



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2023 – 11:36 PM EDT

PDB ID : 4OGL  
Title : X-ray structure uridine phosphorylase from *Vibrio cholerae* in complex with thymine at 1.25 Å resolution  
Authors : Prokofev, I.I.; Lashkov, A.A.; Gabdoulkhakov, A.G.; Betzel, C.; Mikhailov, A.M.  
Deposited on : 2014-01-16  
Resolution : 1.25 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.

The types of validation reports are described at

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

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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 : 2.35.1  
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) : 2.35.1

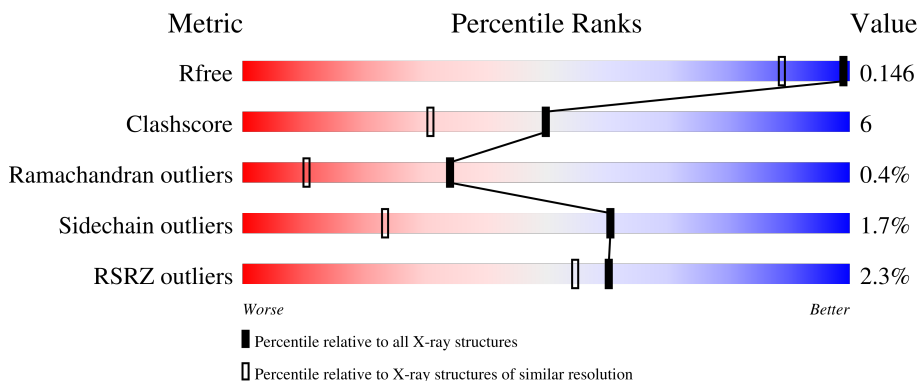
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.25 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	2024 (1.28-1.20)
Clashscore	141614	1007 (1.26-1.22)
Ramachandran outliers	138981	2053 (1.28-1.20)
Sidechain outliers	138945	2051 (1.28-1.20)
RSRZ outliers	127900	1987 (1.28-1.20)

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  $\geq 3$ , 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	 3% 90% 8%
1	B	253	 3% 84% 15%
1	C	253	 % 88% 11%
1	D	253	 88% 11%
1	E	253	 2% 87% 12%

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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	TDR	B	301	-	X	X	-
2	TDR	D	301	-	X	-	-
2	TDR	E	301	-	X	X	-
3	EDO	A	302	-	-	X	-

## 2 Entry composition [i](#)

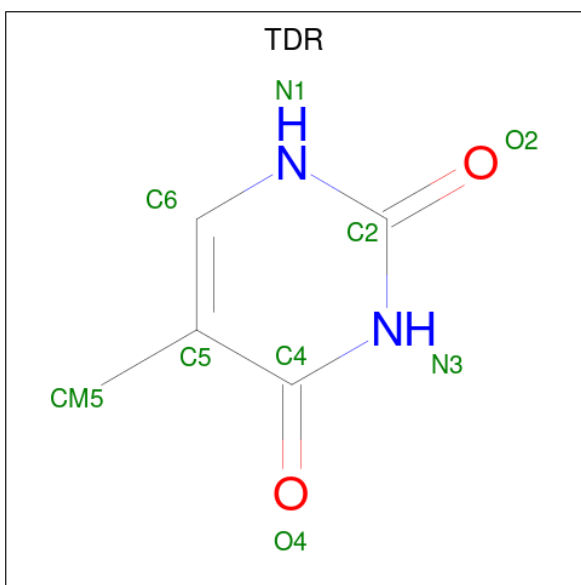
There are 7 unique types of molecules in this entry. The entry contains 14803 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

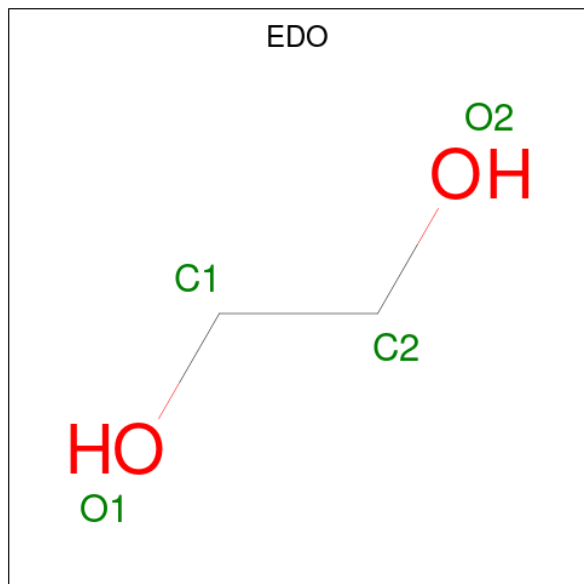
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	247	Total 2020	C 1286	N 347	O 370	S 17	0	29	0
1	B	251	Total 2102	C 1331	N 360	O 394	S 17	0	38	0
1	C	251	Total 2081	C 1322	N 360	O 381	S 18	0	33	0
1	D	251	Total 2079	C 1319	N 360	O 382	S 18	0	34	0
1	E	251	Total 2082	C 1322	N 356	O 386	S 18	0	38	0
1	F	251	Total 2020	C 1283	N 345	O 374	S 18	0	27	0

- Molecule 2 is THYMINE (three-letter code: TDR) (formula: C<sub>5</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	5	2	2		
2	B	1	Total	C	N	O	0	0
			9	5	2	2		
2	C	1	Total	C	N	O	0	0
			9	5	2	2		
2	D	1	Total	C	N	O	0	0
			9	5	2	2		
2	E	1	Total	C	N	O	0	0
			9	5	2	2		
2	F	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



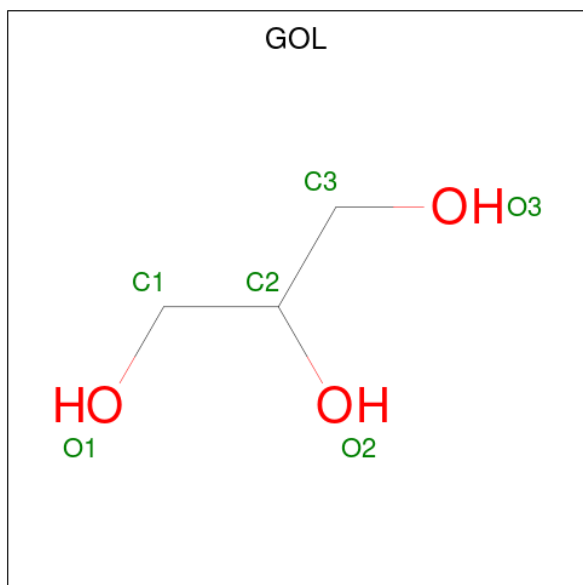
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

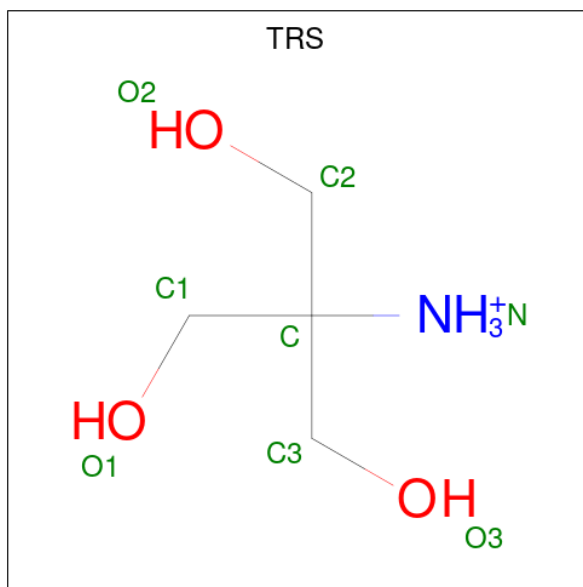


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	351	Total	O	0	23
			374	374		
7	B	348	Total	O	0	16
			366	366		
7	C	391	Total	O	0	17
			409	409		
7	D	393	Total	O	0	12
			405	405		
7	E	369	Total	O	0	21
			391	391		

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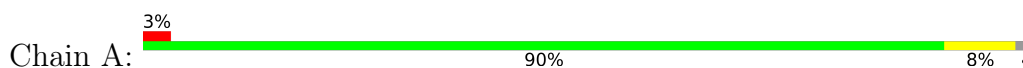
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	F	317	Total 337	O 337	0	18



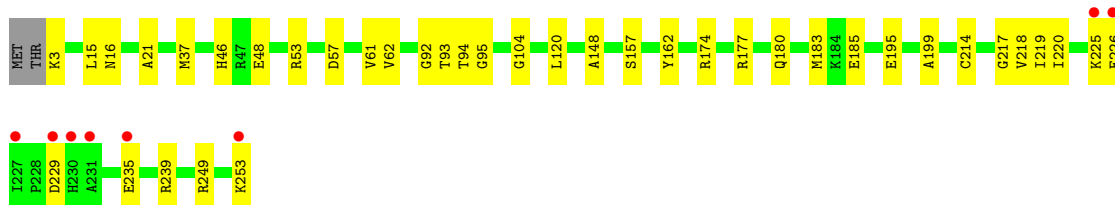
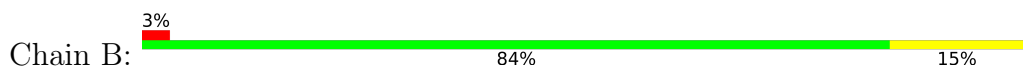
### 3 Residue-property plots [i](#)

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.

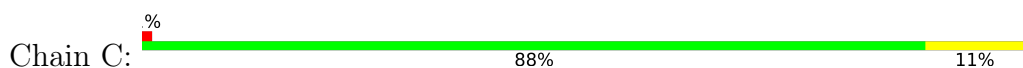
- Molecule 1: Uridine phosphorylase



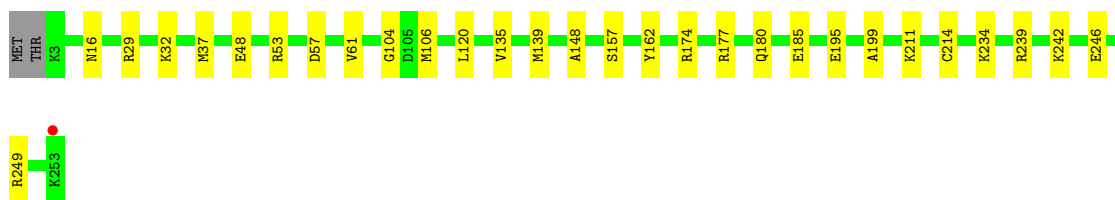
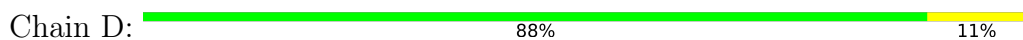
- Molecule 1: Uridine phosphorylase



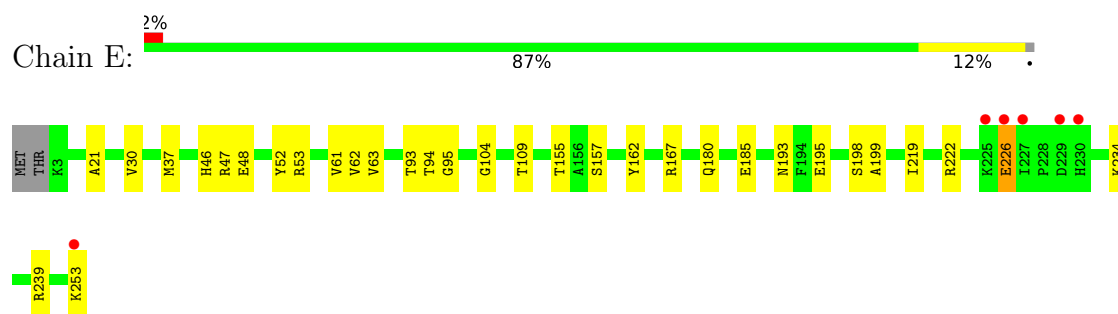
- Molecule 1: Uridine phosphorylase



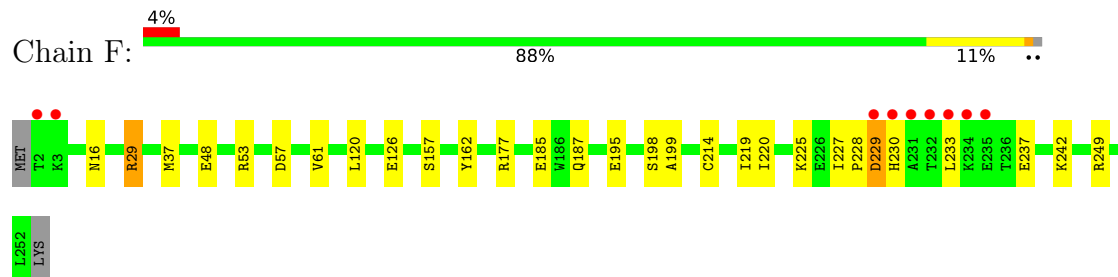
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.75Å 96.50Å 92.78Å 90.00° 119.99° 90.00°	Depositor
Resolution (Å)	8.00 – 1.25 8.00 – 1.25	Depositor EDS
% Data completeness (in resolution range)	98.2 (8.00-1.25) 98.2 (8.00-1.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 1.25Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.115 , 0.147 0.115 , 0.146	Depositor DCC
$R_{free}$ test set	19179 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.6	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.47 , 84.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.155 for l,k,-h-l 0.155 for -h-l,k,h 0.025 for h,-k,-h-l 0.025 for l,-k,h 0.025 for -h-l,-k,l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	14803	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, TDR, EDO, TRS, GOL

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	0.40	0/2132	0.61	0/2876
1	B	0.40	0/2237	0.60	0/3021
1	C	0.40	0/2212	0.62	0/2984
1	D	0.42	0/2206	0.61	0/2974
1	E	0.40	0/2214	0.60	0/2987
1	F	0.40	0/2133	0.60	0/2883
All	All	0.40	0/13134	0.61	0/17725

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	2020	0	2128	17	0
1	B	2102	0	2201	32	0
1	C	2081	0	2206	20	0
1	D	2079	0	2197	27	0
1	E	2082	0	2207	24	0
1	F	2020	0	2122	25	0
2	A	9	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	9	0	6	4	0
2	C	9	0	6	0	0
2	D	9	0	6	0	0
2	E	9	0	6	4	0
2	F	9	0	6	1	0
3	A	4	0	6	4	0
3	B	4	0	6	0	0
3	C	12	0	18	4	0
3	E	8	0	12	1	0
3	F	8	0	12	0	0
4	A	6	0	8	0	0
4	C	6	0	8	0	0
4	D	12	0	16	1	0
4	E	6	0	8	0	0
4	F	6	0	8	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
6	B	8	0	12	2	0
7	A	374	0	0	9	0
7	B	366	0	0	14	0
7	C	409	0	0	10	0
7	D	405	0	0	14	0
7	E	391	0	0	14	0
7	F	337	0	0	10	0
All	All	14803	0	13211	148	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 6.

All (148) 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:E:95[B]:GLY:O	7:E:747:HOH:O	1.88	0.92
1:D:214[B]:CYS:SG	7:D:537[B]:HOH:O	2.27	0.90
1:D:211[B]:LYS:NZ	7:D:557:HOH:O	2.04	0.90
1:B:180[A]:GLN:NE2	7:B:582:HOH:O	2.06	0.87
1:D:174[B]:ARG:NH2	7:D:518:HOH:O	2.06	0.86
1:E:94[A]:THR:HA	7:E:545:HOH:O	1.76	0.85
1:B:214[B]:CYS:SG	7:B:510[B]:HOH:O	2.34	0.85
1:A:174[B]:ARG:NH1	7:A:720:HOH:O	2.05	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106[B]:MET:SD	7:C:478:HOH:O	2.38	0.81
1:C:48[B]:GLU:HG3	1:D:48[B]:GLU:HB3	1.62	0.80
1:D:177[A]:ARG:NH2	7:D:554:HOH:O	2.14	0.80
1:B:53[B]:ARG:NH1	7:B:740:HOH:O	2.15	0.80
1:A:29[B]:ARG:NH2	7:A:540:HOH:O	2.15	0.78
3:C:302:EDO:H12	1:D:120:LEU:HD22	1.65	0.78
1:B:46[B]:HIS:ND1	7:B:726:HOH:O	2.15	0.78
1:F:185[A]:GLU:OE1	7:F:498:HOH:O	2.02	0.78
1:F:214[B]:CYS:SG	7:F:531:HOH:O	2.43	0.76
1:C:177[B]:ARG:NH1	7:C:682:HOH:O	2.18	0.76
1:F:126[B]:GLU:OE2	7:F:578:HOH:O	2.03	0.75
1:C:102:ASN:OD1	7:C:680:HOH:O	2.03	0.75
1:B:177[B]:ARG:NH2	7:B:515:HOH:O	2.19	0.75
1:D:180:GLN:NE2	7:D:670:HOH:O	2.21	0.73
1:B:180[B]:GLN:OE1	7:F:651[B]:HOH:O	2.05	0.73
1:C:214[B]:CYS:SG	7:C:580:HOH:O	2.45	0.73
1:E:180[B]:GLN:OE1	7:E:506:HOH:O	2.07	0.72
1:A:29[B]:ARG:NH2	7:A:718:HOH:O	2.14	0.72
1:C:82:GLN:HG2	3:C:304:EDO:H22	1.72	0.71
1:B:93[B]:THR:HG23	7:B:718:HOH:O	1.91	0.71
2:E:301:TDR:O4	7:E:485:HOH:O	2.08	0.69
2:E:301:TDR:N1	7:E:545:HOH:O	2.25	0.69
1:D:16[A]:ASN:HB2	1:D:53[A]:ARG:HD2	1.74	0.69
1:C:180:GLN:OE1	7:C:561:HOH:O	2.12	0.68
1:D:239[B]:ARG:NH1	7:D:792:HOH:O	2.26	0.68
1:F:177[A]:ARG:NH2	7:F:587:HOH:O	2.27	0.68
1:A:249[B]:ARG:NH2	7:A:742:HOH:O	2.27	0.67
1:B:15:LEU:HD22	1:B:62[B]:VAL:HG11	1.76	0.67
1:B:253:LYS:NZ	7:B:525:HOH:O	2.28	0.67
1:E:104:GLY:O	1:E:239[B]:ARG:NH1	2.26	0.67
1:D:106[B]:MET:SD	7:D:491:HOH:O	2.52	0.67
1:E:185[C]:GLU:OE1	7:E:470:HOH:O	2.08	0.66
1:C:48[B]:GLU:CG	1:D:48[B]:GLU:HB3	2.26	0.66
1:D:185[A]:GLU:OE1	7:D:534:HOH:O	2.12	0.65
1:A:178:ARG:NH2	7:A:449[B]:HOH:O	2.28	0.65
1:B:185[B]:GLU:OE1	7:B:530:HOH:O	2.08	0.65
1:B:92[B]:GLY:O	7:B:718:HOH:O	2.14	0.65
2:B:301:TDR:N1	7:B:732:HOH:O	2.30	0.65
1:B:16[A]:ASN:HB2	1:B:53[A]:ARG:HD2	1.77	0.65
1:E:180[A]:GLN:OE1	7:E:506:HOH:O	2.14	0.64
1:F:16:ASN:HB2	1:F:53[A]:ARG:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187[B]:GLN:NE2	7:F:554:HOH:O	2.30	0.61
2:B:301:TDR:HN1	6:B:303:TRS:H32	1.64	0.61
1:B:148:ALA:HB2	1:B:239[B]:ARG:HD2	1.82	0.59
1:A:39:ASN:OD1	7:A:525:HOH:O	2.16	0.59
1:F:219:ILE:HD13	1:F:233:LEU:HD12	1.85	0.59
1:B:94[A]:THR:HA	7:B:732:HOH:O	2.03	0.58
1:D:180:GLN:OE1	7:D:582:HOH:O	2.17	0.57
1:D:234[B]:LYS:NZ	7:D:516:HOH:O	2.39	0.56
1:A:26:ASP:HB3	1:A:29[A]:ARG:HG2	1.86	0.56
1:A:187[A]:GLN:OE1	7:A:477:HOH:O	2.17	0.56
1:B:94[B]:THR:O	1:B:219:ILE:N	2.32	0.56
1:B:185[A]:GLU:OE1	7:B:530:HOH:O	2.18	0.55
1:E:37:MET:SD	1:E:61[B]:VAL:HG21	2.46	0.55
1:B:94[B]:THR:N	1:B:217:GLY:O	2.35	0.55
1:C:242[A]:LYS:HG2	7:C:764:HOH:O	2.07	0.55
1:B:37:MET:SD	1:B:61[B]:VAL:HG21	2.47	0.55
1:C:16[B]:ASN:HB2	1:C:53:ARG:HD2	1.89	0.54
1:C:26:ASP:HB3	1:C:29[A]:ARG:HG2	1.89	0.54
1:E:222:ARG:HG2	7:E:751:HOH:O	2.08	0.53
1:E:155[B]:THR:HG22	1:E:193:ASN:OD1	2.08	0.53
3:A:302:EDO:H11	1:B:120:LEU:HD22	1.91	0.52
3:E:303:EDO:H22	1:F:120:LEU:HD22	1.91	0.52
1:C:48[A]:GLU:HB3	1:D:48[A]:GLU:HB3	1.91	0.51
1:D:48[B]:GLU:CD	1:D:48[B]:GLU:H	2.11	0.51
1:E:234:LYS:NZ	7:E:694[A]:HOH:O	2.38	0.50
1:D:37:MET:SD	1:D:61[B]:VAL:HG21	2.51	0.50
1:A:48[B]:GLU:HB3	1:B:48:GLU:HB3	1.94	0.49
1:D:185[A]:GLU:OE2	7:D:446:HOH:O	2.20	0.49
1:F:126[A]:GLU:OE2	7:F:626:HOH:O	2.20	0.49
1:E:109:THR:OG1	1:E:155[B]:THR:HG21	2.12	0.49
1:A:26:ASP:HB3	1:A:29[B]:ARG:HG3	1.94	0.49
1:F:37:MET:SD	1:F:61[B]:VAL:HG21	2.53	0.48
1:C:37:MET:SD	1:C:61[B]:VAL:HG21	2.53	0.48
1:F:29[B]:ARG:NH2	1:F:237:GLU:OE2	2.47	0.48
1:F:225[B]:LYS:HZ2	1:F:225[B]:LYS:HB3	1.78	0.48
1:A:48[B]:GLU:H	1:A:48[B]:GLU:CD	2.16	0.48
1:E:167[B]:ARG:NH2	2:E:301:TDR:O4	2.46	0.48
1:F:157[A]:SER:HB3	1:F:199:ALA:HB2	1.95	0.48
3:C:303:EDO:H22	7:C:766[A]:HOH:O	2.14	0.47
1:A:185[B]:GLU:HG3	7:A:442:HOH:O	2.14	0.47
1:D:246[B]:GLU:HG2	7:D:610:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:GLU:H	1:E:226:GLU:CD	2.16	0.47
1:F:157[B]:SER:HB2	1:F:199:ALA:HB2	1.96	0.47
1:A:178:ARG:HD2	3:A:302:EDO:H12	1.97	0.47
1:E:52:TYR:HB2	1:E:63[B]:VAL:HG13	1.97	0.47
1:D:104:GLY:O	1:D:239[A]:ARG:NH2	2.49	0.46
1:A:37:MET:SD	1:A:61[B]:VAL:HG21	2.56	0.46
1:E:53[B]:ARG:NH1	7:E:576:HOH:O	2.49	0.45
1:F:242:LYS:HD2	7:F:538:HOH:O	2.16	0.45
1:A:16[A]:ASN:HB2	1:A:53[A]:ARG:HD2	1.98	0.45
1:B:235[B]:GLU:HG3	7:B:486:HOH:O	2.16	0.45
1:C:157:SER:HB3	1:C:199:ALA:HB2	1.98	0.45
1:E:47[A]:ARG:NH2	7:E:677:HOH:O	2.48	0.45
1:F:229:ASP:OD1	1:F:229:ASP:N	2.48	0.45
1:D:148:ALA:HB2	1:D:239[B]:ARG:HD3	1.98	0.45
1:A:48[A]:GLU:HB3	1:B:48:GLU:HB3	1.99	0.45
1:D:29[A]:ARG:NH1	1:D:32:LYS:HD2	2.31	0.44
1:E:157:SER:HB3	1:E:199:ALA:HB2	1.99	0.44
1:F:157[B]:SER:OG	1:F:198:SER:OG	2.34	0.44
1:A:157:SER:HB3	1:A:199:ALA:HB2	1.99	0.44
1:C:174[D]:ARG:NH1	7:C:785:HOH:O	2.45	0.44
1:E:46:HIS:HE1	7:E:532:HOH:O	2.00	0.44
1:F:229:ASP:O	1:F:230:HIS:ND1	2.51	0.44
1:D:174[B]:ARG:NH1	7:D:498:HOH:O	2.50	0.44
1:F:57:ASP:OD2	1:F:249:ARG:HG3	2.17	0.44
1:B:21:ALA:HB2	1:B:62[B]:VAL:HG23	1.99	0.43
1:E:21:ALA:HB2	1:E:62[B]:VAL:HG13	2.00	0.43
3:A:302:EDO:H11	1:B:120:LEU:HD13	2.00	0.43
1:B:57:ASP:OD2	1:B:249[A]:ARG:HG3	2.19	0.43
1:B:220[A]:ILE:HG12	2:B:301:TDR:H5M2	2.00	0.43
1:E:30:VAL:HG13	1:E:63[B]:VAL:HG22	1.99	0.43
1:F:219:ILE:HD11	2:F:301:TDR:H5M1	1.99	0.43
1:D:157:SER:HB3	1:D:199:ALA:HB2	2.00	0.43
1:B:157:SER:HB3	1:B:199:ALA:HB2	2.01	0.43
2:E:301:TDR:H5M3	7:E:769:HOH:O	2.19	0.43
1:C:4[B]:THR:HG23	7:C:762:HOH:O	2.19	0.42
1:C:47[B]:ARG:NH1	7:D:468[B]:HOH:O	2.32	0.42
1:C:132:ASP:HB2	3:C:303:EDO:H21	2.00	0.42
1:D:242[A]:LYS:HB3	1:D:242[A]:LYS:HE2	1.87	0.42
1:F:233:LEU:HG	1:F:237:GLU:HG3	2.02	0.42
1:D:135:VAL:O	1:D:139[B]:MET:HG2	2.19	0.41
1:E:48:GLU:HB3	1:F:48:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:TDR:N1	6:B:303:TRS:H32	2.33	0.41
7:C:791:HOH:O	4:D:303:GOL:H31	2.21	0.41
1:F:177[A]:ARG:NH1	7:F:707:HOH:O	2.53	0.41
1:B:94[B]:THR:O	1:B:218:VAL:HA	2.20	0.41
1:D:57:ASP:OD2	1:D:249[B]:ARG:HG3	2.21	0.41
1:E:93[B]:THR:HB	1:E:219:ILE:HG23	2.03	0.41
1:B:104:GLY:O	1:B:239[B]:ARG:NH2	2.54	0.41
1:B:174[B]:ARG:HD2	7:F:443[B]:HOH:O	2.21	0.41
1:F:220:ILE:HG13	1:F:225[B]:LYS:HD3	2.03	0.41
1:C:242[A]:LYS:HB2	1:C:242[A]:LYS:HE3	1.81	0.40
1:F:227:ILE:HA	1:F:228:PRO:HD3	1.94	0.40
3:A:302:EDO:H21	7:A:721:HOH:O	2.22	0.40
1:B:235[A]:GLU:HG3	7:B:486:HOH:O	2.20	0.40
1:E:95[A]:GLY:O	1:E:193:ASN:HB2	2.22	0.40
1:E:198[B]:SER:OG	7:E:537:HOH:O	2.20	0.40
1:C:108:VAL:HB	1:C:152:MET:SD	2.61	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	272/253 (108%)	268 (98%)	3 (1%)	1 (0%)	34	10
1	B	289/253 (114%)	286 (99%)	2 (1%)	1 (0%)	41	16
1	C	285/253 (113%)	278 (98%)	6 (2%)	1 (0%)	34	10
1	D	283/253 (112%)	279 (99%)	3 (1%)	1 (0%)	34	10
1	E	286/253 (113%)	282 (99%)	3 (1%)	1 (0%)	41	16
1	F	276/253 (109%)	272 (99%)	3 (1%)	1 (0%)	34	10
All	All	1691/1518 (111%)	1665 (98%)	20 (1%)	6 (0%)	34	10

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 [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	227/203 (112%)	223 (98%)	4 (2%)	59 21
1	B	238/203 (117%)	230 (97%)	8 (3%)	37 5
1	C	236/203 (116%)	229 (97%)	7 (3%)	41 6
1	D	235/203 (116%)	234 (100%)	1 (0%)	91 77
1	E	237/203 (117%)	233 (98%)	4 (2%)	60 23
1	F	228/203 (112%)	224 (98%)	4 (2%)	59 21
All	All	1401/1218 (115%)	1373 (98%)	28 (2%)	60 16

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	GLU
1	A	234[A]	LYS
1	A	234[B]	LYS
1	A	235	GLU
1	B	3	LYS
1	B	183[A]	MET
1	B	183[B]	MET
1	B	195	GLU
1	B	225	LYS
1	B	226[A]	GLU
1	B	226[B]	GLU

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Mol	Chain	Res	Type
1	B	229	ASP
1	C	3	LYS
1	C	90[A]	ARG
1	C	90[B]	ARG
1	C	195	GLU
1	C	234[A]	LYS
1	C	234[B]	LYS
1	C	253	LYS
1	D	195	GLU
1	E	195	GLU
1	E	226	GLU
1	E	253[A]	LYS
1	E	253[B]	LYS
1	F	29[A]	ARG
1	F	29[B]	ARG
1	F	195	GLU
1	F	229	ASP

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

Mol	Chain	Res	Type
1	D	180	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 25 ligands modelled in this entry, 3 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	C	303	-	3,3,3	0.46	0	2,2,2	0.09	0
3	EDO	C	302	-	3,3,3	0.36	0	2,2,2	0.29	0
2	TDR	B	301	-	9,9,9	2.69	5 (55%)	12,12,12	3.22	8 (66%)
4	GOL	D	302	-	5,5,5	0.22	0	5,5,5	0.54	0
3	EDO	A	302	-	3,3,3	0.27	0	2,2,2	0.51	0
2	TDR	E	301	-	9,9,9	2.62	3 (33%)	12,12,12	3.97	8 (66%)
2	TDR	C	301	-	9,9,9	2.25	2 (22%)	12,12,12	1.94	6 (50%)
3	EDO	B	302	-	3,3,3	0.46	0	2,2,2	0.26	0
4	GOL	F	304	-	5,5,5	0.36	0	5,5,5	0.41	0
4	GOL	A	303	-	5,5,5	0.28	0	5,5,5	0.64	0
4	GOL	E	304	-	5,5,5	0.35	0	5,5,5	0.40	0
6	TRS	B	303	-	7,7,7	0.36	0	9,9,9	0.82	0
3	EDO	E	303	-	3,3,3	0.28	0	2,2,2	0.47	0
2	TDR	F	301	-	9,9,9	2.33	2 (22%)	12,12,12	2.38	6 (50%)
4	GOL	D	303	-	5,5,5	0.37	0	5,5,5	0.50	0
3	EDO	F	302	-	3,3,3	0.49	0	2,2,2	0.23	0
3	EDO	C	304	-	3,3,3	0.40	0	2,2,2	0.29	0
3	EDO	F	303	-	3,3,3	0.43	0	2,2,2	0.08	0
2	TDR	A	301	-	9,9,9	2.15	2 (22%)	12,12,12	2.07	4 (33%)
3	EDO	E	302	-	3,3,3	0.39	0	2,2,2	0.17	0
2	TDR	D	301	-	9,9,9	2.26	3 (33%)	12,12,12	2.06	6 (50%)
4	GOL	C	305	-	5,5,5	0.28	0	5,5,5	0.72	0

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
3	EDO	C	303	-	-	1/1/1/1	-
3	EDO	C	302	-	-	1/1/1/1	-
2	TDR	B	301	-	-	-	0/1/1/1
4	GOL	D	302	-	-	1/4/4/4	-
3	EDO	A	302	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TDR	E	301	-	-	-	0/1/1/1
2	TDR	C	301	-	-	-	0/1/1/1
3	EDO	B	302	-	-	1/1/1/1	-
4	GOL	F	304	-	-	0/4/4/4	-
4	GOL	A	303	-	-	1/4/4/4	-
4	GOL	E	304	-	-	2/4/4/4	-
6	TRS	B	303	-	-	6/9/9/9	-
3	EDO	E	303	-	-	0/1/1/1	-
2	TDR	F	301	-	-	-	0/1/1/1
4	GOL	D	303	-	-	4/4/4/4	-
3	EDO	F	302	-	-	1/1/1/1	-
3	EDO	C	304	-	-	0/1/1/1	-
3	EDO	F	303	-	-	1/1/1/1	-
2	TDR	A	301	-	-	-	0/1/1/1
3	EDO	E	302	-	-	1/1/1/1	-
2	TDR	D	301	-	-	-	0/1/1/1
4	GOL	C	305	-	-	0/4/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	TDR	C6-N1	5.29	1.45	1.36
2	B	301	TDR	C6-N1	5.06	1.44	1.36
2	F	301	TDR	C6-N1	4.83	1.44	1.36
2	B	301	TDR	C2-N1	4.57	1.42	1.36
2	C	301	TDR	C2-N1	4.49	1.42	1.36
2	E	301	TDR	C2-N1	4.49	1.42	1.36
2	C	301	TDR	C6-N1	4.40	1.43	1.36
2	D	301	TDR	C6-N1	4.24	1.43	1.36
2	A	301	TDR	C6-N1	4.19	1.43	1.36
2	F	301	TDR	C2-N1	4.11	1.42	1.36
2	D	301	TDR	C2-N1	4.10	1.42	1.36
2	A	301	TDR	C2-N1	3.55	1.41	1.36
2	B	301	TDR	C2-N3	2.34	1.41	1.37
2	E	301	TDR	C2-N3	2.31	1.41	1.37
2	D	301	TDR	C6-C5	2.21	1.37	1.34
2	B	301	TDR	C6-C5	2.12	1.37	1.34
2	B	301	TDR	C4-C5	2.04	1.48	1.44

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	TDR	C6-N1-C2	-7.01	115.52	122.68
2	E	301	TDR	O2-C2-N1	-6.09	116.08	122.79
2	B	301	TDR	N1-C2-N3	5.24	121.07	115.13
2	B	301	TDR	C5-C4-N3	5.10	119.67	115.31
2	E	301	TDR	N1-C2-N3	4.96	120.75	115.13
2	B	301	TDR	C4-N3-C2	-4.58	119.74	126.34
2	E	301	TDR	O4-C4-C5	-4.49	119.69	124.90
2	E	301	TDR	CM5-C5-C6	-4.22	118.49	123.16
2	F	301	TDR	C5-C4-N3	4.09	118.80	115.31
2	E	301	TDR	CM5-C5-C4	3.88	123.04	118.77
2	B	301	TDR	O2-C2-N1	-3.59	118.83	122.79
2	E	301	TDR	C5-C4-N3	3.57	118.36	115.31
2	A	301	TDR	C5-C4-N3	3.55	118.34	115.31
2	C	301	TDR	C5-C4-N3	3.43	118.24	115.31
2	B	301	TDR	C6-N1-C2	-3.32	119.29	122.68
2	F	301	TDR	N1-C2-N3	3.22	118.78	115.13
2	F	301	TDR	C4-N3-C2	-3.13	121.83	126.34
2	B	301	TDR	CM5-C5-C6	-3.08	119.75	123.16
2	D	301	TDR	N1-C2-N3	3.06	118.60	115.13
2	F	301	TDR	O4-C4-C5	-2.93	121.51	124.90
2	E	301	TDR	C4-N3-C2	-2.85	122.24	126.34
2	F	301	TDR	CM5-C5-C6	-2.84	120.01	123.16
2	A	301	TDR	CM5-C5-C6	-2.82	120.04	123.16
2	D	301	TDR	CM5-C5-C6	-2.77	120.10	123.16
2	D	301	TDR	O4-C4-C5	-2.72	121.75	124.90
2	D	301	TDR	C6-N1-C2	-2.71	119.91	122.68
2	A	301	TDR	N1-C2-N3	2.71	118.20	115.13
2	A	301	TDR	C4-N3-C2	-2.70	122.45	126.34
2	D	301	TDR	C5-C4-N3	2.68	117.60	115.31
2	C	301	TDR	CM5-C5-C6	-2.64	120.24	123.16
2	B	301	TDR	O4-C4-C5	-2.55	121.94	124.90
2	F	301	TDR	C6-N1-C2	-2.41	120.22	122.68
2	C	301	TDR	C6-N1-C2	-2.38	120.25	122.68
2	D	301	TDR	C4-N3-C2	-2.29	123.03	126.34
2	C	301	TDR	N1-C2-N3	2.27	117.70	115.13
2	C	301	TDR	O4-C4-C5	-2.21	122.34	124.90
2	C	301	TDR	C4-N3-C2	-2.18	123.20	126.34
2	B	301	TDR	C5-C6-N1	-2.13	119.86	122.43

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	303	GOL	O1-C1-C2-O2
4	D	303	GOL	O1-C1-C2-C3
4	D	303	GOL	C1-C2-C3-O3
6	B	303	TRS	C1-C-C2-O2
6	B	303	TRS	C3-C-C2-O2
6	B	303	TRS	N-C-C2-O2
4	E	304	GOL	C1-C2-C3-O3
6	B	303	TRS	C3-C-C1-O1
4	D	303	GOL	O2-C2-C3-O3
3	B	302	EDO	O1-C1-C2-O2
6	B	303	TRS	N-C-C1-O1
3	F	302	EDO	O1-C1-C2-O2
6	B	303	TRS	C2-C-C1-O1
3	C	302	EDO	O1-C1-C2-O2
3	C	303	EDO	O1-C1-C2-O2
3	E	302	EDO	O1-C1-C2-O2
4	E	304	GOL	O2-C2-C3-O3
4	A	303	GOL	O1-C1-C2-C3
4	D	302	GOL	O1-C1-C2-C3
3	F	303	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	303	EDO	2	0
3	C	302	EDO	1	0
2	B	301	TDR	4	0
3	A	302	EDO	4	0
2	E	301	TDR	4	0
6	B	303	TRS	2	0
3	E	303	EDO	1	0
2	F	301	TDR	1	0
4	D	303	GOL	1	0
3	C	304	EDO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	247/253 (97%)	-0.46	7 (2%) 53 48	7, 12, 24, 51	0
1	B	251/253 (99%)	-0.40	8 (3%) 47 42	7, 12, 28, 53	0
1	C	251/253 (99%)	-0.55	3 (1%) 79 74	7, 11, 19, 40	0
1	D	251/253 (99%)	-0.60	1 (0%) 92 89	7, 10, 19, 32	0
1	E	251/253 (99%)	-0.39	6 (2%) 59 53	7, 12, 28, 53	0
1	F	251/253 (99%)	-0.31	9 (3%) 42 38	7, 12, 28, 76	0
All	All	1502/1518 (98%)	-0.45	34 (2%) 60 55	7, 11, 25, 76	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	232	THR	10.1
1	F	2	THR	10.0
1	F	230	HIS	9.7
1	F	233	LEU	8.1
1	F	229	ASP	7.9
1	A	233	LEU	6.4
1	E	227	ILE	6.1
1	F	234	LYS	5.3
1	E	225	LYS	5.1
1	A	4	THR	5.0
1	F	231	ALA	4.6
1	A	234[A]	LYS	4.0
1	B	225	LYS	3.9
1	B	230[A]	HIS	3.8
1	E	230	HIS	3.7
1	C	4[A]	THR	3.7
1	A	3	LYS	3.4
1	E	253[A]	LYS	3.4
1	F	235	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	229	ASP	3.3
1	B	231	ALA	3.2
1	E	226	GLU	3.2
1	B	227	ILE	3.1
1	D	253[A]	LYS	3.0
1	B	229	ASP	3.0
1	A	6[A]	PHE	2.9
1	B	253	LYS	2.9
1	C	3	LYS	2.8
1	C	253	LYS	2.6
1	A	253	LYS	2.5
1	A	235	GLU	2.4
1	B	226[A]	GLU	2.4
1	B	235[A]	GLU	2.3
1	F	3[A]	LYS	2.2

## 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, 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
3	EDO	C	303	4/4	0.71	0.18	19,22,23,23	4
4	GOL	D	303	6/6	0.79	0.24	49,50,59,67	6
6	TRS	B	303	8/8	0.81	0.14	19,25,28,29	8
3	EDO	B	302	4/4	0.85	0.23	38,39,39,46	0
3	EDO	E	303	4/4	0.85	0.20	16,20,21,25	4
2	TDR	E	301	9/9	0.86	0.16	12,15,18,18	9
4	GOL	F	304	6/6	0.89	0.10	23,23,26,28	6
4	GOL	D	302	6/6	0.90	0.11	23,26,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	F	302	4/4	0.90	0.18	32,37,41,43	0
3	EDO	E	302	4/4	0.91	0.12	23,24,26,27	4
3	EDO	F	303	4/4	0.91	0.11	24,24,27,27	4
3	EDO	C	304	4/4	0.92	0.12	28,29,30,34	4
4	GOL	C	305	6/6	0.92	0.10	22,24,27,31	0
3	EDO	A	302	4/4	0.92	0.16	17,19,21,23	4
3	EDO	C	302	4/4	0.93	0.14	13,15,19,24	4
2	TDR	B	301	9/9	0.93	0.10	11,13,15,16	9
4	GOL	A	303	6/6	0.94	0.08	21,21,25,27	0
4	GOL	E	304	6/6	0.94	0.11	27,31,32,33	0
2	TDR	D	301	9/9	0.98	0.05	9,11,12,12	0
2	TDR	A	301	9/9	0.98	0.06	10,11,13,15	0
2	TDR	C	301	9/9	0.99	0.04	9,10,12,12	0
5	NA	C	306	1/1	0.99	0.04	14,14,14,14	1
5	NA	E	305	1/1	0.99	0.08	14,14,14,14	1
2	TDR	F	301	9/9	0.99	0.04	11,12,13,15	0
5	NA	A	304	1/1	1.00	0.04	15,15,15,15	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.