



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2016 – 12:22 PM EDT

PDB ID : 4YLH  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027674  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027674

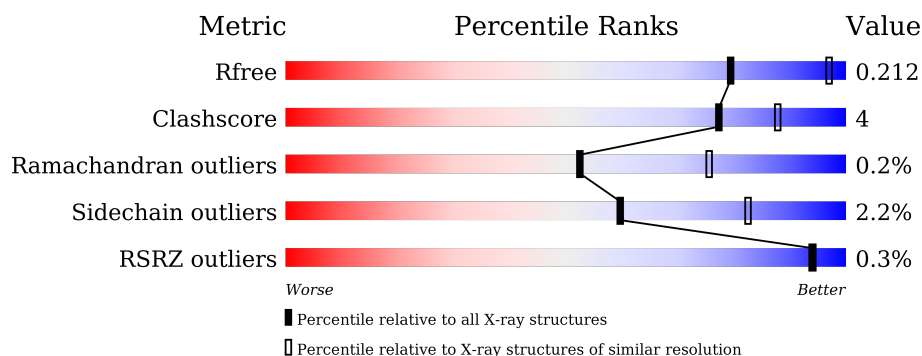
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>86%</div> <div>9%</div> <div>..</div> </div>
1	B	440	<div> <div>88%</div> <div>7%</div> <div>..</div> </div>
1	C	440	<div> <div>86%</div> <div>8%</div> <div>..</div> </div>
1	D	440	<div> <div>86%</div> <div>9%</div> <div>..</div> </div>
1	E	440	<div> <div>86%</div> <div>9%</div> <div>.</div> </div>
1	F	440	<div> <div>83%</div> <div>11%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	440	 87% 8% . .
1	H	440	 86% 9% . .
1	I	440	 85% 10% . .
1	J	440	 2% 86% 9% . .
1	K	440	 88% 7% . .
1	L	440	 86% 8% .. .

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 Q8CLK7
A	0	MET	-	expression tag	UNP Q8CLK7
A	1	GLY	-	expression tag	UNP Q8CLK7
B	-1	ALA	-	expression tag	UNP Q8CLK7
B	0	MET	-	expression tag	UNP Q8CLK7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	expression tag	UNP Q8KLK7
C	-1	ALA	-	expression tag	UNP Q8KLK7
C	0	MET	-	expression tag	UNP Q8KLK7
C	1	GLY	-	expression tag	UNP Q8KLK7
D	-1	ALA	-	expression tag	UNP Q8KLK7
D	0	MET	-	expression tag	UNP Q8KLK7
D	1	GLY	-	expression tag	UNP Q8KLK7
E	-1	ALA	-	expression tag	UNP Q8KLK7
E	0	MET	-	expression tag	UNP Q8KLK7
E	1	GLY	-	expression tag	UNP Q8KLK7
F	-1	ALA	-	expression tag	UNP Q8KLK7
F	0	MET	-	expression tag	UNP Q8KLK7
F	1	GLY	-	expression tag	UNP Q8KLK7
G	-1	ALA	-	expression tag	UNP Q8KLK7
G	0	MET	-	expression tag	UNP Q8KLK7
G	1	GLY	-	expression tag	UNP Q8KLK7
H	-1	ALA	-	expression tag	UNP Q8KLK7
H	0	MET	-	expression tag	UNP Q8KLK7
H	1	GLY	-	expression tag	UNP Q8KLK7
I	-1	ALA	-	expression tag	UNP Q8KLK7
I	0	MET	-	expression tag	UNP Q8KLK7
I	1	GLY	-	expression tag	UNP Q8KLK7
J	-1	ALA	-	expression tag	UNP Q8KLK7
J	0	MET	-	expression tag	UNP Q8KLK7
J	1	GLY	-	expression tag	UNP Q8KLK7
K	-1	ALA	-	expression tag	UNP Q8KLK7
K	0	MET	-	expression tag	UNP Q8KLK7
K	1	GLY	-	expression tag	UNP Q8KLK7
L	-1	ALA	-	expression tag	UNP Q8KLK7
L	0	MET	-	expression tag	UNP Q8KLK7
L	1	GLY	-	expression tag	UNP Q8KLK7

- Molecule 2 is XENON (three-letter code: XE) (formula: Xe).

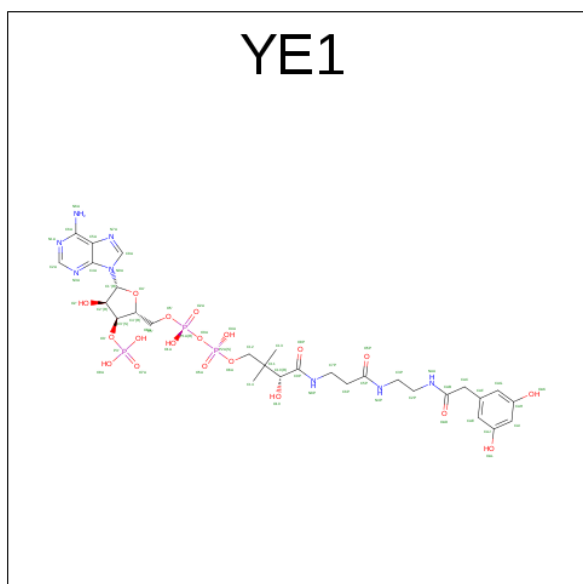
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Xe 1 1	0	1
2	J	1	Total Xe 1 1	0	1
2	D	1	Total Xe 1 1	0	1
2	K	1	Total Xe 1 1	0	1

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Xe	0	1
			1	1		
2	H	1	Total	Xe	0	1
			1	1		
2	B	1	Total	Xe	0	1
			2	2		
2	I	1	Total	Xe	0	1
			1	1		
2	C	1	Total	Xe	0	1
			1	1		
2	A	1	Total	Xe	0	1
			2	2		
2	L	1	Total	Xe	0	1
			1	1		
2	F	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 (three-letter code: YE1) (formula: C<sub>29</sub>H<sub>43</sub>N<sub>8</sub>O<sub>19</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	
			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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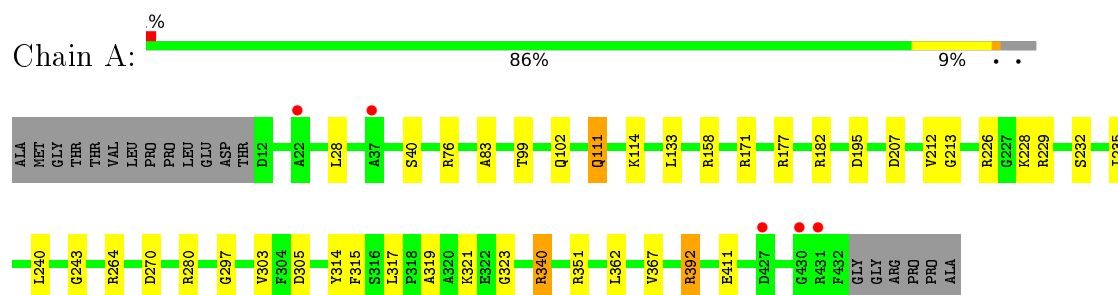
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	65	Total 65	O 65	0	0
4	J	37	Total 37	O 37	0	0
4	K	76	Total 76	O 76	0	0
4	L	57	Total 57	O 57	0	0



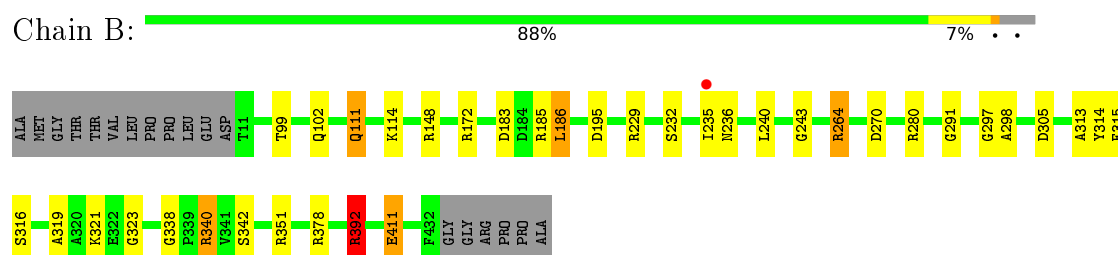
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

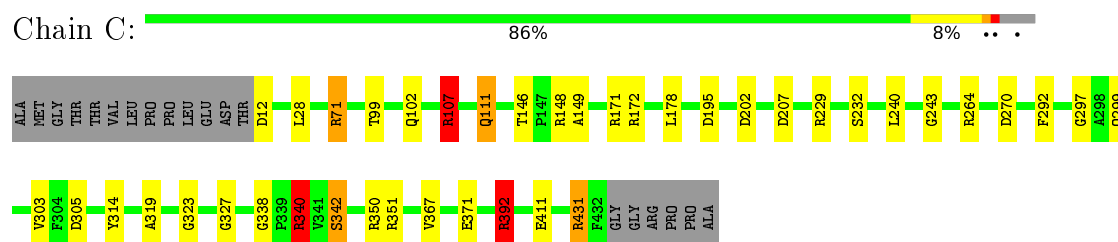
#### • Molecule 1: DpgC



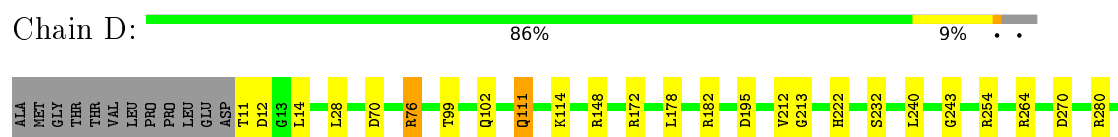
#### • Molecule 1: DpgC



#### • Molecule 1: DpgC



#### • Molecule 1: DpgC





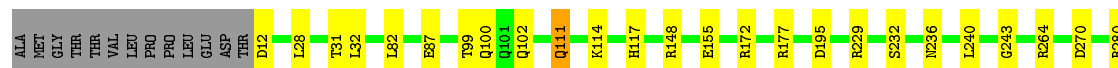
• Molecule 1: DpgC

Chain E: 86% 9% .



• Molecule 1: DpgC

Chain F: 83% 11% . .



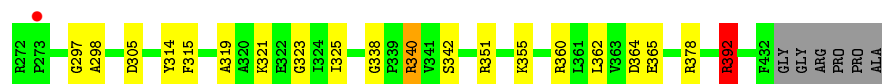
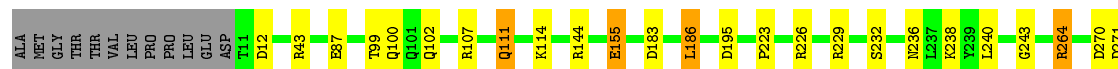
• Molecule 1: DpgC

Chain G: 87% 8% . .



• Molecule 1: DpgC

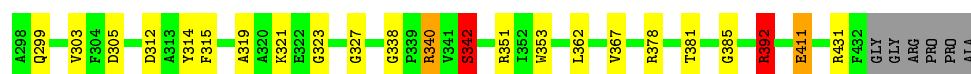
Chain H: 86% 9% . .



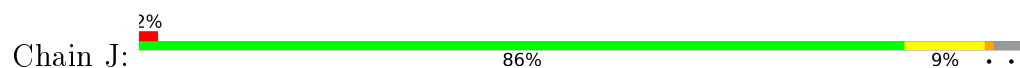
• Molecule 1: DpgC

Chain I: 85% 10% . .

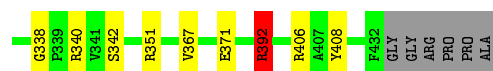




• Molecule 1: DpgC



• Molecule 1: DpgC



• Molecule 1: DpgC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.171 , 0.208 0.176 , 0.212	Depositor DCC
$R_{free}$ test set	11219 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.3	Xtriage
Anisotropy	0.648	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 6.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	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	0.95	EDS
Total number of atoms	40478	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: YE1, XE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.83	1/3277 (0.0%)	1.00	14/4449 (0.3%)
1	B	0.86	1/3330 (0.0%)	1.02	17/4516 (0.4%)
1	C	0.88	0/3327	0.99	11/4511 (0.2%)
1	D	0.91	0/3319	1.00	11/4502 (0.2%)
1	E	0.86	0/3317	1.00	16/4498 (0.4%)
1	F	0.87	1/3320 (0.0%)	1.04	19/4502 (0.4%)
1	G	0.87	0/3312	1.00	11/4494 (0.2%)
1	H	0.83	0/3317	1.02	19/4499 (0.4%)
1	I	0.93	3/3323 (0.1%)	1.00	12/4506 (0.3%)
1	J	0.78	1/3301 (0.0%)	0.98	13/4478 (0.3%)
1	K	0.93	3/3327 (0.1%)	1.11	20/4513 (0.4%)
1	L	0.87	2/3320 (0.1%)	0.97	13/4502 (0.3%)
All	All	0.87	12/39790 (0.0%)	1.01	176/53970 (0.3%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	62	ASP	CB-CG	6.15	1.64	1.51
1	I	225	TYR	CD1-CE1	-6.03	1.30	1.39
1	F	342	SER	CB-OG	-5.97	1.34	1.42
1	J	102	GLN	CG-CD	5.89	1.64	1.51
1	I	342	SER	CB-OG	-5.88	1.34	1.42
1	B	411	GLU	CG-CD	5.86	1.60	1.51
1	L	342	SER	CB-OG	-5.85	1.34	1.42
1	K	340	ARG	CD-NE	-5.69	1.36	1.46
1	I	411	GLU	CD-OE2	5.39	1.31	1.25
1	K	408	TYR	CE2-CZ	-5.16	1.31	1.38
1	A	40	SER	CA-CB	5.13	1.60	1.52
1	L	40	SER	CA-CB	5.07	1.60	1.52

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	406	ARG	NE-CZ-NH1	19.54	130.07	120.30
1	K	406	ARG	NE-CZ-NH2	-13.35	113.62	120.30
1	K	62	ASP	CB-CG-OD2	12.65	129.68	118.30
1	G	392	ARG	NE-CZ-NH2	-11.59	114.51	120.30
1	K	340	ARG	NE-CZ-NH2	-11.55	114.53	120.30
1	J	144	ARG	NE-CZ-NH1	11.30	125.95	120.30
1	B	185	ARG	CB-CA-C	-11.29	87.82	110.40
1	F	406	ARG	NE-CZ-NH2	-10.25	115.17	120.30
1	F	392	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	B	185	ARG	CG-CD-NE	-9.72	91.38	111.80
1	I	28	LEU	CB-CG-CD2	9.66	127.43	111.00
1	A	28	LEU	CB-CG-CD2	9.53	127.21	111.00
1	F	392	ARG	NE-CZ-NH1	9.53	125.07	120.30
1	A	195	ASP	CB-CG-OD1	9.32	126.69	118.30
1	I	340	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	H	340	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	C	28	LEU	CB-CG-CD2	9.30	126.81	111.00
1	G	392	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	A	182	ARG	CG-CD-NE	9.20	131.11	111.80
1	H	195	ASP	CB-CG-OD1	9.17	126.55	118.30
1	E	195	ASP	CB-CG-OD1	9.14	126.52	118.30
1	D	28	LEU	CB-CG-CD2	9.10	126.46	111.00
1	E	392	ARG	NE-CZ-NH2	-8.75	115.92	120.30
1	F	386	ASP	CB-CG-OD2	-8.74	110.44	118.30
1	B	340	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	K	71	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	F	177	ARG	NE-CZ-NH2	-8.57	116.01	120.30
1	J	144	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	K	195	ASP	CB-CG-OD1	8.45	125.90	118.30
1	B	392	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	F	386	ASP	CB-CG-OD1	8.39	125.85	118.30
1	A	182	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	B	392	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	H	392	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	J	392	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	F	406	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	H	186	LEU	CB-CG-CD2	8.05	124.68	111.00
1	D	340	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	F	340	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	G	367	VAL	CA-CB-CG1	-7.90	99.05	110.90
1	G	340	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	H	186	LEU	CB-CG-CD1	-7.78	97.78	111.00
1	E	340	ARG	NE-CZ-NH2	-7.78	116.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	LEU	CB-CG-CD2	7.74	124.16	111.00
1	F	406	ARG	CD-NE-CZ	7.70	134.38	123.60
1	A	340	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	G	378	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	H	107	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	L	340	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	K	340	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	J	340	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	B	186	LEU	CB-CG-CD1	-7.38	98.45	111.00
1	L	107	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	367	VAL	CA-CB-CG1	-7.27	99.99	110.90
1	F	177	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	J	392	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	I	392	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	182	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	E	195	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	E	392	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	K	392	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	H	392	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	C	392	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	C	107	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	H	195	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	K	182	ARG	CG-CD-NE	6.87	126.22	111.80
1	L	392	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	K	155	GLU	OE1-CD-OE2	-6.73	115.22	123.30
1	K	406	ARG	CD-NE-CZ	6.71	132.99	123.60
1	K	392	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	195	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	A	340	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	F	378	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	K	71	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	K	195	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	C	392	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	C	340	ARG	CD-NE-CZ	-6.41	114.63	123.60
1	K	71	ARG	CD-NE-CZ	6.40	132.56	123.60
1	H	340	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	K	62	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	J	12	ASP	CB-CG-OD1	6.35	124.01	118.30
1	B	183	ASP	CB-CG-OD1	6.33	124.00	118.30
1	G	340	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	J	280	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	177	ARG	NE-CZ-NH2	-6.23	117.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	392	ARG	CD-NE-CZ	6.21	132.30	123.60
1	J	183	ASP	CB-CG-OD1	6.20	123.88	118.30
1	H	43	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	H	183	ASP	CB-CG-OD1	6.18	123.86	118.30
1	L	340	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	J	340	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	L	229	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	L	360	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	E	183	ASP	CB-CG-OD1	6.15	123.83	118.30
1	K	229	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	I	367	VAL	CA-CB-CG2	-6.12	101.72	110.90
1	D	280	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	D	431	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	G	378	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	229	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	A	226	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	G	392	ARG	CD-NE-CZ	6.04	132.05	123.60
1	E	226	ARG	CG-CD-NE	6.03	124.47	111.80
1	I	378	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	D	392	ARG	CG-CD-NE	6.00	124.39	111.80
1	G	12	ASP	CB-CG-OD1	6.00	123.70	118.30
1	E	340	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	D	182	ARG	CA-CB-CG	-5.93	100.35	113.40
1	B	340	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	E	229	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	392	ARG	CG-CD-NE	5.85	124.09	111.80
1	C	340	ARG	CB-CG-CD	5.85	126.82	111.60
1	B	378	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	E	182	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	I	26	GLU	CB-CA-C	-5.83	98.75	110.40
1	G	280	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	L	350	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	E	182	ARG	CG-CD-NE	5.78	123.93	111.80
1	L	431	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	H	264	ARG	CB-CG-CD	5.76	126.59	111.60
1	H	378	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	F	172	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	K	43	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	L	172	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	185	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	H	186	LEU	CA-CB-CG	5.69	128.39	115.30
1	A	229	ARG	NE-CZ-NH1	5.67	123.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	12	ASP	CB-CG-OD1	5.66	123.40	118.30
1	A	280	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	J	171	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	I	367	VAL	CA-CB-CG1	5.64	119.36	110.90
1	C	350	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	J	229	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	F	229	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	I	12	ASP	CB-CG-OD1	5.61	123.35	118.30
1	K	76	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	J	378	ARG	CG-CD-NE	-5.60	100.04	111.80
1	F	12	ASP	CB-CG-OD1	5.58	123.32	118.30
1	D	76	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	280	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	D	12	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	186	LEU	CA-CB-CG	5.52	128.00	115.30
1	F	340	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	I	392	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	H	229	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	E	172	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	378	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	I	229	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	431	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	H	12	ASP	CB-CG-OD1	5.40	123.16	118.30
1	I	431	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	J	343	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	L	29	LEU	CB-CG-CD2	5.32	120.05	111.00
1	H	378	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	E	43	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	I	172	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	L	12	ASP	CB-CG-OD1	5.25	123.03	118.30
1	B	229	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	G	270	ASP	CB-CG-OD2	5.24	123.01	118.30
1	F	280	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	F	350	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	L	171	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	172	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	H	271	ASP	CB-CG-OD2	5.21	122.98	118.30
1	K	340	ARG	CD-NE-CZ	5.21	130.89	123.60
1	E	392	ARG	CG-CD-NE	-5.20	100.89	111.80
1	H	107	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	L	392	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	F	406	ARG	CG-CD-NE	5.13	122.57	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	340	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	D	76	ARG	CD-NE-CZ	5.08	130.72	123.60
1	B	172	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	E	411	GLU	CG-CD-OE2	5.07	128.43	118.30
1	E	161	GLU	OE1-CD-OE2	5.06	129.38	123.30
1	B	264	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	D	172	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3216	0	3201	23	0
1	B	3268	0	3266	21	0
1	C	3265	0	3266	26	0
1	D	3258	0	3254	19	0
1	E	3256	0	3255	29	0
1	F	3258	0	3260	27	0
1	G	3251	0	3241	21	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	25	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	0
3	C	59	0	38	2	0
3	D	59	0	38	2	0
3	E	59	0	39	4	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	1	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	2	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	292	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 (292) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:C:107:ARG:HG3	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:A:76:ARG:NH1	1:A:133:LEU:HD22	2.06	0.66
3:H:502:YE1:HAE	3:H:502:YE1:OAD	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:HH11	1:H:144:ARG:HG2	1.63	0.63
1:C:171:ARG:NH1	1:C:207:ASP:OD2	2.31	0.62
1:B:315[A]:PHE:C	2:B:501[A]:XE:XE	3.16	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:HC71	3:J:502:YE1:HN62	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
1:J:384:ASP:HB2	1:L:321:LYS:HZ3	1.68	0.58
1:B:298:ALA:HB1	1:B:315[B]:PHE:CE2	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:238:LYS:NZ	3:E:502:YE1:O9A	2.36	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:HH11	1:G:264:ARG:HG2	1.73	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	1:D:264:ARG:HH11	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:L:315[B]:PHE:C	1:L:315[B]:PHE:CD1	2.85	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:H:360:ARG:CZ	1:H:364:ASP:O	2.60	0.49
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:HH11	1:C:264:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:315[B]:PHE:C	1:A:315[B]:PHE:CD1	2.86	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:298:ALA:HB1	1:F:315[B]:PHE:CE2	2.47	0.48
1:F:82:LEU:HB2	4:F:645:HOH:O	2.11	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: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:HD12	1:G:178:LEU:N	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:K:315[B]:PHE:CD1	1:K:315[B]:PHE:C	2.87	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
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: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:H:360:ARG:HH12	1:H:365:GLU:HA	1.80	0.47
1:F:312:ASP:HB3	1:I:353:TRP:HH2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:238:LYS:HE3	3:J:502:YE1:O2'	2.14	0.47
1:I:264:ARG:HG2	1:I:264:ARG:HH11	1.80	0.47
1:J:264:ARG:HH11	1:J:264:ARG:HG2	1.80	0.47
1:D:178:LEU:HD12	1:D:178:LEU:N	2.29	0.47
1:E:264:ARG:HH11	1:E:264:ARG:HG2	1.79	0.47
1:C:71:ARG:O	1:C:71:ARG:HG3	2.15	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:NH1	1:C:107:ARG:HG3	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:HAE	3:F:502:YE1:OAD	2.15	0.47
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: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: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:I:232:SER:HB3	1:I:297:GLY:HA3	1.98	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ARG:NH1	1:B:195:ASP:OD2	2.48	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:G:305:ASP:CG	1:G:392:ARG:HH11	2.20	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:338:GLY:O	1:E:342:SER:HB3	2.18	0.44
1:E:236:ASN:HA	3:E:502:YE1:N1A	2.32	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
3:C:502:YE1:OAD	3:C:502:YE1:HAE	2.18	0.44
1:J:305:ASP:CG	1:J:392:ARG:HH11	2.22	0.44
1:J:28:LEU:HD22	1:J:32:LEU:HD11	2.00	0.44
1:H:155:GLU:CD	1:H:155:GLU:H	2.21	0.43
1:A:305:ASP:C	1:C:340:ARG:NH2	2.71	0.43
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: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:H:321:LYS:NZ	1:I:381:THR:O	2.36	0.43
1:I:235:ILE:HB	3:I:502:YE1:HAE	2.01	0.42
4:H:606:HOH:O	1:I:385:GLY:CA	2.65	0.42
1:I:305:ASP:CG	1:I:392:ARG:HH11	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:305:ASP:CG	1:L:392:ARG:HH11	2.23	0.41
1:C:178:LEU:N	1:C:178:LEU:HD12	2.36	0.41
1:A:111:GLN:NE2	1:A:114:LYS:HE3	2.35	0.41
1:C:305:ASP:CG	1:C:392:ARG:HH11	2.24	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:E:321:LYS:HZ3	1:F:384:ASP:HB2	1.85	0.41
1:H:305:ASP:CG	1:H:392:ARG:HH11	2.23	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:C:367:VAL:HG12	1:C:371:GLU:HB2	2.03	0.41
1:I:178:LEU:HD12	1:I:178:LEU:N	2.36	0.41
1:K:305:ASP:CG	1:K:392:ARG:HH11	2.24	0.41
1:B:305:ASP:CG	1:B:392:ARG:HH11	2.23	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:L:315[B]:PHE:HD1	1:L:315[B]:PHE:O	2.04	0.41
1:A:212:VAL:HG12	1:A:213:GLY:N	2.35	0.41
1:A:305:ASP:CG	1:A:392:ARG:HE	2.24	0.41
1:B:291:GLY:O	1:B:313:ALA:HA	2.20	0.41
1:E:408:TYR:CE1	1:F:394:MET:HE2	2.55	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
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:E:305:ASP:CG	1:E:392:ARG:HH11	2.25	0.40
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:OAD	3:I:502:YE1:HAE	2.22	0.40
1:D:305:ASP:CG	1:D:392:ARG:HE	2.25	0.40
1:F:148:ARG:NH1	1:F:195:ASP:OD2	2.50	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	420/440 (96%)	411 (98%)	8 (2%)	1 (0%)	52	75
1	B	421/440 (96%)	413 (98%)	7 (2%)	1 (0%)	52	75
1	C	420/440 (96%)	411 (98%)	8 (2%)	1 (0%)	52	75
1	D	422/440 (96%)	414 (98%)	7 (2%)	1 (0%)	52	75
1	E	420/440 (96%)	411 (98%)	8 (2%)	1 (0%)	52	75
1	F	420/440 (96%)	410 (98%)	9 (2%)	1 (0%)	52	75
1	G	421/440 (96%)	412 (98%)	8 (2%)	1 (0%)	52	75
1	H	421/440 (96%)	413 (98%)	7 (2%)	1 (0%)	52	75
1	I	420/440 (96%)	411 (98%)	8 (2%)	1 (0%)	52	75
1	J	421/440 (96%)	413 (98%)	7 (2%)	1 (0%)	52	75
1	K	421/440 (96%)	411 (98%)	9 (2%)	1 (0%)	52	75
1	L	420/440 (96%)	411 (98%)	8 (2%)	1 (0%)	52	75
All	All	5047/5280 (96%)	4941 (98%)	94 (2%)	12 (0%)	52	75

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%)	310 (98%)	6 (2%)	65	85
1	B	328/345 (95%)	322 (98%)	6 (2%)	66	86
1	C	328/345 (95%)	320 (98%)	8 (2%)	57	80
1	D	325/345 (94%)	317 (98%)	8 (2%)	55	79
1	E	326/345 (94%)	321 (98%)	5 (2%)	72	89
1	F	326/345 (94%)	318 (98%)	8 (2%)	55	79
1	G	323/345 (94%)	313 (97%)	10 (3%)	47	74
1	H	325/345 (94%)	319 (98%)	6 (2%)	66	86
1	I	327/345 (95%)	319 (98%)	8 (2%)	57	80
1	J	321/345 (93%)	312 (97%)	9 (3%)	51	77
1	K	327/345 (95%)	321 (98%)	6 (2%)	66	86
1	L	326/345 (94%)	319 (98%)	7 (2%)	61	84
All	All	3898/4140 (94%)	3811 (98%)	87 (2%)	60	82

All (87) 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	321	LYS
1	A	340	ARG
1	A	411	GLU
1	B	111	GLN
1	B	186	LEU
1	B	321	LYS
1	B	340	ARG
1	B	392	ARG
1	B	411	GLU
1	C	71	ARG
1	C	107	ARG

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Mol	Chain	Res	Type
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	D	11	THR
1	D	14	LEU
1	D	111	GLN
1	D	303	VAL
1	D	321	LYS
1	D	340	ARG
1	D	360	ARG
1	D	411	GLU
1	E	40	SER
1	E	111	GLN
1	E	224	ARG
1	E	340	ARG
1	E	392	ARG
1	F	31	THR
1	F	111	GLN
1	F	155	GLU
1	F	303	VAL
1	F	321	LYS
1	F	340	ARG
1	F	342	SER
1	F	392	ARG
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	340	ARG
1	G	360	ARG
1	G	370	ASP
1	G	392	ARG
1	H	111	GLN
1	H	155	GLU
1	H	186	LEU
1	H	264	ARG
1	H	340	ARG

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Mol	Chain	Res	Type
1	H	392	ARG
1	I	111	GLN
1	I	228	LYS
1	I	303	VAL
1	I	321	LYS
1	I	340	ARG
1	I	342	SER
1	I	392	ARG
1	I	411	GLU
1	J	12	ASP
1	J	31	THR
1	J	39	SER
1	J	111	GLN
1	J	303	VAL
1	J	340	ARG
1	J	360	ARG
1	J	392	ARG
1	J	431	ARG
1	K	11	THR
1	K	62	ASP
1	K	111	GLN
1	K	155	GLU
1	K	321	LYS
1	K	392	ARG
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) 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	B	168	HIS

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Mol	Chain	Res	Type
1	C	102	GLN
1	C	111	GLN
1	C	299	GLN
1	D	102	GLN
1	D	111	GLN
1	E	102	GLN
1	E	111	GLN
1	E	222	HIS
1	E	423	HIS
1	F	79	HIS
1	F	100	GLN
1	F	102	GLN
1	F	111	GLN
1	F	117	HIS
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	423	HIS
1	I	79	HIS
1	I	102	GLN
1	I	111	GLN
1	I	299	GLN
1	J	79	HIS
1	J	100	GLN
1	J	111	GLN
1	K	35	HIS
1	K	79	HIS
1	K	102	GLN
1	K	111	GLN
1	L	64	HIS
1	L	102	GLN
1	L	111	GLN
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 ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	A	502	-	53,62,62	1.84	15 (28%)	67,92,92	1.79	17 (25%)
3	YE1	B	502	-	53,62,62	2.27	19 (35%)	67,92,92	1.88	18 (26%)
3	YE1	C	502	-	53,62,62	2.70	22 (41%)	67,92,92	1.75	14 (20%)
3	YE1	D	502	-	53,62,62	2.18	19 (35%)	67,92,92	1.76	14 (20%)
3	YE1	E	502	-	53,62,62	2.05	15 (28%)	67,92,92	1.85	14 (20%)
3	YE1	F	502	-	53,62,62	2.26	19 (35%)	67,92,92	2.27	24 (35%)
3	YE1	G	502	-	53,62,62	2.30	18 (33%)	67,92,92	1.73	16 (23%)
3	YE1	H	502	-	53,62,62	2.30	17 (32%)	67,92,92	2.00	18 (26%)
3	YE1	I	502	-	53,62,62	2.01	16 (30%)	67,92,92	1.74	14 (20%)
3	YE1	J	502	-	53,62,62	1.96	15 (28%)	67,92,92	1.57	12 (17%)
3	YE1	K	502	-	53,62,62	2.00	16 (30%)	67,92,92	1.74	14 (20%)
3	YE1	L	502	-	53,62,62	2.31	20 (37%)	67,92,92	1.74	18 (26%)

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	A	502	-	-	1/51/71/71	0/4/4/4
3	YE1	B	502	-	-	0/51/71/71	0/4/4/4
3	YE1	C	502	-	-	0/51/71/71	0/4/4/4
3	YE1	D	502	-	-	0/51/71/71	0/4/4/4
3	YE1	E	502	-	-	0/51/71/71	0/4/4/4
3	YE1	F	502	-	-	1/51/71/71	0/4/4/4
3	YE1	G	502	-	-	0/51/71/71	0/4/4/4
3	YE1	H	502	-	-	1/51/71/71	0/4/4/4
3	YE1	I	502	-	-	0/51/71/71	0/4/4/4
3	YE1	J	502	-	-	0/51/71/71	0/4/4/4
3	YE1	K	502	-	-	0/51/71/71	0/4/4/4
3	YE1	L	502	-	-	0/51/71/71	0/4/4/4

All (211) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	502	YE1	O10-C10	-6.02	1.30	1.42
3	H	502	YE1	CAE-CAJ	-4.79	1.31	1.39
3	J	502	YE1	C6P-C5P	-4.59	1.42	1.51
3	L	502	YE1	C13-C11	-4.28	1.44	1.53
3	L	502	YE1	C2P-NAA	-4.19	1.36	1.46
3	C	502	YE1	O10-C10	-4.16	1.33	1.42
3	H	502	YE1	O3'-C3'	-4.13	1.31	1.44
3	A	502	YE1	O2'-C2'	-4.06	1.33	1.43
3	C	502	YE1	C2P-NAA	-4.05	1.36	1.46
3	F	502	YE1	C6P-C5P	-3.92	1.43	1.51
3	G	502	YE1	O10-C10	-3.87	1.34	1.42
3	H	502	YE1	O4'-C4'	-3.79	1.36	1.45
3	H	502	YE1	O4'-C1'	-3.77	1.35	1.41
3	F	502	YE1	CAI-CAH	-3.75	1.33	1.39
3	B	502	YE1	O3'-C3'	-3.49	1.33	1.44
3	G	502	YE1	CAI-CAJ	-3.47	1.33	1.39
3	F	502	YE1	CAI-CAJ	-3.44	1.33	1.39
3	D	502	YE1	O3'-C3'	-3.44	1.33	1.44
3	F	502	YE1	O2'-C2'	-3.41	1.34	1.43
3	J	502	YE1	O4'-C1'	-3.37	1.36	1.41
3	D	502	YE1	C6P-C5P	-3.37	1.44	1.51
3	A	502	YE1	C6P-C5P	-3.25	1.45	1.51
3	L	502	YE1	O3'-C3'	-3.23	1.33	1.44
3	I	502	YE1	CAG-CAH	-3.17	1.34	1.39
3	K	502	YE1	CAG-CAH	-3.13	1.34	1.39
3	D	502	YE1	O2'-C2'	-3.03	1.35	1.43
3	A	502	YE1	O3'-C3'	-2.99	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	YE1	C3P-N4P	-2.98	1.39	1.46
3	E	502	YE1	C3P-N4P	-2.77	1.39	1.46
3	D	502	YE1	O6A-C12	-2.72	1.34	1.43
3	F	502	YE1	C4A-N3A	-2.68	1.31	1.35
3	F	502	YE1	P1A-O1A	-2.67	1.43	1.55
3	E	502	YE1	C4A-N3A	-2.67	1.31	1.35
3	B	502	YE1	CAI-CAH	-2.55	1.35	1.39
3	C	502	YE1	O2'-C2'	-2.52	1.37	1.43
3	G	502	YE1	O3'-C3'	-2.51	1.36	1.44
3	I	502	YE1	O4'-C1'	-2.51	1.37	1.41
3	J	502	YE1	O2'-C2'	-2.51	1.37	1.43
3	E	502	YE1	O3'-C3'	-2.49	1.36	1.44
3	L	502	YE1	O4'-C1'	-2.48	1.37	1.41
3	K	502	YE1	O4'-C1'	-2.46	1.37	1.41
3	E	502	YE1	O5'-C5'	-2.41	1.35	1.44
3	B	502	YE1	O6A-C12	-2.39	1.35	1.43
3	F	502	YE1	P2A-O4A	-2.38	1.45	1.55
3	A	502	YE1	P2A-O4A	-2.35	1.45	1.55
3	E	502	YE1	CAI-CAJ	-2.35	1.35	1.39
3	J	502	YE1	O5P-C5P	-2.28	1.18	1.23
3	I	502	YE1	O3'-C3'	-2.12	1.37	1.44
3	K	502	YE1	O3'-C3'	-2.11	1.37	1.44
3	B	502	YE1	C6P-C5P	-2.11	1.47	1.51
3	E	502	YE1	P2A-O4A	-2.08	1.46	1.55
3	L	502	YE1	C5'-C4'	-2.07	1.45	1.51
3	G	502	YE1	CAI-CAH	-2.03	1.36	1.39
3	H	502	YE1	O5'-C5'	-2.02	1.36	1.44
3	F	502	YE1	C5A-N7A	2.01	1.46	1.39
3	D	502	YE1	C5A-C4A	2.02	1.45	1.40
3	C	502	YE1	OAL-CAJ	2.04	1.41	1.37
3	E	502	YE1	CAG-CAF	2.07	1.43	1.39
3	C	502	YE1	P3'-O7A	2.10	1.57	1.50
3	I	502	YE1	C2A-N3A	2.13	1.35	1.32
3	G	502	YE1	P1A-O5'	2.13	1.68	1.59
3	L	502	YE1	C4A-N3A	2.14	1.38	1.35
3	B	502	YE1	C6A-N6A	2.15	1.42	1.34
3	F	502	YE1	C2A-N3A	2.16	1.36	1.32
3	K	502	YE1	C2A-N3A	2.17	1.36	1.32
3	F	502	YE1	CAE-CAF	2.17	1.43	1.39
3	D	502	YE1	CAB-NAA	2.17	1.38	1.33
3	G	502	YE1	CAB-NAA	2.18	1.38	1.33
3	G	502	YE1	O4'-C4'	2.21	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	YE1	OAK-CAH	2.21	1.42	1.37
3	A	502	YE1	CAI-CAJ	2.23	1.42	1.39
3	A	502	YE1	C13-C11	2.24	1.58	1.53
3	E	502	YE1	C3'-C4'	2.24	1.59	1.52
3	B	502	YE1	C7P-N8P	2.25	1.51	1.46
3	L	502	YE1	CAG-CAH	2.25	1.42	1.39
3	L	502	YE1	C9P-N8P	2.27	1.38	1.33
3	K	502	YE1	OAD-CAB	2.28	1.28	1.23
3	I	502	YE1	OAD-CAB	2.29	1.28	1.23
3	B	502	YE1	O4'-C4'	2.31	1.50	1.45
3	H	502	YE1	C2'-C3'	2.32	1.58	1.53
3	J	502	YE1	CAG-CAF	2.33	1.43	1.39
3	L	502	YE1	C5A-C4A	2.33	1.45	1.40
3	H	502	YE1	C9P-N8P	2.36	1.38	1.33
3	A	502	YE1	C2A-N1A	2.36	1.38	1.33
3	B	502	YE1	C2'-C1'	2.39	1.57	1.53
3	G	502	YE1	C7P-N8P	2.42	1.51	1.46
3	I	502	YE1	C5'-C4'	2.42	1.59	1.51
3	D	502	YE1	OAD-CAB	2.43	1.28	1.23
3	K	502	YE1	C5'-C4'	2.44	1.59	1.51
3	J	502	YE1	P1A-O5'	2.44	1.69	1.59
3	D	502	YE1	CAE-CAF	2.46	1.43	1.39
3	G	502	YE1	C6P-C5P	2.49	1.56	1.51
3	F	502	YE1	C5P-N4P	2.50	1.39	1.33
3	H	502	YE1	C13-C11	2.51	1.59	1.53
3	D	502	YE1	C7P-N8P	2.51	1.52	1.46
3	J	502	YE1	OAK-CAH	2.53	1.43	1.37
3	A	502	YE1	C8A-N7A	2.53	1.39	1.34
3	F	502	YE1	C6A-N6A	2.54	1.44	1.34
3	C	502	YE1	C5P-N4P	2.54	1.39	1.33
3	E	502	YE1	C14-C11	2.55	1.59	1.53
3	A	502	YE1	CAB-NAA	2.55	1.39	1.33
3	D	502	YE1	P1A-O5'	2.57	1.70	1.59
3	C	502	YE1	C2'-C3'	2.57	1.58	1.53
3	J	502	YE1	C5P-N4P	2.59	1.39	1.33
3	G	502	YE1	C2'-C1'	2.60	1.57	1.53
3	H	502	YE1	C2P-C3P	2.64	1.64	1.50
3	B	502	YE1	O2'-C2'	2.65	1.49	1.43
3	A	502	YE1	C5A-C4A	2.66	1.46	1.40
3	D	502	YE1	O10-C10	2.66	1.47	1.42
3	C	502	YE1	C14-C11	2.68	1.59	1.53
3	G	502	YE1	CAG-CAF	2.70	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	502	YE1	CAB-NAA	2.71	1.39	1.33
3	L	502	YE1	P2A-O6A	2.71	1.70	1.59
3	K	502	YE1	P2A-O6A	2.72	1.70	1.59
3	I	502	YE1	P2A-O6A	2.72	1.70	1.59
3	J	502	YE1	C2P-C3P	2.74	1.64	1.50
3	C	502	YE1	C2A-N1A	2.78	1.39	1.33
3	H	502	YE1	CAC-CAB	2.78	1.58	1.51
3	H	502	YE1	C2A-N1A	2.79	1.39	1.33
3	E	502	YE1	OAD-CAB	2.79	1.29	1.23
3	L	502	YE1	C5P-N4P	2.79	1.40	1.33
3	C	502	YE1	P1A-O5'	2.82	1.71	1.59
3	L	502	YE1	CAE-CAF	2.83	1.44	1.39
3	K	502	YE1	O4'-C4'	2.89	1.51	1.45
3	C	502	YE1	C3'-C4'	2.89	1.61	1.52
3	I	502	YE1	O4'-C4'	2.90	1.51	1.45
3	G	502	YE1	OAD-CAB	2.90	1.29	1.23
3	D	502	YE1	C3P-N4P	2.90	1.52	1.46
3	G	502	YE1	C5P-N4P	2.91	1.40	1.33
3	F	502	YE1	C14-C11	2.95	1.60	1.53
3	B	502	YE1	C2A-N1A	2.96	1.39	1.33
3	K	502	YE1	C2A-N1A	2.98	1.39	1.33
3	A	502	YE1	CAI-CAH	3.00	1.43	1.39
3	I	502	YE1	C2A-N1A	3.00	1.39	1.33
3	G	502	YE1	C8A-N7A	3.01	1.40	1.34
3	H	502	YE1	C7P-C6P	3.03	1.61	1.51
3	B	502	YE1	C5A-C4A	3.04	1.47	1.40
3	K	502	YE1	CAB-NAA	3.05	1.40	1.33
3	I	502	YE1	CAB-NAA	3.06	1.40	1.33
3	B	502	YE1	C14-C11	3.08	1.60	1.53
3	J	502	YE1	OAD-CAB	3.09	1.29	1.23
3	D	502	YE1	C8A-N7A	3.09	1.40	1.34
3	K	502	YE1	C4A-N3A	3.14	1.40	1.35
3	I	502	YE1	C4A-N3A	3.15	1.40	1.35
3	C	502	YE1	CAB-NAA	3.15	1.41	1.33
3	B	502	YE1	P1A-O5'	3.22	1.72	1.59
3	E	502	YE1	O4'-C4'	3.23	1.52	1.45
3	K	502	YE1	C2'-C3'	3.29	1.60	1.53
3	I	502	YE1	C2'-C3'	3.29	1.60	1.53
3	B	502	YE1	C3'-C4'	3.32	1.62	1.52
3	F	502	YE1	CAE-CAJ	3.36	1.44	1.39
3	F	502	YE1	C3'-C4'	3.42	1.62	1.52
3	J	502	YE1	C3'-C4'	3.46	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	502	YE1	CAG-CAF	3.46	1.45	1.39
3	C	502	YE1	CAC-CAF	3.51	1.57	1.51
3	K	502	YE1	CAG-CAF	3.53	1.45	1.39
3	F	502	YE1	C7P-N8P	3.54	1.54	1.46
3	A	502	YE1	C2P-NAA	3.54	1.54	1.46
3	I	502	YE1	CAG-CAF	3.55	1.45	1.39
3	D	502	YE1	C7P-C6P	3.55	1.62	1.51
3	D	502	YE1	CAE-CAJ	3.55	1.44	1.39
3	L	502	YE1	CAG-CAF	3.56	1.45	1.39
3	J	502	YE1	CAI-CAJ	3.58	1.44	1.39
3	B	502	YE1	CAG-CAF	3.59	1.45	1.39
3	C	502	YE1	CAI-CAJ	3.59	1.44	1.39
3	K	502	YE1	CAE-CAJ	3.62	1.44	1.39
3	G	502	YE1	P2A-O6A	3.63	1.74	1.59
3	I	502	YE1	CAE-CAJ	3.65	1.44	1.39
3	B	502	YE1	OAL-CAJ	3.65	1.45	1.37
3	H	502	YE1	CAB-NAA	3.66	1.42	1.33
3	L	502	YE1	P1A-O5'	3.68	1.74	1.59
3	L	502	YE1	CAC-CAB	3.71	1.61	1.51
3	A	502	YE1	P2A-O6A	3.73	1.75	1.59
3	J	502	YE1	C14-C11	3.81	1.62	1.53
3	A	502	YE1	C14-C11	3.87	1.62	1.53
3	D	502	YE1	P2A-O6A	3.92	1.75	1.59
3	D	502	YE1	OAL-CAJ	3.99	1.46	1.37
3	E	502	YE1	C2'-C1'	4.00	1.60	1.53
3	L	502	YE1	C2'-C1'	4.00	1.60	1.53
3	A	502	YE1	CAG-CAF	4.13	1.46	1.39
3	L	502	YE1	C2'-C3'	4.19	1.62	1.53
3	J	502	YE1	C2'-C1'	4.21	1.60	1.53
3	H	502	YE1	C4A-N3A	4.26	1.41	1.35
3	E	502	YE1	OAL-CAJ	4.26	1.47	1.37
3	H	502	YE1	C5P-N4P	4.28	1.43	1.33
3	C	502	YE1	OAD-CAB	4.38	1.32	1.23
3	K	502	YE1	CAI-CAH	4.43	1.46	1.39
3	I	502	YE1	CAI-CAH	4.43	1.46	1.39
3	C	502	YE1	OAK-CAH	4.47	1.47	1.37
3	G	502	YE1	CAG-CAH	4.48	1.46	1.39
3	G	502	YE1	C2P-NAA	4.57	1.56	1.46
3	F	502	YE1	P2A-O6A	4.59	1.78	1.59
3	J	502	YE1	P2A-O6A	4.74	1.79	1.59
3	F	502	YE1	C2A-N1A	4.75	1.43	1.33
3	L	502	YE1	C14-C11	5.02	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	502	YE1	C5P-N4P	5.37	1.46	1.33
3	C	502	YE1	C6P-C5P	5.38	1.61	1.51
3	C	502	YE1	C2'-C1'	5.48	1.62	1.53
3	B	502	YE1	C2'-C3'	5.52	1.65	1.53
3	C	502	YE1	C7P-C6P	5.67	1.69	1.51
3	C	502	YE1	P2A-O6A	5.76	1.83	1.59
3	B	502	YE1	O4'-C1'	5.78	1.49	1.41
3	I	502	YE1	OAL-CAJ	5.83	1.50	1.37
3	K	502	YE1	OAL-CAJ	5.84	1.51	1.37
3	C	502	YE1	CAG-CAF	5.85	1.49	1.39
3	E	502	YE1	P2A-O6A	6.03	1.84	1.59
3	F	502	YE1	C2'-C1'	6.43	1.63	1.53
3	B	502	YE1	P2A-O6A	6.52	1.87	1.59
3	H	502	YE1	P2A-O6A	6.80	1.88	1.59
3	D	502	YE1	C2'-C1'	6.86	1.64	1.53
3	G	502	YE1	OAK-CAH	8.89	1.58	1.37

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	502	YE1	O3'-P3'-O7A	-7.98	88.43	107.48
3	B	502	YE1	O3'-P3'-O7A	-7.63	89.26	107.48
3	H	502	YE1	C1'-N9A-C4A	-6.50	119.55	126.81
3	F	502	YE1	CAJ-CAE-CAF	-6.14	116.62	120.41
3	A	502	YE1	C1'-N9A-C4A	-6.05	120.06	126.81
3	K	502	YE1	O3'-P3'-O7A	-5.75	93.75	107.48
3	I	502	YE1	O3'-P3'-O7A	-5.75	93.76	107.48
3	G	502	YE1	CAH-CAG-CAF	-5.70	116.89	120.41
3	F	502	YE1	O4'-C1'-N9A	-5.67	97.39	108.11
3	D	502	YE1	O3'-P3'-O7A	-5.33	94.76	107.48
3	L	502	YE1	O3'-P3'-O7A	-5.30	94.83	107.48
3	H	502	YE1	CAH-CAG-CAF	-5.13	117.25	120.41
3	H	502	YE1	O8A-P3'-O3'	-4.93	91.88	106.62
3	G	502	YE1	O3'-P3'-O7A	-4.86	95.87	107.48
3	C	502	YE1	CAC-CAB-NAA	-4.84	109.51	116.09
3	J	502	YE1	C1'-N9A-C4A	-4.73	121.53	126.81
3	B	502	YE1	CAH-CAG-CAF	-4.61	117.56	120.41
3	G	502	YE1	CAC-CAB-NAA	-4.37	110.14	116.09
3	C	502	YE1	O8A-P3'-O3'	-4.36	93.59	106.62
3	E	502	YE1	C7P-C6P-C5P	-4.27	104.89	112.22
3	D	502	YE1	CAC-CAB-NAA	-4.23	110.33	116.09
3	L	502	YE1	CAH-CAG-CAF	-4.21	117.81	120.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	502	YE1	CAC-CAB-NAA	-4.11	110.50	116.09
3	I	502	YE1	CAC-CAB-NAA	-4.09	110.53	116.09
3	K	502	YE1	C1'-N9A-C4A	-4.06	122.27	126.81
3	I	502	YE1	C1'-N9A-C4A	-4.06	122.28	126.81
3	H	502	YE1	C7P-C6P-C5P	-4.00	105.36	112.22
3	I	502	YE1	C7P-C6P-C5P	-3.94	105.46	112.22
3	K	502	YE1	C7P-C6P-C5P	-3.94	105.46	112.22
3	C	502	YE1	CAJ-CAE-CAF	-3.93	117.99	120.41
3	E	502	YE1	CAC-CAB-NAA	-3.85	110.85	116.09
3	L	502	YE1	CAC-CAB-NAA	-3.75	110.99	116.09
3	J	502	YE1	CAC-CAB-NAA	-3.68	111.09	116.09
3	C	502	YE1	C1'-N9A-C4A	-3.50	122.90	126.81
3	A	502	YE1	O3'-P3'-O7A	-3.50	99.13	107.48
3	B	502	YE1	C1'-N9A-C4A	-3.43	122.98	126.81
3	A	502	YE1	CAC-CAB-NAA	-3.42	111.44	116.09
3	J	502	YE1	C7P-C6P-C5P	-3.37	106.44	112.22
3	F	502	YE1	C1'-N9A-C4A	-3.31	123.11	126.81
3	E	502	YE1	CAH-CAG-CAF	-3.29	118.38	120.41
3	C	502	YE1	C6P-C5P-N4P	-3.25	110.80	116.46
3	D	502	YE1	C1'-N9A-C4A	-3.24	123.19	126.81
3	D	502	YE1	C13-C11-C12	-3.23	104.31	108.50
3	A	502	YE1	O2'-C2'-C1'	-3.23	101.51	111.61
3	K	502	YE1	CAC-CAF-CAG	-3.22	114.93	120.37
3	I	502	YE1	CAC-CAF-CAG	-3.20	114.96	120.37
3	D	502	YE1	C7P-C6P-C5P	-3.18	106.77	112.22
3	F	502	YE1	O9A-P3'-O3'	-3.13	97.27	106.62
3	F	502	YE1	C4'-O4'-C1'	-3.12	106.34	109.64
3	E	502	YE1	C6P-C5P-N4P	-3.12	111.03	116.46
3	C	502	YE1	O6A-P2A-O5A	-3.08	96.58	109.21
3	F	502	YE1	OAL-CAJ-CAI	-3.03	111.84	119.80
3	A	502	YE1	CAH-CAG-CAF	-3.00	118.56	120.41
3	G	502	YE1	C1'-N9A-C4A	-2.93	123.54	126.81
3	B	502	YE1	C3'-C2'-C1'	-2.89	93.76	100.06
3	L	502	YE1	C6P-C5P-N4P	-2.89	111.43	116.46
3	D	502	YE1	CAJ-CAE-CAF	-2.82	118.67	120.41
3	E	502	YE1	C1'-N9A-C4A	-2.72	123.78	126.81
3	L	502	YE1	O4A-P2A-O6A	-2.71	95.32	108.24
3	H	502	YE1	C6P-C5P-N4P	-2.70	111.75	116.46
3	J	502	YE1	C2'-C1'-N9A	-2.69	106.26	113.47
3	H	502	YE1	CAC-CAB-NAA	-2.69	112.43	116.09
3	F	502	YE1	CAH-CAG-CAF	-2.69	118.75	120.41
3	L	502	YE1	C1'-N9A-C4A	-2.66	123.84	126.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	502	YE1	P3'-O3'-C3'	-2.65	114.79	121.56
3	K	502	YE1	P3'-O3'-C3'	-2.64	114.81	121.56
3	H	502	YE1	O4'-C1'-N9A	-2.60	103.19	108.11
3	K	502	YE1	C6P-C5P-N4P	-2.58	111.96	116.46
3	I	502	YE1	C6P-C5P-N4P	-2.58	111.98	116.46
3	G	502	YE1	CAJ-CAE-CAF	-2.57	118.83	120.41
3	J	502	YE1	CAJ-CAE-CAF	-2.56	118.83	120.41
3	E	502	YE1	CAJ-CAE-CAF	-2.55	118.84	120.41
3	G	502	YE1	C7P-C6P-C5P	-2.52	107.90	112.22
3	J	502	YE1	O9A-P3'-O3'	-2.51	99.11	106.62
3	L	502	YE1	N6A-C6A-N1A	-2.51	114.31	118.52
3	A	502	YE1	O8A-P3'-O3'	-2.49	99.17	106.62
3	B	502	YE1	C7P-C6P-C5P	-2.45	108.01	112.22
3	F	502	YE1	OAK-CAH-CAI	-2.44	113.38	119.80
3	B	502	YE1	CAJ-CAE-CAF	-2.44	118.91	120.41
3	K	502	YE1	CAH-CAG-CAF	-2.43	118.91	120.41
3	B	502	YE1	C4'-O4'-C1'	-2.42	107.07	109.64
3	I	502	YE1	CAH-CAG-CAF	-2.41	118.92	120.41
3	D	502	YE1	CAH-CAG-CAF	-2.41	118.93	120.41
3	G	502	YE1	OAK-CAH-CAI	-2.40	113.47	119.80
3	A	502	YE1	C2'-C1'-N9A	-2.38	107.09	113.47
3	E	502	YE1	C4'-O4'-C1'	-2.38	107.12	109.64
3	E	502	YE1	O9A-P3'-O3'	-2.35	99.60	106.62
3	L	502	YE1	O6A-P2A-O5A	-2.33	99.66	109.21
3	C	502	YE1	C2'-C3'-C4'	-2.33	98.78	103.25
3	A	502	YE1	O4A-P2A-O6A	-2.32	97.16	108.24
3	F	502	YE1	C6P-C5P-N4P	-2.26	112.52	116.46
3	F	502	YE1	O3'-C3'-C4'	-2.25	101.19	110.09
3	F	502	YE1	C2A-N1A-C6A	-2.19	114.85	118.77
3	B	502	YE1	C6P-C5P-N4P	-2.17	112.68	116.46
3	L	502	YE1	O4'-C1'-N9A	-2.16	104.03	108.11
3	G	502	YE1	C6P-C5P-N4P	-2.15	112.72	116.46
3	H	502	YE1	O3'-P3'-O7A	-2.12	102.43	107.48
3	B	502	YE1	O4'-C1'-N9A	-2.11	104.12	108.11
3	B	502	YE1	OAK-CAH-CAI	-2.09	114.29	119.80
3	I	502	YE1	CAJ-CAE-CAF	-2.07	119.13	120.41
3	G	502	YE1	C2A-N1A-C6A	-2.06	115.08	118.77
3	A	502	YE1	CAC-CAF-CAG	-2.06	116.89	120.37
3	F	502	YE1	CAC-CAF-CAG	-2.06	116.89	120.37
3	L	502	YE1	C7P-C6P-C5P	-2.05	108.69	112.22
3	C	502	YE1	C7P-C6P-C5P	-2.05	108.69	112.22
3	B	502	YE1	C2P-NAA-CAB	-2.04	118.76	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	502	YE1	O4A-P2A-O6A	-2.02	98.63	108.24
3	K	502	YE1	CAJ-CAE-CAF	-2.01	119.17	120.41
3	J	502	YE1	O9A-P3'-O7A	2.00	117.16	110.63
3	H	502	YE1	O5P-C5P-C6P	2.03	125.49	121.97
3	F	502	YE1	OAL-CAJ-CAE	2.03	125.14	119.80
3	B	502	YE1	O4'-C4'-C5'	2.03	116.55	109.29
3	F	502	YE1	C14-C11-C10	2.04	112.89	109.17
3	L	502	YE1	CAF-CAC-CAB	2.04	119.31	112.86
3	H	502	YE1	CAI-CAJ-CAE	2.07	123.53	120.43
3	F	502	YE1	O9A-P3'-O7A	2.13	117.59	110.63
3	H	502	YE1	C13-C11-C12	2.15	111.29	108.50
3	C	502	YE1	OAD-CAB-NAA	2.15	127.23	122.96
3	F	502	YE1	O1A-P1A-O2A	2.16	123.78	112.56
3	G	502	YE1	CAF-CAC-CAB	2.18	119.78	112.86
3	K	502	YE1	O5P-C5P-C6P	2.19	125.77	121.97
3	E	502	YE1	O8A-P3'-O7A	2.19	117.77	110.63
3	H	502	YE1	O9A-P3'-O8A	2.19	115.48	107.44
3	I	502	YE1	O5P-C5P-C6P	2.20	125.78	121.97
3	D	502	YE1	CAC-CAF-CAE	2.20	124.10	120.37
3	H	502	YE1	O8A-P3'-O7A	2.21	117.85	110.63
3	A	502	YE1	O8A-P3'-O7A	2.22	117.86	110.63
3	A	502	YE1	O3'-C3'-C2'	2.22	119.98	111.73
3	K	502	YE1	O4'-C4'-C5'	2.23	117.28	109.29
3	I	502	YE1	O4'-C4'-C5'	2.23	117.28	109.29
3	C	502	YE1	O8A-P3'-O7A	2.24	117.93	110.63
3	A	502	YE1	O9A-P3'-O7A	2.24	117.94	110.63
3	L	502	YE1	C10-C9P-N8P	2.25	121.62	116.31
3	A	502	YE1	O9A-P3'-O8A	2.26	115.72	107.44
3	L	502	YE1	O9A-P3'-O7A	2.26	117.99	110.63
3	F	502	YE1	O10-C10-C9P	2.26	115.88	110.52
3	E	502	YE1	O4A-P2A-O5A	2.27	124.39	112.56
3	F	502	YE1	O4'-C4'-C3'	2.29	110.18	104.89
3	I	502	YE1	CAC-CAF-CAE	2.31	124.28	120.37
3	G	502	YE1	O1A-P1A-O2A	2.32	124.61	112.56
3	G	502	YE1	O9A-P3'-O8A	2.34	116.02	107.44
3	K	502	YE1	CAC-CAF-CAE	2.34	124.33	120.37
3	D	502	YE1	C2P-NAA-CAB	2.35	127.45	122.79
3	J	502	YE1	O9A-P3'-O8A	2.36	116.11	107.44
3	J	502	YE1	O1A-P1A-O2A	2.37	124.90	112.56
3	E	502	YE1	O4A-P2A-O3A	2.39	115.49	105.27
3	L	502	YE1	O2'-C2'-C3'	2.39	118.04	111.13
3	L	502	YE1	O1A-P1A-O2A	2.40	125.03	112.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	YE1	O2'-C2'-C3'	2.43	118.14	111.13
3	D	502	YE1	CAI-CAH-CAG	2.47	124.12	120.43
3	F	502	YE1	CAI-CAH-CAG	2.48	124.14	120.43
3	H	502	YE1	O4A-P2A-O5A	2.48	125.49	112.56
3	B	502	YE1	O4A-P2A-O3A	2.50	115.96	105.27
3	G	502	YE1	O4A-P2A-O5A	2.51	125.64	112.56
3	F	502	YE1	CAC-CAF-CAE	2.56	124.70	120.37
3	D	502	YE1	C13-C11-C10	2.57	113.86	109.17
3	E	502	YE1	O9A-P3'-O7A	2.58	119.05	110.63
3	B	502	YE1	O8A-P3'-O7A	2.59	119.06	110.63
3	A	502	YE1	N3A-C2A-N1A	2.59	130.90	128.87
3	G	502	YE1	O9A-P3'-O7A	2.63	119.22	110.63
3	G	502	YE1	CAI-CAJ-CAE	2.65	124.39	120.43
3	I	502	YE1	O8A-P3'-O7A	2.66	119.32	110.63
3	K	502	YE1	O8A-P3'-O7A	2.66	119.32	110.63
3	G	502	YE1	O5P-C5P-C6P	2.67	126.60	121.97
3	H	502	YE1	O2'-C2'-C3'	2.71	118.95	111.13
3	B	502	YE1	O4A-P2A-O5A	2.72	126.73	112.56
3	C	502	YE1	O1A-P1A-O3A	2.73	116.97	105.27
3	F	502	YE1	O4A-P2A-O5A	2.73	126.79	112.56
3	E	502	YE1	O9A-P3'-O8A	2.77	117.62	107.44
3	J	502	YE1	P3'-O3'-C3'	2.78	128.68	121.56
3	C	502	YE1	O9A-P3'-O8A	2.81	117.75	107.44
3	H	502	YE1	O9A-P3'-O7A	2.81	119.79	110.63
3	D	502	YE1	O1A-P1A-O2A	2.82	127.25	112.56
3	A	502	YE1	O4A-P2A-O5A	2.87	127.52	112.56
3	C	502	YE1	O4A-P2A-O5A	2.88	127.57	112.56
3	H	502	YE1	O3'-C3'-C2'	2.89	122.48	111.73
3	L	502	YE1	O8A-P3'-O7A	2.90	120.10	110.63
3	I	502	YE1	O4A-P2A-O5A	2.91	127.72	112.56
3	K	502	YE1	O4A-P2A-O5A	2.92	127.76	112.56
3	A	502	YE1	CAF-CAC-CAB	3.03	122.46	112.86
3	D	502	YE1	O4A-P2A-O5A	3.05	128.44	112.56
3	B	502	YE1	CAF-CAC-CAB	3.06	122.54	112.86
3	L	502	YE1	O4A-P2A-O5A	3.08	128.58	112.56
3	B	502	YE1	O9A-P3'-O7A	3.13	120.83	110.63
3	J	502	YE1	O4A-P2A-O5A	3.15	128.95	112.56
3	D	502	YE1	O9A-P3'-O7A	3.20	121.08	110.63
3	L	502	YE1	O5P-C5P-C6P	3.42	127.91	121.97
3	A	502	YE1	P3'-O3'-C3'	3.46	130.43	121.56
3	F	502	YE1	C13-C11-C12	3.47	113.00	108.50
3	C	502	YE1	O5P-C5P-C6P	4.13	129.13	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	502	YE1	O3'-C3'-C2'	4.33	127.83	111.73
3	H	502	YE1	P3'-O3'-C3'	4.67	133.51	121.56
3	F	502	YE1	P3'-O3'-C3'	8.37	143.00	121.56

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	502	YE1	P3'-O3'-C3'-C2'
3	A	502	YE1	P3'-O3'-C3'-C2'
3	F	502	YE1	P3'-O3'-C3'-C2'

There are no ring outliers.

11 monomers are involved in 34 short contacts:

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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	421/440 (95%)	-0.09	5 (1%) 81 78	16, 39, 80, 111	0
1	B	422/440 (95%)	-0.23	1 (0%) 95 95	19, 38, 62, 77	0
1	C	421/440 (95%)	-0.20	0 100 100	17, 37, 67, 90	0
1	D	423/440 (96%)	-0.28	1 (0%) 95 95	16, 32, 52, 68	0
1	E	421/440 (95%)	-0.23	1 (0%) 95 95	19, 35, 59, 76	0
1	F	421/440 (95%)	-0.24	0 100 100	16, 34, 56, 74	0
1	G	422/440 (95%)	-0.25	0 100 100	16, 32, 62, 83	0
1	H	422/440 (95%)	-0.14	1 (0%) 95 95	17, 41, 65, 86	0
1	I	421/440 (95%)	-0.24	0 100 100	15, 34, 59, 74	0
1	J	422/440 (95%)	-0.03	7 (1%) 73 69	25, 44, 78, 108	0
1	K	422/440 (95%)	-0.24	0 100 100	13, 33, 59, 77	0
1	L	421/440 (95%)	-0.15	1 (0%) 95 95	18, 38, 72, 103	0
All	All	5059/5280 (95%)	-0.19	17 (0%) 94 94	13, 36, 65, 111	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	427	ASP	3.9
1	J	37	ALA	3.6
1	A	37	ALA	3.6
1	J	430	GLY	3.0
1	J	29	LEU	3.0
1	J	36	GLY	2.7
1	A	430	GLY	2.6
1	H	273	PRO	2.6
1	J	47	ALA	2.4
1	L	36	GLY	2.4
1	B	235	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	38	ARG	2.2
1	A	431	ARG	2.2
1	D	384	ASP	2.1
1	J	30	ALA	2.1
1	E	432	PHE	2.0
1	A	22	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	YE1	I	502	59/59	0.95	0.16	0.84	17,37,47,50	0
3	YE1	E	502	59/59	0.97	0.16	0.39	27,45,59,63	0
3	YE1	G	502	59/59	0.98	0.14	0.16	19,36,54,58	0
3	YE1	H	502	59/59	0.97	0.15	0.03	19,42,67,73	0
3	YE1	A	502	59/59	0.97	0.14	-0.07	29,46,64,73	0
3	YE1	K	502	59/59	0.98	0.14	-0.10	17,37,47,50	0
3	YE1	F	502	59/59	0.98	0.14	-0.13	23,35,44,53	0
3	YE1	L	502	59/59	0.97	0.14	-0.17	23,37,49,63	0
3	YE1	B	502	59/59	0.97	0.13	-0.34	14,43,55,57	0
3	YE1	J	502	59/59	0.96	0.13	-0.39	28,49,68,75	0
3	YE1	C	502	59/59	0.98	0.12	-0.63	13,32,49,55	0
3	YE1	D	502	59/59	0.98	0.12	-0.95	15,28,43,47	0
2	XE	B	501[A]	1/1	0.99	0.12	-1.28	27,27,27,27	1
2	XE	D	501[B]	1/1	0.98	0.10	-1.68	24,24,24,24	1
2	XE	K	501[B]	1/1	0.99	0.08	-1.85	63,63,63,63	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	XE	E	501[B]	1/1	0.99	0.11	-1.94	55,55,55,55	1
2	XE	G	501[B]	1/1	1.00	0.11	-2.01	36,36,36,36	1
2	XE	B	501[B]	1/1	0.99	0.12	-2.13	43,43,43,43	1
2	XE	H	501[B]	1/1	0.98	0.06	-2.17	47,47,47,47	1
2	XE	C	501[B]	1/1	1.00	0.07	-2.65	48,48,48,48	1
2	XE	A	501[A]	1/1	0.99	0.10	-2.74	58,58,58,58	1
2	XE	L	501[B]	1/1	0.99	0.07	-2.75	101,101,101,101	1
2	XE	I	501[B]	1/1	0.99	0.06	-3.01	37,37,37,37	1
2	XE	A	501[B]	1/1	0.99	0.10	-3.37	47,47,47,47	1
2	XE	J	501[B]	1/1	0.99	0.07	-3.48	46,46,46,46	1
2	XE	F	501[B]	1/1	0.99	0.06	-5.34	39,39,39,39	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.