



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 09:05 pm BST

PDB ID : 5LOK  
Title : X-ray structure of uridine phosphorylase from *Vibrio cholerae* in complex with cytidine and cytosine at 1.11 Å resolution  
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Deposited on : 2016-08-09  
Resolution : 1.11 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

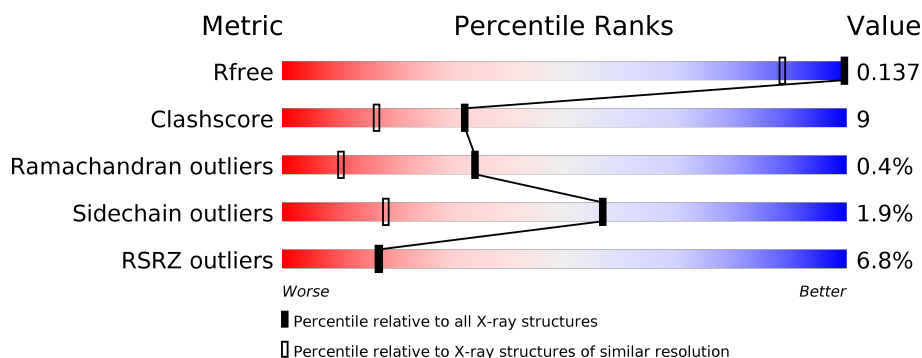
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.11 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))
$R_{free}$	130704	1619 (1.14-1.06)
Clashscore	141614	1671 (1.14-1.06)
Ramachandran outliers	138981	1615 (1.14-1.06)
Sidechain outliers	138945	1613 (1.14-1.06)
RSRZ outliers	127900	1588 (1.14-1.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	<div> <div>4%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	B	253	<div> <div>9%</div> <div>89%</div> <div>11%</div> </div>
1	C	253	<div> <div>4%</div> <div>86%</div> <div>13%</div> </div>
1	D	253	<div> <div>5%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	E	253	<div> <div>9%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	F	253	<div> <div>10%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	301	-	-	X	-
2	EDO	B	303	-	-	X	-
2	EDO	E	303	-	-	X	-
8	CL	E	301	-	-	X	-
8	CL	F	301	-	-	X	-

## 2 Entry composition [i](#)

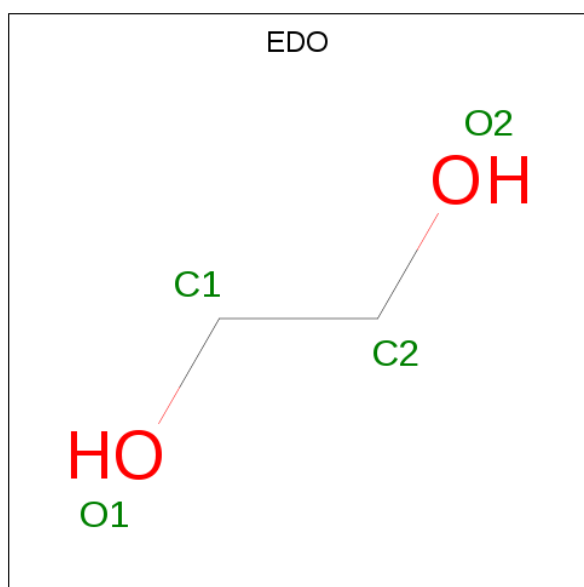
There are 9 unique types of molecules in this entry. The entry contains 27605 atoms, of which 13155 are hydrogens and 0 are deuteriums.

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	251	Total	C	H	N	O	S	0	52	0
			4333	1338	2187	380	409	19			
1	B	252	Total	C	H	N	O	S	0	47	0
			4374	1344	2231	380	401	18			
1	C	252	Total	C	H	N	O	S	0	38	0
			4216	1303	2139	360	396	18			
1	D	251	Total	C	H	N	O	S	0	35	0
			4209	1300	2132	369	391	17			
1	E	252	Total	C	H	N	O	S	0	45	0
			4306	1331	2182	369	407	17			
1	F	251	Total	C	H	N	O	S	0	46	0
			4268	1319	2154	371	408	16			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).

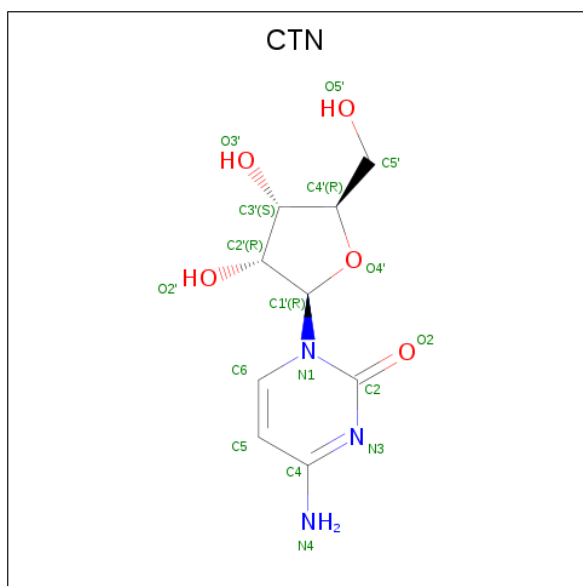


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		
3	E	1	Total	K	0	0
			1	1		

- Molecule 4 is 4-AMINO-1-BETA-D-RIBOFURANOSYL-2(1H)-PYRIMIDINONE (three-letter code: CTN) (formula: C<sub>9</sub>H<sub>13</sub>N<sub>3</sub>O<sub>5</sub>).



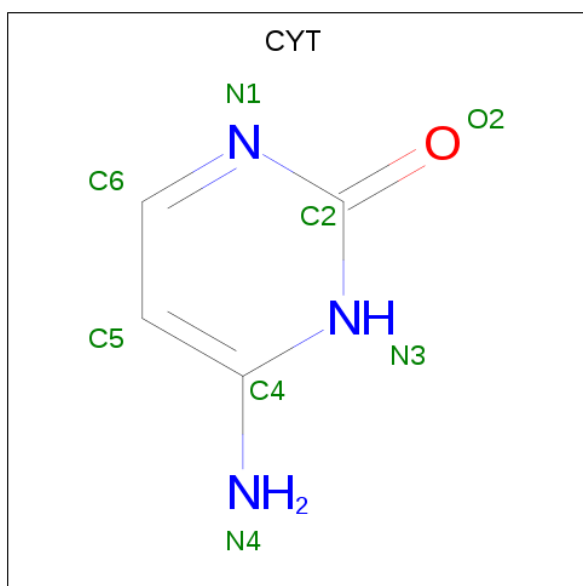
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	1
			30	9	13	3	5		
4	B	1	Total	C	H	N	O	0	1
			30	9	13	3	5		
4	C	1	Total	C	H	N	O	0	1
			30	9	13	3	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	H	N	O	0	1
			30	9	13	3	5		
4	E	1	Total	C	H	N	O	0	1
			30	9	13	3	5		
4	F	1	Total	C	H	N	O	0	1
			30	9	13	3	5		

- Molecule 5 is 6-AMINOPYRIMIDIN-2(1H)-ONE (three-letter code: CYT) (formula:  $C_4H_5N_3O$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	1
			12	4	4	3	1		
5	B	1	Total	C	H	N	O	0	1
			12	4	4	3	1		
5	C	1	Total	C	H	N	O	0	1
			12	4	4	3	1		
5	D	1	Total	C	H	N	O	0	0
			12	4	4	3	1		
5	D	1	Total	C	H	N	O	0	1
			12	4	4	3	1		
5	E	1	Total	C	H	N	O	0	1
			12	4	4	3	1		
5	F	1	Total	C	H	N	O	0	1
			12	4	4	3	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	1
			11	3	5	3		
6	B	1	Total	C	H	O	0	1
			9	3	3	3		
6	C	1	Total	C	H	O	0	1
			10	3	4	3		
6	D	1	Total	C	H	O	0	1
			10	3	4	3		
6	E	1	Total	C	H	O	0	1
			10	3	4	3		
6	F	1	Total	C	H	O	0	1
			10	3	4	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	1
			10	8	2		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Cl	0	0
			2	2		
8	C	1	Total	Cl	0	0
			1	1		
8	F	1	Total	Cl	0	0
			1	1		
8	E	2	Total	Cl	0	0
			2	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	256	Total	O	0	10
			265	265		
9	B	263	Total	O	0	6
			268	268		
9	C	273	Total	O	0	8
			280	280		
9	D	250	Total	O	0	5
			254	254		

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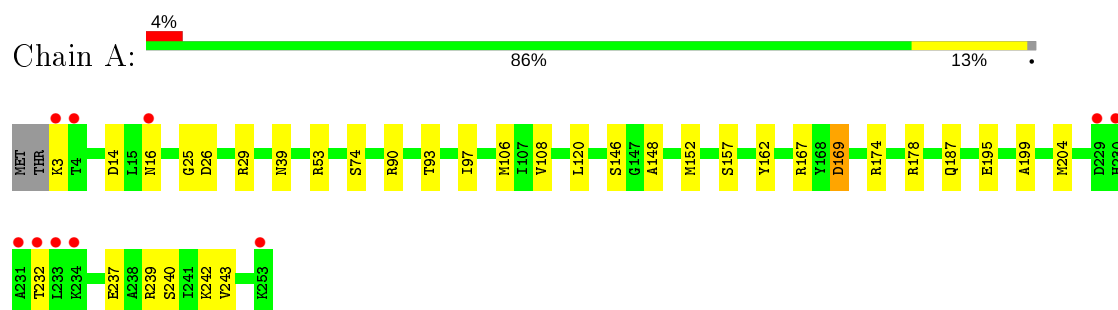
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	244	Total 248	O 248	0	5
9	F	222	Total 229	O 229	0	8

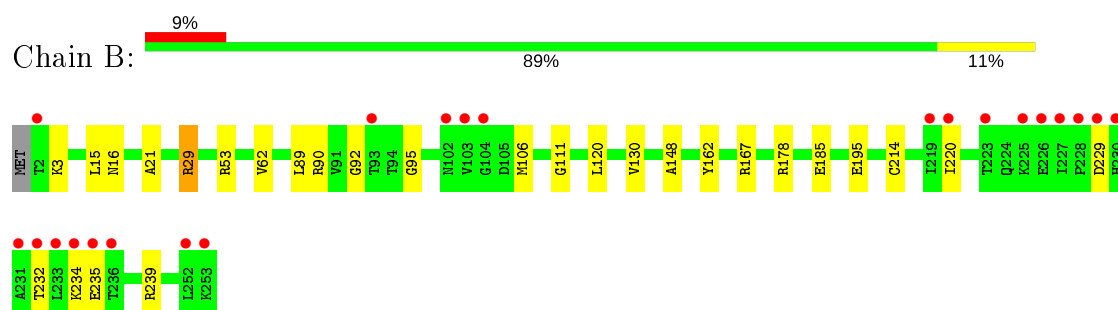
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

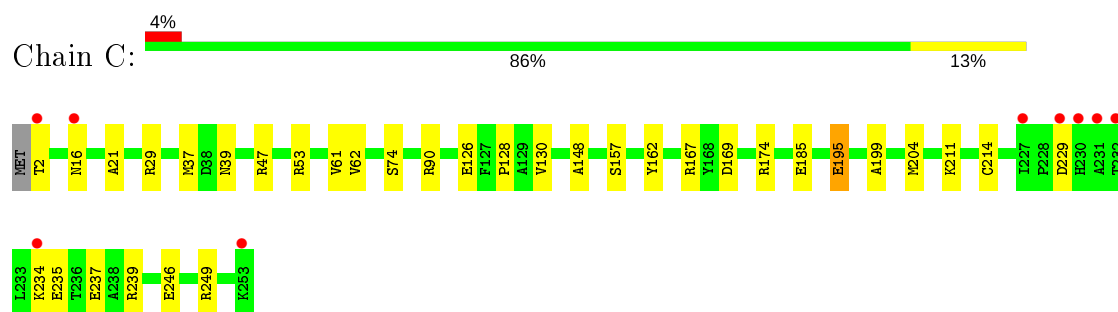
- Molecule 1: Uridine phosphorylase



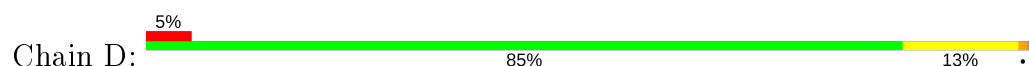
- Molecule 1: Uridine phosphorylase

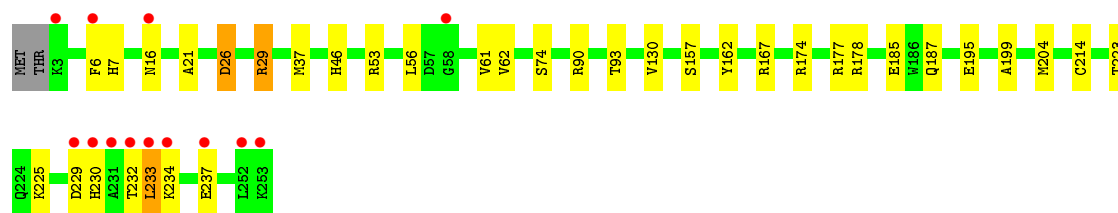


- Molecule 1: Uridine phosphorylase

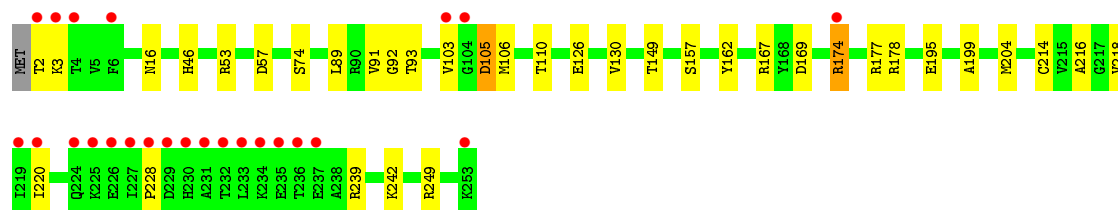
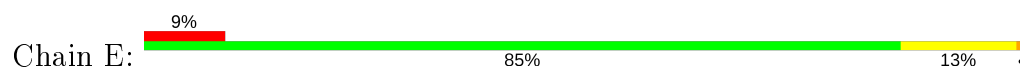


- Molecule 1: Uridine phosphorylase

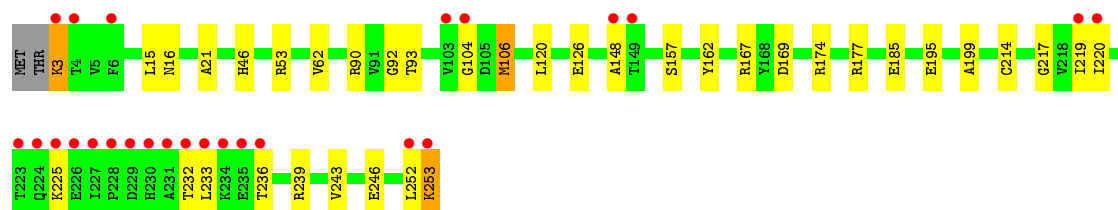
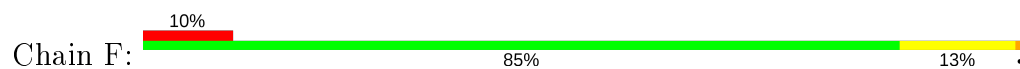




• Molecule 1: Uridine phosphorylase



• Molecule 1: Uridine phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.26 Å 71.77 Å 89.23 Å 69.35° 72.17° 85.78°	Depositor
Resolution (Å)	39.67 – 1.11 44.35 – 1.11	Depositor EDS
% Data completeness (in resolution range)	89.2 (39.67-1.11) 89.2 (44.35-1.11)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 1.11 Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.114 , 0.136 0.115 , 0.137	Depositor DCC
$R_{free}$ test set	5266 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.9	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	27605	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CYT, K, CL, EDO, SO4, CTN

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	0.67	0/2368	0.94	7/3203 (0.2%)
1	B	0.63	0/2317	0.81	1/3126 (0.0%)
1	C	0.64	0/2221	0.84	2/3004 (0.1%)
1	D	0.69	0/2215	0.87	3/2991 (0.1%)
1	E	0.67	0/2267	0.84	7/3069 (0.2%)
1	F	0.63	0/2261	0.80	3/3060 (0.1%)
All	All	0.66	0/13649	0.85	23/18453 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90[A]	ARG	NE-CZ-NH1	-13.52	113.54	120.30
1	A	90[B]	ARG	NE-CZ-NH1	-13.52	113.54	120.30
1	D	90[A]	ARG	NE-CZ-NH1	-8.53	116.04	120.30
1	D	90[B]	ARG	NE-CZ-NH1	-8.53	116.04	120.30
1	B	89	LEU	CB-CG-CD1	7.01	122.93	111.00
1	F	90	ARG	NE-CZ-NH1	-6.73	116.93	120.30
1	A	26	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	C	90	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	C	47	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	169[A]	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	A	169[B]	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	E	89	LEU	CB-CG-CD1	5.58	120.48	111.00
1	E	169[A]	ASP	CB-CG-OD1	5.54	123.29	118.30
1	E	169[B]	ASP	CB-CG-OD1	5.54	123.29	118.30
1	E	177	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	F	174[A]	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	F	174[B]	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	90[A]	ARG	NH1-CZ-NH2	5.23	125.16	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90[B]	ARG	NH1-CZ-NH2	5.23	125.16	119.40
1	E	105[A]	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	E	105[B]	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	E	174	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	D	26	ASP	CB-CG-OD1	5.10	122.89	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2146	2187	1999	38	0
1	B	2143	2231	2109	40	0
1	C	2077	2139	2045	29	0
1	D	2077	2132	2042	40	0
1	E	2124	2182	2101	35	0
1	F	2114	2154	2035	36	0
2	A	4	0	6	6	0
2	B	4	0	6	10	0
2	E	4	0	5	6	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	17	13	13	2	0
4	B	17	13	13	2	0
4	C	17	13	13	2	0
4	D	17	13	13	2	0
4	E	17	13	13	1	0
4	F	17	13	13	2	0
5	A	8	4	4	2	0
5	B	8	4	2	1	0
5	C	8	4	4	1	0
5	D	16	8	8	3	0
5	E	8	4	4	1	0
5	F	8	4	4	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	6	5	8	1	0
6	B	6	3	8	0	0
6	C	6	4	8	0	0
6	D	6	4	8	1	0
6	E	6	4	8	1	0
6	F	6	4	8	1	0
7	A	10	0	0	2	0
8	B	2	0	0	2	0
8	C	1	0	0	0	0
8	E	2	0	0	3	0
8	F	1	0	0	2	0
9	A	265	0	0	13	0
9	B	268	0	0	18	0
9	C	280	0	0	12	0
9	D	254	0	0	19	0
9	E	248	0	0	17	0
9	F	229	0	0	20	0
All	All	14450	13155	12500	228	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (228) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187[A]:GLN:NE2	9:A:401:HOH:O	1.66	1.22
5:D:301:CYT:O2	9:D:401:HOH:O	1.54	1.20
1:D:214[B]:CYS:SG	9:D:571:HOH:O	1.96	1.20
1:F:93[B]:THR:HG23	9:F:408:HOH:O	1.00	1.17
7:A:306[B]:SO4:O3	9:A:402:HOH:O	1.74	1.04
6:E:307[C]:GOL:H11	9:E:405[C]:HOH:O	1.56	1.04
1:D:174[A]:ARG:NH2	9:D:403:HOH:O	1.87	1.04
1:F:185[B]:GLU:OE2	9:F:402:HOH:O	1.75	1.03
1:D:178[B]:ARG:NH2	1:E:126[B]:GLU:OE2	1.93	1.00
1:D:46[B]:HIS:ND1	9:D:404:HOH:O	1.97	0.96
1:F:106[B]:MET:HE1	1:F:243:VAL:HG21	1.47	0.96
1:B:185[B]:GLU:OE1	9:B:401:HOH:O	1.83	0.94
1:C:229[B]:ASP:OD1	9:C:401:HOH:O	1.83	0.94
1:B:53[B]:ARG:NH1	9:B:402:HOH:O	1.96	0.94
1:D:185[A]:GLU:OE1	9:D:402:HOH:O	1.84	0.93
1:F:126[B]:GLU:OE1	9:F:577[B]:HOH:O	1.87	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211[B]:LYS:NZ	9:C:561[B]:HOH:O	2.02	0.91
8:E:302:CL:CL	9:E:466:HOH:O	2.24	0.90
1:E:214[B]:CYS:SG	9:E:566:HOH:O	2.31	0.89
1:E:106[A]:MET:SD	9:E:528:HOH:O	2.32	0.88
1:C:235[B]:GLU:OE1	9:C:402:HOH:O	1.95	0.84
1:E:93[B]:THR:HG23	9:E:401:HOH:O	1.76	0.84
1:A:187[A]:GLN:OE1	9:A:403:HOH:O	1.97	0.82
1:B:90[A]:ARG:NH2	9:B:404:HOH:O	2.08	0.82
1:A:39[B]:ASN:OD1	9:A:404:HOH:O	1.98	0.81
1:D:29[B]:ARG:NH2	9:D:407:HOH:O	2.13	0.81
1:F:53[A]:ARG:NH1	9:F:403:HOH:O	2.09	0.81
1:F:93[B]:THR:CG2	9:F:408:HOH:O	1.74	0.81
8:B:301:CL:CL	9:B:431:HOH:O	2.37	0.79
1:F:214[B]:CYS:SG	9:F:525:HOH:O	2.39	0.79
1:D:225[B]:LYS:NZ	1:D:229[B]:ASP:OD1	2.15	0.79
9:B:437[B]:HOH:O	1:D:177[B]:ARG:NH1	2.14	0.79
1:D:214[B]:CYS:SG	9:D:533:HOH:O	2.42	0.77
1:D:178[B]:ARG:NH1	9:D:406:HOH:O	2.13	0.76
1:B:178:ARG:HD2	2:B:303:EDO:H22	1.67	0.75
6:D:304[C]:GOL:H32	9:D:414[C]:HOH:O	1.87	0.75
1:A:169[B]:ASP:OD2	9:A:405:HOH:O	2.05	0.75
1:A:178:ARG:HD2	2:A:301:EDO:H22	1.70	0.74
1:A:187[A]:GLN:NE2	9:A:403:HOH:O	2.19	0.74
1:F:104[A]:GLY:HA2	1:F:236[A]:THR:HG21	1.69	0.73
1:A:120:LEU:HD22	2:B:303:EDO:H12	1.72	0.71
1:F:93[B]:THR:CA	9:F:408:HOH:O	2.37	0.71
4:A:303[A]:CTN:H2'	4:A:303[A]:CTN:O2	1.92	0.70
1:B:90[A]:ARG:HG2	1:B:214[A]:CYS:SG	2.31	0.69
1:D:130[A]:VAL:HG12	1:E:130[A]:VAL:HG11	1.74	0.69
1:F:232:THR:O	1:F:236[A]:THR:HG23	1.93	0.68
1:C:169[A]:ASP:OD1	9:C:403:HOH:O	2.10	0.68
8:F:301:CL:CL	9:F:429:HOH:O	2.48	0.67
1:B:178:ARG:CD	2:B:303:EDO:H22	2.23	0.67
1:A:167:ARG:HH22	5:A:304[B]:CYT:N4	1.92	0.67
2:A:301:EDO:H12	1:B:120:LEU:HD22	1.77	0.67
2:E:303:EDO:H21	1:F:120:LEU:HD22	1.77	0.67
1:D:185[A]:GLU:OE2	9:D:405:HOH:O	2.12	0.67
1:E:178:ARG:HD2	2:E:303:EDO:H11	1.74	0.67
1:A:146:SER:HB2	1:A:242[B]:LYS:HE2	1.76	0.67
1:C:126[B]:GLU:OE2	9:C:404:HOH:O	2.13	0.66
4:C:303[A]:CTN:H2'	4:C:303[A]:CTN:O2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187[A]:GLN:CD	9:A:403:HOH:O	2.32	0.66
4:F:302[A]:CTN:O2'	9:F:404:HOH:O	2.12	0.65
6:F:304[C]:GOL:H11	9:F:409[C]:HOH:O	1.95	0.65
1:C:53[B]:ARG:NH2	9:C:407:HOH:O	2.28	0.64
4:D:302[A]:CTN:H2'	4:D:302[A]:CTN:O2	1.97	0.64
1:A:16[A]:ASN:HB3	1:A:53[A]:ARG:HD2	1.80	0.64
1:B:178:ARG:HD2	2:B:303:EDO:C2	2.27	0.64
1:A:237[A]:GLU:OE2	9:A:406:HOH:O	2.15	0.64
1:D:29[B]:ARG:NH1	1:D:237[B]:GLU:OE1	2.30	0.64
1:A:29[B]:ARG:NH1	1:A:240[B]:SER:OG	2.31	0.63
1:F:252:LEU:O	1:F:253:LYS:HB2	1.97	0.63
1:B:220[B]:ILE:HG13	8:B:302:CL:CL	2.36	0.63
1:D:130[A]:VAL:HG12	1:E:130[A]:VAL:CG1	2.29	0.62
1:D:130[A]:VAL:CG1	1:E:130[A]:VAL:CG1	2.78	0.62
1:D:46[B]:HIS:CD2	9:D:532:HOH:O	2.53	0.62
4:E:305[A]:CTN:O2	4:E:305[A]:CTN:H2'	1.99	0.61
1:D:230:HIS:HA	1:D:233:LEU:HD22	1.82	0.61
1:E:2:THR:N	9:E:406:HOH:O	2.32	0.61
1:C:128:PRO:HB2	1:C:130[A]:VAL:HG13	1.83	0.60
1:F:92[A]:GLY:HA2	9:F:429:HOH:O	2.01	0.60
1:F:93[B]:THR:N	9:F:408:HOH:O	2.34	0.59
1:D:187[A]:GLN:NE2	9:D:410:HOH:O	2.35	0.59
1:F:93[B]:THR:HB	1:F:219[B]:ILE:HG23	1.85	0.59
1:B:167:ARG:HH22	5:B:305[B]:CYT:N4	2.01	0.58
1:F:167:ARG:HH22	5:F:303[B]:CYT:N4	2.00	0.58
1:D:167:ARG:HH22	5:D:303[B]:CYT:N4	2.02	0.58
1:B:29[A]:ARG:HG2	9:B:611:HOH:O	2.03	0.58
1:A:120:LEU:HD22	2:B:303:EDO:C1	2.34	0.57
1:B:130[A]:VAL:CG1	1:C:130[A]:VAL:HG12	2.34	0.57
1:C:167:ARG:HH22	5:C:304[B]:CYT:N4	2.01	0.57
1:C:214[B]:CYS:SG	9:C:591:HOH:O	2.57	0.57
1:E:167:ARG:HH22	5:E:306[B]:CYT:N4	2.03	0.57
1:E:92[B]:GLY:C	9:E:401:HOH:O	2.42	0.57
1:D:130[A]:VAL:HG11	1:E:130[A]:VAL:HG12	1.86	0.57
1:E:242[A]:LYS:NZ	9:E:402:HOH:O	2.26	0.56
1:E:105[B]:ASP:OD1	1:E:149[B]:THR:OG1	2.24	0.56
1:F:106[B]:MET:HG2	1:F:217[B]:GLY:HA2	1.88	0.56
1:D:223[B]:THR:HG22	9:D:597:HOH:O	2.04	0.56
1:A:106[B]:MET:SD	1:A:243:VAL:HG21	2.46	0.56
1:C:16:ASN:HB2	1:C:53[A]:ARG:HD2	1.87	0.56
1:B:53[B]:ARG:CD	9:B:419:HOH:O	2.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220[B]:ILE:HG13	8:E:301:CL:CL	2.43	0.55
1:F:15:LEU:HD22	1:F:62[B]:VAL:HG11	1.88	0.55
1:B:16:ASN:HB2	1:B:53[B]:ARG:HD2	1.88	0.55
1:B:92[B]:GLY:O	9:B:405:HOH:O	2.18	0.55
1:F:104[A]:GLY:HA2	1:F:236[A]:THR:CG2	2.38	0.54
1:B:92[A]:GLY:HA2	9:B:431:HOH:O	2.07	0.54
1:D:37:MET:SD	1:D:61[B]:VAL:HG21	2.48	0.54
1:D:178[B]:ARG:NH1	9:D:416:HOH:O	2.41	0.53
1:B:106[A]:MET:HE1	1:B:239:ARG:HG2	1.88	0.53
1:E:92[A]:GLY:HA2	9:E:466:HOH:O	2.07	0.53
1:E:53[A]:ARG:NE	9:E:404:HOH:O	2.28	0.53
1:A:178:ARG:CD	2:A:301:EDO:H22	2.38	0.53
1:B:130[A]:VAL:HG11	1:C:130[A]:VAL:HG12	1.91	0.53
1:C:148:ALA:HB2	1:C:239[B]:ARG:HD3	1.91	0.53
1:B:239:ARG:NE	9:B:413:HOH:O	2.42	0.52
1:A:120:LEU:HB3	2:B:303:EDO:H11	1.92	0.52
1:B:95[A]:GLY:HA3	4:B:304[A]:CTN:N4	2.25	0.52
1:B:53[B]:ARG:HG2	9:B:419:HOH:O	2.09	0.51
1:E:57:ASP:OD2	1:E:249[A]:ARG:HG3	2.10	0.51
1:E:103[B]:VAL:HG11	1:E:228:PRO:HB3	1.92	0.51
1:F:92[B]:GLY:C	9:F:408:HOH:O	2.47	0.51
1:B:178:ARG:CZ	2:B:303:EDO:H22	2.41	0.51
1:F:16:ASN:HB2	1:F:53[A]:ARG:HD2	1.94	0.50
1:A:29[B]:ARG:CZ	1:A:237[B]:GLU:HG2	2.41	0.50
1:C:174[A]:ARG:HD2	9:E:548:HOH:O	2.12	0.50
1:D:53[B]:ARG:HG2	9:D:426:HOH:O	2.12	0.50
1:A:16[A]:ASN:ND2	9:A:407[A]:HOH:O	2.16	0.50
1:C:237[B]:GLU:CG	9:C:412:HOH:O	2.58	0.50
1:F:3:LYS:HG3	1:F:3:LYS:O	2.12	0.50
1:F:220[B]:ILE:HD11	5:F:303[B]:CYT:H41	1.77	0.50
1:A:97[A]:ILE:HG23	1:A:187[A]:GLN:HG3	1.94	0.50
1:D:130[A]:VAL:CG1	1:E:130[A]:VAL:HG12	2.40	0.50
9:E:608:HOH:O	8:F:301:CL:CL	2.57	0.50
1:A:239:ARG:HG3	1:A:242[B]:LYS:HZ3	1.77	0.50
2:A:301:EDO:C1	1:B:120:LEU:HD22	2.40	0.50
1:F:246[B]:GLU:HG2	9:F:414:HOH:O	2.11	0.50
1:C:237[B]:GLU:HG3	9:C:412:HOH:O	2.12	0.49
5:D:301:CYT:N4	9:D:411:HOH:O	2.36	0.49
1:D:16[B]:ASN:HB2	1:D:53[B]:ARG:HD2	1.94	0.49
1:E:242[B]:LYS:HE3	9:E:520:HOH:O	2.13	0.49
1:F:169[C]:ASP:OD1	9:F:401:HOH:O	0.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:EDO:C2	9:A:535:HOH:O	2.59	0.49
1:D:46[B]:HIS:HD2	9:D:532:HOH:O	1.91	0.49
1:C:37:MET:SD	1:C:61[B]:VAL:HG21	2.53	0.49
1:A:187[B]:GLN:HG2	9:A:569:HOH:O	2.12	0.48
1:B:178:ARG:NE	2:B:303:EDO:H22	2.28	0.48
1:B:29[A]:ARG:HD2	9:B:611:HOH:O	2.12	0.48
2:A:301:EDO:H11	1:B:120:LEU:HB3	1.95	0.48
1:B:15:LEU:HD22	1:B:62[B]:VAL:HG11	1.94	0.48
1:E:178:ARG:CD	2:E:303:EDO:H11	2.43	0.48
1:B:148:ALA:HB2	1:B:239:ARG:HD2	1.95	0.48
1:A:106[B]:MET:HG3	1:A:148:ALA:HB1	1.95	0.48
1:C:246[A]:GLU:OE1	1:C:249[A]:ARG:NH2	2.42	0.47
1:A:29[A]:ARG:HG3	7:A:306[A]:SO4:O2	2.13	0.47
1:B:21:ALA:HA	1:B:62[B]:VAL:O	2.15	0.47
1:A:174[B]:ARG:HD2	9:C:544:HOH:O	2.14	0.47
1:A:242[B]:LYS:HD2	1:A:243:VAL:N	2.29	0.47
1:C:29[B]:ARG:HD3	1:C:237[B]:GLU:OE2	2.14	0.47
1:C:39:ASN:OD1	9:C:405:HOH:O	2.21	0.47
1:E:46[A]:HIS:HD2	9:E:423:HOH:O	1.99	0.46
1:E:91:VAL:HG22	1:E:92[B]:GLY:N	2.31	0.46
1:A:97[A]:ILE:HG23	1:A:187[A]:GLN:CG	2.45	0.46
1:B:21:ALA:HB2	1:B:62[B]:VAL:HG23	1.97	0.46
1:F:53[B]:ARG:NH1	9:F:412:HOH:O	2.43	0.46
1:F:21:ALA:HA	1:F:62[B]:VAL:O	2.15	0.46
1:C:235[A]:GLU:OE1	1:C:239[A]:ARG:NH1	2.48	0.46
1:E:178:ARG:HD2	2:E:303:EDO:C1	2.43	0.46
1:D:21:ALA:HA	1:D:62[B]:VAL:O	2.17	0.45
1:C:195:GLU:HB2	4:C:303[A]:CTN:O2'	2.16	0.45
1:B:234[B]:LYS:HD2	9:B:609:HOH:O	2.15	0.45
1:A:167:ARG:HH22	5:A:304[B]:CYT:H42	1.62	0.45
1:F:21:ALA:HB2	1:F:62[B]:VAL:HG23	1.99	0.45
1:B:106[A]:MET:CE	1:B:239:ARG:HG2	2.46	0.45
1:E:92[B]:GLY:O	1:E:216[B]:ALA:HA	2.17	0.45
1:E:93[B]:THR:N	9:E:401:HOH:O	2.49	0.45
1:B:95[A]:GLY:HA3	4:B:304[A]:CTN:HN41	1.81	0.44
1:F:177[B]:ARG:NH2	9:F:423:HOH:O	2.50	0.44
1:F:236[A]:THR:HG22	1:F:239[A]:ARG:HH12	1.82	0.44
6:A:305[C]:GOL:H11	9:A:419[C]:HOH:O	2.18	0.44
1:E:157:SER:HB3	1:E:199:ALA:HB2	2.00	0.44
1:E:16[A]:ASN:HB2	1:E:53[A]:ARG:HD2	2.00	0.44
1:A:97[A]:ILE:CG2	1:A:187[A]:GLN:HG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:GLY:HA3	9:A:409:HOH:O	2.18	0.43
1:D:187[A]:GLN:OE1	9:D:408:HOH:O	2.21	0.43
1:A:14:ASP:O	1:A:53[B]:ARG:HD3	2.18	0.43
1:C:21:ALA:HA	1:C:62[B]:VAL:O	2.18	0.43
1:D:6:PHE:HD2	1:D:7:HIS:CE1	2.36	0.43
1:C:234:LYS:HD3	1:C:234:LYS:HA	1.83	0.43
8:E:301:CL:CL	9:E:515:HOH:O	2.59	0.43
1:A:97[A]:ILE:CG2	1:A:187[A]:GLN:CG	2.97	0.42
1:E:178:ARG:HD2	2:E:303:EDO:C2	2.49	0.42
1:A:74:SER:HA	1:A:204[B]:MET:HE1	2.01	0.42
1:D:74:SER:HA	1:D:204[B]:MET:HE1	2.01	0.42
1:D:26:ASP:HB3	1:D:29[B]:ARG:HG3	2.01	0.42
1:E:93[B]:THR:CA	9:E:401:HOH:O	2.66	0.42
1:E:178:ARG:HD2	2:E:303:EDO:H22	2.02	0.42
1:B:53[B]:ARG:NE	9:B:419:HOH:O	2.50	0.42
1:F:157:SER:HB3	1:F:199:ALA:HB2	2.01	0.42
1:A:108:VAL:HB	1:A:152[A]:MET:SD	2.60	0.41
1:D:157:SER:HB3	1:D:199:ALA:HB2	2.03	0.41
1:D:204[B]:MET:HB3	1:D:204[B]:MET:HE3	1.87	0.41
1:F:126[A]:GLU:OE2	9:F:405:HOH:O	2.21	0.41
1:F:106[B]:MET:HE1	1:F:243:VAL:CG2	2.35	0.41
1:F:93[B]:THR:CB	9:F:408:HOH:O	2.33	0.41
1:B:229:ASP:HB2	1:B:232:THR:OG1	2.21	0.41
1:C:185[B]:GLU:HG3	9:C:460:HOH:O	2.20	0.41
1:D:130[B]:VAL:HG11	1:E:110:THR:O	2.20	0.41
1:D:229[A]:ASP:HB3	1:D:232:THR:HG23	2.03	0.41
1:B:239:ARG:CD	9:B:413:HOH:O	2.69	0.41
1:D:93:THR:OG1	4:D:302[A]:CTN:H6	2.20	0.41
1:E:74:SER:HA	1:E:204[B]:MET:HE1	2.03	0.41
4:F:302[A]:CTN:O2	4:F:302[A]:CTN:H2'	2.20	0.41
1:A:157:SER:HB3	1:A:199:ALA:HB2	2.03	0.41
1:A:97[A]:ILE:HG22	1:A:187[A]:GLN:HG2	2.03	0.40
1:A:93:THR:OG1	4:A:303[A]:CTN:H6	2.21	0.40
1:B:29[A]:ARG:CD	9:B:611:HOH:O	2.67	0.40
1:B:178:ARG:NH1	2:B:303:EDO:H22	2.36	0.40
1:D:229[B]:ASP:HB2	1:D:232:THR:HG23	2.03	0.40
2:B:303:EDO:C2	9:B:490:HOH:O	2.69	0.40
1:C:157:SER:HB3	1:C:199:ALA:HB2	2.04	0.40
1:B:111:GLY:HA3	1:C:130[A]:VAL:HG11	2.04	0.40
1:C:169[B]:ASP:N	1:C:169[B]:ASP:OD1	2.48	0.40
1:F:148:ALA:HB2	1:F:239[B]:ARG:HD3	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:HIS:HD2	9:F:428:HOH:O	2.03	0.40
1:C:74:SER:HA	1:C:204[B]:MET:HE1	2.04	0.40
1:D:37:MET:HG2	1:D:56:LEU:HD13	2.04	0.40
1:B:92[B]:GLY:C	9:B:405:HOH:O	2.57	0.40
1:D:53[B]:ARG:NE	9:D:426:HOH:O	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	303/253 (120%)	300 (99%)	2 (1%)	1 (0%)	41	15
1	B	300/253 (119%)	298 (99%)	1 (0%)	1 (0%)	41	15
1	C	288/253 (114%)	285 (99%)	2 (1%)	1 (0%)	41	15
1	D	284/253 (112%)	281 (99%)	2 (1%)	1 (0%)	34	10
1	E	297/253 (117%)	292 (98%)	4 (1%)	1 (0%)	41	15
1	F	295/253 (117%)	291 (99%)	3 (1%)	1 (0%)	41	15
All	All	1767/1518 (116%)	1747 (99%)	14 (1%)	6 (0%)	34	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	162	TYR
1	C	162	TYR
1	D	162	TYR
1	E	162	TYR
1	F	162	TYR
1	A	162	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	252/203 (124%)	249 (99%)	3 (1%)	71	36
1	B	247/203 (122%)	241 (98%)	6 (2%)	49	11
1	C	238/203 (117%)	236 (99%)	2 (1%)	81	52
1	D	234/203 (115%)	229 (98%)	5 (2%)	53	14
1	E	241/203 (119%)	237 (98%)	4 (2%)	60	23
1	F	239/203 (118%)	232 (97%)	7 (3%)	42	7
All	All	1451/1218 (119%)	1424 (98%)	27 (2%)	57	18

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	195	GLU
1	A	232	THR
1	B	3	LYS
1	B	29[A]	ARG
1	B	29[B]	ARG
1	B	195	GLU
1	B	235[A]	GLU
1	B	235[B]	GLU
1	C	2	THR
1	C	195	GLU
1	D	29[A]	ARG
1	D	29[B]	ARG
1	D	195	GLU
1	D	233	LEU
1	D	234	LYS
1	E	3	LYS
1	E	174	ARG
1	E	195	GLU
1	E	239	ARG
1	F	3	LYS
1	F	106[A]	MET

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Mol	Chain	Res	Type
1	F	106[B]	MET
1	F	195	GLU
1	F	225	LYS
1	F	233	LEU
1	F	253	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 9 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	EDO	B	303	-	3,3,3	0.45	0	2,2,2	0.34	0
4	CTN	E	305[A]	-	15,18,18	1.47	4 (26%)	17,26,26	1.69	4 (23%)
6	GOL	F	304[C]	-	5,5,5	0.46	0	5,5,5	0.81	0
4	CTN	B	304[A]	-	15,18,18	1.62	4 (26%)	17,26,26	1.56	3 (17%)
6	GOL	B	306[B]	-	5,5,5	0.36	0	5,5,5	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CTN	F	302[A]	-	15,18,18	1.47	4 (26%)	17,26,26	1.61	4 (23%)
5	CYT	B	305[B]	-	7,8,8	1.45	1 (14%)	8,10,10	6.46	3 (37%)
4	CTN	D	302[A]	-	15,18,18	1.62	4 (26%)	17,26,26	1.63	3 (17%)
6	GOL	D	304[C]	-	5,5,5	0.29	0	5,5,5	1.26	1 (20%)
6	GOL	C	305[B]	-	5,5,5	0.33	0	5,5,5	0.61	0
5	CYT	F	303[B]	-	7,8,8	1.15	0	8,10,10	6.29	3 (37%)
5	CYT	C	304[B]	-	7,8,8	1.69	3 (42%)	8,10,10	5.68	3 (37%)
7	SO4	A	306[A]	-	4,4,4	0.26	0	6,6,6	0.59	0
7	SO4	A	306[B]	-	4,4,4	0.46	0	6,6,6	1.01	0
6	GOL	E	307[C]	-	5,5,5	0.56	0	5,5,5	0.71	0
2	EDO	A	301	-	3,3,3	0.46	0	2,2,2	0.34	0
6	GOL	A	305[C]	-	5,5,5	0.36	0	5,5,5	1.17	1 (20%)
5	CYT	D	303[B]	-	7,8,8	1.09	0	8,10,10	6.35	4 (50%)
5	CYT	A	304[B]	-	7,8,8	1.31	1 (14%)	8,10,10	7.09	4 (50%)
5	CYT	E	306[B]	-	7,8,8	1.37	0	8,10,10	6.17	4 (50%)
5	CYT	D	301	-	7,8,8	1.35	1 (14%)	8,10,10	6.50	4 (50%)
4	CTN	C	303[A]	-	15,18,18	1.39	3 (20%)	17,26,26	1.94	4 (23%)
2	EDO	E	303	-	3,3,3	0.72	0	2,2,2	0.54	0
4	CTN	A	303[A]	-	15,18,18	1.44	3 (20%)	17,26,26	2.53	5 (29%)

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	CYT	C	304[B]	-	-	-	0/1/1/1
4	CTN	E	305[A]	-	-	2/4/22/22	0/2/2/2
6	GOL	F	304[C]	-	-	4/4/4/4	-
6	GOL	B	306[B]	-	-	2/4/4/4	-
4	CTN	B	304[A]	-	-	4/4/22/22	0/2/2/2
4	CTN	F	302[A]	-	-	3/4/22/22	0/2/2/2
5	CYT	B	305[B]	-	-	-	0/1/1/1
4	CTN	D	302[A]	-	-	1/4/22/22	0/2/2/2
6	GOL	D	304[C]	-	-	2/4/4/4	-
6	GOL	C	305[B]	-	-	4/4/4/4	-
5	CYT	F	303[B]	-	-	-	0/1/1/1
2	EDO	B	303	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	E	307[C]	-	-	2/4/4/4	-
2	EDO	A	301	-	-	1/1/1/1	-
6	GOL	A	305[C]	-	-	2/4/4/4	-
5	CYT	D	303[B]	-	-	-	0/1/1/1
5	CYT	A	304[B]	-	-	-	0/1/1/1
5	CYT	E	306[B]	-	-	-	0/1/1/1
5	CYT	D	301	-	-	-	0/1/1/1
4	CTN	C	303[A]	-	-	4/4/22/22	0/2/2/2
2	EDO	E	303	-	-	1/1/1/1	-
4	CTN	A	303[A]	-	-	2/4/22/22	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	302[A]	CTN	C4-N4	3.53	1.45	1.35
4	E	305[A]	CTN	C4-N4	3.39	1.45	1.35
4	C	303[A]	CTN	C4-N4	3.33	1.45	1.35
4	D	302[A]	CTN	C4-N3	-3.03	1.30	1.35
4	A	303[A]	CTN	C4-N3	-2.97	1.30	1.35
4	D	302[A]	CTN	C4-N4	2.94	1.43	1.35
4	B	304[A]	CTN	C4-N4	2.92	1.43	1.35
4	B	304[A]	CTN	C4-N3	-2.88	1.30	1.35
4	B	304[A]	CTN	C6-N1	-2.79	1.32	1.35
4	F	302[A]	CTN	C6-N1	-2.69	1.32	1.35
4	D	302[A]	CTN	C5-C4	-2.63	1.35	1.41
4	B	304[A]	CTN	C5-C4	-2.52	1.35	1.41
5	D	301	CYT	C5-C6	-2.50	1.33	1.38
4	E	305[A]	CTN	C6-N1	-2.49	1.32	1.35
5	C	304[B]	CYT	C6-N1	2.43	1.39	1.34
4	E	305[A]	CTN	C4-N3	-2.39	1.31	1.35
4	C	303[A]	CTN	C5-C4	-2.39	1.35	1.41
5	C	304[B]	CYT	C5-C6	-2.39	1.33	1.38
4	A	303[A]	CTN	C4-N4	2.28	1.41	1.35
4	E	305[A]	CTN	C5-C4	-2.27	1.35	1.41
4	A	303[A]	CTN	C5-C4	-2.24	1.35	1.41
4	F	302[A]	CTN	C5-C4	-2.23	1.36	1.41
4	D	302[A]	CTN	O4'-C1'	-2.18	1.38	1.41
4	F	302[A]	CTN	C4-N3	-2.17	1.32	1.35
4	C	303[A]	CTN	C4-N3	-2.15	1.32	1.35
5	A	304[B]	CYT	C2-N3	-2.09	1.34	1.38
5	B	305[B]	CYT	C4-N4	-2.07	1.29	1.35
5	C	304[B]	CYT	C2-N3	-2.05	1.34	1.38

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	304[B]	CYT	C6-N1-C2	13.99	121.32	114.42
5	E	306[B]	CYT	N1-C2-N3	-13.48	117.72	128.43
5	B	305[B]	CYT	N1-C2-N3	-13.22	117.92	128.43
5	A	304[B]	CYT	N1-C2-N3	-13.06	118.05	128.43
5	D	301	CYT	C6-N1-C2	13.03	120.84	114.42
5	F	303[B]	CYT	N1-C2-N3	-12.99	118.10	128.43
5	D	301	CYT	N1-C2-N3	-12.09	118.81	128.43
5	D	303[B]	CYT	N1-C2-N3	-11.94	118.93	128.43
5	C	304[B]	CYT	N1-C2-N3	-11.76	119.08	128.43
5	D	303[B]	CYT	C6-N1-C2	11.73	120.20	114.42
5	B	305[B]	CYT	C6-N1-C2	11.58	120.13	114.42
5	F	303[B]	CYT	C6-N1-C2	11.21	119.95	114.42
5	C	304[B]	CYT	C6-N1-C2	9.29	119.00	114.42
5	E	306[B]	CYT	C6-N1-C2	9.09	118.90	114.42
4	A	303[A]	CTN	C2-N3-C4	8.23	124.68	116.34
4	C	303[A]	CTN	C2-N3-C4	6.11	122.53	116.34
5	E	306[B]	CYT	C2-N3-C4	5.70	122.12	116.34
5	D	303[B]	CYT	C2-N3-C4	5.69	122.11	116.34
5	A	304[B]	CYT	C2-N3-C4	5.36	121.77	116.34
5	C	304[B]	CYT	C2-N3-C4	5.25	121.66	116.34
4	E	305[A]	CTN	C2-N3-C4	5.17	121.58	116.34
5	B	305[B]	CYT	C2-N3-C4	4.59	120.99	116.34
5	F	303[B]	CYT	C2-N3-C4	4.47	120.87	116.34
4	B	304[A]	CTN	C2-N3-C4	4.46	120.87	116.34
4	D	302[A]	CTN	C2-N3-C4	4.39	120.79	116.34
4	F	302[A]	CTN	C2-N3-C4	4.11	120.51	116.34
4	A	303[A]	CTN	C5-C4-N3	-3.74	117.41	121.72
5	D	301	CYT	C2-N3-C4	3.69	120.08	116.34
4	D	302[A]	CTN	C6-N1-C2	-3.03	116.39	121.20
4	F	302[A]	CTN	C3'-C2'-C1'	2.91	105.36	100.98
4	D	302[A]	CTN	C3'-C2'-C1'	2.76	105.14	100.98
4	A	303[A]	CTN	N4-C4-N3	2.65	120.68	116.49
5	A	304[B]	CYT	C5-C6-N1	-2.59	120.74	123.96
4	A	303[A]	CTN	C6-N1-C2	-2.59	117.09	121.20
4	C	303[A]	CTN	C5-C4-N3	-2.59	118.74	121.72
5	D	301	CYT	C5-C6-N1	-2.55	120.80	123.96
4	B	304[A]	CTN	C3'-C2'-C1'	2.48	104.72	100.98
4	C	303[A]	CTN	C3'-C2'-C1'	2.48	104.71	100.98
4	A	303[A]	CTN	C3'-C2'-C1'	2.31	104.45	100.98
4	F	302[A]	CTN	N4-C4-N3	2.30	120.13	116.49
4	E	305[A]	CTN	C3'-C2'-C1'	2.29	104.42	100.98
4	F	302[A]	CTN	C6-N1-C2	-2.26	117.61	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	305[A]	CTN	C6-N1-C2	-2.26	117.62	121.20
4	E	305[A]	CTN	C5-C4-N3	-2.24	119.13	121.72
5	D	303[B]	CYT	C5-C6-N1	-2.24	121.18	123.96
4	C	303[A]	CTN	C6-N1-C2	-2.21	117.69	121.20
5	E	306[B]	CYT	C6-C5-C4	2.14	118.15	116.91
6	D	304[C]	GOL	O2-C2-C1	2.10	118.36	109.12
4	B	304[A]	CTN	O4'-C4'-C5'	-2.08	104.73	109.21
6	A	305[C]	GOL	O2-C2-C3	2.01	117.99	109.12

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	305[A]	CTN	O4'-C1'-N1-C6
4	E	305[A]	CTN	C2'-C1'-N1-C6
6	F	304[C]	GOL	O1-C1-C2-C3
4	B	304[A]	CTN	O4'-C1'-N1-C6
4	B	304[A]	CTN	C2'-C1'-N1-C6
6	B	306[B]	GOL	O1-C1-C2-C3
4	F	302[A]	CTN	O4'-C1'-N1-C6
4	F	302[A]	CTN	C2'-C1'-N1-C6
4	D	302[A]	CTN	C2'-C1'-N1-C6
6	D	304[C]	GOL	C1-C2-C3-O3
6	C	305[B]	GOL	O1-C1-C2-C3
6	C	305[B]	GOL	C1-C2-C3-O3
6	C	305[B]	GOL	O2-C2-C3-O3
6	E	307[C]	GOL	O1-C1-C2-C3
6	A	305[C]	GOL	O1-C1-C2-C3
4	C	303[A]	CTN	O4'-C1'-N1-C6
4	C	303[A]	CTN	C2'-C1'-N1-C6
4	A	303[A]	CTN	O4'-C1'-N1-C6
4	A	303[A]	CTN	C2'-C1'-N1-C6
4	C	303[A]	CTN	C3'-C4'-C5'-O5'
6	B	306[B]	GOL	O1-C1-C2-O2
4	B	304[A]	CTN	C3'-C4'-C5'-O5'
4	C	303[A]	CTN	O4'-C4'-C5'-O5'
4	B	304[A]	CTN	O4'-C4'-C5'-O5'
6	F	304[C]	GOL	O1-C1-C2-O2
6	D	304[C]	GOL	O2-C2-C3-O3
6	C	305[B]	GOL	O1-C1-C2-O2
6	E	307[C]	GOL	O1-C1-C2-O2
2	E	303	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	303	EDO	O1-C1-C2-O2
6	F	304[C]	GOL	O2-C2-C3-O3
4	F	302[A]	CTN	O4'-C4'-C5'-O5'
6	F	304[C]	GOL	C1-C2-C3-O3
2	A	301	EDO	O1-C1-C2-O2
6	A	305[C]	GOL	O1-C1-C2-O2

There are no ring outliers.

22 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	303	EDO	10	0
4	E	305[A]	CTN	1	0
6	F	304[C]	GOL	1	0
4	B	304[A]	CTN	2	0
4	F	302[A]	CTN	2	0
5	B	305[B]	CYT	1	0
4	D	302[A]	CTN	2	0
6	D	304[C]	GOL	1	0
5	F	303[B]	CYT	2	0
5	C	304[B]	CYT	1	0
7	A	306[A]	SO4	1	0
7	A	306[B]	SO4	1	0
6	E	307[C]	GOL	1	0
2	A	301	EDO	6	0
6	A	305[C]	GOL	1	0
5	D	303[B]	CYT	1	0
5	A	304[B]	CYT	2	0
5	E	306[B]	CYT	1	0
5	D	301	CYT	2	0
4	C	303[A]	CTN	2	0
2	E	303	EDO	6	0
4	A	303[A]	CTN	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	251/253 (99%)	0.10	10 (3%) 38 34	7, 13, 25, 43	0
1	B	252/253 (99%)	0.33	22 (8%) 10 11	6, 13, 38, 69	1 (0%)
1	C	252/253 (99%)	0.05	9 (3%) 42 39	7, 13, 27, 50	0
1	D	251/253 (99%)	0.16	13 (5%) 27 25	7, 14, 29, 57	0
1	E	252/253 (99%)	0.46	24 (9%) 8 9	7, 14, 41, 70	0
1	F	251/253 (99%)	0.56	25 (9%) 7 9	7, 16, 45, 82	0
All	All	1509/1518 (99%)	0.28	103 (6%) 17 17	6, 14, 34, 82	1 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	227	ILE	15.6
1	E	2	THR	11.3
1	E	227	ILE	11.2
1	F	228	PRO	10.7
1	B	227	ILE	9.6
1	F	231	ALA	9.5
1	F	229	ASP	8.3
1	B	229	ASP	7.5
1	B	230	HIS	7.2
1	C	2	THR	7.1
1	E	232	THR	7.1
1	E	225	LYS	7.1
1	F	232	THR	7.0
1	F	230	HIS	6.8
1	D	232	THR	6.7
1	E	229	ASP	6.4
1	D	233	LEU	6.3
1	E	230	HIS	6.3
1	B	228	PRO	6.3

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Mol	Chain	Res	Type	RSRZ
1	E	233	LEU	6.2
1	B	2	THR	6.2
1	F	220[A]	ILE	6.1
1	F	219[A]	ILE	5.8
1	D	230	HIS	5.7
1	E	226	GLU	5.7
1	B	220[A]	ILE	5.7
1	B	232	THR	5.6
1	F	233	LEU	5.6
1	F	226	GLU	5.5
1	E	234	LYS	5.4
1	F	225	LYS	5.4
1	E	231	ALA	5.4
1	D	231	ALA	5.2
1	B	225	LYS	5.1
1	F	253	LYS	5.1
1	E	3	LYS	5.1
1	E	228	PRO	4.9
1	E	220[A]	ILE	4.8
1	B	233	LEU	4.7
1	A	253	LYS	4.7
1	A	231	ALA	4.7
1	B	231	ALA	4.6
1	C	230	HIS	4.5
1	B	226	GLU	4.4
1	C	253	LYS	4.3
1	D	234	LYS	4.3
1	F	103	VAL	4.3
1	E	219[A]	ILE	4.3
1	A	234[A]	LYS	4.3
1	A	232	THR	4.2
1	E	103[A]	VAL	4.2
1	F	148	ALA	4.2
1	E	253	LYS	4.0
1	F	234	LYS	4.0
1	B	103[A]	VAL	4.0
1	F	149[A]	THR	3.9
1	F	235[A]	GLU	3.9
1	F	236[A]	THR	3.8
1	D	253	LYS	3.7
1	E	235	GLU	3.7
1	E	4	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	235[A]	GLU	3.6
1	F	223	THR	3.6
1	A	3	LYS	3.6
1	C	229[A]	ASP	3.6
1	B	219[A]	ILE	3.5
1	F	6	PHE	3.5
1	A	230[A]	HIS	3.4
1	F	3	LYS	3.4
1	B	234[A]	LYS	3.3
1	F	224	GLN	3.3
1	B	253[A]	LYS	3.2
1	E	224	GLN	3.2
1	D	3	LYS	3.1
1	A	233[A]	LEU	3.0
1	F	252	LEU	3.0
1	E	6	PHE	3.0
1	C	232	THR	2.9
1	C	234	LYS	2.9
1	B	236	THR	2.8
1	C	227	ILE	2.8
1	E	237[A]	GLU	2.7
1	C	231	ALA	2.7
1	A	4[A]	THR	2.7
1	B	104[A]	GLY	2.7
1	E	104[A]	GLY	2.6
1	E	236	THR	2.5
1	B	93[A]	THR	2.4
1	F	4	THR	2.4
1	D	237[A]	GLU	2.4
1	B	252[A]	LEU	2.3
1	B	102[A]	ASN	2.3
1	D	16[A]	ASN	2.3
1	A	16[A]	ASN	2.3
1	F	104[A]	GLY	2.2
1	D	6	PHE	2.2
1	D	58	GLY	2.1
1	E	174	ARG	2.1
1	D	252	LEU	2.1
1	A	229[A]	ASP	2.1
1	C	16	ASN	2.0
1	D	229[A]	ASP	2.0
1	B	223	THR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	SO4	A	306[A]	5/5	0.89	0.17	32,32,32,32	5
7	SO4	A	306[B]	5/5	0.89	0.17	27,27,27,28	5
2	EDO	A	301	4/4	0.91	0.20	17,19,23,25	4
5	CYT	D	301	8/8	0.92	0.15	27,30,35,36	12
2	EDO	E	303	4/4	0.92	0.23	16,17,21,21	4
6	GOL	F	304[C]	6/6	0.93	0.09	18,21,23,24	10
2	EDO	B	303	4/4	0.93	0.21	15,18,20,23	4
4	CTN	F	302[A]	17/17	0.95	0.11	23,28,34,34	30
8	CL	E	301	1/1	0.96	0.12	53,53,53,53	0
6	GOL	E	307[C]	6/6	0.96	0.06	18,19,23,23	10
4	CTN	B	304[A]	17/17	0.96	0.10	14,16,20,21	30
6	GOL	D	304[C]	6/6	0.96	0.09	26,27,32,32	10
6	GOL	B	306[B]	6/6	0.96	0.08	17,19,20,22	9
6	GOL	C	305[B]	6/6	0.97	0.10	15,17,20,20	10
5	CYT	F	303[B]	8/8	0.97	0.06	10,13,16,16	12
5	CYT	B	305[B]	8/8	0.97	0.06	10,12,15,16	12
4	CTN	E	305[A]	17/17	0.97	0.10	19,20,24,24	30
4	CTN	C	303[A]	17/17	0.98	0.10	14,15,18,19	30
5	CYT	E	306[B]	8/8	0.98	0.07	9,11,14,15	12
5	CYT	C	304[B]	8/8	0.99	0.07	9,10,13,13	12
6	GOL	A	305[C]	6/6	0.99	0.09	20,22,26,26	11
5	CYT	D	303[B]	8/8	0.99	0.08	7,8,10,11	12
5	CYT	A	304[B]	8/8	0.99	0.10	6,8,9,10	12
8	CL	B	302	1/1	0.99	0.09	32,32,32,32	1
8	CL	B	301	1/1	0.99	0.08	22,22,22,22	1
8	CL	E	302	1/1	0.99	0.05	21,21,21,21	1
4	CTN	D	302[A]	17/17	0.99	0.09	9,11,14,15	30

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CTN	A	303[A]	17/17	0.99	0.10	7,9,11,12	30
3	K	A	302	1/1	1.00	0.14	11,11,11,11	1
3	K	E	304	1/1	1.00	0.13	11,11,11,11	1
3	K	C	302	1/1	1.00	0.11	13,13,13,13	1
8	CL	C	301	1/1	1.00	0.09	16,16,16,16	1
8	CL	F	301	1/1	1.00	0.05	25,25,25,25	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.