Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 12:25 PM BST

PDB ID	:	6Z9Z
Title	:	Atomic resolution X-ray structure of the Uridine phosphorylase from Vibrio cholerae on crystals grown under microgravity
Authors	:	Eistrikh-Heller, P.A.; Rubinsky, S.V.; Samygina, V.R.; Gabdulkhakov, A.G.; Lashkov, A.A.
Deposited on	:	2020-06-04
Resolution	:	1.04 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

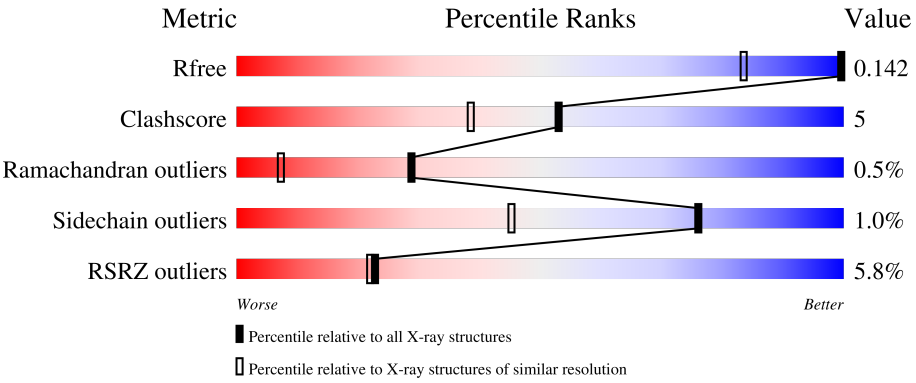
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.20
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

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 1.04 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	1596 (1.10-0.98)
Clashscore	141614	1677 (1.10-0.98)
Ramachandran outliers	138981	1591 (1.10-0.98)
Sidechain outliers	138945	1589 (1.10-0.98)
RSRZ outliers	127900	1557 (1.10-0.98)

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	4% 88% 11%
1	B	253	2% 91% 8%
1	C	253	6% 93% 6%
1	D	253	11% 85% 11%
1	E	253	6% 91% 6%

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Mol	Chain	Length	Quality of chain
1	F	253	6% 90% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NA	E	304	-	-	-	X
5	PEG	D	306	-	-	X	-

2 Entry composition

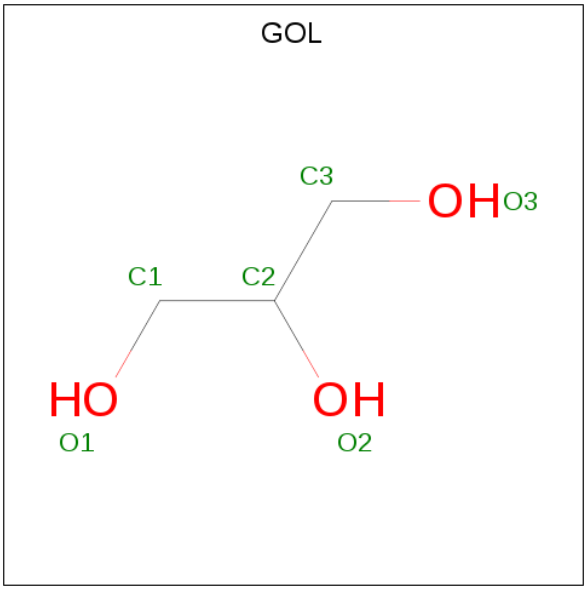
There are 7 unique types of molecules in this entry. The entry contains 27335 atoms, of which 13041 are hydrogens and 0 are deuteriums.

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.

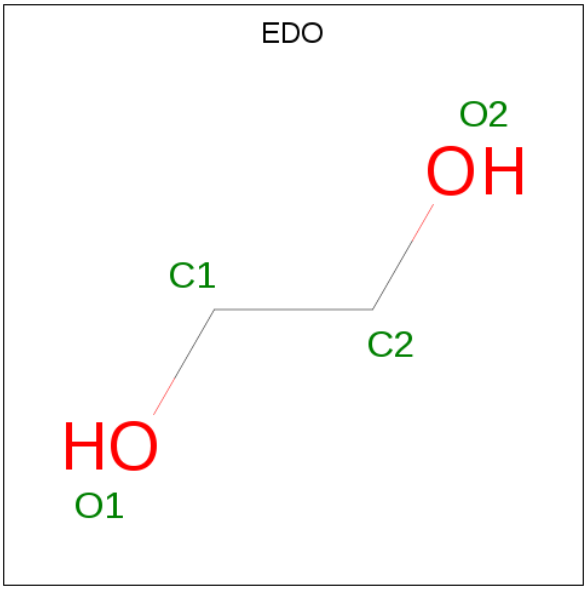
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	251	Total	C	H	N	O	S	0	38	0
			4267	1318	2178	362	392	17			
1	B	252	Total	C	H	N	O	S	0	39	0
			4246	1317	2161	356	395	17			
1	C	251	Total	C	H	N	O	S	0	31	0
			4137	1278	2095	362	384	18			
1	D	246	Total	C	H	N	O	S	0	59	0
			4445	1375	2255	383	413	19			
1	E	247	Total	C	H	N	O	S	0	32	0
			4028	1249	2038	342	381	18			
1	F	252	Total	C	H	N	O	S	0	45	0
			4287	1321	2182	372	394	18			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	E	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		

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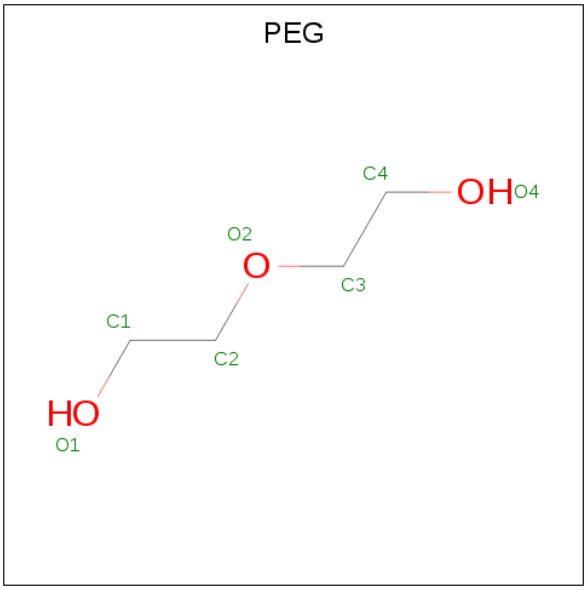
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C H O 10 2 6 2	0	0
3	E	1	Total C H O 10 2 6 2	0	0
3	E	1	Total C H O 10 2 6 2	0	0
3	F	1	Total C H O 10 2 6 2	0	0
3	F	1	Total C H O 10 2 6 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		
6	E	1	Total	Mg	0	0
			1	1		

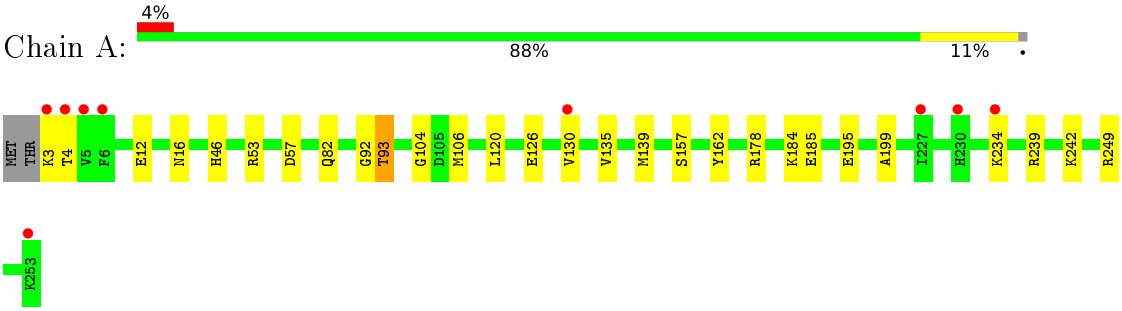
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	314	Total	O	0	4
			318	318		
7	B	335	Total	O	0	3
			338	338		
7	C	322	Total	O	0	6
			328	328		
7	D	227	Total	O	0	2
			229	229		
7	E	220	Total	O	0	3
			223	223		
7	F	250	Total	O	0	2
			252	252		

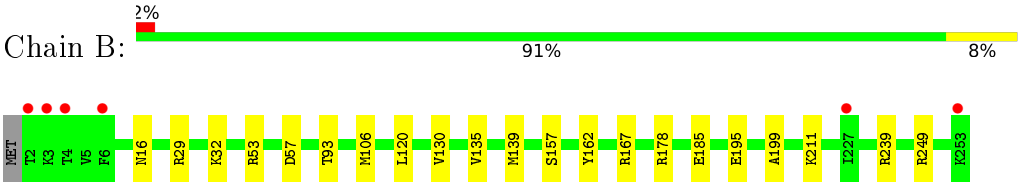
3 Residue-property plots (i)

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.

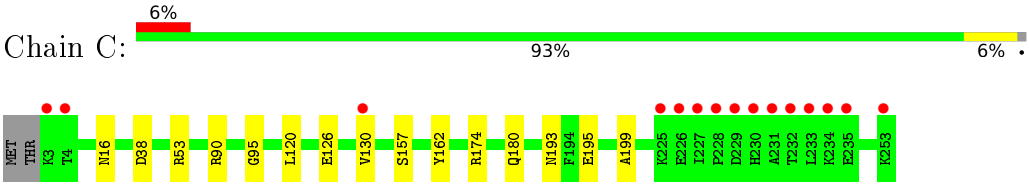
- Molecule 1: Uridine phosphorylase



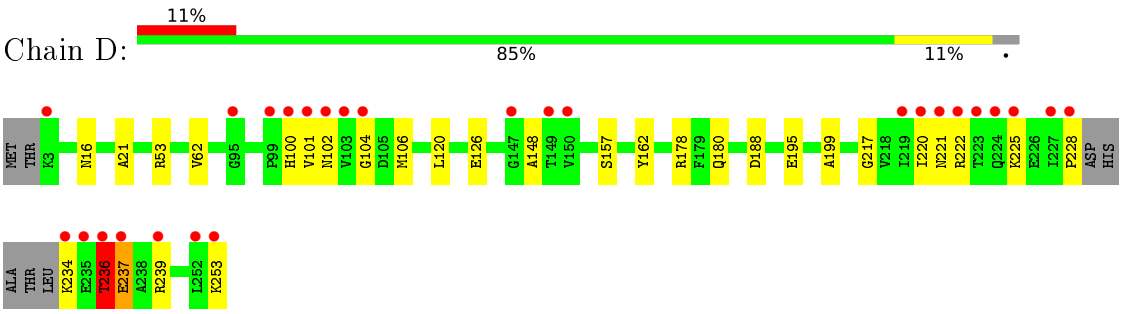
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase

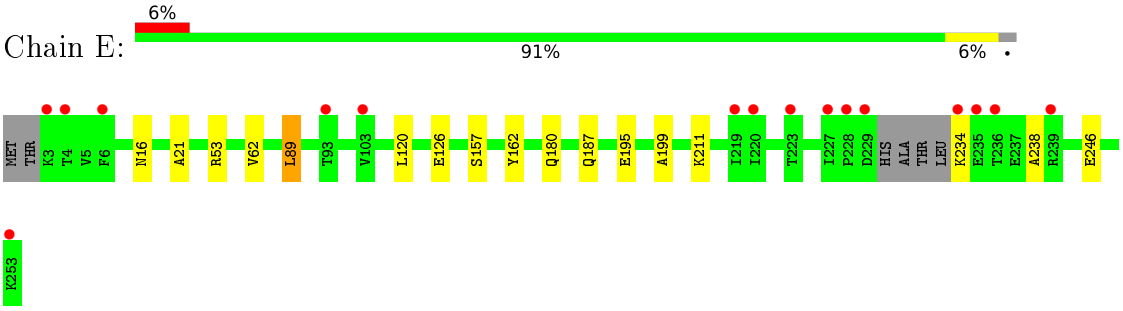


- Molecule 1: Uridine phosphorylase



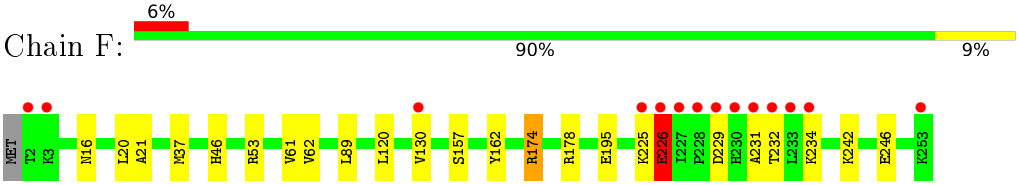
- Molecule 1: Uridine phosphorylase

Chain E:



• Molecule 1: Uridine phosphorylase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.19Å 97.06Å 93.23Å 90.00° 119.97° 90.00°	Depositor
Resolution (Å)	46.61 – 1.04 46.61 – 1.04	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.61-1.04) 99.0 (46.61-1.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 1.04Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.126 , 0.142 0.126 , 0.142	Depositor DCC
R_{free} test set	34041 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	10.2	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.105 for -h-l,k,h 0.105 for l,k,-h-l 0.012 for h,-k,-h-l 0.011 for -h-l,-k,l 0.011 for l,-k,h	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	27335	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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

5.1 Standard geometry

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

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	0.35	0/2227	0.61	2/3004 (0.1%)
1	B	0.31	0/2237	0.57	0/3024
1	C	0.31	0/2177	0.56	0/2941
1	D	0.46	2/2312 (0.1%)	0.66	2/3125 (0.1%)
1	E	0.31	0/2120	0.61	2/2863 (0.1%)
1	F	0.40	0/2291	0.65	3/3093 (0.1%)
All	All	0.36	2/13364 (0.0%)	0.61	9/18050 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	236[A]	THR	CA-C	10.22	1.79	1.52
1	D	236[B]	THR	CA-C	10.22	1.79	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	236[A]	THR	CA-C-O	-10.45	98.17	120.10
1	D	236[B]	THR	CA-C-O	-10.45	98.17	120.10
1	F	174[A]	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	F	174[B]	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	E	89[A]	LEU	CA-CB-CG	6.11	129.34	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	89[B]	LEU	CA-CB-CG	6.11	129.34	115.30
1	A	93[A]	THR	CB-CA-C	-5.64	96.37	111.60
1	A	93[B]	THR	CB-CA-C	-5.64	96.37	111.60
1	F	226	GLU	CB-CA-C	5.12	120.63	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	236[A]	THR	Mainchain
1	D	236[B]	THR	Mainchain

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	2089	2178	2133	37	0
1	B	2085	2161	2095	23	0
1	C	2042	2095	2013	16	0
1	D	2190	2255	2194	39	0
1	E	1990	2038	1944	12	0
1	F	2105	2182	2046	22	0
2	A	6	8	8	0	0
2	B	6	8	8	0	0
2	C	6	8	8	0	0
2	D	6	8	8	0	0
2	E	6	8	8	0	0
3	A	8	12	12	2	0
3	B	12	18	18	4	0
3	C	8	12	12	1	0
3	D	4	6	6	0	0
3	E	8	12	12	1	1
3	F	8	12	12	2	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	3	0	0	0	0
5	C	7	10	8	2	1
5	D	7	10	9	5	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
7	A	318	0	0	17	0
7	B	338	0	0	11	0
7	C	328	0	0	4	0
7	D	229	0	0	14	0
7	E	223	0	0	6	0
7	F	252	0	0	4	0
All	All	14294	13041	12554	138	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (138) 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:D:102[B]:ASN:HB2	7:D:415:HOH:O	1.42	1.16
1:A:3[B]:LYS:HG3	7:A:673:HOH:O	1.49	1.11
1:C:120:LEU:HD13	5:D:306:PEG:H21	1.33	1.09
1:C:38:ASP:OD2	5:C:307:PEG:H42	1.51	1.08
1:E:246[A]:GLU:HG2	7:E:422:HOH:O	1.53	1.04
1:A:184[B]:LYS:HE2	7:B:649[B]:HOH:O	1.58	1.01
1:A:93[B]:THR:HG23	7:A:406:HOH:O	1.61	1.00
1:A:93[B]:THR:CG2	7:A:406:HOH:O	2.11	0.99
1:A:130[A]:VAL:CG2	1:F:130[A]:VAL:CG2	2.42	0.97
1:D:180[A]:GLN:NE2	7:D:403:HOH:O	2.01	0.93
1:D:104[B]:GLY:HA2	1:D:239:ARG:HH22	1.32	0.89
1:A:130[A]:VAL:HG22	1:F:130[A]:VAL:HG21	1.54	0.89
1:A:3[B]:LYS:HE2	7:A:673:HOH:O	1.72	0.89
1:A:130[A]:VAL:HG21	1:F:130[A]:VAL:HG22	1.59	0.84
1:E:180[A]:GLN:NE2	7:E:403:HOH:O	2.15	0.79
1:D:101[B]:VAL:O	1:D:221[B]:ASN:ND2	2.16	0.78
1:A:234[A]:LYS:HG2	7:A:432:HOH:O	1.83	0.78
1:A:130[A]:VAL:HG21	1:F:130[A]:VAL:CG2	2.12	0.78
1:C:38:ASP:OD2	5:C:307:PEG:C4	2.31	0.77
3:E:301:EDO:H21	1:F:120:LEU:HD22	1.67	0.77
1:C:120:LEU:HD22	5:D:306:PEG:H31	1.68	0.76
1:D:104[B]:GLY:HA2	1:D:239:ARG:NH2	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53[A]:ARG:CD	7:D:408:HOH:O	2.34	0.75
1:A:130[A]:VAL:HG22	1:F:130[A]:VAL:CG2	2.13	0.75
1:A:130[A]:VAL:CG2	1:F:130[A]:VAL:HG21	2.14	0.74
3:A:303:EDO:H21	1:B:120:LEU:HD22	1.71	0.73
1:B:130[A]:VAL:CG1	1:C:130[A]:VAL:CG2	2.66	0.73
1:E:126[B]:GLU:OE2	7:E:401:HOH:O	2.06	0.73
1:B:93[B]:THR:CG2	7:B:428:HOH:O	2.36	0.72
1:A:120:LEU:HD22	3:B:304:EDO:H21	1.70	0.72
1:A:126[B]:GLU:OE1	7:A:404:HOH:O	2.07	0.72
3:C:302:EDO:H21	1:D:120:LEU:HD22	1.71	0.71
1:C:126[B]:GLU:OE2	7:C:402:HOH:O	2.09	0.71
1:B:130[A]:VAL:HG12	1:C:130[A]:VAL:CG2	2.22	0.70
1:D:53[A]:ARG:HG2	7:D:408:HOH:O	1.91	0.70
1:B:93[B]:THR:HG23	7:B:428:HOH:O	1.90	0.69
1:D:100[B]:HIS:O	7:D:404:HOH:O	2.09	0.69
1:E:120:LEU:HD22	3:F:302:EDO:H12	1.73	0.69
1:C:180:GLN:NE2	7:C:404:HOH:O	2.24	0.69
1:B:130[A]:VAL:HG12	1:C:130[A]:VAL:HG21	1.74	0.68
1:A:104:GLY:O	1:A:239[A]:ARG:NH1	2.26	0.68
1:B:185[B]:GLU:OE1	7:B:401:HOH:O	2.10	0.68
1:A:3[B]:LYS:CE	7:A:673:HOH:O	2.32	0.67
1:A:185[B]:GLU:OE1	7:A:405:HOH:O	2.12	0.67
1:C:53[B]:ARG:NH1	7:C:406:HOH:O	2.29	0.66
1:E:187[B]:GLN:OE1	7:E:402:HOH:O	2.14	0.66
1:D:53[A]:ARG:NH1	7:D:406:HOH:O	2.27	0.66
1:B:130[A]:VAL:HG11	1:C:130[A]:VAL:HG22	1.77	0.66
1:A:130[A]:VAL:CG2	1:F:130[A]:VAL:HG22	2.19	0.64
1:B:130[A]:VAL:CG1	1:C:130[A]:VAL:HG22	2.27	0.64
1:A:3[A]:LYS:NZ	7:A:412:HOH:O	2.32	0.63
1:E:211[B]:LYS:NZ	7:E:404:HOH:O	2.30	0.63
1:B:178:ARG:HD2	3:B:304:EDO:H11	1.81	0.62
1:A:93[B]:THR:HG22	7:A:406:HOH:O	1.88	0.62
1:A:178:ARG:HD2	3:A:303:EDO:H11	1.82	0.61
1:F:37:MET:SD	1:F:61[B]:VAL:HG21	2.41	0.61
1:D:53[A]:ARG:CG	7:D:408:HOH:O	2.49	0.60
1:D:16:ASN:HB2	1:D:53[A]:ARG:HD2	1.85	0.59
1:B:106[B]:MET:SD	7:B:419:HOH:O	2.57	0.59
1:F:16[A]:ASN:HB2	1:F:53[A]:ARG:HD2	1.84	0.59
1:E:16:ASN:HB2	1:E:53[A]:ARG:HD2	1.84	0.58
1:A:92[A]:GLY:O	7:A:406:HOH:O	2.16	0.58
1:E:234:LYS:NZ	1:E:238:ALA:HB2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ASN:HB2	1:C:53[A]:ARG:HD2	1.87	0.56
1:A:92[B]:GLY:O	7:A:406:HOH:O	2.17	0.56
1:A:3[A]:LYS:HD2	7:A:673:HOH:O	2.05	0.56
1:D:53[A]:ARG:NE	7:D:408:HOH:O	2.36	0.56
1:A:16[A]:ASN:HB2	1:A:53:ARG:HD2	1.86	0.56
1:B:167:ARG:HA	3:B:302:EDO:H11	1.87	0.55
1:F:231:ALA:O	1:F:234[B]:LYS:HG3	2.07	0.55
1:F:46[B]:HIS:NE2	7:F:404:HOH:O	2.28	0.55
1:B:16[A]:ASN:HB2	1:B:53:ARG:HD2	1.89	0.54
1:B:185[B]:GLU:OE2	7:B:402:HOH:O	2.18	0.54
1:A:93[A]:THR:HG23	7:A:636:HOH:O	2.08	0.54
5:D:306:PEG:H41	7:D:536:HOH:O	2.07	0.53
1:E:187[B]:GLN:NE2	7:E:405:HOH:O	2.33	0.53
1:D:236[B]:THR:CA	1:D:237:GLU:N	2.65	0.51
1:D:236[B]:THR:HG22	1:D:239:ARG:NH2	2.26	0.51
1:D:236[A]:THR:CA	1:D:237:GLU:N	2.65	0.50
1:A:184[B]:LYS:CE	7:B:649[B]:HOH:O	2.32	0.50
1:B:93[B]:THR:HG22	7:B:428:HOH:O	2.04	0.49
1:D:220[B]:ILE:HD12	1:D:228:PRO:HA	1.94	0.49
1:D:102[B]:ASN:CB	7:D:415:HOH:O	2.23	0.49
1:F:226:GLU:HG2	7:F:458:HOH:O	2.13	0.48
1:F:229:ASP:OD1	1:F:232:THR:HG22	2.13	0.48
1:A:57:ASP:OD2	1:A:249[A]:ARG:HG3	2.14	0.47
1:E:234:LYS:HZ3	1:E:238:ALA:HB2	1.78	0.47
1:A:46[A]:HIS:HB2	7:A:403:HOH:O	2.15	0.47
1:F:178:ARG:HD2	3:F:302:EDO:H22	1.96	0.47
1:D:53[B]:ARG:NH2	7:D:413:HOH:O	2.46	0.47
1:F:246[B]:GLU:HG2	7:F:408:HOH:O	2.15	0.46
1:D:157:SER:HB3	1:D:199:ALA:HB2	1.98	0.46
1:B:135:VAL:O	1:B:139[B]:MET:HG2	2.17	0.45
1:B:211[A]:LYS:NZ	7:B:420:HOH:O	2.49	0.45
1:A:242:LYS:HE3	1:A:242:LYS:HB3	1.75	0.45
1:D:178:ARG:HD2	5:D:306:PEG:H41	1.98	0.45
1:C:157:SER:HB3	1:C:199:ALA:HB2	1.99	0.45
1:D:126:GLU:OE2	7:D:405:HOH:O	2.21	0.44
1:D:239:ARG:HE	1:D:239:ARG:HB3	1.55	0.44
1:B:157:SER:HB3	1:B:199:ALA:HB2	1.99	0.44
1:E:157:SER:HB3	1:E:199:ALA:HB2	1.99	0.44
1:B:239:ARG:NH2	7:B:419:HOH:O	2.49	0.44
1:A:106[B]:MET:SD	7:A:512:HOH:O	2.60	0.44
5:D:306:PEG:C4	7:D:536:HOH:O	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102[B]:ASN:ND2	7:D:415:HOH:O	2.47	0.43
1:A:157:SER:HB3	1:A:199:ALA:HB2	2.00	0.43
1:F:242[B]:LYS:HE3	7:F:536:HOH:O	2.19	0.43
1:A:135:VAL:O	1:A:139[B]:MET:HG2	2.19	0.43
1:A:82:GLN:HG2	3:B:303:EDO:H21	2.00	0.43
1:A:234[B]:LYS:HB3	1:A:234[B]:LYS:HE3	1.76	0.43
1:D:21:ALA:HA	1:D:62[B]:VAL:O	2.19	0.42
1:A:185[B]:GLU:OE2	7:A:407:HOH:O	2.22	0.42
1:F:21:ALA:HB2	1:F:62[B]:VAL:HG13	2.01	0.42
1:F:21:ALA:HA	1:F:62[B]:VAL:O	2.19	0.42
1:C:95[B]:GLY:O	1:C:193:ASN:HB2	2.19	0.42
1:C:174[B]:ARG:HD2	7:C:636:HOH:O	2.20	0.42
1:D:220[B]:ILE:HD11	1:D:225[B]:LYS:HE2	2.02	0.42
1:D:106[A]:MET:HG3	1:D:148[A]:ALA:HB1	2.02	0.41
1:E:21:ALA:HB2	1:E:62[B]:VAL:HG13	2.01	0.41
1:A:3[A]:LYS:N	1:A:12:GLU:H	2.18	0.41
1:B:29:ARG:HD2	1:B:32[A]:LYS:HE3	2.01	0.41
1:B:57:ASP:OD2	1:B:249[A]:ARG:HG3	2.21	0.41
1:D:188:ASP:HB3	1:F:174[A]:ARG:HD3	2.03	0.41
1:D:234:LYS:HD2	1:D:234:LYS:C	2.41	0.41
1:B:185[B]:GLU:OE2	7:B:403:HOH:O	2.22	0.40
1:F:20:LEU:HD21	1:F:89[B]:LEU:HD13	2.02	0.40
1:D:106[B]:MET:SD	1:D:217[B]:GLY:HA2	2.61	0.40
1:B:29:ARG:HH21	1:B:32[A]:LYS:NZ	2.19	0.40
1:D:236[B]:THR:HG22	1:D:239:ARG:HH21	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:307:PEG:O1	3:E:303:EDO:O1[1_656]	2.06	0.14

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	287/253 (113%)	280 (98%)	4 (1%)	3 (1%)	15 2
1	B	289/253 (114%)	285 (99%)	3 (1%)	1 (0%)	41 14
1	C	280/253 (111%)	276 (99%)	3 (1%)	1 (0%)	34 11
1	D	301/253 (119%)	294 (98%)	4 (1%)	3 (1%)	15 2
1	E	275/253 (109%)	273 (99%)	1 (0%)	1 (0%)	34 11
1	F	295/253 (117%)	290 (98%)	4 (1%)	1 (0%)	41 14
All	All	1727/1518 (114%)	1698 (98%)	19 (1%)	10 (1%)	29 5

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	162	TYR
1	A	4[A]	THR
1	A	4[B]	THR
1	A	162	TYR
1	B	162	TYR
1	C	162	TYR
1	D	162	TYR
1	E	162	TYR
1	D	222[A]	ARG
1	D	222[B]	ARG

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	236/203 (116%)	235 (100%)	1 (0%)	91 72
1	B	238/203 (117%)	237 (100%)	1 (0%)	91 72
1	C	230/203 (113%)	227 (99%)	3 (1%)	69 34
1	D	246/203 (121%)	243 (99%)	3 (1%)	71 38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	225/203 (111%)	222 (99%)	3 (1%)	69 34
1	F	243/203 (120%)	240 (99%)	3 (1%)	71 38
All	All	1418/1218 (116%)	1404 (99%)	14 (1%)	76 45

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	GLU
1	B	195	GLU
1	C	90[A]	ARG
1	C	90[B]	ARG
1	C	195	GLU
1	D	195	GLU
1	D	237	GLU
1	D	253	LYS
1	E	89[A]	LEU
1	E	89[B]	LEU
1	E	195	GLU
1	F	195	GLU
1	F	225	LYS
1	F	226	GLU

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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 13 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	B	301	-	5,5,5	0.89	0	5,5,5	0.96	0
3	EDO	C	302	-	3,3,3	0.43	0	2,2,2	0.38	0
3	EDO	A	303	-	3,3,3	0.36	0	2,2,2	0.17	0
3	EDO	B	304	-	3,3,3	0.37	0	2,2,2	0.20	0
3	EDO	B	303	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	B	302	-	3,3,3	0.37	0	2,2,2	0.42	0
2	GOL	E	302	-	5,5,5	0.87	0	5,5,5	1.01	0
3	EDO	F	302	-	3,3,3	0.40	0	2,2,2	0.36	0
3	EDO	C	301	-	3,3,3	0.43	0	2,2,2	0.34	0
3	EDO	A	302	-	3,3,3	0.38	0	2,2,2	0.47	0
2	GOL	C	303	-	5,5,5	0.91	0	5,5,5	0.99	0
2	GOL	D	301	-	5,5,5	0.84	0	5,5,5	1.04	1 (20%)
3	EDO	E	303	-	3,3,3	0.44	0	2,2,2	0.33	0
3	EDO	E	301	-	3,3,3	0.43	0	2,2,2	0.37	0
5	PEG	C	307	-	6,6,6	1.09	0	5,5,5	0.23	0
5	PEG	D	306	-	6,6,6	1.67	1 (16%)	5,5,5	0.52	0
3	EDO	D	302	-	3,3,3	0.46	0	2,2,2	0.30	0
2	GOL	A	301	-	5,5,5	0.89	0	5,5,5	0.98	0
3	EDO	F	301	-	3,3,3	0.41	0	2,2,2	0.44	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
2	GOL	B	301	-	-	0/4/4/4	-
3	EDO	C	302	-	-	0/1/1/1	-
3	EDO	A	303	-	-	1/1/1/1	-
3	EDO	B	304	-	-	1/1/1/1	-
3	EDO	B	303	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	302	-	-	1/1/1/1	-
2	GOL	E	302	-	-	3/4/4/4	-
3	EDO	F	302	-	-	1/1/1/1	-
3	EDO	C	301	-	-	1/1/1/1	-
3	EDO	A	302	-	-	1/1/1/1	-
2	GOL	C	303	-	-	0/4/4/4	-
2	GOL	D	301	-	-	2/4/4/4	-
3	EDO	E	303	-	-	0/1/1/1	-
3	EDO	E	301	-	-	0/1/1/1	-
5	PEG	C	307	-	-	2/4/4/4	-
5	PEG	D	306	-	-	2/4/4/4	-
3	EDO	D	302	-	-	1/1/1/1	-
2	GOL	A	301	-	-	0/4/4/4	-
3	EDO	F	301	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	306	PEG	O4-C4	-3.58	1.23	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	GOL	C3-C2-C1	-2.08	103.61	111.70

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	GOL	C1-C2-C3-O3
5	D	306	PEG	O1-C1-C2-O2
2	D	301	GOL	O2-C2-C3-O3
3	A	303	EDO	O1-C1-C2-O2
3	D	302	EDO	O1-C1-C2-O2
3	F	302	EDO	O1-C1-C2-O2
3	A	302	EDO	O1-C1-C2-O2
3	B	302	EDO	O1-C1-C2-O2
5	C	307	PEG	C1-C2-O2-C3
2	E	302	GOL	O1-C1-C2-C3
3	B	304	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	C	307	PEG	O2-C3-C4-O4
5	D	306	PEG	C4-C3-O2-C2
2	E	302	GOL	O1-C1-C2-O2
3	C	301	EDO	O1-C1-C2-O2
2	E	302	GOL	C1-C2-C3-O3
3	B	303	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	302	EDO	1	0
3	A	303	EDO	2	0
3	B	304	EDO	2	0
3	B	303	EDO	1	0
3	B	302	EDO	1	0
3	F	302	EDO	2	0
3	E	303	EDO	0	1
3	E	301	EDO	1	0
5	C	307	PEG	2	1
5	D	306	PEG	5	0

5.7 Other polymers

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^{th} 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%)	-0.04	9 (3%) 42 36	8, 11, 19, 45	0
1	B	252/253 (99%)	-0.07	6 (2%) 59 52	8, 11, 20, 60	0
1	C	251/253 (99%)	0.05	15 (5%) 21 21	8, 11, 25, 52	0
1	D	246/253 (97%)	0.26	27 (10%) 5 9	8, 13, 28, 74	0
1	E	247/253 (97%)	0.16	16 (6%) 18 19	8, 13, 25, 65	0
1	F	252/253 (99%)	0.17	14 (5%) 24 23	7, 12, 28, 62	0
All	All	1499/1518 (98%)	0.09	87 (5%) 23 22	7, 12, 25, 74	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	231	ALA	10.0
1	F	2	THR	9.2
1	F	227	ILE	8.6
1	A	4[A]	THR	8.2
1	F	230	HIS	7.9
1	C	227	ILE	7.8
1	E	229	ASP	7.7
1	F	225	LYS	6.5
1	B	2	THR	6.2
1	F	226	GLU	6.0
1	D	236[A]	THR	5.8
1	D	234	LYS	5.8
1	E	4	THR	5.6
1	C	225	LYS	5.5
1	D	253	LYS	5.5
1	D	103[A]	VAL	5.4
1	E	234	LYS	5.3
1	F	232	THR	5.3
1	F	253	LYS	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	3[A]	LYS	4.9
1	C	226	GLU	4.9
1	A	253	LYS	4.9
1	F	233	LEU	4.8
1	F	229	ASP	4.6
1	F	228	PRO	4.6
1	D	224[A]	GLN	4.6
1	D	227	ILE	4.5
1	E	235	GLU	4.5
1	D	235	GLU	4.5
1	E	236	THR	4.3
1	E	227	ILE	4.3
1	C	253	LYS	4.2
1	C	3	LYS	4.1
1	D	228	PRO	4.1
1	D	102[A]	ASN	4.1
1	C	230	HIS	4.0
1	B	4	THR	4.0
1	E	220	ILE	3.9
1	A	6[A]	PHE	3.7
1	F	234[A]	LYS	3.7
1	E	93[A]	THR	3.6
1	E	3	LYS	3.6
1	C	229	ASP	3.6
1	D	225[A]	LYS	3.5
1	D	223[A]	THR	3.4
1	B	227	ILE	3.4
1	D	239	ARG	3.3
1	C	231	ALA	3.2
1	E	253	LYS	3.1
1	A	227	ILE	3.1
1	E	223	THR	3.1
1	D	101[A]	VAL	3.0
1	D	220[A]	ILE	3.0
1	D	104[A]	GLY	3.0
1	C	228	PRO	2.9
1	C	234	LYS	2.9
1	B	3	LYS	2.9
1	E	219	ILE	2.9
1	C	232	THR	2.9
1	D	147[A]	GLY	2.8
1	D	219[A]	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	234[A]	LYS	2.8
1	E	228	PRO	2.8
1	B	6[A]	PHE	2.8
1	D	3	LYS	2.8
1	C	130[A]	VAL	2.7
1	D	149[A]	THR	2.7
1	E	103	VAL	2.7
1	F	130[A]	VAL	2.6
1	D	252	LEU	2.6
1	C	4	THR	2.6
1	D	95[A]	GLY	2.6
1	B	253	LYS	2.4
1	A	230	HIS	2.4
1	E	239	ARG	2.4
1	F	3	LYS	2.4
1	D	237	GLU	2.4
1	A	130[A]	VAL	2.3
1	C	235[A]	GLU	2.3
1	D	99[A]	PRO	2.2
1	D	150[A]	VAL	2.2
1	D	221[A]	ASN	2.1
1	E	6	PHE	2.1
1	D	222[A]	ARG	2.1
1	C	233	LEU	2.1
1	A	5[A]	VAL	2.1
1	D	100[A]	HIS	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, 95^{th} 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
2	GOL	C	303	6/6	0.62	0.22	50,60,61,61	0
3	EDO	E	303	4/4	0.63	0.16	48,58,58,58	0
4	NA	A	304	1/1	0.71	0.16	41,41,41,41	0
3	EDO	D	302	4/4	0.72	0.28	47,57,58,58	0
3	EDO	B	303	4/4	0.73	0.19	45,55,55,55	0
4	NA	E	304	1/1	0.76	0.40	74,74,74,74	0
5	PEG	C	307	7/7	0.80	0.29	42,51,52,53	0
3	EDO	C	301	4/4	0.82	0.16	31,38,40,41	0
2	GOL	E	302	6/6	0.82	0.14	33,40,46,46	0
2	GOL	D	301	6/6	0.82	0.14	28,35,42,42	0
5	PEG	D	306	7/7	0.86	0.23	32,41,48,49	0
3	EDO	F	302	4/4	0.87	0.22	19,23,28,29	10
3	EDO	F	301	4/4	0.88	0.12	26,31,35,36	0
3	EDO	C	302	4/4	0.88	0.20	26,32,37,39	0
3	EDO	E	301	4/4	0.89	0.17	24,29,35,37	0
3	EDO	B	304	4/4	0.90	0.16	24,29,34,37	0
3	EDO	A	303	4/4	0.90	0.22	25,31,35,38	0
3	EDO	A	302	4/4	0.91	0.17	20,26,31,31	0
4	NA	C	306	1/1	0.91	0.21	29,29,29,29	1
2	GOL	B	301	6/6	0.91	0.12	17,25,30,32	0
3	EDO	B	302	4/4	0.91	0.20	21,25,29,29	0
2	GOL	A	301	6/6	0.91	0.11	14,20,24,26	14
4	NA	C	305	1/1	0.95	0.17	17,17,17,17	1
4	NA	D	304	1/1	0.97	0.15	29,29,29,29	0
4	NA	B	305	1/1	0.98	0.18	16,16,16,16	1
4	NA	E	305	1/1	0.98	0.15	26,26,26,26	0
4	NA	E	307	1/1	0.99	0.12	12,12,12,12	1
6	MG	E	306	1/1	0.99	0.05	16,16,16,16	1
4	NA	C	304	1/1	1.00	0.11	12,12,12,12	1
4	NA	D	303	1/1	1.00	0.06	13,13,13,13	0
6	MG	D	305	1/1	1.00	0.04	15,15,15,15	1
4	NA	A	305	1/1	1.00	0.03	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.