



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 04:41 PM UTC

PDB ID : 4APZ / pdb_00004apz
Title : Structure of B. subtilis genomic dUTPase YncF in complex with dU, PPi and Mg in P1
Authors : Garcia-Nafria, J.; Timm, J.; Harrison, C.; Turkenburg, J.P.; Wilson, K.S.
Deposited on : 2012-04-11
Resolution : 2.01 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
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

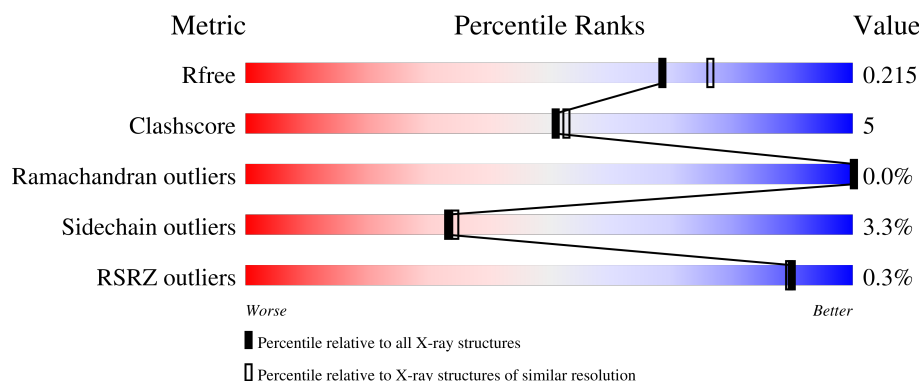
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	1	144	2% 90% 7% ..
1	2	144	92% ..
1	3	144	89% 8% ...
1	4	144	88% 8% ..
1	5	144	2% 88% 8% ..

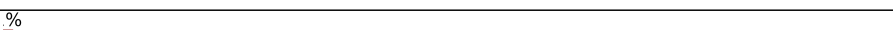
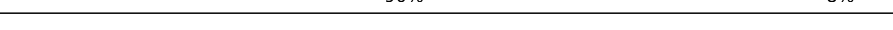
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Mol	Chain	Length	Quality of chain
1	6	144	% 90% 7% ..
1	7	144	% 90% 8% ..
1	8	144	% 83% 14% ..
1	9	144	88% 9% ..
1	A	144	% 89% 10% ..
1	B	144	87% 10% ..
1	C	144	% 88% 10% ..
1	D	144	% 88% 10% ..
1	E	144	83% 15% ..
1	F	144	% 88% 11% ..
1	G	144	87% 10% ..
1	H	144	% 85% 11% ...
1	I	144	90% 8% ..
1	J	144	88% 10% .
1	K	144	88% 10% ..
1	L	144	91% 7% ..
1	M	144	88% 9% ..
1	N	144	90% 9% .
1	O	144	84% 14% ..
1	P	144	85% 12% ..
1	Q	144	85% 15% .
1	R	144	85% 12% ..
1	S	144	89% 7% ..
1	T	144	89% 9% ..
1	U	144	88% 10% ..

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Mol	Chain	Length	Quality of chain
1	V	144	 85% 12% ..
1	W	144	 88% 10% ..
1	X	144	 92% 6% ..
1	Y	144	 88% 10% ..
1	Z	144	 86% 12% ..
1	a	144	 90% 8% ..
1	b	144	 85% 13% ..
1	c	144	 89% 8% ..
1	d	144	 88% 8% ..
1	e	144	 85% 13% ..
1	f	144	 87% 10% ..
1	g	144	 86% 12% ..
1	h	144	 88% 8% ..
1	i	144	 90% 8% ..
1	j	144	 88% 10% ..
1	k	144	 75% 23% ..
1	l	144	 91% 7% ..
1	m	144	 88% 10% ..

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	DUR	J	1145	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 60911 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 PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	142	Total	C	N	O	S	9	2	0
			1148	730	193	218	7			
1	2	142	Total	C	N	O	S	0	2	0
			1149	730	194	218	7			
1	3	142	Total	C	N	O	S	3	0	0
			1136	721	191	218	6			
1	4	142	Total	C	N	O	S	0	4	0
			1162	739	196	220	7			
1	5	142	Total	C	N	O	S	7	1	0
			1141	725	191	218	7			
1	6	142	Total	C	N	O	S	11	1	0
			1141	725	191	218	7			
1	7	142	Total	C	N	O	S	0	0	0
			1136	721	191	218	6			
1	8	142	Total	C	N	O	S	0	1	0
			1141	725	191	218	7			
1	9	142	Total	C	N	O	S	3	2	0
			1150	731	193	219	7			
1	A	143	Total	C	N	O	S	4	2	0
			1151	731	192	221	7			
1	B	142	Total	C	N	O	S	4	2	0
			1148	730	193	218	7			
1	C	142	Total	C	N	O	S	6	2	0
			1148	729	193	220	6			
1	D	142	Total	C	N	O	S	7	1	0
			1141	725	191	218	7			
1	E	142	Total	C	N	O	S	3	1	0
			1143	726	193	218	6			
1	F	143	Total	C	N	O	S	3	2	0
			1155	734	194	220	7			
1	G	142	Total	C	N	O	S	6	2	0
			1152	732	195	219	6			

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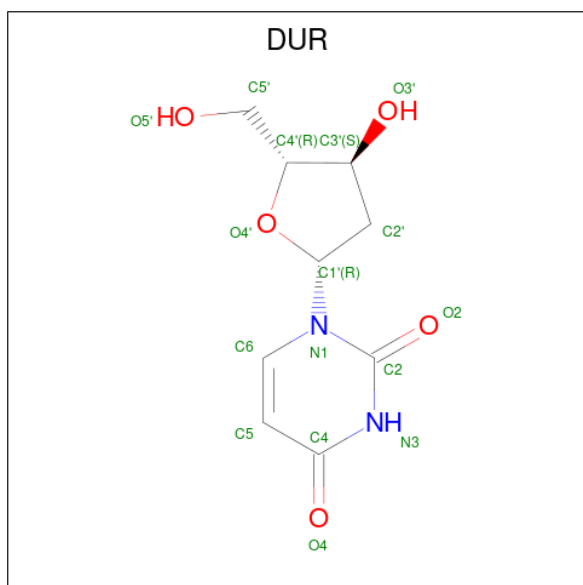
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	142	Total	C	N	O	S	3	0	0
			1136	721	191	218	6			
1	I	142	Total	C	N	O	S	7	1	0
			1141	725	191	218	7			
1	J	142	Total	C	N	O	S	2	1	0
			1143	726	193	218	6			
1	K	142	Total	C	N	O	S	11	1	0
			1142	725	191	220	6			
1	L	142	Total	C	N	O	S	0	0	0
			1136	721	191	218	6			
1	M	142	Total	C	N	O	S	2	1	0
			1139	723	191	219	6			
1	N	142	Total	C	N	O	S	3	0	0
			1136	721	191	218	6			
1	O	142	Total	C	N	O	S	0	0	0
			1136	721	191	218	6			
1	P	142	Total	C	N	O	S	2	2	0
			1150	731	193	219	7			
1	Q	143	Total	C	N	O	S	0	1	0
			1150	730	194	220	6			
1	R	142	Total	C	N	O	S	3	1	0
			1143	726	193	218	6			
1	S	142	Total	C	N	O	S	0	2	0
			1148	730	193	218	7			
1	T	142	Total	C	N	O	S	4	2	0
			1148	730	193	218	7			
1	U	142	Total	C	N	O	S	0	2	0
			1148	730	193	218	7			
1	V	142	Total	C	N	O	S	3	1	0
			1141	725	191	218	7			
1	W	142	Total	C	N	O	S	0	0	0
			1136	721	191	218	6			
1	X	142	Total	C	N	O	S	0	3	0
			1151	732	193	219	7			
1	Y	142	Total	C	N	O	S	3	1	0
			1141	725	191	218	7			
1	Z	142	Total	C	N	O	S	8	2	0
			1150	731	193	219	7			
1	a	143	Total	C	N	O	S	7	1	0
			1148	729	192	220	7			
1	b	143	Total	C	N	O	S	3	0	0
			1143	725	192	220	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	c	142	Total	C	N	O	S	8	2	0
			1148	730	193	218	7			
1	d	142	Total	C	N	O	S	0	1	0
			1141	725	191	218	7			
1	e	142	Total	C	N	O	S	0	1	0
			1141	725	191	218	7			
1	f	142	Total	C	N	O	S	0	1	0
			1141	725	191	218	7			
1	g	142	Total	C	N	O	S	3	2	0
			1153	732	194	220	7			
1	h	142	Total	C	N	O	S	4	0	0
			1136	721	191	218	6			
1	i	142	Total	C	N	O	S	4	1	0
			1141	725	191	218	7			
1	j	143	Total	C	N	O	S	2	1	0
			1148	729	192	220	7			
1	k	142	Total	C	N	O	S	4	1	0
			1141	725	191	218	7			
1	l	142	Total	C	N	O	S	0	2	0
			1148	730	193	218	7			
1	m	142	Total	C	N	O	S	0	1	0
			1141	725	191	218	7			

- Molecule 2 is 2'-DEOXYURIDINE (CCD ID: DUR) (formula: $C_9H_{12}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	1	1	Total	C	N	O	0	0
			16	9	2	5		
2	2	1	Total	C	N	O	0	0
			16	9	2	5		
2	3	1	Total	C	N	O	0	0
			16	9	2	5		
2	4	1	Total	C	N	O	0	0
			16	9	2	5		
2	5	1	Total	C	N	O	0	0
			16	9	2	5		
2	6	1	Total	C	N	O	0	0
			16	9	2	5		
2	7	1	Total	C	N	O	0	0
			16	9	2	5		
2	8	1	Total	C	N	O	0	0
			16	9	2	5		
2	9	1	Total	C	N	O	0	0
			16	9	2	5		
2	A	1	Total	C	N	O	0	0
			16	9	2	5		
2	B	1	Total	C	N	O	0	0
			16	9	2	5		
2	C	1	Total	C	N	O	0	0
			16	9	2	5		
2	D	1	Total	C	N	O	0	0
			16	9	2	5		
2	E	1	Total	C	N	O	0	0
			16	9	2	5		
2	F	1	Total	C	N	O	0	0
			16	9	2	5		
2	G	1	Total	C	N	O	0	0
			16	9	2	5		
2	H	1	Total	C	N	O	0	0
			16	9	2	5		
2	I	1	Total	C	N	O	0	0
			16	9	2	5		
2	J	1	Total	C	N	O	0	0
			16	9	2	5		
2	K	1	Total	C	N	O	0	0
			16	9	2	5		
2	L	1	Total	C	N	O	0	0
			16	9	2	5		
2	M	1	Total	C	N	O	0	0
			16	9	2	5		

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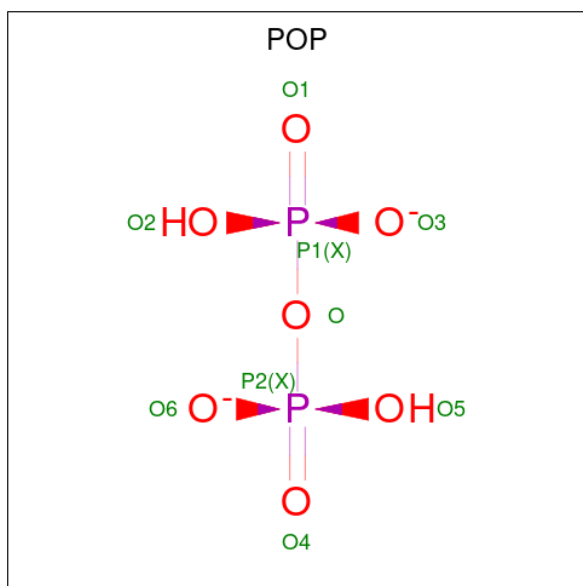
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	N	1	Total	C	N	O	0	0
			16	9	2	5		
2	O	1	Total	C	N	O	0	0
			16	9	2	5		
2	P	1	Total	C	N	O	0	0
			16	9	2	5		
2	Q	1	Total	C	N	O	0	0
			16	9	2	5		
2	R	1	Total	C	N	O	0	0
			16	9	2	5		
2	S	1	Total	C	N	O	0	0
			16	9	2	5		
2	T	1	Total	C	N	O	0	0
			16	9	2	5		
2	U	1	Total	C	N	O	0	0
			16	9	2	5		
2	V	1	Total	C	N	O	0	0
			16	9	2	5		
2	W	1	Total	C	N	O	0	0
			16	9	2	5		
2	X	1	Total	C	N	O	0	0
			16	9	2	5		
2	Y	1	Total	C	N	O	0	0
			16	9	2	5		
2	Z	1	Total	C	N	O	0	0
			16	9	2	5		
2	a	1	Total	C	N	O	0	0
			16	9	2	5		
2	b	1	Total	C	N	O	0	0
			16	9	2	5		
2	c	1	Total	C	N	O	0	0
			16	9	2	5		
2	d	1	Total	C	N	O	0	0
			16	9	2	5		
2	e	1	Total	C	N	O	0	0
			16	9	2	5		
2	f	1	Total	C	N	O	0	0
			16	9	2	5		
2	g	1	Total	C	N	O	0	0
			16	9	2	5		
2	h	1	Total	C	N	O	0	0
			16	9	2	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	i	1	Total	C	N	O	0	0
			16	9	2	5		
2	j	1	Total	C	N	O	0	0
			16	9	2	5		
2	k	1	Total	C	N	O	0	0
			16	9	2	5		
2	l	1	Total	C	N	O	0	0
			16	9	2	5		
2	m	1	Total	C	N	O	0	0
			16	9	2	5		

- Molecule 3 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1	1	Total	O P	0	0
			9 7 2			
3	2	1	Total	O P	0	0
			9 7 2			
3	3	1	Total	O P	0	0
			9 7 2			
3	4	1	Total	O P	0	0
			9 7 2			
3	5	1	Total	O P	0	0
			9 7 2			
3	6	1	Total	O P	0	0
			9 7 2			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	7	1	Total 9	O 7	P 2	0	0
3	8	1	Total 9	O 7	P 2	0	0
3	9	1	Total 9	O 7	P 2	0	0
3	A	1	Total 9	O 7	P 2	0	0
3	B	1	Total 9	O 7	P 2	0	0
3	C	1	Total 9	O 7	P 2	0	0
3	D	1	Total 9	O 7	P 2	0	0
3	E	1	Total 9	O 7	P 2	0	0
3	F	1	Total 9	O 7	P 2	0	0
3	G	1	Total 9	O 7	P 2	0	0
3	H	1	Total 9	O 7	P 2	0	0
3	I	1	Total 9	O 7	P 2	0	0
3	J	1	Total 9	O 7	P 2	0	0
3	K	1	Total 9	O 7	P 2	0	0
3	L	1	Total 9	O 7	P 2	0	0
3	M	1	Total 9	O 7	P 2	0	0
3	N	1	Total 9	O 7	P 2	0	0
3	O	1	Total 9	O 7	P 2	0	0
3	P	1	Total 9	O 7	P 2	0	0
3	Q	1	Total 9	O 7	P 2	0	0
3	R	1	Total 9	O 7	P 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	1	Total	O	P	0	0
			9	7	2		
3	T	1	Total	O	P	0	0
			9	7	2		
3	U	1	Total	O	P	0	0
			9	7	2		
3	V	1	Total	O	P	0	0
			9	7	2		
3	W	1	Total	O	P	0	0
			9	7	2		
3	X	1	Total	O	P	0	0
			9	7	2		
3	Y	1	Total	O	P	0	0
			9	7	2		
3	Z	1	Total	O	P	0	0
			9	7	2		
3	a	1	Total	O	P	0	0
			9	7	2		
3	b	1	Total	O	P	0	0
			9	7	2		
3	c	1	Total	O	P	0	0
			9	7	2		
3	d	1	Total	O	P	0	0
			9	7	2		
3	e	1	Total	O	P	0	0
			9	7	2		
3	f	1	Total	O	P	0	0
			9	7	2		
3	g	1	Total	O	P	0	0
			9	7	2		
3	h	1	Total	O	P	0	0
			9	7	2		
3	i	1	Total	O	P	0	0
			9	7	2		
3	j	1	Total	O	P	0	0
			9	7	2		
3	k	1	Total	O	P	0	0
			9	7	2		
3	l	1	Total	O	P	0	0
			9	7	2		
3	m	1	Total	O	P	0	0
			9	7	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1	1	Total 1	Mg 1	0	0
4	2	1	Total 1	Mg 1	0	0
4	3	1	Total 1	Mg 1	0	0
4	4	1	Total 1	Mg 1	0	0
4	5	1	Total 1	Mg 1	0	0
4	6	1	Total 1	Mg 1	0	0
4	7	1	Total 1	Mg 1	0	0
4	8	1	Total 1	Mg 1	0	0
4	9	1	Total 1	Mg 1	0	0
4	A	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0
4	E	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0
4	G	1	Total 1	Mg 1	0	0
4	H	1	Total 1	Mg 1	0	0
4	I	1	Total 1	Mg 1	0	0
4	J	1	Total 1	Mg 1	0	0
4	K	1	Total 1	Mg 1	0	0
4	L	1	Total 1	Mg 1	0	0

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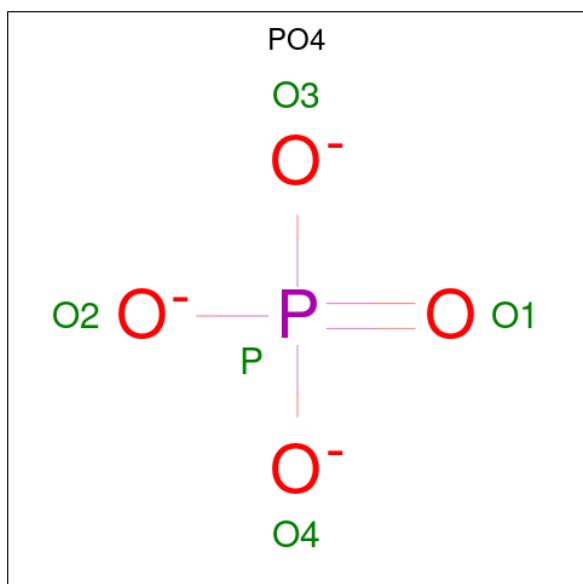
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total 1	Mg 1	0	0
4	N	1	Total 1	Mg 1	0	0
4	O	1	Total 1	Mg 1	0	0
4	P	1	Total 1	Mg 1	0	0
4	Q	1	Total 1	Mg 1	0	0
4	R	1	Total 1	Mg 1	0	0
4	S	1	Total 1	Mg 1	0	0
4	T	1	Total 1	Mg 1	0	0
4	U	1	Total 1	Mg 1	0	0
4	V	1	Total 1	Mg 1	0	0
4	W	1	Total 1	Mg 1	0	0
4	X	1	Total 1	Mg 1	0	0
4	Y	1	Total 1	Mg 1	0	0
4	Z	1	Total 1	Mg 1	0	0
4	a	1	Total 1	Mg 1	0	0
4	b	1	Total 1	Mg 1	0	0
4	c	1	Total 1	Mg 1	0	0
4	d	1	Total 1	Mg 1	0	0
4	e	1	Total 1	Mg 1	0	0
4	f	1	Total 1	Mg 1	0	0
4	g	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	h	1	Total	Mg	0	0
			1	1		
4	i	1	Total	Mg	0	0
			1	1		
4	j	1	Total	Mg	0	0
			1	1		
4	k	1	Total	Mg	0	0
			1	1		
4	l	1	Total	Mg	0	0
			1	1		
4	m	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	e	1	Total	O	P	0	0
			5	4	1		
5	l	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	120	Total	O	0	0
			120	120		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	2	139	Total 139	O 139	0	0
6	3	102	Total 102	O 102	0	0
6	4	85	Total 85	O 85	0	0
6	5	109	Total 109	O 109	0	0
6	6	93	Total 93	O 93	0	0
6	7	69	Total 69	O 69	0	0
6	8	136	Total 136	O 136	0	0
6	9	101	Total 101	O 101	0	0
6	A	122	Total 122	O 122	0	0
6	A	3	Total 3	O 3	0	0
6	B	96	Total 96	O 96	0	0
6	C	67	Total 67	O 67	0	0
6	D	133	Total 133	O 133	0	0
6	E	111	Total 111	O 111	0	0
6	F	86	Total 86	O 86	0	0
6	G	141	Total 141	O 141	0	0
6	H	123	Total 123	O 123	0	0
6	I	84	Total 84	O 84	0	0
6	J	116	Total 116	O 116	0	0
6	K	95	Total 95	O 95	0	0
6	L	70	Total 70	O 70	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	M	124	Total O 124 124	0	0
6	N	98	Total O 98 98	0	0
6	O	68	Total O 68 68	0	0
6	P	142	Total O 142 142	0	0
6	Q	103	Total O 103 103	0	0
6	R	75	Total O 75 75	0	0
6	S	133	Total O 133 133	0	0
6	T	90	Total O 90 90	0	0
6	U	62	Total O 62 62	0	0
6	V	118	Total O 118 118	0	0
6	W	97	Total O 97 97	0	0
6	X	70	Total O 70 70	0	0
6	Y	94	Total O 94 94	0	0
6	Z	60	Total O 60 60	0	0
6	a	1	Total O 1 1	0	0
6	a	69	Total O 69 69	0	0
6	b	127	Total O 127 127	0	0
6	c	105	Total O 105 105	0	0
6	d	63	Total O 63 63	0	0
6	e	128	Total O 128 128	0	0
6	f	92	Total O 92 92	0	0

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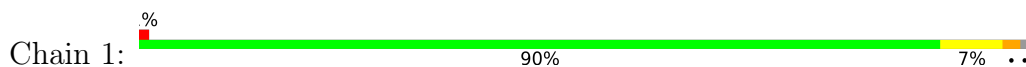
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	g	74	Total 74	O 74	0	0
6	h	143	Total 143	O 143	0	0
6	i	99	Total 99	O 99	0	0
6	j	63	Total 63	O 63	0	0
6	k	109	Total 109	O 109	0	0
6	l	69	Total 69	O 69	0	0
6	m	49	Total 49	O 49	0	0

3 Residue-property plots [i](#)

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

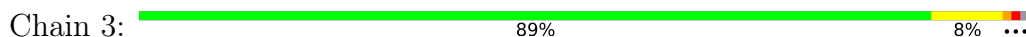
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



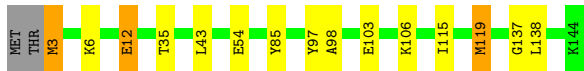
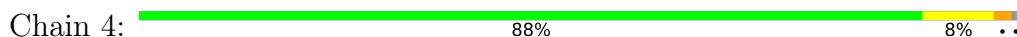
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



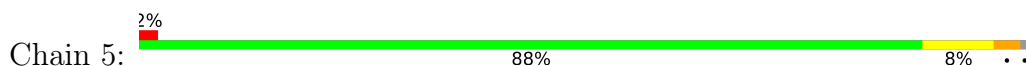
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

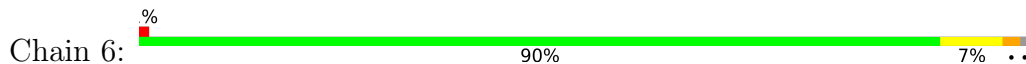


- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

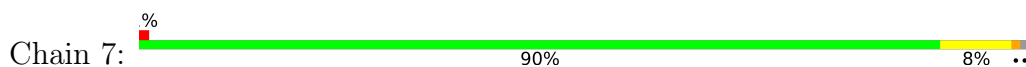




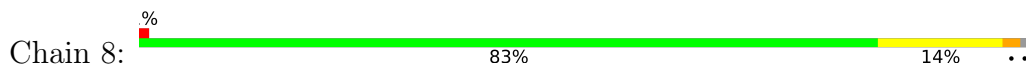
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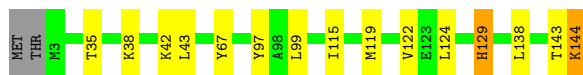
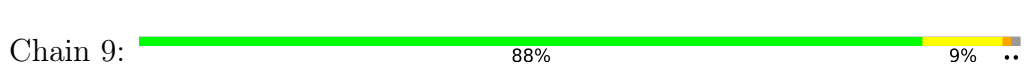
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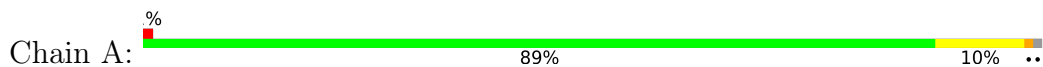
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- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

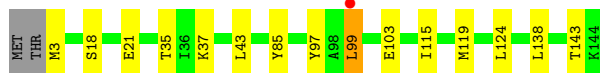
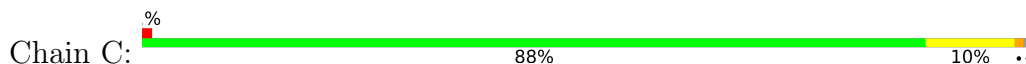


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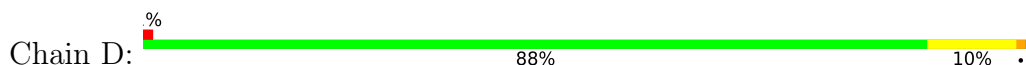




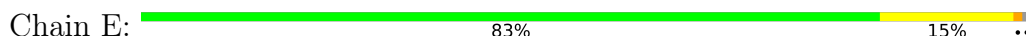
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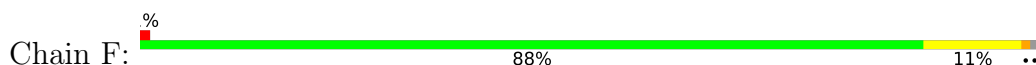
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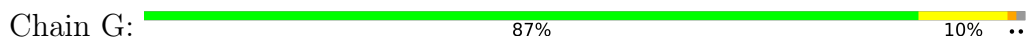
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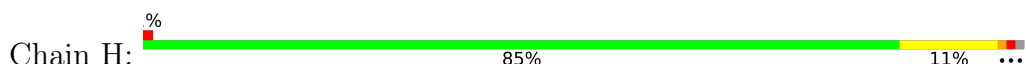
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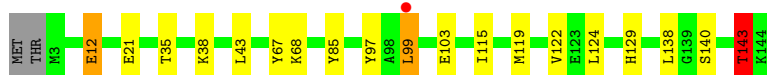


- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



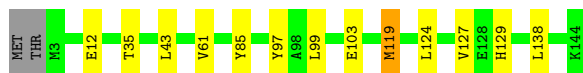
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF





- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain I: 90% 8% ..



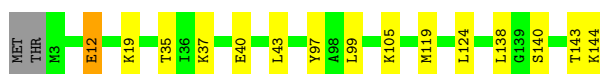
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain J: 88% 10% ..



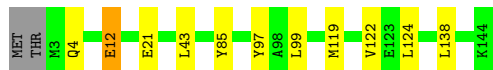
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain K: 88% 10% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain L: 91% 7% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain M: 88% 9% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain N: 90% 9% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain O: 84% 14% ..



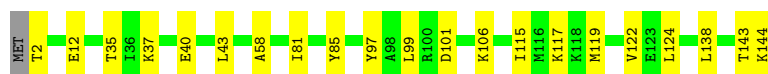
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain P: 85% 12% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain Q: 85% 15% .



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain R: 85% 12% ..



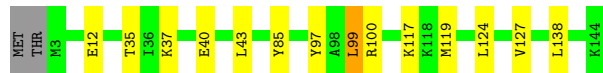
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain S: 89% 7% ..



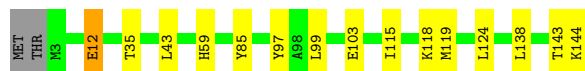
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain T: 89% 9% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain U:  88% 10% ..



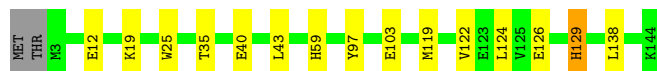
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain V:  85% 12% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain W:  88% 10% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain X:  92% 6% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain Y:  88% 10% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain Z:  86% 12% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain a:  90% 8% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain b:  85% 13% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain c:  89% 8% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain d:  88% 8% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain e:  85% 13% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain f:  87% 10% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain g:  86% 12% ..



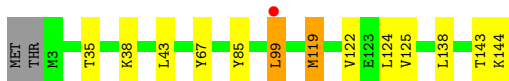
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain h: 88% 8% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain i: 90% 8% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain j: 88% 10% ..



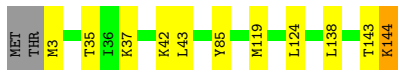
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain k: 75% 23% ..



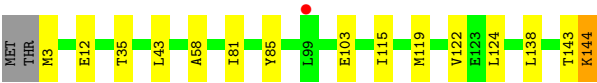
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain l: 91% 7% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain m: 88% 10% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	97.06Å 97.07Å 193.85Å 89.72° 88.47° 90.11°	Depositor
Resolution (Å)	36.44 – 2.01 36.44 – 2.01	Depositor EDS
% Data completeness (in resolution range)	96.7 (36.44-2.01) 96.7 (36.44-2.01)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.169 , 0.212 0.174 , 0.215	Depositor DCC
R_{free} test set	22967 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.044 for k,-h,l 0.044 for -k,h,l 0.046 for h,-k,-l 0.048 for -h,k,-l 0.044 for -h,-k,l 0.039 for k,h,-l 0.115 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	60911	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DUR, POP, PO4, MG

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	1	1.06	0/1176	0.92	0/1582
1	2	1.16	0/1176	0.96	2/1581 (0.1%)
1	3	1.19	3/1157 (0.3%)	0.98	1/1556 (0.1%)
1	4	1.20	4/1196 (0.3%)	0.99	1/1608 (0.1%)
1	5	1.12	2/1165 (0.2%)	0.96	3/1567 (0.2%)
1	6	1.13	2/1165 (0.2%)	0.95	1/1567 (0.1%)
1	7	1.08	1/1157 (0.1%)	0.92	0/1556
1	8	1.16	5/1165 (0.4%)	0.93	0/1567
1	9	1.15	0/1173	0.93	0/1575
1	A	1.05	2/1178 (0.2%)	0.91	0/1585
1	B	1.12	2/1176 (0.2%)	0.92	0/1582
1	C	1.06	0/1171	0.92	0/1572
1	D	1.14	1/1165 (0.1%)	1.00	0/1567
1	E	1.17	5/1168 (0.4%)	0.98	1/1571 (0.1%)
1	F	1.17	2/1183 (0.2%)	1.00	0/1592
1	G	1.19	3/1176 (0.3%)	0.95	0/1579
1	H	1.23	3/1157 (0.3%)	1.04	1/1556 (0.1%)
1	I	1.19	1/1165 (0.1%)	0.99	0/1567
1	J	1.14	1/1168 (0.1%)	0.98	0/1571
1	K	1.15	1/1166 (0.1%)	0.96	0/1568
1	L	1.14	0/1157	0.96	0/1556
1	M	1.17	1/1163 (0.1%)	0.91	0/1564
1	N	1.07	1/1157 (0.1%)	0.94	0/1556
1	O	1.16	2/1157 (0.2%)	0.90	0/1556
1	P	1.24	5/1173 (0.4%)	0.95	0/1575
1	Q	1.24	1/1175 (0.1%)	1.03	0/1581
1	R	1.24	3/1168 (0.3%)	0.96	0/1571
1	S	1.17	1/1176 (0.1%)	0.95	0/1582
1	T	1.12	0/1176	0.96	1/1582 (0.1%)
1	U	1.12	2/1176 (0.2%)	0.95	0/1582
1	V	1.22	4/1165 (0.3%)	0.99	1/1567 (0.1%)
1	W	1.20	4/1157 (0.3%)	0.95	0/1556

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	X	1.17	0/1182	1.02	0/1590
1	Y	1.15	1/1165 (0.1%)	0.95	0/1567
1	Z	1.11	1/1173 (0.1%)	0.93	0/1575
1	a	1.18	1/1172 (0.1%)	0.97	0/1577
1	b	1.18	3/1164 (0.3%)	0.96	0/1566
1	c	1.10	1/1176 (0.1%)	0.93	0/1582
1	d	1.15	1/1165 (0.1%)	0.98	2/1567 (0.1%)
1	e	1.15	1/1165 (0.1%)	0.93	0/1567
1	f	1.21	3/1165 (0.3%)	0.99	1/1567 (0.1%)
1	g	1.14	1/1173 (0.1%)	0.94	0/1575
1	h	1.21	2/1157 (0.2%)	0.97	0/1556
1	i	1.19	1/1165 (0.1%)	0.99	4/1567 (0.3%)
1	j	1.21	1/1172 (0.1%)	0.97	0/1577
1	k	1.23	1/1165 (0.1%)	1.17	0/1567
1	l	1.05	0/1176	0.89	0/1582
1	m	1.02	0/1165	0.92	0/1567
All	All	1.16	80/56103 (0.1%)	0.96	19/75446 (0.0%)

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	59	HIS	ND1-CE1	8.16	1.40	1.32
1	6	108	ASP	C-O	-7.96	1.14	1.23
1	g	134	ASP	C-O	-7.17	1.15	1.23
1	Z	59	HIS	ND1-CE1	6.98	1.39	1.32
1	V	122	VAL	C-O	-6.97	1.17	1.24
1	5	59	HIS	CE1-NE2	6.71	1.39	1.32
1	b	59	HIS	ND1-CE1	6.57	1.39	1.32
1	Y	59	HIS	CG-CD2	6.35	1.42	1.35
1	8	59	HIS	CE1-NE2	6.28	1.38	1.32
1	U	59	HIS	ND1-CE1	6.17	1.38	1.32
1	P	95	PRO	CA-C	-6.05	1.46	1.52
1	8	48	VAL	C-O	6.03	1.30	1.24
1	V	25	TRP	NE1-CE2	-6.02	1.30	1.37
1	4	119[A]	MET	C-O	-6.01	1.16	1.23
1	4	119[B]	MET	C-O	-6.01	1.16	1.23
1	I	61	VAL	C-O	5.94	1.28	1.24
1	W	25	TRP	NE1-CE2	-5.90	1.30	1.37
1	h	74	GLN	C-O	5.89	1.31	1.24
1	E	62	PRO	C-O	-5.88	1.16	1.23
1	f	64	SER	C-O	-5.86	1.16	1.24
1	6	129	HIS	CG-CD2	5.83	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	h	44	VAL	N-CA	-5.79	1.42	1.46
1	A	25	TRP	NE1-CE2	-5.79	1.31	1.37
1	O	68	LYS	C-O	-5.78	1.17	1.24
1	d	59	HIS	ND1-CE1	5.77	1.38	1.32
1	E	115	ILE	C-O	5.71	1.31	1.24
1	A	105	LYS	C-O	-5.70	1.17	1.23
1	H	68	LYS	C-O	-5.68	1.17	1.24
1	E	70	PHE	C-O	-5.67	1.17	1.24
1	P	19	LYS	C-O	5.66	1.30	1.24
1	J	59	HIS	CD2-NE2	-5.61	1.31	1.37
1	3	129	HIS	CG-CD2	5.59	1.42	1.35
1	P	32	GLU	C-O	-5.57	1.17	1.23
1	8	59	HIS	CG-CD2	5.52	1.42	1.35
1	B	119[A]	MET	C-O	-5.48	1.17	1.24
1	B	119[B]	MET	C-O	-5.48	1.17	1.24
1	E	140	SER	C-O	-5.46	1.17	1.24
1	V	25	TRP	C-O	-5.44	1.16	1.23
1	D	94	PHE	C-O	-5.42	1.20	1.25
1	K	140	SER	C-O	-5.42	1.17	1.24
1	4	98	ALA	N-CA	5.41	1.53	1.46
1	F	59	HIS	CD2-NE2	-5.41	1.31	1.37
1	G	105	LYS	C-O	-5.41	1.17	1.23
1	M	72	VAL	C-O	-5.40	1.18	1.24
1	7	59	HIS	CG-CD2	5.33	1.41	1.35
1	V	129	HIS	CG-CD2	5.32	1.41	1.35
1	8	57	GLU	CA-C	5.28	1.59	1.52
1	P	25	TRP	NE1-CE2	-5.28	1.31	1.37
1	N	140	SER	C-O	-5.27	1.17	1.24
1	5	129	HIS	CG-CD2	5.26	1.41	1.35
1	R	48	VAL	C-O	-5.25	1.18	1.24
1	b	59	HIS	CG-CD2	5.24	1.41	1.35
1	W	126	GLU	CA-C	5.24	1.59	1.52
1	3	84	SER	C-O	-5.23	1.17	1.24
1	H	140	SER	C-O	-5.23	1.17	1.24
1	E	59	HIS	CG-ND1	-5.23	1.32	1.38
1	8	86	LYS	C-O	-5.20	1.17	1.24
1	k	59	HIS	ND1-CE1	5.19	1.37	1.32
1	a	64	SER	C-O	-5.18	1.17	1.24
1	f	138	LEU	C-O	-5.18	1.17	1.23
1	e	59	HIS	CE1-NE2	5.16	1.37	1.32
1	f	129	HIS	CG-CD2	5.16	1.41	1.35
1	c	37	LYS	CB-CG	-5.15	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	59	HIS	ND1-CE1	5.15	1.37	1.32
1	U	118	LYS	C-O	-5.15	1.17	1.23
1	j	134	ASP	C-O	-5.15	1.17	1.24
1	G	75	THR	C-O	-5.14	1.17	1.24
1	F	61	VAL	CA-C	-5.13	1.48	1.52
1	R	78	MET	CA-C	-5.13	1.46	1.52
1	R	92	TRP	C-O	-5.12	1.17	1.23
1	H	129	HIS	CG-CD2	5.09	1.41	1.35
1	4	137	GLY	C-O	-5.08	1.18	1.23
1	G	62	PRO	C-O	-5.07	1.17	1.23
1	Q	122	VAL	C-O	-5.06	1.19	1.24
1	b	48	VAL	CA-C	-5.04	1.46	1.52
1	W	129	HIS	CG-CD2	5.04	1.41	1.35
1	3	93	PHE	CA-C	5.02	1.58	1.52
1	i	125	VAL	C-O	-5.02	1.18	1.24
1	P	59	HIS	ND1-CE1	5.01	1.37	1.32
1	S	25	TRP	NE1-CE2	-5.00	1.31	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	6	LYS	CG-CD-CE	7.43	128.39	111.30
1	d	43	LEU	CA-C-N	-6.22	118.11	122.59
1	d	43	LEU	C-N-CA	-6.22	118.11	122.59
1	f	40	GLU	CA-CB-CG	6.12	126.33	114.10
1	6	99	LEU	CD1-CG-CD2	-5.90	97.82	110.80
1	H	143	THR	N-CA-CB	-5.66	103.37	110.90
1	3	99	LEU	CD1-CG-CD2	-5.56	98.57	110.80
1	V	99	LEU	CD1-CG-CD2	-5.52	98.65	110.80
1	5	12	GLU	CA-CB-CG	5.47	125.03	114.10
1	E	54	GLU	CB-CG-CD	5.35	121.69	112.60
1	i	119[A]	MET	CA-C-N	-5.34	114.74	120.03
1	i	119[A]	MET	C-N-CA	-5.34	114.74	120.03
1	i	119[B]	MET	CA-C-N	-5.34	114.74	120.03
1	i	119[B]	MET	C-N-CA	-5.34	114.74	120.03
1	5	52	LEU	CA-C-N	-5.13	114.50	119.78
1	5	52	LEU	C-N-CA	-5.13	114.50	119.78
1	T	99	LEU	CD1-CG-CD2	-5.11	99.57	110.80
1	2	43	LEU	CA-C-N	-5.10	118.92	122.59
1	2	43	LEU	C-N-CA	-5.10	118.92	122.59

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	1	1148	0	1146	22	0
1	2	1149	0	1152	17	0
1	3	1136	0	1130	11	0
1	4	1162	0	1165	13	0
1	5	1141	0	1139	22	0
1	6	1141	0	1139	15	0
1	7	1136	0	1130	20	0
1	8	1141	0	1139	23	0
1	9	1150	0	1152	19	0
1	A	1151	0	1151	24	0
1	B	1148	0	1146	26	0
1	C	1148	0	1148	25	0
1	D	1141	0	1139	19	0
1	E	1143	0	1137	22	0
1	F	1155	0	1153	25	0
1	G	1152	0	1150	17	0
1	H	1136	0	1130	19	0
1	I	1141	0	1139	10	0
1	J	1143	0	1137	12	0
1	K	1142	0	1136	14	0
1	L	1136	0	1130	10	0
1	M	1139	0	1135	21	0
1	N	1136	0	1130	16	0
1	O	1136	0	1130	22	0
1	P	1150	0	1152	18	0
1	Q	1150	0	1144	21	0
1	R	1143	0	1137	19	0
1	S	1148	0	1146	13	0
1	T	1148	0	1146	12	0
1	U	1148	0	1146	11	0
1	V	1141	0	1139	12	0
1	W	1136	0	1130	10	0
1	X	1151	0	1151	10	0
1	Y	1141	0	1139	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	1150	0	1152	20	0
1	a	1148	0	1146	14	0
1	b	1143	0	1137	14	0
1	c	1148	0	1146	13	0
1	d	1141	0	1139	12	0
1	e	1141	0	1139	15	0
1	f	1141	0	1139	15	0
1	g	1153	0	1152	16	0
1	h	1136	0	1130	16	0
1	i	1141	0	1139	15	0
1	j	1148	0	1146	17	0
1	k	1141	0	1139	23	0
1	l	1148	0	1146	10	0
1	m	1141	0	1139	15	0
2	1	16	0	12	0	0
2	2	16	0	12	3	0
2	3	16	0	12	0	0
2	4	16	0	12	1	0
2	5	16	0	12	1	0
2	6	16	0	12	0	0
2	7	16	0	12	2	0
2	8	16	0	12	2	0
2	9	16	0	12	0	0
2	A	16	0	12	1	0
2	B	16	0	12	2	0
2	C	16	0	12	2	0
2	D	16	0	12	0	0
2	E	16	0	12	0	0
2	F	16	0	12	2	0
2	G	16	0	12	2	0
2	H	16	0	12	2	0
2	I	16	0	12	1	0
2	J	16	0	12	0	0
2	K	16	0	12	0	0
2	L	16	0	12	1	0
2	M	16	0	12	1	0
2	N	16	0	12	1	0
2	O	16	0	12	2	0
2	P	16	0	12	1	0
2	Q	16	0	12	2	0
2	R	16	0	12	1	0
2	S	16	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	16	0	12	2	0
2	U	16	0	12	1	0
2	V	16	0	12	0	0
2	W	16	0	12	0	0
2	X	16	0	12	2	0
2	Y	16	0	12	2	0
2	Z	16	0	12	0	0
2	a	16	0	12	0	0
2	b	16	0	12	1	0
2	c	16	0	12	0	0
2	d	16	0	12	1	0
2	e	16	0	12	1	0
2	f	16	0	12	1	0
2	g	16	0	12	1	0
2	h	16	0	12	2	0
2	i	16	0	12	2	0
2	j	16	0	12	2	0
2	k	16	0	12	0	0
2	l	16	0	12	1	0
2	m	16	0	12	2	0
3	1	9	0	0	0	0
3	2	9	0	0	0	0
3	3	9	0	0	0	0
3	4	9	0	0	0	0
3	5	9	0	0	0	0
3	6	9	0	0	0	0
3	7	9	0	0	0	0
3	8	9	0	0	0	0
3	9	9	0	0	0	0
3	A	9	0	0	0	0
3	B	9	0	0	0	0
3	C	9	0	0	0	0
3	D	9	0	0	0	0
3	E	9	0	0	0	0
3	F	9	0	0	0	0
3	G	9	0	0	0	0
3	H	9	0	0	0	0
3	I	9	0	0	0	0
3	J	9	0	0	0	0
3	K	9	0	0	0	0
3	L	9	0	0	0	0
3	M	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	9	0	0	0	0
3	O	9	0	0	0	0
3	P	9	0	0	0	0
3	Q	9	0	0	0	0
3	R	9	0	0	0	0
3	S	9	0	0	0	0
3	T	9	0	0	0	0
3	U	9	0	0	0	0
3	V	9	0	0	0	0
3	W	9	0	0	0	0
3	X	9	0	0	0	0
3	Y	9	0	0	0	0
3	Z	9	0	0	0	0
3	a	9	0	0	0	0
3	b	9	0	0	0	0
3	c	9	0	0	0	0
3	d	9	0	0	0	0
3	e	9	0	0	0	0
3	f	9	0	0	0	0
3	g	9	0	0	0	0
3	h	9	0	0	0	0
3	i	9	0	0	0	0
3	j	9	0	0	0	0
3	k	9	0	0	0	0
3	l	9	0	0	0	0
3	m	9	0	0	0	0
4	1	1	0	0	0	0
4	2	1	0	0	0	0
4	3	1	0	0	0	0
4	4	1	0	0	0	0
4	5	1	0	0	0	0
4	6	1	0	0	0	0
4	7	1	0	0	0	0
4	8	1	0	0	0	0
4	9	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
4	T	1	0	0	0	0
4	U	1	0	0	0	0
4	V	1	0	0	0	0
4	W	1	0	0	0	0
4	X	1	0	0	0	0
4	Y	1	0	0	0	0
4	Z	1	0	0	0	0
4	a	1	0	0	0	0
4	b	1	0	0	0	0
4	c	1	0	0	0	0
4	d	1	0	0	0	0
4	e	1	0	0	0	0
4	f	1	0	0	0	0
4	g	1	0	0	0	0
4	h	1	0	0	0	0
4	i	1	0	0	0	0
4	j	1	0	0	0	0
4	k	1	0	0	0	0
4	l	1	0	0	0	0
4	m	1	0	0	0	0
5	e	5	0	0	0	0
5	l	5	0	0	0	0
6	1	120	0	0	7	0
6	2	139	0	0	1	0
6	3	102	0	0	2	0
6	4	85	0	0	2	0
6	5	109	0	0	0	0
6	6	93	0	0	2	0
6	7	69	0	0	1	0
6	8	136	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	9	101	0	0	0	0
6	A	125	0	0	2	0
6	B	96	0	0	3	0
6	C	67	0	0	0	0
6	D	133	0	0	1	0
6	E	111	0	0	7	0
6	F	86	0	0	2	0
6	G	141	0	0	4	0
6	H	123	0	0	2	0
6	I	84	0	0	0	0
6	J	116	0	0	0	0
6	K	95	0	0	1	0
6	L	70	0	0	1	0
6	M	124	0	0	3	0
6	N	98	0	0	2	0
6	O	68	0	0	2	0
6	P	142	0	0	5	0
6	Q	103	0	0	3	0
6	R	75	0	0	6	0
6	S	133	0	0	0	0
6	T	90	0	0	1	0
6	U	62	0	0	0	0
6	V	118	0	0	3	0
6	W	97	0	0	1	0
6	X	70	0	0	1	0
6	Y	94	0	0	0	0
6	Z	60	0	0	1	0
6	a	70	0	0	1	0
6	b	127	0	0	0	0
6	c	105	0	0	5	0
6	d	63	0	0	2	0
6	e	128	0	0	6	0
6	f	92	0	0	3	0
6	g	74	0	0	4	0
6	h	143	0	0	6	0
6	i	99	0	0	3	0
6	j	63	0	0	1	0
6	k	109	0	0	2	0
6	l	69	0	0	3	0
6	m	49	0	0	2	0
All	All	60911	0	55378	582	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 5.

All (582) 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:Q:119:MET:CE	1:R:115:ILE:HG12	1.64	1.25
1:M:119:MET:CE	1:O:115:ILE:HG12	1.67	1.23
1:c:3:MET:HA	6:c:2001:HOH:O	1.42	1.18
1:1:119[A]:MET:HE3	1:Z:115:ILE:HG12	1.18	1.17
1:M:115:ILE:HG12	1:N:119:MET:CE	1.77	1.15
1:E:99:LEU:HD22	1:F:97:TYR:CE2	1.81	1.13
1:M:119:MET:HE3	1:O:115:ILE:HG12	1.27	1.11
1:8:35:THR:HG23	1:8:103:GLU:HG3	1.34	1.09
1:W:19:LYS:HE2	6:W:2019:HOH:O	1.49	1.09
1:A:105:LYS:HE2	6:A:2134:HOH:O	1.51	1.09
1:3:16:ARG:HG2	6:3:2017:HOH:O	1.52	1.08
1:A:2:THR:HG1	1:J:3:MET:N	1.50	1.08
1:G:119:MET:HE3	1:H:115:ILE:HG12	1.27	1.08
1:8:3:MET:N	1:b:2:THR:HG1	1.52	1.07
1:A:99:LEU:HD23	1:C:97:TYR:CZ	1.90	1.06
1:N:115:ILE:HG12	1:O:119:MET:HE3	1.37	1.06
1:M:115:ILE:HG12	1:N:119:MET:HE3	1.06	1.05
1:2:35:THR:HG23	1:2:103:GLU:HG3	1.36	1.04
1:3:35:THR:HG23	1:3:103:GLU:HG3	1.39	1.04
1:6:35:THR:HG23	1:6:103:GLU:HG3	1.38	1.04
1:1:99:LEU:HD22	1:Y:97:TYR:CE2	1.93	1.03
1:i:119[A]:MET:HE3	1:j:115:ILE:HG12	1.36	1.03
1:B:97:TYR:CE2	1:C:99:LEU:HD22	1.92	1.03
1:Q:119:MET:HE3	1:R:115:ILE:HG12	1.03	1.02
1:1:99:LEU:HD23	1:Y:97:TYR:CZ	1.95	1.01
1:1:119[A]:MET:CE	1:Z:115:ILE:HG12	1.90	1.01
1:1:99:LEU:CD2	1:Y:97:TYR:CZ	2.44	1.00
1:Q:2:THR:HG1	1:V:3:MET:N	1.59	0.99
1:Q:119:MET:HE3	1:R:115:ILE:CG1	1.91	0.99
1:g:143:THR:HG22	6:g:2206:HOH:O	1.62	0.99
1:A:99:LEU:CD2	1:C:97:TYR:CE2	2.46	0.98
1:A:119[A]:MET:HE3	1:B:115:ILE:HG12	1.44	0.98
1:5:35:THR:CG2	1:5:103:GLU:HG3	1.94	0.97
1:7:35:THR:HG23	1:7:103:GLU:HG3	1.43	0.97
1:S:35:THR:HG23	1:S:103:GLU:HG3	1.44	0.96
1:B:97:TYR:CZ	1:C:99:LEU:CD2	2.49	0.96
1:A:115:ILE:HG12	1:C:119:MET:HE3	1.47	0.95
1:M:115:ILE:CG1	1:N:119:MET:HE3	1.95	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:TYR:CE2	1:C:99:LEU:CD2	2.50	0.93
1:B:97:TYR:CZ	1:C:99:LEU:HD23	2.03	0.93
1:F:2:THR:HG21	1:R:121:ALA:O	1.67	0.93
1:E:143:THR:HG21	6:E:2230:HOH:O	1.67	0.93
1:d:3:MET:N	1:j:2:THR:HG23	1.84	0.92
1:A:97:TYR:CE2	1:B:99:LEU:HD22	2.05	0.92
1:1:99:LEU:CD2	1:Y:97:TYR:CE2	2.53	0.92
6:B:2162:HOH:O	1:C:143:THR:HG21	1.69	0.92
1:A:99:LEU:HD23	1:C:97:TYR:CE2	2.05	0.92
1:P:143:THR:HG21	6:P:2136:HOH:O	1.70	0.92
1:D:97:TYR:CZ	1:F:99:LEU:HD22	2.04	0.91
1:i:67:TYR:CE1	1:i:99:LEU:HD23	2.06	0.91
1:c:143:THR:HG21	6:c:2169:HOH:O	1.69	0.90
1:D:99:LEU:HD13	1:E:97:TYR:CE2	2.07	0.89
1:J:115:ILE:HG12	1:K:119:MET:HE3	1.51	0.89
1:E:99:LEU:CD2	1:F:97:TYR:CZ	2.54	0.89
1:b:115:ILE:HG12	1:d:119[A]:MET:HE3	1.54	0.89
1:8:119[A]:MET:HE3	1:a:115:ILE:HG12	1.54	0.88
1:j:143:THR:HG23	1:j:144:LYS:HD3	1.53	0.88
1:D:119[A]:MET:HE3	1:F:115:ILE:HG12	1.55	0.88
1:d:143:THR:HG21	6:d:2191:HOH:O	1.73	0.88
1:Z:67:TYR:CE1	1:Z:99:LEU:HD23	2.08	0.87
1:A:97:TYR:CZ	1:B:99:LEU:CD2	2.57	0.87
1:9:99:LEU:HD13	1:a:97:TYR:CE2	2.10	0.86
1:Y:115:ILE:HG12	1:Z:119[A]:MET:HE3	1.57	0.86
1:M:119:MET:HE1	1:O:115:ILE:HG12	1.57	0.86
1:l:119[A]:MET:HE3	1:m:115:ILE:HG12	1.56	0.86
1:5:99:LEU:HD13	1:7:97:TYR:CE2	2.10	0.85
1:1:35:THR:HG22	1:1:103:GLU:HG3	1.57	0.85
1:8:67:TYR:CE1	1:8:99:LEU:HD12	2.12	0.85
1:A:99:LEU:CD2	1:C:97:TYR:CZ	2.61	0.83
1:i:67:TYR:HE1	1:i:99:LEU:HD23	1.41	0.83
1:2:35:THR:HG23	1:2:103:GLU:CG	2.10	0.82
1:5:35:THR:HG22	1:5:103:GLU:HG3	1.62	0.82
1:R:6:LYS:HE2	6:R:2003:HOH:O	1.79	0.82
1:i:143:THR:HG21	6:i:2182:HOH:O	1.80	0.82
1:H:67:TYR:CE1	1:H:99:LEU:HD23	2.14	0.82
1:A:97:TYR:CZ	1:B:99:LEU:HD22	2.15	0.81
1:S:35:THR:CG2	1:S:103:GLU:HG3	2.09	0.81
1:7:35:THR:CG2	1:7:103:GLU:HG3	2.11	0.81
1:f:119[A]:MET:HE3	1:g:115:ILE:HG12	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:2080:HOH:O	1:W:129:HIS:HB3	1.82	0.80
1:H:12:GLU:CD	1:H:12:GLU:H	1.89	0.80
6:1:2014:HOH:O	1:g:16:ARG:HG2	1.81	0.80
1:f:143:THR:HG21	6:f:2176:HOH:O	1.82	0.80
1:8:67:TYR:HE1	1:8:99:LEU:HD12	1.47	0.79
1:Z:67:TYR:HE1	1:Z:99:LEU:HD23	1.44	0.79
1:G:3:MET:HE3	6:G:2045:HOH:O	1.81	0.79
1:O:12:GLU:CD	1:O:12:GLU:H	1.88	0.79
1:Z:37:LYS:HB2	1:Z:40:GLU:CD	2.08	0.79
1:5:99:LEU:HD13	1:7:97:TYR:CZ	2.18	0.78
1:1:35:THR:HG21	6:1:2086:HOH:O	1.84	0.78
1:7:35:THR:HG23	1:7:103:GLU:CG	2.12	0.78
1:6:35:THR:HG23	1:6:103:GLU:CG	2.14	0.78
1:E:99:LEU:CD2	1:F:97:TYR:CE2	2.64	0.78
1:E:99:LEU:HD22	1:F:97:TYR:CZ	2.15	0.78
1:2:138:LEU:HD22	1:4:43:LEU:HD11	1.64	0.77
1:h:12:GLU:CD	1:h:12:GLU:H	1.90	0.77
1:S:143:THR:HG22	1:S:144:LYS:HD3	1.66	0.77
1:b:143:THR:HG23	1:b:144:LYS:HD3	1.67	0.77
1:c:16:ARG:HG2	6:l:2031:HOH:O	1.82	0.77
1:h:114:ARG:HB2	1:j:119[B]:MET:HG3	1.66	0.77
1:5:35:THR:HG23	1:5:103:GLU:HG3	1.67	0.77
1:Z:67:TYR:CE1	1:Z:99:LEU:CD2	2.67	0.77
1:Z:67:TYR:HE1	1:Z:99:LEU:CD2	1.98	0.77
1:R:12:GLU:CD	1:R:12:GLU:H	1.93	0.77
1:S:35:THR:HG23	1:S:103:GLU:CG	2.13	0.76
1:D:67:TYR:CE1	1:D:99:LEU:HD12	2.22	0.75
1:g:143:THR:HG23	1:g:144[A]:LYS:HD3	1.68	0.75
1:M:43:LEU:HD11	1:N:138:LEU:HD22	1.66	0.75
1:T:119[A]:MET:HE3	1:U:115:ILE:HG12	1.67	0.75
1:G:119:MET:CE	1:H:115:ILE:HG12	2.13	0.75
1:e:143:THR:HG23	1:e:144:LYS:HD3	1.68	0.75
1:X:143:THR:HG22	6:X:2070:HOH:O	1.86	0.74
1:S:115:ILE:HG12	1:U:119[A]:MET:HE3	1.68	0.73
1:h:40:GLU:HG2	6:h:2094:HOH:O	1.87	0.73
1:8:129:HIS:ND1	6:8:2117:HOH:O	2.22	0.73
1:W:43:LEU:HD11	1:X:138:LEU:HD22	1.71	0.73
1:P:43:LEU:HD11	1:R:138:LEU:HD22	1.69	0.73
1:P:119[A]:MET:HE3	1:Q:115:ILE:HG12	1.68	0.73
1:1:35:THR:CG2	1:1:103:GLU:HG3	2.19	0.72
1:1:119[A]:MET:HE3	1:Z:115:ILE:CG1	2.10	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:12:GLU:CD	1:U:12:GLU:H	1.97	0.72
1:6:35:THR:CG2	1:6:103:GLU:HG3	2.19	0.72
1:5:35:THR:HG23	1:5:103:GLU:CG	2.20	0.71
1:e:115:ILE:HG12	1:g:119[B]:MET:HE3	1.70	0.71
1:9:99:LEU:HD13	1:a:97:TYR:CZ	2.26	0.71
1:5:97:TYR:CZ	1:6:99:LEU:HD23	2.26	0.71
1:A:99:LEU:HD22	1:C:97:TYR:CE2	2.23	0.71
1:D:67:TYR:HE1	1:D:99:LEU:HD12	1.54	0.71
1:R:143:THR:HG21	6:R:2073:HOH:O	1.91	0.71
1:e:138:LEU:HD22	1:f:43:LEU:HD11	1.72	0.71
6:8:2098:HOH:O	1:9:129:HIS:ND1	2.24	0.71
1:c:143:THR:HG23	1:c:144:LYS:HD3	1.74	0.70
1:4:106:LYS:NZ	6:4:2006:HOH:O	2.24	0.70
1:a:143:THR:HG23	1:a:144:LYS:HD3	1.71	0.70
1:Q:2:THR:OG1	1:V:3:MET:N	2.24	0.70
1:M:119:MET:HE3	1:O:115:ILE:CG1	2.14	0.69
6:i:2148:HOH:O	1:j:2:THR:HA	1.92	0.69
1:5:99:LEU:CD1	1:7:97:TYR:CE2	2.75	0.69
1:D:43:LEU:HD11	1:E:138:LEU:HD22	1.74	0.69
1:G:99:LEU:HD23	1:I:97:TYR:CE2	2.27	0.69
1:B:12:GLU:OE2	6:B:2014:HOH:O	2.09	0.69
1:d:143:THR:HG23	1:d:144:LYS:HD3	1.75	0.69
1:2:99:LEU:HD22	1:3:97:TYR:CZ	2.28	0.68
1:Q:106:LYS:HE2	6:Q:2077:HOH:O	1.93	0.68
1:m:143:THR:HG23	1:m:144:LYS:HD3	1.75	0.68
1:F:2:THR:CG2	1:P:3:MET:N	2.57	0.68
1:B:138:LEU:HD22	1:C:43:LEU:HD11	1.74	0.68
1:d:12:GLU:CD	1:d:12:GLU:H	2.02	0.68
1:f:119[A]:MET:CE	1:g:115:ILE:HG12	2.24	0.68
1:H:67:TYR:HE1	1:H:99:LEU:HD23	1.56	0.67
1:i:119[A]:MET:CE	1:j:115:ILE:HG12	2.19	0.67
1:8:99:LEU:HD13	1:9:97:TYR:CE2	2.30	0.67
1:1:3:MET:HA	6:1:2001:HOH:O	1.94	0.67
1:A:119[A]:MET:CE	1:B:115:ILE:HG12	2.23	0.67
1:A:138:LEU:HD22	1:B:43:LEU:HD11	1.75	0.67
1:d:3:MET:N	1:j:2:THR:CG2	2.56	0.67
1:i:67:TYR:HE1	1:i:99:LEU:CD2	2.08	0.67
1:J:43:LEU:HD11	1:K:138:LEU:HD22	1.77	0.67
1:S:143:THR:CG2	1:S:144:LYS:HD3	2.24	0.66
1:k:68:LYS:HD3	6:k:2054:HOH:O	1.94	0.66
1:E:16:ARG:HG2	6:E:2025:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:GLU:CD	1:F:12:GLU:H	2.03	0.66
1:G:143:THR:HG22	6:G:2204:HOH:O	1.95	0.66
1:S:138:LEU:HD22	1:T:43:LEU:HD11	1.78	0.66
1:i:38:LYS:HG3	1:i:99:LEU:O	1.96	0.66
1:S:115:ILE:HG12	1:U:119[A]:MET:CE	2.24	0.66
1:f:143:THR:HG23	1:f:144:LYS:HD3	1.76	0.66
1:k:138:LEU:HD22	1:l:43:LEU:HD11	1.77	0.66
1:M:138:LEU:HD22	1:O:43:LEU:HD11	1.77	0.65
1:V:43:LEU:HD11	1:W:138:LEU:HD22	1.78	0.65
6:1:2077:HOH:O	1:Y:129:HIS:CG	2.48	0.65
1:5:35:THR:CG2	1:5:103:GLU:CG	2.72	0.65
1:9:143:THR:HG23	1:9:144[A]:LYS:HD3	1.79	0.65
1:l:143:THR:HG23	1:l:144:LYS:HD3	1.79	0.65
1:i:67:TYR:CE1	1:i:99:LEU:CD2	2.79	0.64
1:Y:43:LEU:HD11	1:Z:138:LEU:HD22	1.80	0.64
1:7:67:TYR:CE1	1:7:99:LEU:HD12	2.32	0.64
1:3:43:LEU:HD11	1:4:138:LEU:HD22	1.80	0.64
1:5:43:LEU:HD11	1:7:138:LEU:HD22	1.78	0.64
1:T:117:LYS:HE2	6:T:2070:HOH:O	1.98	0.64
1:N:43:LEU:HD11	1:O:138:LEU:HD22	1.80	0.64
1:l:119[A]:MET:CE	1:m:115:ILE:HG12	2.28	0.64
1:l:138:LEU:HD22	1:m:43:LEU:HD11	1.79	0.64
1:D:138:LEU:HD22	1:F:43:LEU:HD11	1.80	0.63
1:8:138:LEU:HD22	1:a:43:LEU:HD11	1.78	0.63
1:S:43:LEU:HD11	1:U:138:LEU:HD22	1.80	0.63
1:D:119[A]:MET:CE	1:F:115:ILE:HG12	2.27	0.63
1:K:37:LYS:O	1:K:40:GLU:HG3	1.98	0.63
1:b:138:LEU:HD22	1:c:43:LEU:HD11	1.81	0.62
1:2:119[A]:MET:CE	1:4:115:ILE:HG12	2.29	0.62
1:6:97:TYR:CE2	1:7:99:LEU:HD13	2.34	0.62
1:Z:38:LYS:HG3	1:Z:99:LEU:O	1.99	0.62
1:6:138:LEU:HD22	1:7:43:LEU:HD11	1.81	0.62
1:F:2:THR:CG2	1:R:121:ALA:O	2.44	0.62
1:P:138:LEU:HD22	1:Q:43:LEU:HD11	1.81	0.62
1:Q:119:MET:HE1	1:R:115:ILE:HG12	1.72	0.62
1:G:43:LEU:HD11	1:I:138:LEU:HD22	1.80	0.62
1:a:143:THR:HG22	6:a:2187:HOH:O	2.00	0.62
1:l:43:LEU:HD11	1:Y:138:LEU:HD22	1.81	0.62
6:M:2060:HOH:O	1:O:143:THR:HG21	1.98	0.61
1:P:143:THR:HG23	1:P:144[A]:LYS:HD3	1.82	0.61
1:h:143:THR:HG23	1:h:144:LYS:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:138:LEU:CD2	1:4:43:LEU:HD11	2.30	0.61
1:f:3:MET:N	6:f:2001:HOH:O	2.32	0.61
1:7:67:TYR:HE1	1:7:99:LEU:HD12	1.65	0.61
1:E:19:LYS:HE2	6:E:2046:HOH:O	2.00	0.61
1:5:138:LEU:HD22	1:6:43:LEU:HD11	1.82	0.61
1:8:3:MET:N	1:b:2:THR:OG1	2.29	0.60
1:A:115:ILE:HG12	1:C:119:MET:CE	2.24	0.60
1:6:119[A]:MET:HE3	1:7:115:ILE:HG12	1.82	0.60
1:K:43:LEU:HD11	1:L:138:LEU:HD22	1.81	0.60
1:T:37:LYS:HB2	1:T:40:GLU:CD	2.26	0.60
1:X:143:THR:HG23	1:X:144:LYS:HD3	1.83	0.60
1:b:37:LYS:HB2	1:b:40:GLU:CD	2.26	0.60
1:g:54:GLU:HG2	6:g:2105:HOH:O	2.01	0.60
1:R:143:THR:HG23	1:R:144:LYS:HD3	1.83	0.60
1:c:138:LEU:HD22	1:d:43:LEU:HD11	1.83	0.60
1:A:43:LEU:HD11	1:C:138:LEU:HD22	1.84	0.60
1:G:119:MET:HE3	1:H:115:ILE:CG1	2.17	0.60
1:M:43:LEU:HD11	1:N:138:LEU:CD2	2.32	0.60
6:A:2030:HOH:O	1:J:16:ARG:HG2	2.01	0.59
1:a:12:GLU:CD	1:a:12:GLU:H	2.10	0.59
1:m:3:MET:HA	6:m:2002:HOH:O	2.01	0.59
1:D:115:ILE:HG12	1:E:119:MET:CE	2.33	0.59
1:8:103:GLU:HG2	6:8:2045:HOH:O	2.03	0.58
1:H:38:LYS:HG3	1:H:99:LEU:O	2.03	0.58
1:2:119[A]:MET:HE3	1:4:115:ILE:HG12	1.84	0.58
1:P:43:LEU:HD11	1:R:138:LEU:CD2	2.34	0.58
1:Q:138:LEU:HD22	1:R:43:LEU:HD11	1.84	0.58
1:B:97:TYR:CD2	1:C:99:LEU:HD22	2.37	0.58
1:e:43:LEU:HD11	1:g:138:LEU:HD22	1.84	0.58
1:1:138:LEU:HD22	1:Z:43:LEU:HD11	1.86	0.58
1:j:3:MET:HA	6:j:2002:HOH:O	2.02	0.58
1:6:129:HIS:HB3	6:6:2087:HOH:O	2.03	0.57
1:T:138:LEU:HD22	1:U:43:LEU:HD11	1.85	0.57
1:k:119[A]:MET:HE1	1:k:122:VAL:HG11	1.87	0.57
1:D:38:LYS:HG3	1:D:99:LEU:O	2.05	0.57
1:2:127:VAL:HG12	1:a:21:GLU:HB2	1.86	0.57
1:E:67:TYR:CE1	1:E:99:LEU:HD13	2.40	0.57
1:i:138:LEU:HD22	1:j:43:LEU:HD11	1.87	0.57
1:N:115:ILE:CG1	1:O:119:MET:HE3	2.25	0.57
1:H:119:MET:HE3	1:H:122:VAL:CG1	2.35	0.56
1:N:43:LEU:HD11	1:O:138:LEU:CD2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:138:LEU:HD22	1:i:43:LEU:HD11	1.86	0.56
1:3:35:THR:HG23	1:3:103:GLU:CG	2.26	0.56
1:R:117:LYS:HD3	6:R:2018:HOH:O	2.04	0.56
1:1:99:LEU:HD22	1:Y:97:TYR:CD2	2.37	0.56
1:l:37:LYS:HD3	6:l:2058:HOH:O	2.05	0.56
1:F:85:TYR:CD2	2:F:1145:DUR:H2'2	2.41	0.56
1:A:97:TYR:CZ	1:B:99:LEU:HD23	2.41	0.56
1:Z:143:THR:HG23	1:Z:144[B]:LYS:HD3	1.86	0.56
1:8:143:THR:HG23	1:8:144:LYS:HD3	1.86	0.56
1:M:128:GLU:OE1	1:M:129:HIS:CD2	2.58	0.56
1:H:138:LEU:HD22	1:I:43:LEU:HD11	1.86	0.56
1:k:43:LEU:HD11	1:m:138:LEU:HD22	1.88	0.56
1:g:4:GLN:NE2	6:g:2006:HOH:O	2.39	0.55
1:f:138:LEU:HD22	1:g:43:LEU:HD11	1.88	0.55
1:k:6:LYS:NZ	1:k:51:GLU:CD	2.65	0.55
1:2:43:LEU:HD11	1:3:138:LEU:HD22	1.87	0.55
1:N:115:ILE:HG12	1:O:119:MET:CE	2.24	0.55
1:9:67:TYR:CE1	1:9:99:LEU:HD12	2.41	0.55
1:W:119:MET:CE	1:W:122:VAL:HG11	2.37	0.55
1:j:11:ASP:HB2	1:j:12:GLU:OE2	2.07	0.54
1:8:35:THR:HG23	1:8:103:GLU:CG	2.24	0.54
1:9:119[A]:MET:HE1	1:9:122:VAL:HG11	1.89	0.54
1:e:119[A]:MET:HE3	1:f:115:ILE:HG12	1.88	0.54
1:1:99:LEU:HD23	1:Y:97:TYR:OH	2.06	0.54
1:A:99:LEU:CD2	1:C:97:TYR:CD2	2.91	0.54
1:h:143:THR:CG2	1:h:144:LYS:HD3	2.37	0.54
1:6:119[A]:MET:CE	1:7:115:ILE:HG12	2.37	0.54
1:H:119:MET:HE3	1:H:122:VAL:HG13	1.89	0.54
1:f:12:GLU:CD	1:f:12:GLU:H	2.14	0.54
1:Z:106:LYS:NZ	6:Z:2004:HOH:O	2.40	0.54
1:9:119[A]:MET:CE	1:9:122:VAL:CG1	2.86	0.54
6:E:2047:HOH:O	1:F:119[A]:MET:HG2	2.08	0.54
1:7:100:ARG:NE	6:7:2043:HOH:O	2.24	0.53
1:F:2:THR:HG21	1:P:3:MET:N	2.22	0.53
1:h:3:MET:HA	6:h:2002:HOH:O	2.08	0.53
1:W:43:LEU:HD11	1:X:138:LEU:CD2	2.38	0.53
1:Z:143:THR:HG23	1:Z:144[A]:LYS:HD3	1.90	0.53
1:d:85:TYR:CD2	2:d:1145:DUR:H2'2	2.44	0.53
1:e:106:LYS:NZ	6:e:2013:HOH:O	2.38	0.53
1:H:97:TYR:CE2	1:I:99:LEU:HD23	2.43	0.53
1:H:143:THR:HG22	6:H:2257:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:35:THR:HG23	6:h:2079:HOH:O	2.08	0.53
1:B:119[A]:MET:HE3	1:C:115:ILE:HG12	1.90	0.53
1:Q:143:THR:HG23	1:Q:144:LYS:HD3	1.91	0.53
1:h:143:THR:HG23	1:h:144:LYS:CD	2.39	0.53
1:5:67:TYR:CE1	1:5:99:LEU:HD12	2.44	0.53
1:d:19:LYS:HE2	6:d:2036:HOH:O	2.07	0.53
1:E:100:ARG:NE	6:E:2121:HOH:O	2.39	0.53
1:K:12:GLU:CD	1:K:12:GLU:H	2.14	0.53
1:K:12:GLU:HG3	6:K:2017:HOH:O	2.08	0.53
1:P:119[A]:MET:CE	1:Q:115:ILE:HG12	2.38	0.53
1:V:138:LEU:HD22	1:X:43:LEU:HD11	1.90	0.53
1:k:7:ILE:HD11	1:k:48:VAL:CG1	2.38	0.52
1:1:35:THR:CG2	1:1:103:GLU:CG	2.86	0.52
1:m:3:MET:N	6:m:2001:HOH:O	2.41	0.52
1:9:43:LEU:HD11	1:a:138:LEU:HD22	1.91	0.52
6:1:2077:HOH:O	1:Y:129:HIS:HB3	2.08	0.52
1:C:85:TYR:CG	2:C:1145:DUR:H2'2	2.44	0.52
1:Z:37:LYS:HB2	1:Z:40:GLU:OE2	2.07	0.52
1:C:85:TYR:CD2	2:C:1145:DUR:H2'2	2.45	0.52
1:f:35:THR:O	1:f:42:LYS:NZ	2.41	0.52
1:g:58:ALA:HB3	1:g:81:ILE:HB	1.92	0.52
1:D:115:ILE:HG12	1:E:119:MET:HE3	1.91	0.52
2:i:1145:DUR:H5	6:i:2111:HOH:O	2.10	0.52
1:E:43:LEU:HD11	1:F:138:LEU:HD22	1.92	0.52
1:9:67:TYR:HE1	1:9:99:LEU:HD12	1.76	0.51
1:D:12:GLU:CD	1:D:12:GLU:H	2.18	0.51
1:P:35:THR:CG2	6:P:2049:HOH:O	2.58	0.51
1:M:12:GLU:CD	1:M:12:GLU:H	2.18	0.51
1:L:4:GLN:NE2	6:L:2005:HOH:O	2.44	0.51
1:k:11:ASP:OD1	1:k:13:THR:N	2.33	0.51
1:k:76:ASN:O	1:k:77:SER:HB2	2.10	0.51
1:S:97:TYR:CE2	1:T:99:LEU:HD23	2.46	0.51
1:A:99:LEU:HD22	1:C:97:TYR:CD2	2.46	0.51
1:l:3:MET:HA	6:l:2001:HOH:O	2.10	0.51
1:A:138:LEU:CD2	1:B:43:LEU:HD11	2.41	0.51
1:9:115:ILE:HG12	1:a:119[A]:MET:HE3	1.93	0.50
1:Z:67:TYR:CE1	1:Z:99:LEU:HD22	2.44	0.50
1:K:99:LEU:HD23	1:L:97:TYR:CE2	2.46	0.50
1:k:138:LEU:CD2	1:l:43:LEU:HD11	2.42	0.50
1:9:119[A]:MET:CE	1:9:122:VAL:HG11	2.42	0.50
1:U:12:GLU:CD	1:U:12:GLU:N	2.68	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:85:TYR:CD2	2:X:1145:DUR:H2'2	2.47	0.50
1:h:35:THR:CG2	6:h:2079:HOH:O	2.59	0.50
1:J:138:LEU:HD22	1:L:43:LEU:HD11	1.94	0.49
1:G:138:LEU:HD22	1:H:43:LEU:HD11	1.93	0.49
1:P:105:LYS:HE3	6:P:2046:HOH:O	2.12	0.49
1:Q:97:TYR:CE2	1:R:99:LEU:HD23	2.47	0.49
1:9:43:LEU:HD11	1:a:138:LEU:CD2	2.42	0.49
1:A:2:THR:OG1	1:J:3:MET:N	2.30	0.49
1:G:3:MET:CE	6:G:2045:HOH:O	2.51	0.49
1:k:7:ILE:HD11	1:k:48:VAL:HG11	1.93	0.49
1:E:99:LEU:HD23	1:F:97:TYR:CZ	2.46	0.49
1:B:138:LEU:CD2	1:C:43:LEU:HD11	2.43	0.49
1:F:38:LYS:HG3	1:F:99:LEU:O	2.12	0.49
1:J:43:LEU:HD11	1:K:138:LEU:CD2	2.41	0.49
1:O:100:ARG:NH1	1:O:101:ASP:O	2.46	0.49
1:e:100:ARG:NE	6:e:2123:HOH:O	2.30	0.49
2:2:1145:DUR:O5'	2:2:1145:DUR:H6	2.12	0.49
1:B:85:TYR:CD2	2:B:1145:DUR:H2'2	2.47	0.49
1:G:99:LEU:HD23	1:I:97:TYR:CD2	2.48	0.49
1:P:97:TYR:CE2	1:Q:99:LEU:HD23	2.47	0.49
1:D:138:LEU:CD2	1:F:43:LEU:HD11	2.43	0.48
1:e:37:LYS:HB2	1:e:40:GLU:CD	2.37	0.48
1:e:138:LEU:CD2	1:f:43:LEU:HD11	2.42	0.48
1:Q:101:ASP:HB3	6:Q:2074:HOH:O	2.12	0.48
1:S:138:LEU:CD2	1:T:43:LEU:HD11	2.43	0.48
1:b:119:MET:HE1	1:b:122:VAL:HG11	1.95	0.48
1:H:85:TYR:CG	2:H:1145:DUR:H2'2	2.48	0.48
1:m:85:TYR:CD2	2:m:1145:DUR:H2'2	2.48	0.48
1:c:119[A]:MET:HE3	1:d:115:ILE:HG12	1.96	0.48
1:T:97:TYR:CE2	1:U:99:LEU:HD23	2.49	0.48
1:b:119:MET:CE	1:b:122:VAL:CG1	2.91	0.48
1:j:143:THR:CG2	1:j:144:LYS:HD3	2.34	0.48
1:B:38:LYS:HG3	1:B:99:LEU:O	2.14	0.48
1:I:127:VAL:HG12	1:X:21:GLU:HB2	1.95	0.48
1:O:85:TYR:CG	2:O:1145:DUR:H2'2	2.49	0.48
1:8:43:LEU:HD11	1:9:138:LEU:HD22	1.94	0.48
1:b:43:LEU:HD11	1:d:138:LEU:HD22	1.96	0.48
1:j:85:TYR:CD2	2:j:1145:DUR:H2'2	2.49	0.48
1:k:6:LYS:HZ3	1:k:51:GLU:CD	2.20	0.48
1:5:43:LEU:HD11	1:7:138:LEU:CD2	2.44	0.48
1:G:143:THR:HG23	1:G:144[A]:LYS:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:58:ALA:HB3	1:V:81:ILE:HB	1.95	0.48
1:G:35:THR:HG22	1:G:103:GLU:HG3	1.96	0.47
1:8:67:TYR:HE1	1:8:99:LEU:CD1	2.22	0.47
1:1:43:LEU:HD11	1:Y:138:LEU:CD2	2.45	0.47
6:F:2028:HOH:O	1:P:16:ARG:HG2	2.14	0.47
1:3:99:LEU:HD22	1:4:97:TYR:CZ	2.50	0.47
1:8:138:LEU:CD2	1:a:43:LEU:HD11	2.43	0.47
1:A:143:THR:HG23	1:A:144:LYS:HD3	1.96	0.47
1:B:85:TYR:CG	2:B:1145:DUR:H2'2	2.49	0.47
1:M:99:LEU:HD23	1:N:97:TYR:CE2	2.50	0.47
1:Q:117:LYS:HE2	6:Q:2024:HOH:O	2.14	0.47
1:k:38:LYS:HE2	1:k:99:LEU:O	2.15	0.47
1:2:35:THR:HG23	1:2:103:GLU:CD	2.40	0.47
1:B:97:TYR:OH	1:C:99:LEU:HD23	2.13	0.47
1:P:138:LEU:CD2	1:Q:43:LEU:HD11	2.45	0.47
1:e:3:MET:CE	6:e:2007:HOH:O	2.62	0.47
1:2:119[A]:MET:HE3	1:2:119[A]:MET:HB2	1.30	0.47
1:D:99:LEU:HD13	1:E:97:TYR:CD2	2.47	0.47
1:k:98:ALA:HB1	1:k:100:ARG:O	2.15	0.47
1:5:99:LEU:CD1	1:7:97:TYR:CD2	2.98	0.47
1:K:105:LYS:HA	1:K:105:LYS:HD2	1.79	0.47
1:7:85:TYR:CG	2:7:1145:DUR:H2'2	2.50	0.46
1:D:43:LEU:HD11	1:E:138:LEU:CD2	2.44	0.46
1:F:85:TYR:CG	2:F:1145:DUR:H2'2	2.50	0.46
1:H:12:GLU:CD	1:H:12:GLU:N	2.67	0.46
1:Q:37:LYS:HB2	1:Q:40:GLU:OE1	2.14	0.46
1:2:119[A]:MET:HE1	1:4:115:ILE:HG12	1.97	0.46
1:5:38:LYS:HG3	1:5:99:LEU:O	2.15	0.46
1:8:58:ALA:HB3	1:8:81:ILE:HB	1.96	0.46
1:S:12:GLU:CD	1:S:12:GLU:H	2.23	0.46
1:1:117:LYS:HE3	6:1:2054:HOH:O	2.16	0.46
1:5:35:THR:HG23	1:5:103:GLU:HG2	1.94	0.46
1:M:35:THR:HG23	6:M:2053:HOH:O	2.15	0.46
1:4:12:GLU:H	1:4:12:GLU:CD	2.23	0.46
1:5:119[A]:MET:HE3	1:6:115:ILE:HG12	1.97	0.46
2:8:1145:DUR:H6	2:8:1145:DUR:O5'	2.15	0.46
1:M:85:TYR:CD2	2:M:1145:DUR:H2'2	2.51	0.46
1:Y:85:TYR:CG	2:Y:1145:DUR:H2'2	2.50	0.46
1:j:143:THR:HG23	1:j:144:LYS:CD	2.37	0.46
1:k:27:ASP:OD2	1:k:109:ARG:HD2	2.15	0.46
1:7:38:LYS:HG3	1:7:99:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:103:GLU:HG2	6:N:2028:HOH:O	2.15	0.46
1:e:43:LEU:HD11	1:g:138:LEU:CD2	2.45	0.46
6:H:2216:HOH:O	1:K:19:LYS:HE3	2.14	0.46
1:Q:85:TYR:CD2	2:Q:1145:DUR:H2'2	2.51	0.46
1:Y:43:LEU:HD11	1:Z:138:LEU:CD2	2.44	0.46
1:8:99:LEU:HD13	1:9:97:TYR:CD2	2.50	0.46
1:9:38:LYS:HG3	1:9:99:LEU:O	2.15	0.46
1:D:99:LEU:HD13	1:E:97:TYR:CZ	2.47	0.46
1:J:115:ILE:HG12	1:K:119:MET:CE	2.35	0.46
1:8:85:TYR:CG	2:8:1145:DUR:H2'2	2.51	0.46
1:J:3:MET:HB3	1:J:3:MET:HE2	1.65	0.46
1:O:85:TYR:CD2	2:O:1145:DUR:H2'2	2.51	0.46
1:9:143:THR:HG23	1:9:144[B]:LYS:HD3	1.98	0.46
1:V:43:LEU:HD11	1:W:138:LEU:CD2	2.45	0.46
1:V:97:TYR:CE2	1:X:99:LEU:HD23	2.51	0.46
1:l:138:LEU:CD2	1:m:43:LEU:HD11	2.45	0.46
1:5:127:VAL:HG12	1:Z:21:GLU:HB2	1.98	0.45
1:O:119:MET:HE2	1:O:122:VAL:CG1	2.46	0.45
1:N:99:LEU:HD23	1:O:97:TYR:CE2	2.51	0.45
1:b:85:TYR:CD2	2:b:1145:DUR:H2'2	2.51	0.45
1:L:21:GLU:HB2	1:T:127:VAL:HG12	1.98	0.45
1:M:100:ARG:NE	6:M:2100:HOH:O	2.21	0.45
1:O:58:ALA:HB3	1:O:81:ILE:HB	1.98	0.45
1:2:35:THR:CG2	1:2:103:GLU:CD	2.90	0.45
1:V:3:MET:HA	6:V:2002:HOH:O	2.15	0.45
1:g:3:MET:HE2	1:g:3:MET:HB3	1.82	0.45
1:6:138:LEU:CD2	1:7:43:LEU:HD11	2.45	0.45
1:X:85:TYR:CG	2:X:1145:DUR:H2'2	2.52	0.45
1:h:105:LYS:HD3	6:h:2084:HOH:O	2.16	0.45
1:b:35:THR:HG22	1:b:103:GLU:CG	2.46	0.45
1:c:37:LYS:O	1:c:40:GLU:HB2	2.16	0.45
1:6:37:LYS:O	1:6:38:LYS:C	2.59	0.45
1:I:85:TYR:CG	2:I:1145:DUR:H2'2	2.50	0.45
1:k:19:LYS:HD2	6:k:2043:HOH:O	2.16	0.45
1:1:103:GLU:HG2	6:1:2087:HOH:O	2.15	0.45
1:M:119:MET:HE3	1:M:119:MET:HB2	1.76	0.45
1:e:85:TYR:CG	2:e:1145:DUR:H2'2	2.51	0.45
1:k:17:ILE:HG21	1:k:28:LEU:HD23	1.98	0.45
1:W:119:MET:CE	1:W:122:VAL:CG1	2.95	0.45
1:E:127:VAL:HG12	1:H:21:GLU:HB2	1.99	0.44
1:e:102:THR:OG1	6:e:2151:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:99:LEU:CD1	1:a:97:TYR:CE2	2.94	0.44
1:F:10:LEU:O	6:F:2011:HOH:O	2.20	0.44
1:i:85:TYR:CD2	2:i:1145:DUR:H2'2	2.52	0.44
1:i:143:THR:HG23	1:i:144:LYS:HD3	1.99	0.44
1:1:99:LEU:CD2	1:Y:97:TYR:CE1	2.95	0.44
1:E:100:ARG:NH2	6:E:2121:HOH:O	2.49	0.44
1:K:43:LEU:HD11	1:L:138:LEU:CD2	2.48	0.44
1:2:35:THR:CG2	1:2:103:GLU:OE2	2.65	0.44
1:4:3:MET:HA	6:4:2001:HOH:O	2.18	0.44
1:G:85:TYR:CD2	2:G:1145:DUR:H2'2	2.52	0.44
6:G:2147:HOH:O	1:I:129:HIS:CG	2.71	0.44
1:J:97:TYR:CE2	1:L:99:LEU:HD23	2.53	0.44
1:M:115:ILE:HG12	1:N:119:MET:HE1	1.85	0.44
1:g:85:TYR:CD2	2:g:1145:DUR:H2'2	2.53	0.44
1:i:138:LEU:CD2	1:j:43:LEU:HD11	2.47	0.44
1:k:119[A]:MET:CE	1:k:122:VAL:CG1	2.96	0.44
1:4:35:THR:HG22	1:4:103:GLU:HG2	2.00	0.44
1:8:38:LYS:HG3	1:8:99:LEU:O	2.18	0.44
1:G:43:LEU:HD11	1:I:138:LEU:CD2	2.47	0.44
1:T:85:TYR:CG	2:T:1145:DUR:H2'2	2.53	0.44
1:J:143:THR:HG23	1:J:144:LYS:HD3	2.00	0.44
1:h:6:LYS:CD	6:h:2114:HOH:O	2.66	0.44
1:b:58:ALA:HB3	1:b:81:ILE:HB	1.99	0.44
1:f:103:GLU:HG2	6:f:2061:HOH:O	2.18	0.44
1:L:12:GLU:H	1:L:12:GLU:CD	2.26	0.43
1:O:143:THR:HG22	6:O:2068:HOH:O	2.17	0.43
1:P:35:THR:HG22	6:P:2049:HOH:O	2.17	0.43
1:X:12:GLU:H	1:X:12:GLU:CD	2.26	0.43
1:g:19:LYS:NZ	6:g:2041:HOH:O	2.48	0.43
1:j:85:TYR:CG	2:j:1145:DUR:H2'2	2.52	0.43
1:m:119[A]:MET:CE	1:m:122:VAL:HG11	2.47	0.43
1:R:32:GLU:OE2	6:R:2022:HOH:O	2.21	0.43
1:k:119[A]:MET:HE1	1:k:122:VAL:CG1	2.48	0.43
1:m:85:TYR:CG	2:m:1145:DUR:H2'2	2.53	0.43
1:5:85:TYR:CD2	2:5:1145:DUR:H2'2	2.53	0.43
1:3:115:ILE:HG12	1:4:119[A]:MET:HE3	2.00	0.43
1:A:38:LYS:HG3	1:A:99:LEU:O	2.19	0.43
1:5:67:TYR:HE1	1:5:99:LEU:HD12	1.83	0.43
1:c:119[A]:MET:HE3	1:c:119[A]:MET:HB2	1.89	0.43
1:k:115:ILE:HG12	1:m:119[A]:MET:HE3	2.01	0.43
1:l:85:TYR:CD2	2:l:1145:DUR:H2'2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:119:MET:HE2	6:3:2083:HOH:O	2.17	0.43
1:L:119:MET:CE	1:L:122:VAL:HG11	2.48	0.43
1:U:85:TYR:CD2	2:U:1145:DUR:H2'2	2.53	0.43
1:Y:99:LEU:HD23	1:Z:97:TYR:CE2	2.54	0.43
1:h:85:TYR:CD2	2:h:1145:DUR:H2'2	2.53	0.43
1:V:37:LYS:O	1:V:40:GLU:HB2	2.18	0.43
1:b:119:MET:CE	1:b:122:VAL:HG11	2.48	0.43
1:G:85:TYR:CG	2:G:1145:DUR:H2'2	2.53	0.43
1:N:82:ASP:CG	6:N:2055:HOH:O	2.61	0.43
1:H:119:MET:CE	1:H:122:VAL:CG1	2.97	0.43
1:K:143:THR:HG23	1:K:144:LYS:HD3	2.01	0.43
1:S:99:LEU:HD23	1:U:97:TYR:CE2	2.53	0.43
1:b:35:THR:HG22	1:b:103:GLU:HG2	2.01	0.43
1:c:119[A]:MET:HG2	6:c:2090:HOH:O	2.19	0.43
1:R:85:TYR:CD2	2:R:1145:DUR:H2'2	2.54	0.43
1:c:68:LYS:HB2	6:c:2097:HOH:O	2.19	0.43
1:H:85:TYR:CD2	2:H:1145:DUR:H2'2	2.54	0.42
1:m:58:ALA:HB3	1:m:81:ILE:HB	2.01	0.42
1:4:85:TYR:CD2	2:4:1145:DUR:H2'2	2.55	0.42
2:A:1145:DUR:H6	2:A:1145:DUR:O5'	2.18	0.42
1:Y:58:ALA:HB3	1:Y:81:ILE:HB	2.01	0.42
1:h:85:TYR:CG	2:h:1145:DUR:H2'2	2.55	0.42
1:7:85:TYR:CD2	2:7:1145:DUR:H2'2	2.54	0.42
1:M:128:GLU:OE1	1:M:129:HIS:HD2	2.02	0.42
1:f:138:LEU:CD2	1:g:43:LEU:HD11	2.48	0.42
1:9:119[A]:MET:CE	1:9:122:VAL:HG13	2.49	0.42
1:D:40:GLU:OE2	6:D:2069:HOH:O	2.21	0.42
1:2:119[A]:MET:HG2	6:2:2065:HOH:O	2.19	0.42
1:F:2:THR:HG22	1:P:3:MET:N	2.31	0.42
1:F:67:TYR:CE1	1:F:99:LEU:HD13	2.55	0.42
1:e:32:GLU:HB3	6:e:2062:HOH:O	2.20	0.42
6:B:2162:HOH:O	1:C:143:THR:CG2	2.44	0.42
1:E:119:MET:HE3	1:E:119:MET:HB2	1.48	0.42
1:j:119[A]:MET:CE	1:j:122:VAL:CG1	2.98	0.42
1:P:85:TYR:CD2	2:P:1145:DUR:H2'2	2.55	0.42
1:h:43:LEU:HD11	1:j:138:LEU:HD22	2.00	0.42
1:5:138:LEU:CD2	1:6:43:LEU:HD11	2.48	0.42
1:Q:58:ALA:HB3	1:Q:81:ILE:HB	2.01	0.42
1:R:117:LYS:CD	6:R:2018:HOH:O	2.66	0.42
1:T:37:LYS:HE2	1:T:37:LYS:HB3	1.89	0.42
1:Y:85:TYR:CD2	2:Y:1145:DUR:H2'2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:58:ALA:HB3	1:k:81:ILE:HB	2.02	0.41
1:3:119:MET:HE1	1:3:122:VAL:HG21	2.02	0.41
1:A:97:TYR:CE1	1:B:99:LEU:CD2	3.01	0.41
1:L:85:TYR:CD2	2:L:1145:DUR:H2'2	2.55	0.41
1:V:99:LEU:HD23	1:W:97:TYR:CE2	2.55	0.41
1:V:117:LYS:HD2	6:V:2036:HOH:O	2.20	0.41
1:8:3:MET:HE2	1:8:53:PRO:HB3	2.03	0.41
1:O:101:ASP:HB3	6:O:2028:HOH:O	2.20	0.41
1:R:6:LYS:CE	6:R:2003:HOH:O	2.53	0.41
1:2:85:TYR:CD2	2:2:1145:DUR:H2'2	2.56	0.41
1:J:99:LEU:HD23	1:K:97:TYR:CE2	2.55	0.41
1:M:58:ALA:HB3	1:M:81:ILE:HB	2.02	0.41
1:P:103:GLU:HG2	6:P:2048:HOH:O	2.20	0.41
1:T:85:TYR:CD2	2:T:1145:DUR:H2'2	2.56	0.41
1:B:58:ALA:HB3	1:B:81:ILE:HB	2.02	0.41
1:C:21:GLU:HB2	1:O:127:VAL:HG12	2.03	0.41
1:E:119:MET:HE2	1:E:120:PRO:O	2.21	0.41
1:B:143:THR:HG23	1:B:144:LYS:HD3	2.02	0.41
1:U:143:THR:HG23	1:U:144:LYS:HD3	2.02	0.41
1:Y:12:GLU:H	1:Y:12:GLU:CD	2.28	0.41
1:h:138:LEU:CD2	1:i:43:LEU:HD11	2.51	0.41
1:3:119:MET:HE3	1:3:122:VAL:HG13	2.02	0.41
1:B:97:TYR:CE1	1:C:99:LEU:CD2	3.01	0.41
1:1:127:VAL:HG12	1:6:21:GLU:HB2	2.03	0.41
1:2:85:TYR:CG	2:2:1145:DUR:H2'2	2.56	0.41
1:D:58:ALA:HB3	1:D:81:ILE:HB	2.03	0.41
1:Q:85:TYR:CG	2:Q:1145:DUR:H2'2	2.55	0.41
1:c:129[A]:HIS:CE1	6:c:2149:HOH:O	2.74	0.41
1:e:75:THR:OG1	6:e:2133:HOH:O	2.22	0.41
1:f:85:TYR:CD2	2:f:1145:DUR:H2'2	2.56	0.41
1:k:11:ASP:OD1	1:k:11:ASP:C	2.62	0.41
1:k:119[A]:MET:CE	1:k:122:VAL:HG13	2.51	0.41
1:5:129:HIS:HB3	6:6:2062:HOH:O	2.21	0.41
1:i:122:VAL:HG23	1:i:122:VAL:O	2.21	0.41
1:m:35:THR:HG22	1:m:103:GLU:CG	2.51	0.41
1:G:26:ILE:HD12	1:I:119[A]:MET:HE1	2.02	0.40
1:f:3:MET:HE2	1:f:3:MET:HB3	1.96	0.40
1:8:3:MET:HE2	1:8:53:PRO:CB	2.51	0.40
1:8:67:TYR:CE1	1:8:99:LEU:CD1	2.94	0.40
1:M:138:LEU:CD2	1:O:43:LEU:HD11	2.47	0.40
1:m:119[A]:MET:CE	1:m:122:VAL:CG1	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:38:LYS:HG3	1:1:99:LEU:O	2.20	0.40
1:B:21:GLU:HB2	1:F:127:VAL:HG12	2.03	0.40
1:H:99:LEU:HD12	1:H:99:LEU:HA	1.86	0.40
1:N:85:TYR:CD2	2:N:1145:DUR:H2'2	2.56	0.40
1:8:21:GLU:HB2	1:d:127:VAL:HG12	2.04	0.40
1:D:97:TYR:CE2	1:F:99:LEU:HD22	2.52	0.40
1:V:115:ILE:HG12	1:W:119:MET:HE3	2.04	0.40
1:a:3:MET:HE2	1:a:3:MET:HB3	1.96	0.40
1:k:36:ILE:HG22	1:k:37:LYS:N	2.36	0.40
6:E:2188:HOH:O	1:G:122:VAL:HG23	2.21	0.40
1:c:115:ILE:HD13	1:c:115:ILE:HG21	1.79	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	1	142/144 (99%)	140 (99%)	1 (1%)	1 (1%)	18	14
1	2	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
1	3	140/144 (97%)	138 (99%)	2 (1%)	0	100	100
1	4	144/144 (100%)	142 (99%)	2 (1%)	0	100	100
1	5	141/144 (98%)	140 (99%)	1 (1%)	0	100	100
1	6	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	7	140/144 (97%)	138 (99%)	2 (1%)	0	100	100
1	8	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	9	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	A	143/144 (99%)	141 (99%)	2 (1%)	0	100	100
1	B	142/144 (99%)	141 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	141/144 (98%)	140 (99%)	1 (1%)	0	100	100
1	D	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	E	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	F	143/144 (99%)	141 (99%)	2 (1%)	0	100	100
1	G	141/144 (98%)	138 (98%)	3 (2%)	0	100	100
1	H	140/144 (97%)	139 (99%)	1 (1%)	0	100	100
1	I	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	J	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	K	141/144 (98%)	140 (99%)	1 (1%)	0	100	100
1	L	140/144 (97%)	139 (99%)	1 (1%)	0	100	100
1	M	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	N	140/144 (97%)	138 (99%)	2 (1%)	0	100	100
1	O	140/144 (97%)	139 (99%)	1 (1%)	0	100	100
1	P	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	Q	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
1	R	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	S	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
1	T	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
1	U	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
1	V	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	W	140/144 (97%)	138 (99%)	2 (1%)	0	100	100
1	X	143/144 (99%)	142 (99%)	1 (1%)	0	100	100
1	Y	141/144 (98%)	140 (99%)	1 (1%)	0	100	100
1	Z	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	a	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
1	b	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	c	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
1	d	141/144 (98%)	139 (99%)	1 (1%)	1 (1%)	18	14
1	e	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	f	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	g	141/144 (98%)	139 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	h	140/144 (97%)	138 (99%)	2 (1%)	0	100	100
1	i	141/144 (98%)	137 (97%)	4 (3%)	0	100	100
1	j	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
1	k	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
1	l	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
1	m	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
All	All	6780/6912 (98%)	6685 (99%)	93 (1%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	77	SER
1	d	77	SER

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	1	125/125 (100%)	120 (96%)	5 (4%)	28	27
1	2	125/125 (100%)	122 (98%)	3 (2%)	43	47
1	3	123/125 (98%)	120 (98%)	3 (2%)	43	47
1	4	127/125 (102%)	124 (98%)	3 (2%)	43	47
1	5	124/125 (99%)	120 (97%)	4 (3%)	34	35
1	6	124/125 (99%)	123 (99%)	1 (1%)	73	80
1	7	123/125 (98%)	121 (98%)	2 (2%)	55	62
1	8	124/125 (99%)	119 (96%)	5 (4%)	28	27
1	9	125/125 (100%)	119 (95%)	6 (5%)	23	21
1	A	126/125 (101%)	123 (98%)	3 (2%)	43	47
1	B	125/125 (100%)	121 (97%)	4 (3%)	34	35
1	C	125/125 (100%)	117 (94%)	8 (6%)	16	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	124/125 (99%)	120 (97%)	4 (3%)	34	35
1	E	124/125 (99%)	119 (96%)	5 (4%)	28	27
1	F	126/125 (101%)	123 (98%)	3 (2%)	43	47
1	G	125/125 (100%)	121 (97%)	4 (3%)	34	35
1	H	123/125 (98%)	117 (95%)	6 (5%)	22	20
1	I	124/125 (99%)	118 (95%)	6 (5%)	23	21
1	J	124/125 (99%)	119 (96%)	5 (4%)	28	27
1	K	124/125 (99%)	121 (98%)	3 (2%)	43	47
1	L	123/125 (98%)	121 (98%)	2 (2%)	55	62
1	M	124/125 (99%)	121 (98%)	3 (2%)	43	47
1	N	123/125 (98%)	120 (98%)	3 (2%)	43	47
1	O	123/125 (98%)	117 (95%)	6 (5%)	22	20
1	P	125/125 (100%)	121 (97%)	4 (3%)	34	35
1	Q	125/125 (100%)	122 (98%)	3 (2%)	43	47
1	R	124/125 (99%)	119 (96%)	5 (4%)	28	27
1	S	125/125 (100%)	117 (94%)	8 (6%)	16	12
1	T	125/125 (100%)	121 (97%)	4 (3%)	34	35
1	U	125/125 (100%)	121 (97%)	4 (3%)	34	35
1	V	124/125 (99%)	119 (96%)	5 (4%)	28	27
1	W	123/125 (98%)	118 (96%)	5 (4%)	27	26
1	X	126/125 (101%)	124 (98%)	2 (2%)	55	62
1	Y	124/125 (99%)	119 (96%)	5 (4%)	28	27
1	Z	125/125 (100%)	121 (97%)	4 (3%)	34	35
1	a	125/125 (100%)	121 (97%)	4 (3%)	34	35
1	b	124/125 (99%)	120 (97%)	4 (3%)	34	35
1	c	125/125 (100%)	122 (98%)	3 (2%)	43	47
1	d	124/125 (99%)	120 (97%)	4 (3%)	34	35
1	e	124/125 (99%)	119 (96%)	5 (4%)	28	27
1	f	124/125 (99%)	120 (97%)	4 (3%)	34	35
1	g	125/125 (100%)	120 (96%)	5 (4%)	28	27
1	h	123/125 (98%)	119 (97%)	4 (3%)	33	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	i	124/125 (99%)	121 (98%)	3 (2%)	43	47
1	j	125/125 (100%)	120 (96%)	5 (4%)	28	27
1	k	124/125 (99%)	117 (94%)	7 (6%)	19	16
1	l	125/125 (100%)	121 (97%)	4 (3%)	34	35
1	m	124/125 (99%)	121 (98%)	3 (2%)	43	47
All	All	5970/6000 (100%)	5769 (97%)	201 (3%)	33	33

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	12	GLU
1	1	35	THR
1	1	99	LEU
1	1	103	GLU
1	1	128	GLU
1	2	35	THR
1	2	103	GLU
1	2	124	LEU
1	3	12	GLU
1	3	35	THR
1	3	99	LEU
1	4	3	MET
1	4	12	GLU
1	4	54	GLU
1	5	12	GLU
1	5	35	THR
1	5	103	GLU
1	5	128	GLU
1	6	35	THR
1	7	35	THR
1	7	124	LEU
1	8	3	MET
1	8	12	GLU
1	8	35	THR
1	8	42	LYS
1	8	144	LYS
1	9	35	THR
1	9	42	LYS
1	9	124	LEU
1	9	129	HIS

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Mol	Chain	Res	Type
1	9	144[A]	LYS
1	9	144[B]	LYS
1	A	12	GLU
1	A	35	THR
1	A	124	LEU
1	B	35	THR
1	B	99	LEU
1	B	103	GLU
1	B	124	LEU
1	C	3	MET
1	C	18[A]	SER
1	C	18[B]	SER
1	C	35	THR
1	C	37	LYS
1	C	99	LEU
1	C	103	GLU
1	C	124	LEU
1	D	12	GLU
1	D	100	ARG
1	D	124	LEU
1	D	126	GLU
1	E	12	GLU
1	E	35	THR
1	E	99	LEU
1	E	103	GLU
1	E	124	LEU
1	F	12	GLU
1	F	35	THR
1	F	124	LEU
1	G	12	GLU
1	G	35	THR
1	G	103	GLU
1	G	124	LEU
1	H	12	GLU
1	H	35	THR
1	H	99	LEU
1	H	103	GLU
1	H	124	LEU
1	H	143	THR
1	I	12	GLU
1	I	35	THR
1	I	103	GLU

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Mol	Chain	Res	Type
1	I	119[A]	MET
1	I	119[B]	MET
1	I	124	LEU
1	J	12	GLU
1	J	35	THR
1	J	54	GLU
1	J	103	GLU
1	J	124	LEU
1	K	12	GLU
1	K	35	THR
1	K	124	LEU
1	L	12	GLU
1	L	124	LEU
1	M	12	GLU
1	M	35	THR
1	M	124	LEU
1	N	12	GLU
1	N	35	THR
1	N	124	LEU
1	O	12	GLU
1	O	18	SER
1	O	32	GLU
1	O	35	THR
1	O	99	LEU
1	O	124	LEU
1	P	12	GLU
1	P	35	THR
1	P	103	GLU
1	P	124	LEU
1	Q	12	GLU
1	Q	35	THR
1	Q	124	LEU
1	R	12	GLU
1	R	35	THR
1	R	103	GLU
1	R	105	LYS
1	R	124	LEU
1	S	12	GLU
1	S	35	THR
1	S	103	GLU
1	S	105	LYS
1	S	124	LEU

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Mol	Chain	Res	Type
1	S	129[A]	HIS
1	S	129[B]	HIS
1	S	143	THR
1	T	12	GLU
1	T	35	THR
1	T	100	ARG
1	T	124	LEU
1	U	12	GLU
1	U	35	THR
1	U	103	GLU
1	U	124	LEU
1	V	35	THR
1	V	42	LYS
1	V	103	GLU
1	V	124	LEU
1	V	128	GLU
1	W	12	GLU
1	W	35	THR
1	W	40	GLU
1	W	103	GLU
1	W	124	LEU
1	X	12	GLU
1	X	124	LEU
1	Y	12	GLU
1	Y	35	THR
1	Y	100	ARG
1	Y	124	LEU
1	Y	143	THR
1	Z	12	GLU
1	Z	35	THR
1	Z	99	LEU
1	Z	124	LEU
1	a	12	GLU
1	a	40	GLU
1	a	124	LEU
1	a	144	LYS
1	b	12	GLU
1	b	54	GLU
1	b	124	LEU
1	b	144	LYS
1	c	35	THR
1	c	124	LEU

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Mol	Chain	Res	Type
1	c	144	LYS
1	d	3	MET
1	d	12	GLU
1	d	35	THR
1	d	124	LEU
1	e	12	GLU
1	e	35	THR
1	e	42	LYS
1	e	124	LEU
1	e	144	LYS
1	f	12	GLU
1	f	35	THR
1	f	37	LYS
1	f	124	LEU
1	g	35	THR
1	g	42	LYS
1	g	124	LEU
1	g	144[A]	LYS
1	g	144[B]	LYS
1	h	12	GLU
1	h	35	THR
1	h	124	LEU
1	h	144	LYS
1	i	35	THR
1	i	99	LEU
1	i	124	LEU
1	j	12	GLU
1	j	35	THR
1	j	54	GLU
1	j	124	LEU
1	j	144	LYS
1	k	3	MET
1	k	12	GLU
1	k	42	LYS
1	k	99	LEU
1	k	102	THR
1	k	124	LEU
1	k	144	LYS
1	l	35	THR
1	l	42	LYS
1	l	124	LEU
1	l	144	LYS

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Mol	Chain	Res	Type
1	m	12	GLU
1	m	124	LEU
1	m	144	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	4	GLN
1	2	4	GLN
1	2	112	GLN
1	3	4	GLN
1	3	129	HIS
1	4	112	GLN
1	5	129	HIS
1	6	4	GLN
1	6	129	HIS
1	7	129	HIS
1	B	4	GLN
1	D	4	GLN
1	E	4	GLN
1	F	4	GLN
1	G	4	GLN
1	I	4	GLN
1	I	112	GLN
1	J	4	GLN
1	L	4	GLN
1	M	4	GLN
1	M	129	HIS
1	N	4	GLN
1	Q	4	GLN
1	S	4	GLN
1	T	4	GLN
1	U	4	GLN
1	V	4	GLN
1	V	129	HIS
1	W	4	GLN
1	Z	4	GLN
1	Z	129	HIS
1	a	129	HIS
1	b	129	HIS
1	d	4	GLN
1	e	129	HIS

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Mol	Chain	Res	Type
1	g	4	GLN
1	i	129	HIS
1	k	4	GLN
1	l	4	GLN
1	m	4	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 146 ligands modelled in this entry, 48 are monoatomic - leaving 98 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DUR	V	1145	-	17,17,17	1.64	4 (23%)	24,24,24	2.34	7 (29%)
3	POP	4	1146	4	6,8,8	1.20	1 (16%)	12,13,13	1.68	3 (25%)
3	POP	e	1146	4	6,8,8	1.30	1 (16%)	12,13,13	1.37	3 (25%)
3	POP	m	1146	4	6,8,8	0.89	0	12,13,13	1.53	1 (8%)
3	POP	N	1146	4	6,8,8	1.22	1 (16%)	12,13,13	1.35	2 (16%)
2	DUR	b	1145	-	17,17,17	1.68	4 (23%)	24,24,24	2.05	7 (29%)
2	DUR	J	1145	-	17,17,17	1.60	3 (17%)	24,24,24	2.33	8 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DUR	M	1145	-	17,17,17	1.53	3 (17%)	24,24,24	2.51	6 (25%)
2	DUR	8	1145	-	17,17,17	1.79	4 (23%)	24,24,24	1.57	6 (25%)
2	DUR	F	1145	-	17,17,17	1.86	3 (17%)	24,24,24	1.32	5 (20%)
2	DUR	A	1145	-	17,17,17	1.81	4 (23%)	24,24,24	2.15	6 (25%)
3	POP	W	1146	4	6,8,8	0.83	0	12,13,13	1.42	2 (16%)
3	POP	6	1146	4	6,8,8	0.79	0	12,13,13	1.30	1 (8%)
2	DUR	E	1145	-	17,17,17	1.35	3 (17%)	24,24,24	2.17	8 (33%)
2	DUR	C	1145	-	17,17,17	1.61	5 (29%)	24,24,24	2.51	7 (29%)
3	POP	M	1146	4	6,8,8	1.16	1 (16%)	12,13,13	1.65	3 (25%)
2	DUR	7	1145	-	17,17,17	1.53	4 (23%)	24,24,24	2.21	8 (33%)
3	POP	X	1146	4	6,8,8	0.98	0	12,13,13	1.51	3 (25%)
2	DUR	c	1145	-	17,17,17	1.57	4 (23%)	24,24,24	1.79	7 (29%)
3	POP	I	1146	4	6,8,8	1.57	2 (33%)	12,13,13	1.49	2 (16%)
3	POP	K	1146	4	6,8,8	1.46	2 (33%)	12,13,13	0.95	0
2	DUR	f	1145	-	17,17,17	1.27	3 (17%)	24,24,24	1.96	7 (29%)
3	POP	S	1146	4	6,8,8	1.38	1 (16%)	12,13,13	0.89	0
3	POP	E	1146	4	6,8,8	0.83	0	12,13,13	1.17	1 (8%)
3	POP	l	1146	4	6,8,8	0.81	0	12,13,13	1.08	1 (8%)
3	POP	D	1146	4	6,8,8	1.11	1 (16%)	12,13,13	1.40	3 (25%)
3	POP	c	1146	4	6,8,8	0.61	0	12,13,13	1.74	3 (25%)
3	POP	h	1146	4	6,8,8	1.32	1 (16%)	12,13,13	1.40	2 (16%)
2	DUR	R	1145	-	17,17,17	1.74	3 (17%)	24,24,24	1.77	5 (20%)
2	DUR	I	1145	-	17,17,17	1.72	2 (11%)	24,24,24	2.10	5 (20%)
3	POP	5	1146	4	6,8,8	1.06	0	12,13,13	1.18	3 (25%)
3	POP	L	1146	4	6,8,8	0.93	0	12,13,13	1.25	1 (8%)
2	DUR	T	1145	-	17,17,17	1.16	3 (17%)	24,24,24	2.31	7 (29%)
2	DUR	2	1145	-	17,17,17	1.33	3 (17%)	24,24,24	1.91	5 (20%)
3	POP	i	1146	4	6,8,8	1.05	0	12,13,13	1.33	2 (16%)
2	DUR	Y	1145	-	17,17,17	1.57	3 (17%)	24,24,24	2.10	7 (29%)
2	DUR	S	1145	-	17,17,17	1.64	4 (23%)	24,24,24	1.83	6 (25%)
3	POP	U	1146	4	6,8,8	0.94	0	12,13,13	1.20	0
3	POP	C	1146	4	6,8,8	0.59	0	12,13,13	1.38	3 (25%)
3	POP	1	1146	4	6,8,8	0.93	0	12,13,13	1.49	4 (33%)
2	DUR	9	1145	-	17,17,17	1.28	2 (11%)	24,24,24	2.04	6 (25%)
2	DUR	D	1145	-	17,17,17	0.86	0	24,24,24	2.03	8 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DUR	1	1145	-	17,17,17	1.82	6 (35%)	24,24,24	1.25	4 (16%)
3	POP	Z	1146	4	6,8,8	0.73	0	12,13,13	1.33	3 (25%)
3	POP	F	1146	4	6,8,8	1.04	1 (16%)	12,13,13	1.45	1 (8%)
2	DUR	h	1145	-	17,17,17	2.16	7 (41%)	24,24,24	2.19	6 (25%)
3	POP	J	1146	4	6,8,8	0.87	0	12,13,13	1.05	1 (8%)
3	POP	8	1146	4	6,8,8	1.19	0	12,13,13	1.26	1 (8%)
2	DUR	m	1145	-	17,17,17	1.39	3 (17%)	24,24,24	1.46	5 (20%)
2	DUR	H	1145	-	17,17,17	1.61	4 (23%)	24,24,24	2.23	9 (37%)
3	POP	V	1146	4	6,8,8	0.92	0	12,13,13	1.76	3 (25%)
3	POP	9	1146	4	6,8,8	0.99	0	12,13,13	1.05	0
3	POP	B	1146	4	6,8,8	1.21	0	12,13,13	1.74	5 (41%)
3	POP	k	1146	4	6,8,8	0.82	0	12,13,13	1.62	3 (25%)
3	POP	O	1146	4	6,8,8	1.19	0	12,13,13	1.28	2 (16%)
2	DUR	j	1145	-	17,17,17	1.65	5 (29%)	24,24,24	2.26	7 (29%)
2	DUR	Q	1145	-	17,17,17	1.22	1 (5%)	24,24,24	2.17	4 (16%)
2	DUR	5	1145	-	17,17,17	1.37	4 (23%)	24,24,24	2.48	7 (29%)
3	POP	7	1146	4	6,8,8	0.84	0	12,13,13	1.26	2 (16%)
2	DUR	4	1145	-	17,17,17	1.30	3 (17%)	24,24,24	2.06	7 (29%)
3	POP	d	1146	4	6,8,8	0.91	0	12,13,13	1.79	6 (50%)
2	DUR	B	1145	-	17,17,17	1.47	3 (17%)	24,24,24	1.98	5 (20%)
2	DUR	N	1145	-	17,17,17	1.19	2 (11%)	24,24,24	2.28	9 (37%)
2	DUR	W	1145	-	17,17,17	1.44	2 (11%)	24,24,24	1.82	6 (25%)
2	DUR	L	1145	-	17,17,17	1.61	4 (23%)	24,24,24	1.97	7 (29%)
3	POP	3	1146	4	6,8,8	1.23	0	12,13,13	1.40	3 (25%)
3	POP	Y	1146	4	6,8,8	0.96	1 (16%)	12,13,13	1.62	4 (33%)
5	PO4	e	1148	-	4,4,4	0.61	0	6,6,6	0.84	0
5	PO4	l	1148	-	4,4,4	1.33	0	6,6,6	1.16	1 (16%)
3	POP	H	1146	4	6,8,8	1.31	0	12,13,13	1.23	1 (8%)
3	POP	2	1146	4	6,8,8	1.10	0	12,13,13	0.85	0
3	POP	g	1146	4	6,8,8	0.75	0	12,13,13	1.48	2 (16%)
2	DUR	g	1145	-	17,17,17	1.37	3 (17%)	24,24,24	1.86	6 (25%)
3	POP	b	1146	4	6,8,8	1.16	0	12,13,13	1.35	2 (16%)
2	DUR	i	1145	-	17,17,17	1.25	1 (5%)	24,24,24	2.68	9 (37%)
3	POP	R	1146	4	6,8,8	0.64	0	12,13,13	1.57	3 (25%)
2	DUR	k	1145	-	17,17,17	1.19	1 (5%)	24,24,24	2.25	7 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POP	G	1146	4	6,8,8	1.38	2 (33%)	12,13,13	1.78	5 (41%)
2	DUR	d	1145	-	17,17,17	1.39	2 (11%)	24,24,24	1.73	5 (20%)
3	POP	P	1146	4	6,8,8	1.24	0	12,13,13	1.62	4 (33%)
2	DUR	G	1145	-	17,17,17	1.60	4 (23%)	24,24,24	1.71	7 (29%)
2	DUR	3	1145	-	17,17,17	1.48	3 (17%)	24,24,24	2.28	8 (33%)
3	POP	Q	1146	4	6,8,8	1.10	1 (16%)	12,13,13	1.05	1 (8%)
2	DUR	6	1145	-	17,17,17	1.43	2 (11%)	24,24,24	1.86	7 (29%)
2	DUR	U	1145	-	17,17,17	1.51	2 (11%)	24,24,24	2.54	8 (33%)
2	DUR	e	1145	-	17,17,17	1.93	3 (17%)	24,24,24	1.94	6 (25%)
2	DUR	Z	1145	-	17,17,17	1.49	2 (11%)	24,24,24	2.46	7 (29%)
2	DUR	O	1145	-	17,17,17	1.61	2 (11%)	24,24,24	1.89	7 (29%)
3	POP	f	1146	4	6,8,8	0.67	0	12,13,13	1.68	4 (33%)
3	POP	j	1146	4	6,8,8	0.77	0	12,13,13	1.71	3 (25%)
2	DUR	a	1145	-	17,17,17	1.38	2 (11%)	24,24,24	2.46	9 (37%)
2	DUR	l	1145	-	17,17,17	1.66	5 (29%)	24,24,24	1.97	7 (29%)
3	POP	a	1146	4	6,8,8	0.88	0	12,13,13	1.32	1 (8%)
2	DUR	K	1145	-	17,17,17	1.27	1 (5%)	24,24,24	2.46	8 (33%)
3	POP	T	1146	4	6,8,8	1.07	0	12,13,13	1.55	3 (25%)
2	DUR	P	1145	-	17,17,17	1.24	2 (11%)	24,24,24	2.24	9 (37%)
3	POP	A	1146	4	6,8,8	1.14	0	12,13,13	1.21	1 (8%)
2	DUR	X	1145	-	17,17,17	1.70	4 (23%)	24,24,24	1.99	6 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DUR	V	1145	-	-	0/6/18/18	0/2/2/2
3	POP	4	1146	4	-	2/6/6/6	-
3	POP	e	1146	4	-	2/6/6/6	-
3	POP	m	1146	4	-	2/6/6/6	-
3	POP	N	1146	4	-	2/6/6/6	-
2	DUR	b	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	J	1145	-	1/1/3/3	2/6/18/18	0/2/2/2
2	DUR	M	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	8	1145	-	-	0/6/18/18	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DUR	F	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	A	1145	-	-	0/6/18/18	0/2/2/2
3	POP	W	1146	4	-	3/6/6/6	-
3	POP	6	1146	4	-	2/6/6/6	-
2	DUR	E	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	C	1145	-	-	0/6/18/18	0/2/2/2
3	POP	M	1146	4	-	2/6/6/6	-
2	DUR	7	1145	-	-	0/6/18/18	0/2/2/2
3	POP	X	1146	4	-	2/6/6/6	-
2	DUR	c	1145	-	-	0/6/18/18	0/2/2/2
3	POP	I	1146	4	-	3/6/6/6	-
3	POP	K	1146	4	-	2/6/6/6	-
2	DUR	f	1145	-	-	0/6/18/18	0/2/2/2
3	POP	S	1146	4	-	2/6/6/6	-
3	POP	E	1146	4	-	2/6/6/6	-
3	POP	l	1146	4	-	2/6/6/6	-
3	POP	D	1146	4	-	3/6/6/6	-
3	POP	c	1146	4	-	3/6/6/6	-
3	POP	h	1146	4	-	3/6/6/6	-
2	DUR	R	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	I	1145	-	-	0/6/18/18	0/2/2/2
3	POP	5	1146	4	-	2/6/6/6	-
3	POP	L	1146	4	-	2/6/6/6	-
2	DUR	T	1145	-	-	2/6/18/18	0/2/2/2
2	DUR	2	1145	-	-	0/6/18/18	0/2/2/2
3	POP	i	1146	4	-	2/6/6/6	-
2	DUR	Y	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	S	1145	-	-	0/6/18/18	0/2/2/2
3	POP	U	1146	4	-	3/6/6/6	-
3	POP	C	1146	4	-	3/6/6/6	-
3	POP	1	1146	4	-	2/6/6/6	-
2	DUR	9	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	D	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	1	1145	-	-	0/6/18/18	0/2/2/2
3	POP	Z	1146	4	-	2/6/6/6	-
3	POP	F	1146	4	-	2/6/6/6	-
2	DUR	h	1145	-	-	0/6/18/18	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POP	J	1146	4	-	3/6/6/6	-
3	POP	8	1146	4	-	2/6/6/6	-
2	DUR	m	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	H	1145	-	-	0/6/18/18	0/2/2/2
3	POP	V	1146	4	-	3/6/6/6	-
3	POP	9	1146	4	-	2/6/6/6	-
3	POP	B	1146	4	-	3/6/6/6	-
3	POP	k	1146	4	-	2/6/6/6	-
3	POP	O	1146	4	-	2/6/6/6	-
2	DUR	j	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	Q	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	5	1145	-	-	0/6/18/18	0/2/2/2
3	POP	7	1146	4	-	2/6/6/6	-
2	DUR	4	1145	-	-	0/6/18/18	0/2/2/2
3	POP	d	1146	4	-	3/6/6/6	-
2	DUR	B	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	N	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	W	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	L	1145	-	-	0/6/18/18	0/2/2/2
3	POP	3	1146	4	-	2/6/6/6	-
3	POP	Y	1146	4	-	3/6/6/6	-
3	POP	H	1146	4	-	2/6/6/6	-
3	POP	2	1146	4	-	2/6/6/6	-
3	POP	g	1146	4	-	2/6/6/6	-
2	DUR	g	1145	-	-	0/6/18/18	0/2/2/2
3	POP	b	1146	4	-	3/6/6/6	-
2	DUR	i	1145	-	-	0/6/18/18	0/2/2/2
3	POP	R	1146	4	-	3/6/6/6	-
2	DUR	k	1145	-	-	0/6/18/18	0/2/2/2
3	POP	G	1146	4	-	3/6/6/6	-
2	DUR	d	1145	-	-	0/6/18/18	0/2/2/2
3	POP	P	1146	4	-	2/6/6/6	-
2	DUR	G	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	3	1145	-	-	0/6/18/18	0/2/2/2
3	POP	Q	1146	4	-	2/6/6/6	-
2	DUR	6	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	U	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	e	1145	-	-	0/6/18/18	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DUR	Z	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	O	1145	-	-	0/6/18/18	0/2/2/2
3	POP	f	1146	4	-	2/6/6/6	-
3	POP	j	1146	4	-	3/6/6/6	-
2	DUR	a	1145	-	-	0/6/18/18	0/2/2/2
2	DUR	l	1145	-	-	0/6/18/18	0/2/2/2
3	POP	a	1146	4	-	2/6/6/6	-
2	DUR	K	1145	-	-	0/6/18/18	0/2/2/2
3	POP	T	1146	4	-	3/6/6/6	-
2	DUR	P	1145	-	-	0/6/18/18	0/2/2/2
3	POP	A	1146	4	-	2/6/6/6	-
2	DUR	X	1145	-	-	0/6/18/18	0/2/2/2

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	h	1145	DUR	C2-N3	-5.74	1.28	1.38
2	F	1145	DUR	C2-N3	-5.18	1.28	1.38
2	I	1145	DUR	C2-N3	-5.07	1.29	1.38
2	J	1145	DUR	C2-N3	-5.01	1.29	1.38
2	A	1145	DUR	C4-N3	-4.81	1.30	1.38
2	e	1145	DUR	C2-N3	-4.64	1.29	1.38
2	b	1145	DUR	C2-N3	-4.46	1.30	1.38
2	e	1145	DUR	C4-N3	-4.37	1.31	1.38
2	8	1145	DUR	C2-N3	-4.31	1.30	1.38
2	O	1145	DUR	C2-N3	-4.31	1.30	1.38
2	L	1145	DUR	C2-N3	-4.25	1.30	1.38
2	M	1145	DUR	C4-N3	-4.23	1.31	1.38
2	R	1145	DUR	C4-N3	-4.01	1.31	1.38
2	U	1145	DUR	C4-N3	-3.98	1.31	1.38
2	Z	1145	DUR	C2-N3	-3.94	1.31	1.38
2	X	1145	DUR	C4-N3	-3.85	1.32	1.38
2	R	1145	DUR	C6-N1	-3.82	1.29	1.38
2	S	1145	DUR	C2-N3	-3.77	1.31	1.38
2	c	1145	DUR	C4-N3	-3.75	1.32	1.38
2	1	1145	DUR	C6-C5	3.71	1.43	1.35
2	X	1145	DUR	C2-N3	-3.61	1.31	1.38
2	Y	1145	DUR	C2-N3	-3.59	1.31	1.38
2	H	1145	DUR	C4-N3	-3.57	1.32	1.38
2	j	1145	DUR	C4-N3	-3.56	1.32	1.38
2	C	1145	DUR	C4-N3	-3.55	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	1145	DUR	C4-N3	-3.51	1.32	1.38
2	P	1145	DUR	C4-N3	-3.49	1.32	1.38
2	V	1145	DUR	C2-N3	-3.49	1.31	1.38
2	3	1145	DUR	C5-C4	-3.45	1.36	1.43
2	E	1145	DUR	C2-N3	-3.44	1.32	1.38
2	d	1145	DUR	C4-N3	-3.39	1.32	1.38
2	A	1145	DUR	C2-N3	-3.34	1.32	1.38
2	G	1145	DUR	O4-C4	3.34	1.31	1.24
2	9	1145	DUR	C4-N3	-3.31	1.32	1.38
2	5	1145	DUR	C6-N1	-3.27	1.30	1.38
2	c	1145	DUR	C6-N1	-3.24	1.30	1.38
2	l	1145	DUR	O4-C4	3.23	1.30	1.24
2	W	1145	DUR	C4-N3	-3.21	1.33	1.38
2	e	1145	DUR	C5-C4	-3.18	1.36	1.43
2	b	1145	DUR	C5-C4	-3.17	1.36	1.43
2	Z	1145	DUR	C4-N3	-3.17	1.33	1.38
2	I	1145	DUR	C6-N1	-3.16	1.30	1.38
2	3	1145	DUR	C2-N3	-3.15	1.32	1.38
2	8	1145	DUR	O2-C2	3.12	1.28	1.23
2	V	1145	DUR	C4-N3	-3.12	1.33	1.38
2	W	1145	DUR	C2-N3	-3.11	1.32	1.38
2	l	1145	DUR	C2-N3	-3.11	1.32	1.38
2	F	1145	DUR	C5-C4	-3.11	1.37	1.43
2	8	1145	DUR	C2-N1	3.10	1.43	1.38
2	2	1145	DUR	C4-N3	-3.09	1.33	1.38
2	M	1145	DUR	C2-N3	-3.08	1.32	1.38
2	1	1145	DUR	O2-C2	3.06	1.28	1.23
2	7	1145	DUR	C5-C4	-3.03	1.37	1.43
2	j	1145	DUR	C2-N3	-3.01	1.32	1.38
2	l	1145	DUR	O4'-C1'	3.00	1.49	1.42
2	f	1145	DUR	C4-N3	-2.97	1.33	1.38
2	Y	1145	DUR	C4-N3	-2.95	1.33	1.38
2	m	1145	DUR	C4-N3	-2.91	1.33	1.38
2	h	1145	DUR	O2-C2	2.91	1.28	1.23
2	2	1145	DUR	C2-N3	-2.88	1.33	1.38
2	B	1145	DUR	C2-N1	2.86	1.42	1.38
2	V	1145	DUR	C6-N1	-2.85	1.31	1.38
2	A	1145	DUR	C6-C5	2.83	1.41	1.35
2	E	1145	DUR	C4-N3	-2.82	1.33	1.38
2	V	1145	DUR	C2-N1	2.80	1.42	1.38
2	c	1145	DUR	C5-C4	-2.78	1.37	1.43
2	6	1145	DUR	C2-N3	-2.77	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1145	DUR	C5-C4	-2.76	1.37	1.43
2	5	1145	DUR	C4-N3	-2.75	1.33	1.38
2	a	1145	DUR	C2-N3	-2.74	1.33	1.38
2	N	1145	DUR	C5-C4	-2.71	1.37	1.43
2	7	1145	DUR	C4-N3	-2.71	1.34	1.38
2	P	1145	DUR	O2-C2	2.71	1.27	1.23
2	H	1145	DUR	C2-N3	-2.69	1.33	1.38
2	m	1145	DUR	C5-C4	-2.68	1.37	1.43
2	g	1145	DUR	C4-N3	-2.66	1.34	1.38
2	6	1145	DUR	C4-N3	-2.66	1.34	1.38
2	B	1145	DUR	C4-N3	-2.66	1.34	1.38
2	a	1145	DUR	C5-C4	-2.62	1.38	1.43
2	S	1145	DUR	C2-N1	2.61	1.42	1.38
2	O	1145	DUR	C4-N3	-2.61	1.34	1.38
2	d	1145	DUR	C2-N3	-2.59	1.33	1.38
2	3	1145	DUR	C4-N3	-2.57	1.34	1.38
2	L	1145	DUR	C4-N3	-2.57	1.34	1.38
2	h	1145	DUR	C2-N1	2.57	1.42	1.38
2	G	1145	DUR	O2-C2	2.55	1.27	1.23
2	K	1145	DUR	C2-N3	-2.55	1.33	1.38
2	h	1145	DUR	C5-C4	-2.53	1.38	1.43
2	G	1145	DUR	C4-N3	-2.52	1.34	1.38
2	T	1145	DUR	C2-N3	-2.50	1.33	1.38
2	h	1145	DUR	C6-C5	2.50	1.40	1.35
2	H	1145	DUR	C2-N1	2.50	1.42	1.38
2	R	1145	DUR	C5-C4	-2.49	1.38	1.43
2	7	1145	DUR	C2-N3	-2.47	1.33	1.38
2	S	1145	DUR	C6-C5	2.45	1.40	1.35
2	7	1145	DUR	C6-N1	-2.43	1.32	1.38
2	g	1145	DUR	C2-N1	2.42	1.42	1.38
2	m	1145	DUR	C2-N3	-2.41	1.33	1.38
3	I	1146	POP	P2-O6	-2.40	1.45	1.54
2	A	1145	DUR	C2-N1	2.40	1.42	1.38
2	l	1145	DUR	C4-N3	-2.39	1.34	1.38
2	4	1145	DUR	C4-N3	-2.39	1.34	1.38
3	h	1146	POP	P2-O5	-2.38	1.46	1.54
2	J	1145	DUR	C2'-C3'	-2.37	1.46	1.52
2	j	1145	DUR	O4-C4	2.36	1.29	1.24
2	l	1145	DUR	O4-C4	2.36	1.29	1.24
2	f	1145	DUR	C5-C4	-2.36	1.38	1.43
2	B	1145	DUR	C2-N3	-2.34	1.33	1.38
2	k	1145	DUR	C2-N3	-2.32	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	1145	DUR	C5-C4	-2.32	1.38	1.43
2	g	1145	DUR	C2-N3	-2.31	1.33	1.38
2	1	1145	DUR	C5-C4	-2.31	1.38	1.43
3	F	1146	POP	P2-O4	-2.30	1.43	1.50
2	L	1145	DUR	C5-C4	-2.30	1.38	1.43
2	1	1145	DUR	O4'-C4'	-2.28	1.39	1.45
3	e	1146	POP	P2-O6	-2.28	1.46	1.54
2	L	1145	DUR	C6-N1	-2.28	1.32	1.38
2	N	1145	DUR	C6-C5	2.27	1.40	1.35
2	c	1145	DUR	C2-N3	-2.27	1.34	1.38
2	Y	1145	DUR	O2-C2	2.27	1.27	1.23
2	4	1145	DUR	O4-C4	2.26	1.28	1.24
2	h	1145	DUR	C6-N1	-2.26	1.32	1.38
2	J	1145	DUR	C5-C4	-2.25	1.38	1.43
2	h	1145	DUR	C4-N3	-2.23	1.34	1.38
2	8	1145	DUR	C4-N3	-2.23	1.34	1.38
2	i	1145	DUR	C2-N3	-2.22	1.34	1.38
2	C	1145	DUR	C6-C5	2.22	1.40	1.35
2	j	1145	DUR	C5-C4	-2.22	1.38	1.43
2	S	1145	DUR	C5-C4	-2.21	1.38	1.43
2	C	1145	DUR	C2-N3	-2.20	1.34	1.38
3	I	1146	POP	P1-O2	-2.20	1.46	1.54
2	C	1145	DUR	C6-N1	-2.18	1.32	1.38
2	b	1145	DUR	C2-N1	-2.17	1.35	1.38
2	G	1145	DUR	C5-C4	-2.16	1.39	1.43
3	N	1146	POP	P2-O6	-2.15	1.46	1.54
3	Q	1146	POP	P2-O5	-2.14	1.46	1.54
3	4	1146	POP	P1-O1	2.14	1.57	1.50
2	F	1145	DUR	O3'-C3'	2.13	1.47	1.43
3	G	1146	POP	P2-O6	-2.11	1.47	1.54
3	M	1146	POP	P1-O2	-2.11	1.47	1.54
2	Q	1145	DUR	C2-N3	-2.10	1.34	1.38
2	2	1145	DUR	C2-N1	2.10	1.41	1.38
2	l	1145	DUR	C5-C4	-2.10	1.39	1.43
3	D	1146	POP	P1-O2	-2.10	1.47	1.54
2	j	1145	DUR	C6-C5	2.08	1.39	1.35
3	G	1146	POP	P2-O4	2.07	1.56	1.50
3	Y	1146	POP	P2-O5	-2.07	1.47	1.54
2	5	1145	DUR	C2-N3	-2.06	1.34	1.38
2	U	1145	DUR	C2-N3	-2.06	1.34	1.38
2	b	1145	DUR	C4-N3	-2.06	1.35	1.38
3	S	1146	POP	P2-O4	2.05	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	9	1145	DUR	O4-C4	2.05	1.28	1.24
3	K	1146	POP	P1-O3	-2.05	1.47	1.54
2	X	1145	DUR	C2-N1	2.04	1.41	1.38
2	T	1145	DUR	C5-C4	-2.03	1.39	1.43
3	K	1146	POP	P2-O5	-2.03	1.47	1.54
2	X	1145	DUR	C6-N1	-2.03	1.33	1.38
2	M	1145	DUR	C6-N1	-2.02	1.33	1.38
2	f	1145	DUR	C6-N1	-2.02	1.33	1.38
2	H	1145	DUR	O4-C4	2.02	1.28	1.24
2	4	1145	DUR	C2-N3	-2.02	1.34	1.38
2	T	1145	DUR	C2-N1	2.01	1.41	1.38
2	E	1145	DUR	C6-C5	2.00	1.39	1.35

All (431) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	1145	DUR	N3-C2-N1	6.51	123.37	114.89
2	U	1145	DUR	C4-N3-C2	-6.48	118.57	126.61
2	M	1145	DUR	C4-N3-C2	-6.32	118.77	126.61
2	A	1145	DUR	N3-C2-N1	6.13	122.87	114.89
2	j	1145	DUR	N3-C2-N1	6.00	122.70	114.89
2	C	1145	DUR	C4-N3-C2	-5.96	119.21	126.61
2	V	1145	DUR	N3-C2-N1	5.94	122.62	114.89
2	Q	1145	DUR	C4-N3-C2	-5.86	119.34	126.61
2	Z	1145	DUR	C4-N3-C2	-5.85	119.34	126.61
2	C	1145	DUR	N3-C2-N1	5.81	122.45	114.89
2	K	1145	DUR	C4-N3-C2	-5.79	119.42	126.61
2	5	1145	DUR	O2-C2-N1	-5.76	115.30	122.80
2	9	1145	DUR	N3-C2-N1	5.75	122.37	114.89
2	i	1145	DUR	O4-C4-C5	-5.74	115.27	125.16
2	4	1145	DUR	N3-C2-N1	5.71	122.32	114.89
2	U	1145	DUR	N3-C2-N1	5.69	122.30	114.89
2	J	1145	DUR	C5-C4-N3	5.66	122.72	114.80
2	a	1145	DUR	N3-C2-N1	5.58	122.15	114.89
2	V	1145	DUR	C4-N3-C2	-5.52	119.76	126.61
2	K	1145	DUR	O4-C4-C5	-5.51	115.66	125.16
2	Q	1145	DUR	C5-C4-N3	5.45	122.44	114.80
2	M	1145	DUR	C5-C4-N3	5.44	122.42	114.80
2	k	1145	DUR	C4-N3-C2	-5.37	119.94	126.61
2	h	1145	DUR	C4-N3-C2	-5.33	119.99	126.61
2	i	1145	DUR	C4-N3-C2	-5.30	120.03	126.61
2	N	1145	DUR	N3-C2-N1	5.27	121.75	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	k	1145	DUR	N3-C2-N1	5.26	121.74	114.89
2	U	1145	DUR	C5-C4-N3	5.25	122.16	114.80
2	I	1145	DUR	C4-N3-C2	-5.24	120.11	126.61
2	a	1145	DUR	C4-N3-C2	-5.21	120.14	126.61
2	T	1145	DUR	C4-N3-C2	-5.15	120.22	126.61
2	h	1145	DUR	N3-C2-N1	5.12	121.56	114.89
2	M	1145	DUR	N3-C2-N1	5.11	121.55	114.89
2	7	1145	DUR	C4-N3-C2	-5.05	120.34	126.61
2	M	1145	DUR	O2-C2-N1	-5.04	116.24	122.80
2	5	1145	DUR	O4-C4-C5	-4.99	116.56	125.16
2	E	1145	DUR	N3-C2-N1	4.97	121.36	114.89
2	D	1145	DUR	N3-C2-N1	4.97	121.36	114.89
2	3	1145	DUR	O4-C4-C5	-4.96	116.61	125.16
2	5	1145	DUR	C4-N3-C2	-4.94	120.47	126.61
2	O	1145	DUR	N3-C2-N1	4.93	121.31	114.89
2	b	1145	DUR	C5-C4-N3	4.88	121.64	114.80
2	7	1145	DUR	O4-C4-C5	-4.87	116.75	125.16
2	H	1145	DUR	N3-C2-N1	4.86	121.22	114.89
2	X	1145	DUR	N3-C2-N1	4.85	121.21	114.89
2	3	1145	DUR	C5-C4-N3	4.81	121.53	114.80
2	e	1145	DUR	N3-C2-N1	4.79	121.12	114.89
2	L	1145	DUR	C4-N3-C2	-4.73	120.74	126.61
2	P	1145	DUR	C4-N3-C2	-4.72	120.76	126.61
2	P	1145	DUR	N3-C2-N1	4.71	121.02	114.89
2	i	1145	DUR	C5-C4-N3	4.70	121.39	114.80
2	3	1145	DUR	C4-N3-C2	-4.68	120.80	126.61
2	K	1145	DUR	C5-C4-N3	4.68	121.35	114.80
2	5	1145	DUR	N3-C2-N1	4.64	120.93	114.89
2	T	1145	DUR	C5-C4-N3	4.64	121.29	114.80
2	4	1145	DUR	C4-N3-C2	-4.63	120.86	126.61
2	N	1145	DUR	C4-N3-C2	-4.63	120.87	126.61
2	2	1145	DUR	C4-N3-C2	-4.63	120.87	126.61
2	I	1145	DUR	O4-C4-C5	-4.62	117.19	125.16
2	B	1145	DUR	C4-N3-C2	-4.62	120.88	126.61
2	W	1145	DUR	C5-C4-N3	4.61	121.26	114.80
2	B	1145	DUR	N3-C2-N1	4.59	120.86	114.89
2	T	1145	DUR	O4-C4-C5	-4.56	117.29	125.16
2	9	1145	DUR	C4-N3-C2	-4.55	120.97	126.61
2	N	1145	DUR	O2-C2-N1	-4.54	116.88	122.80
2	j	1145	DUR	C4-N3-C2	-4.54	120.98	126.61
2	i	1145	DUR	N3-C2-N1	4.50	120.75	114.89
2	T	1145	DUR	N3-C2-N1	4.49	120.73	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	1145	DUR	C4-N3-C2	-4.40	121.15	126.61
2	d	1145	DUR	N3-C2-N1	4.37	120.58	114.89
2	C	1145	DUR	C5-C4-N3	4.36	120.90	114.80
2	g	1145	DUR	N3-C2-N1	4.36	120.56	114.89
2	7	1145	DUR	C5-C4-N3	4.33	120.86	114.80
2	a	1145	DUR	C1'-N1-C2	4.29	126.06	117.66
2	Y	1145	DUR	N3-C2-N1	4.29	120.48	114.89
2	E	1145	DUR	C4-N3-C2	-4.28	121.30	126.61
2	D	1145	DUR	C4-N3-C2	-4.25	121.34	126.61
2	A	1145	DUR	C6-N1-C2	-4.20	115.88	121.00
2	m	1145	DUR	C5-C4-N3	4.19	120.67	114.80
2	L	1145	DUR	C5-C4-N3	4.18	120.66	114.80
2	5	1145	DUR	O4-C4-N3	4.17	125.32	119.27
2	I	1145	DUR	C5-C4-N3	4.17	120.64	114.80
2	2	1145	DUR	C5-C4-N3	4.12	120.58	114.80
2	h	1145	DUR	C5-C4-N3	4.12	120.57	114.80
2	O	1145	DUR	O2-C2-N3	-4.11	113.91	121.49
2	S	1145	DUR	N3-C2-N1	4.11	120.24	114.89
2	f	1145	DUR	N3-C2-N1	4.11	120.24	114.89
3	m	1146	POP	O6-P2-O5	4.10	123.17	107.80
2	8	1145	DUR	C5-C4-N3	4.08	120.51	114.80
2	l	1145	DUR	N3-C2-N1	4.07	120.19	114.89
3	V	1146	POP	O6-P2-O5	4.07	123.06	107.80
2	7	1145	DUR	N3-C2-N1	4.07	120.19	114.89
2	i	1145	DUR	O2-C2-N1	-4.06	117.51	122.80
2	H	1145	DUR	C4-N3-C2	-4.03	121.60	126.61
2	l	1145	DUR	O4-C4-C5	-4.00	118.26	125.16
2	K	1145	DUR	N3-C2-N1	4.00	120.10	114.89
2	J	1145	DUR	C4-N3-C2	-4.00	121.65	126.61
2	J	1145	DUR	C6-C5-C4	-3.98	114.45	119.53
2	f	1145	DUR	C4-N3-C2	-3.96	121.69	126.61
2	P	1145	DUR	O4-C4-C5	-3.96	118.33	125.16
2	M	1145	DUR	O4-C4-C5	-3.96	118.33	125.16
2	P	1145	DUR	O2-C2-N1	-3.95	117.65	122.80
2	G	1145	DUR	O4-C4-C5	-3.95	118.35	125.16
2	k	1145	DUR	O2-C2-N1	-3.95	117.66	122.80
2	J	1145	DUR	O3'-C3'-C4'	3.95	125.03	110.07
2	X	1145	DUR	C4-N3-C2	-3.93	121.73	126.61
2	N	1145	DUR	O4-C4-C5	-3.92	118.41	125.16
2	b	1145	DUR	C6-C5-C4	-3.92	114.53	119.53
2	Q	1145	DUR	N3-C2-N1	3.91	119.98	114.89
2	2	1145	DUR	N3-C2-N1	3.89	119.96	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	1145	DUR	C5-C4-N3	3.87	120.23	114.80
2	A	1145	DUR	O2-C2-N3	-3.85	114.38	121.49
2	3	1145	DUR	O2-C2-N1	-3.85	117.79	122.80
2	E	1145	DUR	C5-C4-N3	3.83	120.16	114.80
2	c	1145	DUR	C4-N3-C2	-3.82	121.88	126.61
2	d	1145	DUR	O2-C2-N1	-3.79	117.86	122.80
2	e	1145	DUR	C5-C4-N3	3.79	120.11	114.80
2	3	1145	DUR	N3-C2-N1	3.79	119.83	114.89
2	H	1145	DUR	O4-C4-C5	-3.78	118.65	125.16
2	l	1145	DUR	C4-N3-C2	-3.76	121.94	126.61
2	S	1145	DUR	C4-N3-C2	-3.74	121.97	126.61
2	Z	1145	DUR	O2-C2-N1	-3.73	117.95	122.80
2	4	1145	DUR	O2-C2-N1	-3.69	117.99	122.80
2	I	1145	DUR	N3-C2-N1	3.66	119.66	114.89
2	C	1145	DUR	O4-C4-C5	-3.65	118.86	125.16
2	R	1145	DUR	C5-C4-N3	3.63	119.89	114.80
2	e	1145	DUR	C4-N3-C2	-3.63	122.11	126.61
2	g	1145	DUR	C4-N3-C2	-3.59	122.16	126.61
2	Y	1145	DUR	C5-C4-N3	3.59	119.83	114.80
2	Y	1145	DUR	C4-N3-C2	-3.57	122.18	126.61
2	Y	1145	DUR	O4-C4-C5	-3.56	119.02	125.16
2	L	1145	DUR	O4-C4-C5	-3.56	119.02	125.16
2	U	1145	DUR	O4-C4-C5	-3.56	119.03	125.16
2	c	1145	DUR	N3-C2-N1	3.55	119.52	114.89
2	f	1145	DUR	O4-C4-C5	-3.54	119.05	125.16
2	g	1145	DUR	O4-C4-C5	-3.54	119.05	125.16
2	L	1145	DUR	N3-C2-N1	3.53	119.49	114.89
2	a	1145	DUR	O4-C4-C5	-3.51	119.11	125.16
2	6	1145	DUR	C5-C4-N3	3.50	119.70	114.80
2	a	1145	DUR	O2-C2-N3	-3.50	115.04	121.49
2	R	1145	DUR	N3-C2-N1	3.46	119.39	114.89
2	6	1145	DUR	C4-N3-C2	-3.43	122.36	126.61
2	6	1145	DUR	N3-C2-N1	3.42	119.35	114.89
2	k	1145	DUR	C5-C4-N3	3.36	119.51	114.80
2	Q	1145	DUR	O4-C4-C5	-3.35	119.38	125.16
3	j	1146	POP	O5-P2-O4	3.34	123.85	110.83
2	B	1145	DUR	C5-C4-N3	3.31	119.44	114.80
2	i	1145	DUR	O4'-C1'-N1	3.31	113.74	107.86
2	W	1145	DUR	C4-N3-C2	-3.31	122.50	126.61
3	k	1146	POP	O6-P2-O	3.31	115.74	104.64
3	c	1146	POP	O2-P1-O1	3.30	123.70	110.83
2	K	1145	DUR	O2-C2-N1	-3.30	118.50	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	1145	DUR	N3-C2-N1	3.29	119.18	114.89
2	2	1145	DUR	O4-C4-C5	-3.29	119.50	125.16
3	g	1146	POP	O3-P1-O	3.28	115.63	104.64
2	h	1145	DUR	O4-C4-C5	-3.25	119.55	125.16
2	f	1145	DUR	C5-C4-N3	3.25	119.35	114.80
2	c	1145	DUR	C1'-N1-C2	3.25	124.01	117.66
2	g	1145	DUR	C5-C4-N3	3.25	119.34	114.80
2	X	1145	DUR	O4-C4-C5	-3.24	119.57	125.16
2	h	1145	DUR	C5-C6-N1	-3.24	116.57	121.84
2	h	1145	DUR	O2-C2-N3	-3.24	115.51	121.49
2	j	1145	DUR	O2-C2-N1	-3.23	118.59	122.80
2	Y	1145	DUR	C1'-N1-C2	3.21	123.94	117.66
3	G	1146	POP	O5-P2-O4	3.21	123.34	110.83
2	W	1145	DUR	N3-C2-N1	3.21	119.06	114.89
2	H	1145	DUR	C6-N1-C2	-3.19	117.11	121.00
2	Z	1145	DUR	C5-C4-N3	3.19	119.27	114.80
2	V	1145	DUR	C1'-N1-C2	3.17	123.86	117.66
2	H	1145	DUR	C5-C4-N3	3.16	119.23	114.80
2	J	1145	DUR	C2'-C3'-C4'	3.14	109.18	102.80
2	P	1145	DUR	C5-C4-N3	3.13	119.18	114.80
3	4	1146	POP	O3-P1-O1	3.13	123.02	110.83
2	6	1145	DUR	C1'-N1-C2	3.12	123.77	117.66
3	D	1146	POP	O6-P2-O5	3.11	119.46	107.80
2	V	1145	DUR	C5-C4-N3	3.09	119.13	114.80
2	G	1145	DUR	O4-C4-N3	3.09	123.75	119.27
3	M	1146	POP	O5-P2-O4	3.08	122.84	110.83
2	b	1145	DUR	O4-C4-C5	-3.07	119.87	125.16
3	T	1146	POP	O3-P1-O2	3.06	119.28	107.80
2	1	1145	DUR	C6-N1-C2	-3.05	117.28	121.00
2	G	1145	DUR	C1'-N1-C2	3.05	123.63	117.66
3	a	1146	POP	O5-P2-O4	3.05	122.72	110.83
2	d	1145	DUR	C4-N3-C2	-3.04	122.83	126.61
2	V	1145	DUR	C6-N1-C2	-3.04	117.30	121.00
2	D	1145	DUR	C6-N1-C2	-3.03	117.31	121.00
2	k	1145	DUR	O4-C4-C5	-3.03	119.94	125.16
3	R	1146	POP	O2-P1-O1	3.02	122.60	110.83
2	S	1145	DUR	O3'-C3'-C4'	3.00	121.44	110.07
2	C	1145	DUR	C1'-N1-C2	3.00	123.52	117.66
2	E	1145	DUR	O2-C2-N1	-2.97	118.93	122.80
2	j	1145	DUR	C5-C4-N3	2.96	118.94	114.80
2	1	1145	DUR	N3-C2-N1	2.96	118.74	114.89
2	O	1145	DUR	C6-N1-C2	-2.95	117.41	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	f	1146	POP	O-P1-O1	-2.95	95.53	111.04
3	c	1146	POP	O5-P2-O4	2.95	122.32	110.83
3	j	1146	POP	O3-P1-O1	2.95	122.31	110.83
2	b	1145	DUR	C4-N3-C2	-2.95	122.96	126.61
3	i	1146	POP	O6-P2-O5	2.92	118.75	107.80
2	V	1145	DUR	O2-C2-N3	-2.92	116.11	121.49
2	X	1145	DUR	O2-C2-N1	-2.90	119.02	122.80
2	Z	1145	DUR	O4-C4-C5	-2.90	120.16	125.16
2	A	1145	DUR	C1'-N1-C2	2.90	123.33	117.66
2	6	1145	DUR	O4-C4-C5	-2.89	120.18	125.16
2	P	1145	DUR	C2'-C3'-C4'	-2.87	96.98	102.80
2	l	1145	DUR	C1'-N1-C2	2.87	123.27	117.66
2	j	1145	DUR	C6-N1-C2	-2.87	117.50	121.00
2	H	1145	DUR	C2'-C3'-C4'	-2.86	97.01	102.80
2	E	1145	DUR	O4-C4-C5	-2.84	120.26	125.16
3	f	1146	POP	O2-P1-O1	2.84	121.89	110.83
2	H	1145	DUR	C1'-N1-C2	2.84	123.21	117.66
2	f	1145	DUR	O2-C2-N1	-2.84	119.10	122.80
2	O	1145	DUR	C4-N3-C2	-2.83	123.11	126.61
2	P	1145	DUR	C1'-N1-C2	2.82	123.17	117.66
2	X	1145	DUR	C5-C4-N3	2.81	118.74	114.80
2	f	1145	DUR	O3'-C3'-C2'	2.81	120.65	110.88
2	c	1145	DUR	O2-C2-N3	-2.80	116.33	121.49
2	a	1145	DUR	C1'-N1-C6	-2.79	116.04	121.53
2	a	1145	DUR	C5-C4-N3	2.79	118.71	114.80
2	l	1145	DUR	O4-C4-N3	2.79	123.32	119.27
2	D	1145	DUR	C1'-N1-C2	2.78	123.10	117.66
2	N	1145	DUR	O4-C4-N3	2.78	123.31	119.27
3	Y	1146	POP	O2-P1-O	2.77	113.92	104.64
2	i	1145	DUR	O4-C4-N3	2.76	123.28	119.27
2	B	1145	DUR	O4-C4-C5	-2.76	120.40	125.16
3	E	1146	POP	O6-P2-O5	2.76	118.15	107.80
2	e	1145	DUR	O2-C2-N3	-2.76	116.41	121.49
2	g	1145	DUR	C6-N1-C2	-2.73	117.67	121.00
2	b	1145	DUR	O4'-C4'-C3'	-2.73	99.42	105.65
2	D	1145	DUR	O4-C4-C5	-2.73	120.45	125.16
3	P	1146	POP	O3-P1-O1	2.73	121.46	110.83
2	J	1145	DUR	O4'-C4'-C5'	2.72	114.97	109.22
3	B	1146	POP	O6-P2-O5	2.71	117.97	107.80
2	T	1145	DUR	C5'-C4'-C3'	2.71	121.58	114.82
2	e	1145	DUR	C6-N1-C2	-2.71	117.70	121.00
2	9	1145	DUR	O2-C2-N1	-2.70	119.29	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1145	DUR	O4-C4-C5	-2.69	120.52	125.16
2	G	1145	DUR	N3-C2-N1	2.69	118.39	114.89
2	F	1145	DUR	N3-C2-N1	2.69	118.39	114.89
2	d	1145	DUR	O4-C4-C5	-2.69	120.52	125.16
2	m	1145	DUR	O4-C4-C5	-2.69	120.53	125.16
3	3	1146	POP	O3-P1-O1	2.68	121.29	110.83
2	j	1145	DUR	O4-C4-C5	-2.67	120.55	125.16
3	X	1146	POP	O-P1-O1	-2.67	97.00	111.04
3	O	1146	POP	O2-P1-O1	2.67	121.23	110.83
2	W	1145	DUR	O4-C4-C5	-2.67	120.56	125.16
3	R	1146	POP	O3-P1-O2	2.66	117.79	107.80
2	c	1145	DUR	C5-C4-N3	2.65	118.51	114.80
2	2	1145	DUR	O2-C2-N1	-2.65	119.35	122.80
2	A	1145	DUR	C4-N3-C2	-2.64	123.34	126.61
3	X	1146	POP	O3-P1-O1	2.63	121.08	110.83
2	m	1145	DUR	C4-N3-C2	-2.63	123.35	126.61
2	8	1145	DUR	N3-C2-N1	2.62	118.30	114.89
2	a	1145	DUR	C6-N1-C2	-2.60	117.83	121.00
2	i	1145	DUR	C1'-N1-C2	2.60	122.74	117.66
2	H	1145	DUR	O2-C2-N1	-2.60	119.42	122.80
2	O	1145	DUR	C5-C4-N3	2.59	118.43	114.80
3	h	1146	POP	O-P1-O1	-2.59	97.42	111.04
2	k	1145	DUR	O4'-C1'-C2'	2.59	111.08	106.25
3	d	1146	POP	O2-P1-O	2.58	113.29	104.64
2	l	1145	DUR	C5-C4-N3	2.58	118.41	114.80
2	J	1145	DUR	N3-C2-N1	2.58	118.25	114.89
2	H	1145	DUR	O3'-C3'-C4'	2.57	119.80	110.07
2	K	1145	DUR	C1'-N1-C2	2.56	122.66	117.66
2	U	1145	DUR	O3'-C3'-C2'	2.55	119.75	110.88
2	X	1145	DUR	O4'-C4'-C5'	-2.55	103.82	109.22
2	K	1145	DUR	O4-C4-N3	2.55	122.97	119.27
2	k	1145	DUR	C2'-C1'-N1	-2.54	107.46	113.81
2	8	1145	DUR	C4-N3-C2	-2.53	123.47	126.61
2	Y	1145	DUR	C6-N1-C2	-2.53	117.91	121.00
2	9	1145	DUR	C1'-N1-C2	2.52	122.60	117.66
3	B	1146	POP	O5-P2-O4	2.52	120.65	110.83
3	I	1146	POP	O3-P1-O1	-2.51	101.05	110.83
3	d	1146	POP	O3-P1-O2	2.51	117.22	107.80
2	V	1145	DUR	O4-C4-C5	-2.51	120.84	125.16
2	E	1145	DUR	C3'-C2'-C1'	2.50	108.73	102.60
2	4	1145	DUR	C5-C4-N3	2.49	118.29	114.80
3	1	1146	POP	O3-P1-O2	2.49	117.14	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1145	DUR	C5-C4-N3	2.49	118.28	114.80
2	W	1145	DUR	C6-C5-C4	-2.48	116.36	119.53
2	D	1145	DUR	O2-C2-N1	-2.48	119.57	122.80
3	Y	1146	POP	O6-P2-O5	2.48	117.10	107.80
2	F	1145	DUR	C6-C5-C4	-2.48	116.37	119.53
2	8	1145	DUR	O4-C4-C5	-2.48	120.89	125.16
3	I	1146	POP	O2-P1-O	2.47	112.93	104.64
2	K	1145	DUR	C1'-N1-C6	-2.46	116.69	121.53
3	T	1146	POP	O6-P2-O5	2.46	117.03	107.80
2	B	1145	DUR	O2-C2-N3	-2.46	116.95	121.49
3	F	1146	POP	O3-P1-O1	2.46	120.42	110.83
3	M	1146	POP	O3-P1-O	2.46	112.88	104.64
3	k	1146	POP	O5-P2-O4	2.46	120.42	110.83
2	b	1145	DUR	O4'-C1'-N1	-2.46	103.50	107.86
3	R	1146	POP	O-P1-O1	-2.45	98.16	111.04
3	M	1146	POP	O-P1-O1	-2.45	98.16	111.04
2	4	1145	DUR	O4-C4-C5	-2.44	120.95	125.16
2	c	1145	DUR	O4-C4-C5	-2.43	120.97	125.16
3	b	1146	POP	O-P1-O1	-2.43	98.28	111.04
3	b	1146	POP	O6-P2-O5	2.43	116.89	107.80
3	f	1146	POP	O6-P2-O	2.42	112.77	104.64
2	D	1145	DUR	C5-C4-N3	2.42	118.19	114.80
3	D	1146	POP	O-P1-O1	-2.42	98.31	111.04
3	4	1146	POP	O-P1-O1	-2.42	98.32	111.04
2	4	1145	DUR	C6-N1-C2	-2.41	118.06	121.00
3	N	1146	POP	O-P1-O1	-2.40	98.39	111.04
2	F	1145	DUR	C5-C4-N3	2.40	118.16	114.80
2	W	1145	DUR	C1'-N1-C2	2.40	122.34	117.66
2	R	1145	DUR	O4-C4-C5	-2.39	121.03	125.16
3	P	1146	POP	O5-P2-O4	2.39	120.15	110.83
3	W	1146	POP	O-P2-O4	-2.39	98.48	111.04
2	S	1145	DUR	O4-C4-C5	-2.39	121.05	125.16
2	m	1145	DUR	N3-C2-N1	2.38	118.00	114.89
3	G	1146	POP	O-P1-O1	-2.38	98.53	111.04
2	a	1145	DUR	O3'-C3'-C4'	2.37	119.05	110.07
3	g	1146	POP	O6-P2-O5	2.37	116.69	107.80
3	7	1146	POP	O5-P2-O	2.37	112.58	104.64
2	e	1145	DUR	C3'-C2'-C1'	2.36	108.38	102.60
3	O	1146	POP	O6-P2-O5	2.36	116.66	107.80
2	5	1145	DUR	C5-C4-N3	2.36	118.10	114.80
3	G	1146	POP	O6-P2-O5	2.36	116.63	107.80
2	T	1145	DUR	C1'-N1-C2	2.35	122.26	117.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	i	1145	DUR	C6-C5-C4	-2.35	116.53	119.53
2	Z	1145	DUR	C5-C6-N1	-2.35	118.03	121.84
3	1	1146	POP	O6-P2-O5	2.34	116.56	107.80
2	6	1145	DUR	C1'-N1-C6	-2.34	116.94	121.53
2	d	1145	DUR	C5-C4-N3	2.34	118.07	114.80
3	1	1146	POP	O3-P1-O	2.34	112.47	104.64
3	V	1146	POP	O6-P2-O4	-2.33	101.75	110.83
2	l	1145	DUR	C1'-N1-C6	-2.33	116.95	121.53
3	N	1146	POP	O3-P1-O1	2.33	119.91	110.83
3	V	1146	POP	O2-P1-O	2.32	112.42	104.64
3	8	1146	POP	O6-P2-O5	2.32	116.50	107.80
2	G	1145	DUR	C4-N3-C2	-2.32	123.73	126.61
2	E	1145	DUR	O4'-C1'-N1	-2.32	103.75	107.86
3	d	1146	POP	O5-P2-O4	2.31	119.85	110.83
3	Y	1146	POP	O-P2-O4	-2.30	98.94	111.04
2	A	1145	DUR	C5-C4-N3	2.29	118.00	114.80
2	L	1145	DUR	C2'-C3'-C4'	-2.28	98.18	102.80
3	c	1146	POP	O-P1-O1	-2.28	99.05	111.04
2	L	1145	DUR	C3'-C2'-C1'	2.28	108.17	102.60
2	N	1145	DUR	C6-N1-C2	-2.27	118.23	121.00
2	Z	1145	DUR	C5'-C4'-C3'	-2.27	109.16	114.82
2	C	1145	DUR	C6-N1-C2	-2.27	118.23	121.00
2	f	1145	DUR	C6-N1-C2	-2.27	118.23	121.00
2	c	1145	DUR	C1'-N1-C6	-2.26	117.09	121.53
2	C	1145	DUR	O2-C2-N3	-2.26	117.32	121.49
3	5	1146	POP	O2-P1-O	2.26	112.20	104.64
3	B	1146	POP	O2-P1-O	2.26	112.20	104.64
2	N	1145	DUR	C4'-O4'-C1'	2.26	114.87	109.51
3	6	1146	POP	O3-P1-O1	2.25	119.60	110.83
3	C	1146	POP	O6-P2-O5	2.25	116.22	107.80
3	P	1146	POP	O-P2-O4	-2.24	99.23	111.04
3	f	1146	POP	O5-P2-O4	2.24	119.58	110.83
2	E	1145	DUR	C2'-C1'-N1	-2.23	108.23	113.81
2	T	1145	DUR	O4'-C4'-C5'	-2.23	104.51	109.22
2	j	1145	DUR	C5-C6-N1	-2.22	118.23	121.84
2	Y	1145	DUR	O4'-C4'-C5'	2.22	113.91	109.22
3	B	1146	POP	O-P2-O4	-2.22	99.37	111.04
3	5	1146	POP	O-P1-O1	-2.21	99.39	111.04
3	Y	1146	POP	O-P1-O1	-2.21	99.39	111.04
2	O	1145	DUR	O4'-C1'-N1	2.21	111.79	107.86
3	e	1146	POP	O-P1-O1	-2.21	99.43	111.04
2	G	1145	DUR	C5-C4-N3	2.20	117.89	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1146	POP	O6-P2-O5	2.20	116.06	107.80
2	6	1145	DUR	O2-C2-N3	-2.19	117.44	121.49
2	P	1145	DUR	O4-C4-N3	2.19	122.45	119.27
3	A	1146	POP	O6-P2-O5	2.19	116.02	107.80
2	8	1145	DUR	O2-C2-N3	-2.19	117.45	121.49
2	1	1145	DUR	C1'-N1-C2	2.19	121.94	117.66
2	U	1145	DUR	O2-C2-N1	-2.19	119.95	122.80
3	Z	1146	POP	O-P2-O4	-2.19	99.54	111.04
2	5	1145	DUR	C6-N1-C2	-2.19	118.34	121.00
3	4	1146	POP	O6-P2-O5	2.18	115.98	107.80
3	J	1146	POP	O6-P2-O5	2.18	115.97	107.80
3	Z	1146	POP	O5-P2-O4	2.17	119.29	110.83
2	R	1145	DUR	C1'-N1-C2	2.17	121.90	117.66
3	H	1146	POP	O-P1-O1	-2.17	99.63	111.04
3	Q	1146	POP	O2-P1-O1	2.17	119.28	110.83
3	G	1146	POP	O3-P1-O1	2.16	119.25	110.83
2	U	1145	DUR	C6-N1-C2	-2.16	118.37	121.00
2	4	1145	DUR	O3'-C3'-C4'	2.16	118.24	110.07
3	T	1146	POP	O2-P1-O	2.15	111.86	104.64
2	D	1145	DUR	O4'-C1'-N1	2.15	111.68	107.86
2	3	1145	DUR	C6-C5-C4	-2.15	116.79	119.53
3	e	1146	POP	O3-P1-O1	2.15	119.20	110.83
3	h	1146	POP	O6-P2-O5	2.15	115.85	107.80
2	I	1145	DUR	C1'-N1-C6	-2.14	117.32	121.53
3	e	1146	POP	O6-P2-O4	-2.14	102.50	110.83
5	l	1148	PO4	O4-P-O2	2.14	114.56	107.91
2	G	1145	DUR	C1'-N1-C6	-2.13	117.33	121.53
2	L	1145	DUR	O2-C2-N1	-2.13	120.02	122.80
3	5	1146	POP	O3-P1-O2	2.13	115.78	107.80
2	7	1145	DUR	O4-C4-N3	2.13	122.36	119.27
3	C	1146	POP	O3-P1-O1	2.11	119.07	110.83
3	d	1146	POP	O6-P2-O5	2.11	115.70	107.80
3	7	1146	POP	O3-P1-O2	2.10	115.68	107.80
3	d	1146	POP	O3-P1-O1	2.10	119.02	110.83
2	9	1145	DUR	C5-C6-N1	-2.10	118.43	121.84
3	C	1146	POP	O-P1-O1	-2.10	100.00	111.04
2	7	1145	DUR	C2'-C3'-C4'	-2.09	98.55	102.80
3	D	1146	POP	O2-P1-O1	2.09	118.98	110.83
2	F	1145	DUR	O3'-C3'-C2'	2.09	118.14	110.88
3	Z	1146	POP	O3-P1-O1	2.09	118.97	110.83
2	7	1145	DUR	O2-C2-N1	-2.09	120.08	122.80
3	1	1146	POP	O-P1-O1	-2.08	100.08	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	k	1146	POP	O3-P1-O2	2.08	115.60	107.80
3	3	1146	POP	O-P2-O4	-2.08	100.11	111.04
2	M	1145	DUR	C6-C5-C4	-2.07	116.89	119.53
2	3	1145	DUR	C6-N1-C2	-2.07	118.48	121.00
2	g	1145	DUR	O2-C2-N1	-2.07	120.10	122.80
3	l	1146	POP	O3-P1-O1	2.07	118.89	110.83
2	8	1145	DUR	C6-C5-C4	-2.07	116.89	119.53
2	1	1145	DUR	C5'-C4'-C3'	2.06	119.96	114.82
2	3	1145	DUR	O4'-C1'-N1	-2.06	104.21	107.86
3	X	1146	POP	O-P2-O4	-2.06	100.21	111.04
3	B	1146	POP	O3-P1-O2	2.06	115.52	107.80
2	9	1145	DUR	O3'-C3'-C4'	2.06	117.86	110.07
2	S	1145	DUR	O2-C2-N3	-2.06	117.69	121.49
3	j	1146	POP	O6-P2-O5	2.06	115.51	107.80
3	L	1146	POP	O6-P2-O	2.05	111.52	104.64
3	i	1146	POP	O3-P1-O	2.05	111.52	104.64
2	P	1145	DUR	C6-N1-C2	-2.05	118.50	121.00
3	W	1146	POP	O6-P2-O5	2.05	115.48	107.80
2	N	1145	DUR	O4'-C1'-N1	2.05	111.50	107.86
2	m	1145	DUR	C6-C5-C4	-2.05	116.92	119.53
2	F	1145	DUR	O4-C4-C5	-2.04	121.64	125.16
3	3	1146	POP	O6-P2-O5	2.04	115.45	107.80
2	7	1145	DUR	O3'-C3'-C4'	2.04	117.80	110.07
2	U	1145	DUR	O2-C2-N3	-2.03	117.75	121.49
3	G	1146	POP	O-P2-O4	-2.03	100.38	111.04
3	d	1146	POP	O2-P1-O1	-2.01	103.00	110.83
2	O	1145	DUR	C1'-N1-C2	2.00	121.58	117.66

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	J	1145	DUR	C3'

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	1	1146	POP	P1-O-P2-O5
3	2	1146	POP	P1-O-P2-O5
3	3	1146	POP	P1-O-P2-O5
3	4	1146	POP	P1-O-P2-O5
3	5	1146	POP	P1-O-P2-O5
3	6	1146	POP	P1-O-P2-O5

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Mol	Chain	Res	Type	Atoms
3	7	1146	POP	P1-O-P2-O5
3	8	1146	POP	P1-O-P2-O5
3	9	1146	POP	P1-O-P2-O5
3	A	1146	POP	P1-O-P2-O5
3	B	1146	POP	P1-O-P2-O5
3	C	1146	POP	P1-O-P2-O5
3	D	1146	POP	P1-O-P2-O5
3	F	1146	POP	P1-O-P2-O5
3	G	1146	POP	P1-O-P2-O5
3	H	1146	POP	P1-O-P2-O5
3	I	1146	POP	P1-O-P2-O5
3	J	1146	POP	P1-O-P2-O5
3	K	1146	POP	P1-O-P2-O5
3	L	1146	POP	P1-O-P2-O5
3	M	1146	POP	P1-O-P2-O5
3	N	1146	POP	P1-O-P2-O5
3	O	1146	POP	P1-O-P2-O5
3	P	1146	POP	P1-O-P2-O5
3	Q	1146	POP	P1-O-P2-O5
3	R	1146	POP	P1-O-P2-O5
3	S	1146	POP	P1-O-P2-O5
3	T	1146	POP	P1-O-P2-O5
3	U	1146	POP	P1-O-P2-O5
3	V	1146	POP	P1-O-P2-O5
3	W	1146	POP	P1-O-P2-O5
3	X	1146	POP	P1-O-P2-O5
3	Y	1146	POP	P1-O-P2-O5
3	Z	1146	POP	P1-O-P2-O5
3	a	1146	POP	P1-O-P2-O5
3	b	1146	POP	P1-O-P2-O5
3	c	1146	POP	P1-O-P2-O5
3	d	1146	POP	P1-O-P2-O5
3	e	1146	POP	P1-O-P2-O5
3	f	1146	POP	P1-O-P2-O5
3	g	1146	POP	P1-O-P2-O5
3	h	1146	POP	P1-O-P2-O5
3	i	1146	POP	P1-O-P2-O5
3	j	1146	POP	P1-O-P2-O5
3	k	1146	POP	P1-O-P2-O5
3	l	1146	POP	P1-O-P2-O5
2	T	1145	DUR	C3'-C4'-C5'-O5'
2	J	1145	DUR	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	J	1145	DUR	C3'-C4'-C5'-O5'
3	6	1146	POP	P1-O-P2-O4
3	E	1146	POP	P1-O-P2-O4
3	M	1146	POP	P1-O-P2-O4
3	P	1146	POP	P1-O-P2-O4
3	g	1146	POP	P1-O-P2-O4
2	T	1145	DUR	O4'-C4'-C5'-O5'
3	f	1146	POP	P1-O-P2-O4
3	m	1146	POP	P1-O-P2-O4
3	E	1146	POP	P1-O-P2-O5
3	m	1146	POP	P1-O-P2-O5
3	F	1146	POP	P1-O-P2-O4
3	Z	1146	POP	P1-O-P2-O4
3	i	1146	POP	P1-O-P2-O4
3	4	1146	POP	P1-O-P2-O4
3	8	1146	POP	P1-O-P2-O4
3	L	1146	POP	P1-O-P2-O4
3	X	1146	POP	P1-O-P2-O4
3	Y	1146	POP	P1-O-P2-O4
3	j	1146	POP	P1-O-P2-O4
3	2	1146	POP	P1-O-P2-O4
3	5	1146	POP	P1-O-P2-O4
3	7	1146	POP	P1-O-P2-O4
3	C	1146	POP	P1-O-P2-O4
3	D	1146	POP	P1-O-P2-O4
3	H	1146	POP	P1-O-P2-O4
3	I	1146	POP	P1-O-P2-O4
3	J	1146	POP	P1-O-P2-O4
3	N	1146	POP	P1-O-P2-O4
3	Q	1146	POP	P1-O-P2-O4
3	R	1146	POP	P1-O-P2-O4
3	T	1146	POP	P1-O-P2-O4
3	U	1146	POP	P1-O-P2-O4
3	W	1146	POP	P1-O-P2-O4
3	b	1146	POP	P1-O-P2-O4
3	d	1146	POP	P1-O-P2-O4
3	h	1146	POP	P1-O-P2-O4
3	k	1146	POP	P1-O-P2-O4
3	A	1146	POP	P1-O-P2-O6
3	B	1146	POP	P1-O-P2-O6
3	C	1146	POP	P1-O-P2-O6
3	D	1146	POP	P1-O-P2-O6

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Mol	Chain	Res	Type	Atoms
3	G	1146	POP	P1-O-P2-O6
3	I	1146	POP	P1-O-P2-O6
3	J	1146	POP	P1-O-P2-O6
3	O	1146	POP	P1-O-P2-O6
3	R	1146	POP	P1-O-P2-O6
3	S	1146	POP	P1-O-P2-O6
3	T	1146	POP	P1-O-P2-O6
3	U	1146	POP	P1-O-P2-O6
3	V	1146	POP	P1-O-P2-O6
3	W	1146	POP	P1-O-P2-O6
3	Y	1146	POP	P1-O-P2-O6
3	b	1146	POP	P1-O-P2-O6
3	c	1146	POP	P1-O-P2-O6
3	d	1146	POP	P1-O-P2-O6
3	h	1146	POP	P1-O-P2-O6
3	j	1146	POP	P1-O-P2-O6
3	l	1146	POP	P1-O-P2-O6
3	1	1146	POP	P1-O-P2-O4
3	3	1146	POP	P1-O-P2-O4
3	9	1146	POP	P1-O-P2-O4
3	B	1146	POP	P1-O-P2-O4
3	G	1146	POP	P1-O-P2-O4
3	K	1146	POP	P1-O-P2-O4
3	V	1146	POP	P1-O-P2-O4
3	a	1146	POP	P1-O-P2-O4
3	c	1146	POP	P1-O-P2-O4
3	e	1146	POP	P1-O-P2-O4

There are no ring outliers.

33 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	b	1145	DUR	1	0
2	M	1145	DUR	1	0
2	8	1145	DUR	2	0
2	F	1145	DUR	2	0
2	A	1145	DUR	1	0
2	C	1145	DUR	2	0
2	7	1145	DUR	2	0
2	f	1145	DUR	1	0
2	R	1145	DUR	1	0
2	I	1145	DUR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	1145	DUR	2	0
2	2	1145	DUR	3	0
2	Y	1145	DUR	2	0
2	h	1145	DUR	2	0
2	m	1145	DUR	2	0
2	H	1145	DUR	2	0
2	j	1145	DUR	2	0
2	Q	1145	DUR	2	0
2	5	1145	DUR	1	0
2	4	1145	DUR	1	0
2	B	1145	DUR	2	0
2	N	1145	DUR	1	0
2	L	1145	DUR	1	0
2	g	1145	DUR	1	0
2	i	1145	DUR	2	0
2	d	1145	DUR	1	0
2	G	1145	DUR	2	0
2	U	1145	DUR	1	0
2	e	1145	DUR	1	0
2	O	1145	DUR	2	0
2	l	1145	DUR	1	0
2	P	1145	DUR	1	0
2	X	1145	DUR	2	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, 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	1	142/144 (98%)	-0.29	2 (1%) 73 73	14, 24, 44, 53	5 (3%)
1	2	142/144 (98%)	-0.42	0 100 100	12, 23, 39, 50	2 (1%)
1	3	142/144 (98%)	-0.47	0 100 100	11, 21, 36, 44	1 (0%)
1	4	142/144 (98%)	-0.44	0 100 100	12, 21, 35, 49	4 (2%)
1	5	142/144 (98%)	-0.19	3 (2%) 63 63	12, 26, 48, 56	3 (2%)
1	6	142/144 (98%)	-0.13	2 (1%) 73 73	14, 26, 46, 58	4 (2%)
1	7	142/144 (98%)	-0.21	1 (0%) 84 84	16, 27, 47, 60	0
1	8	142/144 (98%)	-0.44	1 (0%) 84 84	12, 21, 40, 53	1 (0%)
1	9	142/144 (98%)	-0.41	0 100 100	11, 22, 38, 53	3 (2%)
1	A	143/144 (99%)	-0.18	1 (0%) 84 84	13, 26, 44, 55	4 (2%)
1	B	142/144 (98%)	-0.27	0 100 100	13, 25, 43, 51	4 (2%)
1	C	142/144 (98%)	-0.26	1 (0%) 84 84	15, 25, 45, 57	4 (2%)
1	D	142/144 (98%)	-0.45	1 (0%) 84 84	11, 22, 38, 54	3 (2%)
1	E	142/144 (98%)	-0.44	0 100 100	12, 22, 37, 57	2 (1%)
1	F	143/144 (99%)	-0.44	1 (0%) 84 84	10, 21, 40, 48	3 (2%)
1	G	142/144 (98%)	-0.47	0 100 100	11, 20, 37, 50	4 (2%)
1	H	142/144 (98%)	-0.45	1 (0%) 84 84	11, 20, 38, 48	1 (0%)
1	I	142/144 (98%)	-0.50	0 100 100	12, 20, 35, 47	3 (2%)
1	J	142/144 (98%)	-0.38	0 100 100	13, 22, 42, 51	2 (1%)
1	K	142/144 (98%)	-0.34	0 100 100	13, 24, 40, 52	5 (3%)
1	L	142/144 (98%)	-0.42	0 100 100	14, 23, 39, 55	0
1	M	142/144 (98%)	-0.36	0 100 100	13, 23, 40, 48	2 (1%)
1	N	142/144 (98%)	-0.36	0 100 100	15, 25, 44, 52	1 (0%)
1	O	142/144 (98%)	-0.30	0 100 100	16, 24, 41, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	P	142/144 (98%)	-0.50	0 100 100	11, 20, 38, 48	3 (2%)
1	Q	143/144 (99%)	-0.41	0 100 100	13, 22, 40, 46	1 (0%)
1	R	142/144 (98%)	-0.45	0 100 100	11, 21, 40, 50	2 (1%)
1	S	142/144 (98%)	-0.40	0 100 100	13, 23, 39, 54	2 (1%)
1	T	142/144 (98%)	-0.35	0 100 100	12, 24, 41, 56	3 (2%)
1	U	142/144 (98%)	-0.42	0 100 100	13, 23, 42, 50	2 (1%)
1	V	142/144 (98%)	-0.39	0 100 100	10, 23, 41, 50	2 (1%)
1	W	142/144 (98%)	-0.41	0 100 100	11, 22, 41, 51	0
1	X	142/144 (98%)	-0.39	0 100 100	12, 21, 41, 50	3 (2%)
1	Y	142/144 (98%)	-0.36	0 100 100	12, 24, 44, 54	2 (1%)
1	Z	142/144 (98%)	-0.26	2 (1%) 73 73	13, 25, 43, 66	4 (2%)
1	a	143/144 (99%)	-0.51	0 100 100	13, 22, 36, 44	3 (2%)
1	b	143/144 (99%)	-0.31	0 100 100	12, 24, 45, 51	1 (0%)
1	c	142/144 (98%)	-0.31	0 100 100	13, 24, 42, 58	4 (2%)
1	d	142/144 (98%)	-0.32	1 (0%) 84 84	12, 25, 45, 60	1 (0%)
1	e	142/144 (98%)	-0.38	0 100 100	12, 23, 44, 53	1 (0%)
1	f	142/144 (98%)	-0.30	0 100 100	13, 24, 42, 49	1 (0%)
1	g	142/144 (98%)	-0.33	0 100 100	9, 23, 42, 57	3 (2%)
1	h	142/144 (98%)	-0.44	0 100 100	10, 21, 40, 48	1 (0%)
1	i	142/144 (98%)	-0.40	1 (0%) 84 84	10, 21, 39, 46	2 (1%)
1	j	143/144 (99%)	-0.35	0 100 100	13, 22, 43, 51	2 (1%)
1	k	142/144 (98%)	-0.32	0 100 100	15, 27, 45, 58	2 (1%)
1	l	142/144 (98%)	-0.14	0 100 100	14, 28, 50, 63	2 (1%)
1	m	142/144 (98%)	-0.16	1 (0%) 84 84	13, 28, 49, 57	1 (0%)
All	All	6822/6912 (98%)	-0.36	19 (0%) 90 89	9, 24, 43, 66	109 (1%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	99	LEU	3.5
1	A	99	LEU	3.4
1	i	99	LEU	3.2
1	5	99	LEU	3.1
1	H	99	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	99	LEU	2.8
1	1	99	LEU	2.7
1	C	99	LEU	2.5
1	Z	12	GLU	2.4
1	7	99	LEU	2.3
1	d	129	HIS	2.2
1	D	99	LEU	2.2
1	6	67	TYR	2.1
1	5	143	THR	2.1
1	m	99	LEU	2.0
1	5	129	HIS	2.0
1	6	133	GLU	2.0
1	8	99	LEU	2.0
1	1	35	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PO4	l	1148	5/5	0.87	0.32	40,46,51,61	0
5	PO4	e	1148	5/5	0.88	0.12	49,54,55,61	0
2	DUR	Y	1145	16/16	0.95	0.06	14,17,20,20	0
2	DUR	C	1145	16/16	0.95	0.05	16,18,22,22	0
2	DUR	J	1145	16/16	0.95	0.06	13,14,16,16	0
2	DUR	I	1145	16/16	0.96	0.05	10,13,14,15	0
2	DUR	3	1145	16/16	0.96	0.05	12,13,15,16	0
2	DUR	K	1145	16/16	0.96	0.05	14,16,18,18	0
2	DUR	V	1145	16/16	0.96	0.05	12,14,16,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DUR	B	1145	16/16	0.96	0.05	18,19,20,20	0
2	DUR	Z	1145	16/16	0.96	0.05	17,19,22,22	0
2	DUR	c	1145	16/16	0.96	0.05	16,17,19,21	0
2	DUR	e	1145	16/16	0.96	0.05	14,15,16,16	0
2	DUR	h	1145	16/16	0.96	0.05	11,13,14,14	0
2	DUR	i	1145	16/16	0.96	0.05	15,16,19,19	0
2	DUR	j	1145	16/16	0.96	0.05	14,16,17,20	0
2	DUR	l	1145	16/16	0.96	0.05	14,18,19,20	0
2	DUR	D	1145	16/16	0.96	0.05	13,14,17,20	0
2	DUR	N	1145	16/16	0.97	0.04	15,17,20,20	0
2	DUR	O	1145	16/16	0.97	0.05	16,18,21,21	0
2	DUR	Q	1145	16/16	0.97	0.04	14,15,17,20	0
2	DUR	R	1145	16/16	0.97	0.04	12,13,15,15	0
2	DUR	S	1145	16/16	0.97	0.04	12,15,17,17	0
2	DUR	T	1145	16/16	0.97	0.05	14,18,20,20	0
2	DUR	U	1145	16/16	0.97	0.04	15,16,17,18	0
2	DUR	A	1145	16/16	0.97	0.04	16,18,20,20	0
2	DUR	W	1145	16/16	0.97	0.05	14,15,17,17	0
2	DUR	X	1145	16/16	0.97	0.05	12,14,15,20	0
2	DUR	2	1145	16/16	0.97	0.04	12,14,17,18	0
2	DUR	4	1145	16/16	0.97	0.05	11,12,13,14	0
2	DUR	a	1145	16/16	0.97	0.04	15,16,17,17	0
2	DUR	b	1145	16/16	0.97	0.05	13,15,17,19	0
2	DUR	5	1145	16/16	0.97	0.04	17,20,22,22	0
2	DUR	E	1145	16/16	0.97	0.04	13,14,15,15	0
2	DUR	f	1145	16/16	0.97	0.04	15,16,19,22	0
2	DUR	g	1145	16/16	0.97	0.05	14,16,18,19	0
2	DUR	F	1145	16/16	0.97	0.04	12,14,15,16	0
2	DUR	H	1145	16/16	0.97	0.04	12,14,15,15	0
2	DUR	6	1145	16/16	0.97	0.05	19,21,23,23	0
2	DUR	k	1145	16/16	0.97	0.04	17,18,20,20	0
2	DUR	l	1145	16/16	0.97	0.05	17,20,23,23	0
2	DUR	m	1145	16/16	0.97	0.04	15,20,23,23	0
4	MG	d	1147	1/1	0.97	0.04	22,22,22,22	0
2	DUR	8	1145	16/16	0.97	0.04	12,13,14,15	0
2	DUR	9	1145	16/16	0.97	0.04	13,14,16,17	0
2	DUR	G	1145	16/16	0.98	0.04	11,13,14,14	0
2	DUR	P	1145	16/16	0.98	0.04	13,14,16,17	0
2	DUR	L	1145	16/16	0.98	0.04	14,15,18,19	0
3	POP	B	1146	9/9	0.98	0.04	16,18,20,23	0
3	POP	k	1146	9/9	0.98	0.04	19,23,24,25	0
4	MG	6	1147	1/1	0.98	0.04	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	E	1147	1/1	0.98	0.02	17,17,17,17	0
4	MG	M	1147	1/1	0.98	0.02	19,19,19,19	0
4	MG	O	1147	1/1	0.98	0.02	20,20,20,20	0
4	MG	S	1147	1/1	0.98	0.02	14,14,14,14	0
4	MG	T	1147	1/1	0.98	0.03	17,17,17,17	0
4	MG	a	1147	1/1	0.98	0.02	15,15,15,15	0
4	MG	b	1147	1/1	0.98	0.03	16,16,16,16	0
2	DUR	M	1145	16/16	0.98	0.04	14,17,18,19	0
4	MG	e	1147	1/1	0.98	0.02	18,18,18,18	0
4	MG	f	1147	1/1	0.98	0.02	17,17,17,17	0
4	MG	m	1147	1/1	0.98	0.05	17,17,17,17	0
2	DUR	7	1145	16/16	0.98	0.04	15,18,21,24	0
2	DUR	d	1145	16/16	0.98	0.04	14,15,17,18	0
3	POP	H	1146	9/9	0.99	0.03	14,15,16,17	0
3	POP	I	1146	9/9	0.99	0.04	11,13,15,17	0
3	POP	J	1146	9/9	0.99	0.03	15,18,19,20	0
3	POP	K	1146	9/9	0.99	0.03	13,15,18,21	0
3	POP	L	1146	9/9	0.99	0.03	16,17,19,21	0
3	POP	M	1146	9/9	0.99	0.03	13,19,20,20	0
3	POP	N	1146	9/9	0.99	0.03	16,18,19,20	0
3	POP	O	1146	9/9	0.99	0.03	16,17,22,23	0
3	POP	P	1146	9/9	0.99	0.02	14,15,17,17	0
3	POP	Q	1146	9/9	0.99	0.03	11,12,14,14	0
3	POP	R	1146	9/9	0.99	0.03	13,14,15,16	0
3	POP	S	1146	9/9	0.99	0.04	13,15,18,21	0
3	POP	T	1146	9/9	0.99	0.03	13,16,18,19	0
3	POP	U	1146	9/9	0.99	0.03	16,17,19,19	0
3	POP	V	1146	9/9	0.99	0.04	14,16,17,20	0
3	POP	W	1146	9/9	0.99	0.03	10,13,15,16	0
3	POP	X	1146	9/9	0.99	0.03	15,16,18,19	0
3	POP	Y	1146	9/9	0.99	0.02	15,17,18,19	0
3	POP	Z	1146	9/9	0.99	0.04	16,18,19,20	0
3	POP	a	1146	9/9	0.99	0.03	13,15,16,17	0
3	POP	b	1146	9/9	0.99	0.03	15,17,20,21	0
3	POP	c	1146	9/9	0.99	0.02	14,16,18,18	0
3	POP	d	1146	9/9	0.99	0.03	19,20,22,23	0
3	POP	e	1146	9/9	0.99	0.04	16,18,20,20	0
3	POP	f	1146	9/9	0.99	0.03	13,15,17,17	0
3	POP	g	1146	9/9	0.99	0.04	13,15,16,19	0
3	POP	h	1146	9/9	0.99	0.03	17,18,19,19	0
3	POP	j	1146	9/9	0.99	0.03	13,14,16,17	0
3	POP	2	1146	9/9	0.99	0.04	13,14,16,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	POP	l	1146	9/9	0.99	0.03	15,19,22,23	0
3	POP	m	1146	9/9	0.99	0.03	18,20,21,22	0
4	MG	1	1147	1/1	0.99	0.02	18,18,18,18	0
4	MG	2	1147	1/1	0.99	0.01	11,11,11,11	0
4	MG	3	1147	1/1	0.99	0.03	17,17,17,17	0
4	MG	4	1147	1/1	0.99	0.02	15,15,15,15	0
3	POP	3	1146	9/9	0.99	0.03	14,16,17,18	0
4	MG	7	1147	1/1	0.99	0.05	20,20,20,20	0
4	MG	8	1147	1/1	0.99	0.01	17,17,17,17	0
4	MG	9	1147	1/1	0.99	0.03	17,17,17,17	0
4	MG	B	1147	1/1	0.99	0.04	18,18,18,18	0
4	MG	C	1147	1/1	0.99	0.01	13,13,13,13	0
4	MG	D	1147	1/1	0.99	0.03	15,15,15,15	0
3	POP	4	1146	9/9	0.99	0.03	14,14,16,17	0
4	MG	F	1147	1/1	0.99	0.02	14,14,14,14	0
4	MG	G	1147	1/1	0.99	0.03	14,14,14,14	0
4	MG	H	1147	1/1	0.99	0.03	16,16,16,16	0
4	MG	I	1147	1/1	0.99	0.03	11,11,11,11	0
4	MG	J	1147	1/1	0.99	0.07	17,17,17,17	0
4	MG	K	1147	1/1	0.99	0.01	15,15,15,15	0
3	POP	5	1146	9/9	0.99	0.04	17,19,20,20	0
4	MG	N	1147	1/1	0.99	0.02	14,14,14,14	0
3	POP	6	1146	9/9	0.99	0.04	18,21,22,24	0
4	MG	P	1147	1/1	0.99	0.04	13,13,13,13	0
4	MG	Q	1147	1/1	0.99	0.01	10,10,10,10	0
4	MG	R	1147	1/1	0.99	0.04	12,12,12,12	0
3	POP	7	1146	9/9	0.99	0.05	18,20,22,23	0
3	POP	8	1146	9/9	0.99	0.02	14,16,17,17	0
4	MG	U	1147	1/1	0.99	0.03	15,15,15,15	0
4	MG	V	1147	1/1	0.99	0.02	14,14,14,14	0
4	MG	W	1147	1/1	0.99	0.02	12,12,12,12	0
4	MG	X	1147	1/1	0.99	0.02	16,16,16,16	0
4	MG	Y	1147	1/1	0.99	0.01	16,16,16,16	0
4	MG	Z	1147	1/1	0.99	0.02	21,21,21,21	0
3	POP	9	1146	9/9	0.99	0.03	14,14,16,16	0
3	POP	A	1146	9/9	0.99	0.03	18,19,21,25	0
4	MG	c	1147	1/1	0.99	0.02	15,15,15,15	0
3	POP	1	1146	9/9	0.99	0.03	18,19,21,24	0
3	POP	C	1146	9/9	0.99	0.04	17,18,22,22	0
3	POP	D	1146	9/9	0.99	0.03	11,15,17,17	0
4	MG	g	1147	1/1	0.99	0.05	16,16,16,16	0
4	MG	h	1147	1/1	0.99	0.02	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	j	1147	1/1	0.99	0.01	13,13,13,13	0
4	MG	k	1147	1/1	0.99	0.04	21,21,21,21	0
4	MG	l	1147	1/1	0.99	0.01	18,18,18,18	0
3	POP	E	1146	9/9	0.99	0.03	15,16,17,18	0
3	POP	F	1146	9/9	0.99	0.03	11,13,13,13	0
3	POP	G	1146	9/9	0.99	0.03	12,14,15,16	0
4	MG	L	1147	1/1	1.00	0.01	17,17,17,17	0
4	MG	5	1147	1/1	1.00	0.04	18,18,18,18	0
4	MG	A	1147	1/1	1.00	0.03	21,21,21,21	0
4	MG	i	1147	1/1	1.00	0.01	14,14,14,14	0
3	POP	i	1146	9/9	1.00	0.04	13,16,19,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.