Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:31 am BST

PDB ID	:	6EH5
Title	:	003 Human T-Cell Receptor specific for HIV GAG epitope SLYNTVATL carried by Human Leukocyte Antigen HLA-A*0201
Authors	:	Rizkallah, P.J.; Cole, D.K.
Deposited on	:	2017-09-12
Resolution	:	1.29 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:

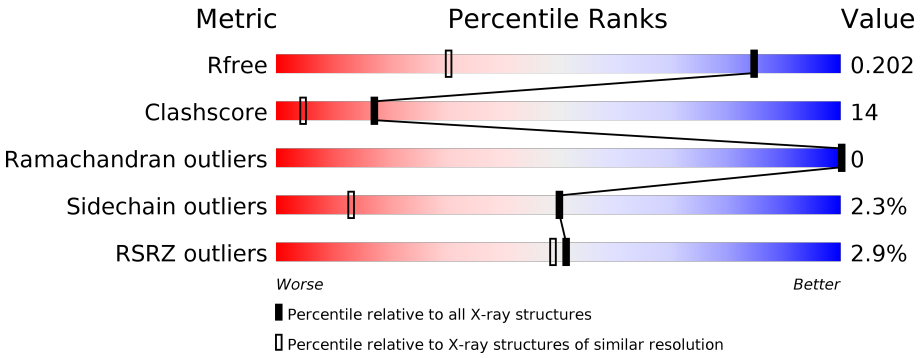
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.29 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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	202	2% 76% 21%
2	B	244	3% 80% 17%

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	EDO	A	304	-	-	X	-
4	EDO	A	310	-	-	X	-
4	EDO	A	314	-	X	-	-
4	EDO	A	315	-	X	X	-
4	EDO	A	316	-	X	-	-
4	EDO	B	311	-	-	-	X
5	PG4	B	301	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4317 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.

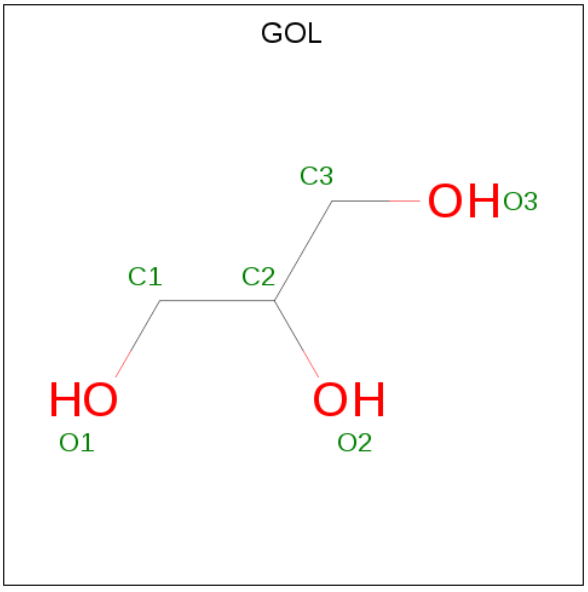
- Molecule 1 is a protein called Human T Cell Receptor Alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	9	0
			1631	1017	270	336	8			

- Molecule 2 is a protein called Human T Cell Receptor Beta Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	14	0
			2061	1291	372	391	7			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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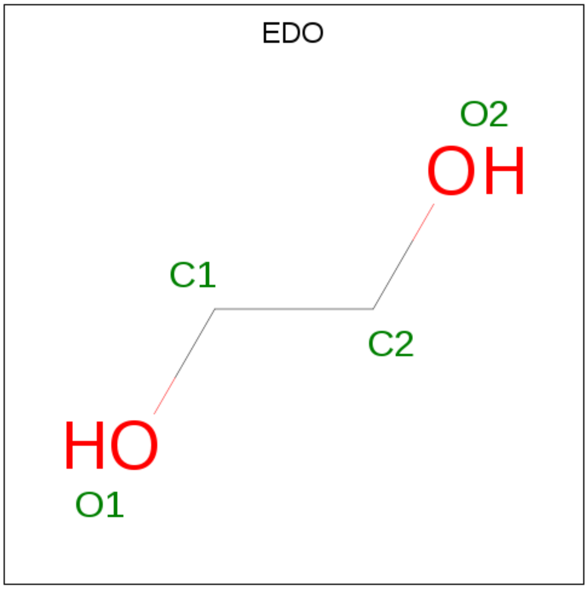
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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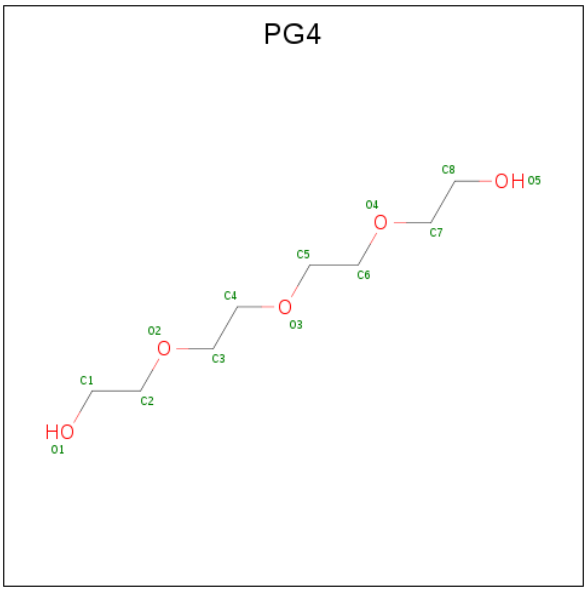
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0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

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 13 8 5	0	0

- Molecule 6 is water.

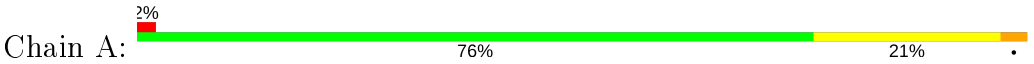
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	227	Total O 227 227	0	0
6	B	259	Total O 259 259	0	0

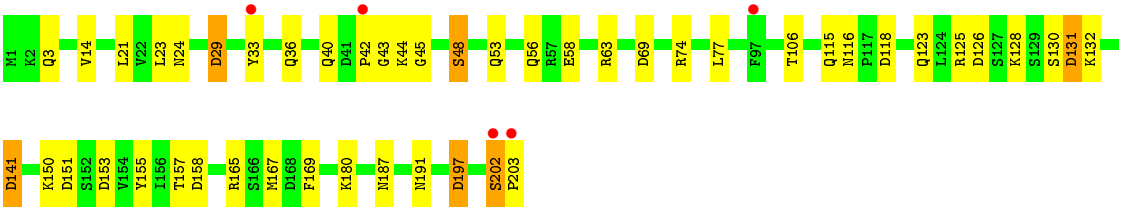
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Human T Cell Receptor Alpha Chain

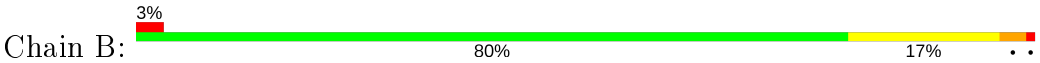
Chain A:

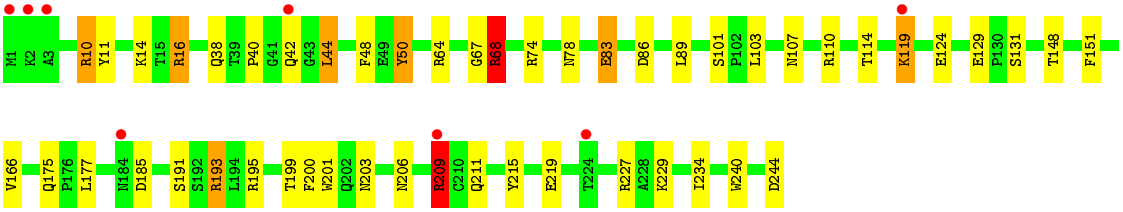




- Molecule 2: Human T Cell Receptor Beta Chain

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	43.15Å 81.17Å 64.90Å 90.00° 90.33° 90.00°	Depositor
Resolution (Å)	50.69 – 1.29 50.69 – 1.29	Depositor EDS
% Data completeness (in resolution range)	94.9 (50.69-1.29) 94.9 (50.69-1.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 1.29Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.168 , 0.195 0.176 , 0.202	Depositor DCC
R_{free} test set	5313 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	14.3	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4317	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% 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, PG4, EDO

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	1.44	11/1674 (0.7%)	1.43	21/2269 (0.9%)
2	B	1.55	25/2142 (1.2%)	1.39	26/2904 (0.9%)
All	All	1.50	36/3816 (0.9%)	1.41	47/5173 (0.9%)

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
2	B	0	1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	119	LYS	CE-NZ	14.25	1.84	1.49
2	B	83[A]	GLU	CD-OE1	9.69	1.36	1.25
2	B	83[B]	GLU	CD-OE1	9.69	1.36	1.25
2	B	83[A]	GLU	CG-CD	9.01	1.65	1.51
2	B	83[B]	GLU	CG-CD	9.01	1.65	1.51
2	B	193	ARG	CZ-NH2	-8.25	1.22	1.33
2	B	219	GLU	CD-OE1	-7.97	1.16	1.25
1	A	155	TYR	CE1-CZ	-7.42	1.28	1.38
2	B	129	GLU	CD-OE1	-7.00	1.18	1.25
2	B	119	LYS	CD-CE	6.87	1.68	1.51
2	B	101	SER	CB-OG	-6.83	1.33	1.42
1	A	141[A]	ASP	CB-CG	6.77	1.66	1.51
1	A	141[B]	ASP	CB-CG	6.77	1.66	1.51
1	A	141[C]	ASP	CB-CG	6.77	1.66	1.51
2	B	83[A]	GLU	CD-OE2	6.69	1.33	1.25
2	B	83[B]	GLU	CD-OE2	6.69	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	68[A]	ARG	CZ-NH2	6.61	1.41	1.33
2	B	68[B]	ARG	CZ-NH2	6.61	1.41	1.33
2	B	131	SER	CB-OG	-6.53	1.33	1.42
2	B	124	GLU	CG-CD	6.43	1.61	1.51
2	B	67	GLY	N-CA	6.40	1.55	1.46
2	B	215	TYR	CG-CD1	6.21	1.47	1.39
2	B	215	TYR	CZ-OH	6.11	1.48	1.37
2	B	50	TYR	CE1-CZ	-6.07	1.30	1.38
2	B	166	VAL	CB-CG2	-5.70	1.40	1.52
1	A	141[A]	ASP	CG-OD1	5.30	1.37	1.25
1	A	141[B]	ASP	CG-OD1	5.30	1.37	1.25
1	A	141[C]	ASP	CG-OD1	5.30	1.37	1.25
2	B	11	TYR	CG-CD2	-5.28	1.32	1.39
1	A	48	SER	N-CA	-5.28	1.35	1.46
2	B	215	TYR	CE1-CZ	-5.27	1.31	1.38
1	A	187	ASN	CB-CG	5.27	1.63	1.51
2	B	14	LYS	CD-CE	-5.21	1.38	1.51
1	A	58	GLU	CG-CD	5.12	1.59	1.51
2	B	193	ARG	NE-CZ	-5.06	1.26	1.33
1	A	58	GLU	CB-CG	-5.06	1.42	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	44	LEU	CB-CG-CD1	-13.52	88.02	111.00
2	B	68[A]	ARG	NE-CZ-NH2	-12.47	114.06	120.30
2	B	68[B]	ARG	NE-CZ-NH2	-12.47	114.06	120.30
1	A	131	ASP	CB-CG-OD2	-12.13	107.38	118.30
2	B	193	ARG	NE-CZ-NH1	-10.49	115.06	120.30
1	A	118	ASP	CB-CG-OD1	9.52	126.87	118.30
1	A	197	ASP	CB-CG-OD2	9.51	126.86	118.30
1	A	69	ASP	CB-CG-OD1	8.78	126.20	118.30
2	B	16	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	A	158	ASP	CB-CG-OD1	8.62	126.06	118.30
2	B	64	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	A	131	ASP	CB-CG-OD1	7.42	124.98	118.30
2	B	68[A]	ARG	CG-CD-NE	7.32	127.17	111.80
2	B	68[B]	ARG	CG-CD-NE	7.32	127.17	111.80
2	B	244	ASP	CB-CG-OD1	7.31	124.88	118.30
2	B	195	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	74	ARG	NE-CZ-NH1	-7.09	116.75	120.30
1	A	141[A]	ASP	CB-CG-OD1	6.95	124.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	141[B]	ASP	CB-CG-OD1	6.95	124.56	118.30
1	A	141[C]	ASP	CB-CG-OD1	6.95	124.56	118.30
1	A	125	ARG	NE-CZ-NH1	-6.86	116.87	120.30
2	B	10[A]	ARG	NE-CZ-NH1	-6.79	116.90	120.30
2	B	10[B]	ARG	NE-CZ-NH1	-6.79	116.90	120.30
2	B	10[C]	ARG	NE-CZ-NH1	-6.79	116.90	120.30
1	A	141[A]	ASP	N-CA-CB	-6.50	98.90	110.60
1	A	141[B]	ASP	N-CA-CB	-6.50	98.90	110.60
1	A	141[C]	ASP	N-CA-CB	-6.50	98.90	110.60
2	B	131	SER	N-CA-CB	-6.10	101.35	110.50
2	B	83[A]	GLU	OE1-CD-OE2	-6.09	116.00	123.30
2	B	83[B]	GLU	OE1-CD-OE2	-6.09	116.00	123.30
1	A	29	ASP	CB-CG-OD1	6.08	123.78	118.30
2	B	209[A]	ARG	NE-CZ-NH2	6.00	123.30	120.30
2	B	209[B]	ARG	NE-CZ-NH2	6.00	123.30	120.30
2	B	209[C]	ARG	NE-CZ-NH2	6.00	123.30	120.30
2	B	209[D]	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	A	125	ARG	NE-CZ-NH2	5.99	123.29	120.30
1	A	141[A]	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	141[B]	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	141[C]	ASP	CB-CG-OD2	-5.92	112.97	118.30
2	B	151	PHE	CB-CG-CD1	-5.71	116.80	120.80
2	B	227	ARG	NE-CZ-NH2	5.67	123.13	120.30
1	A	202	SER	CA-CB-OG	-5.51	96.32	111.20
2	B	74	ARG	NE-CZ-NH2	5.43	123.02	120.30
2	B	119	LYS	CG-CD-CE	5.42	128.16	111.90
1	A	63	ARG	NE-CZ-NH1	-5.39	117.60	120.30
2	B	86	ASP	CB-CG-OD1	5.34	123.11	118.30
2	B	193	ARG	NE-CZ-NH2	5.22	122.91	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	50	TYR	Sidechain

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	1631	0	1571	50	0
2	B	2061	0	1984	41	0
3	A	18	0	24	6	0
4	A	52	0	64	30	0
4	B	56	0	83	6	0
5	B	13	0	18	8	0
6	A	227	0	0	15	0
6	B	259	0	0	17	1
All	All	4317	0	3744	104	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 14.

All (104) 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)
2:B:119:LYS:CE	2:B:119:LYS:NZ	1.84	1.41
2:B:78:ASN:HB3	6:B:404:HOH:O	1.32	1.25
1:A:167:MET:HG2	6:A:616:HOH:O	1.37	1.21
1:A:131:ASP:OD1	6:A:402:HOH:O	1.67	1.11
4:A:315:EDO:O1	4:A:315:EDO:C2	1.99	1.10
2:B:240[B]:TRP:CZ3	6:B:617:HOH:O	2.07	1.07
4:A:315:EDO:O2	4:A:315:EDO:C1	2.05	1.04
2:B:240[B]:TRP:CH2	6:B:617:HOH:O	2.10	1.01
2:B:10[A]:ARG:NH1	6:B:403:HOH:O	1.97	0.97
1:A:151[A]:ASP:OD1	1:A:153[A]:ASP:OD1	1.86	0.93
4:A:315:EDO:H22	4:A:315:EDO:C1	1.38	0.90
4:A:315:EDO:H21	4:A:315:EDO:C1	1.38	0.89
1:A:40:GLN:HE22	2:B:38:GLN:HE22	1.18	0.89
4:A:315:EDO:H11	4:A:315:EDO:C2	1.34	0.85
4:A:315:EDO:H12	4:A:315:EDO:C2	1.34	0.85
2:B:206:ASN:HD21	5:B:301:PG4:H52	1.42	0.83
4:B:303:EDO:H21	6:B:529:HOH:O	1.79	0.82
4:A:304:EDO:O2	2:B:110:ARG:NH2	2.16	0.79
4:A:315:EDO:C1	4:A:315:EDO:C2	0.76	0.76
1:A:21[B]:LEU:CD1	1:A:23[B]:LEU:CD1	2.64	0.75
1:A:24:ASN:HB3	4:A:314:EDO:H21	1.66	0.75
1:A:123:GLN:NE2	6:A:404:HOH:O	2.20	0.74
1:A:151[A]:ASP:OD2	1:A:180:LYS:NZ	2.22	0.73
4:A:310:EDO:C1	6:A:407:HOH:O	2.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:310:EDO:H12	6:A:407:HOH:O	1.88	0.73
1:A:43:GLY:C	4:A:304:EDO:H12	2.09	0.73
1:A:45:GLY:H	2:B:107:ASN:HD22	1.36	0.73
1:A:203:PRO:HA	3:A:301:GOL:O1	1.90	0.71
1:A:157[A]:THR:HG21	2:B:191:SER:OG	1.94	0.68
1:A:128:LYS:HA	4:A:310:EDO:H22	1.74	0.68
2:B:177[A]:LEU:HD12	2:B:177[A]:LEU:O	1.92	0.68
1:A:197:ASP:O	4:A:309:EDO:H12	1.94	0.68
1:A:167:MET:CE	6:A:616:HOH:O	2.41	0.67
4:A:309:EDO:C2	6:A:406:HOH:O	2.41	0.67
4:B:304:EDO:H22	6:B:441:HOH:O	1.95	0.67
2:B:68[A]:ARG:CZ	6:B:414:HOH:O	2.44	0.66
1:A:21[B]:LEU:CD1	1:A:23[B]:LEU:HD11	2.25	0.66
1:A:21[B]:LEU:HD12	1:A:23[B]:LEU:CD1	2.24	0.66
1:A:3:GLN:HE22	1:A:29:ASP:H	1.43	0.64
4:A:309:EDO:H21	6:A:406:HOH:O	1.98	0.62
1:A:167:MET:CG	6:A:616:HOH:O	2.12	0.61
2:B:177[A]:LEU:HD12	2:B:177[A]:LEU:C	2.21	0.61
1:A:44:LYS:N	4:A:304:EDO:H12	2.16	0.61
2:B:114:THR:OG1	2:B:119:LYS:HE2	2.01	0.61
2:B:16:ARG:NH2	2:B:83[B]:GLU:OE1	2.27	0.61
2:B:16:ARG:NH2	6:B:406:HOH:O	2.27	0.60
2:B:209[D]:ARG:NH2	6:B:401:HOH:O	2.32	0.59
4:A:306:EDO:H21	6:A:615:HOH:O	2.03	0.58
4:A:315:EDO:H12	4:A:315:EDO:H21	1.22	0.58
2:B:203:ASN:HD22	5:B:301:PG4:C5	2.17	0.57
1:A:167:MET:HE2	6:A:616:HOH:O	2.00	0.57
1:A:21[B]:LEU:HD13	1:A:23[B]:LEU:HD11	1.88	0.55
1:A:24:ASN:CB	4:A:314:EDO:H21	2.34	0.55
2:B:68[B]:ARG:NH2	6:B:410:HOH:O	2.39	0.54
4:A:304:EDO:HO2	2:B:110:ARG:HH21	1.50	0.54
1:A:132:LYS:NZ	6:A:402:HOH:O	2.41	0.54
1:A:132:LYS:HE2	2:B:148:THR:HG21	1.90	0.53
2:B:10[A]:ARG:CZ	6:B:403:HOH:O	2.49	0.53
1:A:14:VAL:HG21	1:A:21[A]:LEU:HD21	1.90	0.53
2:B:16:ARG:HE	2:B:83[B]:GLU:CD	2.13	0.52
1:A:36[B]:GLN:HE22	2:B:103:LEU:H	1.59	0.51
2:B:206:ASN:ND2	5:B:301:PG4:H52	2.21	0.51
2:B:203:ASN:HD22	5:B:301:PG4:H51	1.75	0.51
2:B:229:LYS:HD3	4:B:307:EDO:H11	1.92	0.51
1:A:23[A]:LEU:HD22	1:A:106:THR:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LYS:HE2	3:A:303:GOL:H12	1.93	0.50
1:A:53[B]:GLN:H	1:A:56:GLN:NE2	2.10	0.50
1:A:3:GLN:NE2	1:A:29:ASP:H	2.09	0.49
1:A:150[A]:LYS:HE3	1:A:191:ASN:HB2	1.95	0.49
2:B:199:THR:HB	5:B:301:PG4:H12	1.95	0.49
1:A:53[A]:GLN:H	1:A:56:GLN:NE2	2.11	0.49
2:B:78:ASN:CB	6:B:404:HOH:O	2.17	0.48
1:A:167:MET:HG3	4:A:313:EDO:O1	2.15	0.47
2:B:119:LYS:HE3	2:B:185:ASP:CB	2.46	0.46
4:A:313:EDO:H21	6:B:511:HOH:O	2.16	0.46
1:A:23[A]:LEU:HD12	1:A:77:LEU:HD23	1.97	0.46
2:B:68[A]:ARG:NE	6:B:414:HOH:O	2.48	0.45
2:B:211[A]:GLN:NE2	2:B:234:ILE:HD13	2.31	0.45
4:B:310:EDO:C1	6:B:405:HOH:O	2.62	0.45
1:A:169:PHE:HA	3:A:302:GOL:H11	1.99	0.45
2:B:40:PRO:N	4:B:303:EDO:H12	2.32	0.44
2:B:200:PHE:CE1	5:B:301:PG4:H61	2.52	0.44
1:A:132:LYS:CE	3:A:303:GOL:H12	2.48	0.44
2:B:119:LYS:HE3	2:B:185:ASP:HB3	2.00	0.44
2:B:209[D]:ARG:HD2	6:B:401:HOH:O	2.17	0.44
1:A:36[A]:GLN:HE22	2:B:103:LEU:H	1.65	0.44
1:A:45:GLY:H	2:B:107:ASN:ND2	2.10	0.44
1:A:130:SER:HA	4:A:312:EDO:H11	1.98	0.44
5:B:301:PG4:H22	6:B:415:HOH:O	2.16	0.44
1:A:115:GLN:HG3	1:A:116:ASN:ND2	2.33	0.43
1:A:33:TYR:N	1:A:33:TYR:CD1	2.86	0.43
1:A:53[B]:GLN:H	1:A:56:GLN:HE21	1.65	0.43
2:B:199:THR:HG22	5:B:301:PG4:H31	2.00	0.43
4:A:314:EDO:C2	6:A:466:HOH:O	2.65	0.43
4:A:304:EDO:H11	2:B:89:LEU:HD22	1.99	0.43
1:A:202:SER:N	4:A:307:EDO:H12	2.35	0.42
1:A:48:SER:HB3	4:A:308:EDO:O1	2.20	0.42
1:A:42:PRO:HD3	6:A:474:HOH:O	2.20	0.41
1:A:53[A]:GLN:H	1:A:56:GLN:HE21	1.66	0.41
2:B:201:TRP:NE1	4:B:304:EDO:H11	2.34	0.41
1:A:126:ASP:HB3	4:A:310:EDO:H11	2.01	0.41
3:A:302:GOL:C3	6:A:405:HOH:O	2.64	0.41
1:A:115:GLN:HE21	3:A:302:GOL:H32	1.85	0.41
1:A:202:SER:H	4:A:307:EDO:H12	1.87	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)
6:B:444:HOH:O	6:B:576:HOH:O[1_556]	2.05	0.15

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	210/202 (104%)	208 (99%)	2 (1%)	0	100 100
2	B	259/244 (106%)	253 (98%)	6 (2%)	0	100 100
All	All	469/446 (105%)	461 (98%)	8 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	190/180 (106%)	186 (98%)	4 (2%)	53 16
2	B	231/214 (108%)	220 (95%)	11 (5%)	25 2
All	All	421/394 (107%)	406 (96%)	15 (4%)	50 4

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

Mol	Chain	Res	Type
1	A	141[A]	ASP
1	A	141[B]	ASP
1	A	141[C]	ASP

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Mol	Chain	Res	Type
1	A	165	ARG
2	B	42	GLN
2	B	44	LEU
2	B	48	PHE
2	B	68[A]	ARG
2	B	68[B]	ARG
2	B	175	GLN
2	B	193	ARG
2	B	209[A]	ARG
2	B	209[B]	ARG
2	B	209[C]	ARG
2	B	209[D]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	40	GLN
1	A	56	GLN
1	A	59	GLN
1	A	65	ASN
1	A	115	GLN
1	A	116	ASN
1	A	123	GLN
1	A	148	GLN
2	B	45	GLN
2	B	57	ASN
2	B	107	ASN
2	B	213	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

31 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	B	312	-	3,3,3	0.50	0	2,2,2	0.62	0
4	EDO	B	302	-	3,3,3	0.61	0	2,2,2	0.40	0
3	GOL	A	303	-	5,5,5	0.63	0	5,5,5	1.05	0
4	EDO	B	303	-	3,3,3	0.72	0	2,2,2	0.67	0
4	EDO	B	306	-	3,3,3	0.52	0	2,2,2	0.76	0
4	EDO	B	308	-	3,3,3	0.88	0	2,2,2	1.48	1 (50%)
4	EDO	B	307	-	3,3,3	0.35	0	2,2,2	0.65	0
4	EDO	A	312	-	3,3,3	0.34	0	2,2,2	0.68	0
5	PG4	B	301	-	12,12,12	0.57	0	11,11,11	1.22	2 (18%)
4	EDO	A	316	-	3,3,3	5.77	2 (66%)	2,2,2	4.13	1 (50%)
4	EDO	A	304	-	3,3,3	0.61	0	2,2,2	1.07	0
3	GOL	A	301	-	5,5,5	0.47	0	5,5,5	1.02	1 (20%)
4	EDO	A	314	-	3,3,3	6.55	2 (66%)	2,2,2	1.52	1 (50%)
4	EDO	A	315	-	3,3,3	6.03	1 (33%)	2,2,2	3.67	2 (100%)
3	GOL	A	302	-	5,5,5	0.84	0	5,5,5	2.15	2 (40%)
4	EDO	B	313	-	3,3,3	0.65	0	2,2,2	0.33	0
4	EDO	A	308	-	3,3,3	0.22	0	2,2,2	1.36	0
4	EDO	B	311	-	3,3,3	0.52	0	2,2,2	0.11	0
4	EDO	B	310	-	3,3,3	0.50	0	2,2,2	0.36	0
4	EDO	B	315	-	3,3,3	0.48	0	2,2,2	0.28	0
4	EDO	B	314	-	3,3,3	0.72	0	2,2,2	0.74	0
4	EDO	A	305	-	3,3,3	0.92	0	2,2,2	0.47	0
4	EDO	A	307	-	3,3,3	1.24	0	2,2,2	1.71	1 (50%)
4	EDO	B	305	-	3,3,3	0.30	0	2,2,2	1.02	0
4	EDO	A	311	-	3,3,3	0.65	0	2,2,2	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	A	306	-	3,3,3	0.44	0	2,2,2	0.19	0
4	EDO	A	313	-	3,3,3	0.54	0	2,2,2	0.97	0
4	EDO	A	309	-	3,3,3	0.88	0	2,2,2	0.98	0
4	EDO	B	309	-	3,3,3	0.63	0	2,2,2	0.24	0
4	EDO	B	304	-	3,3,3	0.68	0	2,2,2	0.44	0
4	EDO	A	310	-	3,3,3	0.57	0	2,2,2	0.83	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
4	EDO	B	312	-	-	0/1/1/1	-
4	EDO	B	302	-	-	0/1/1/1	-
3	GOL	A	303	-	-	2/4/4/4	-
4	EDO	B	303	-	-	1/1/1/1	-
4	EDO	B	306	-	-	0/1/1/1	-
4	EDO	B	308	-	-	1/1/1/1	-
4	EDO	B	307	-	-	1/1/1/1	-
4	EDO	A	312	-	-	1/1/1/1	-
5	PG4	B	301	-	-	7/10/10/10	-
4	EDO	A	316	-	-	0/1/1/1	-
4	EDO	A	304	-	-	1/1/1/1	-
3	GOL	A	301	-	-	2/4/4/4	-
4	EDO	A	314	-	-	1/1/1/1	-
4	EDO	A	315	-	-	1/1/1/1	-
3	GOL	A	302	-	-	2/4/4/4	-
4	EDO	B	313	-	-	0/1/1/1	-
4	EDO	A	308	-	-	0/1/1/1	-
4	EDO	B	311	-	-	1/1/1/1	-
4	EDO	B	310	-	-	0/1/1/1	-
4	EDO	B	315	-	-	1/1/1/1	-
4	EDO	B	314	-	-	0/1/1/1	-
4	EDO	A	305	-	-	0/1/1/1	-
4	EDO	A	307	-	-	1/1/1/1	-
4	EDO	B	305	-	-	0/1/1/1	-
4	EDO	A	311	-	-	1/1/1/1	-
4	EDO	A	306	-	-	1/1/1/1	-
4	EDO	A	313	-	-	1/1/1/1	-
4	EDO	A	309	-	-	1/1/1/1	-
4	EDO	B	309	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	304	-	-	0/1/1/1	-
4	EDO	A	310	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	314	EDO	O1-C1	-10.93	0.85	1.42
4	A	315	EDO	C2-C1	-10.24	0.76	1.48
4	A	316	EDO	O1-C1	-9.29	0.94	1.42
4	A	316	EDO	O2-C2	3.59	1.60	1.42
4	A	314	EDO	O2-C2	2.97	1.57	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	316	EDO	O1-C1-C2	5.79	153.58	111.91
4	A	315	EDO	O1-C1-C2	4.49	144.18	111.91
3	A	302	GOL	O3-C3-C2	-3.98	91.09	110.20
4	A	315	EDO	O2-C2-C1	2.60	130.61	111.91
4	A	307	EDO	O1-C1-C2	-2.30	95.37	111.91
3	A	302	GOL	O2-C2-C3	2.30	119.24	109.12
5	B	301	PG4	C5-O3-C4	2.26	123.09	113.29
5	B	301	PG4	O3-C4-C3	-2.10	100.91	110.39
3	A	301	GOL	O2-C2-C1	2.09	118.31	109.12
4	B	308	EDO	O1-C1-C2	2.01	126.38	111.91
4	A	314	EDO	O1-C1-C2	2.00	126.32	111.91

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	GOL	O1-C1-C2-C3
3	A	302	GOL	O1-C1-C2-C3
3	A	302	GOL	C1-C2-C3-O3
3	A	301	GOL	O1-C1-C2-O2
5	B	301	PG4	O2-C3-C4-O3
5	B	301	PG4	O4-C7-C8-O5
5	B	301	PG4	O3-C5-C6-O4
5	B	301	PG4	C8-C7-O4-C6
3	A	303	GOL	O1-C1-C2-C3
4	B	303	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	307	EDO	O1-C1-C2-O2
4	A	314	EDO	O1-C1-C2-O2
4	A	307	EDO	O1-C1-C2-O2
4	A	306	EDO	O1-C1-C2-O2
5	B	301	PG4	O1-C1-C2-O2
4	A	313	EDO	O1-C1-C2-O2
4	A	310	EDO	O1-C1-C2-O2
4	B	309	EDO	O1-C1-C2-O2
5	B	301	PG4	C5-C6-O4-C7
3	A	303	GOL	O1-C1-C2-O2
5	B	301	PG4	C4-C3-O2-C2
4	A	312	EDO	O1-C1-C2-O2
4	A	304	EDO	O1-C1-C2-O2
4	A	315	EDO	O1-C1-C2-O2
4	B	315	EDO	O1-C1-C2-O2
4	B	311	EDO	O1-C1-C2-O2
4	A	309	EDO	O1-C1-C2-O2
4	B	308	EDO	O1-C1-C2-O2
4	A	311	EDO	O1-C1-C2-O2

There are no ring outliers.

18 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	GOL	2	0
4	B	303	EDO	2	0
4	B	307	EDO	1	0
4	A	312	EDO	1	0
5	B	301	PG4	8	0
4	A	304	EDO	5	0
3	A	301	GOL	1	0
4	A	314	EDO	3	0
4	A	315	EDO	8	0
3	A	302	GOL	3	0
4	A	308	EDO	1	0
4	B	310	EDO	1	0
4	A	307	EDO	2	0
4	A	306	EDO	1	0
4	A	313	EDO	2	0
4	A	309	EDO	3	0
4	B	304	EDO	2	0
4	A	310	EDO	4	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	202/202 (100%)	-0.14	5 (2%) 57 56	11, 17, 31, 50	0
2	B	244/244 (100%)	-0.07	8 (3%) 46 44	9, 15, 34, 64	0
All	All	446/446 (100%)	-0.10	13 (2%) 51 49	9, 16, 32, 64	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	TYR	5.0
2	B	1	MET	4.4
1	A	97	PHE	3.3
2	B	209[A]	ARG	3.3
2	B	2	LYS	3.3
2	B	184	ASN	3.0
2	B	119	LYS	2.6
1	A	203	PRO	2.5
2	B	224	THR	2.3
1	A	42	PRO	2.2
2	B	3	ALA	2.1
2	B	42	GLN	2.1
1	A	202	SER	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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
4	EDO	B	311	4/4	0.10	1.55	92,94,96,100	0
4	EDO	B	313	4/4	0.61	0.31	39,47,49,51	0
4	EDO	A	306	4/4	0.63	0.16	32,35,39,40	0
4	EDO	A	312	4/4	0.65	0.32	35,40,43,49	0
4	EDO	B	310	4/4	0.66	0.35	58,64,64,65	0
4	EDO	B	309	4/4	0.68	0.26	30,33,34,35	0
4	EDO	A	311	4/4	0.77	0.18	36,36,36,38	0
4	EDO	B	307	4/4	0.80	0.27	35,41,41,41	0
4	EDO	A	304	4/4	0.80	0.19	24,28,32,37	0
4	EDO	B	308	4/4	0.83	0.18	25,27,31,34	0
4	EDO	B	302	4/4	0.85	0.10	20,20,21,21	0
4	EDO	A	313	4/4	0.86	0.19	22,29,30,32	0
4	EDO	B	315	4/4	0.86	0.17	34,35,35,36	0
3	GOL	A	303	6/6	0.87	0.27	20,29,36,48	0
3	GOL	A	302	6/6	0.87	0.25	24,31,32,40	0
5	PG4	B	301	13/13	0.88	0.35	19,35,47,49	0
3	GOL	A	301	6/6	0.89	0.19	24,31,35,43	0
4	EDO	B	303	4/4	0.89	0.13	16,25,26,28	0
4	EDO	B	312	4/4	0.91	0.15	34,36,36,37	0
4	EDO	B	314	4/4	0.91	0.25	24,26,28,34	0
4	EDO	B	304	4/4	0.91	0.18	24,27,32,38	0
4	EDO	A	305	4/4	0.92	0.15	19,22,23,25	0
4	EDO	A	309	4/4	0.93	0.25	22,26,27,43	0
4	EDO	A	310	4/4	0.93	0.14	17,22,23,33	0
4	EDO	B	305	4/4	0.94	0.21	21,31,37,37	0
4	EDO	A	308	4/4	0.94	0.24	22,22,26,32	0
4	EDO	B	306	4/4	0.95	0.14	22,31,34,35	0
4	EDO	A	315	4/4	0.95	0.23	4,6,24,25	0
4	EDO	A	307	4/4	0.97	0.21	23,26,27,30	0
4	EDO	A	314	4/4	0.97	0.19	5,15,23,35	0
4	EDO	A	316	4/4	0.97	0.21	5,17,22,34	0

6.5 Other polymers

There are no such residues in this entry.