



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:53 PM UTC

PDB ID : 5LOK / pdb_00005lok
Title : X-ray structure of uridine phosphorylase from *Vibrio cholerae* in complex with cytidine and cytosine at 1.11 Å resolution
Authors : Prokofev, I.I.; Lashkov, A.A.; Gabdoulkhakov, A.G.; Dontsova, M.V.; Betzel, C.; Mikhailov, A.M.
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.

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

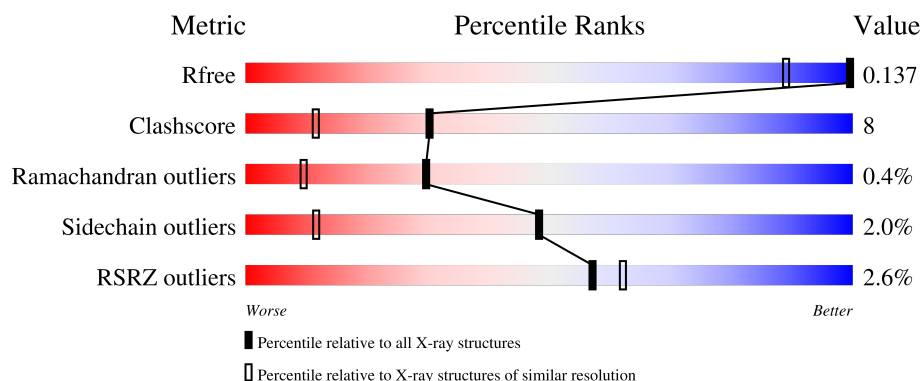
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1625 (1.12-1.08)
Clashscore	190562	1656 (1.12-1.08)
Ramachandran outliers	187476	1616 (1.12-1.08)
Sidechain outliers	187428	1612 (1.12-1.08)
RSRZ outliers	180081	1625 (1.12-1.08)

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	86% 13% .
1	B	253	3% 89% 10% .
1	C	253	87% 12%
1	D	253	3% 85% 14% ..
1	E	253	3% 86% 13%

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Mol	Chain	Length	Quality of chain
1	F	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
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](#)

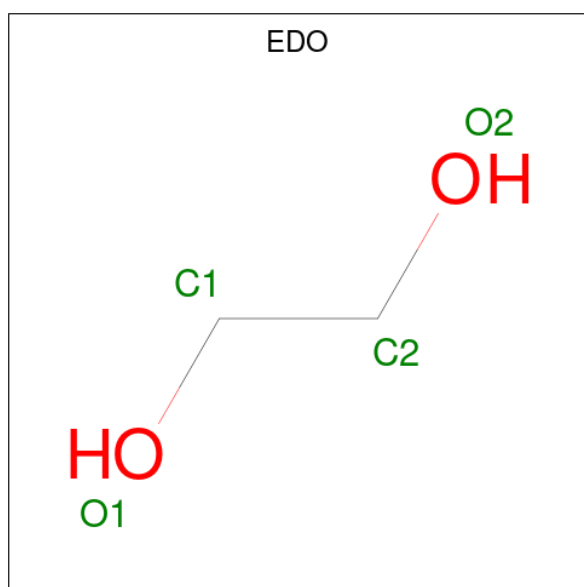
There are 9 unique types of molecules in this entry. The entry contains 27605 atoms, of which 13155 are hydrogens and 0 are deuteriums.

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 (CCD ID: EDO) (formula: C₂H₆O₂).

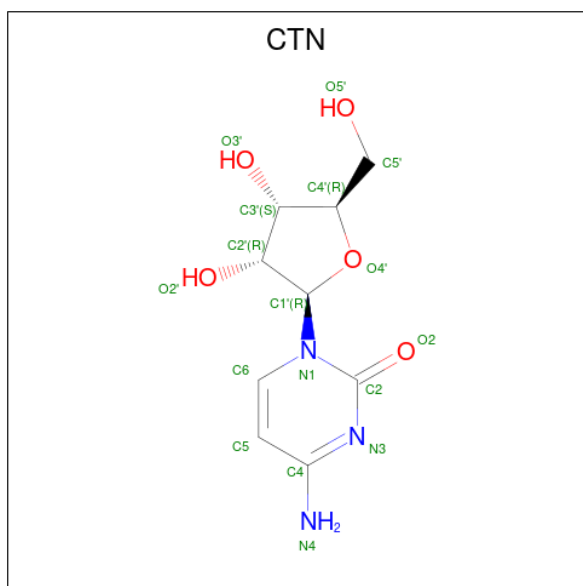


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is POTASSIUM ION (CCD ID: 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 (CCD ID: CTN) (formula: C₉H₁₃N₃O₅).



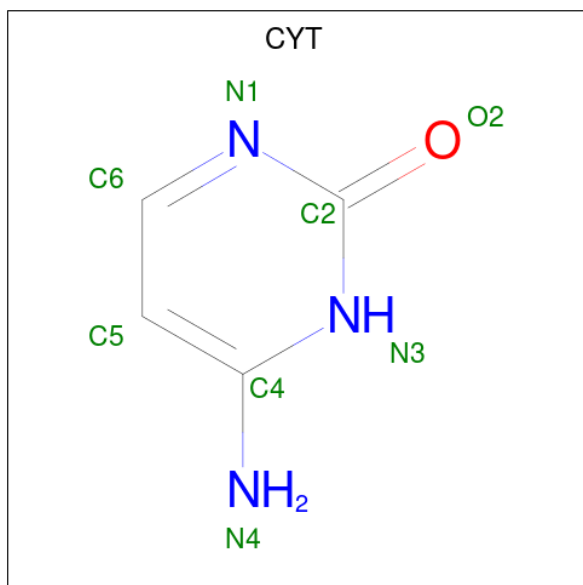
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	1
			30	9	13	3	5		
4	B	1	Total	C	H	N	O	0	1
			30	9	13	3	5		
4	C	1	Total	C	H	N	O	0	1
			30	9	13	3	5		

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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 (CCD ID: 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 (CCD ID: 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 (CCD ID: SO4) (formula: O₄S).



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

- Molecule 8 is CHLORIDE ION (CCD ID: 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	E	2	Total	Cl	0	0
			2	2		
8	F	1	Total	Cl	0	0
			1	1		

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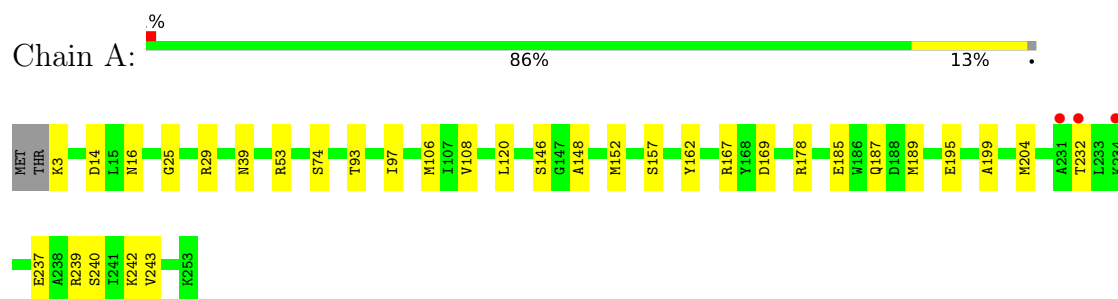
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	244	Total 248	O 248	0	5
9	F	222	Total 229	O 229	0	8

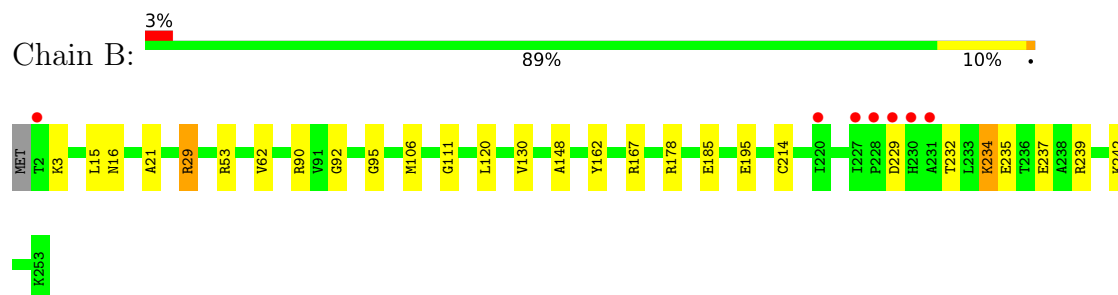
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

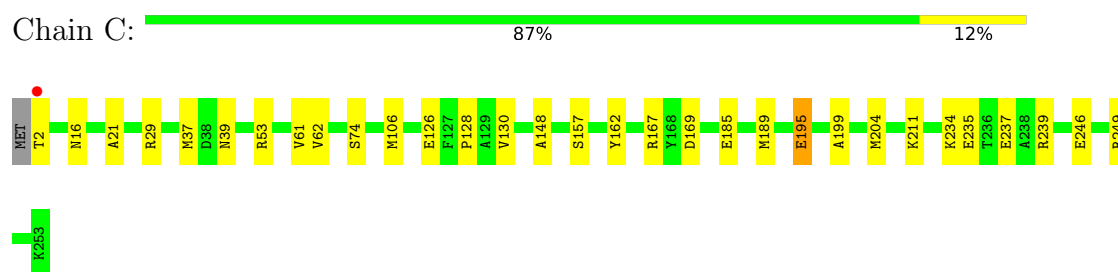
- Molecule 1: Uridine phosphorylase



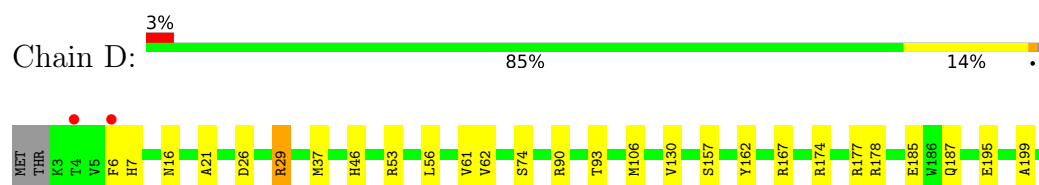
- Molecule 1: Uridine phosphorylase

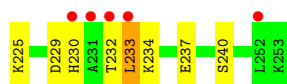


- Molecule 1: Uridine phosphorylase

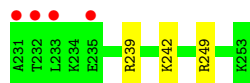
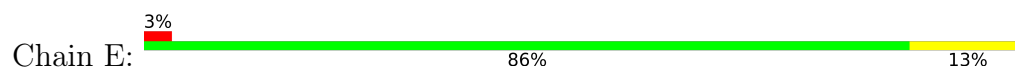


- Molecule 1: Uridine phosphorylase

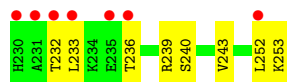
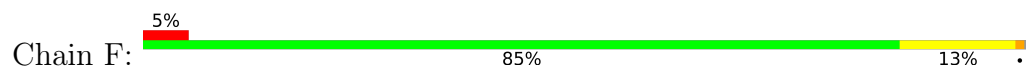




- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.26Å 71.77Å 89.23Å 69.35° 72.17° 85.78°	Depositor
Resolution (Å)	39.67 – 1.11 39.67 – 1.11	Depositor EDS
% Data completeness (in resolution range)	89.2 (39.67-1.11) 89.2 (39.67-1.11)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.11Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.114 , 0.136 0.116 , 0.137	Depositor DCC
R_{free} test set	5266 reflections (0.94%)	wwPDB-VP
Wilson B-factor (Å ²)	9.9	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

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: CYT, CL, GOL, EDO, K, 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	0.63	0/2368	0.79	0/3203
1	B	0.60	0/2317	0.75	0/3126
1	C	0.62	0/2221	0.79	0/3004
1	D	0.62	0/2215	0.77	2/2991 (0.1%)
1	E	0.61	0/2267	0.76	0/3069
1	F	0.60	0/2261	0.75	0/3060
All	All	0.61	0/13649	0.77	2/18453 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	90[A]	ARG	NE-CZ-NH1	-5.20	116.30	121.50
1	D	90[B]	ARG	NE-CZ-NH1	-5.20	116.30	121.50

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	36	0
1	B	2143	2231	2109	41	0
1	C	2077	2139	2045	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2077	2132	2042	36	0
1	E	2124	2182	2101	37	0
1	F	2114	2154	2035	30	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	3	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	1	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
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	1	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	9	0
9	B	268	0	0	20	0
9	C	280	0	0	9	0
9	D	254	0	0	15	0
9	E	248	0	0	15	0
9	F	229	0	0	10	0
All	All	14450	13155	12500	220	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 8.

All (220) 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)
5:D:301:CYT:O2	9:D:401:HOH:O	1.54	1.20
7:A:306[B]:SO4:O3	9:A:402:HOH:O	1.74	1.04
1:D:174[A]:ARG:NH2	9:D:403:HOH:O	1.87	1.04
6:E:307[C]:GOL:H11	9:E:405[C]:HOH:O	1.56	1.04
1:D:178[B]:ARG:NH2	1:E:126[B]:GLU:OE2	1.93	1.00
1:B:185[B]:GLU:OE1	9:B: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
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:106[A]:MET:SD	9:E:528:HOH:O	2.32	0.88
1:D:46[B]:HIS:ND1	9:D:404:HOH:O	1.97	0.86
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: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
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: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: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
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
4:B:304[A]:CTN:O2'	9:B:403:HOH:O	2.05	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O2	4:C:303[A]:CTN:H2'	1.95	0.66
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:O2	4:D:302[A]:CTN:H2'	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: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:E:92[B]:GLY:C	9:E:401:HOH:O	2.42	0.62
4:E:305[A]:CTN:H2'	4:E:305[A]:CTN:O2	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:106[B]:MET:HE1	1:F:243:VAL:HG11	1.83	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:F:106[B]:MET:HE1	1:F:243:VAL:HG21	1.84	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:A:74:SER:HA	1:A:204[B]:MET:HE1	1.86	0.58
1:E:185[B]:GLU:HG2	1:E:189:MET:HE3	1.85	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:E:167:ARG:HH22	5:E:306[B]:CYT:N4	2.03	0.57
1:D:130[A]:VAL:HG11	1:E:130[A]:VAL:HG12	1.86	0.57
1:E:105[B]:ASP:OD1	1:E:149[B]:THR:OG1	2.24	0.56
1:C:74:SER:HA	1:C:204[B]:MET:HE1	1.87	0.56
1:F:106[B]:MET:HG2	1:F:217[B]:GLY:HA2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:74:SER:HA	1:E:204[B]:MET:HE1	1.87	0.55
1:B:92[B]:GLY:O	9:B:405:HOH:O	2.18	0.55
1:D:74:SER:HA	1:D:204[B]:MET:HE1	1.88	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:C:185[B]:GLU:HG2	1:C:189:MET:HE3	1.91	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:E:242[A]:LYS:NZ	9:E:402:HOH:O	2.26	0.53
1:A:106[B]:MET:HE1	1:A:240[B]:SER:HA	1.91	0.52
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:74:SER:HA	1:F:204[B]:MET:HE1	1.92	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: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:O	1:F:3:LYS:HG3	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
2:A:301:EDO:C1	1:B:120:LEU:HD22	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237[B]:GLU:HG3	9:C:412:HOH:O	2.12	0.49
1:F:106[B]:MET:CE	1:F:243:VAL:HG21	2.42	0.49
1:D:16[B]:ASN:HB2	1:D:53[B]:ARG:HD2	1.94	0.49
5:D:301:CYT:N4	9:D:411:HOH:O	2.36	0.49
1:E:242[B]:LYS:HE3	9:E:520:HOH:O	2.13	0.49
2:A:301:EDO:C2	9:A:535:HOH:O	2.59	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:B:92[B]:GLY:C	9:B:405:HOH:O	2.57	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:C:185[B]:GLU:CG	1:C:189:MET:HE3	2.45	0.46
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:B:106[A]:MET:CE	1:B:239:ARG:HG2	2.46	0.45
1:A:239:ARG:HG3	1:A:242[B]:LYS:HZ3	1.81	0.45
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: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:E:185[B]:GLU:CG	1:E:189:MET:HE3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:185[B]:GLU:HG2	1:A:189:MET:HE3	1.98	0.44
1:A:97[A]:ILE:CG2	1:A:187[A]:GLN:HG2	2.48	0.43
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: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:106[A]:MET:HE1	1:F:240[A]:SER:OG	2.20	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:F:126[A]:GLU:OE2	9:F:405:HOH:O	2.21	0.41
1:B:106[A]:MET:HE1	1:B:239:ARG:HG2	2.02	0.41
1:A:185[B]:GLU:CG	1:A:189:MET:HE3	2.51	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:106[B]:MET:HE1	1:D:240:SER:HA	2.03	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:106[A]:MET:HE3	1:B:239:ARG:HH11	1.86	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
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:93:THR:OG1	4:A:303[A]:CTN:H6	2.21	0.40
1:A:97[A]:ILE:HG22	1:A:187[A]:GLN:HG2	2.03	0.40
1:B:29[A]:ARG:CD	9:B:611:HOH:O	2.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ARG:NH1	2:B:303:EDO:H22	2.36	0.40
1:B:242[A]:LYS:NZ	9:B:408:HOH:O	2.24	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:OD1	1:C:169[B]:ASP:N	2.48	0.40
1:F:46:HIS:HD2	9:F:428:HOH:O	2.03	0.40
1:F:148:ALA:HB2	1:F:239[B]:ARG:HD3	2.01	0.40
1:D:37:MET:HG2	1:D:56:LEU:HD13	2.04	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%)	36	13
1	B	300/253 (119%)	298 (99%)	1 (0%)	1 (0%)	36	13
1	C	288/253 (114%)	285 (99%)	2 (1%)	1 (0%)	36	13
1	D	284/253 (112%)	281 (99%)	2 (1%)	1 (0%)	30	9
1	E	297/253 (117%)	292 (98%)	4 (1%)	1 (0%)	36	13
1	F	295/253 (117%)	291 (99%)	3 (1%)	1 (0%)	36	13
All	All	1767/1518 (116%)	1747 (99%)	14 (1%)	6 (0%)	30	13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	162	TYR

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Mol	Chain	Res	Type
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%)	63	26
1	B	247/203 (122%)	237 (96%)	10 (4%)	28	2
1	C	238/203 (117%)	236 (99%)	2 (1%)	73	40
1	D	234/203 (115%)	229 (98%)	5 (2%)	47	11
1	E	241/203 (119%)	237 (98%)	4 (2%)	53	18
1	F	239/203 (118%)	233 (98%)	6 (2%)	42	8
All	All	1451/1218 (119%)	1421 (98%)	30 (2%)	48	11

All (30) 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	234[A]	LYS
1	B	234[B]	LYS
1	B	235[A]	GLU
1	B	235[B]	GLU
1	B	237[A]	GLU
1	B	237[B]	GLU

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	102	ASN
1	C	224	GLN
1	D	180	GLN
1	E	224	GLN
1	F	59	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 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
4	CTN	B	304[A]	-	18,18,18	1.88	5 (27%)	26,26,26	1.55	5 (19%)
7	SO4	A	306[A]	-	4,4,4	0.20	0	6,6,6	0.60	0
6	GOL	B	306[B]	-	5,5,5	0.37	0	5,5,5	0.55	0
2	EDO	A	301	-	3,3,3	0.43	0	2,2,2	0.38	0
5	CYT	A	304[B]	-	7,8,8	1.93	3 (42%)	7,10,10	3.19	3 (42%)
5	CYT	B	305[B]	-	7,8,8	2.02	3 (42%)	7,10,10	3.38	4 (57%)
4	CTN	C	303[A]	-	18,18,18	1.58	3 (16%)	26,26,26	1.60	4 (15%)
7	SO4	A	306[B]	-	4,4,4	0.49	0	6,6,6	1.00	0
4	CTN	D	302[A]	-	18,18,18	1.67	3 (16%)	26,26,26	1.40	3 (11%)
5	CYT	D	303[B]	-	7,8,8	1.74	2 (28%)	7,10,10	2.23	2 (28%)
6	GOL	F	304[C]	-	5,5,5	0.48	0	5,5,5	0.87	0
4	CTN	A	303[A]	-	18,18,18	1.48	2 (11%)	26,26,26	1.49	5 (19%)
6	GOL	E	307[C]	-	5,5,5	0.57	0	5,5,5	0.75	0
6	GOL	A	305[C]	-	5,5,5	0.36	0	5,5,5	1.25	1 (20%)
6	GOL	C	305[B]	-	5,5,5	0.34	0	5,5,5	0.65	0
4	CTN	E	305[A]	-	18,18,18	1.71	4 (22%)	26,26,26	1.61	4 (15%)
5	CYT	E	306[B]	-	7,8,8	1.87	3 (42%)	7,10,10	2.48	4 (57%)
2	EDO	E	303	-	3,3,3	0.73	0	2,2,2	0.51	0
4	CTN	F	302[A]	-	18,18,18	1.70	4 (22%)	26,26,26	1.76	5 (19%)
6	GOL	D	304[C]	-	5,5,5	0.30	0	5,5,5	1.35	1 (20%)
5	CYT	C	304[B]	-	7,8,8	1.84	3 (42%)	7,10,10	2.10	2 (28%)
5	CYT	F	303[B]	-	7,8,8	1.89	3 (42%)	7,10,10	3.18	4 (57%)
2	EDO	B	303	-	3,3,3	0.42	0	2,2,2	0.38	0
5	CYT	D	301	-	7,8,8	1.87	3 (42%)	7,10,10	3.52	3 (42%)

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
4	CTN	B	304[A]	-	-	6/6/22/22	0/2/2/2
6	GOL	B	306[B]	-	-	2/4/4/4	-
2	EDO	A	301	-	-	1/1/1/1	-
5	CYT	A	304[B]	-	-	-	0/1/1/1
5	CYT	B	305[B]	-	-	-	0/1/1/1
4	CTN	C	303[A]	-	-	4/6/22/22	0/2/2/2
4	CTN	D	302[A]	-	-	2/6/22/22	0/2/2/2
5	CYT	D	303[B]	-	-	-	0/1/1/1
6	GOL	F	304[C]	-	-	4/4/4/4	-
4	CTN	A	303[A]	-	-	2/6/22/22	0/2/2/2
6	GOL	E	307[C]	-	-	2/4/4/4	-
6	GOL	A	305[C]	-	-	2/4/4/4	-
6	GOL	C	305[B]	-	-	4/4/4/4	-
4	CTN	E	305[A]	-	-	2/6/22/22	0/2/2/2
5	CYT	E	306[B]	-	-	-	0/1/1/1
2	EDO	E	303	-	-	1/1/1/1	-
4	CTN	F	302[A]	-	-	4/6/22/22	0/2/2/2
6	GOL	D	304[C]	-	-	2/4/4/4	-
5	CYT	C	304[B]	-	-	-	0/1/1/1
5	CYT	F	303[B]	-	-	-	0/1/1/1
2	EDO	B	303	-	-	1/1/1/1	-
5	CYT	D	301	-	-	-	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	302[A]	CTN	C4-N4	4.82	1.45	1.33
4	E	305[A]	CTN	C4-N4	4.65	1.45	1.33
4	C	303[A]	CTN	C4-N4	4.58	1.45	1.33
4	B	304[A]	CTN	O2-C2	-4.23	1.15	1.23
4	D	302[A]	CTN	C4-N4	4.10	1.43	1.33
4	B	304[A]	CTN	C4-N4	4.08	1.43	1.33
4	D	302[A]	CTN	C5-C4	-3.41	1.35	1.42
4	E	305[A]	CTN	O2-C2	-3.33	1.17	1.23
4	F	302[A]	CTN	O2-C2	-3.30	1.17	1.23
4	A	303[A]	CTN	C4-N4	3.30	1.41	1.33
4	B	304[A]	CTN	C5-C4	-3.29	1.35	1.42
5	E	306[B]	CYT	C4-N3	-3.28	1.32	1.37
4	C	303[A]	CTN	C5-C4	-3.16	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	303[B]	CYT	C4-N3	-3.04	1.33	1.37
4	E	305[A]	CTN	C5-C4	-3.04	1.35	1.42
4	A	303[A]	CTN	C5-C4	-3.01	1.35	1.42
4	F	302[A]	CTN	C5-C4	-3.00	1.36	1.42
5	A	304[B]	CYT	C4-N3	-2.91	1.33	1.37
5	B	305[B]	CYT	C4-N3	-2.86	1.33	1.37
5	B	305[B]	CYT	C4-N4	-2.80	1.29	1.34
5	D	301	CYT	C5-C6	-2.74	1.33	1.39
5	C	304[B]	CYT	C5-C6	-2.65	1.33	1.39
5	D	301	CYT	C4-N3	-2.63	1.33	1.37
5	F	303[B]	CYT	O2-C2	-2.48	1.19	1.24
5	D	303[B]	CYT	C4-N3	-2.46	1.33	1.37
5	A	304[B]	CYT	C4-N4	-2.45	1.29	1.34
5	C	304[B]	CYT	C4-N4	-2.44	1.29	1.34
4	B	304[A]	CTN	C6-N1	-2.39	1.32	1.38
4	F	302[A]	CTN	C6-N1	-2.34	1.32	1.38
5	E	306[B]	CYT	C5-C6	-2.26	1.34	1.39
5	A	304[B]	CYT	C2-N3	-2.26	1.34	1.39
4	C	303[A]	CTN	O2-C2	-2.25	1.19	1.23
5	D	303[B]	CYT	C5-C4	2.25	1.42	1.39
4	E	305[A]	CTN	C6-N1	-2.23	1.32	1.38
5	C	304[B]	CYT	C2-N3	-2.21	1.34	1.39
4	B	304[A]	CTN	C2-N1	-2.17	1.35	1.40
5	F	303[B]	CYT	C5-C6	-2.16	1.34	1.39
5	B	305[B]	CYT	C5-C6	-2.06	1.35	1.39
5	D	301	CYT	C5-C4	2.04	1.42	1.39
4	D	302[A]	CTN	C4-N3	-2.03	1.30	1.34
5	E	306[B]	CYT	C4-N4	-2.01	1.30	1.34

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	305[B]	CYT	C5-C4-N3	6.97	122.01	118.04
5	D	301	CYT	C5-C4-N3	6.75	121.88	118.04
5	F	303[B]	CYT	C5-C4-N3	6.63	121.82	118.04
5	A	304[B]	CYT	C5-C4-N3	5.48	121.16	118.04
5	A	304[B]	CYT	C5-C6-N1	-5.07	120.74	124.75
5	D	301	CYT	C5-C6-N1	-5.00	120.80	124.75
5	E	306[B]	CYT	C5-C4-N3	4.85	120.81	118.04
4	F	302[A]	CTN	C1'-N1-C2	4.84	129.13	118.44
5	D	303[B]	CYT	C5-C6-N1	-4.51	121.18	124.75
4	E	305[A]	CTN	O2-C2-N3	-4.35	115.47	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	302[A]	CTN	O2-C2-N3	-4.33	115.50	122.33
4	E	305[A]	CTN	C1'-N1-C2	4.22	127.76	118.44
5	B	305[B]	CYT	C5-C6-N1	-4.05	121.55	124.75
4	C	303[A]	CTN	C1'-N1-C2	3.99	127.26	118.44
5	C	304[B]	CYT	C5-C4-N3	3.94	120.28	118.04
4	C	303[A]	CTN	O2-C2-N3	-3.89	116.20	122.33
4	D	302[A]	CTN	O2-C2-N3	-3.86	116.24	122.33
4	B	304[A]	CTN	C1'-N1-C2	3.84	126.92	118.44
4	B	304[A]	CTN	C1'-N1-C6	-3.58	113.12	120.78
4	F	302[A]	CTN	C1'-N1-C6	-3.52	113.26	120.78
5	D	301	CYT	C5-C4-N4	-3.40	120.57	123.88
5	D	303[B]	CYT	C5-C4-N3	3.28	119.91	118.04
5	A	304[B]	CYT	C5-C4-N4	-3.25	120.72	123.88
5	F	303[B]	CYT	C5-C4-N4	-3.23	120.74	123.88
5	C	304[B]	CYT	C5-C6-N1	-3.21	122.21	124.75
5	F	303[B]	CYT	C5-C6-N1	-3.17	122.24	124.75
5	E	306[B]	CYT	C5-C6-N1	-3.13	122.28	124.75
4	B	304[A]	CTN	O4'-C1'-N1	-3.11	101.30	108.36
4	D	302[A]	CTN	C1'-N1-C2	3.04	125.17	118.44
5	B	305[B]	CYT	C5-C4-N4	-2.98	120.98	123.88
4	E	305[A]	CTN	C1'-N1-C6	-2.88	114.62	120.78
4	A	303[A]	CTN	O2-C2-N3	-2.83	117.87	122.33
4	C	303[A]	CTN	O2-C2-N1	2.81	124.41	118.90
4	A	303[A]	CTN	C4-N3-C2	2.81	124.68	120.26
4	E	305[A]	CTN	O2-C2-N1	2.79	124.37	118.90
4	A	303[A]	CTN	C1'-N1-C2	2.73	124.47	118.44
4	C	303[A]	CTN	C1'-N1-C6	-2.69	115.04	120.78
4	F	302[A]	CTN	O2-C2-N1	2.55	123.90	118.90
4	A	303[A]	CTN	O2-C2-N1	2.51	123.82	118.90
4	D	302[A]	CTN	C6-N1-C2	-2.41	116.39	120.46
5	F	303[B]	CYT	O2-C2-N3	2.33	123.06	118.58
4	A	303[A]	CTN	C5-C4-N3	-2.32	117.41	121.32
4	B	304[A]	CTN	O2-C2-N3	-2.32	118.67	122.33
5	B	305[B]	CYT	O2-C2-N3	2.26	122.93	118.58
6	D	304[C]	GOL	O2-C2-C1	2.22	118.36	109.18
5	E	306[B]	CYT	O2-C2-N3	2.18	122.77	118.58
6	A	305[C]	GOL	O2-C2-C3	2.13	117.99	109.18
4	B	304[A]	CTN	O4'-C4'-C5'	-2.12	104.73	109.22
5	E	306[B]	CYT	C5-C4-N4	-2.10	121.83	123.88
4	F	302[A]	CTN	C3'-C2'-C1'	2.06	105.36	101.46

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	302[A]	CTN	C2'-C1'-N1-C2
6	A	305[C]	GOL	O1-C1-C2-C3
6	B	306[B]	GOL	O1-C1-C2-C3
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	D	304[C]	GOL	C1-C2-C3-O3
6	E	307[C]	GOL	O1-C1-C2-C3
6	F	304[C]	GOL	O1-C1-C2-C3
4	A	303[A]	CTN	C2'-C1'-N1-C6
4	C	303[A]	CTN	C2'-C1'-N1-C6
4	D	302[A]	CTN	C2'-C1'-N1-C6
4	A	303[A]	CTN	C2'-C1'-N1-C2
4	C	303[A]	CTN	C2'-C1'-N1-C2
4	D	302[A]	CTN	C2'-C1'-N1-C2
4	E	305[A]	CTN	C2'-C1'-N1-C2
4	C	303[A]	CTN	C3'-C4'-C5'-O5'
4	B	304[A]	CTN	C2'-C1'-N1-C6
4	E	305[A]	CTN	C2'-C1'-N1-C6
4	F	302[A]	CTN	C2'-C1'-N1-C6
6	B	306[B]	GOL	O1-C1-C2-O2
4	C	303[A]	CTN	O4'-C4'-C5'-O5'
4	B	304[A]	CTN	C3'-C4'-C5'-O5'
4	B	304[A]	CTN	O4'-C4'-C5'-O5'
6	C	305[B]	GOL	O1-C1-C2-O2
6	D	304[C]	GOL	O2-C2-C3-O3
6	E	307[C]	GOL	O1-C1-C2-O2
6	F	304[C]	GOL	O1-C1-C2-O2
4	B	304[A]	CTN	C2'-C1'-N1-C2
2	B	303	EDO	O1-C1-C2-O2
2	E	303	EDO	O1-C1-C2-O2
6	F	304[C]	GOL	O2-C2-C3-O3
4	F	302[A]	CTN	O4'-C4'-C5'-O5'
2	A	301	EDO	O1-C1-C2-O2
4	B	304[A]	CTN	O4'-C1'-N1-C6
4	B	304[A]	CTN	O4'-C1'-N1-C2
6	F	304[C]	GOL	C1-C2-C3-O3
6	A	305[C]	GOL	O1-C1-C2-O2
4	F	302[A]	CTN	O4'-C1'-N1-C6

There are no ring outliers.

22 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	304[A]	CTN	3	0
7	A	306[A]	SO4	1	0
2	A	301	EDO	6	0
5	A	304[B]	CYT	2	0
5	B	305[B]	CYT	1	0
4	C	303[A]	CTN	2	0
7	A	306[B]	SO4	1	0
4	D	302[A]	CTN	2	0
5	D	303[B]	CYT	1	0
6	F	304[C]	GOL	1	0
4	A	303[A]	CTN	2	0
6	E	307[C]	GOL	1	0
6	A	305[C]	GOL	1	0
4	E	305[A]	CTN	1	0
5	E	306[B]	CYT	1	0
2	E	303	EDO	6	0
4	F	302[A]	CTN	1	0
6	D	304[C]	GOL	1	0
5	C	304[B]	CYT	1	0
5	F	303[B]	CYT	2	0
2	B	303	EDO	10	0
5	D	301	CYT	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	251/253 (99%)	-0.46	3 (1%) 76 81	5, 13, 25, 49	33 (13%)
1	B	252/253 (99%)	-0.43	7 (2%) 55 60	4, 12, 40, 76	35 (13%)
1	C	252/253 (99%)	-0.38	1 (0%) 88 90	5, 14, 28, 56	27 (10%)
1	D	251/253 (99%)	-0.38	7 (2%) 55 60	5, 14, 31, 63	26 (10%)
1	E	252/253 (99%)	-0.32	8 (3%) 50 55	5, 13, 46, 76	35 (13%)
1	F	251/253 (99%)	-0.14	13 (5%) 33 36	5, 16, 46, 88	33 (13%)
All	All	1509/1518 (99%)	-0.35	39 (2%) 57 62	4, 14, 36, 88	189 (12%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	THR	4.1
1	F	233	LEU	4.0
1	F	228	PRO	4.0
1	D	233	LEU	3.9
1	F	227	ILE	3.9
1	D	232	THR	3.9
1	F	231	ALA	3.9
1	E	2	THR	3.6
1	F	220[A]	ILE	3.2
1	F	236[A]	THR	3.1
1	E	231	ALA	3.1
1	D	230	HIS	3.0
1	D	231	ALA	2.9
1	B	227	ILE	2.9
1	B	230	HIS	2.9
1	B	2	THR	2.8
1	B	220[A]	ILE	2.7
1	F	232	THR	2.6
1	B	228	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	232	THR	2.6
1	F	230	HIS	2.6
1	E	233	LEU	2.5
1	F	252	LEU	2.4
1	E	228	PRO	2.4
1	E	232	THR	2.4
1	F	235[A]	GLU	2.3
1	A	231	ALA	2.2
1	E	174	ARG	2.2
1	D	4	THR	2.1
1	E	227	ILE	2.1
1	B	229	ASP	2.1
1	A	234[A]	LYS	2.1
1	D	6	PHE	2.1
1	F	229	ASP	2.1
1	E	235	GLU	2.1
1	F	223	THR	2.1
1	B	231	ALA	2.1
1	F	6	PHE	2.0
1	D	252	LEU	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(Å ²)	Q<0.9
4	CTN	F	302[A]	17/17	0.87	0.13	23,28,34,34	30
4	CTN	E	305[A]	17/17	0.88	0.14	19,20,24,24	30
4	CTN	C	303[A]	17/17	0.92	0.10	14,15,18,19	30

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	B	303	4/4	0.92	0.15	15,18,20,23	4
4	CTN	B	304[A]	17/17	0.92	0.09	14,16,20,21	30
5	CYT	D	301	8/8	0.92	0.12	27,30,35,36	12
7	SO4	A	306[A]	5/5	0.92	0.12	32,32,32,32	5
7	SO4	A	306[B]	5/5	0.92	0.12	27,27,27,28	5
2	EDO	E	303	4/4	0.93	0.13	16,17,21,21	4
2	EDO	A	301	4/4	0.93	0.12	17,19,23,25	4
6	GOL	D	304[C]	6/6	0.94	0.09	26,27,32,32	10
6	GOL	F	304[C]	6/6	0.95	0.07	18,21,23,24	10
8	CL	E	301	1/1	0.95	0.12	53,53,53,53	0
6	GOL	A	305[C]	6/6	0.96	0.07	20,22,26,26	11
6	GOL	B	306[B]	6/6	0.97	0.06	17,19,20,22	9
6	GOL	C	305[B]	6/6	0.97	0.06	15,17,20,20	10
4	CTN	D	302[A]	17/17	0.97	0.06	9,11,14,15	30
6	GOL	E	307[C]	6/6	0.97	0.06	18,19,23,23	10
4	CTN	A	303[A]	17/17	0.98	0.04	7,9,11,12	30
5	CYT	B	305[B]	8/8	0.98	0.05	10,12,15,16	12
5	CYT	F	303[B]	8/8	0.99	0.04	10,13,16,16	12
5	CYT	C	304[B]	8/8	0.99	0.03	9,10,13,13	12
5	CYT	A	304[B]	8/8	0.99	0.03	6,8,9,10	12
5	CYT	D	303[B]	8/8	0.99	0.03	7,8,10,11	12
8	CL	B	301	1/1	0.99	0.06	22,22,22,22	1
8	CL	B	302	1/1	0.99	0.06	32,32,32,32	1
5	CYT	E	306[B]	8/8	0.99	0.04	9,11,14,15	12
8	CL	E	302	1/1	0.99	0.04	21,21,21,21	1
8	CL	F	301	1/1	0.99	0.04	25,25,25,25	1
8	CL	C	301	1/1	1.00	0.03	16,16,16,16	1
3	K	E	304	1/1	1.00	0.03	11,11,11,11	1
3	K	A	302	1/1	1.00	0.03	11,11,11,11	1
3	K	C	302	1/1	1.00	0.02	13,13,13,13	1

6.5 Other polymers ⓘ

There are no such residues in this entry.