Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 12:11 am GMT

PDB ID	:	5EFO
Title	:	X-ray structure uridine phosphorylase from Vibrio cholerae in complex with cytidine and cytosine at 1.63A.
Authors	:	Prokofev, I.I.; Lashkov, A.A.; Gabdoulkhakov, A.G.; Betzel, C.; Mikhailov, A.M.
Deposited on	:	2015-10-24
Resolution	:	1.63 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 (i) 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 (i)) were used in the production of this report:

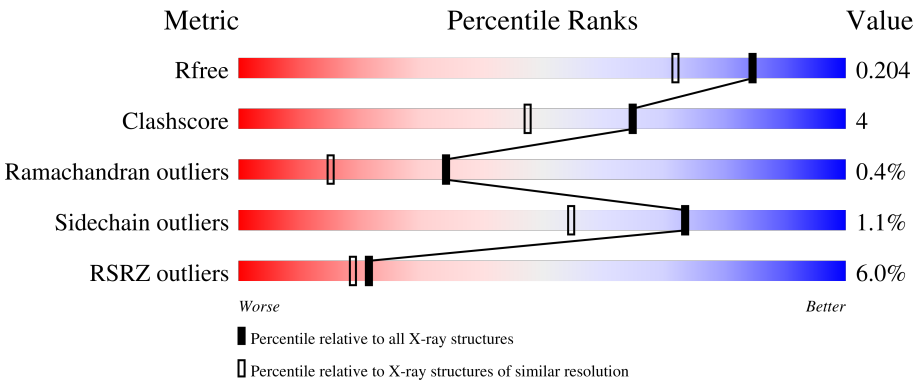
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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 <=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	6% 93% 5% •
1	B	253	5% 90% 9% •
1	C	253	7% 92% 7% •
1	D	253	7% 94% 6% •
1	E	253	6% 90% 9% •

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Mol	Chain	Length	Quality of chain
1	F	253	5% 93% 6%

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
5	GOL	E	302[A]	-	-	X	-
7	EDO	F	302	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 13396 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.

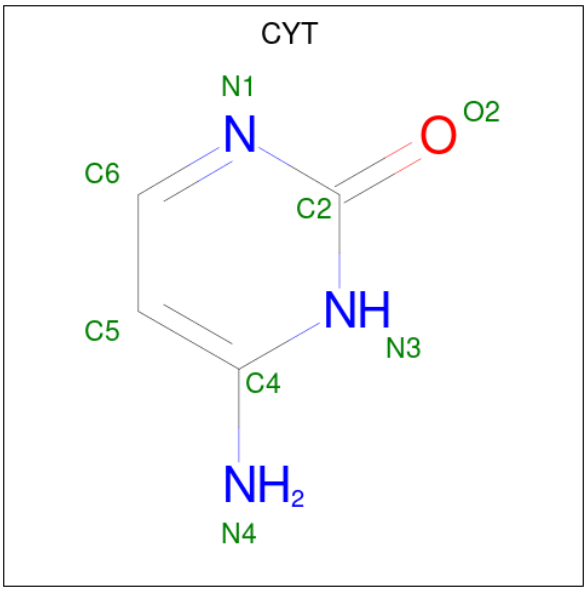
- Molecule 1 is a protein called Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	248	1931	1218	330	369	14	0	14	0
1	B	253	1980	1248	338	379	15	0	15	0
1	C	251	1967	1237	342	372	16	0	15	0
1	D	251	1955	1230	337	372	16	0	13	0
1	E	251	1956	1230	339	370	17	0	13	0
1	F	251	1929	1213	333	368	15	0	9	0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

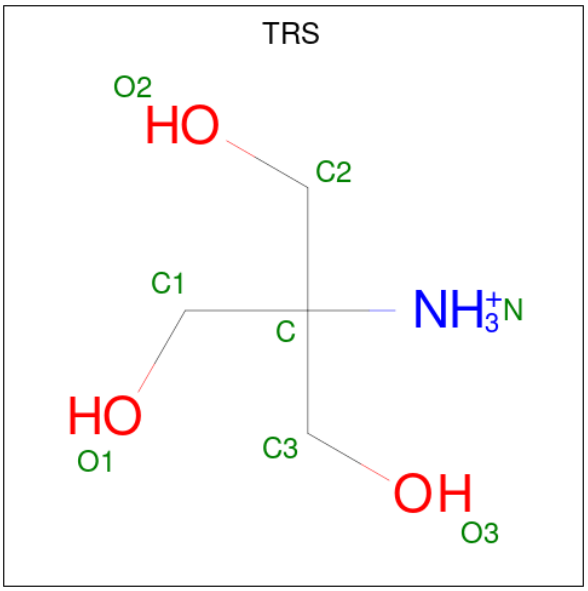
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0
2	C	1	1	1	0	0
2	E	1	1	1	0	0

- Molecule 3 is 6-AMINOPYRIMIDIN-2(1H)-ONE (three-letter code: CYT) (formula: $C_4H_5N_3O$).



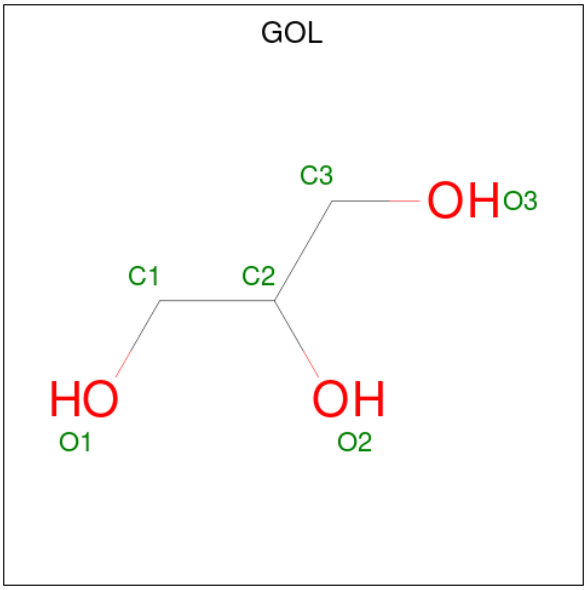
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	8	4	3	1	0	0
3	B	1	8	4	3	1	0	0
3	C	1	8	4	3	1	0	1
3	C	1	8	4	3	1	0	0
3	D	1	8	4	3	1	0	0
3	D	1	8	4	3	1	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	8	4	1	3	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	12	6	6	0	1
5	C	1	12	6	6	0	1
5	D	1	12	6	6	0	1

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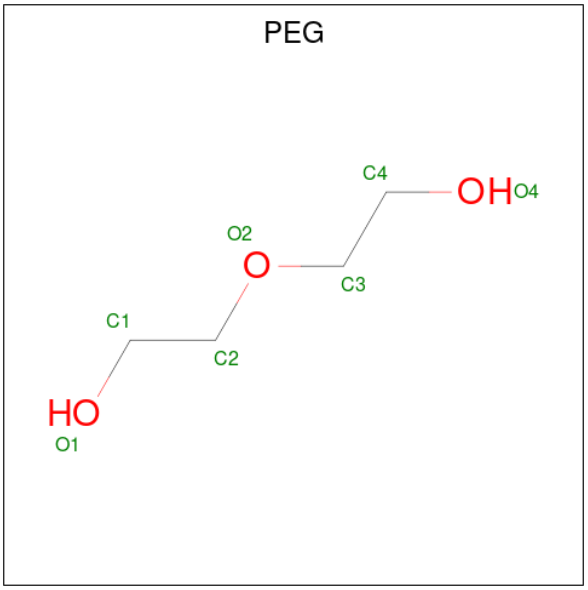
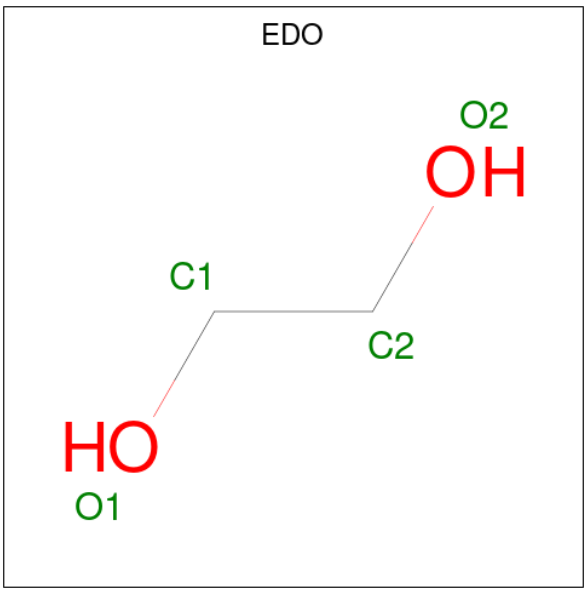
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	E	1	12	6	6	0	1

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



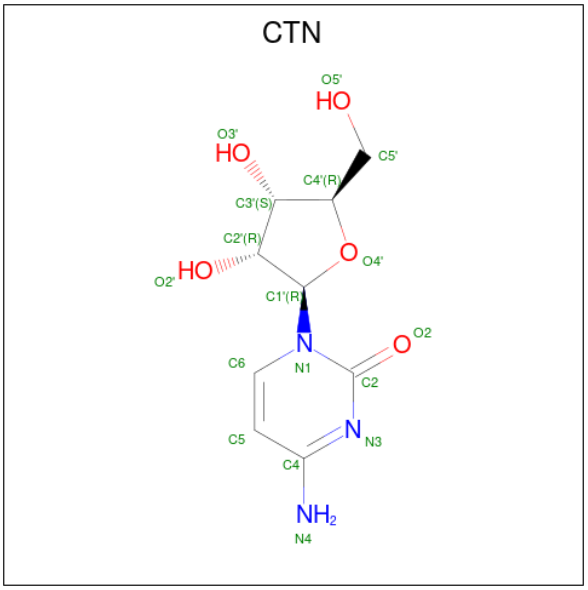
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	C	1	7	4	3	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
7	D	1	4	2	2		0	0
			Total	C	O			
7	F	1	4	2	2		0	0
			Total	C	O			
7	F	1	4	2	2		0	0

- Molecule 8 is 4-AMINO-1-BETA-D-RIBOFURANOSYL-2(1H)-PYRIMIDINONE (three-letter code: CTN) (formula: $C_9H_{13}N_3O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	E	1	17	9	3	5	0	0
			Total	C	N	O		
8	F	1	17	9	3	5	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	245	245	245	0	0
			Total	O		
9	B	261	262	262	0	1
			Total	O		
9	C	268	271	271	0	3
			Total	O		
9	D	259	260	260	0	1

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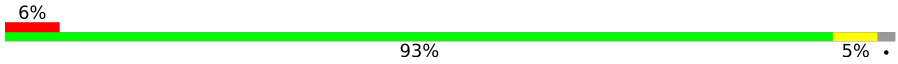
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	E	212	214	214	0	2
			Total	O		
9	F	264	266	266	0	2

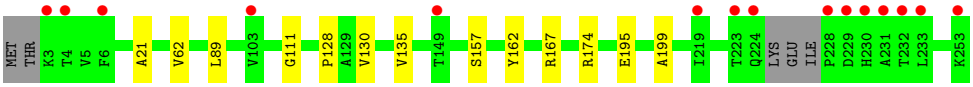
3 Residue-property plots (i)

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

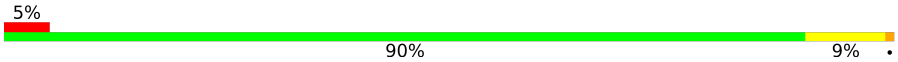
Chain A:

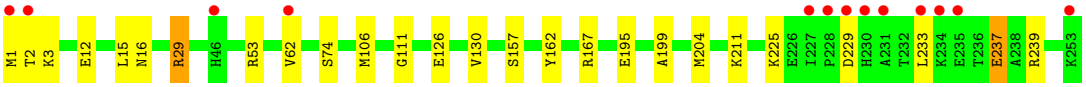




- Molecule 1: Uridine phosphorylase

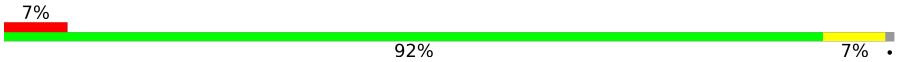
Chain B:





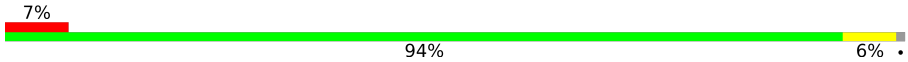
- Molecule 1: Uridine phosphorylase

Chain C:



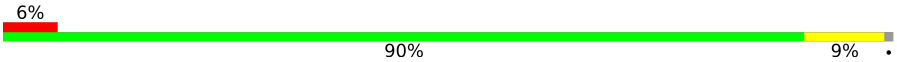
- Molecule 1: Uridine phosphorylase

Chain D:



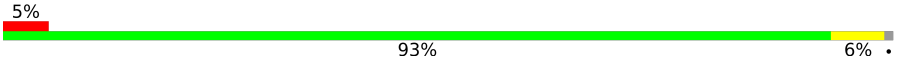
- Molecule 1: Uridine phosphorylase

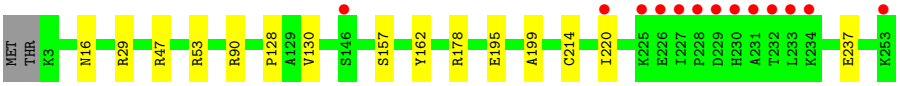
Chain E:



• Molecule 1: Uridine phosphorylase

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.95Å 76.34Å 89.69Å 67.54° 73.74° 84.92°	Depositor
Resolution (Å)	19.97 – 1.63 19.97 – 1.63	Depositor EDS
% Data completeness (in resolution range)	92.2 (19.97-1.63) 92.2 (19.97-1.63)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.163 , 0.207 0.159 , 0.204	Depositor DCC
R_{free} test set	8011 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	14.3	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13396	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, GOL, NA, PEG, EDO, TRS, 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	0.38	0/2001	0.56	0/2709
1	B	0.38	0/2054	0.58	0/2781
1	C	0.38	0/2044	0.58	0/2765
1	D	0.38	0/2022	0.57	0/2738
1	E	0.39	0/2024	0.55	0/2740
1	F	0.38	0/1988	0.56	0/2693
All	All	0.38	0/12133	0.57	0/16426

There are no bond length outliers.

There are no bond angle outliers.

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	1931	0	1964	11	0
1	B	1980	0	2018	19	0
1	C	1967	0	2012	15	0
1	D	1955	0	1993	18	0
1	E	1956	0	1990	27	0
1	F	1929	0	1955	15	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	E	1	0	0	0	0
3	A	8	0	4	3	0
3	B	8	0	4	1	0
3	C	16	0	8	6	0
3	D	16	0	8	4	0
4	A	8	0	12	1	0
5	B	12	0	16	0	0
5	C	12	0	16	0	0
5	D	12	0	16	0	0
5	E	12	0	16	8	0
6	C	7	0	10	0	0
7	D	4	0	6	0	0
7	F	8	0	12	5	0
8	E	17	0	13	1	0
8	F	17	0	13	2	0
9	A	245	0	0	2	0
9	B	262	0	0	0	0
9	C	271	0	0	4	0
9	D	260	0	0	3	0
9	E	214	0	0	4	0
9	F	266	0	0	2	0
All	All	13396	0	12086	97	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (97) 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)
3:C:303[A]:CYT:N1	9:C:401:HOH:O	1.81	1.14
1:B:1:MET:HA	1:B:12:GLU:HB3	1.33	1.08
1:F:214[B]:CYS:SG	9:F:597:HOH:O	2.14	1.06
1:E:29[A]:ARG:NH1	5:E:302[A]:GOL:O1	1.97	0.98
1:E:214[B]:CYS:SG	9:E:498:HOH:O	2.21	0.93
1:E:29[A]:ARG:HH12	5:E:302[A]:GOL:H12	1.37	0.90
1:E:29[A]:ARG:HH12	5:E:302[A]:GOL:C1	1.90	0.85
1:E:29[A]:ARG:NH1	5:E:302[A]:GOL:C1	2.39	0.84
1:F:178:ARG:HD2	7:F:302:EDO:H11	1.60	0.81
8:E:303:CTN:O2	8:E:303:CTN:H2'	1.88	0.73
1:D:130[A]:VAL:HG11	1:E:130[A]:VAL:HG12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:PRO:HB2	1:F:130[A]:VAL:HG23	1.71	0.72
1:E:29[A]:ARG:NH1	5:E:302[A]:GOL:H12	2.03	0.71
1:D:130[A]:VAL:CG1	1:E:130[A]:VAL:CG1	2.70	0.69
1:A:167:ARG:HH22	3:A:302:CYT:N4	1.90	0.69
1:D:130[A]:VAL:CG1	1:E:130[A]:VAL:HG12	2.23	0.68
1:B:126[A]:GLU:OE2	3:C:304:CYT:C2	2.47	0.68
3:C:303[A]:CYT:C6	9:C:401:HOH:O	2.35	0.67
1:A:174[A]:ARG:NH2	9:A:401:HOH:O	2.29	0.65
8:F:303:CTN:H2'	8:F:303:CTN:O2	1.98	0.63
1:B:130[B]:VAL:CG2	1:C:130[B]:VAL:HG22	2.29	0.62
1:F:29[B]:ARG:NH2	1:F:237:GLU:O	2.32	0.62
1:C:128:PRO:HB2	1:C:130[B]:VAL:HG23	1.81	0.62
1:D:174[B]:ARG:NH1	9:D:403:HOH:O	2.33	0.61
1:F:16:ASN:HB2	1:F:53:ARG:HD2	1.83	0.61
1:A:167:ARG:HH22	3:A:302:CYT:H42	1.48	0.61
1:B:29:ARG:HD3	1:B:237[A]:GLU:OE2	2.00	0.61
1:E:174[A]:ARG:HD2	9:E:597:HOH:O	2.03	0.58
1:B:167:ARG:HH22	3:B:302:CYT:N4	2.01	0.58
1:B:126[A]:GLU:OE2	3:C:304:CYT:O2	2.23	0.57
1:C:167:ARG:HH22	3:C:303[A]:CYT:N4	2.03	0.57
1:F:90:ARG:HG2	1:F:214[B]:CYS:SG	2.44	0.56
1:D:167:ARG:HH22	3:D:302:CYT:N4	2.03	0.56
1:D:185[B]:GLU:OE1	3:D:303:CYT:N1	2.39	0.56
1:D:174[B]:ARG:NH2	9:D:404:HOH:O	2.35	0.55
1:D:130[A]:VAL:HG12	1:E:130[A]:VAL:CG1	2.36	0.55
1:D:29[A]:ARG:HH12	1:D:92:GLY:HA2	1.72	0.55
1:E:120:LEU:HD22	7:F:302:EDO:H12	1.90	0.54
1:E:16:ASN:HB2	1:E:53:ARG:HD2	1.89	0.54
1:F:128:PRO:HB2	1:F:130[A]:VAL:CG2	2.36	0.54
1:D:130[B]:VAL:HG21	1:E:110:THR:O	2.08	0.54
1:C:174[A]:ARG:HD3	1:E:188:ASP:HB3	1.91	0.52
5:E:302[A]:GOL:H31	1:F:47:ARG:HH22	1.74	0.52
1:C:15:LEU:HG	1:C:62:VAL:HG21	1.92	0.51
1:C:16:ASN:HB2	1:C:53:ARG:HD2	1.91	0.51
1:A:174[A]:ARG:NH1	9:A:403:HOH:O	2.39	0.51
1:B:15:LEU:HD13	1:B:62[A]:VAL:HG21	1.94	0.50
1:B:157:SER:HB3	1:B:199:ALA:HB2	1.94	0.50
1:D:130[A]:VAL:HG12	1:E:130[A]:VAL:HG11	1.92	0.50
1:D:174[B]:ARG:NH2	9:D:408:HOH:O	2.45	0.49
1:E:37:MET:HG2	1:E:56:LEU:HD13	1.94	0.49
1:A:130[A]:VAL:CG1	1:F:130[A]:VAL:HG22	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130[B]:VAL:HG21	1:C:130[B]:VAL:HG22	1.93	0.49
1:C:208:SER:HA	1:D:174[A]:ARG:HH22	1.77	0.49
1:E:211:LYS:NZ	9:E:403:HOH:O	2.45	0.48
1:F:157:SER:HB3	1:F:199:ALA:HB2	1.95	0.48
1:E:157:SER:HB3	1:E:199:ALA:HB2	1.96	0.47
1:B:130[A]:VAL:HG21	1:C:110:THR:O	2.15	0.47
1:C:222[B]:ARG:NH1	9:C:406:HOH:O	2.46	0.47
1:A:111:GLY:HA3	1:F:130[A]:VAL:HG21	1.97	0.47
1:A:157:SER:HB3	1:A:199:ALA:HB2	1.96	0.47
1:D:29[A]:ARG:NH1	1:D:92:GLY:HA2	2.30	0.47
1:F:29[B]:ARG:NH2	1:F:237:GLU:HG3	2.30	0.47
1:B:16:ASN:HB2	1:B:53:ARG:HD2	1.97	0.47
1:B:74:SER:HA	1:B:204[B]:MET:HE1	1.98	0.46
1:B:1:MET:HA	1:B:12:GLU:CB	2.24	0.46
1:B:239[A]:ARG:HG3	1:B:239[A]:ARG:NH1	2.30	0.46
1:A:21:ALA:HB2	1:A:62[A]:VAL:HG13	1.97	0.46
3:D:303:CYT:N4	1:E:126:GLU:OE1	2.48	0.46
1:D:16:ASN:HB2	1:D:53:ARG:HD2	1.97	0.46
3:A:302:CYT:N1	4:A:303:TRS:H21	2.30	0.46
1:C:15:LEU:HG	1:C:62:VAL:CG2	2.46	0.46
1:E:120:LEU:HB3	7:F:302:EDO:H12	1.98	0.45
1:D:106[B]:MET:HE3	1:D:143:ALA:HB1	1.97	0.45
1:B:126[B]:GLU:OE2	3:C:304:CYT:O2	2.36	0.44
1:B:111:GLY:HA3	1:C:130[B]:VAL:HG21	1.99	0.44
7:F:302:EDO:H21	9:F:593:HOH:O	2.18	0.43
1:E:29[B]:ARG:NH1	1:E:237:GLU:HB3	2.33	0.43
1:F:178:ARG:CD	7:F:302:EDO:H11	2.38	0.43
1:C:157:SER:HB3	1:C:199:ALA:HB2	2.01	0.43
1:E:128:PRO:HB2	1:E:130[A]:VAL:HG13	2.01	0.42
1:E:93:THR:H	5:E:302[A]:GOL:H32	1.84	0.42
1:D:182:SER:O	1:D:185[B]:GLU:HG2	2.20	0.42
1:B:239[A]:ARG:HG3	1:B:239[A]:ARG:HH11	1.85	0.42
1:B:229:ASP:O	1:B:233:LEU:HG	2.19	0.42
1:B:106[A]:MET:HB3	1:B:106[A]:MET:HE2	1.80	0.41
1:A:89:LEU:HD22	1:A:135:VAL:HG13	2.03	0.41
1:A:128:PRO:HB2	1:A:130[A]:VAL:HG13	2.02	0.41
1:E:29[A]:ARG:CZ	5:E:302[A]:GOL:O1	2.64	0.41
1:A:174[A]:ARG:NH1	1:A:174[A]:ARG:HB3	2.36	0.41
1:C:220:ILE:HG23	9:C:406:HOH:O	2.21	0.41
1:F:220:ILE:HD11	8:F:303:CTN:HN41	1.85	0.41
1:E:224[B]:GLN:NE2	9:E:401:HOH:O	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:MET:O	1:E:187[B]:GLN:HG3	2.21	0.40
1:F:29[B]:ARG:CZ	1:F:237:GLU:HG3	2.51	0.40
1:C:122:PHE:CE1	1:C:204[A]:MET:HG3	2.57	0.40
1:D:178:ARG:HE	3:D:303:CYT:H41	1.69	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	258/253 (102%)	255 (99%)	2 (1%)	1 (0%)	34	15
1	B	266/253 (105%)	262 (98%)	3 (1%)	1 (0%)	34	15
1	C	264/253 (104%)	262 (99%)	1 (0%)	1 (0%)	34	15
1	D	262/253 (104%)	259 (99%)	2 (1%)	1 (0%)	34	15
1	E	262/253 (104%)	261 (100%)	0	1 (0%)	34	15
1	F	258/253 (102%)	257 (100%)	0	1 (0%)	34	15
All	All	1570/1518 (103%)	1556 (99%)	8 (0%)	6 (0%)	34	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	162	TYR
1	D	162	TYR
1	E	162	TYR
1	F	162	TYR
1	A	162	TYR
1	B	162	TYR

5.3.2 Protein sidechains (i)

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	212/203 (104%)	211 (100%)	1 (0%)	88	80
1	B	217/203 (107%)	208 (96%)	9 (4%)	30	7
1	C	216/203 (106%)	215 (100%)	1 (0%)	88	80
1	D	214/203 (105%)	213 (100%)	1 (0%)	88	80
1	E	214/203 (105%)	212 (99%)	2 (1%)	78	63
1	F	210/203 (103%)	209 (100%)	1 (0%)	88	80
All	All	1283/1218 (105%)	1268 (99%)	15 (1%)	73	51

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	GLU
1	B	2	THR
1	B	3	LYS
1	B	29	ARG
1	B	195	GLU
1	B	211[A]	LYS
1	B	211[B]	LYS
1	B	225	LYS
1	B	237[A]	GLU
1	B	237[B]	GLU
1	C	195	GLU
1	D	195	GLU
1	E	195	GLU
1	E	233	LEU
1	F	195	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
5	GOL	B	301[A]	-	5,5,5	0.26	0	5,5,5	0.39	0
3	CYT	C	304	-	7,8,8	0.85	0	8,10,10	5.94	6 (75%)
8	CTN	F	303	-	15,18,18	0.75	1 (6%)	17,26,26	2.00	6 (35%)
3	CYT	A	302	-	7,8,8	0.81	0	8,10,10	6.56	6 (75%)
7	EDO	F	302	-	3,3,3	0.34	0	2,2,2	0.38	0
3	CYT	D	303	-	7,8,8	0.88	0	8,10,10	6.16	5 (62%)
3	CYT	C	303[A]	-	7,8,8	0.83	0	8,10,10	6.36	5 (62%)
8	CTN	E	303	-	15,18,18	0.67	0	17,26,26	2.22	6 (35%)
5	GOL	E	302[B]	-	5,5,5	0.26	0	5,5,5	0.23	0
6	PEG	C	302	-	6,6,6	0.50	0	5,5,5	0.21	0
7	EDO	D	301	-	3,3,3	0.48	0	2,2,2	0.33	0
5	GOL	E	302[A]	-	5,5,5	0.27	0	5,5,5	0.24	0
5	GOL	D	304[B]	-	5,5,5	0.31	0	5,5,5	0.25	0
3	CYT	B	302	-	7,8,8	0.74	0	8,10,10	6.09	6 (75%)
5	GOL	D	304[A]	-	5,5,5	0.28	0	5,5,5	0.30	0
7	EDO	F	301	-	3,3,3	0.45	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	C	301[B]	-	5,5,5	0.30	0	5,5,5	0.19	0
4	TRS	A	303	-	7,7,7	0.45	0	9,9,9	0.74	0
5	GOL	B	301[B]	-	5,5,5	0.28	0	5,5,5	0.51	0
5	GOL	C	301[A]	-	5,5,5	0.28	0	5,5,5	0.33	0
3	CYT	D	302	-	7,8,8	0.83	0	8,10,10	6.42	6 (75%)

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	GOL	B	301[A]	-	-	2/4/4/4	-
3	CYT	C	304	-	-	-	0/1/1/1
8	CTN	F	303	-	-	2/4/22/22	0/2/2/2
3	CYT	A	302	-	-	-	0/1/1/1
7	EDO	F	302	-	-	1/1/1/1	-
3	CYT	D	303	-	-	-	0/1/1/1
3	CYT	C	303[A]	-	-	-	0/1/1/1
8	CTN	E	303	-	-	4/4/22/22	0/2/2/2
5	GOL	E	302[B]	-	-	2/4/4/4	-
6	PEG	C	302	-	-	4/4/4/4	-
7	EDO	D	301	-	-	0/1/1/1	-
5	GOL	E	302[A]	-	-	1/4/4/4	-
5	GOL	D	304[B]	-	-	4/4/4/4	-
3	CYT	B	302	-	-	-	0/1/1/1
5	GOL	D	304[A]	-	-	2/4/4/4	-
7	EDO	F	301	-	-	1/1/1/1	-
5	GOL	C	301[B]	-	-	0/4/4/4	-
4	TRS	A	303	-	-	0/9/9/9	-
5	GOL	B	301[B]	-	-	4/4/4/4	-
5	GOL	C	301[A]	-	-	2/4/4/4	-
3	CYT	D	302	-	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	303	CTN	O4'-C1'	2.10	1.44	1.41

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302	CYT	C6-N1-C2	14.12	121.38	114.42
3	C	303[A]	CYT	C6-N1-C2	13.65	121.15	114.42
3	D	302	CYT	C6-N1-C2	13.62	121.14	114.42
3	D	303	CYT	C6-N1-C2	13.18	120.92	114.42
3	C	304	CYT	C6-N1-C2	12.63	120.65	114.42
3	B	302	CYT	C6-N1-C2	12.31	120.49	114.42
3	A	302	CYT	N3-C2-N1	-9.99	120.49	128.43
3	B	302	CYT	N3-C2-N1	-9.70	120.72	128.43
3	D	302	CYT	N3-C2-N1	-9.65	120.76	128.43
3	C	303[A]	CYT	N3-C2-N1	-9.58	120.81	128.43
3	D	303	CYT	N3-C2-N1	-9.24	121.09	128.43
3	C	304	CYT	N3-C2-N1	-8.65	121.55	128.43
8	E	303	CTN	C4-N3-C2	5.24	121.66	116.34
3	B	302	CYT	C4-N3-C2	4.18	120.58	116.34
8	F	303	CTN	C4-N3-C2	4.17	120.56	116.34
3	D	302	CYT	C5-C6-N1	-4.11	118.86	123.96
8	E	303	CTN	C3'-C2'-C1'	4.09	107.14	100.98
3	C	303[A]	CYT	C5-C6-N1	-4.06	118.92	123.96
3	A	302	CYT	C5-C6-N1	-4.05	118.93	123.96
3	C	304	CYT	C5-C6-N1	-4.04	118.94	123.96
3	D	303	CYT	C5-C6-N1	-4.00	118.98	123.96
8	F	303	CTN	C3'-C2'-C1'	3.97	106.96	100.98
3	D	302	CYT	C4-N3-C2	3.79	120.18	116.34
3	A	302	CYT	C4-N3-C2	3.74	120.13	116.34
3	C	303[A]	CYT	C4-N3-C2	3.73	120.12	116.34
3	D	303	CYT	C4-N3-C2	3.72	120.11	116.34
3	C	304	CYT	C6-C5-C4	3.70	119.05	116.91
3	D	302	CYT	C6-C5-C4	3.46	118.92	116.91
3	B	302	CYT	C5-C6-N1	-3.45	119.67	123.96
3	B	302	CYT	C6-C5-C4	3.35	118.85	116.91
3	C	304	CYT	C4-N3-C2	3.15	119.53	116.34
3	D	303	CYT	C6-C5-C4	3.13	118.72	116.91
8	F	303	CTN	C6-N1-C2	-3.12	116.24	121.20
3	C	303[A]	CYT	C6-C5-C4	3.05	118.68	116.91
8	E	303	CTN	C6-N1-C2	-2.99	116.44	121.20
3	A	302	CYT	C6-C5-C4	2.85	118.56	116.91
8	E	303	CTN	C5'-C4'-C3'	-2.83	108.26	115.09
3	B	302	CYT	N4-C4-N3	2.61	120.61	116.49
8	E	303	CTN	C5-C4-N3	-2.58	118.74	121.72
8	F	303	CTN	C5'-C4'-C3'	-2.42	109.25	115.09
3	C	304	CYT	N4-C4-N3	2.40	120.28	116.49
8	F	303	CTN	C5-C4-N3	-2.31	119.05	121.72
3	D	302	CYT	N4-C4-N3	2.30	120.12	116.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302	CYT	N4-C4-N3	2.12	119.85	116.49
8	E	303	CTN	N4-C4-N3	2.01	119.66	116.49
8	F	303	CTN	N4-C4-N3	2.00	119.66	116.49

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	301[A]	GOL	O1-C1-C2-O2
5	B	301[A]	GOL	O1-C1-C2-C3
5	B	301[B]	GOL	O1-C1-C2-C3
5	C	301[A]	GOL	O1-C1-C2-C3
5	D	304[A]	GOL	O1-C1-C2-C3
5	D	304[B]	GOL	O1-C1-C2-C3
5	D	304[B]	GOL	C1-C2-C3-O3
5	E	302[B]	GOL	C1-C2-C3-O3
8	E	303	CTN	O4'-C1'-N1-C6
8	E	303	CTN	C2'-C1'-N1-C6
8	F	303	CTN	O4'-C1'-N1-C6
8	F	303	CTN	C2'-C1'-N1-C6
5	D	304[B]	GOL	O2-C2-C3-O3
6	C	302	PEG	O2-C3-C4-O4
8	E	303	CTN	C3'-C4'-C5'-O5'
8	E	303	CTN	O4'-C4'-C5'-O5'
6	C	302	PEG	O1-C1-C2-O2
5	B	301[B]	GOL	C1-C2-C3-O3
5	B	301[B]	GOL	O1-C1-C2-O2
5	B	301[B]	GOL	O2-C2-C3-O3
5	C	301[A]	GOL	O1-C1-C2-O2
5	D	304[A]	GOL	O1-C1-C2-O2
5	D	304[B]	GOL	O1-C1-C2-O2
5	E	302[B]	GOL	O2-C2-C3-O3
7	F	302	EDO	O1-C1-C2-O2
6	C	302	PEG	C1-C2-O2-C3
6	C	302	PEG	C4-C3-O2-C2
7	F	301	EDO	O1-C1-C2-O2
5	E	302[A]	GOL	C1-C2-C3-O3

There are no ring outliers.

11 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	304	CYT	3	0
8	F	303	CTN	2	0
3	A	302	CYT	3	0
7	F	302	EDO	5	0
3	D	303	CYT	3	0
3	C	303[A]	CYT	3	0
8	E	303	CTN	1	0
5	E	302[A]	GOL	8	0
3	B	302	CYT	1	0
4	A	303	TRS	1	0
3	D	302	CYT	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	248/253 (98%)	0.44	15 (6%)	21	19	8, 16, 34, 81	0
1	B	253/253 (100%)	0.37	13 (5%)	28	25	8, 15, 37, 66	0
1	C	251/253 (99%)	0.40	17 (6%)	17	15	8, 15, 43, 71	0
1	D	251/253 (99%)	0.49	17 (6%)	17	15	8, 16, 43, 72	0
1	E	251/253 (99%)	0.32	15 (5%)	21	19	8, 15, 33, 67	0
1	F	251/253 (99%)	0.37	13 (5%)	27	25	8, 16, 39, 74	0
All	All	1505/1518 (99%)	0.40	90 (5%)	21	19	8, 16, 40, 81	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	ILE	11.1
1	A	231	ALA	10.4
1	D	227	ILE	8.0
1	F	230	HIS	7.0
1	B	231	ALA	6.9
1	B	230	HIS	6.8
1	C	227	ILE	6.7
1	F	231	ALA	6.5
1	F	227	ILE	6.5
1	A	230	HIS	6.2
1	C	4	THR	5.9
1	B	228	PRO	5.8
1	C	230	HIS	5.7
1	A	233	LEU	5.6
1	A	228	PRO	5.4
1	F	233	LEU	5.3
1	F	229	ASP	5.3
1	A	232	THR	5.2
1	C	229	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	231	ALA	5.1
1	C	225	LYS	5.1
1	E	4	THR	5.0
1	A	4	THR	4.9
1	C	233	LEU	4.8
1	F	228	PRO	4.8
1	D	230	HIS	4.8
1	C	231	ALA	4.7
1	E	234	LYS	4.7
1	B	2	THR	4.7
1	E	232	THR	4.7
1	C	228	PRO	4.6
1	D	226	GLU	4.6
1	D	229	ASP	4.5
1	E	230	HIS	4.4
1	D	233	LEU	4.4
1	B	229	ASP	4.4
1	B	233	LEU	4.4
1	E	231	ALA	4.3
1	D	225	LYS	4.2
1	A	229	ASP	4.2
1	D	232	THR	4.2
1	B	1	MET	4.1
1	E	3	LYS	4.1
1	D	234	LYS	3.8
1	F	234	LYS	3.6
1	B	253	LYS	3.5
1	C	3	LYS	3.5
1	F	226	GLU	3.5
1	A	253	LYS	3.4
1	F	225	LYS	3.3
1	E	6	PHE	3.3
1	C	149	THR	3.2
1	E	235	GLU	3.2
1	F	232	THR	3.2
1	B	234	LYS	3.1
1	F	253	LYS	3.0
1	D	228	PRO	3.0
1	E	224[A]	GLN	3.0
1	C	232	THR	3.0
1	A	224	GLN	2.9
1	B	235[A]	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	234	LYS	2.9
1	E	227	ILE	2.8
1	D	58	GLY	2.7
1	E	253	LYS	2.7
1	D	218	VAL	2.7
1	E	228	PRO	2.7
1	C	219	ILE	2.6
1	E	229	ASP	2.6
1	D	252	LEU	2.6
1	C	253	LYS	2.5
1	A	103[A]	VAL	2.5
1	D	46	HIS	2.4
1	A	3	LYS	2.4
1	D	148	ALA	2.4
1	C	235	GLU	2.4
1	A	223	THR	2.4
1	C	6	PHE	2.3
1	D	219	ILE	2.3
1	F	220	ILE	2.2
1	F	146	SER	2.2
1	E	233	LEU	2.2
1	C	46[A]	HIS	2.1
1	A	219	ILE	2.1
1	A	149	THR	2.1
1	A	6[A]	PHE	2.1
1	B	46[A]	HIS	2.1
1	B	62[A]	VAL	2.0
1	D	224	GLN	2.0
1	E	16	ASN	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 monosaccharides 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
3	CYT	C	304	8/8	0.58	0.24	24,27,31,31	8
6	PEG	C	302	7/7	0.65	0.29	34,44,51,53	0
7	EDO	F	301	4/4	0.68	0.16	39,42,42,45	4
3	CYT	D	303	8/8	0.75	0.22	20,21,25,28	8
5	GOL	E	302[A]	6/6	0.81	0.20	36,44,45,45	6
7	EDO	D	301	4/4	0.81	0.18	29,32,38,41	0
5	GOL	E	302[B]	6/6	0.81	0.20	41,44,46,47	6
8	CTN	F	303	17/17	0.84	0.19	13,21,29,31	17
3	CYT	A	302	8/8	0.87	0.21	13,26,31,31	8
4	TRS	A	303	8/8	0.88	0.13	19,28,32,35	0
5	GOL	C	301[A]	6/6	0.89	0.14	12,20,23,24	6
5	GOL	C	301[B]	6/6	0.89	0.14	23,23,25,26	6
3	CYT	D	302	8/8	0.90	0.20	13,23,26,27	8
5	GOL	D	304[A]	6/6	0.90	0.13	20,21,21,23	6
8	CTN	E	303	17/17	0.90	0.24	9,14,30,32	17
5	GOL	D	304[B]	6/6	0.90	0.13	13,19,21,25	6
5	GOL	B	301[B]	6/6	0.91	0.13	18,29,33,38	6
5	GOL	B	301[A]	6/6	0.91	0.13	23,29,33,33	6
3	CYT	C	303[A]	8/8	0.93	0.17	16,20,24,25	8
7	EDO	F	302	4/4	0.95	0.18	17,18,24,31	4
3	CYT	B	302	8/8	0.96	0.07	14,16,17,17	0
2	NA	A	301	1/1	0.99	0.05	24,24,24,24	0
2	NA	C	305	1/1	0.99	0.07	28,28,28,28	0
2	NA	E	301	1/1	0.99	0.07	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.