



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 11:53 AM EDT

PDB ID : 1RXS / pdb_00001rxs
Title : E. coli uridine phosphorylase: 2'-deoxyuridine phosphate complex
Authors : Caradoc-Davies, T.T.; Cutfield, S.M.; Lamont, I.L.; Cutfield, J.F.
Deposited on : 2003-12-18
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

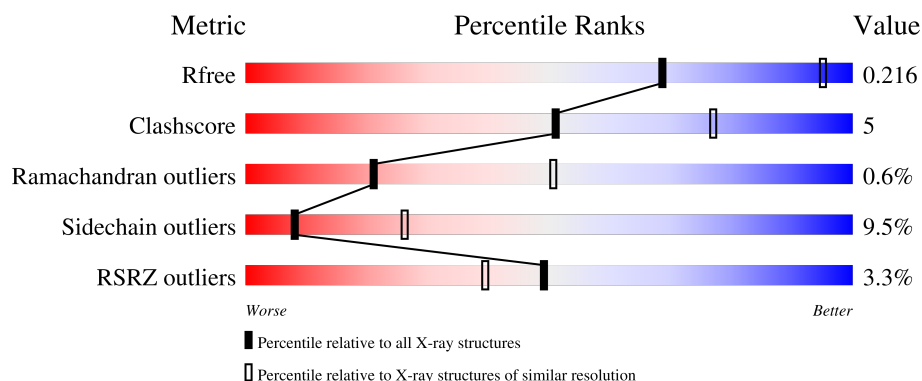
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	253	% 80% 16% ..
1	B	253	% 82% 12% ..
1	C	253	4% 79% 16% ..
1	D	253	4% 80% 15% ..
1	E	253	82% 14% ..

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Mol	Chain	Length	Quality of chain
1	F	253	
1	G	253	
1	H	253	
1	I	253	
1	J	253	
1	K	253	
1	L	253	
1	M	253	
1	N	253	
1	O	253	
1	P	253	
1	Q	253	
1	R	253	
1	a	253	
1	b	253	
1	c	253	
1	d	253	
1	e	253	
1	h	253	
1	i	253	
1	j	253	
1	k	253	
1	l	253	
1	m	253	
1	o	253	

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
4	PO4	P	3121	-	-	X	-
5	DUR	B	2012	X	-	-	-
5	DUR	C	2022	X	-	-	-
5	DUR	D	2032	X	-	-	-
5	DUR	E	2042	X	-	-	-
5	DUR	F	2052	X	-	-	-
5	DUR	G	3052	X	-	-	-
5	DUR	H	2062	X	-	-	-
5	DUR	I	3072	X	-	-	-
5	DUR	J	2082	X	-	-	-
5	DUR	K	2092	X	-	-	-
5	DUR	M	3112	X	-	-	-
5	DUR	N	2102	X	-	-	-
5	DUR	O	2112	X	-	-	-
5	DUR	P	3122	X	-	-	-
5	DUR	Q	2122	X	-	-	-
5	DUR	R	2132	X	-	-	-
5	DUR	a	3012	X	-	-	-
5	DUR	b	3022	X	-	-	-
5	DUR	c	3032	X	-	-	-
5	DUR	e	3042	X	-	-	-
5	DUR	h	3062	X	-	-	-
5	DUR	i	2072	X	-	-	-
5	DUR	j	3082	X	-	-	-
5	DUR	k	3092	X	-	-	-
5	DUR	l	3102	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 57608 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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	a	242	Total	C	N	O	S	0	0	0
			1817	1141	318	348	10			
1	B	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	b	242	Total	C	N	O	S	0	0	0
			1817	1141	318	348	10			
1	C	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	c	242	Total	C	N	O	S	0	0	0
			1817	1141	318	348	10			
1	D	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	d	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	E	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	e	242	Total	C	N	O	S	0	0	0
			1817	1141	318	348	10			
1	F	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	R	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	G	242	Total	C	N	O	S	0	0	0
			1817	1141	318	348	10			
1	P	242	Total	C	N	O	S	0	0	0
			1817	1141	318	348	10			
1	H	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	h	242	Total	C	N	O	S	0	0	0
			1817	1141	318	348	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	242	Total	C	N	O	S	0	0	0
			1817	1141	318	348	10			
1	i	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	J	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	j	242	Total	C	N	O	S	0	0	0
			1817	1141	318	348	10			
1	K	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	k	242	Total	C	N	O	S	0	0	0
			1817	1141	318	348	10			
1	L	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	l	242	Total	C	N	O	S	0	0	0
			1817	1141	318	348	10			
1	M	242	Total	C	N	O	S	0	0	0
			1817	1141	318	348	10			
1	m	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	N	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	Q	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	O	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	o	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

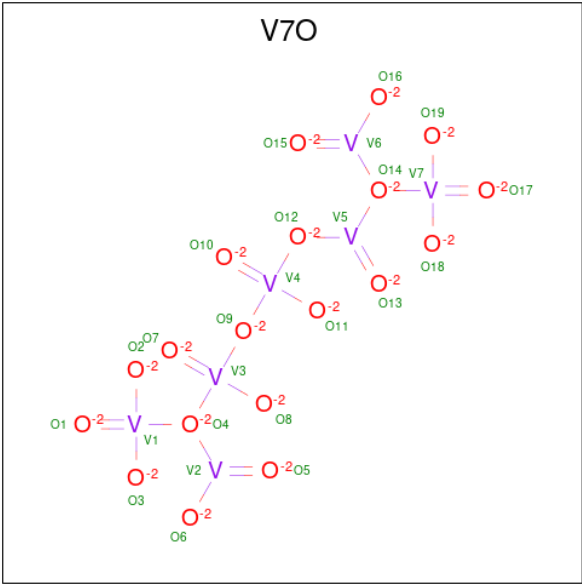
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		
2	E	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	R	1	Total	K	0	0
			1	1		
2	G	1	Total	K	0	0
			1	1		
2	h	1	Total	K	0	0
			1	1		
2	i	1	Total	K	0	0
			1	1		
2	J	1	Total	K	0	0
			1	1		
2	K	1	Total	K	0	0
			1	1		
2	L	1	Total	K	0	0
			1	1		
2	M	1	Total	K	0	0
			1	1		
2	N	1	Total	K	0	0
			1	1		
2	o	1	Total	K	0	0
			1	1		

- Molecule 3 is META VANADATE (CCD ID: V7O) (formula: O₁₉V₇).



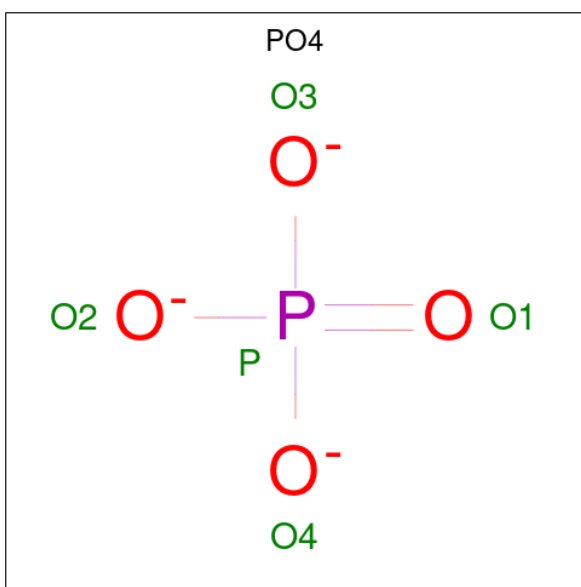
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	V	0	0
			11	8	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	V	0	0
			11	8	3		
3	b	1	Total	O	V	0	0
			11	8	3		
3	c	1	Total	O	V	0	0
			11	8	3		
3	D	1	Total	O	V	0	0
			11	8	3		
3	D	1	Total	O	V	0	0
			11	8	3		
3	e	1	Total	O	V	0	0
			11	8	3		
3	R	1	Total	O	V	0	0
			11	8	3		
3	H	1	Total	O	V	0	0
			11	8	3		
3	h	1	Total	O	V	0	0
			11	8	3		
3	I	1	Total	O	V	0	0
			11	8	3		
3	i	1	Total	O	V	0	0
			11	8	3		
3	J	1	Total	O	V	0	0
			11	8	3		
3	j	1	Total	O	V	0	0
			11	8	3		
3	k	1	Total	O	V	0	0
			11	8	3		
3	L	1	Total	O	V	0	0
			11	8	3		
3	M	1	Total	O	V	0	0
			11	8	3		
3	M	1	Total	O	V	0	0
			11	8	3		
3	Q	1	Total	O	V	0	0
			11	8	3		
3	o	1	Total	O	V	0	0
			11	8	3		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



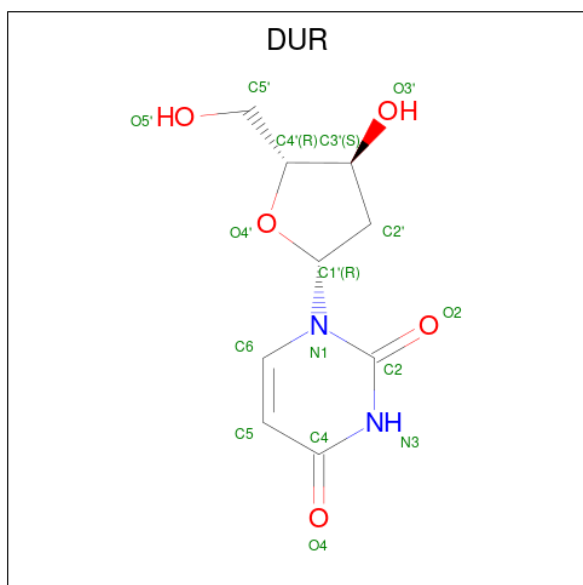
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	a	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	b	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	c	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	e	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	R	1	Total	O	P	0	0
			5	4	1		
4	G	1	Total	O	P	0	0
			5	4	1		
4	P	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		
4	h	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	I	1	Total	O	P	0	0
			5	4	1		
4	i	1	Total	O	P	0	0
			5	4	1		
4	J	1	Total	O	P	0	0
			5	4	1		
4	j	1	Total	O	P	0	0
			5	4	1		
4	K	1	Total	O	P	0	0
			5	4	1		
4	k	1	Total	O	P	0	0
			5	4	1		
4	l	1	Total	O	P	0	0
			5	4	1		
4	M	1	Total	O	P	0	0
			5	4	1		
4	N	1	Total	O	P	0	0
			5	4	1		
4	Q	1	Total	O	P	0	0
			5	4	1		
4	O	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 2'-DEOXYURIDINE (CCD ID: DUR) (formula: $C_9H_{12}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	a	1	Total	C	N	O	0	0
			16	9	2	5		
5	B	1	Total	C	N	O	0	0
			16	9	2	5		
5	b	1	Total	C	N	O	0	0
			16	9	2	5		
5	C	1	Total	C	N	O	0	0
			16	9	2	5		
5	c	1	Total	C	N	O	0	0
			16	9	2	5		
5	D	1	Total	C	N	O	0	0
			16	9	2	5		
5	E	1	Total	C	N	O	0	0
			16	9	2	5		
5	e	1	Total	C	N	O	0	0
			16	9	2	5		
5	F	1	Total	C	N	O	0	0
			16	9	2	5		
5	R	1	Total	C	N	O	0	0
			16	9	2	5		
5	G	1	Total	C	N	O	0	0
			16	9	2	5		
5	P	1	Total	C	N	O	0	0
			16	9	2	5		
5	H	1	Total	C	N	O	0	0
			16	9	2	5		
5	h	1	Total	C	N	O	0	0
			16	9	2	5		
5	I	1	Total	C	N	O	0	0
			16	9	2	5		
5	i	1	Total	C	N	O	0	0
			16	9	2	5		
5	J	1	Total	C	N	O	0	0
			16	9	2	5		
5	j	1	Total	C	N	O	0	0
			16	9	2	5		
5	K	1	Total	C	N	O	0	0
			16	9	2	5		
5	k	1	Total	C	N	O	0	0
			16	9	2	5		
5	l	1	Total	C	N	O	0	0
			16	9	2	5		
5	M	1	Total	C	N	O	0	0
			16	9	2	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	N	1	Total	C	N	O	0	0
			16	9	2	5		
5	Q	1	Total	C	N	O	0	0
			16	9	2	5		
5	O	1	Total	C	N	O	0	0
			16	9	2	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	54	Total	O	0	0
			54	54		
6	a	52	Total	O	0	0
			52	52		
6	B	55	Total	O	0	0
			55	55		
6	b	48	Total	O	0	0
			48	48		
6	C	52	Total	O	0	0
			52	52		
6	c	54	Total	O	0	0
			54	54		
6	D	52	Total	O	0	0
			52	52		
6	d	56	Total	O	0	0
			56	56		
6	E	51	Total	O	0	0
			51	51		
6	e	49	Total	O	0	0
			49	49		
6	F	59	Total	O	0	0
			59	59		
6	R	52	Total	O	0	0
			52	52		
6	G	46	Total	O	0	0
			46	46		
6	P	51	Total	O	0	0
			51	51		
6	H	51	Total	O	0	0
			51	51		
6	h	55	Total	O	0	0
			55	55		

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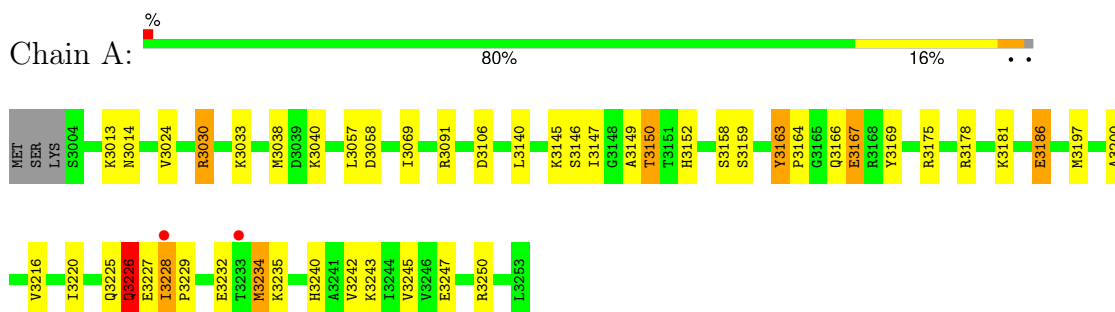
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	51	Total 51	O 51	0	0
6	i	56	Total 56	O 56	0	0
6	J	52	Total 52	O 52	0	0
6	j	51	Total 51	O 51	0	0
6	K	50	Total 50	O 50	0	0
6	k	53	Total 53	O 53	0	0
6	L	58	Total 58	O 58	0	0
6	l	51	Total 51	O 51	0	0
6	M	48	Total 48	O 48	0	0
6	m	53	Total 53	O 53	0	0
6	N	58	Total 58	O 58	0	0
6	Q	50	Total 50	O 50	0	0
6	O	56	Total 56	O 56	0	0
6	o	57	Total 57	O 57	0	0

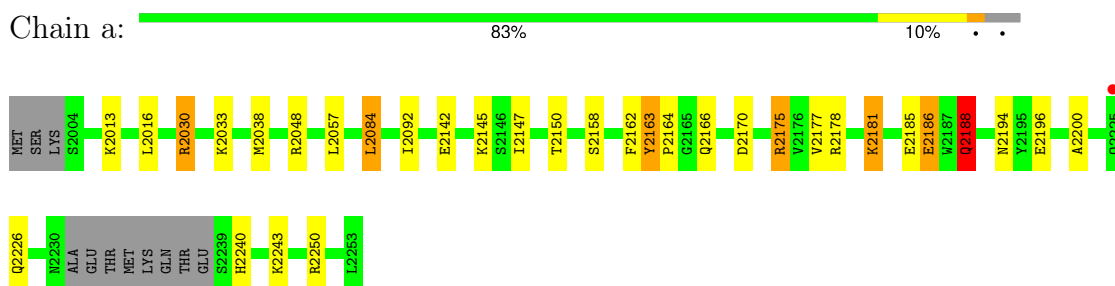
3 Residue-property plots

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

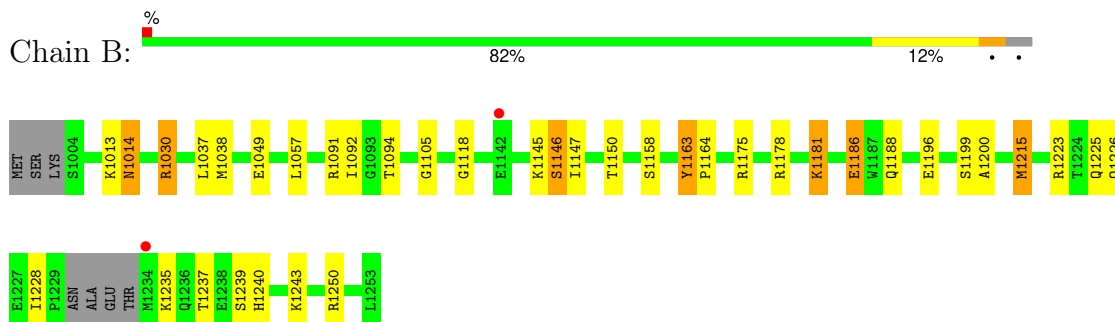
- Molecule 1: Uridine phosphorylase



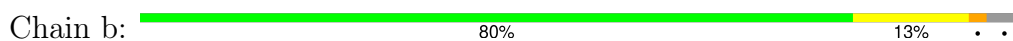
- Molecule 1: Uridine phosphorylase

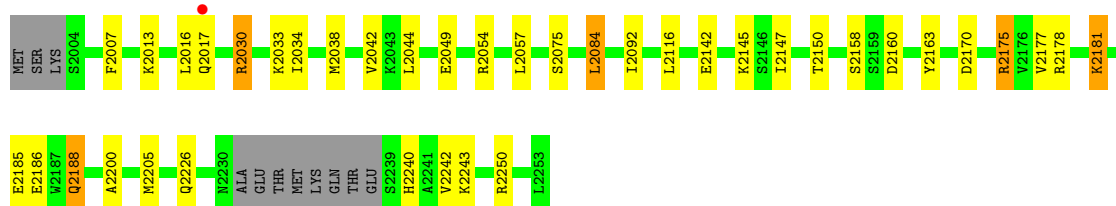


- Molecule 1: Uridine phosphorylase

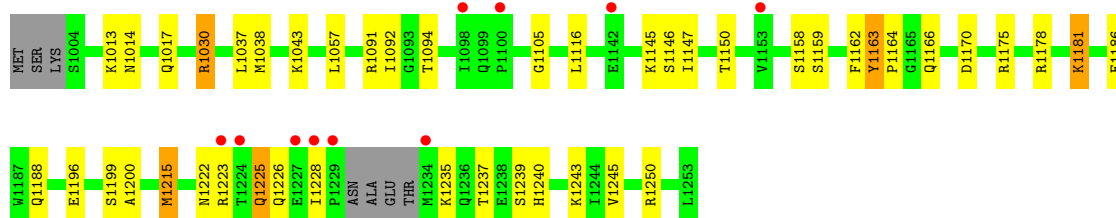
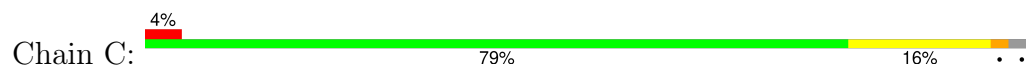


- Molecule 1: Uridine phosphorylase

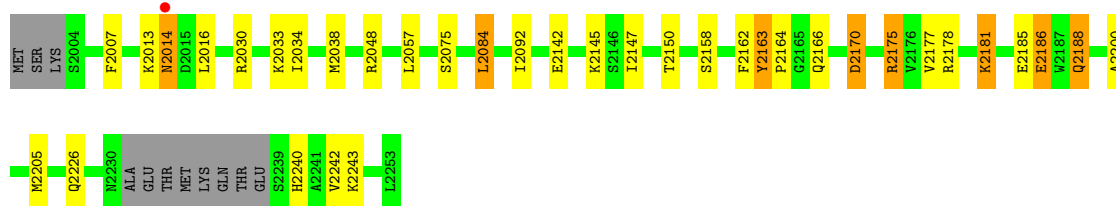
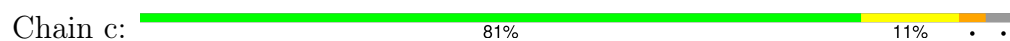




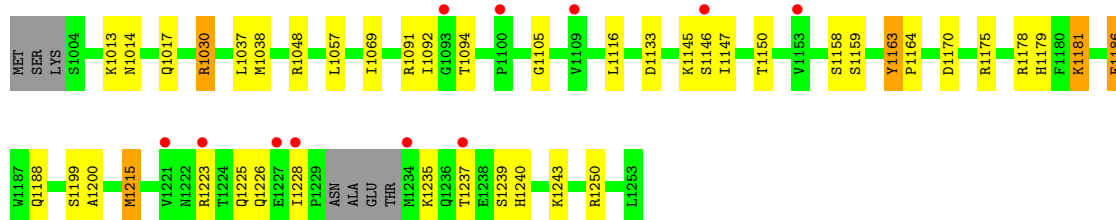
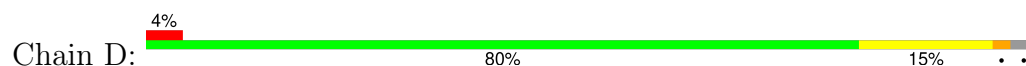
- Molecule 1: Uridine phosphorylase



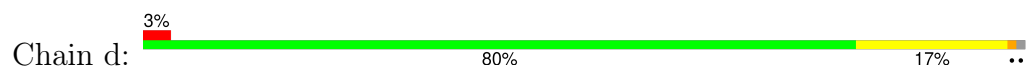
- Molecule 1: Uridine phosphorylase

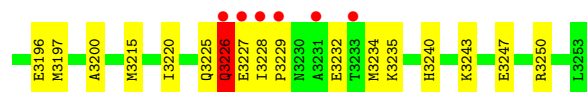


- Molecule 1: Uridine phosphorylase



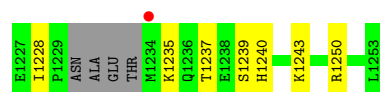
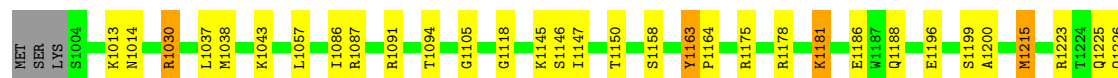
- Molecule 1: Uridine phosphorylase





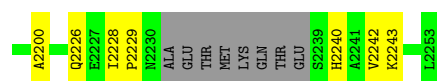
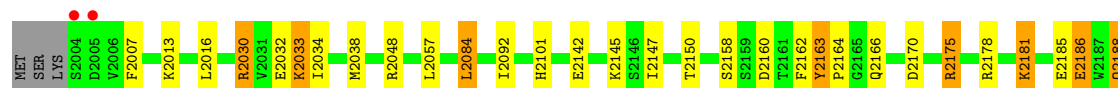
- Molecule 1: Uridine phosphorylase

Chain E: 82% 14%



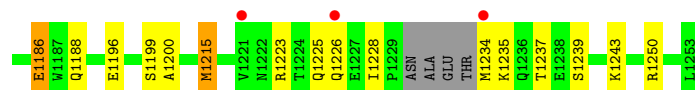
- Molecule 1: Uridine phosphorylase

Chain e: 81% 11%



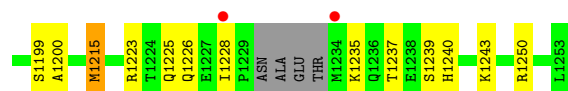
- Molecule 1: Uridine phosphorylase

Chain F: 79% 17%



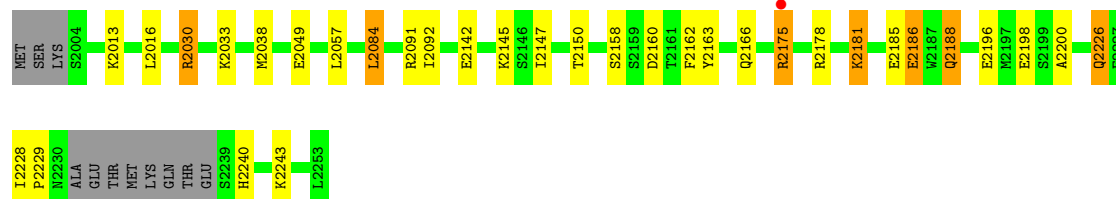
- Molecule 1: Uridine phosphorylase

Chain R: 80% 15%



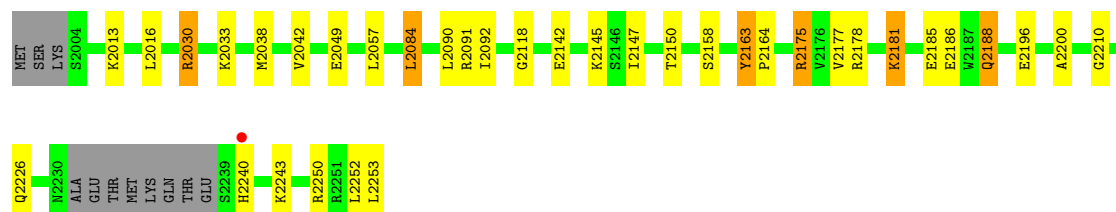
- Molecule 1: Uridine phosphorylase

Chain G:  83% 10% . .



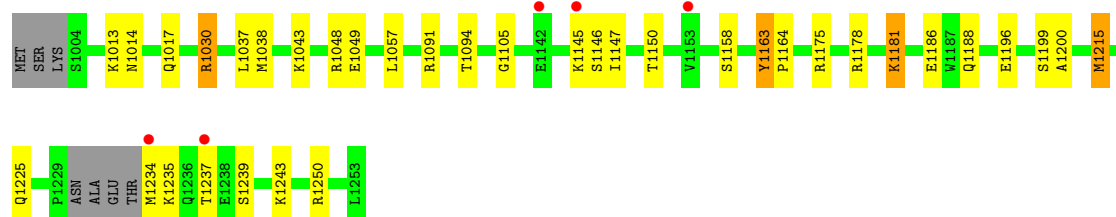
• Molecule 1: Uridine phosphorylase

Chain P:  81% 12% . .



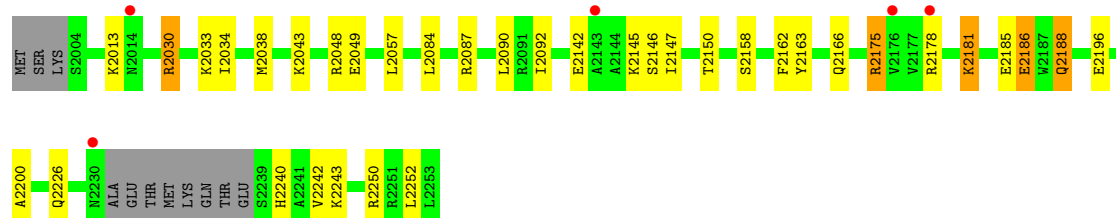
• Molecule 1: Uridine phosphorylase

Chain H:  83% 13% . .



• Molecule 1: Uridine phosphorylase

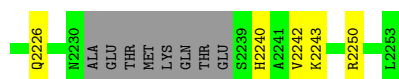
Chain h:  81% 12% . .



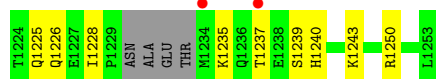
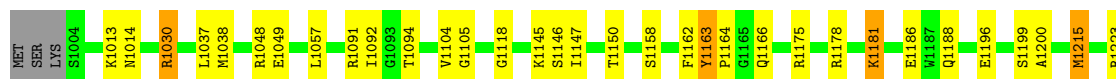
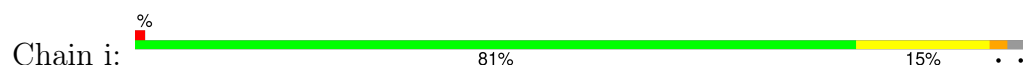
• Molecule 1: Uridine phosphorylase

Chain I:  82% 12% . .

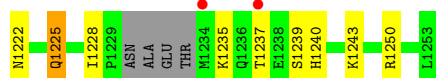
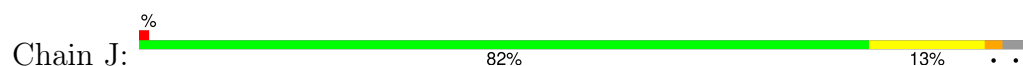




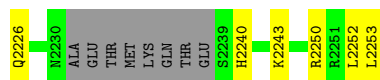
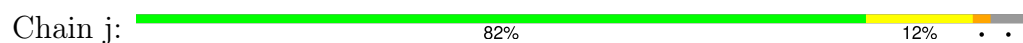
- Molecule 1: Uridine phosphorylase



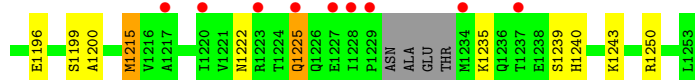
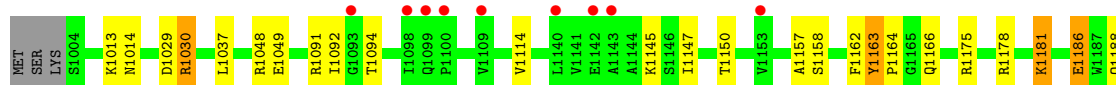
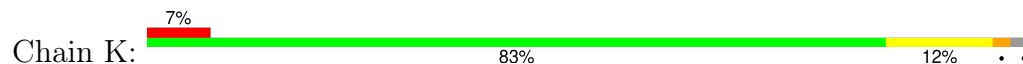
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase

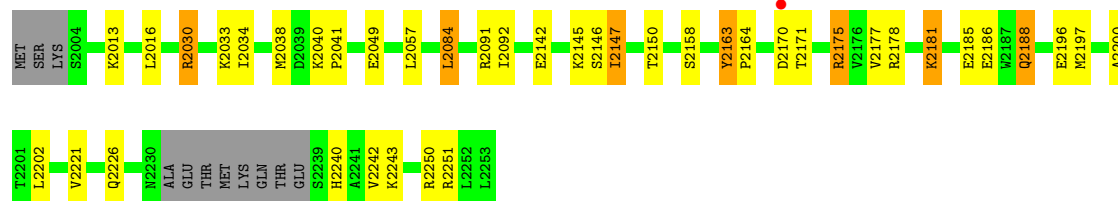


- Molecule 1: Uridine phosphorylase



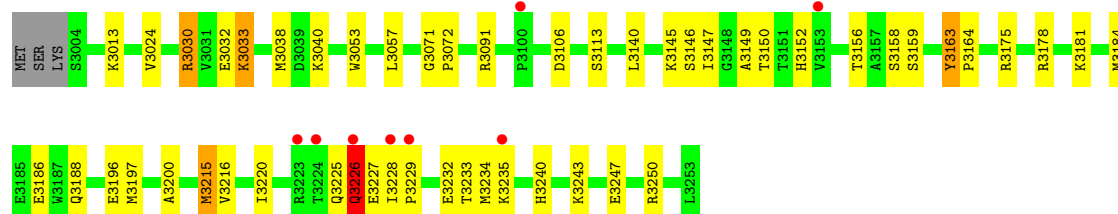
- Molecule 1: Uridine phosphorylase

Chain k:  79% 13% • •



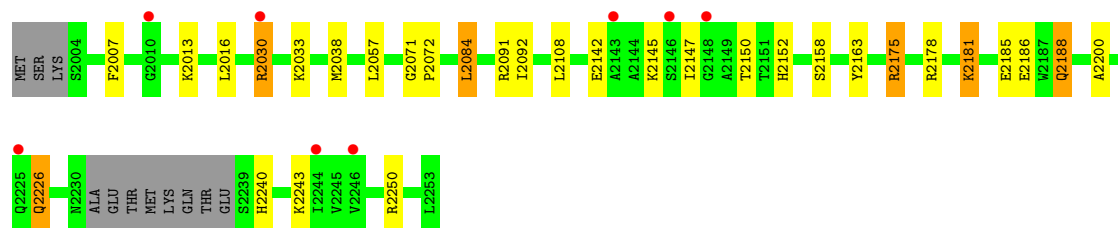
• Molecule 1: Uridine phosphorylase

Chain L:  79% 18% • •



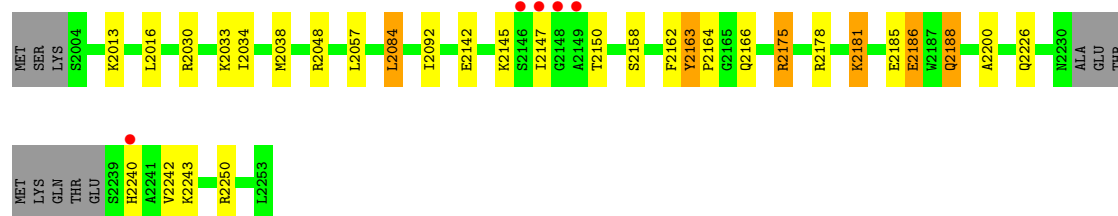
• Molecule 1: Uridine phosphorylase

Chain l:  83% 10% • •



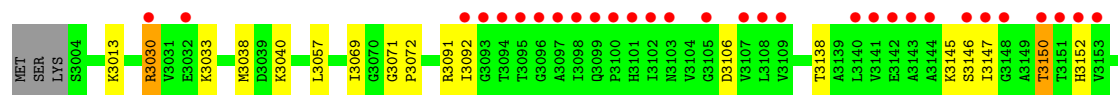
• Molecule 1: Uridine phosphorylase

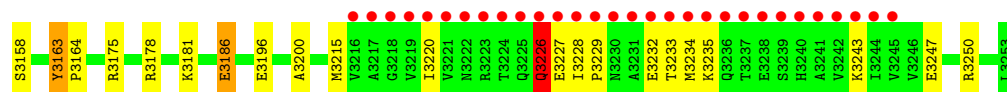
Chain M:  83% 10% • •



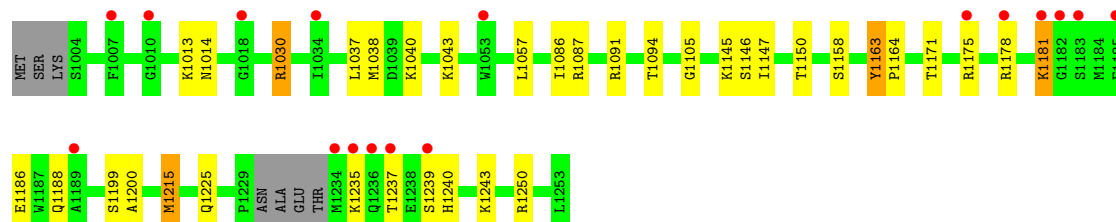
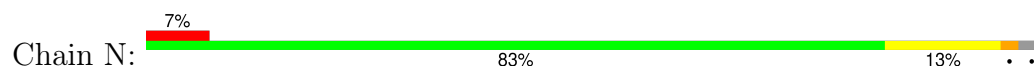
• Molecule 1: Uridine phosphorylase

Chain m:  83% 14% • •

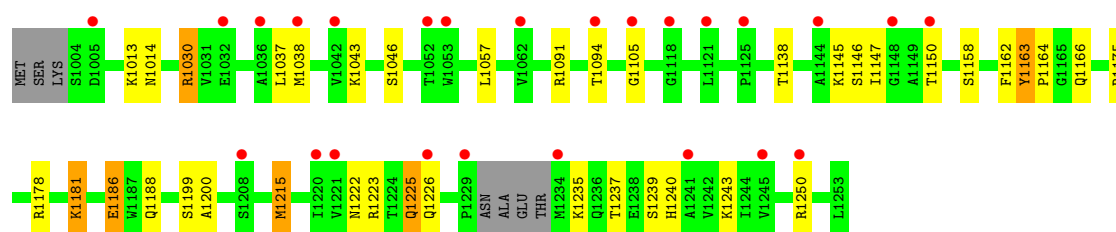
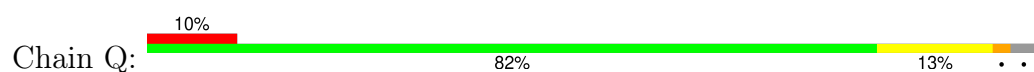




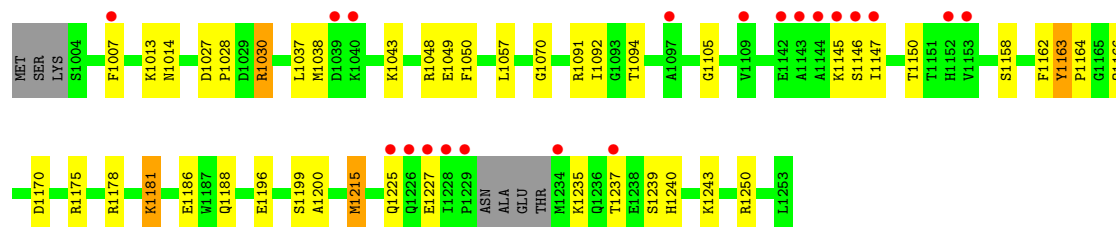
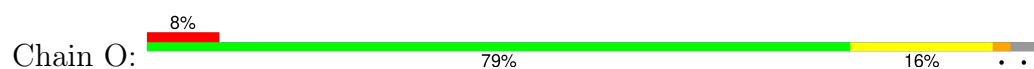
• Molecule 1: Uridine phosphorylase



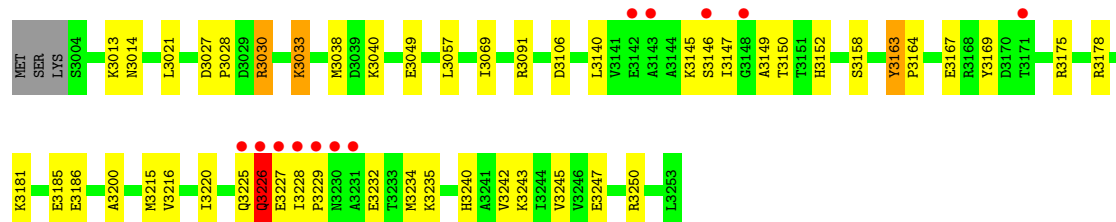
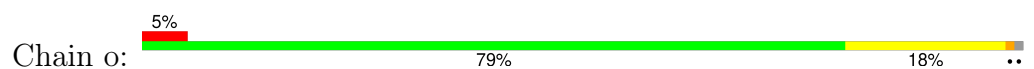
• Molecule 1: Uridine phosphorylase



• Molecule 1: Uridine phosphorylase



• Molecule 1: Uridine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	160.96Å 98.21Å 242.73Å 90.00° 109.09° 90.00°	Depositor
Resolution (Å)	26.75 – 2.80 26.75 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (26.75-2.80) 99.0 (26.75-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.176 , 0.218 0.177 , 0.216	Depositor DCC
R_{free} test set	8725 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	57608	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, V7O, DUR, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.92	3/1912 (0.2%)	1.04	2/2595 (0.1%)
1	B	0.84	0/1882	0.95	1/2552 (0.0%)
1	C	0.84	0/1882	0.94	0/2552
1	D	0.76	0/1882	0.92	0/2552
1	E	0.75	0/1882	0.93	0/2552
1	F	0.83	1/1882 (0.1%)	0.93	1/2552 (0.0%)
1	G	0.78	0/1848	1.00	0/2508
1	H	0.80	1/1882 (0.1%)	0.91	0/2552
1	I	0.71	0/1848	0.95	0/2508
1	J	0.72	0/1882	0.92	0/2552
1	K	0.76	0/1882	0.92	0/2552
1	L	0.76	1/1912 (0.1%)	0.97	0/2595
1	M	0.69	0/1848	0.96	0/2508
1	N	0.65	0/1882	0.91	0/2552
1	O	0.68	0/1882	0.91	1/2552 (0.0%)
1	P	0.88	0/1848	0.99	0/2508
1	Q	0.64	0/1882	0.88	0/2552
1	R	0.81	0/1882	0.94	0/2552
1	a	0.88	0/1848	1.03	3/2508 (0.1%)
1	b	0.86	0/1848	1.01	1/2508 (0.0%)
1	c	0.82	0/1848	1.00	2/2508 (0.1%)
1	d	0.79	1/1912 (0.1%)	0.97	0/2595
1	e	0.76	0/1848	0.96	0/2508
1	h	0.70	0/1848	0.96	0/2508
1	i	0.74	0/1882	0.94	0/2552
1	j	0.85	0/1848	1.00	1/2508 (0.0%)
1	k	0.81	1/1848 (0.1%)	0.98	1/2508 (0.0%)
1	l	0.67	0/1848	0.92	0/2508
1	m	0.72	1/1912 (0.1%)	0.93	0/2595
1	o	0.69	0/1912	0.95	0/2595
All	All	0.77	9/56202 (0.0%)	0.95	13/76247 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	o	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3234	MET	SD-CE	6.53	1.95	1.79
1	H	1234	MET	SD-CE	5.86	1.94	1.79
1	A	3150	THR	CA-CB	5.82	1.61	1.53
1	L	3215	MET	CG-SD	-5.56	1.66	1.80
1	m	3150	THR	CA-CB	5.41	1.60	1.53
1	d	3193	MET	SD-CE	5.22	1.92	1.79
1	k	2197	MET	SD-CE	5.08	1.92	1.79
1	F	1234	MET	SD-CE	5.06	1.92	1.79
1	A	3228	ILE	CA-CB	5.02	1.60	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	1070	GLY	N-CA-C	6.75	119.85	112.29
1	a	2194	ASN	N-CA-C	5.86	117.04	108.14
1	B	1014	ASN	N-CA-C	5.74	117.54	111.28
1	b	2170	ASP	CB-CA-C	-5.38	103.34	112.00
1	A	3167	GLU	N-CA-C	5.33	118.74	111.39
1	a	2170	ASP	CB-CA-C	-5.25	103.55	112.00
1	a	2188	GLN	N-CA-CB	5.25	117.84	110.12
1	c	2170	ASP	CB-CA-C	-5.24	103.44	111.83
1	c	2014	ASN	N-CA-C	5.22	116.97	111.28
1	F	1070	GLY	N-CA-C	5.18	118.09	112.29
1	A	3166	GLN	N-CA-C	-5.13	106.26	112.88
1	k	2170	ASP	CB-CA-C	-5.08	103.70	111.83
1	j	2170	ASP	CB-CA-C	-5.04	103.23	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	o	3226	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1880	0	1884	28	0
1	B	1851	0	1860	18	0
1	C	1851	0	1860	20	0
1	D	1851	0	1860	25	0
1	E	1851	0	1860	14	0
1	F	1851	0	1860	29	0
1	G	1817	0	1822	16	1
1	H	1851	0	1860	14	0
1	I	1817	0	1823	17	0
1	J	1851	0	1859	20	0
1	K	1851	0	1859	19	0
1	L	1880	0	1884	30	0
1	M	1817	0	1822	15	0
1	N	1851	0	1860	27	0
1	O	1851	0	1860	25	0
1	P	1817	0	1822	18	1
1	Q	1851	0	1860	19	0
1	R	1851	0	1860	21	1
1	a	1817	0	1823	14	0
1	b	1817	0	1822	27	0
1	c	1817	0	1822	18	1
1	d	1880	0	1884	39	1
1	e	1817	0	1822	31	5
1	h	1817	0	1822	21	0
1	i	1851	0	1859	19	2
1	j	1817	0	1823	17	0
1	k	1817	0	1822	29	1
1	l	1817	0	1823	14	0
1	m	1880	0	1885	23	2
1	o	1880	0	1884	31	5
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
2	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	R	1	0	0	0	0
2	h	1	0	0	0	0
2	i	1	0	0	0	0
2	o	1	0	0	0	0
3	A	11	0	0	1	0
3	B	11	0	0	1	0
3	D	22	0	0	4	0
3	H	11	0	0	2	0
3	I	11	0	0	3	0
3	J	11	0	0	5	0
3	L	11	0	0	1	0
3	M	22	0	0	4	0
3	Q	11	0	0	1	0
3	R	11	0	0	2	0
3	b	11	0	0	2	0
3	c	11	0	0	2	0
3	e	11	0	0	2	0
3	h	11	0	0	3	0
3	i	11	0	0	2	0
3	j	11	0	0	0	0
3	k	11	0	0	0	0
3	o	11	0	0	1	0
4	B	5	0	0	0	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	1	0
4	H	5	0	0	1	0
4	I	5	0	0	0	0
4	J	5	0	0	0	0
4	K	5	0	0	0	0
4	M	5	0	0	0	0
4	N	5	0	0	0	0
4	O	5	0	0	1	0
4	P	5	0	0	2	0
4	Q	5	0	0	0	0
4	R	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	a	5	0	0	0	0
4	b	5	0	0	0	0
4	c	5	0	0	0	0
4	e	5	0	0	0	0
4	h	5	0	0	0	0
4	i	5	0	0	0	0
4	j	5	0	0	0	0
4	k	5	0	0	1	0
4	l	5	0	0	1	0
5	B	16	0	11	0	0
5	C	16	0	11	1	0
5	D	16	0	11	0	0
5	E	16	0	11	0	0
5	F	16	0	11	0	0
5	G	16	0	11	1	0
5	H	16	0	11	0	0
5	I	16	0	11	0	0
5	J	16	0	11	0	0
5	K	16	0	11	0	0
5	M	16	0	11	0	0
5	N	16	0	11	0	0
5	O	16	0	11	0	0
5	P	16	0	11	1	0
5	Q	16	0	11	0	0
5	R	16	0	11	0	0
5	a	16	0	11	0	0
5	b	16	0	11	0	0
5	c	16	0	11	0	0
5	e	16	0	11	0	0
5	h	16	0	11	0	0
5	i	16	0	11	0	0
5	j	16	0	11	0	0
5	k	16	0	11	0	0
5	l	16	0	11	0	0
6	A	54	0	0	2	0
6	B	55	0	0	0	1
6	C	52	0	0	3	0
6	D	52	0	0	4	0
6	E	51	0	0	1	0
6	F	59	0	0	2	0
6	G	46	0	0	4	0
6	H	51	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	51	0	0	5	0
6	J	52	0	0	3	0
6	K	50	0	0	3	0
6	L	58	0	0	2	0
6	M	48	0	0	3	0
6	N	58	0	0	1	0
6	O	56	0	0	5	0
6	P	51	0	0	4	0
6	Q	50	0	0	6	0
6	R	52	0	0	3	0
6	a	52	0	0	4	0
6	b	48	0	0	4	0
6	c	54	0	0	5	0
6	d	56	0	0	4	0
6	e	49	0	0	5	0
6	h	55	0	0	7	0
6	i	56	0	0	3	0
6	j	51	0	0	3	0
6	k	53	0	0	6	0
6	l	51	0	0	3	0
6	m	53	0	0	2	0
6	o	57	0	0	3	0
All	All	57608	0	55741	586	11

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 (586) 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:b:2042:VAL:HG11	1:d:3250:ARG:NH2	1.18	1.50
1:G:2181:LYS:HD2	6:G:684:HOH:O	1.26	1.33
1:J:1178:ARG:HD3	3:J:5042:V7O:O15	1.29	1.26
1:m:3226:GLN:CG	1:m:3227:GLU:H	1.55	1.19
1:d:3226:GLN:CG	1:d:3227:GLU:H	1.57	1.18
1:d:3226:GLN:HG2	1:d:3227:GLU:H	1.06	1.17
1:b:2017:GLN:NE2	1:d:3058:ASP:HA	1.59	1.17
1:b:2042:VAL:CG1	1:d:3250:ARG:HH22	1.58	1.15
1:e:2032:GLU:HG2	1:N:1040:LYS:HE2	1.29	1.13
3:H:5031:V7O:O17	3:I:5032:V7O:O13	1.67	1.11
1:b:2042:VAL:CG1	1:d:3250:ARG:NH2	2.11	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:3226:GLN:CG	1:o:3227:GLU:H	1.57	1.11
1:L:3226:GLN:CG	1:L:3227:GLU:H	1.64	1.09
1:m:3226:GLN:HG2	1:m:3227:GLU:H	1.12	1.08
1:L:3226:GLN:HG2	1:L:3227:GLU:H	1.20	1.06
1:A:3226:GLN:CG	1:A:3227:GLU:H	1.67	1.04
1:F:1043:LYS:HD3	1:k:2146:SER:O	1.56	1.04
1:A:3226:GLN:HG2	1:A:3227:GLU:H	1.23	1.04
1:h:2043:LYS:HE3	6:h:823:HOH:O	1.57	1.03
1:k:2181:LYS:HD2	6:k:1151:HOH:O	1.65	0.96
3:J:5042:V7O:O18	1:L:3178:ARG:HD3	1.66	0.95
1:c:2175:ARG:NE	6:c:300:HOH:O	2.00	0.94
1:G:2175:ARG:NE	6:G:670:HOH:O	1.95	0.94
1:d:3226:GLN:HG2	1:d:3227:GLU:N	1.81	0.94
1:o:3226:GLN:HG2	1:o:3227:GLU:H	1.31	0.93
1:R:1181:LYS:HD2	6:R:631:HOH:O	1.69	0.92
1:C:1199:SER:HB3	1:C:1215:MET:HE2	1.52	0.92
1:k:2030:ARG:HB2	6:k:1133:HOH:O	1.70	0.91
1:m:3226:GLN:CG	1:m:3227:GLU:N	2.26	0.90
1:d:3226:GLN:CG	1:d:3227:GLU:N	2.29	0.88
3:D:5022:V7O:O18	1:F:1178:ARG:HD3	1.73	0.87
1:P:2181:LYS:HD2	6:P:735:HOH:O	1.74	0.87
1:K:1199:SER:HB3	1:K:1215:MET:HE2	1.56	0.87
1:h:2181:LYS:HD2	6:h:839:HOH:O	1.75	0.87
1:J:1178:ARG:CD	3:J:5042:V7O:O15	2.21	0.85
1:J:1199:SER:HB3	1:J:1215:MET:HE2	1.59	0.84
1:R:1199:SER:HB3	1:R:1215:MET:HE2	1.56	0.84
1:H:1199:SER:HB3	1:H:1215:MET:HE2	1.59	0.84
1:L:3226:GLN:CG	1:L:3227:GLU:N	2.37	0.84
1:o:3226:GLN:CG	1:o:3227:GLU:N	2.32	0.83
1:A:3226:GLN:CG	1:A:3227:GLU:N	2.38	0.83
1:m:3226:GLN:HG2	1:m:3227:GLU:N	1.87	0.83
1:O:1199:SER:HB3	1:O:1215:MET:HE2	1.61	0.82
1:e:2032:GLU:HG2	1:N:1040:LYS:CE	2.08	0.82
1:Q:1199:SER:HB3	1:Q:1215:MET:HE2	1.61	0.82
1:o:3226:GLN:HG3	1:o:3227:GLU:H	1.41	0.82
1:b:2042:VAL:HG11	1:d:3250:ARG:HH21	1.41	0.81
1:e:2032:GLU:CG	1:N:1040:LYS:HE2	2.09	0.80
1:F:1199:SER:HB3	1:F:1215:MET:HE2	1.64	0.80
1:e:2032:GLU:HB3	1:N:1040:LYS:HZ3	1.47	0.79
1:m:3226:GLN:HG3	1:m:3227:GLU:H	1.47	0.79
1:a:2030:ARG:HD3	6:a:88:HOH:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:2181:LYS:HD2	6:c:314:HOH:O	1.84	0.78
1:A:3226:GLN:HG2	1:A:3227:GLU:N	1.98	0.78
1:L:3226:GLN:HG2	1:L:3227:GLU:N	1.97	0.77
1:D:1178:ARG:NH2	1:E:1181:LYS:O	2.16	0.76
1:B:1199:SER:HB3	1:B:1215:MET:HE2	1.67	0.76
1:I:2175:ARG:NE	6:I:876:HOH:O	2.18	0.76
1:D:1199:SER:HB3	1:D:1215:MET:HE2	1.67	0.76
1:K:1181:LYS:HD2	6:K:4154:HOH:O	1.86	0.76
3:h:5033:V7O:O15	3:i:5034:V7O:O18	2.03	0.75
1:b:2017:GLN:NE2	1:d:3058:ASP:CA	2.47	0.75
1:a:2178:ARG:NH2	1:c:2181:LYS:O	2.21	0.74
1:I:2178:ARG:NH1	3:I:5032:V7O:O15	2.20	0.74
1:k:2038:MET:HG2	1:k:2057:LEU:HD13	1.69	0.74
1:j:2030:ARG:HD3	6:j:1029:HOH:O	1.88	0.73
1:M:2178:ARG:NH2	1:N:1181:LYS:O	2.20	0.73
1:D:1048:ARG:NH1	6:D:330:HOH:O	2.15	0.73
1:i:1199:SER:HB3	1:i:1215:MET:HE2	1.70	0.72
1:l:2158:SER:HB3	1:l:2200:ALA:HB2	1.71	0.72
1:e:2175:ARG:NE	6:e:513:HOH:O	2.19	0.72
1:P:2178:ARG:NH2	1:i:1181:LYS:O	2.24	0.71
1:N:1199:SER:HB3	1:N:1215:MET:HE2	1.72	0.71
1:d:3181:LYS:O	1:e:2178:ARG:NH2	2.23	0.71
1:K:1178:ARG:NH2	1:L:3181:LYS:O	2.23	0.70
1:G:2178:ARG:NH2	1:H:1181:LYS:O	2.24	0.70
1:J:1178:ARG:NH2	1:K:1181:LYS:O	2.25	0.70
1:b:2030:ARG:HD3	6:b:192:HOH:O	1.91	0.70
1:C:1181:LYS:HD2	6:C:261:HOH:O	1.90	0.69
1:e:2186:GLU:HG3	6:R:633:HOH:O	1.92	0.69
1:F:1043:LYS:CD	1:k:2146:SER:O	2.36	0.69
1:L:3226:GLN:HG3	1:L:3227:GLU:H	1.58	0.68
3:b:5013:V7O:O12	3:c:5014:V7O:O18	2.11	0.68
1:L:3038:MET:HG2	1:L:3057:LEU:HD13	1.75	0.68
1:E:1199:SER:HB3	1:E:1215:MET:HE2	1.75	0.67
1:k:2181:LYS:O	1:l:2178:ARG:NH2	2.26	0.67
1:h:2038:MET:HG2	1:h:2057:LEU:HD13	1.77	0.67
1:J:1181:LYS:O	1:L:3178:ARG:NH2	2.27	0.67
1:A:3226:GLN:HG3	1:A:3227:GLU:H	1.59	0.67
3:J:5042:V7O:O17	3:L:5041:V7O:O17	2.12	0.67
1:A:3178:ARG:NH2	1:B:1181:LYS:O	2.27	0.66
1:o:3226:GLN:HG2	1:o:3227:GLU:N	2.03	0.66
1:D:1178:ARG:HD3	3:D:5022:V7O:O15	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1181:LYS:O	1:F:1178:ARG:NH2	2.28	0.65
1:l:2181:LYS:HD2	6:l:1258:HOH:O	1.94	0.65
1:Q:1158:SER:HB3	1:Q:1200:ALA:HB2	1.76	0.65
1:h:2175:ARG:NE	6:h:825:HOH:O	2.23	0.65
3:e:5023:V7O:O15	3:R:5024:V7O:O18	2.13	0.65
1:P:2158:SER:HB3	1:P:2200:ALA:HB2	1.79	0.65
3:b:5013:V7O:O15	3:c:5014:V7O:O18	2.14	0.65
1:F:1158:SER:HB3	1:F:1200:ALA:HB2	1.79	0.65
1:I:2038:MET:HG2	1:I:2057:LEU:HD13	1.78	0.65
1:e:2038:MET:HG2	1:e:2057:LEU:HD13	1.78	0.64
1:G:2038:MET:HG2	1:G:2057:LEU:HD13	1.78	0.64
3:M:5052:V7O:O18	1:O:1178:ARG:HD3	1.97	0.64
1:B:1158:SER:HB3	1:B:1200:ALA:HB2	1.80	0.64
1:P:2038:MET:HG2	1:P:2057:LEU:HD13	1.79	0.64
1:j:2158:SER:HB3	1:j:2200:ALA:HB2	1.79	0.64
1:K:1158:SER:HB3	1:K:1200:ALA:HB2	1.80	0.64
1:o:3158:SER:HB3	1:o:3200:ALA:HB2	1.78	0.64
1:a:2181:LYS:HD2	6:a:106:HOH:O	1.97	0.64
1:m:3178:ARG:NH2	1:o:3181:LYS:O	2.29	0.64
1:M:2048:ARG:NH1	6:M:1287:HOH:O	2.26	0.64
1:H:1048:ARG:HD2	6:H:773:HOH:O	1.98	0.63
1:P:2030:ARG:HD3	6:P:717:HOH:O	1.97	0.63
1:e:2158:SER:HB3	1:e:2200:ALA:HB2	1.80	0.63
1:o:3226:GLN:HB3	1:o:3227:GLU:HG3	1.78	0.63
1:j:2038:MET:HG2	1:j:2057:LEU:HD13	1.80	0.63
1:P:2181:LYS:O	1:h:2178:ARG:NH2	2.31	0.63
1:b:2017:GLN:HE21	1:d:3058:ASP:HA	1.60	0.63
3:J:5042:V7O:O18	1:L:3178:ARG:CD	2.44	0.63
1:N:1178:ARG:NH2	1:O:1181:LYS:O	2.32	0.63
1:M:2181:LYS:HD2	6:M:1309:HOH:O	1.99	0.62
1:j:2178:ARG:NH2	1:l:2181:LYS:O	2.32	0.62
1:b:2175:ARG:NE	6:b:196:HOH:O	2.31	0.62
1:N:1181:LYS:HD2	6:N:1416:HOH:O	1.99	0.62
6:a:93:HOH:O	1:c:2186:GLU:HG3	1.98	0.62
1:l:2038:MET:HG2	1:l:2057:LEU:HD13	1.81	0.62
1:h:2158:SER:HB3	1:h:2200:ALA:HB2	1.82	0.61
1:B:1178:ARG:NH2	1:C:1181:LYS:O	2.34	0.61
1:O:1170:ASP:HB3	6:O:1489:HOH:O	2.00	0.61
1:c:2158:SER:HB3	1:c:2200:ALA:HB2	1.82	0.61
1:d:3226:GLN:HG3	1:d:3227:GLU:H	1.57	0.61
1:d:3178:ARG:NH2	1:R:1181:LYS:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1158:SER:HB3	1:E:1200:ALA:HB2	1.83	0.60
1:A:3181:LYS:O	1:C:1178:ARG:NH2	2.35	0.60
1:G:2181:LYS:O	1:I:2178:ARG:NH2	2.35	0.60
1:I:2158:SER:HB3	1:I:2200:ALA:HB2	1.84	0.60
1:l:2175:ARG:NE	6:l:1244:HOH:O	2.29	0.60
1:a:2158:SER:HB3	1:a:2200:ALA:HB2	1.83	0.60
1:b:2181:LYS:HD2	6:b:210:HOH:O	2.00	0.60
1:d:3186:GLU:HG3	6:e:514:HOH:O	2.01	0.60
1:j:2181:LYS:HD2	6:j:1047:HOH:O	2.00	0.60
1:m:3038:MET:HG2	1:m:3057:LEU:HD13	1.83	0.60
1:M:2181:LYS:O	1:O:1178:ARG:NH2	2.35	0.60
1:G:2186:GLU:HG3	6:I:877:HOH:O	2.02	0.60
1:Q:1046:SER:N	6:Q:1454:HOH:O	2.30	0.59
1:L:3163:TYR:HB2	1:L:3164:PRO:HD3	1.85	0.59
1:M:2186:GLU:HG3	6:O:1524:HOH:O	2.00	0.59
1:O:1158:SER:HB3	1:O:1200:ALA:HB2	1.82	0.59
1:C:1158:SER:HB3	1:C:1200:ALA:HB2	1.85	0.59
1:N:1158:SER:HB3	1:N:1200:ALA:HB2	1.85	0.59
1:M:2158:SER:HB3	1:M:2200:ALA:HB2	1.85	0.59
3:h:5033:V7O:O12	3:i:5034:V7O:O18	2.21	0.58
1:b:2017:GLN:NE2	1:d:3058:ASP:OD1	2.36	0.58
1:F:1053:TRP:CZ2	1:k:2146:SER:HA	2.38	0.58
1:C:1199:SER:CB	1:C:1215:MET:HE2	2.32	0.58
1:R:1042:VAL:HG13	1:k:2041:PRO:HD2	1.84	0.58
1:J:1186:GLU:HG3	6:L:1207:HOH:O	2.03	0.58
3:D:5021:V7O:O16	3:D:5022:V7O:O13	2.22	0.58
1:O:1105:GLY:HA2	1:O:1237:THR:HG23	1.85	0.58
1:A:3158:SER:HB3	1:A:3200:ALA:HB2	1.85	0.58
1:A:3181:LYS:HE2	6:A:54:HOH:O	2.02	0.58
1:m:3158:SER:HB3	1:m:3200:ALA:HB2	1.86	0.58
1:o:3038:MET:HG2	1:o:3057:LEU:HD13	1.86	0.58
1:D:1158:SER:HB3	1:D:1200:ALA:HB2	1.86	0.58
1:F:1228:ILE:HD12	1:R:1007:PHE:HB2	1.86	0.58
3:Q:5053:V7O:O15	3:o:5054:V7O:O18	2.21	0.57
1:H:1158:SER:HB3	1:H:1200:ALA:HB2	1.85	0.57
3:M:5051:V7O:O16	3:M:5052:V7O:O13	2.21	0.57
6:d:423:HOH:O	1:R:1186:GLU:HG3	2.05	0.57
1:m:3226:GLN:HG3	1:m:3227:GLU:N	2.10	0.56
1:k:2158:SER:HB3	1:k:2200:ALA:HB2	1.87	0.56
1:R:1199:SER:CB	1:R:1215:MET:HE2	2.32	0.56
1:F:1043:LYS:HE2	1:k:2147:ILE:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:3163:TYR:HB2	1:m:3164:PRO:HD3	1.88	0.55
1:G:2158:SER:HB3	1:G:2200:ALA:HB2	1.88	0.55
1:K:1049:GLU:HB3	1:k:2049:GLU:HB3	1.88	0.55
6:A:55:HOH:O	1:B:1186:GLU:HG3	2.06	0.55
1:a:2038:MET:HG2	1:a:2057:LEU:HD13	1.87	0.55
1:L:3247:GLU:O	1:L:3250:ARG:HB2	2.07	0.55
1:b:2158:SER:HB3	1:b:2200:ALA:HB2	1.88	0.55
1:Q:1181:LYS:O	1:o:3178:ARG:NH2	2.40	0.55
1:O:1227:GLU:OE2	6:O:1489:HOH:O	2.18	0.55
1:A:3058:ASP:OD2	1:A:3250:ARG:HD2	2.07	0.55
6:E:476:HOH:O	1:F:1186:GLU:HG3	2.07	0.55
1:e:2033:LYS:HD2	1:N:1040:LYS:HG2	1.88	0.55
1:J:1158:SER:HB3	1:J:1200:ALA:HB2	1.88	0.55
1:m:3106:ASP:OD1	1:m:3152:HIS:HE1	1.90	0.55
1:m:3181:LYS:O	1:Q:1178:ARG:NH2	2.40	0.55
1:A:3220:ILE:HB	1:A:3234:MET:HG2	1.87	0.55
1:J:1105:GLY:HA2	1:J:1237:THR:HG23	1.88	0.55
1:a:2186:GLU:HG3	6:b:197:HOH:O	2.06	0.54
1:E:1105:GLY:HA2	1:E:1237:THR:HG23	1.88	0.54
1:c:2038:MET:HG2	1:c:2057:LEU:HD13	1.90	0.54
1:A:3186:GLU:HG3	6:C:263:HOH:O	2.07	0.54
1:D:1105:GLY:HA2	1:D:1237:THR:HG23	1.90	0.54
1:a:2181:LYS:O	1:b:2178:ARG:NH2	2.40	0.54
6:L:1188:HOH:O	1:l:2007:PHE:HZ	1.91	0.54
1:H:1038:MET:HG2	1:H:1057:LEU:HD13	1.89	0.54
1:b:2038:MET:HG2	1:b:2057:LEU:HD13	1.89	0.54
1:e:2033:LYS:HD2	1:N:1040:LYS:HE3	1.89	0.54
1:m:3186:GLU:HG3	6:Q:1471:HOH:O	2.07	0.54
1:m:3220:ILE:HB	1:m:3234:MET:HG2	1.89	0.54
1:j:2181:LYS:O	1:k:2178:ARG:NH2	2.41	0.53
1:K:1030:ARG:HH21	1:K:1094:THR:HG23	1.73	0.53
1:h:2146:SER:HA	1:L:3053:TRP:CZ2	2.43	0.53
3:M:5051:V7O:O17	3:M:5052:V7O:O13	2.26	0.53
1:O:1163:TYR:HB2	1:O:1164:PRO:CD	2.39	0.53
1:P:2210:GLY:N	6:P:708:HOH:O	2.41	0.53
1:R:1091:ARG:HG2	1:R:1215:MET:SD	2.48	0.53
1:B:1146:SER:O	1:m:3250:ARG:NH2	2.42	0.53
1:R:1158:SER:HB3	1:R:1200:ALA:HB2	1.90	0.53
1:H:1178:ARG:NH2	1:I:2181:LYS:O	2.42	0.53
1:I:2185:GLU:HA	1:I:2188:GLN:HG3	1.91	0.53
1:A:3038:MET:HG2	1:A:3057:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1105:GLY:HA2	1:F:1237:THR:HG23	1.91	0.53
1:Q:1091:ARG:HG2	1:Q:1215:MET:SD	2.49	0.53
1:F:1007:PHE:HB2	1:R:1228:ILE:HD12	1.91	0.53
1:M:2038:MET:HG2	1:M:2057:LEU:HD13	1.89	0.53
1:M:2175:ARG:NE	6:M:1295:HOH:O	2.40	0.53
1:Q:1186:GLU:HG3	6:Q:1580:HOH:O	2.09	0.53
3:A:5011:V7O:O16	3:B:5012:V7O:O13	2.27	0.53
1:d:3220:ILE:HB	1:d:3234:MET:HG2	1.90	0.53
1:O:1038:MET:HG2	1:O:1057:LEU:HD13	1.90	0.53
1:o:3163:TYR:HB2	1:o:3164:PRO:HD3	1.91	0.53
6:J:5084:HOH:O	1:K:1186:GLU:HG3	2.07	0.53
1:l:2185:GLU:HA	1:l:2188:GLN:HG3	1.91	0.53
1:o:3247:GLU:O	1:o:3250:ARG:HB2	2.09	0.53
1:A:3140:LEU:HD22	1:A:3216:VAL:HB	1.91	0.52
1:d:3149:ALA:HB2	1:d:3240:HIS:CE1	2.44	0.52
1:K:1163:TYR:HB2	1:K:1164:PRO:CD	2.39	0.52
1:o:3106:ASP:OD1	1:o:3152:HIS:HE1	1.92	0.52
1:o:3185:GLU:HB2	6:o:1536:HOH:O	2.08	0.52
1:N:1030:ARG:HH21	1:N:1094:THR:HG23	1.75	0.52
1:i:1105:GLY:HA2	1:i:1237:THR:HG23	1.91	0.52
1:L:3220:ILE:HB	1:L:3234:MET:HG2	1.90	0.52
1:N:1038:MET:HG2	1:N:1057:LEU:HD13	1.92	0.52
1:F:1030:ARG:HH21	1:F:1094:THR:HG23	1.76	0.52
1:O:1050:PHE:O	6:O:1510:HOH:O	2.18	0.52
1:e:2033:LYS:HD2	1:N:1040:LYS:CE	2.40	0.51
1:N:1105:GLY:HA2	1:N:1237:THR:HG23	1.91	0.51
1:Q:1030:ARG:HH21	1:Q:1094:THR:HG23	1.75	0.51
1:C:1170:ASP:HB3	6:C:228:HOH:O	2.10	0.51
1:d:3158:SER:HB3	1:d:3200:ALA:HB2	1.92	0.51
1:D:1170:ASP:HB3	6:D:332:HOH:O	2.10	0.51
1:e:2032:GLU:CB	1:N:1040:LYS:HZ3	2.19	0.51
1:I:2030:ARG:HD3	6:I:872:HOH:O	2.11	0.51
1:L:3149:ALA:HB2	1:L:3240:HIS:CE1	2.45	0.51
1:b:2181:LYS:O	1:c:2178:ARG:NH2	2.44	0.51
1:Q:1181:LYS:HD2	6:Q:1469:HOH:O	2.09	0.51
1:a:2185:GLU:HA	1:a:2188:GLN:HG3	1.92	0.51
1:d:3038:MET:HG2	1:d:3057:LEU:HD13	1.93	0.51
1:J:1030:ARG:HH21	1:J:1094:THR:HG23	1.76	0.51
1:R:1091:ARG:HB3	1:R:1215:MET:HG2	1.92	0.51
1:o:3220:ILE:HB	1:o:3234:MET:HG2	1.91	0.51
1:b:2016:LEU:HD22	1:b:2084:LEU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1030:ARG:HH21	1:R:1094:THR:HG23	1.75	0.51
1:i:1158:SER:HB3	1:i:1200:ALA:HB2	1.92	0.51
4:P:3121:PO4:O4	5:P:3122:DUR:H2'2	2.11	0.51
1:B:1105:GLY:HA2	1:B:1237:THR:HG23	1.93	0.50
1:C:1163:TYR:HB2	1:C:1164:PRO:CD	2.41	0.50
1:F:1199:SER:CB	1:F:1215:MET:HE2	2.37	0.50
1:M:2162:PHE:HA	1:M:2166:GLN:NE2	2.26	0.50
1:Q:1038:MET:HG2	1:Q:1057:LEU:HD13	1.94	0.50
1:a:2162:PHE:HA	1:a:2166:GLN:NE2	2.26	0.50
1:P:2175:ARG:NE	6:P:721:HOH:O	2.32	0.50
1:L:3158:SER:HB3	1:L:3200:ALA:HB2	1.93	0.50
1:Q:1199:SER:CB	1:Q:1215:MET:HE2	2.38	0.50
1:d:3094:THR:OG1	6:d:413:HOH:O	2.00	0.50
1:H:1030:ARG:HH21	1:H:1094:THR:HG23	1.76	0.50
1:i:1030:ARG:HH21	1:i:1094:THR:HG23	1.75	0.50
1:G:2091:ARG:NH2	1:G:2198:GLU:OE1	2.44	0.50
1:c:2185:GLU:HA	1:c:2188:GLN:HG3	1.94	0.50
1:O:1030:ARG:HH21	1:O:1094:THR:HG23	1.76	0.50
1:o:3225:GLN:NE2	6:o:1567:HOH:O	2.43	0.50
1:D:1186:GLU:HG3	6:F:580:HOH:O	2.11	0.49
1:J:1152:HIS:HA	6:J:5066:HOH:O	2.11	0.49
1:D:1163:TYR:HB2	1:D:1164:PRO:CD	2.41	0.49
1:l:2030:ARG:O	1:l:2030:ARG:HG3	2.12	0.49
1:P:2185:GLU:HA	1:P:2188:GLN:HG3	1.94	0.49
1:i:1048:ARG:NH1	6:i:906:HOH:O	2.38	0.49
1:K:1199:SER:CB	1:K:1215:MET:HE2	2.35	0.49
1:m:3138:THR:HG23	6:m:1335:HOH:O	2.12	0.49
1:Q:1163:TYR:HB2	1:Q:1164:PRO:CD	2.43	0.49
1:i:1163:TYR:HB2	1:i:1164:PRO:CD	2.42	0.49
1:C:1223:ARG:HA	1:C:1226:GLN:O	2.12	0.49
1:F:1038:MET:HG2	1:F:1057:LEU:HD13	1.93	0.49
1:L:3106:ASP:OD1	1:L:3152:HIS:HE1	1.96	0.49
1:R:1038:MET:HG2	1:R:1057:LEU:HD13	1.95	0.49
3:M:5051:V7O:O17	3:M:5052:V7O:O17	2.30	0.49
1:A:3106:ASP:OD1	1:A:3152:HIS:HE1	1.95	0.49
1:c:2170:ASP:HB2	6:c:297:HOH:O	2.13	0.49
1:d:3247:GLU:O	1:d:3250:ARG:HB2	2.13	0.49
4:C:2021:PO4:O4	5:C:2022:DUR:H2'2	2.13	0.49
1:N:1163:TYR:HB2	1:N:1164:PRO:CD	2.42	0.49
1:B:1163:TYR:HB2	1:B:1164:PRO:CD	2.43	0.48
1:i:1091:ARG:HG2	1:i:1215:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1091:ARG:HG2	1:N:1215:MET:SD	2.52	0.48
1:O:1007:PHE:HE1	6:o:1561:HOH:O	1.95	0.48
1:d:3163:TYR:HB2	1:d:3164:PRO:HD3	1.95	0.48
3:e:5023:V7O:O12	3:R:5024:V7O:O13	2.31	0.48
1:h:2030:ARG:HD3	6:h:821:HOH:O	2.12	0.48
1:j:2016:LEU:HD22	1:j:2084:LEU:HB3	1.95	0.48
1:j:2175:ARG:NE	6:j:1033:HOH:O	2.44	0.48
1:j:2185:GLU:HA	1:j:2188:GLN:HG3	1.95	0.48
1:b:2042:VAL:HG11	1:d:3250:ARG:HH22	0.69	0.48
1:b:2185:GLU:HA	1:b:2188:GLN:HG3	1.95	0.48
1:c:2175:ARG:CD	6:c:300:HOH:O	2.57	0.48
1:d:3106:ASP:OD1	1:d:3152:HIS:HE1	1.96	0.48
6:d:527:HOH:O	1:e:2181:LYS:HD2	2.13	0.48
1:h:2178:ARG:HG2	3:h:5033:V7O:O17	2.13	0.48
1:A:3247:GLU:O	1:A:3250:ARG:HB2	2.13	0.48
1:e:2185:GLU:HA	1:e:2188:GLN:HG3	1.95	0.48
1:L:3163:TYR:HB2	1:L:3164:PRO:CD	2.43	0.48
1:k:2163:TYR:HB2	1:k:2164:PRO:CD	2.44	0.48
1:k:2221:VAL:HG23	6:k:1119:HOH:O	2.12	0.48
1:C:1091:ARG:HB3	1:C:1215:MET:HG2	1.96	0.48
1:c:2048:ARG:NH1	6:c:292:HOH:O	2.41	0.48
1:D:1069:ILE:HD11	1:d:3048:ARG:HD3	1.95	0.48
1:e:2170:ASP:HB2	6:e:510:HOH:O	2.12	0.48
1:E:1091:ARG:HG2	1:E:1215:MET:SD	2.54	0.48
1:F:1032:GLU:CD	1:k:2251:ARG:HH22	2.21	0.48
1:I:2181:LYS:HD2	6:I:890:HOH:O	2.14	0.48
1:M:2185:GLU:HA	1:M:2188:GLN:HG3	1.94	0.48
1:Q:1138:THR:HG21	6:Q:1429:HOH:O	2.13	0.48
1:B:1030:ARG:HH21	1:B:1094:THR:HG23	1.78	0.47
1:H:1199:SER:CB	1:H:1215:MET:HE2	2.37	0.47
1:e:2033:LYS:HB3	6:e:508:HOH:O	2.13	0.47
1:l:2071:GLY:N	1:l:2072:PRO:CD	2.77	0.47
1:O:1048:ARG:HD3	1:o:3069:ILE:HD11	1.96	0.47
1:a:2175:ARG:NE	6:a:92:HOH:O	2.46	0.47
1:H:1049:GLU:HB3	1:h:2049:GLU:HB3	1.97	0.47
1:O:1199:SER:CB	1:O:1215:MET:HE2	2.38	0.47
1:A:3069:ILE:HD11	1:a:2048:ARG:HD3	1.95	0.47
1:F:1043:LYS:HE2	1:k:2147:ILE:C	2.39	0.47
1:k:2016:LEU:HD22	1:k:2084:LEU:HB3	1.96	0.47
1:K:1048:ARG:HD2	6:K:4142:HOH:O	2.15	0.47
1:B:1199:SER:CB	1:B:1215:MET:HE2	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1105:GLY:HA2	1:C:1237:THR:HG23	1.97	0.47
1:d:3163:TYR:HB2	1:d:3164:PRO:CD	2.44	0.47
1:Q:1105:GLY:HA2	1:Q:1237:THR:HG23	1.97	0.47
1:b:2116:LEU:HB2	1:b:2158:SER:O	2.15	0.47
1:I:2030:ARG:HB2	6:I:872:HOH:O	2.14	0.47
1:E:1178:ARG:NH2	1:F:1181:LYS:O	2.48	0.47
1:I:2162:PHE:HA	1:I:2166:GLN:NE2	2.30	0.47
1:J:1091:ARG:HB3	1:J:1215:MET:HG2	1.97	0.47
1:B:1118:GLY:HA3	1:b:2160:ASP:OD2	2.15	0.46
1:b:2017:GLN:HE22	1:d:3058:ASP:HA	1.64	0.46
1:e:2181:LYS:O	1:R:1178:ARG:NH2	2.48	0.46
1:R:1162:PHE:HA	1:R:1166:GLN:NE2	2.30	0.46
1:G:2016:LEU:HD22	1:G:2084:LEU:HB3	1.96	0.46
4:G:3051:PO4:O4	5:G:3052:DUR:H2'2	2.15	0.46
1:J:1228:ILE:HD12	1:j:2007:PHE:HB2	1.97	0.46
1:A:3163:TYR:HB2	1:A:3164:PRO:CD	2.45	0.46
1:H:1163:TYR:HB2	1:H:1164:PRO:CD	2.45	0.46
1:K:1163:TYR:CB	1:K:1164:PRO:CD	2.93	0.46
1:i:1048:ARG:HD2	6:i:928:HOH:O	2.15	0.46
1:E:1030:ARG:HH21	1:E:1094:THR:HG23	1.80	0.46
1:o:3226:GLN:HG3	1:o:3227:GLU:N	2.15	0.46
1:O:1049:GLU:HB3	1:o:3049:GLU:HB3	1.96	0.46
1:k:2163:TYR:CB	1:k:2164:PRO:CD	2.94	0.46
1:N:1163:TYR:HB2	1:N:1164:PRO:HD3	1.97	0.46
1:O:1163:TYR:CB	1:O:1164:PRO:CD	2.93	0.46
1:J:1162:PHE:HA	1:J:1166:GLN:NE2	2.31	0.46
1:i:1038:MET:HG2	1:i:1057:LEU:HD13	1.96	0.46
1:o:3030:ARG:NH2	1:o:3030:ARG:HB3	2.31	0.46
1:h:2090:LEU:HD11	1:h:2252:LEU:HD12	1.97	0.45
1:H:1091:ARG:HG2	1:H:1215:MET:SD	2.56	0.45
1:J:1038:MET:HG2	1:J:1057:LEU:HD13	1.98	0.45
1:o:3163:TYR:HB2	1:o:3164:PRO:CD	2.46	0.45
1:d:3181:LYS:HE2	6:d:422:HOH:O	2.16	0.45
1:C:1030:ARG:HH21	1:C:1094:THR:HG23	1.80	0.45
1:A:3226:GLN:HG3	1:A:3227:GLU:N	2.25	0.45
1:c:2016:LEU:HD22	1:c:2084:LEU:HB3	1.98	0.45
1:D:1030:ARG:HH21	1:D:1094:THR:HG23	1.81	0.45
1:d:3159:SER:O	1:d:3197:MET:HG2	2.17	0.45
1:h:2185:GLU:HA	1:h:2188:GLN:HG3	1.97	0.45
1:J:1163:TYR:HB2	1:J:1164:PRO:CD	2.46	0.45
1:R:1223:ARG:HA	1:R:1226:GLN:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1091:ARG:HB3	1:Q:1215:MET:HG2	1.98	0.45
1:A:3167:GLU:HG2	1:A:3169:TYR:CE2	2.50	0.45
1:e:2030:ARG:O	1:e:2030:ARG:HG3	2.17	0.45
1:F:1163:TYR:HB2	1:F:1164:PRO:CD	2.46	0.45
1:P:2016:LEU:HD22	1:P:2084:LEU:HB3	1.97	0.45
1:P:2177:VAL:O	1:P:2178:ARG:C	2.58	0.45
1:h:2043:LYS:CE	6:h:823:HOH:O	2.37	0.45
1:I:2086:ILE:O	1:I:2087:ARG:NH1	2.49	0.45
1:o:3149:ALA:HB2	1:o:3240:HIS:CE1	2.52	0.45
1:b:2034:ILE:HG12	1:b:2242:VAL:HG13	1.99	0.45
1:C:1163:TYR:HB2	1:C:1164:PRO:HD3	1.97	0.45
1:l:2016:LEU:HD22	1:l:2084:LEU:HB3	1.98	0.45
1:o:3226:GLN:CB	1:o:3227:GLU:HG3	2.46	0.45
1:C:1228:ILE:HD12	1:c:2007:PHE:HB2	1.99	0.45
1:o:3030:ARG:HB3	1:o:3030:ARG:CZ	2.47	0.45
1:C:1038:MET:HG2	1:C:1057:LEU:HD13	1.98	0.45
1:F:1091:ARG:HB3	1:F:1215:MET:HG2	1.97	0.45
1:K:1029:ASP:OD2	6:K:4135:HOH:O	2.21	0.45
1:D:1038:MET:HG2	1:D:1057:LEU:HD13	2.00	0.44
1:D:1228:ILE:HD12	1:d:3007:PHE:HB2	1.98	0.44
1:e:2016:LEU:HD22	1:e:2084:LEU:HB3	1.99	0.44
1:F:1043:LYS:HE2	1:k:2147:ILE:CA	2.47	0.44
1:F:1053:TRP:HZ2	1:k:2146:SER:HA	1.79	0.44
1:e:2033:LYS:N	1:N:1040:LYS:HZ1	2.15	0.44
1:h:2087:ARG:HB3	6:h:832:HOH:O	2.16	0.44
1:k:2185:GLU:HA	1:k:2188:GLN:HG3	1.99	0.44
1:A:3163:TYR:HB2	1:A:3164:PRO:HD3	1.99	0.44
1:B:1049:GLU:HB3	1:b:2049:GLU:HB3	2.00	0.44
1:B:1038:MET:HG2	1:B:1057:LEU:HD13	1.99	0.44
1:D:1091:ARG:HG2	1:D:1215:MET:SD	2.57	0.44
1:R:1170:ASP:HB3	6:R:598:HOH:O	2.17	0.44
1:k:2034:ILE:HG12	1:k:2242:VAL:HG13	2.00	0.44
1:E:1163:TYR:HB2	1:E:1164:PRO:CD	2.48	0.44
1:K:1222:ASN:HB3	1:K:1225:GLN:HE21	1.83	0.44
1:A:3242:VAL:O	1:A:3245:VAL:HG12	2.17	0.44
1:B:1091:ARG:HB3	1:B:1215:MET:HG2	2.00	0.44
1:C:1163:TYR:CB	1:C:1164:PRO:CD	2.96	0.44
1:D:1163:TYR:CB	1:D:1164:PRO:CD	2.96	0.44
1:R:1163:TYR:HB2	1:R:1164:PRO:CD	2.47	0.44
1:K:1091:ARG:HG2	1:K:1215:MET:SD	2.58	0.44
1:L:3030:ARG:HE	1:L:3033:LYS:NZ	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:2032:GLU:CD	1:N:1040:LYS:HE2	2.43	0.44
1:H:1105:GLY:HA2	1:H:1237:THR:HG23	2.00	0.44
1:i:1162:PHE:HA	1:i:1166:GLN:NE2	2.33	0.44
1:A:3024:VAL:O	1:A:3091:ARG:HD2	2.17	0.44
1:B:1163:TYR:CB	1:B:1164:PRO:CD	2.95	0.44
1:h:2181:LYS:O	1:i:1178:ARG:NH2	2.50	0.44
1:i:1163:TYR:CB	1:i:1164:PRO:CD	2.95	0.44
1:L:3140:LEU:HD22	1:L:3216:VAL:HB	1.99	0.44
1:E:1223:ARG:HA	1:E:1226:GLN:O	2.17	0.43
1:P:2163:TYR:HB2	1:P:2164:PRO:CD	2.48	0.43
1:h:2186:GLU:HG3	6:i:943:HOH:O	2.18	0.43
1:K:1048:ARG:HB3	1:K:1049:GLU:OE2	2.18	0.43
1:k:2175:ARG:NE	6:k:1137:HOH:O	2.37	0.43
1:P:2253:LEU:HD23	1:P:2253:LEU:HA	1.84	0.43
1:J:1105:GLY:HA2	1:J:1237:THR:CG2	2.47	0.43
1:j:2030:ARG:O	1:j:2030:ARG:HG3	2.17	0.43
1:b:2044:LEU:HD11	1:b:2054:ARG:HB2	2.00	0.43
1:G:2049:GLU:HB3	1:P:2049:GLU:HB3	2.00	0.43
1:k:2091:ARG:HB2	1:k:2202:LEU:HD22	2.00	0.43
1:G:2030:ARG:HD3	6:G:666:HOH:O	2.18	0.43
1:h:2146:SER:HB3	1:L:3032:GLU:OE1	2.19	0.43
1:L:3113:SER:HA	1:L:3156:THR:O	2.18	0.43
1:m:3071:GLY:N	1:m:3072:PRO:CD	2.81	0.43
1:a:2016:LEU:HD22	1:a:2084:LEU:HB3	2.01	0.43
1:b:2177:VAL:O	1:b:2178:ARG:C	2.62	0.43
1:D:1199:SER:CB	1:D:1215:MET:HE2	2.43	0.43
1:e:2034:ILE:HG12	1:e:2242:VAL:HG13	2.01	0.43
1:G:2228:ILE:HA	1:G:2229:PRO:HD3	1.93	0.43
1:k:2030:ARG:HD3	6:k:1133:HOH:O	2.17	0.43
1:O:1105:GLY:HA2	1:O:1237:THR:CG2	2.47	0.43
1:D:1181:LYS:HD2	6:D:365:HOH:O	2.18	0.43
1:O:1091:ARG:HG2	1:O:1215:MET:SD	2.58	0.43
1:A:3159:SER:O	1:A:3197:MET:HG2	2.18	0.43
1:B:1228:ILE:HD12	1:b:2007:PHE:HB2	2.00	0.43
1:d:3091:ARG:HG2	1:d:3215:MET:SD	2.59	0.43
1:F:1116:LEU:HB2	1:F:1159:SER:HA	2.01	0.43
1:M:2048:ARG:HD3	1:m:3069:ILE:HD11	2.00	0.43
1:m:3163:TYR:HB2	1:m:3164:PRO:CD	2.49	0.43
1:o:3140:LEU:HD22	1:o:3216:VAL:HB	2.00	0.43
1:A:3149:ALA:HB2	1:A:3240:HIS:CE1	2.54	0.43
1:c:2075:SER:HA	1:c:2205:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1048:ARG:HD3	1:d:3069:ILE:HD11	2.00	0.43
1:e:2162:PHE:HA	1:e:2166:GLN:NE2	2.34	0.43
1:N:1091:ARG:HB3	1:N:1215:MET:HG2	2.01	0.43
1:D:1091:ARG:HB3	1:D:1215:MET:HG2	2.01	0.42
1:I:2016:LEU:HD22	1:I:2084:LEU:HB3	2.00	0.42
1:M:2034:ILE:HG12	1:M:2242:VAL:HG13	2.01	0.42
1:R:1031:VAL:HG13	1:R:1064:VAL:HG12	2.01	0.42
1:P:2163:TYR:CB	1:P:2164:PRO:CD	2.97	0.42
1:i:1091:ARG:HB3	1:i:1215:MET:HG2	2.01	0.42
1:J:1091:ARG:HG2	1:J:1215:MET:SD	2.59	0.42
1:j:2253:LEU:HD23	1:j:2253:LEU:HA	1.91	0.42
1:k:2091:ARG:NH2	4:k:3091:PO4:O4	2.52	0.42
1:l:2226:GLN:NE2	6:l:1226:HOH:O	2.52	0.42
1:N:1163:TYR:CB	1:N:1164:PRO:CD	2.96	0.42
1:k:2177:VAL:HG22	6:k:1150:HOH:O	2.18	0.42
1:a:2177:VAL:O	1:a:2178:ARG:C	2.63	0.42
1:F:1223:ARG:HA	1:F:1226:GLN:O	2.19	0.42
1:C:1162:PHE:HA	1:C:1166:GLN:NE2	2.35	0.42
1:F:1163:TYR:CB	1:F:1164:PRO:CD	2.97	0.42
1:h:2034:ILE:HG12	1:h:2242:VAL:HG13	2.02	0.42
1:L:3091:ARG:HG2	1:L:3215:MET:SD	2.59	0.42
1:m:3091:ARG:HG2	1:m:3215:MET:SD	2.60	0.42
1:A:3225:GLN:HB3	1:A:3227:GLU:OE1	2.20	0.42
1:D:1091:ARG:HG3	1:D:1092:ILE:N	2.34	0.42
1:d:3226:GLN:HG3	1:d:3227:GLU:N	2.23	0.42
1:j:2090:LEU:HD11	1:j:2252:LEU:HD12	2.00	0.42
1:l:2091:ARG:NH2	4:l:3101:PO4:O4	2.53	0.42
1:Q:1163:TYR:CB	1:Q:1164:PRO:CD	2.97	0.42
1:O:1027:ASP:HA	1:O:1028:PRO:HD2	1.94	0.42
1:A:3030:ARG:HB3	1:A:3030:ARG:CZ	2.49	0.42
1:b:2075:SER:HA	1:b:2205:MET:SD	2.59	0.42
1:E:1086:ILE:O	1:E:1087:ARG:NH2	2.52	0.42
1:E:1118:GLY:HA3	1:e:2160:ASP:OD2	2.20	0.42
1:L:3184:MET:O	1:L:3188:GLN:HG3	2.20	0.42
1:M:2016:LEU:HD22	1:M:2084:LEU:HB3	2.01	0.42
1:o:3030:ARG:HE	1:o:3033:LYS:NZ	2.17	0.42
1:D:1116:LEU:HB2	1:D:1159:SER:HA	2.02	0.42
1:d:3147:ILE:HD11	1:d:3240:HIS:CE1	2.54	0.42
1:R:1105:GLY:HA2	1:R:1237:THR:HG23	2.02	0.42
6:J:5092:HOH:O	1:j:2177:VAL:HB	2.20	0.42
1:L:3149:ALA:HB2	1:L:3240:HIS:HE1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1163:TYR:HB2	1:O:1164:PRO:HD3	2.02	0.42
1:e:2228:ILE:HA	1:e:2229:PRO:HD3	1.90	0.42
1:K:1114:VAL:HB	1:K:1157:ALA:HA	2.02	0.42
1:M:2163:TYR:HB2	1:M:2164:PRO:CD	2.50	0.42
1:O:1162:PHE:HA	1:O:1166:GLN:NE2	2.35	0.42
1:F:1048:ARG:NH1	6:F:543:HOH:O	2.46	0.42
1:L:3071:GLY:N	1:L:3072:PRO:CD	2.82	0.42
1:o:3027:ASP:HA	1:o:3028:PRO:HD2	1.85	0.42
1:e:2033:LYS:H	1:N:1040:LYS:HZ1	1.68	0.41
1:G:2185:GLU:HA	1:G:2188:GLN:HG3	2.01	0.41
1:H:1091:ARG:HB3	1:H:1215:MET:HG2	2.01	0.41
1:h:2030:ARG:HB2	6:h:821:HOH:O	2.20	0.41
1:i:1223:ARG:HA	1:i:1226:GLN:O	2.20	0.41
1:m:3247:GLU:O	1:m:3250:ARG:HB2	2.20	0.41
1:N:1086:ILE:O	1:N:1087:ARG:NH2	2.53	0.41
1:O:1091:ARG:HG3	1:O:1092:ILE:N	2.35	0.41
1:d:3163:TYR:CB	1:d:3164:PRO:CD	2.98	0.41
1:e:2048:ARG:NH1	6:e:505:HOH:O	2.50	0.41
4:H:2061:PO4:O3	1:h:2048:ARG:NH2	2.46	0.41
1:j:2189:ALA:HB1	1:k:2175:ARG:HD3	2.02	0.41
1:o:3021:LEU:C	1:o:3021:LEU:HD23	2.45	0.41
1:o:3091:ARG:HG2	1:o:3215:MET:SD	2.60	0.41
1:c:2163:TYR:HB2	1:c:2164:PRO:CD	2.50	0.41
1:D:1133:ASP:OD2	6:D:359:HOH:O	2.22	0.41
1:k:2040:LYS:N	1:k:2041:PRO:CD	2.83	0.41
1:C:1116:LEU:HB2	1:C:1159:SER:HA	2.02	0.41
1:D:1179:HIS:ND1	3:D:5021:V7O:O12	2.38	0.41
1:e:2033:LYS:HD2	1:N:1040:LYS:CG	2.51	0.41
1:P:2091:ARG:NH2	4:P:3121:PO4:O4	2.52	0.41
1:E:1105:GLY:HA2	1:E:1237:THR:CG2	2.50	0.41
1:Q:1162:PHE:HA	1:Q:1166:GLN:NE2	2.35	0.41
1:B:1223:ARG:HA	1:B:1226:GLN:O	2.21	0.41
1:F:1162:PHE:HA	1:F:1166:GLN:NE2	2.36	0.41
1:G:2160:ASP:OD2	1:P:2118:GLY:HA3	2.21	0.41
1:i:1091:ARG:HG3	1:i:1092:ILE:N	2.35	0.41
1:L:3226:GLN:HG3	1:L:3227:GLU:N	2.25	0.41
1:O:1048:ARG:NH1	6:O:1487:HOH:O	2.42	0.41
1:o:3167:GLU:HG2	1:o:3169:TYR:CE2	2.56	0.41
1:E:1038:MET:HG2	1:E:1057:LEU:HD13	2.02	0.41
1:e:2163:TYR:HB2	1:e:2164:PRO:CD	2.51	0.41
1:F:1091:ARG:HG2	1:F:1215:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1163:TYR:HB2	1:R:1164:PRO:HD3	2.02	0.41
1:h:2162:PHE:HA	1:h:2166:GLN:NE2	2.36	0.41
1:J:1049:GLU:HB3	1:j:2049:GLU:HB3	2.03	0.41
1:J:1222:ASN:HB3	1:J:1225:GLN:HE21	1.86	0.41
1:K:1091:ARG:HG3	1:K:1092:ILE:N	2.35	0.41
1:L:3024:VAL:O	1:L:3091:ARG:HD2	2.21	0.41
1:m:3138:THR:CG2	6:m:1335:HOH:O	2.69	0.41
1:O:1091:ARG:NH1	4:O:2111:PO4:O4	2.54	0.41
1:A:3163:TYR:CB	1:A:3164:PRO:CD	2.99	0.41
1:I:2160:ASP:OD2	1:i:1118:GLY:HA3	2.21	0.41
1:Q:1223:ARG:HA	1:Q:1226:GLN:O	2.21	0.41
1:C:1222:ASN:HB3	1:C:1225:GLN:HE21	1.86	0.40
1:c:2034:ILE:HG12	1:c:2242:VAL:HG13	2.03	0.40
1:c:2162:PHE:HA	1:c:2166:GLN:NE2	2.36	0.40
1:d:3024:VAL:HG23	1:d:3024:VAL:O	2.22	0.40
1:E:1228:ILE:HD12	1:e:2007:PHE:HB2	2.02	0.40
1:I:2049:GLU:HB3	1:i:1049:GLU:HB3	2.03	0.40
1:J:1118:GLY:HA3	1:j:2160:ASP:OD2	2.21	0.40
1:L:3159:SER:O	1:L:3197:MET:HG2	2.21	0.40
1:d:3225:GLN:HB3	1:d:3227:GLU:OE1	2.21	0.40
1:F:1007:PHE:HD2	1:F:1008:HIS:CE1	2.39	0.40
1:G:2162:PHE:HA	1:G:2166:GLN:NE2	2.36	0.40
1:P:2090:LEU:HD11	1:P:2252:LEU:HD12	2.03	0.40
3:H:5031:V7O:O16	3:I:5032:V7O:O12	2.38	0.40
1:K:1162:PHE:HA	1:K:1166:GLN:NE2	2.36	0.40
1:m:3030:ARG:HB3	1:m:3030:ARG:NH2	2.35	0.40
1:o:3242:VAL:O	1:o:3245:VAL:HG12	2.21	0.40
1:d:3149:ALA:HB2	1:d:3240:HIS:HE1	1.82	0.40
1:G:2175:ARG:CD	6:G:670:HOH:O	2.61	0.40
1:I:2007:PHE:HB2	1:i:1228:ILE:HD12	2.04	0.40
1:I:2034:ILE:HG12	1:I:2242:VAL:HG13	2.04	0.40
1:a:2163:TYR:HB2	1:a:2164:PRO:CD	2.51	0.40
1:C:1091:ARG:HG3	1:C:1092:ILE:N	2.35	0.40
1:D:1223:ARG:HA	1:D:1226:GLN:O	2.21	0.40
1:M:2163:TYR:CB	1:M:2164:PRO:CD	3.00	0.40
1:Q:1222:ASN:HB3	1:Q:1225:GLN:HE21	1.86	0.40
1:B:1091:ARG:HG2	1:B:1215:MET:SD	2.62	0.40
1:c:2177:VAL:O	1:c:2178:ARG:C	2.65	0.40
1:H:1163:TYR:HB2	1:H:1164:PRO:HD3	2.02	0.40
1:L:3163:TYR:CB	1:L:3164:PRO:CD	3.00	0.40
1:l:2108:LEU:HD22	1:l:2152:HIS:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1171:THR:HB	6:Q:1374:HOH:O	2.20	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:1104:VAL:O	1:m:3226:GLN:NE2[2_546]	1.65	0.55
1:e:2101:HIS:CE1	1:o:3226:GLN:CD[2_546]	1.71	0.49
1:e:2101:HIS:NE2	1:o:3226:GLN:NE2[2_546]	1.79	0.41
1:d:3005:ASP:O	1:d:3226:GLN:OE1[2_656]	1.85	0.35
1:e:2101:HIS:CE1	1:o:3226:GLN:CG[2_546]	1.93	0.27
1:c:2014:ASN:OD1	1:k:2171:THR:O[2_656]	1.96	0.24
1:i:1104:VAL:CB	1:m:3226:GLN:OE1[2_546]	1.99	0.21
1:G:2226:GLN:OE1	6:B:148:HOH:O[2_556]	2.06	0.14
1:e:2101:HIS:NE2	1:o:3226:GLN:CB[2_546]	2.09	0.11
1:e:2101:HIS:CE1	1:o:3226:GLN:NE2[2_546]	2.10	0.10
1:R:1039:ASP:OD2	1:P:2042:VAL:CG2[1_655]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/253 (98%)	242 (98%)	3 (1%)	3 (1%)	10	34
1	B	242/253 (96%)	239 (99%)	2 (1%)	1 (0%)	30	60
1	C	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	30	60
1	D	242/253 (96%)	238 (98%)	3 (1%)	1 (0%)	30	60
1	E	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	30	60
1	F	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	30	60
1	G	238/253 (94%)	233 (98%)	4 (2%)	1 (0%)	30	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	242/253 (96%)	239 (99%)	2 (1%)	1 (0%)	30	60
1	I	238/253 (94%)	235 (99%)	2 (1%)	1 (0%)	30	60
1	J	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	30	60
1	K	242/253 (96%)	236 (98%)	5 (2%)	1 (0%)	30	60
1	L	248/253 (98%)	240 (97%)	5 (2%)	3 (1%)	10	34
1	M	238/253 (94%)	235 (99%)	2 (1%)	1 (0%)	30	60
1	N	242/253 (96%)	239 (99%)	2 (1%)	1 (0%)	30	60
1	O	242/253 (96%)	238 (98%)	3 (1%)	1 (0%)	30	60
1	P	238/253 (94%)	233 (98%)	4 (2%)	1 (0%)	30	60
1	Q	242/253 (96%)	238 (98%)	3 (1%)	1 (0%)	30	60
1	R	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	30	60
1	a	238/253 (94%)	233 (98%)	4 (2%)	1 (0%)	30	60
1	b	238/253 (94%)	234 (98%)	3 (1%)	1 (0%)	30	60
1	c	238/253 (94%)	236 (99%)	1 (0%)	1 (0%)	30	60
1	d	248/253 (98%)	240 (97%)	5 (2%)	3 (1%)	10	34
1	e	238/253 (94%)	233 (98%)	4 (2%)	1 (0%)	30	60
1	h	238/253 (94%)	235 (99%)	2 (1%)	1 (0%)	30	60
1	i	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	30	60
1	j	238/253 (94%)	233 (98%)	4 (2%)	1 (0%)	30	60
1	k	238/253 (94%)	235 (99%)	2 (1%)	1 (0%)	30	60
1	l	238/253 (94%)	234 (98%)	3 (1%)	1 (0%)	30	60
1	m	248/253 (98%)	240 (97%)	5 (2%)	3 (1%)	10	34
1	o	248/253 (98%)	240 (97%)	5 (2%)	3 (1%)	10	34
All	All	7242/7590 (95%)	7100 (98%)	102 (1%)	40 (1%)	21	51

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3163	TYR
1	A	3229	PRO
1	b	2163	TYR
1	c	2163	TYR
1	d	3163	TYR
1	d	3229	PRO

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Mol	Chain	Res	Type
1	e	2163	TYR
1	G	2163	TYR
1	P	2163	TYR
1	h	2163	TYR
1	i	1163	TYR
1	j	2163	TYR
1	K	1163	TYR
1	k	2163	TYR
1	L	3163	TYR
1	L	3229	PRO
1	M	2163	TYR
1	m	3229	PRO
1	o	3163	TYR
1	o	3229	PRO
1	A	3226	GLN
1	a	2163	TYR
1	B	1163	TYR
1	C	1163	TYR
1	D	1163	TYR
1	E	1163	TYR
1	F	1163	TYR
1	R	1163	TYR
1	I	2163	TYR
1	J	1163	TYR
1	L	3226	GLN
1	l	2163	TYR
1	m	3163	TYR
1	m	3226	GLN
1	N	1163	TYR
1	Q	1163	TYR
1	O	1163	TYR
1	o	3226	GLN
1	d	3226	GLN
1	H	1163	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/204 (98%)	185 (92%)	16 (8%)	11	34
1	B	198/204 (97%)	177 (89%)	21 (11%)	6	22
1	C	198/204 (97%)	175 (88%)	23 (12%)	5	18
1	D	198/204 (97%)	178 (90%)	20 (10%)	7	23
1	E	198/204 (97%)	177 (89%)	21 (11%)	6	22
1	F	198/204 (97%)	178 (90%)	20 (10%)	7	23
1	G	194/204 (95%)	177 (91%)	17 (9%)	9	29
1	H	198/204 (97%)	177 (89%)	21 (11%)	6	22
1	I	194/204 (95%)	176 (91%)	18 (9%)	8	27
1	J	198/204 (97%)	178 (90%)	20 (10%)	7	23
1	K	198/204 (97%)	179 (90%)	19 (10%)	8	26
1	L	201/204 (98%)	183 (91%)	18 (9%)	9	28
1	M	194/204 (95%)	177 (91%)	17 (9%)	9	29
1	N	198/204 (97%)	178 (90%)	20 (10%)	7	23
1	O	198/204 (97%)	177 (89%)	21 (11%)	6	22
1	P	194/204 (95%)	176 (91%)	18 (9%)	8	27
1	Q	198/204 (97%)	178 (90%)	20 (10%)	7	23
1	R	198/204 (97%)	178 (90%)	20 (10%)	7	23
1	a	194/204 (95%)	176 (91%)	18 (9%)	8	27
1	b	194/204 (95%)	177 (91%)	17 (9%)	9	29
1	c	194/204 (95%)	178 (92%)	16 (8%)	10	33
1	d	201/204 (98%)	184 (92%)	17 (8%)	10	31
1	e	194/204 (95%)	178 (92%)	16 (8%)	10	33
1	h	194/204 (95%)	176 (91%)	18 (9%)	8	27
1	i	198/204 (97%)	178 (90%)	20 (10%)	7	23
1	j	194/204 (95%)	176 (91%)	18 (9%)	8	27
1	k	194/204 (95%)	176 (91%)	18 (9%)	8	27
1	l	194/204 (95%)	177 (91%)	17 (9%)	9	29
1	m	201/204 (98%)	183 (91%)	18 (9%)	9	28
1	o	201/204 (98%)	185 (92%)	16 (8%)	11	34
All	All	5907/6120 (96%)	5348 (90%)	559 (10%)	8	26

All (559) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3013	LYS
1	A	3014	ASN
1	A	3030	ARG
1	A	3033	LYS
1	A	3040	LYS
1	A	3145	LYS
1	A	3146	SER
1	A	3147	ILE
1	A	3150	THR
1	A	3175	ARG
1	A	3186	GLU
1	A	3226	GLN
1	A	3228	ILE
1	A	3232	GLU
1	A	3235	LYS
1	A	3243	LYS
1	a	2013	LYS
1	a	2030	ARG
1	a	2033	LYS
1	a	2084	LEU
1	a	2092	ILE
1	a	2142	GLU
1	a	2145	LYS
1	a	2147	ILE
1	a	2150	THR
1	a	2175	ARG
1	a	2181	LYS
1	a	2186	GLU
1	a	2188	GLN
1	a	2196	GLU
1	a	2226	GLN
1	a	2240	HIS
1	a	2243	LYS
1	a	2250	ARG
1	B	1013	LYS
1	B	1014	ASN
1	B	1030	ARG
1	B	1037	LEU
1	B	1092	ILE
1	B	1145	LYS
1	B	1146	SER
1	B	1147	ILE
1	B	1150	THR

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Mol	Chain	Res	Type
1	B	1175	ARG
1	B	1181	LYS
1	B	1186	GLU
1	B	1188	GLN
1	B	1196	GLU
1	B	1215	MET
1	B	1225	GLN
1	B	1235	LYS
1	B	1239	SER
1	B	1240	HIS
1	B	1243	LYS
1	B	1250	ARG
1	b	2013	LYS
1	b	2030	ARG
1	b	2033	LYS
1	b	2084	LEU
1	b	2092	ILE
1	b	2142	GLU
1	b	2145	LYS
1	b	2147	ILE
1	b	2150	THR
1	b	2175	ARG
1	b	2181	LYS
1	b	2186	GLU
1	b	2188	GLN
1	b	2226	GLN
1	b	2240	HIS
1	b	2243	LYS
1	b	2250	ARG
1	C	1013	LYS
1	C	1014	ASN
1	C	1017	GLN
1	C	1030	ARG
1	C	1037	LEU
1	C	1043	LYS
1	C	1145	LYS
1	C	1146	SER
1	C	1147	ILE
1	C	1150	THR
1	C	1175	ARG
1	C	1181	LYS
1	C	1186	GLU

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Mol	Chain	Res	Type
1	C	1188	GLN
1	C	1196	GLU
1	C	1215	MET
1	C	1225	GLN
1	C	1235	LYS
1	C	1239	SER
1	C	1240	HIS
1	C	1243	LYS
1	C	1245	VAL
1	C	1250	ARG
1	c	2013	LYS
1	c	2030	ARG
1	c	2033	LYS
1	c	2084	LEU
1	c	2092	ILE
1	c	2142	GLU
1	c	2145	LYS
1	c	2147	ILE
1	c	2150	THR
1	c	2175	ARG
1	c	2181	LYS
1	c	2186	GLU
1	c	2188	GLN
1	c	2226	GLN
1	c	2240	HIS
1	c	2243	LYS
1	D	1013	LYS
1	D	1014	ASN
1	D	1017	GLN
1	D	1030	ARG
1	D	1037	LEU
1	D	1145	LYS
1	D	1146	SER
1	D	1147	ILE
1	D	1150	THR
1	D	1175	ARG
1	D	1181	LYS
1	D	1186	GLU
1	D	1188	GLN
1	D	1215	MET
1	D	1225	GLN
1	D	1235	LYS

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Mol	Chain	Res	Type
1	D	1239	SER
1	D	1240	HIS
1	D	1243	LYS
1	D	1250	ARG
1	d	3013	LYS
1	d	3014	ASN
1	d	3030	ARG
1	d	3033	LYS
1	d	3040	LYS
1	d	3145	LYS
1	d	3146	SER
1	d	3147	ILE
1	d	3150	THR
1	d	3175	ARG
1	d	3186	GLU
1	d	3196	GLU
1	d	3226	GLN
1	d	3228	ILE
1	d	3232	GLU
1	d	3235	LYS
1	d	3243	LYS
1	E	1013	LYS
1	E	1014	ASN
1	E	1030	ARG
1	E	1037	LEU
1	E	1043	LYS
1	E	1145	LYS
1	E	1146	SER
1	E	1147	ILE
1	E	1150	THR
1	E	1175	ARG
1	E	1181	LYS
1	E	1186	GLU
1	E	1188	GLN
1	E	1196	GLU
1	E	1215	MET
1	E	1225	GLN
1	E	1235	LYS
1	E	1239	SER
1	E	1240	HIS
1	E	1243	LYS
1	E	1250	ARG

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Mol	Chain	Res	Type
1	e	2013	LYS
1	e	2030	ARG
1	e	2033	LYS
1	e	2084	LEU
1	e	2092	ILE
1	e	2142	GLU
1	e	2145	LYS
1	e	2147	ILE
1	e	2150	THR
1	e	2175	ARG
1	e	2181	LYS
1	e	2186	GLU
1	e	2188	GLN
1	e	2226	GLN
1	e	2240	HIS
1	e	2243	LYS
1	F	1013	LYS
1	F	1014	ASN
1	F	1017	GLN
1	F	1030	ARG
1	F	1037	LEU
1	F	1145	LYS
1	F	1146	SER
1	F	1147	ILE
1	F	1150	THR
1	F	1175	ARG
1	F	1181	LYS
1	F	1186	GLU
1	F	1188	GLN
1	F	1196	GLU
1	F	1215	MET
1	F	1225	GLN
1	F	1235	LYS
1	F	1239	SER
1	F	1243	LYS
1	F	1250	ARG
1	R	1013	LYS
1	R	1014	ASN
1	R	1017	GLN
1	R	1030	ARG
1	R	1037	LEU
1	R	1145	LYS

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Mol	Chain	Res	Type
1	R	1146	SER
1	R	1147	ILE
1	R	1150	THR
1	R	1175	ARG
1	R	1181	LYS
1	R	1186	GLU
1	R	1188	GLN
1	R	1215	MET
1	R	1225	GLN
1	R	1235	LYS
1	R	1239	SER
1	R	1240	HIS
1	R	1243	LYS
1	R	1250	ARG
1	G	2013	LYS
1	G	2030	ARG
1	G	2033	LYS
1	G	2084	LEU
1	G	2092	ILE
1	G	2142	GLU
1	G	2145	LYS
1	G	2147	ILE
1	G	2150	THR
1	G	2175	ARG
1	G	2181	LYS
1	G	2186	GLU
1	G	2188	GLN
1	G	2196	GLU
1	G	2226	GLN
1	G	2240	HIS
1	G	2243	LYS
1	P	2013	LYS
1	P	2030	ARG
1	P	2033	LYS
1	P	2084	LEU
1	P	2092	ILE
1	P	2142	GLU
1	P	2145	LYS
1	P	2147	ILE
1	P	2150	THR
1	P	2175	ARG
1	P	2181	LYS

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Mol	Chain	Res	Type
1	P	2186	GLU
1	P	2188	GLN
1	P	2196	GLU
1	P	2226	GLN
1	P	2240	HIS
1	P	2243	LYS
1	P	2250	ARG
1	H	1013	LYS
1	H	1014	ASN
1	H	1017	GLN
1	H	1030	ARG
1	H	1037	LEU
1	H	1043	LYS
1	H	1145	LYS
1	H	1146	SER
1	H	1147	ILE
1	H	1150	THR
1	H	1175	ARG
1	H	1181	LYS
1	H	1186	GLU
1	H	1188	GLN
1	H	1196	GLU
1	H	1215	MET
1	H	1225	GLN
1	H	1235	LYS
1	H	1239	SER
1	H	1243	LYS
1	H	1250	ARG
1	h	2013	LYS
1	h	2030	ARG
1	h	2033	LYS
1	h	2084	LEU
1	h	2092	ILE
1	h	2142	GLU
1	h	2145	LYS
1	h	2147	ILE
1	h	2150	THR
1	h	2175	ARG
1	h	2181	LYS
1	h	2186	GLU
1	h	2188	GLN
1	h	2196	GLU

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Mol	Chain	Res	Type
1	h	2226	GLN
1	h	2240	HIS
1	h	2243	LYS
1	h	2250	ARG
1	I	2013	LYS
1	I	2030	ARG
1	I	2033	LYS
1	I	2084	LEU
1	I	2092	ILE
1	I	2142	GLU
1	I	2145	LYS
1	I	2147	ILE
1	I	2150	THR
1	I	2175	ARG
1	I	2181	LYS
1	I	2186	GLU
1	I	2188	GLN
1	I	2196	GLU
1	I	2226	GLN
1	I	2240	HIS
1	I	2243	LYS
1	I	2250	ARG
1	i	1013	LYS
1	i	1014	ASN
1	i	1030	ARG
1	i	1037	LEU
1	i	1145	LYS
1	i	1146	SER
1	i	1147	ILE
1	i	1150	THR
1	i	1175	ARG
1	i	1181	LYS
1	i	1186	GLU
1	i	1188	GLN
1	i	1196	GLU
1	i	1215	MET
1	i	1225	GLN
1	i	1235	LYS
1	i	1239	SER
1	i	1240	HIS
1	i	1243	LYS
1	i	1250	ARG

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Mol	Chain	Res	Type
1	J	1013	LYS
1	J	1014	ASN
1	J	1030	ARG
1	J	1037	LEU
1	J	1043	LYS
1	J	1145	LYS
1	J	1147	ILE
1	J	1150	THR
1	J	1175	ARG
1	J	1181	LYS
1	J	1186	GLU
1	J	1188	GLN
1	J	1196	GLU
1	J	1215	MET
1	J	1225	GLN
1	J	1235	LYS
1	J	1239	SER
1	J	1240	HIS
1	J	1243	LYS
1	J	1250	ARG
1	j	2013	LYS
1	j	2030	ARG
1	j	2033	LYS
1	j	2084	LEU
1	j	2092	ILE
1	j	2142	GLU
1	j	2145	LYS
1	j	2147	ILE
1	j	2150	THR
1	j	2175	ARG
1	j	2181	LYS
1	j	2186	GLU
1	j	2188	GLN
1	j	2196	GLU
1	j	2226	GLN
1	j	2240	HIS
1	j	2243	LYS
1	j	2250	ARG
1	K	1013	LYS
1	K	1014	ASN
1	K	1030	ARG
1	K	1037	LEU

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Mol	Chain	Res	Type
1	K	1145	LYS
1	K	1147	ILE
1	K	1150	THR
1	K	1175	ARG
1	K	1181	LYS
1	K	1186	GLU
1	K	1188	GLN
1	K	1196	GLU
1	K	1215	MET
1	K	1225	GLN
1	K	1235	LYS
1	K	1239	SER
1	K	1240	HIS
1	K	1243	LYS
1	K	1250	ARG
1	k	2013	LYS
1	k	2030	ARG
1	k	2033	LYS
1	k	2084	LEU
1	k	2092	ILE
1	k	2142	GLU
1	k	2145	LYS
1	k	2147	ILE
1	k	2150	THR
1	k	2175	ARG
1	k	2181	LYS
1	k	2186	GLU
1	k	2188	GLN
1	k	2196	GLU
1	k	2226	GLN
1	k	2240	HIS
1	k	2243	LYS
1	k	2250	ARG
1	L	3013	LYS
1	L	3030	ARG
1	L	3033	LYS
1	L	3040	LYS
1	L	3145	LYS
1	L	3146	SER
1	L	3147	ILE
1	L	3150	THR
1	L	3175	ARG

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Mol	Chain	Res	Type
1	L	3186	GLU
1	L	3196	GLU
1	L	3225	GLN
1	L	3226	GLN
1	L	3228	ILE
1	L	3232	GLU
1	L	3233	THR
1	L	3235	LYS
1	L	3243	LYS
1	l	2013	LYS
1	l	2030	ARG
1	l	2033	LYS
1	l	2084	LEU
1	l	2092	ILE
1	l	2142	GLU
1	l	2145	LYS
1	l	2147	ILE
1	l	2150	THR
1	l	2175	ARG
1	l	2181	LYS
1	l	2186	GLU
1	l	2188	GLN
1	l	2226	GLN
1	l	2240	HIS
1	l	2243	LYS
1	l	2250	ARG
1	M	2013	LYS
1	M	2030	ARG
1	M	2033	LYS
1	M	2084	LEU
1	M	2092	ILE
1	M	2142	GLU
1	M	2145	LYS
1	M	2147	ILE
1	M	2150	THR
1	M	2175	ARG
1	M	2181	LYS
1	M	2186	GLU
1	M	2188	GLN
1	M	2226	GLN
1	M	2240	HIS
1	M	2243	LYS

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Mol	Chain	Res	Type
1	M	2250	ARG
1	m	3013	LYS
1	m	3030	ARG
1	m	3033	LYS
1	m	3040	LYS
1	m	3092	ILE
1	m	3145	LYS
1	m	3146	SER
1	m	3147	ILE
1	m	3150	THR
1	m	3175	ARG
1	m	3186	GLU
1	m	3196	GLU
1	m	3226	GLN
1	m	3228	ILE
1	m	3232	GLU
1	m	3233	THR
1	m	3235	LYS
1	m	3243	LYS
1	N	1013	LYS
1	N	1014	ASN
1	N	1030	ARG
1	N	1037	LEU
1	N	1043	LYS
1	N	1145	LYS
1	N	1146	SER
1	N	1147	ILE
1	N	1150	THR
1	N	1175	ARG
1	N	1181	LYS
1	N	1186	GLU
1	N	1188	GLN
1	N	1215	MET
1	N	1225	GLN
1	N	1235	LYS
1	N	1239	SER
1	N	1240	HIS
1	N	1243	LYS
1	N	1250	ARG
1	Q	1013	LYS
1	Q	1014	ASN
1	Q	1030	ARG

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Mol	Chain	Res	Type
1	Q	1037	LEU
1	Q	1043	LYS
1	Q	1145	LYS
1	Q	1146	SER
1	Q	1147	ILE
1	Q	1150	THR
1	Q	1175	ARG
1	Q	1181	LYS
1	Q	1186	GLU
1	Q	1188	GLN
1	Q	1215	MET
1	Q	1225	GLN
1	Q	1235	LYS
1	Q	1239	SER
1	Q	1240	HIS
1	Q	1243	LYS
1	Q	1250	ARG
1	O	1013	LYS
1	O	1014	ASN
1	O	1030	ARG
1	O	1037	LEU
1	O	1043	LYS
1	O	1145	LYS
1	O	1146	SER
1	O	1147	ILE
1	O	1150	THR
1	O	1175	ARG
1	O	1181	LYS
1	O	1186	GLU
1	O	1188	GLN
1	O	1196	GLU
1	O	1215	MET
1	O	1225	GLN
1	O	1235	LYS
1	O	1239	SER
1	O	1240	HIS
1	O	1243	LYS
1	O	1250	ARG
1	o	3013	LYS
1	o	3014	ASN
1	o	3030	ARG
1	o	3033	LYS

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Mol	Chain	Res	Type
1	o	3040	LYS
1	o	3145	LYS
1	o	3146	SER
1	o	3147	ILE
1	o	3150	THR
1	o	3175	ARG
1	o	3186	GLU
1	o	3226	GLN
1	o	3228	ILE
1	o	3232	GLU
1	o	3235	LYS
1	o	3243	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3152	HIS
1	A	3225	GLN
1	A	3226	GLN
1	A	3240	HIS
1	a	2226	GLN
1	B	1103	ASN
1	b	2017	GLN
1	b	2226	GLN
1	D	1103	ASN
1	D	1225	GLN
1	d	3152	HIS
1	d	3225	GLN
1	d	3226	GLN
1	d	3240	HIS
1	E	1103	ASN
1	e	2179	HIS
1	R	1103	ASN
1	H	1240	HIS
1	h	2179	HIS
1	i	1179	HIS
1	J	1103	ASN
1	J	1179	HIS
1	J	1225	GLN
1	J	1240	HIS
1	j	2179	HIS
1	j	2226	GLN

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Mol	Chain	Res	Type
1	K	1225	GLN
1	L	3152	HIS
1	L	3225	GLN
1	L	3226	GLN
1	L	3240	HIS
1	m	3152	HIS
1	m	3225	GLN
1	m	3226	GLN
1	m	3240	HIS
1	N	1103	ASN
1	N	1240	HIS
1	Q	1103	ASN
1	Q	1225	GLN
1	O	1103	ASN
1	O	1179	HIS
1	o	3152	HIS
1	o	3225	GLN
1	o	3240	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 85 ligands modelled in this entry, 15 are monoatomic - leaving 70 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	V7O	B	5012	3	0,10,25	-	-	-		
5	DUR	i	2072	-	17,17,17	1.92	6 (35%)	24,24,24	3.50	8 (33%)
3	V7O	J	5042	3	0,10,25	-	-	-		
5	DUR	C	2022	-	17,17,17	1.92	7 (41%)	24,24,24	4.00	10 (41%)
5	DUR	D	2032	-	17,17,17	1.82	3 (17%)	24,24,24	3.59	8 (33%)
5	DUR	c	3032	-	17,17,17	2.13	5 (29%)	24,24,24	4.23	11 (45%)
5	DUR	I	3072	-	17,17,17	1.88	4 (23%)	24,24,24	3.56	7 (29%)
5	DUR	E	2042	-	17,17,17	1.91	5 (29%)	24,24,24	3.63	8 (33%)
4	PO4	C	2021	-	4,4,4	0.87	0	6,6,6	0.54	0
4	PO4	Q	2121	-	4,4,4	0.99	0	6,6,6	0.57	0
3	V7O	D	5022	3	0,10,25	-	-	-		
4	PO4	F	2051	-	4,4,4	0.89	0	6,6,6	0.37	0
3	V7O	L	5041	3	0,10,25	-	-	-		
3	V7O	b	5013	3	0,10,25	-	-	-		
5	DUR	j	3082	-	17,17,17	1.89	3 (17%)	24,24,24	3.89	11 (45%)
3	V7O	I	5032	3	0,10,25	-	-	-		
4	PO4	b	3021	-	4,4,4	0.83	0	6,6,6	0.58	0
5	DUR	b	3022	-	17,17,17	1.76	4 (23%)	24,24,24	3.78	9 (37%)
4	PO4	N	2101	-	4,4,4	0.92	0	6,6,6	0.56	0
3	V7O	e	5023	3	0,10,25	-	-	-		
4	PO4	B	2011	-	4,4,4	0.86	0	6,6,6	0.64	0
4	PO4	h	3061	-	4,4,4	0.91	0	6,6,6	0.53	0
5	DUR	J	2082	-	17,17,17	2.07	5 (29%)	24,24,24	3.70	7 (29%)
5	DUR	R	2132	-	17,17,17	1.94	5 (29%)	24,24,24	3.71	10 (41%)
4	PO4	k	3091	-	4,4,4	0.84	0	6,6,6	0.84	0
3	V7O	Q	5053	3	0,10,25	-	-	-		
3	V7O	k	5043	3	0,10,25	-	-	-		
5	DUR	K	2092	-	17,17,17	1.88	5 (29%)	24,24,24	3.41	9 (37%)
4	PO4	G	3051	-	4,4,4	0.91	0	6,6,6	0.65	0
3	V7O	h	5033	3	0,10,25	-	-	-		
5	DUR	P	3122	-	17,17,17	1.69	3 (17%)	24,24,24	3.83	11 (45%)
4	PO4	O	2111	-	4,4,4	0.92	0	6,6,6	0.50	0
5	DUR	G	3052	-	17,17,17	1.74	3 (17%)	24,24,24	3.54	9 (37%)
5	DUR	H	2062	-	17,17,17	1.78	3 (17%)	24,24,24	3.35	6 (25%)
4	PO4	j	3081	-	4,4,4	0.84	0	6,6,6	0.68	0
3	V7O	R	5024	3	0,10,25	-	-	-		
3	V7O	A	5011	3	0,10,25	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DUR	k	3092	-	17,17,17	1.95	5 (29%)	24,24,24	3.62	7 (29%)
4	PO4	i	2071	-	4,4,4	0.87	0	6,6,6	0.51	0
4	PO4	e	3041	-	4,4,4	0.81	0	6,6,6	0.73	0
3	V7O	c	5014	3	0,10,25	-	-	-	-	-
5	DUR	M	3112	-	17,17,17	1.78	3 (17%)	24,24,24	3.64	7 (29%)
3	V7O	o	5054	3	0,10,25	-	-	-	-	-
4	PO4	l	3101	-	4,4,4	0.89	0	6,6,6	0.54	0
4	PO4	M	3111	-	4,4,4	0.85	0	6,6,6	0.83	0
3	V7O	M	5051	3	0,10,25	-	-	-	-	-
4	PO4	P	3121	-	4,4,4	0.89	0	6,6,6	0.55	0
4	PO4	R	2131	-	4,4,4	0.95	0	6,6,6	0.38	0
3	V7O	j	5044	3	0,10,25	-	-	-	-	-
4	PO4	c	3031	-	4,4,4	0.99	0	6,6,6	0.97	1 (16%)
5	DUR	N	2102	-	17,17,17	1.77	4 (23%)	24,24,24	3.36	9 (37%)
3	V7O	M	5052	3	0,10,25	-	-	-	-	-
3	V7O	H	5031	3	0,10,25	-	-	-	-	-
4	PO4	a	3011	-	4,4,4	0.76	0	6,6,6	0.68	0
5	DUR	F	2052	-	17,17,17	1.90	6 (35%)	24,24,24	3.66	9 (37%)
4	PO4	K	2091	-	4,4,4	0.93	0	6,6,6	0.41	0
3	V7O	D	5021	3	0,10,25	-	-	-	-	-
5	DUR	e	3042	-	17,17,17	1.67	3 (17%)	24,24,24	3.55	7 (29%)
4	PO4	I	3071	-	4,4,4	0.78	0	6,6,6	0.75	0
5	DUR	l	3102	-	17,17,17	1.76	3 (17%)	24,24,24	3.50	9 (37%)
4	PO4	J	2081	-	4,4,4	0.87	0	6,6,6	0.48	0
4	PO4	H	2061	-	4,4,4	0.87	0	6,6,6	0.56	0
5	DUR	h	3062	-	17,17,17	1.97	6 (35%)	24,24,24	3.39	6 (25%)
5	DUR	a	3012	-	17,17,17	2.01	5 (29%)	24,24,24	3.83	9 (37%)
5	DUR	O	2112	-	17,17,17	1.92	6 (35%)	24,24,24	3.29	6 (25%)
4	PO4	D	2031	-	4,4,4	0.86	0	6,6,6	0.53	0
4	PO4	E	2041	-	4,4,4	0.82	0	6,6,6	0.67	0
5	DUR	B	2012	-	17,17,17	2.01	6 (35%)	24,24,24	3.66	8 (33%)
3	V7O	i	5034	3	0,10,25	-	-	-	-	-
5	DUR	Q	2122	-	17,17,17	1.77	5 (29%)	24,24,24	3.27	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
5	DUR	i	2072	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	C	2022	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	D	2032	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	c	3032	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	I	3072	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	E	2042	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	j	3082	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	b	3022	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	J	2082	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	R	2132	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	K	2092	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	H	2062	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	P	3122	-	1/1/3/3	2/6/18/18	0/2/2/2
5	DUR	k	3092	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	G	3052	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	M	3112	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	N	2102	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	F	2052	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	e	3042	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	l	3102	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	h	3062	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	a	3012	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	O	2112	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	B	2012	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	Q	2122	-	1/1/3/3	4/6/18/18	0/2/2/2

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	a	3012	DUR	C6-C5	5.38	1.47	1.35
5	J	2082	DUR	C6-C5	5.34	1.47	1.35
5	c	3032	DUR	C6-C5	5.17	1.47	1.35
5	i	2072	DUR	C6-C5	5.16	1.47	1.35
5	D	2032	DUR	C6-C5	5.09	1.46	1.35
5	E	2042	DUR	C6-C5	5.07	1.46	1.35
5	O	2112	DUR	C6-C5	5.00	1.46	1.35
5	C	2022	DUR	C6-C5	5.00	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	2132	DUR	C6-C5	4.99	1.46	1.35
5	h	3062	DUR	C6-C5	4.95	1.46	1.35
5	I	3072	DUR	C6-C5	4.92	1.46	1.35
5	F	2052	DUR	C6-C5	4.86	1.46	1.35
5	Q	2122	DUR	C6-C5	4.84	1.46	1.35
5	j	3082	DUR	C6-C5	4.79	1.46	1.35
5	l	3102	DUR	C6-C5	4.76	1.46	1.35
5	M	3112	DUR	C6-C5	4.71	1.46	1.35
5	N	2102	DUR	C6-C5	4.70	1.46	1.35
5	B	2012	DUR	C6-C5	4.67	1.45	1.35
5	H	2062	DUR	C6-C5	4.65	1.45	1.35
5	K	2092	DUR	C6-C5	4.63	1.45	1.35
5	k	3092	DUR	C6-C5	4.63	1.45	1.35
5	b	3022	DUR	C6-C5	4.60	1.45	1.35
5	P	3122	DUR	C6-C5	4.60	1.45	1.35
5	e	3042	DUR	C6-C5	4.38	1.45	1.35
5	G	3052	DUR	C6-C5	4.26	1.45	1.35
5	c	3032	DUR	C2'-C1'	3.79	1.62	1.52
5	G	3052	DUR	C2'-C1'	3.65	1.62	1.52
5	a	3012	DUR	C2'-C1'	3.63	1.62	1.52
5	j	3082	DUR	C2'-C1'	3.58	1.62	1.52
5	P	3122	DUR	C2'-C1'	3.51	1.61	1.52
5	k	3092	DUR	C2'-C1'	3.47	1.61	1.52
5	J	2082	DUR	C2'-C1'	3.36	1.61	1.52
5	H	2062	DUR	C2'-C1'	3.32	1.61	1.52
5	J	2082	DUR	C2-N1	3.30	1.43	1.38
5	R	2132	DUR	C2'-C1'	3.21	1.61	1.52
5	b	3022	DUR	C2'-C1'	3.19	1.61	1.52
5	I	3072	DUR	C2'-C1'	3.18	1.61	1.52
5	i	2072	DUR	C2'-C1'	3.17	1.61	1.52
5	F	2052	DUR	C2'-C1'	3.14	1.60	1.52
5	B	2012	DUR	C2'-C1'	3.11	1.60	1.52
5	h	3062	DUR	C2-N3	3.09	1.43	1.38
5	e	3042	DUR	C2'-C1'	3.03	1.60	1.52
5	K	2092	DUR	C2'-C1'	3.00	1.60	1.52
5	l	3102	DUR	C2'-C1'	2.99	1.60	1.52
5	h	3062	DUR	C4-N3	2.98	1.43	1.38
5	D	2032	DUR	C2'-C1'	2.97	1.60	1.52
5	h	3062	DUR	C2'-C1'	2.97	1.60	1.52
5	M	3112	DUR	C2'-C1'	2.86	1.60	1.52
5	E	2042	DUR	C2'-C1'	2.86	1.60	1.52
5	B	2012	DUR	C2-N1	2.85	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	2102	DUR	C2'-C1'	2.84	1.60	1.52
5	O	2112	DUR	C2'-C1'	2.83	1.60	1.52
5	B	2012	DUR	C4-N3	2.81	1.43	1.38
5	K	2092	DUR	C2-N1	2.80	1.42	1.38
5	C	2022	DUR	C2'-C1'	2.80	1.60	1.52
5	B	2012	DUR	C5-C4	2.72	1.49	1.43
5	R	2132	DUR	C2-N1	2.72	1.42	1.38
5	M	3112	DUR	C2-N1	2.68	1.42	1.38
5	R	2132	DUR	C4-N3	2.65	1.43	1.38
5	E	2042	DUR	C2-N1	2.64	1.42	1.38
5	c	3032	DUR	C2-N1	2.62	1.42	1.38
5	Q	2122	DUR	C2'-C1'	2.59	1.59	1.52
5	F	2052	DUR	C4-N3	2.59	1.43	1.38
5	O	2112	DUR	C2-N3	2.59	1.42	1.38
5	k	3092	DUR	C4-N3	2.58	1.43	1.38
5	C	2022	DUR	C2-N1	2.56	1.42	1.38
5	I	3072	DUR	C2-N3	2.53	1.42	1.38
5	a	3012	DUR	C2-N3	2.49	1.42	1.38
5	c	3032	DUR	C2'-C3'	2.49	1.59	1.52
5	O	2112	DUR	C4-N3	2.48	1.42	1.38
5	N	2102	DUR	C2-N1	2.47	1.42	1.38
5	c	3032	DUR	C2-N3	2.46	1.42	1.38
5	C	2022	DUR	C2-N3	2.45	1.42	1.38
5	O	2112	DUR	C2-N1	2.39	1.42	1.38
5	C	2022	DUR	C5-C4	2.38	1.48	1.43
5	P	3122	DUR	C2'-C3'	2.37	1.58	1.52
5	K	2092	DUR	C4-N3	2.36	1.42	1.38
5	k	3092	DUR	C2'-C3'	2.33	1.58	1.52
5	j	3082	DUR	C2'-C3'	2.32	1.58	1.52
5	E	2042	DUR	C2-N3	2.32	1.42	1.38
5	h	3062	DUR	C5-C4	2.32	1.48	1.43
5	b	3022	DUR	C4-N3	2.30	1.42	1.38
5	i	2072	DUR	C2-N3	2.30	1.42	1.38
5	E	2042	DUR	C5-C4	2.28	1.48	1.43
5	e	3042	DUR	C2-N1	2.28	1.42	1.38
5	B	2012	DUR	C2'-C3'	2.27	1.58	1.52
5	i	2072	DUR	C2-N1	2.26	1.42	1.38
5	F	2052	DUR	C2-N3	2.24	1.41	1.38
5	k	3092	DUR	C5-C4	2.23	1.48	1.43
5	J	2082	DUR	C5-C4	2.21	1.48	1.43
5	F	2052	DUR	C2-N1	2.20	1.41	1.38
5	Q	2122	DUR	C4-N3	2.20	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	a	3012	DUR	C4-N3	2.20	1.42	1.38
5	D	2032	DUR	C2-N1	2.17	1.41	1.38
5	C	2022	DUR	C2'-C3'	2.16	1.58	1.52
5	b	3022	DUR	C2'-C3'	2.12	1.58	1.52
5	l	3102	DUR	C2'-C3'	2.11	1.58	1.52
5	I	3072	DUR	C4-N3	2.10	1.42	1.38
5	G	3052	DUR	C2-N1	2.10	1.41	1.38
5	O	2112	DUR	C5-C4	2.10	1.48	1.43
5	F	2052	DUR	C5-C4	2.09	1.48	1.43
5	i	2072	DUR	C5-C4	2.09	1.48	1.43
5	N	2102	DUR	C4-N3	2.09	1.42	1.38
5	Q	2122	DUR	C5-C4	2.09	1.48	1.43
5	H	2062	DUR	C2-N1	2.05	1.41	1.38
5	J	2082	DUR	C2'-C3'	2.05	1.58	1.52
5	h	3062	DUR	C2-N1	2.04	1.41	1.38
5	K	2092	DUR	C5-C4	2.03	1.48	1.43
5	Q	2122	DUR	C2-N3	2.02	1.41	1.38
5	i	2072	DUR	C2'-C3'	2.02	1.58	1.52
5	a	3012	DUR	C2'-C3'	2.02	1.58	1.52
5	R	2132	DUR	C2-N3	2.02	1.41	1.38
5	C	2022	DUR	C4-N3	2.02	1.42	1.38

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2022	DUR	C2'-C1'-N1	15.46	152.46	113.81
5	c	3032	DUR	C2'-C1'-N1	15.21	151.85	113.81
5	F	2052	DUR	C2'-C1'-N1	14.67	150.50	113.81
5	I	3072	DUR	C2'-C1'-N1	14.44	149.91	113.81
5	j	3082	DUR	C2'-C1'-N1	14.33	149.65	113.81
5	h	3062	DUR	C2'-C1'-N1	14.30	149.56	113.81
5	P	3122	DUR	C2'-C1'-N1	14.22	149.37	113.81
5	B	2012	DUR	C2'-C1'-N1	14.17	149.24	113.81
5	b	3022	DUR	C2'-C1'-N1	14.12	149.12	113.81
5	J	2082	DUR	C2'-C1'-N1	14.09	149.05	113.81
5	i	2072	DUR	C2'-C1'-N1	14.09	149.05	113.81
5	K	2092	DUR	C2'-C1'-N1	14.08	149.02	113.81
5	e	3042	DUR	C2'-C1'-N1	14.07	148.99	113.81
5	M	3112	DUR	C2'-C1'-N1	14.07	148.98	113.81
5	R	2132	DUR	C2'-C1'-N1	14.00	148.82	113.81
5	k	3092	DUR	C2'-C1'-N1	13.91	148.60	113.81
5	D	2032	DUR	C2'-C1'-N1	13.88	148.51	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	3012	DUR	C2'-C1'-N1	13.73	148.14	113.81
5	Q	2122	DUR	C2'-C1'-N1	13.71	148.08	113.81
5	O	2112	DUR	C2'-C1'-N1	13.62	147.87	113.81
5	E	2042	DUR	C2'-C1'-N1	13.61	147.84	113.81
5	G	3052	DUR	C2'-C1'-N1	13.56	147.72	113.81
5	l	3102	DUR	C2'-C1'-N1	13.44	147.43	113.81
5	N	2102	DUR	C2'-C1'-N1	13.41	147.34	113.81
5	H	2062	DUR	C2'-C1'-N1	13.24	146.92	113.81
5	c	3032	DUR	O4'-C1'-C2'	-7.01	93.16	106.25
5	C	2022	DUR	O4'-C1'-C2'	-6.59	93.94	106.25
5	j	3082	DUR	N3-C2-N1	6.48	123.33	114.89
5	P	3122	DUR	O4'-C1'-C2'	-6.06	94.91	106.25
5	b	3022	DUR	O4'-C1'-C2'	-6.06	94.92	106.25
5	a	3012	DUR	O4'-C1'-C2'	-6.00	95.03	106.25
5	M	3112	DUR	O4'-C1'-C2'	-5.82	95.37	106.25
5	c	3032	DUR	N3-C2-N1	5.81	122.46	114.89
5	E	2042	DUR	O4'-C1'-C2'	-5.81	95.39	106.25
5	c	3032	DUR	C6-N1-C2	-5.76	113.99	121.00
5	B	2012	DUR	O4'-C1'-C2'	-5.73	95.55	106.25
5	J	2082	DUR	O4'-C1'-C2'	-5.52	95.94	106.25
5	k	3092	DUR	N3-C2-N1	5.44	121.97	114.89
5	a	3012	DUR	C6-N1-C2	-5.43	114.39	121.00
5	R	2132	DUR	O4'-C1'-C2'	-5.36	96.24	106.25
5	E	2042	DUR	N3-C2-N1	5.29	121.78	114.89
5	e	3042	DUR	O4'-C1'-C2'	-5.29	96.36	106.25
5	C	2022	DUR	N3-C2-N1	5.29	121.77	114.89
5	j	3082	DUR	O4'-C1'-C2'	-5.27	96.40	106.25
5	a	3012	DUR	N3-C2-N1	5.21	121.67	114.89
5	P	3122	DUR	C6-N1-C2	-5.17	114.71	121.00
5	b	3022	DUR	C6-N1-C2	-5.15	114.73	121.00
5	l	3102	DUR	N3-C2-N1	5.12	121.56	114.89
5	k	3092	DUR	O4'-C1'-C2'	-5.12	96.69	106.25
5	M	3112	DUR	N3-C2-N1	5.06	121.48	114.89
5	D	2032	DUR	N3-C2-N1	4.94	121.33	114.89
5	i	2072	DUR	N3-C2-N1	4.93	121.31	114.89
5	P	3122	DUR	N3-C2-N1	4.92	121.30	114.89
5	B	2012	DUR	N3-C2-N1	4.87	121.23	114.89
5	a	3012	DUR	O4'-C1'-N1	4.85	116.47	107.86
5	J	2082	DUR	N3-C2-N1	4.82	121.16	114.89
5	G	3052	DUR	O4'-C1'-C2'	-4.80	97.27	106.25
5	D	2032	DUR	O4'-C1'-C2'	-4.80	97.27	106.25
5	F	2052	DUR	O4'-C1'-C2'	-4.75	97.37	106.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	3072	DUR	O4'-C1'-C2'	-4.71	97.44	106.25
5	F	2052	DUR	N3-C2-N1	4.64	120.92	114.89
5	J	2082	DUR	C6-N1-C2	-4.62	115.38	121.00
5	I	3072	DUR	N3-C2-N1	4.58	120.86	114.89
5	i	2072	DUR	O4'-C1'-C2'	-4.56	97.72	106.25
5	Q	2122	DUR	N3-C2-N1	4.56	120.83	114.89
5	e	3042	DUR	N3-C2-N1	4.53	120.79	114.89
5	R	2132	DUR	N3-C2-N1	4.51	120.76	114.89
5	D	2032	DUR	C6-N1-C2	-4.48	115.55	121.00
5	R	2132	DUR	C6-N1-C2	-4.48	115.55	121.00
5	l	3102	DUR	O4'-C1'-C2'	-4.46	97.92	106.25
5	j	3082	DUR	C6-N1-C2	-4.46	115.57	121.00
5	E	2042	DUR	O4'-C1'-N1	4.41	115.69	107.86
5	H	2062	DUR	O4'-C1'-C2'	-4.37	98.09	106.25
5	N	2102	DUR	N3-C2-N1	4.35	120.55	114.89
5	j	3082	DUR	O2-C2-N3	-4.33	113.50	121.49
5	k	3092	DUR	C6-N1-C2	-4.32	115.74	121.00
5	H	2062	DUR	N3-C2-N1	4.29	120.48	114.89
5	l	3102	DUR	C6-N1-C2	-4.19	115.89	121.00
5	J	2082	DUR	O2-C2-N3	-4.19	113.76	121.49
5	b	3022	DUR	O4'-C1'-N1	4.14	115.22	107.86
5	c	3032	DUR	O4'-C4'-C5'	-4.10	100.56	109.22
5	E	2042	DUR	C6-N1-C2	-4.10	116.01	121.00
5	C	2022	DUR	C5'-C4'-C3'	4.09	125.02	114.82
5	O	2112	DUR	N3-C2-N1	4.06	120.17	114.89
5	G	3052	DUR	O4'-C4'-C5'	-4.02	100.72	109.22
5	O	2112	DUR	O4'-C1'-C2'	-4.01	98.76	106.25
5	R	2132	DUR	O4'-C1'-N1	3.99	114.95	107.86
5	K	2092	DUR	N3-C2-N1	3.96	120.04	114.89
5	G	3052	DUR	C6-N1-C2	-3.91	116.23	121.00
5	F	2052	DUR	C6-N1-C2	-3.88	116.28	121.00
5	c	3032	DUR	O4'-C1'-N1	3.85	114.70	107.86
5	H	2062	DUR	O4'-C1'-N1	3.83	114.66	107.86
5	b	3022	DUR	N3-C2-N1	3.82	119.87	114.89
5	K	2092	DUR	O4'-C1'-C2'	-3.80	99.14	106.25
5	G	3052	DUR	O4'-C1'-N1	3.80	114.61	107.86
5	h	3062	DUR	O4'-C1'-C2'	-3.80	99.15	106.25
5	i	2072	DUR	C6-N1-C2	-3.79	116.38	121.00
5	C	2022	DUR	C6-N1-C2	-3.79	116.39	121.00
5	G	3052	DUR	N3-C2-N1	3.77	119.81	114.89
5	M	3112	DUR	C6-N1-C2	-3.75	116.44	121.00
5	l	3102	DUR	O4'-C1'-N1	3.70	114.43	107.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	2102	DUR	C6-N1-C2	-3.67	116.53	121.00
5	B	2012	DUR	O2-C2-N3	-3.65	114.77	121.49
5	I	3072	DUR	C6-N1-C2	-3.62	116.59	121.00
5	P	3122	DUR	O4'-C1'-N1	3.58	114.21	107.86
5	c	3032	DUR	O2-C2-N3	-3.56	114.93	121.49
5	N	2102	DUR	O4'-C1'-C2'	-3.55	99.61	106.25
5	H	2062	DUR	C6-N1-C2	-3.54	116.68	121.00
5	j	3082	DUR	O4'-C4'-C5'	-3.52	101.76	109.22
5	h	3062	DUR	C5'-C4'-C3'	3.51	123.57	114.82
5	M	3112	DUR	O2-C2-N3	-3.38	115.26	121.49
5	h	3062	DUR	N3-C2-N1	3.35	119.26	114.89
5	j	3082	DUR	O4'-C1'-N1	3.32	113.76	107.86
5	R	2132	DUR	O2-C2-N3	-3.30	115.40	121.49
5	D	2032	DUR	O4'-C1'-N1	3.30	113.71	107.86
5	e	3042	DUR	O2-C2-N3	-3.28	115.43	121.49
5	e	3042	DUR	O4'-C1'-N1	3.27	113.66	107.86
5	B	2012	DUR	O4'-C1'-N1	3.21	113.56	107.86
5	N	2102	DUR	O2-C2-N3	-3.20	115.59	121.49
5	b	3022	DUR	C5-C6-N1	3.20	127.04	121.84
5	e	3042	DUR	C6-N1-C2	-3.19	117.11	121.00
5	k	3092	DUR	O3'-C3'-C2'	3.18	121.93	110.88
5	F	2052	DUR	C5'-C4'-C3'	3.18	122.75	114.82
5	P	3122	DUR	O2-C2-N3	-3.18	115.63	121.49
5	k	3092	DUR	O4'-C1'-N1	3.15	113.46	107.86
5	h	3062	DUR	O4'-C4'-C5'	-3.14	102.59	109.22
5	c	3032	DUR	C5'-C4'-C3'	3.11	122.58	114.82
5	Q	2122	DUR	O4'-C1'-C2'	-3.10	100.45	106.25
5	K	2092	DUR	O2-C2-N3	-3.09	115.79	121.49
5	l	3102	DUR	O2-C2-N3	-3.08	115.81	121.49
5	J	2082	DUR	O4'-C1'-N1	3.07	113.31	107.86
5	I	3072	DUR	C5'-C4'-C3'	3.07	122.47	114.82
5	M	3112	DUR	O4'-C1'-N1	3.06	113.30	107.86
5	B	2012	DUR	C6-N1-C2	-3.05	117.29	121.00
5	B	2012	DUR	C5'-C4'-C3'	3.03	122.39	114.82
5	R	2132	DUR	C1'-N1-C2	3.03	123.58	117.66
5	Q	2122	DUR	C6-N1-C2	-3.00	117.34	121.00
5	O	2112	DUR	C6-N1-C2	-2.96	117.40	121.00
5	O	2112	DUR	O4'-C1'-N1	2.93	113.07	107.86
5	N	2102	DUR	O4'-C1'-N1	2.92	113.05	107.86
5	F	2052	DUR	O4'-C4'-C5'	-2.90	103.08	109.22
5	D	2032	DUR	O2-C2-N3	-2.90	116.14	121.49
5	G	3052	DUR	C5'-C4'-C3'	2.87	121.99	114.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	3012	DUR	C5-C4-N3	-2.86	110.78	114.80
5	D	2032	DUR	C5'-C4'-C3'	2.84	121.89	114.82
5	E	2042	DUR	O2-C2-N3	-2.80	116.32	121.49
5	H	2062	DUR	O2-C2-N3	-2.79	116.34	121.49
5	c	3032	DUR	C1'-N1-C2	2.78	123.10	117.66
5	k	3092	DUR	O2-C2-N3	-2.78	116.35	121.49
5	e	3042	DUR	C5'-C4'-C3'	2.72	121.61	114.82
5	c	3032	DUR	C5-C6-N1	2.70	126.23	121.84
5	K	2092	DUR	C5'-C4'-C3'	2.70	121.55	114.82
5	i	2072	DUR	O2-C2-N3	-2.68	116.54	121.49
5	c	3032	DUR	O3'-C3'-C2'	2.64	120.05	110.88
5	G	3052	DUR	O2-C2-N3	-2.63	116.64	121.49
5	P	3122	DUR	O3'-C3'-C2'	2.61	119.95	110.88
5	K	2092	DUR	C6-N1-C2	-2.60	117.83	121.00
5	C	2022	DUR	O2-C2-N3	-2.60	116.70	121.49
5	K	2092	DUR	O4'-C4'-C5'	-2.58	103.75	109.22
5	F	2052	DUR	O2-C2-N3	-2.57	116.74	121.49
5	b	3022	DUR	O2-C2-N3	-2.55	116.79	121.49
5	a	3012	DUR	O2-C2-N3	-2.54	116.80	121.49
5	R	2132	DUR	C5'-C4'-C3'	2.52	121.12	114.82
5	j	3082	DUR	O3'-C3'-C2'	2.51	119.59	110.88
5	C	2022	DUR	O4'-C1'-N1	2.50	112.31	107.86
5	i	2072	DUR	O4'-C1'-N1	2.50	112.30	107.86
5	l	3102	DUR	C5'-C4'-C3'	2.46	120.96	114.82
5	E	2042	DUR	C5'-C4'-C3'	2.42	120.85	114.82
5	P	3122	DUR	O4-C4-C5	2.40	129.30	125.16
5	P	3122	DUR	C5-C6-N1	2.39	125.73	121.84
5	I	3072	DUR	O4'-C4'-C5'	-2.38	104.18	109.22
5	i	2072	DUR	O3'-C3'-C2'	2.38	119.15	110.88
5	B	2012	DUR	O4'-C4'-C5'	-2.37	104.20	109.22
5	P	3122	DUR	O4'-C4'-C5'	-2.37	104.21	109.22
5	h	3062	DUR	C6-N1-C2	-2.36	118.12	121.00
5	b	3022	DUR	O4'-C4'-C5'	-2.35	104.25	109.22
5	N	2102	DUR	C1'-N1-C2	2.35	122.25	117.66
5	j	3082	DUR	C5'-C4'-C3'	2.34	120.66	114.82
5	E	2042	DUR	O4'-C4'-C5'	-2.33	104.29	109.22
5	i	2072	DUR	C5'-C4'-C3'	2.32	120.61	114.82
5	R	2132	DUR	O4'-C4'-C5'	-2.31	104.33	109.22
5	F	2052	DUR	C1'-N1-C2	2.31	122.17	117.66
5	I	3072	DUR	O4'-C1'-N1	2.29	111.93	107.86
5	Q	2122	DUR	O3'-C3'-C2'	2.28	118.81	110.88
5	K	2092	DUR	C1'-N1-C2	2.28	122.11	117.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	3012	DUR	C5-C6-N1	2.28	125.54	121.84
5	R	2132	DUR	C5-C6-N1	2.27	125.52	121.84
5	D	2032	DUR	O4'-C4'-C5'	-2.25	104.46	109.22
5	O	2112	DUR	C5'-C4'-C3'	2.25	120.43	114.82
5	j	3082	DUR	C1'-N1-C2	2.24	122.03	117.66
5	P	3122	DUR	C1'-N1-C6	2.21	125.88	121.53
5	a	3012	DUR	O3'-C3'-C2'	2.21	118.56	110.88
5	M	3112	DUR	O3'-C3'-C2'	2.20	118.53	110.88
5	Q	2122	DUR	O2-C2-N3	-2.20	117.43	121.49
5	C	2022	DUR	O4'-C4'-C5'	-2.19	104.58	109.22
5	G	3052	DUR	O3'-C3'-C2'	2.19	118.47	110.88
5	j	3082	DUR	C4-N3-C2	-2.19	123.90	126.61
5	F	2052	DUR	O4'-C1'-N1	2.18	111.73	107.86
4	c	3031	PO4	O4-P-O2	2.14	114.57	107.91
5	C	2022	DUR	O4'-C4'-C3'	-2.13	100.78	105.65
5	l	3102	DUR	O4'-C4'-C5'	-2.09	104.80	109.22
5	l	3102	DUR	O3'-C3'-C2'	2.08	118.11	110.88
5	N	2102	DUR	C5'-C4'-C3'	2.07	119.99	114.82
5	J	2082	DUR	O3'-C3'-C4'	-2.05	102.29	110.07
5	b	3022	DUR	C1'-N1-C2	2.05	121.67	117.66
5	N	2102	DUR	O4'-C4'-C5'	-2.04	104.90	109.22
5	K	2092	DUR	O4'-C1'-N1	2.01	111.44	107.86
5	C	2022	DUR	O3'-C3'-C4'	-2.01	102.45	110.07

All (25) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	a	3012	DUR	C1'
5	B	2012	DUR	C1'
5	b	3022	DUR	C1'
5	C	2022	DUR	C1'
5	c	3032	DUR	C1'
5	D	2032	DUR	C1'
5	E	2042	DUR	C1'
5	e	3042	DUR	C1'
5	F	2052	DUR	C1'
5	R	2132	DUR	C1'
5	G	3052	DUR	C1'
5	P	3122	DUR	C1'
5	H	2062	DUR	C1'
5	h	3062	DUR	C1'
5	I	3072	DUR	C1'

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Mol	Chain	Res	Type	Atom
5	i	2072	DUR	C1'
5	J	2082	DUR	C1'
5	j	3082	DUR	C1'
5	K	2092	DUR	C1'
5	k	3092	DUR	C1'
5	l	3102	DUR	C1'
5	M	3112	DUR	C1'
5	N	2102	DUR	C1'
5	Q	2122	DUR	C1'
5	O	2112	DUR	C1'

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	3112	DUR	C2'-C1'-N1-C2
5	k	3092	DUR	C3'-C4'-C5'-O5'
5	Q	2122	DUR	C3'-C4'-C5'-O5'
5	k	3092	DUR	O4'-C4'-C5'-O5'
5	Q	2122	DUR	O4'-C4'-C5'-O5'
5	F	2052	DUR	C3'-C4'-C5'-O5'
5	h	3062	DUR	C3'-C4'-C5'-O5'
5	I	3072	DUR	C3'-C4'-C5'-O5'
5	J	2082	DUR	C3'-C4'-C5'-O5'
5	K	2092	DUR	C3'-C4'-C5'-O5'
5	N	2102	DUR	C3'-C4'-C5'-O5'
5	O	2112	DUR	C3'-C4'-C5'-O5'
5	M	3112	DUR	C2'-C1'-N1-C6
5	b	3022	DUR	C2'-C1'-N1-C2
5	C	2022	DUR	C2'-C1'-N1-C2
5	c	3032	DUR	C2'-C1'-N1-C2
5	E	2042	DUR	C2'-C1'-N1-C2
5	e	3042	DUR	C2'-C1'-N1-C2
5	P	3122	DUR	C2'-C1'-N1-C2
5	I	3072	DUR	C2'-C1'-N1-C2
5	J	2082	DUR	C2'-C1'-N1-C2
5	k	3092	DUR	C2'-C1'-N1-C2
5	I	3072	DUR	O4'-C4'-C5'-O5'
5	K	2092	DUR	O4'-C4'-C5'-O5'
5	i	2072	DUR	C3'-C4'-C5'-O5'
5	F	2052	DUR	O4'-C4'-C5'-O5'
5	h	3062	DUR	O4'-C4'-C5'-O5'
5	i	2072	DUR	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	J	2082	DUR	O4'-C4'-C5'-O5'
5	N	2102	DUR	O4'-C4'-C5'-O5'
5	C	2022	DUR	C2'-C1'-N1-C6
5	E	2042	DUR	C2'-C1'-N1-C6
5	e	3042	DUR	C2'-C1'-N1-C6
5	P	3122	DUR	C2'-C1'-N1-C6
5	J	2082	DUR	C2'-C1'-N1-C6
5	a	3012	DUR	C2'-C1'-N1-C2
5	B	2012	DUR	C2'-C1'-N1-C2
5	D	2032	DUR	C2'-C1'-N1-C2
5	F	2052	DUR	C2'-C1'-N1-C2
5	R	2132	DUR	C2'-C1'-N1-C2
5	H	2062	DUR	C2'-C1'-N1-C2
5	h	3062	DUR	C2'-C1'-N1-C2
5	i	2072	DUR	C2'-C1'-N1-C2
5	j	3082	DUR	C2'-C1'-N1-C2
5	O	2112	DUR	C2'-C1'-N1-C2
5	O	2112	DUR	O4'-C4'-C5'-O5'
5	e	3042	DUR	O4'-C4'-C5'-O5'
5	H	2062	DUR	O4'-C4'-C5'-O5'
5	l	3102	DUR	O4'-C4'-C5'-O5'
5	M	3112	DUR	O4'-C4'-C5'-O5'
5	l	3102	DUR	C3'-C4'-C5'-O5'
5	M	3112	DUR	C3'-C4'-C5'-O5'
5	a	3012	DUR	O4'-C4'-C5'-O5'
5	F	2052	DUR	C2'-C1'-N1-C6
5	G	3052	DUR	C2'-C1'-N1-C2
5	K	2092	DUR	C2'-C1'-N1-C2
5	a	3012	DUR	C3'-C4'-C5'-O5'
5	c	3032	DUR	C3'-C4'-C5'-O5'
5	e	3042	DUR	C3'-C4'-C5'-O5'
5	H	2062	DUR	C3'-C4'-C5'-O5'
5	j	3082	DUR	C3'-C4'-C5'-O5'
5	R	2132	DUR	C3'-C4'-C5'-O5'
5	B	2012	DUR	C2'-C1'-N1-C6
5	b	3022	DUR	C2'-C1'-N1-C6
5	c	3032	DUR	C2'-C1'-N1-C6
5	D	2032	DUR	C2'-C1'-N1-C6
5	H	2062	DUR	C2'-C1'-N1-C6
5	I	3072	DUR	C2'-C1'-N1-C6
5	i	2072	DUR	C2'-C1'-N1-C6
5	K	2092	DUR	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
5	k	3092	DUR	C2'-C1'-N1-C6
5	O	2112	DUR	C2'-C1'-N1-C6
5	l	3102	DUR	C2'-C1'-N1-C2
5	Q	2122	DUR	C2'-C1'-N1-C2
5	j	3082	DUR	O4'-C4'-C5'-O5'
5	c	3032	DUR	O4'-C4'-C5'-O5'
5	R	2132	DUR	O4'-C4'-C5'-O5'
5	B	2012	DUR	C3'-C4'-C5'-O5'
5	a	3012	DUR	C2'-C1'-N1-C6
5	R	2132	DUR	C2'-C1'-N1-C6
5	G	3052	DUR	C2'-C1'-N1-C6
5	h	3062	DUR	C2'-C1'-N1-C6
5	j	3082	DUR	C2'-C1'-N1-C6
5	Q	2122	DUR	C2'-C1'-N1-C6
5	N	2102	DUR	C2'-C1'-N1-C2
5	E	2042	DUR	O4'-C4'-C5'-O5'
5	l	3102	DUR	C2'-C1'-N1-C6
5	E	2042	DUR	C3'-C4'-C5'-O5'
5	G	3052	DUR	C3'-C4'-C5'-O5'
5	G	3052	DUR	O4'-C4'-C5'-O5'
5	N	2102	DUR	C2'-C1'-N1-C6
5	D	2032	DUR	O4'-C4'-C5'-O5'
5	B	2012	DUR	O4'-C4'-C5'-O5'
5	C	2022	DUR	C3'-C4'-C5'-O5'
5	D	2032	DUR	C3'-C4'-C5'-O5'
5	C	2022	DUR	O4'-C4'-C5'-O5'
5	b	3022	DUR	C3'-C4'-C5'-O5'
5	b	3022	DUR	O4'-C4'-C5'-O5'

There are no ring outliers.

28 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5012	V7O	1	0
3	J	5042	V7O	5	0
5	C	2022	DUR	1	0
4	C	2021	PO4	1	0
3	D	5022	V7O	3	0
3	L	5041	V7O	1	0
3	b	5013	V7O	2	0
3	I	5032	V7O	3	0
3	e	5023	V7O	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	k	3091	PO4	1	0
3	Q	5053	V7O	1	0
4	G	3051	PO4	1	0
3	h	5033	V7O	3	0
5	P	3122	DUR	1	0
4	O	2111	PO4	1	0
5	G	3052	DUR	1	0
3	R	5024	V7O	2	0
3	A	5011	V7O	1	0
3	c	5014	V7O	2	0
3	o	5054	V7O	1	0
4	l	3101	PO4	1	0
3	M	5051	V7O	3	0
4	P	3121	PO4	2	0
3	M	5052	V7O	4	0
3	H	5031	V7O	2	0
3	D	5021	V7O	2	0
4	H	2061	PO4	1	0
3	i	5034	V7O	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	A	250/253 (98%)	-0.35	2 (0%) 82 75	4, 15, 31, 46	0
1	B	246/253 (97%)	-0.42	2 (0%) 82 75	4, 14, 29, 63	0
1	C	246/253 (97%)	-0.05	10 (4%) 41 33	4, 14, 29, 63	0
1	D	246/253 (97%)	0.05	11 (4%) 38 30	4, 14, 29, 63	0
1	E	246/253 (97%)	-0.07	1 (0%) 88 84	4, 14, 29, 63	0
1	F	246/253 (97%)	-0.20	4 (1%) 70 61	4, 14, 29, 63	0
1	G	242/253 (95%)	-0.34	1 (0%) 88 84	6, 13, 25, 37	0
1	H	246/253 (97%)	-0.17	5 (2%) 65 56	4, 14, 29, 63	0
1	I	242/253 (95%)	-0.04	0 100 100	5, 13, 25, 37	0
1	J	246/253 (97%)	-0.16	2 (0%) 82 75	4, 14, 29, 63	0
1	K	246/253 (97%)	0.17	18 (7%) 21 15	4, 14, 29, 63	0
1	L	250/253 (98%)	0.19	8 (3%) 50 40	4, 15, 31, 46	0
1	M	242/253 (95%)	0.09	5 (2%) 63 54	5, 13, 25, 37	0
1	N	246/253 (97%)	0.60	17 (6%) 23 16	4, 14, 29, 63	0
1	O	246/253 (97%)	0.56	20 (8%) 18 13	4, 14, 29, 63	0
1	P	242/253 (95%)	-0.56	1 (0%) 88 84	6, 13, 25, 37	0
1	Q	246/253 (97%)	0.99	25 (10%) 12 9	4, 14, 29, 63	0
1	R	246/253 (97%)	-0.21	6 (2%) 59 49	4, 14, 29, 63	0
1	a	242/253 (95%)	-0.56	1 (0%) 88 84	6, 13, 25, 37	0
1	b	242/253 (95%)	-0.54	1 (0%) 88 84	5, 13, 25, 37	0
1	c	242/253 (95%)	-0.50	1 (0%) 88 84	5, 13, 25, 37	0
1	d	250/253 (98%)	-0.03	8 (3%) 50 40	4, 15, 31, 46	0
1	e	242/253 (95%)	-0.25	2 (0%) 82 75	6, 13, 25, 37	0
1	h	242/253 (95%)	0.32	5 (2%) 63 54	6, 13, 25, 37	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	i	246/253 (97%)	-0.35	2 (0%) 82 75	4, 14, 29, 63	0
1	j	242/253 (95%)	-0.48	0 100 100	5, 13, 25, 37	0
1	k	242/253 (95%)	-0.38	1 (0%) 88 84	6, 13, 25, 37	0
1	l	242/253 (95%)	0.46	8 (3%) 49 39	5, 13, 25, 37	0
1	m	250/253 (98%)	0.82	60 (24%) 2 1	4, 15, 31, 46	0
1	o	250/253 (98%)	0.20	12 (4%) 35 28	4, 15, 31, 46	0
All	All	7352/7590 (96%)	-0.04	239 (3%) 49 39	4, 14, 28, 63	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	m	3153	VAL	6.7
1	Q	1229	PRO	6.1
1	m	3142	GLU	5.9
1	m	3093	GLY	5.8
1	m	3228	ILE	5.6
1	m	3233	THR	5.4
1	m	3098	ILE	5.3
1	o	3226	GLN	5.2
1	d	3226	GLN	4.9
1	m	3223	ARG	4.9
1	m	3217	ALA	4.8
1	m	3109	VAL	4.7
1	O	1228	ILE	4.6
1	N	1239	SER	4.5
1	m	3097	ALA	4.5
1	m	3234	MET	4.5
1	O	1142	GLU	4.4
1	m	3140	LEU	4.2
1	m	3225	GLN	4.2
1	m	3231	ALA	4.2
1	M	2148	GLY	4.1
1	m	3108	LEU	4.1
1	m	3226	GLN	4.0
1	O	1225	GLN	4.0
1	m	3216	VAL	3.9
1	Q	1226	GLN	3.8
1	m	3241	ALA	3.8
1	m	3092	ILE	3.7
1	m	3099	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	m	3151	THR	3.7
1	e	2004	SER	3.7
1	m	3245	VAL	3.7
1	R	1039	ASP	3.6
1	K	1153	VAL	3.6
1	O	1229	PRO	3.6
1	Q	1053	TRP	3.6
1	C	1153	VAL	3.6
1	K	1234	MET	3.5
1	N	1234	MET	3.5
1	o	3229	PRO	3.5
1	m	3230	ASN	3.5
1	K	1225	GLN	3.5
1	e	2005	ASP	3.5
1	m	3222	ASN	3.4
1	D	1228	ILE	3.4
1	H	1145	LYS	3.4
1	m	3143	ALA	3.4
1	m	3152	HIS	3.4
1	H	1234	MET	3.3
1	m	3095	THR	3.3
1	m	3224	THR	3.3
1	o	3228	ILE	3.3
1	M	2149	ALA	3.3
1	m	3101	HIS	3.3
1	m	3148	GLY	3.3
1	m	3227	GLU	3.2
1	Q	1032	GLU	3.2
1	E	1234	MET	3.2
1	N	1034	ILE	3.2
1	d	3227	GLU	3.2
1	N	1189	ALA	3.1
1	m	3239	SER	3.1
1	L	3226	GLN	3.1
1	m	3100	PRO	3.1
1	L	3223	ARG	3.1
1	N	1237	THR	3.1
1	m	3221	VAL	3.0
1	Q	1105	GLY	3.0
1	K	1229	PRO	2.9
1	o	3230	ASN	2.9
1	Q	1208	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	l	2143	ALA	2.9
1	J	1237	THR	2.9
1	m	3218	GLY	2.9
1	O	1234	MET	2.9
1	m	3242	VAL	2.9
1	m	3150	THR	2.9
1	M	2147	ILE	2.9
1	N	1236	GLN	2.9
1	c	2014	ASN	2.9
1	m	3141	VAL	2.9
1	O	1040	LYS	2.8
1	O	1227	GLU	2.8
1	Q	1245	VAL	2.8
1	h	2230	ASN	2.8
1	N	1007	PHE	2.8
1	m	3144	ALA	2.8
1	A	3228	ILE	2.8
1	K	1237	THR	2.8
1	N	1235	LYS	2.8
1	K	1109	VAL	2.8
1	C	1098	ILE	2.8
1	Q	1125	PRO	2.8
1	D	1153	VAL	2.8
1	R	1014	ASN	2.8
1	m	3237	THR	2.8
1	o	3146	SER	2.8
1	o	3231	ALA	2.7
1	Q	1036	ALA	2.7
1	H	1237	THR	2.7
1	i	1237	THR	2.7
1	K	1099	GLN	2.7
1	O	1153	VAL	2.7
1	O	1145	LYS	2.7
1	D	1234	MET	2.7
1	o	3142	GLU	2.7
1	Q	1220	ILE	2.7
1	C	1229	PRO	2.7
1	K	1093	GLY	2.7
1	L	3224	THR	2.7
1	N	1010	GLY	2.7
1	b	2017	GLN	2.7
1	L	3153	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	m	3220	ILE	2.6
1	d	3146	SER	2.6
1	O	1146	SER	2.6
1	C	1228	ILE	2.6
1	K	1227	GLU	2.6
1	M	2240	HIS	2.6
1	R	1228	ILE	2.6
1	Q	1038	MET	2.6
1	m	3240	HIS	2.6
1	C	1224	THR	2.6
1	K	1098	ILE	2.6
1	Q	1221	VAL	2.6
1	o	3227	GLU	2.6
1	K	1223	ARG	2.5
1	m	3096	GLY	2.5
1	K	1228	ILE	2.5
1	D	1237	THR	2.5
1	K	1143	ALA	2.5
1	l	2010	GLY	2.5
1	J	1234	MET	2.5
1	m	3102	ILE	2.5
1	O	1144	ALA	2.5
1	h	2178	ARG	2.5
1	O	1147	ILE	2.5
1	d	3233	THR	2.5
1	B	1234	MET	2.5
1	Q	1234	MET	2.5
1	l	2244	ILE	2.5
1	m	3146	SER	2.5
1	N	1183	SER	2.5
1	m	3094	THR	2.5
1	C	1142	GLU	2.4
1	O	1143	ALA	2.4
1	Q	1052	THR	2.4
1	O	1152	HIS	2.4
1	L	3228	ILE	2.4
1	N	1053	TRP	2.4
1	O	1007	PHE	2.4
1	h	2143	ALA	2.4
1	L	3100	PRO	2.4
1	m	3235	LYS	2.4
1	H	1142	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	m	3238	GLU	2.4
1	D	1093	GLY	2.3
1	o	3148	GLY	2.3
1	N	1185	GLU	2.3
1	o	3225	GLN	2.3
1	R	1234	MET	2.3
1	C	1227	GLU	2.3
1	K	1217	ALA	2.3
1	a	2225	GLN	2.3
1	F	1226	GLN	2.3
1	m	3147	ILE	2.3
1	D	1100	PRO	2.3
1	L	3229	PRO	2.3
1	Q	1121	LEU	2.3
1	m	3243	LYS	2.3
1	N	1175	ARG	2.3
1	C	1100	PRO	2.3
1	F	1221	VAL	2.3
1	m	3229	PRO	2.3
1	N	1018	GLY	2.3
1	N	1182	GLY	2.3
1	C	1234	MET	2.3
1	l	2225	GLN	2.3
1	K	1220	ILE	2.3
1	N	1178	ARG	2.3
1	Q	1094	THR	2.3
1	Q	1150	THR	2.3
1	h	2014	ASN	2.2
1	o	3143	ALA	2.2
1	m	3236	GLN	2.2
1	d	3229	PRO	2.2
1	l	2146	SER	2.2
1	M	2146	SER	2.2
1	d	3231	ALA	2.2
1	l	2030	ARG	2.2
1	m	3219	VAL	2.2
1	m	3232	GLU	2.2
1	Q	1144	ALA	2.2
1	m	3103	ASN	2.2
1	m	3244	ILE	2.2
1	D	1109	VAL	2.2
1	F	1234	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	R	1153	VAL	2.2
1	m	3105	GLY	2.2
1	D	1146	SER	2.2
1	d	3142	GLU	2.2
1	m	3032	GLU	2.2
1	i	1234	MET	2.1
1	l	2148	GLY	2.1
1	o	3171	THR	2.1
1	Q	1241	ALA	2.1
1	O	1097	ALA	2.1
1	d	3228	ILE	2.1
1	O	1226	GLN	2.1
1	P	2240	HIS	2.1
1	K	1100	PRO	2.1
1	D	1223	ARG	2.1
1	B	1142	GLU	2.1
1	D	1227	GLU	2.1
1	D	1221	VAL	2.1
1	H	1153	VAL	2.1
1	m	3107	VAL	2.1
1	A	3233	THR	2.1
1	k	2170	ASP	2.1
1	Q	1148	GLY	2.1
1	O	1237	THR	2.1
1	R	1142	GLU	2.1
1	L	3235	LYS	2.1
1	Q	1062	VAL	2.1
1	K	1140	LEU	2.1
1	G	2175	ARG	2.1
1	K	1142	GLU	2.1
1	F	1153	VAL	2.0
1	h	2176	VAL	2.0
1	l	2246	VAL	2.0
1	C	1223	ARG	2.0
1	Q	1250	ARG	2.0
1	Q	1005	ASP	2.0
1	O	1039	ASP	2.0
1	Q	1042	VAL	2.0
1	O	1109	VAL	2.0
1	m	3030	ARG	2.0
1	Q	1118	GLY	2.0
1	N	1181	LYS	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
4	PO4	C	2021	5/5	0.40	0.28	147,148,148,148	0
4	PO4	Q	2121	5/5	0.51	0.21	131,131,132,132	0
4	PO4	R	2131	5/5	0.68	0.24	136,136,137,137	0
4	PO4	D	2031	5/5	0.69	0.25	135,135,135,136	0
4	PO4	E	2041	5/5	0.69	0.23	127,128,128,128	0
4	PO4	N	2101	5/5	0.71	0.21	126,126,126,127	0
4	PO4	I	3071	5/5	0.71	0.21	120,121,121,122	0
4	PO4	i	2071	5/5	0.73	0.24	127,128,128,128	0
4	PO4	O	2111	5/5	0.75	0.24	126,126,126,127	0
4	PO4	h	3061	5/5	0.76	0.18	124,125,125,125	0
5	DUR	N	2102	16/16	0.76	0.20	86,88,89,89	0
5	DUR	Q	2122	16/16	0.77	0.22	104,107,107,107	0
4	PO4	l	3101	5/5	0.78	0.17	107,107,108,108	0
4	PO4	H	2061	5/5	0.78	0.21	118,119,119,119	0
4	PO4	K	2091	5/5	0.78	0.20	114,114,115,115	0
4	PO4	J	2081	5/5	0.79	0.20	127,128,128,128	0
5	DUR	D	2032	16/16	0.79	0.15	68,72,73,74	0
5	DUR	I	3072	16/16	0.80	0.16	57,63,65,65	0
5	DUR	K	2092	16/16	0.80	0.19	77,81,83,83	0
5	DUR	C	2022	16/16	0.80	0.19	57,69,73,74	0
4	PO4	M	3111	5/5	0.80	0.22	106,106,107,108	0
3	V7O	o	5054	11/26	0.81	0.12	105,107,108,109	0
3	V7O	D	5021	11/26	0.81	0.13	91,94,95,96	0
5	DUR	O	2112	16/16	0.81	0.17	77,81,82,82	0
3	V7O	i	5034	11/26	0.82	0.12	86,88,90,91	0
4	PO4	G	3051	5/5	0.82	0.19	105,105,106,106	0
5	DUR	i	2072	16/16	0.82	0.16	72,75,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DUR	J	2082	16/16	0.82	0.15	50,55,61,62	0
5	DUR	R	2132	16/16	0.83	0.16	63,67,70,71	0
5	DUR	l	3102	16/16	0.83	0.14	61,66,67,68	0
4	PO4	F	2051	5/5	0.83	0.21	108,109,109,110	0
5	DUR	E	2042	16/16	0.83	0.14	59,65,67,67	0
5	DUR	F	2052	16/16	0.83	0.16	57,62,66,67	0
5	DUR	h	3062	16/16	0.84	0.13	53,60,63,64	0
5	DUR	B	2012	16/16	0.84	0.16	44,51,55,55	0
3	V7O	R	5024	11/26	0.84	0.11	86,88,89,92	0
5	DUR	e	3042	16/16	0.85	0.15	55,62,66,67	0
5	DUR	k	3092	16/16	0.85	0.14	43,47,52,53	0
5	DUR	H	2062	16/16	0.85	0.14	57,60,61,62	0
3	V7O	H	5031	11/26	0.86	0.11	96,97,98,99	0
4	PO4	k	3091	5/5	0.86	0.20	106,106,107,107	0
3	V7O	c	5014	11/26	0.86	0.11	84,86,88,89	0
5	DUR	c	3032	16/16	0.86	0.13	38,43,49,50	0
3	V7O	j	5044	11/26	0.87	0.11	88,89,93,94	0
3	V7O	L	5041	11/26	0.87	0.12	91,94,95,95	0
5	DUR	G	3052	16/16	0.88	0.12	42,46,52,53	0
3	V7O	A	5011	11/26	0.88	0.11	78,83,84,88	0
5	DUR	a	3012	16/16	0.89	0.12	35,43,51,51	0
3	V7O	M	5051	11/26	0.89	0.10	87,89,90,90	0
4	PO4	B	2011	5/5	0.89	0.18	101,102,102,102	0
5	DUR	M	3112	16/16	0.90	0.11	55,58,61,61	0
4	PO4	a	3011	5/5	0.90	0.15	67,68,70,70	0
4	PO4	c	3031	5/5	0.91	0.15	74,74,75,75	0
4	PO4	j	3081	5/5	0.91	0.17	81,81,82,82	0
2	K	o	4151	1/1	0.91	0.09	66,66,66,66	0
3	V7O	Q	5053	11/26	0.91	0.10	88,91,94,95	0
5	DUR	j	3082	16/16	0.91	0.11	38,42,47,47	0
4	PO4	P	3121	5/5	0.91	0.17	94,94,95,95	0
5	DUR	b	3022	16/16	0.92	0.11	36,41,46,48	0
3	V7O	M	5052	11/26	0.92	0.12	74,76,78,78	0
2	K	N	4141	1/1	0.92	0.07	61,61,61,61	0
3	V7O	B	5012	11/26	0.92	0.11	73,76,78,78	0
5	DUR	P	3122	16/16	0.92	0.10	31,37,43,45	0
3	V7O	e	5023	11/26	0.92	0.10	70,73,74,74	0
3	V7O	h	5033	11/26	0.93	0.12	76,78,80,80	0
3	V7O	b	5013	11/26	0.93	0.10	63,66,68,69	0
4	PO4	e	3041	5/5	0.93	0.12	87,87,88,88	0
2	K	L	4121	1/1	0.94	0.08	58,58,58,58	0
2	K	R	4061	1/1	0.94	0.08	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	V7O	D	5022	11/26	0.94	0.09	74,77,78,79	0
2	K	h	4081	1/1	0.94	0.07	51,51,51,51	0
3	V7O	J	5042	11/26	0.94	0.10	69,73,74,77	0
4	PO4	b	3021	5/5	0.95	0.12	80,80,81,81	0
3	V7O	k	5043	11/26	0.95	0.09	64,67,69,70	0
3	V7O	I	5032	11/26	0.95	0.08	76,79,80,82	0
2	K	D	4041	1/1	0.96	0.06	64,64,64,64	0
2	K	K	4111	1/1	0.97	0.04	47,47,47,47	0
2	K	M	4131	1/1	0.97	0.06	55,55,55,55	0
2	K	A	4011	1/1	0.98	0.09	34,34,34,34	0
2	K	G	4071	1/1	0.98	0.03	40,40,40,40	0
2	K	E	4051	1/1	0.98	0.04	49,49,49,49	0
2	K	i	4091	1/1	0.98	0.06	45,45,45,45	0
2	K	J	4101	1/1	0.98	0.09	32,32,32,32	0
2	K	B	4021	1/1	0.99	0.04	36,36,36,36	0
2	K	C	4031	1/1	0.99	0.06	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.