'-O5'-P1A-O1A
3	D	502	YE1	C5'-O5'-P1A-O1A
3	E	502	YE1	C5'-O5'-P1A-O1A
3	F	502	YE1	C5'-O5'-P1A-O1A
3	G	502	YE1	C5'-O5'-P1A-O1A
3	G	502	YE1	C5'-O5'-P1A-O3A
3	J	502	YE1	C5'-O5'-P1A-O1A
3	E	502	YE1	C4'-C5'-O5'-P1A
3	H	502	YE1	C4'-C5'-O5'-P1A
3	L	502	YE1	C4'-C3'-O3'-P3'
3	B	502	YE1	CAB-CAC-CAF-CAG
3	J	502	YE1	O4'-C4'-C5'-O5'
3	E	502	YE1	CAB-CAC-CAF-CAG
3	A	502	YE1	C5P-C6P-C7P-N8P
3	H	502	YE1	O10-C10-C11-C13
3	H	502	YE1	P1A-O3A-P2A-O4A
3	G	502	YE1	C3'-O3'-P3'-O9A
3	A	502	YE1	C4'-C5'-O5'-P1A
3	C	502	YE1	O10-C10-C9P-N8P
3	A	502	YE1	C6P-C7P-N8P-C9P
3	E	502	YE1	CAB-CAC-CAF-CAE
3	B	502	YE1	C4'-C5'-O5'-P1A

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Mol	Chain	Res	Type	Atoms
3	E	502	YE1	C3'-O3'-P3'-O7A
3	D	502	YE1	P2A-O3A-P1A-O1A
3	F	502	YE1	C4'-C5'-O5'-P1A
3	B	502	YE1	C3P-C2P-NAA-CAB
3	D	502	YE1	C4'-C5'-O5'-P1A
3	H	502	YE1	O10-C10-C11-C14
3	D	502	YE1	P2A-O3A-P1A-O2A
3	J	502	YE1	P2A-O3A-P1A-O2A
3	L	502	YE1	P2A-O3A-P1A-O2A
3	B	502	YE1	CAB-CAC-CAF-CAE
3	H	502	YE1	C11-C10-C9P-O9P
3	L	502	YE1	C11-C10-C9P-O9P
3	J	502	YE1	C3'-O3'-P3'-O8A
3	E	502	YE1	C13-C11-C12-O6A
3	L	502	YE1	C11-C10-C9P-N8P
3	A	502	YE1	P2A-O3A-P1A-O2A

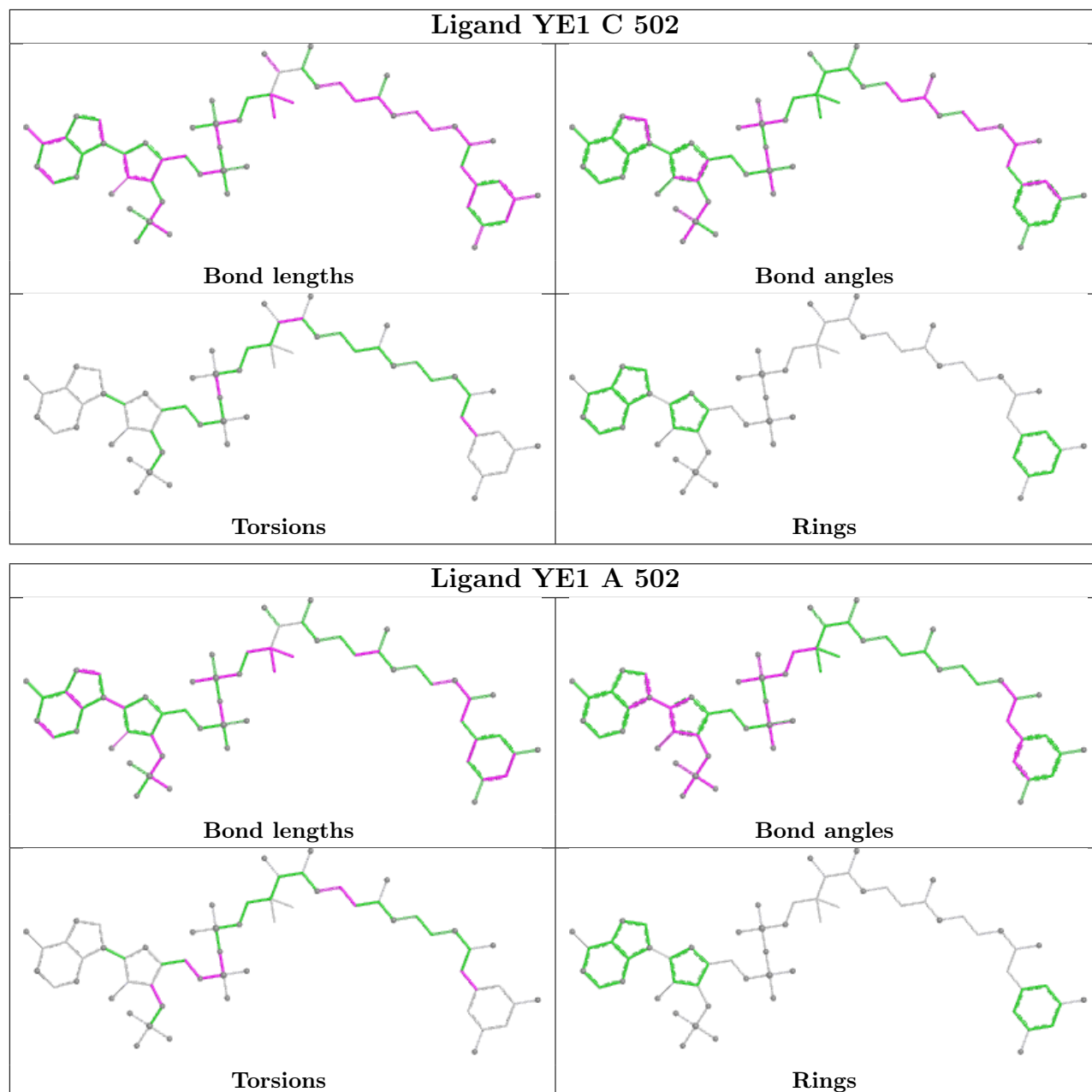
There are no ring outliers.

11 monomers are involved in 36 short contacts:

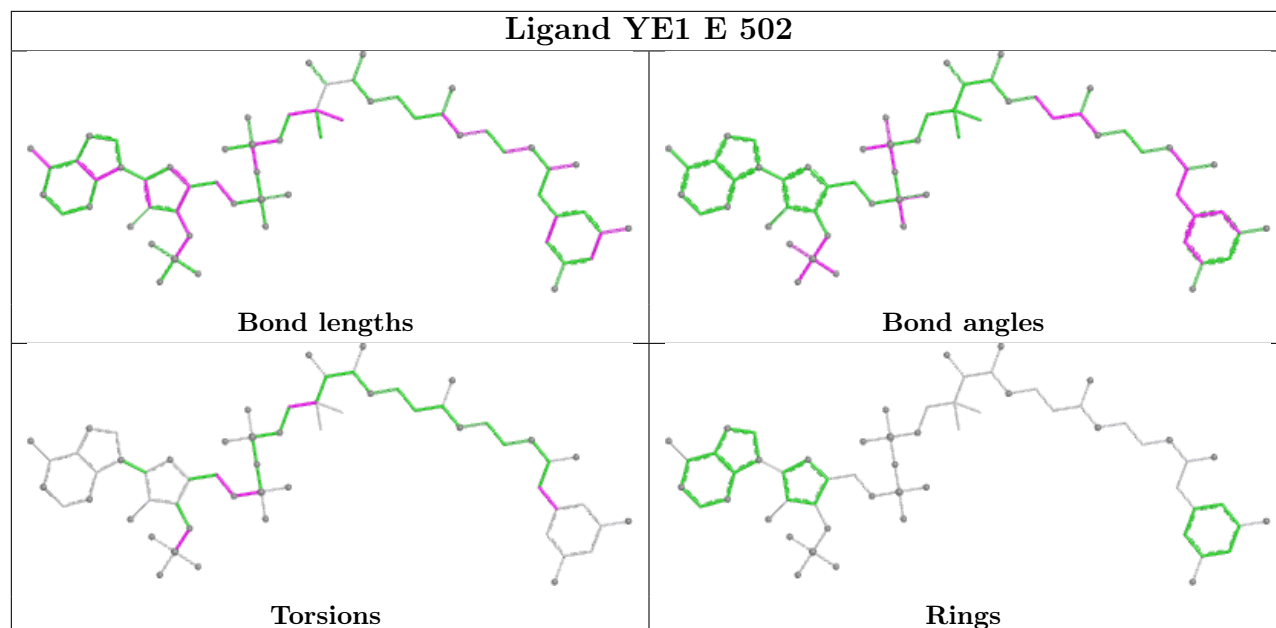
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	YE1	2	0
3	A	502	YE1	1	0
3	E	502	YE1	5	0
3	F	502	YE1	2	0
3	B	502	YE1	4	0
3	G	502	YE1	2	0
3	I	502	YE1	4	0
3	D	502	YE1	2	0
3	H	502	YE1	4	0
3	J	502	YE1	9	0
3	L	502	YE1	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

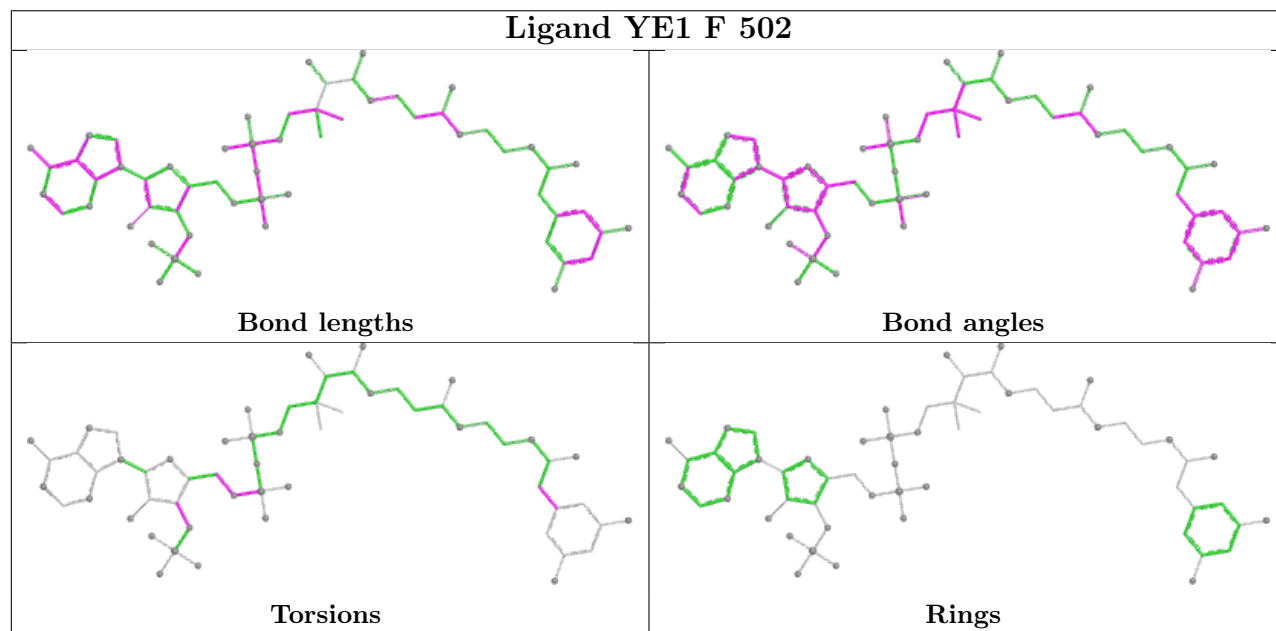
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



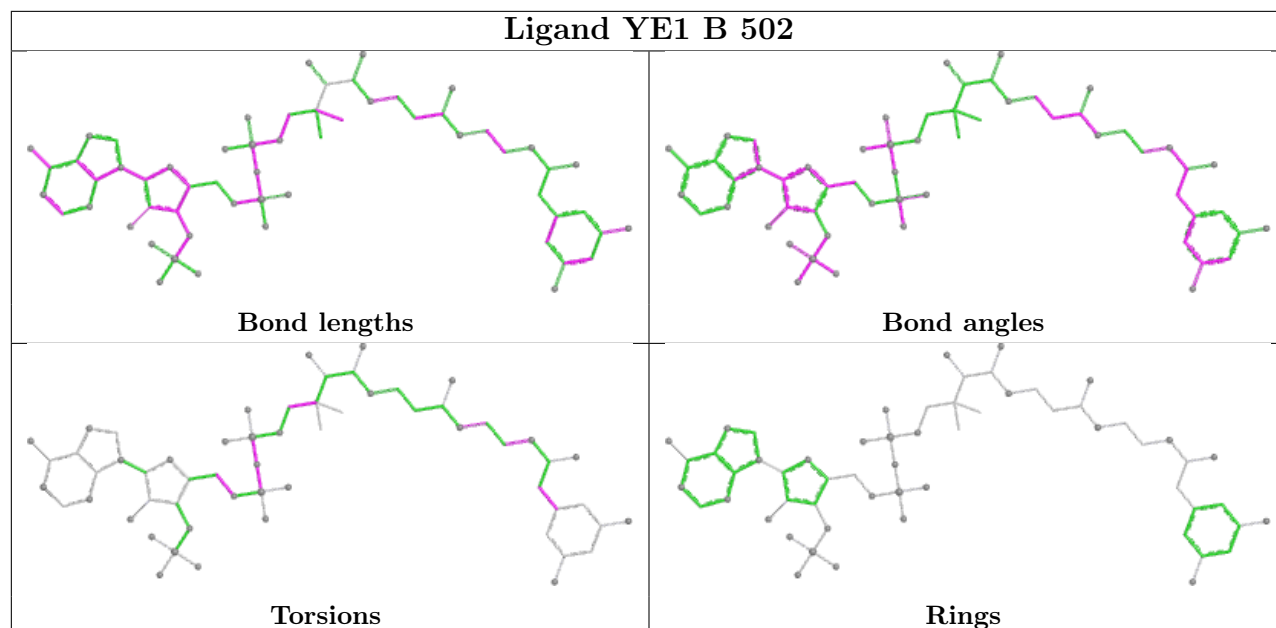
Ligand YE1 E 502



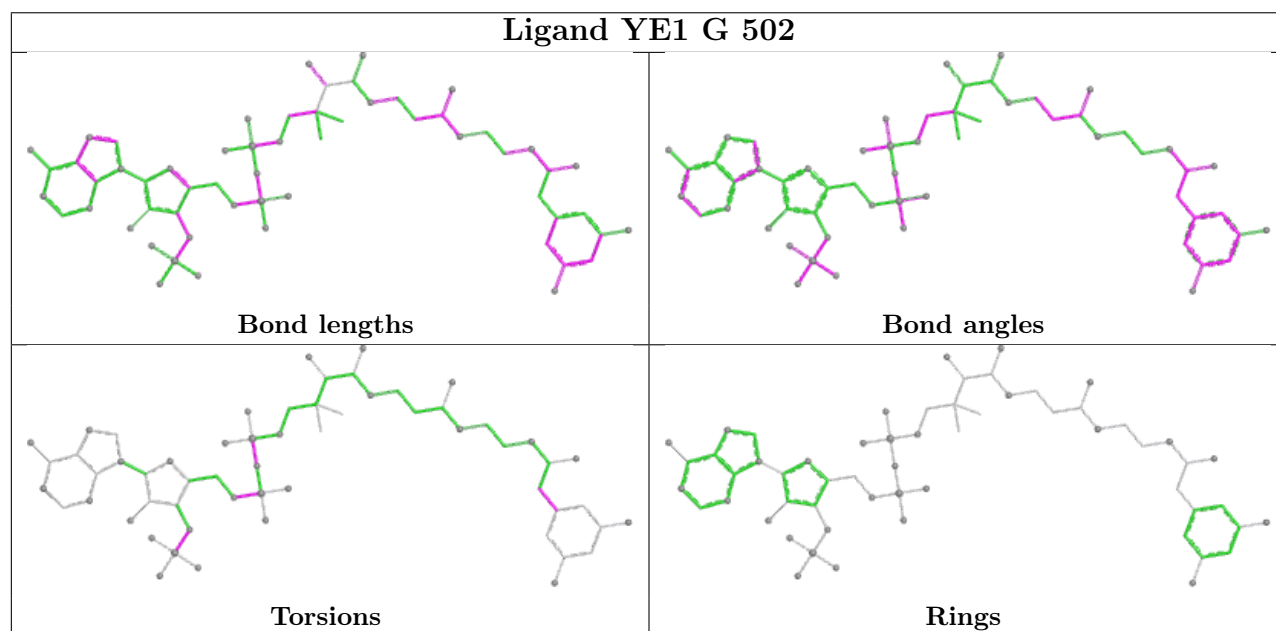
Ligand YE1 F 502

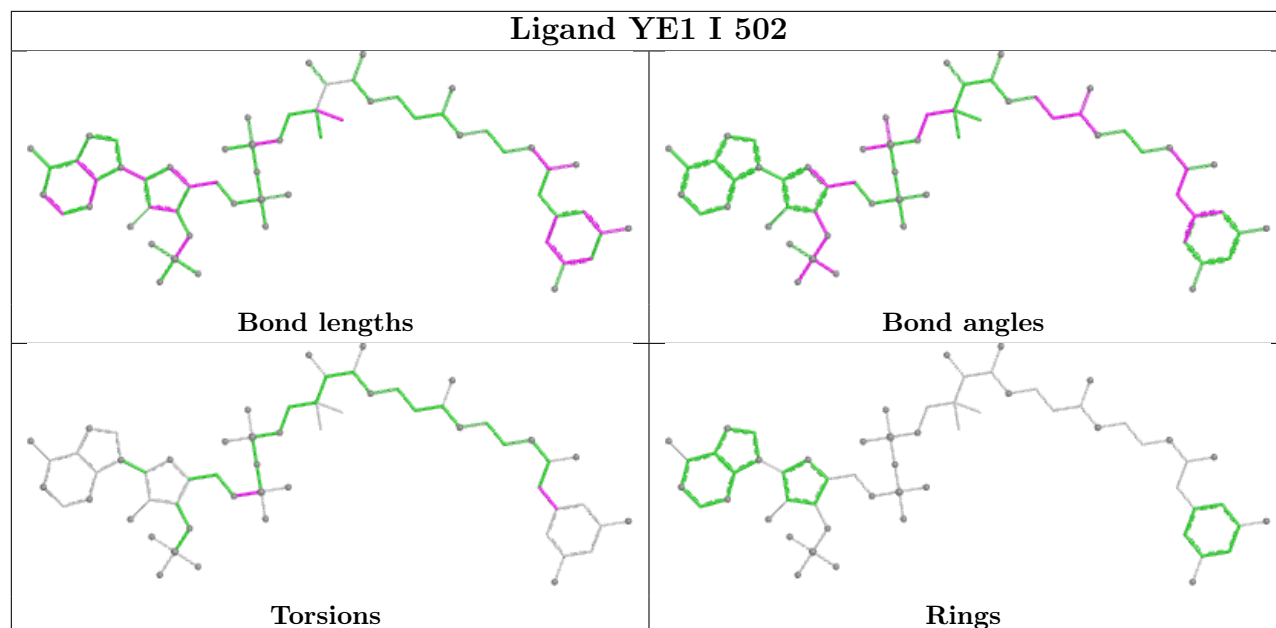
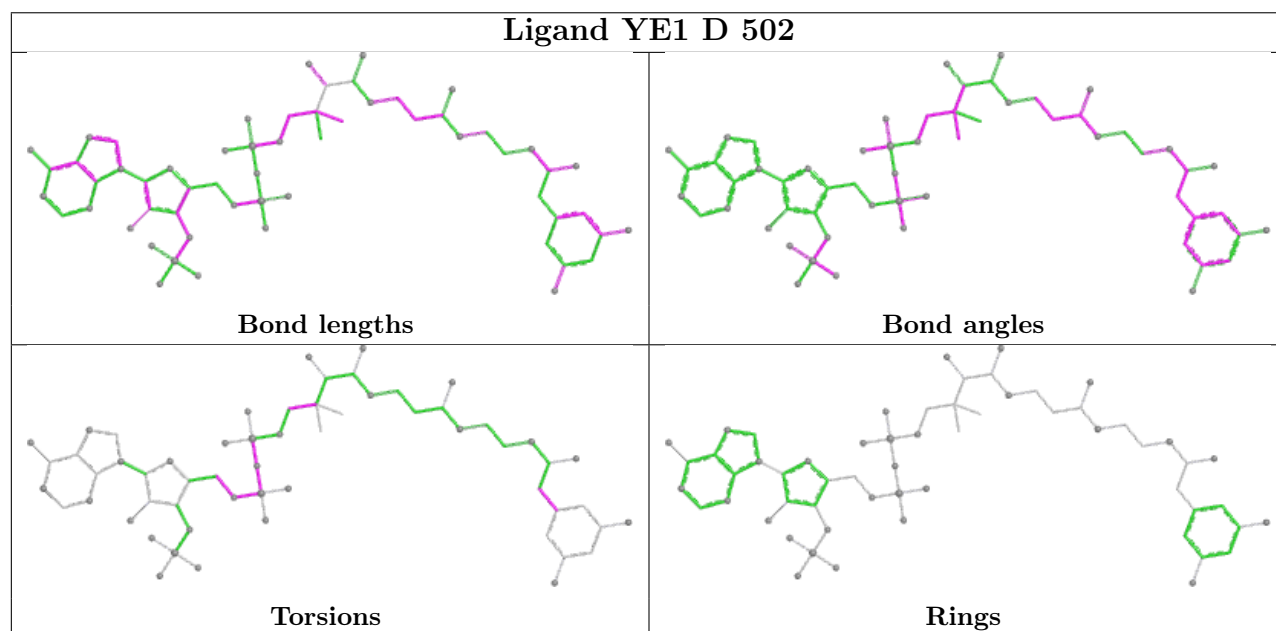


Ligand YE1 B 502

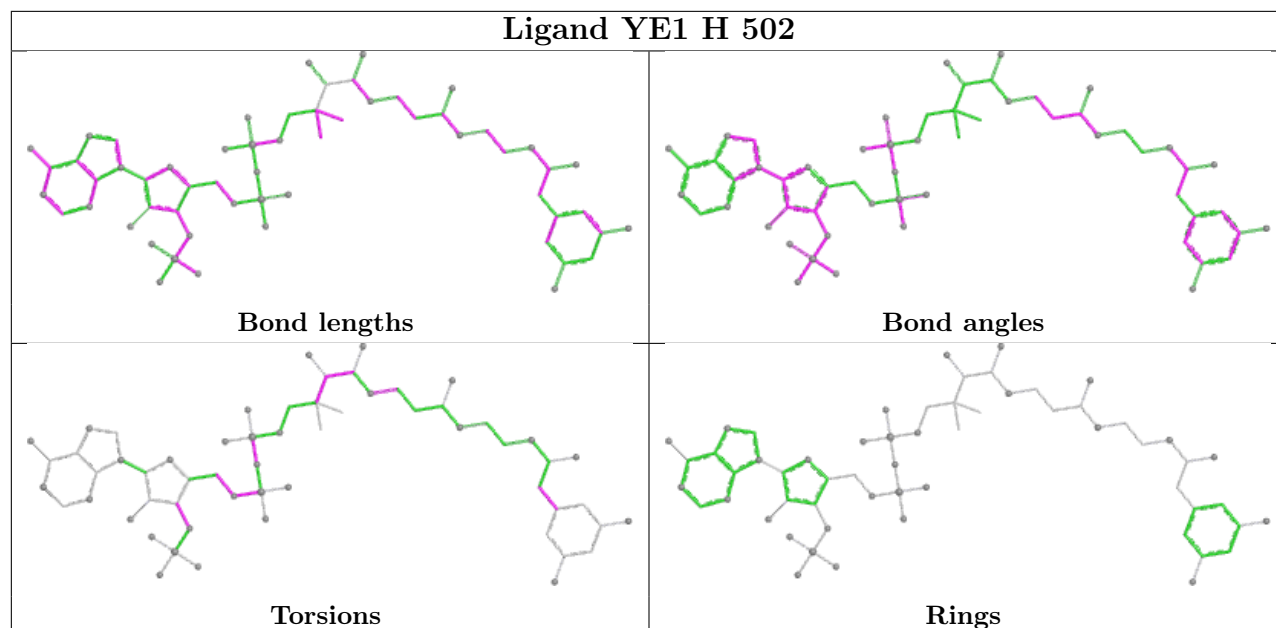


Ligand YE1 G 502

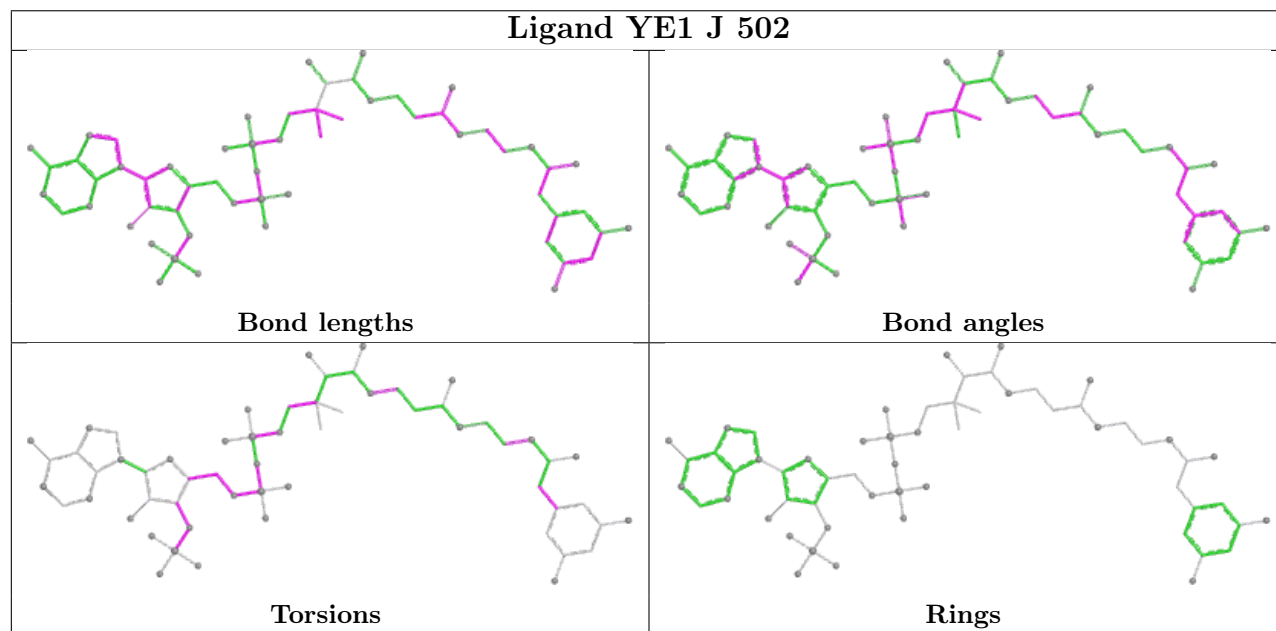


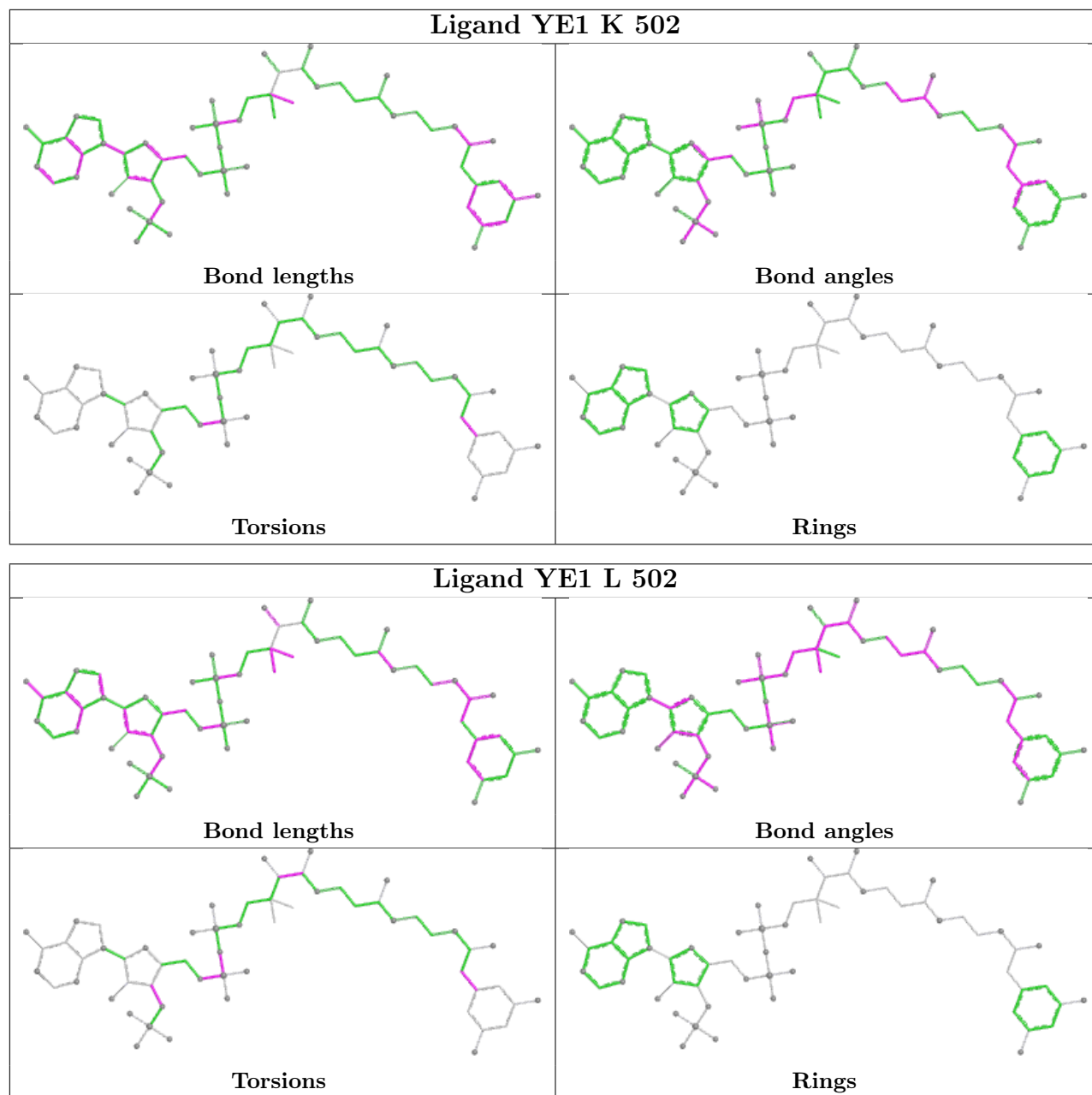
Ligand YE1 I 502**Ligand YE1 D 502**

Ligand YE1 H 502



Ligand YE1 J 502





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	421/440 (95%)	-1.31	0 100 100	11, 39, 80, 111	1 (0%)
1	B	422/440 (95%)	-1.38	0 100 100	13, 38, 62, 77	1 (0%)
1	C	421/440 (95%)	-1.36	0 100 100	12, 37, 67, 90	1 (0%)
1	D	423/440 (96%)	-1.39	0 100 100	11, 32, 52, 68	1 (0%)
1	E	421/440 (95%)	-1.42	0 100 100	11, 35, 59, 76	1 (0%)
1	F	421/440 (95%)	-1.40	0 100 100	15, 34, 56, 74	1 (0%)
1	G	422/440 (95%)	-1.42	0 100 100	11, 32, 62, 83	1 (0%)
1	H	422/440 (95%)	-1.32	0 100 100	10, 41, 65, 86	1 (0%)
1	I	421/440 (95%)	-1.41	0 100 100	13, 34, 59, 74	1 (0%)
1	J	422/440 (95%)	-1.28	0 100 100	16, 44, 78, 108	1 (0%)
1	K	422/440 (95%)	-1.38	0 100 100	13, 33, 59, 77	1 (0%)
1	L	421/440 (95%)	-1.32	0 100 100	9, 38, 72, 103	1 (0%)
All	All	5059/5280 (95%)	-1.37	0 100 100	9, 36, 65, 111	12 (0%)

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 ⓘ

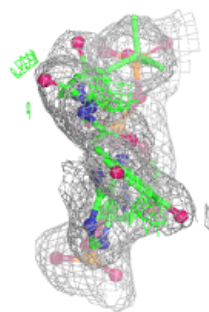
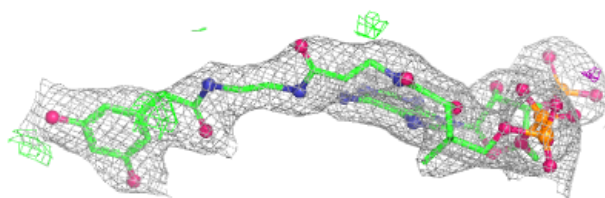
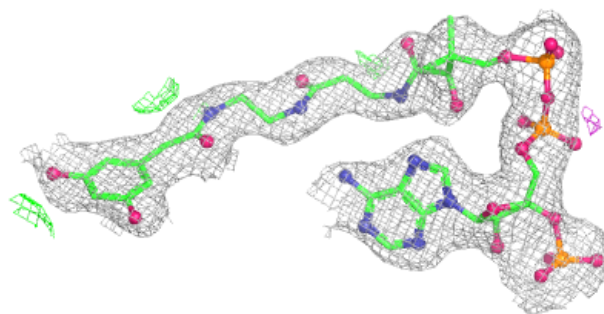
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	XE	A	501[A]	1/1	0.98	0.06	58,58,58,58	1
2	XE	A	501[B]	1/1	0.98	0.06	47,47,47,47	1
2	XE	B	501[A]	1/1	0.99	0.02	27,27,27,27	1
2	XE	B	501[B]	1/1	0.99	0.02	43,43,43,43	1
3	YE1	A	502	59/59	0.99	0.04	29,46,64,73	0
3	YE1	B	502	59/59	0.99	0.04	14,43,55,57	0
3	YE1	C	502	59/59	0.99	0.03	13,32,49,55	0
3	YE1	D	502	59/59	0.99	0.03	15,28,43,47	0
3	YE1	E	502	59/59	0.99	0.04	27,45,59,63	0
3	YE1	F	502	59/59	0.99	0.03	23,35,44,53	0
3	YE1	G	502	59/59	0.99	0.03	19,36,54,58	0
3	YE1	H	502	59/59	0.99	0.04	19,42,67,73	0
3	YE1	I	502	59/59	0.99	0.04	17,37,47,50	0
3	YE1	J	502	59/59	0.99	0.04	28,49,68,75	0
3	YE1	K	502	59/59	0.99	0.03	17,37,47,50	0
3	YE1	L	502	59/59	0.99	0.04	23,37,49,63	0
2	XE	E	501[B]	1/1	1.00	0.02	55,55,55,55	1
2	XE	F	501[B]	1/1	1.00	0.03	39,39,39,39	1
2	XE	G	501[B]	1/1	1.00	0.03	36,36,36,36	1
2	XE	H	501[B]	1/1	1.00	0.05	47,47,47,47	1
2	XE	I	501[B]	1/1	1.00	0.03	37,37,37,37	1
2	XE	J	501[B]	1/1	1.00	0.02	46,46,46,46	1
2	XE	K	501[B]	1/1	1.00	0.01	63,63,63,63	1
2	XE	L	501[B]	1/1	1.00	0.07	101,101,101,101	1
2	XE	C	501[B]	1/1	1.00	0.02	48,48,48,48	1
2	XE	D	501[B]	1/1	1.00	0.02	24,24,24,24	1

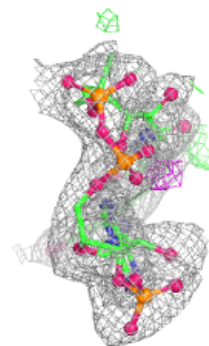
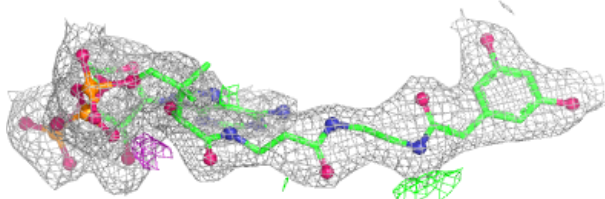
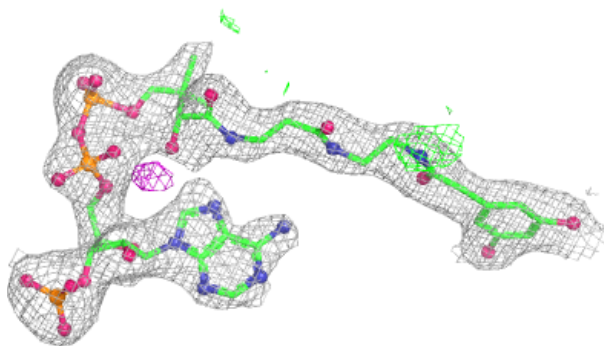
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around YE1 A 502:

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

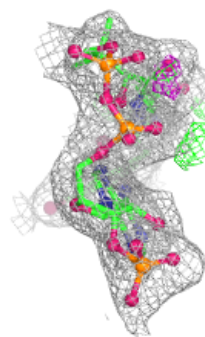
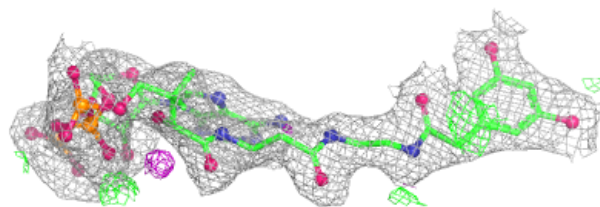
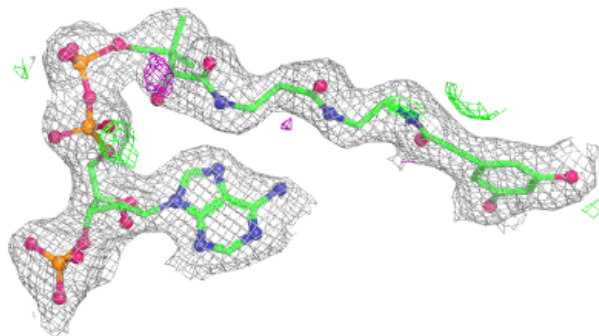
**Electron density around YE1 B 502:**

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

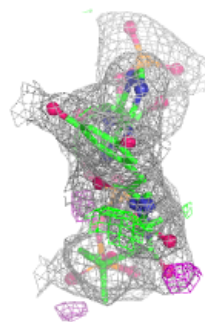
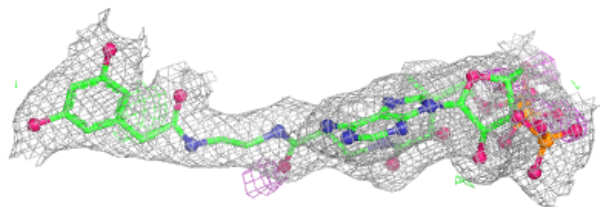
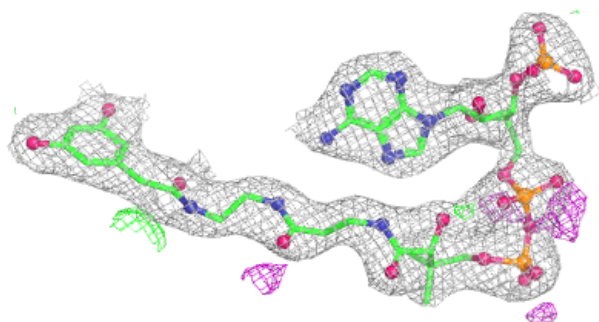


Electron density around YE1 C 502:

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

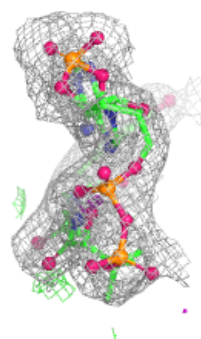
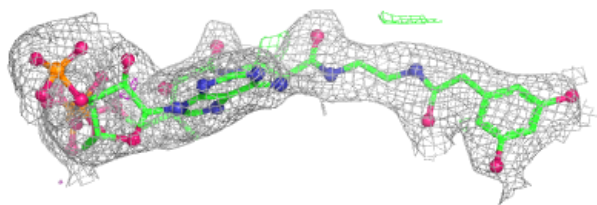
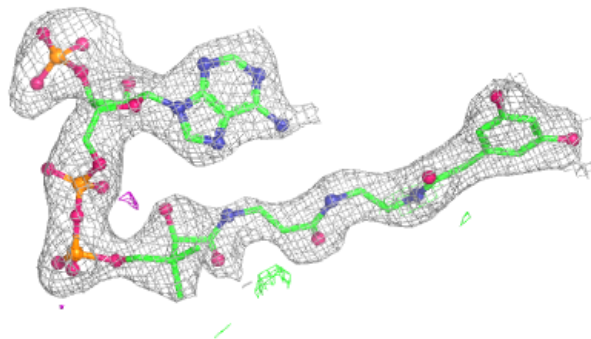
**Electron density around YE1 D 502:**

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

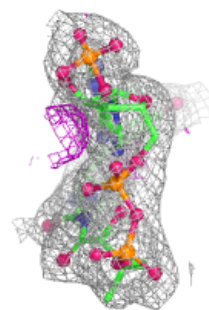
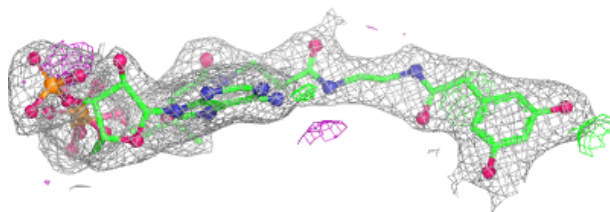
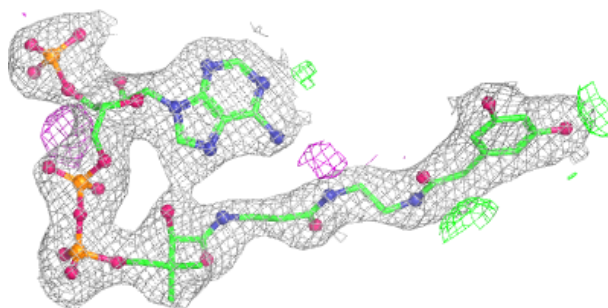


Electron density around YE1 E 502:

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

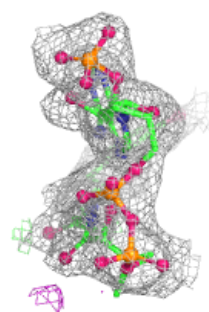
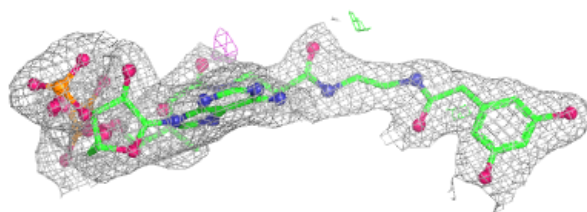
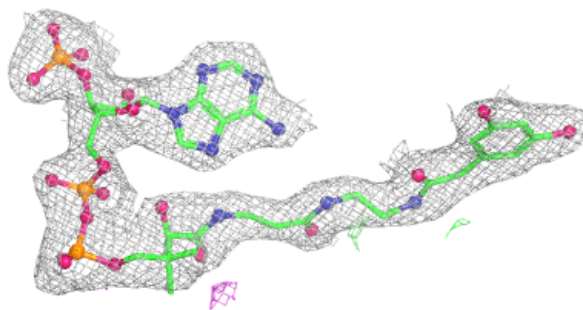
**Electron density around YE1 F 502:**

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

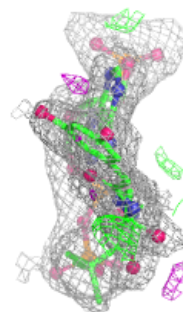
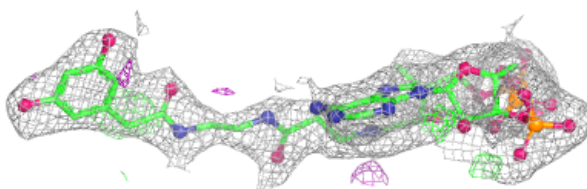
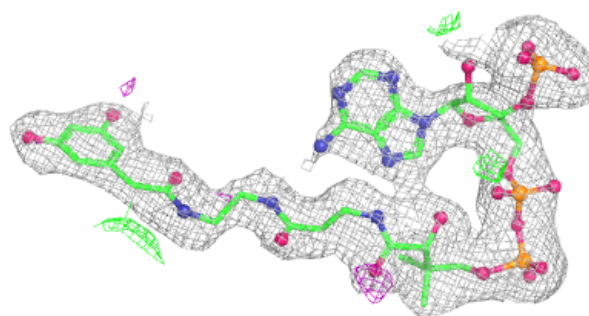


Electron density around YE1 G 502:

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

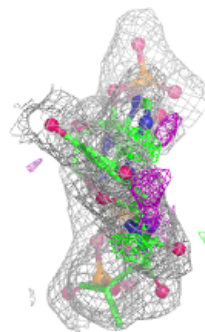
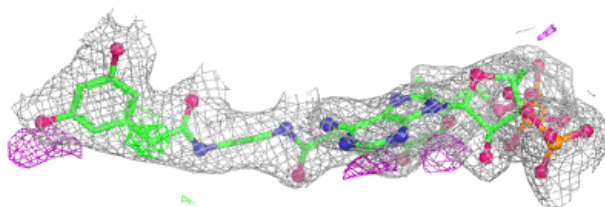
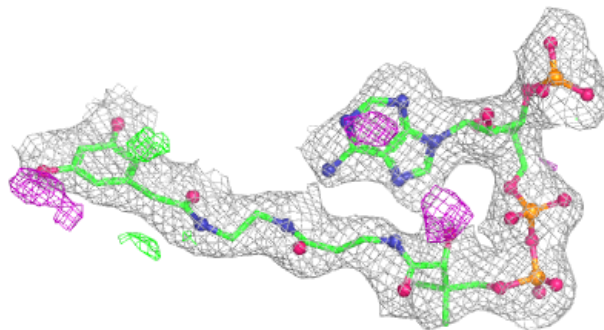
**Electron density around YE1 H 502:**

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

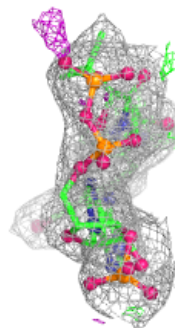
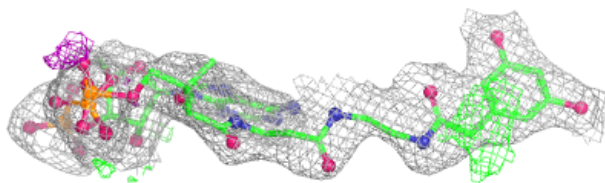
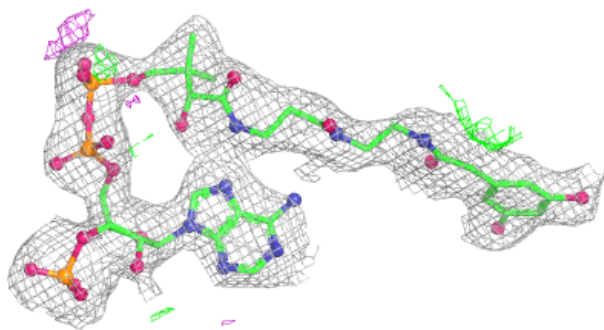


Electron density around YE1 I 502:

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

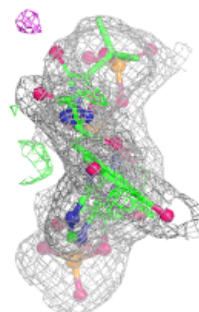
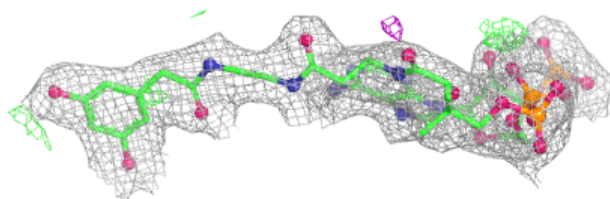
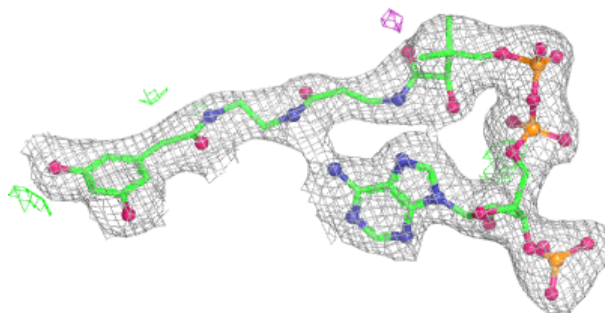
**Electron density around YE1 J 502:**

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

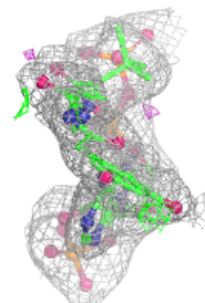
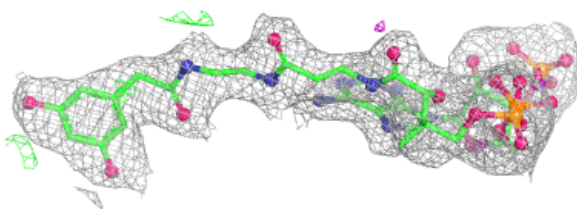
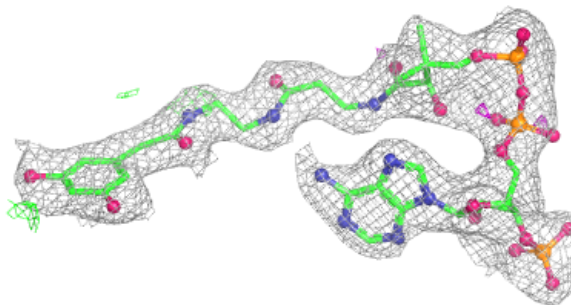


Electron density around YE1 K 502:

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

**Electron density around YE1 L 502:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.