Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:41 PM GMT

PDB ID	:	4MES
Title	:	Crystal structure of ThiT complexed with LMG116
Authors	:	Swier, L.J.Y.M.; Guskov, A.; Slotboom, D.J.
Deposited on	:	2013-08-27
Resolution	:	2.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

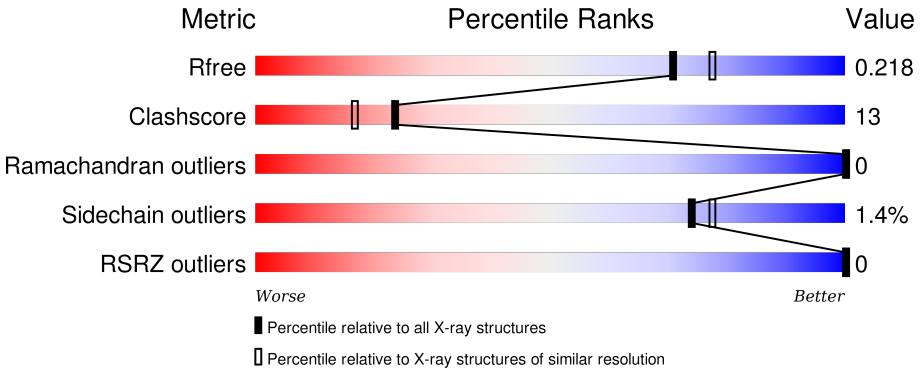
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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. 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	182	85% 12% ·
1	B	182	85% 13% ·

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	BNG	A	201	-	-	-	X
2	BNG	A	202	-	-	-	X
2	BNG	B	203	-	-	-	X
2	BNG	B	204	-	-	-	X
4	PG4	A	204	-	-	-	X
4	PG4	A	205	-	-	-	X
4	PG4	A	206	-	-	-	X
4	PG4	A	207	-	-	-	X
4	PG4	A	210	-	-	-	X
4	PG4	A	211	-	-	X	X
4	PG4	B	207	-	-	-	X
4	PG4	B	208	-	-	-	X
4	PG4	B	209	-	-	X	X
5	PEG	A	213	-	-	X	X
5	PEG	A	214	-	-	-	X
5	PEG	A	215	-	-	-	X
5	PEG	B	210	-	-	-	X
5	PEG	B	213	-	-	-	X
5	PEG	B	214	-	-	-	X
5	PEG	B	217	-	-	X	-
5	PEG	B	221	-	-	-	X
6	PG0	A	217	-	-	-	X
7	P6G	A	218	-	-	-	X
7	P6G	A	219	-	-	-	X
7	P6G	A	220[A]	-	-	-	X
7	P6G	A	220[B]	-	-	-	X
7	P6G	A	221	-	-	-	X
7	P6G	B	224	-	-	-	X
7	P6G	B	225	-	-	-	X
7	P6G	B	226	-	-	-	X
8	1PE	B	222	-	-	-	X

2 Entry composition

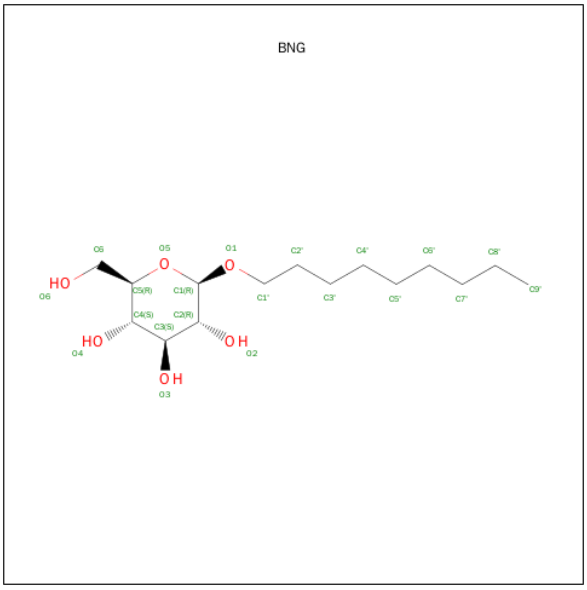
There are 9 unique types of molecules in this entry. The entry contains 3551 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thiamine transporter ThiT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	1	0
			1374	942	214	215	3			
1	B	177	Total	C	N	O	S	0	0	0
			1377	945	214	215	3			

- Molecule 2 is SUGAR (B-NONYLGLUCOSIDE) (three-letter code: BNG) (formula: $C_{15}H_{30}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			21	15	6			
2	A	1	Total	C	O		0	0
			21	15	6			
2	B	1	Total	C	O		0	0
			21	15	6			
2	B	1	Total	C	O		0	0
			21	15	6			

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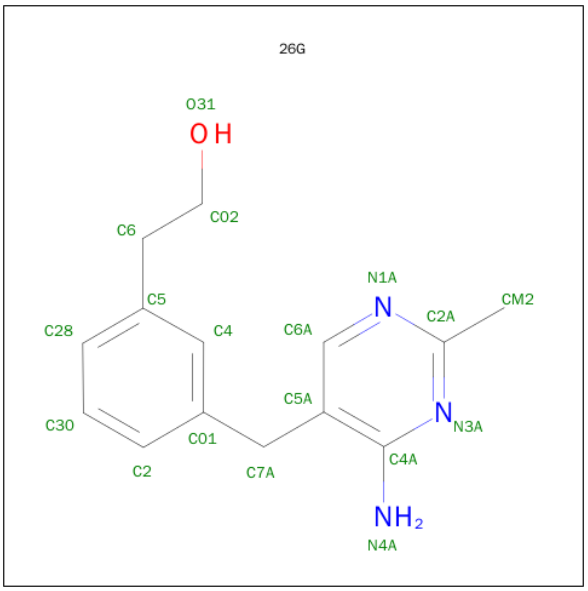
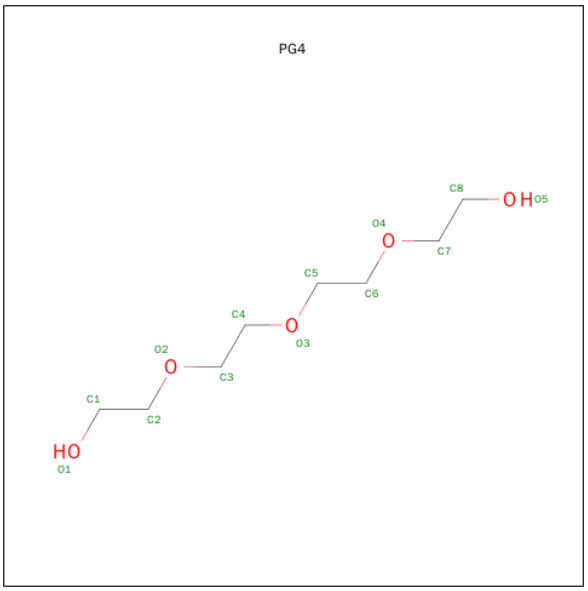
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 21 15 6	0	0
2	B	1	Total C O 21 15 6	0	0
2	B	1	Total C O 21 15 6	0	0

- Molecule 3 is 2-{3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]PHENYL}ETHANOL (three-letter code: 26G) (formula: $C_{14}H_{17}N_3O$).



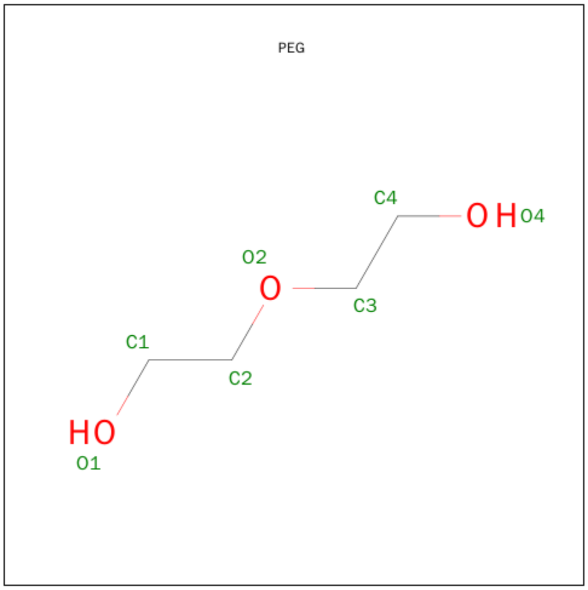
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 18 14 3 1	0	0
3	B	1	Total C N O 18 14 3 1	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 8 5	0	0
4	A	1	Total C O 13 8 5	0	0
4	A	1	Total C O 13 8 5	0	0
4	A	1	Total C O 13 8 5	0	0
4	A	1	Total C O 13 8 5	0	0
4	A	1	Total C O 13 8 5	0	0
4	A	1	Total C O 13 8 5	0	0
4	A	1	Total C O 13 8 5	0	0
4	B	1	Total C O 13 8 5	0	0
4	B	1	Total C O 13 8 5	0	0
4	B	1	Total C O 13 8 5	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	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0

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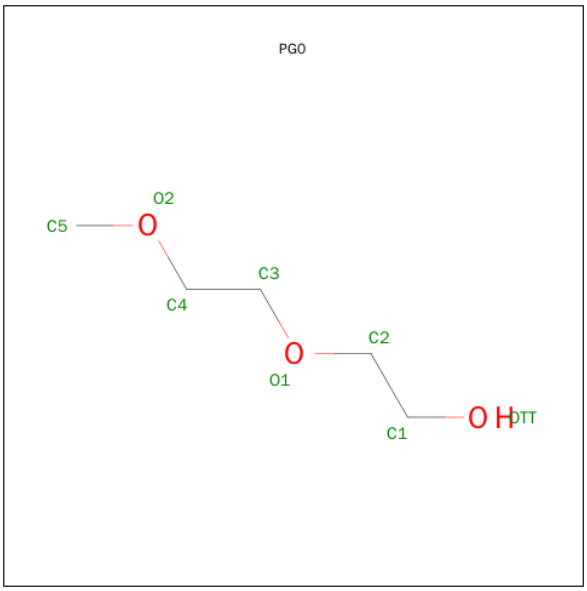
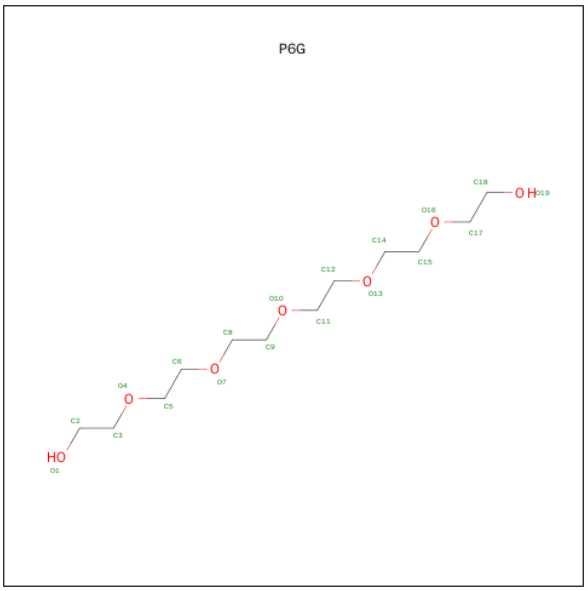
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0

- Molecule 6 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



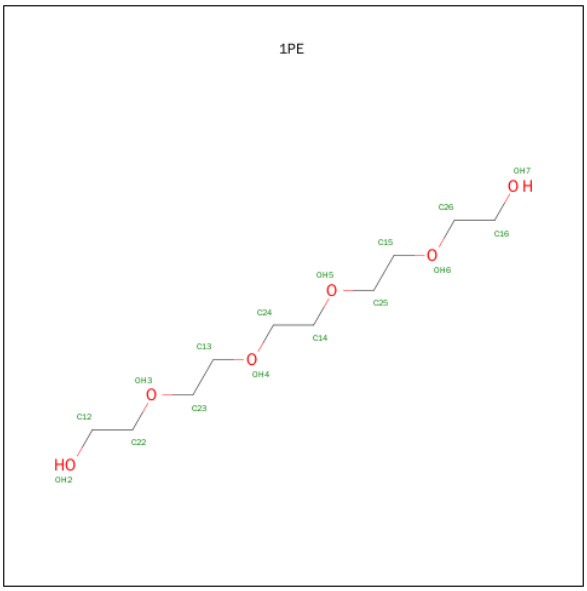
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 8 5 3	0	0
6	B	1	Total C O 8 5 3	0	0

- Molecule 7 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 19 12 7	0	0
7	A	1	Total C O 19 12 7	0	0
7	A	1	Total C O 38 24 14	0	1
7	A	1	Total C O 19 12 7	0	0
7	B	1	Total C O 19 12 7	0	0
7	B	1	Total C O 19 12 7	0	0
7	B	1	Total C O 19 12 7	0	0

- Molecule 8 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 16 10 6	0	0

- Molecule 9 is water.

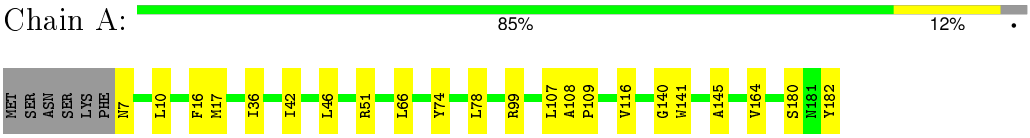
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	70	Total O 72 72	0	2
9	B	99	Total O 99 99	0	0

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 errors 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.

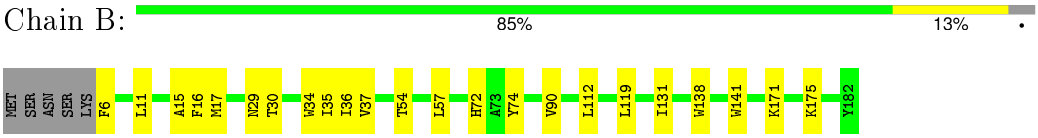
- Molecule 1: Thiamine transporter ThiT

Chain A:



- Molecule 1: Thiamine transporter ThiT

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	61.53Å 84.20Å 127.21Å 90.00° 93.52° 90.00°	Depositor
Resolution (Å)	42.32 – 2.00 47.01 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.32-2.00) 99.8 (47.01-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.174 , 0.208 0.189 , 0.218	Depositor DCC
R_{free} test set	2186 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 64.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 43725 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3551	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 26G, PG0, 1PE, PG4, P6G, PEG, BNG

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	0.60	0/1412	0.62	0/1925
1	B	0.59	0/1416	0.61	0/1930
All	All	0.60	0/2828	0.61	0/3855

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

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	1374	0	1472	33	0
1	B	1377	0	1471	29	0
2	A	42	0	60	5	0
2	B	105	0	150	9	0
3	A	18	0	17	0	0
3	B	18	0	17	1	0
4	A	104	0	144	20	0
4	B	39	0	54	11	0
5	A	35	0	45	9	0
5	B	84	0	108	21	0
6	A	8	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	8	0	12	0	0
7	A	95	0	130	8	0
7	B	57	0	78	7	0
8	B	16	0	22	3	0
9	A	72	0	0	4	0
9	B	99	0	0	3	0
All	All	3551	0	3792	95	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 13.

All (95) 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:B:36:ILE:HG21	4:B:209:PG4:H62	1.54	0.89
1:A:180:SER:HB2	9:A:356:HOH:O	1.77	0.84
1:B:35:ILE:CD1	2:B:201:BNG:H3'2	2.11	0.81
1:A:164:VAL:HG13	4:A:206:PG4:H71	1.65	0.76
1:B:36:ILE:CG2	4:B:209:PG4:H62	2.16	0.76
1:B:119:LEU:HD11	5:B:217:PEG:H42	1.71	0.73
4:A:211:PG4:H52	9:A:307:HOH:O	1.87	0.72
7:A:218:P6G:H21	7:A:218:P6G:H112	1.72	0.71
4:B:209:PG4:H61	9:B:352:HOH:O	1.91	0.70
1:A:145:ALA:H	6:A:217:PG0:H31	1.56	0.70
7:A:218:P6G:H182	7:A:219:P6G:H62	1.74	0.69
1:A:78:LEU:CD2	7:A:218:P6G:H171	2.23	0.67
5:A:214:PEG:H32	5:B:212:PEG:H21	1.78	0.66
1:A:46:LEU:HD23	7:A:220[A]:P6G:H141	1.78	0.65
1:A:10:LEU:HD21	4:A:211:PG4:H32	1.78	0.64
1:B:175:LYS:HB2	5:B:216:PEG:H32	1.80	0.63
1:A:116:VAL:CG1	2:A:202:BNG:H7'2	2.29	0.62
3:B:206:26G:C30	4:B:209:PG4:H81	2.32	0.60
4:A:209:PG4:H82	9:A:367:HOH:O	2.02	0.58
1:B:34:TRP:CE3	4:B:209:PG4:H42	2.39	0.58
1:A:107:LEU:HB3	5:A:213:PEG:H21	1.86	0.58
1:B:35:ILE:HD13	2:B:201:BNG:H3'2	1.86	0.58
1:B:29:ASN:HA	5:B:214:PEG:H22	1.85	0.58
1:A:164:VAL:CG1	4:A:206:PG4:H71	2.34	0.56
1:A:107:LEU:N	5:A:213:PEG:H12	2.20	0.56
1:A:51:ARG:HA	4:A:211:PG4:H81	1.88	0.56
4:A:204:PG4:H51	4:A:208:PG4:H32	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:217:PEG:O4	7:B:225:P6G:H61	2.05	0.56
1:B:6:PHE:N	9:B:359:HOH:O	2.39	0.55
1:A:107:LEU:H	5:A:213:PEG:H32	1.72	0.55
1:B:74:TYR:OH	4:B:209:PG4:H51	2.07	0.54
1:A:108:ALA:H	5:A:213:PEG:H12	1.73	0.54
5:B:219:PEG:H21	5:B:220:PEG:O2	2.07	0.54
1:A:42:ILE:HD12	7:A:220[A]:P6G:H81	1.91	0.53
1:B:37:VAL:HB	5:B:214:PEG:H31	1.90	0.52
5:B:213:PEG:H41	7:B:226:P6G:H21	1.90	0.52
1:A:74:TYR:HE2	4:A:210:PG4:H52	1.75	0.52
1:A:141:TRP:HE1	4:A:209:PG4:H81	1.74	0.52
1:A:116:VAL:HG11	2:A:202:BNG:H7'2	1.93	0.51
1:B:90:VAL:HG11	7:B:224:P6G:H81	1.93	0.50
1:B:30:THR:OG1	4:B:209:PG4:H52	2.12	0.49
4:A:204:PG4:C5	4:A:208:PG4:H32	2.42	0.49
4:B:209:PG4:H21	4:B:209:PG4:H41	1.40	0.49
1:A:10:LEU:HD21	4:A:211:PG4:H51	1.95	0.48
4:A:205:PG4:H81	4:A:205:PG4:H61	1.47	0.48
1:B:34:TRP:CD2	4:B:209:PG4:H42	2.49	0.48
4:A:210:PG4:H52	4:A:210:PG4:H81	1.96	0.48
1:A:36:ILE:HG21	4:A:210:PG4:H51	1.95	0.47
5:B:210:PEG:H22	8:B:222:1PE:H231	1.96	0.47
1:A:99:ARG:NH1	4:A:211:PG4:H82	2.29	0.47
4:A:210:PG4:H62	4:A:210:PG4:H41	1.69	0.47
1:A:182:TYR:OXT	5:A:216:PEG:H22	2.14	0.47
1:B:138:TRP:CG	2:B:201:BNG:H5	2.50	0.47
1:B:57:LEU:HD12	4:B:207:PG4:H41	1.97	0.47
1:B:119:LEU:HA	7:B:225:P6G:H182	1.97	0.47
1:B:15:ALA:HB1	2:B:203:BNG:H4	1.98	0.46
2:A:201:BNG:H5'2	2:A:201:BNG:H2'1	1.68	0.46
5:B:220:PEG:H31	5:B:220:PEG:H12	1.53	0.46
1:A:108:ALA:HB1	2:B:201:BNG:H2'1	1.97	0.46
1:A:182:TYR:OXT	5:A:216:PEG:O1	2.34	0.46
1:B:112:LEU:HD22	5:B:212:PEG:H11	1.98	0.45
1:A:145:ALA:N	6:A:217:PG0:H31	2.30	0.45
1:A:107:LEU:H	5:A:213:PEG:H12	1.81	0.45
1:B:119:LEU:CD1	5:B:217:PEG:H42	2.43	0.45
1:B:141:TRP:CZ3	2:B:202:BNG:H6'1	2.52	0.45
4:A:205:PG4:H41	4:A:205:PG4:H61	1.60	0.45
1:B:131:ILE:HG12	5:B:219:PEG:H11	1.99	0.45
1:B:90:VAL:CG1	7:B:224:P6G:H81	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:202:BNG:H2	2:B:202:BNG:O3	2.17	0.45
7:B:226:P6G:H61	7:B:226:P6G:H92	1.70	0.45
1:A:16:PHE:CD1	1:A:17:MET:CE	3.00	0.44
1:B:54:THR:CG2	5:B:221:PEG:H41	2.48	0.44
5:B:216:PEG:H21	5:B:218:PEG:H42	2.00	0.44
1:B:54:THR:HG21	5:B:221:PEG:H41	2.00	0.44
1:A:10:LEU:CD2	4:A:211:PG4:H32	2.48	0.43
5:B:210:PEG:H22	8:B:222:1PE:H222	2.00	0.43
1:B:35:ILE:HD13	2:B:201:BNG:C3'	2.47	0.43
5:B:210:PEG:H22	8:B:222:1PE:C23	2.48	0.43
2:A:202:BNG:H6'2	2:B:202:BNG:H4'2	2.00	0.43
7:A:221:P6G:H111	7:A:221:P6G:H141	1.83	0.43
1:A:46:LEU:CD2	7:A:220[A]:P6G:H141	2.48	0.42
1:A:140:GLY:O	9:A:338:HOH:O	2.21	0.42
5:B:216:PEG:H32	5:B:216:PEG:H11	1.82	0.42
6:A:217:PG0:H11	6:A:217:PG0:H32	1.18	0.42
1:B:72:HIS:ND1	9:B:371:HOH:O	2.37	0.42
1:B:16:PHE:CD1	1:B:17:MET:CE	3.03	0.42
1:A:108:ALA:HB3	1:A:109:PRO:HD3	2.02	0.41
1:B:119:LEU:HD21	5:B:217:PEG:H42	2.01	0.41
4:A:211:PG4:H51	4:A:211:PG4:H32	1.75	0.41
1:A:16:PHE:CD1	1:A:17:MET:HE2	2.56	0.41
4:B:209:PG4:H51	4:B:209:PG4:H31	1.86	0.41
7:A:220[B]:P6G:H62	7:A:220[B]:P6G:H31	1.92	0.41
1:A:107:LEU:N	5:A:213:PEG:H32	2.35	0.40
1:A:141:TRP:NE1	4:A:209:PG4:H81	2.35	0.40
5:B:213:PEG:C4	7:B:226:P6G:H21	2.51	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	175/182 (96%)	171 (98%)	4 (2%)	0	100	100
1	B	175/182 (96%)	173 (99%)	2 (1%)	0	100	100
All	All	350/364 (96%)	344 (98%)	6 (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	141/146 (97%)	139 (99%)	2 (1%)	74	77
1	B	141/146 (97%)	139 (99%)	2 (1%)	74	77
All	All	282/292 (97%)	278 (99%)	4 (1%)	74	77

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	66	LEU
1	B	11	LEU
1	B	171	LYS

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

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

48 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	$\#\|Z\| > 2$
2	BNG	A	201	-	21,21,21	0.88	1 (4%)	26,26,26	1.66	3 (11%)
2	BNG	A	202	-	21,21,21	0.75	0	26,26,26	1.14	3 (11%)
3	26G	A	203	-	19,19,19	1.10	2 (10%)	25,25,25	1.30	3 (12%)
4	PG4	A	204	-	12,12,12	0.71	0	11,11,11	0.38	0
4	PG4	A	205	-	12,12,12	0.72	0	11,11,11	0.48	0
4	PG4	A	206	-	12,12,12	0.73	0	11,11,11	0.43	0
4	PG4	A	207	-	12,12,12	0.73	0	11,11,11	0.30	0
4	PG4	A	208	-	12,12,12	0.73	0	11,11,11	0.35	0
4	PG4	A	209	-	12,12,12	0.77	0	11,11,11	0.24	0
4	PG4	A	210	-	12,12,12	0.72	0	11,11,11	0.38	0
4	PG4	A	211	-	12,12,12	0.74	0	11,11,11	0.36	0
5	PEG	A	212	-	6,6,6	0.53	0	5,5,5	0.55	0
5	PEG	A	213	-	6,6,6	0.57	0	5,5,5	0.56	0
5	PEG	A	214	-	6,6,6	0.56	0	5,5,5	0.34	0
5	PEG	A	215	-	6,6,6	0.57	0	5,5,5	0.49	0
5	PEG	A	216	-	6,6,6	0.54	0	5,5,5	0.56	0
6	PG0	A	217	-	7,7,7	0.31	0	6,6,6	0.43	0
7	P6G	A	218	-	18,18,18	0.83	0	17,17,17	0.34	0
7	P6G	A	219	-	18,18,18	0.75	0	17,17,17	0.31	0
7	P6G	A	220[A]	-	18,18,18	0.73	0	17,17,17	0.26	0
7	P6G	A	220[B]	-	18,18,18	0.75	0	17,17,17	0.21	0
7	P6G	A	221	-	18,18,18	0.70	0	17,17,17	0.44	0
2	BNG	B	201	-	21,21,21	0.81	0	26,26,26	1.04	2 (7%)
2	BNG	B	202	-	21,21,21	0.75	0	26,26,26	1.36	4 (15%)
2	BNG	B	203	-	21,21,21	0.85	0	26,26,26	1.39	2 (7%)
2	BNG	B	204	-	21,21,21	0.84	0	26,26,26	1.16	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BNG	B	205	-	21,21,21	0.85	0	26,26,26	0.87	1 (3%)
3	26G	B	206	-	19,19,19	1.01	2 (10%)	25,25,25	1.21	2 (8%)
4	PG4	B	207	-	12,12,12	0.76	0	11,11,11	0.35	0
4	PG4	B	208	-	12,12,12	0.75	0	11,11,11	0.36	0
4	PG4	B	209	-	12,12,12	0.74	0	11,11,11	0.34	0
5	PEG	B	210	-	6,6,6	0.56	0	5,5,5	0.39	0
5	PEG	B	211	-	6,6,6	0.61	0	5,5,5	0.32	0
5	PEG	B	212	-	6,6,6	0.55	0	5,5,5	0.41	0
5	PEG	B	213	-	6,6,6	0.58	0	5,5,5	0.77	0
5	PEG	B	214	-	6,6,6	0.56	0	5,5,5	0.30	0
5	PEG	B	215	-	6,6,6	0.55	0	5,5,5	0.30	0
5	PEG	B	216	-	6,6,6	0.55	0	5,5,5	0.48	0
5	PEG	B	217	-	6,6,6	0.54	0	5,5,5	0.42	0
5	PEG	B	218	-	6,6,6	0.55	0	5,5,5	0.42	0
5	PEG	B	219	-	6,6,6	0.56	0	5,5,5	0.43	0
5	PEG	B	220	-	6,6,6	0.58	0	5,5,5	0.31	0
5	PEG	B	221	-	6,6,6	0.57	0	5,5,5	0.44	0
8	1PE	B	222	-	15,15,15	0.71	0	14,14,14	0.45	0
6	PG0	B	223	-	7,7,7	0.34	0	6,6,6	0.29	0
7	P6G	B	224	-	18,18,18	0.77	0	17,17,17	0.25	0
7	P6G	B	225	-	18,18,18	0.72	0	17,17,17	0.33	0
7	P6G	B	226	-	18,18,18	0.78	0	17,17,17	0.25	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	BNG	A	201	-	-	0/12/32/32	0/1/1/1
2	BNG	A	202	-	-	0/12/32/32	0/1/1/1
3	26G	A	203	-	-	0/7/7/7	0/2/2/2
4	PG4	A	204	-	-	0/10/10/10	0/0/0/0
4	PG4	A	205	-	-	0/10/10/10	0/0/0/0
4	PG4	A	206	-	-	0/10/10/10	0/0/0/0
4	PG4	A	207	-	-	0/10/10/10	0/0/0/0
4	PG4	A	208	-	-	0/10/10/10	0/0/0/0
4	PG4	A	209	-	-	0/10/10/10	0/0/0/0
4	PG4	A	210	-	-	0/10/10/10	0/0/0/0
4	PG4	A	211	-	-	0/10/10/10	0/0/0/0
5	PEG	A	212	-	-	0/4/4/4	0/0/0/0
5	PEG	A	213	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	A	214	-	-	0/4/4/4	0/0/0/0
5	PEG	A	215	-	-	0/4/4/4	0/0/0/0
5	PEG	A	216	-	-	0/4/4/4	0/0/0/0
6	PG0	A	217	-	-	0/5/5/5	0/0/0/0
7	P6G	A	218	-	-	0/16/16/16	0/0/0/0
7	P6G	A	219	-	-	0/16/16/16	0/0/0/0
7	P6G	A	220[A]	-	-	0/16/16/16	0/0/0/0
7	P6G	A	220[B]	-	-	0/16/16/16	0/0/0/0
7	P6G	A	221	-	-	0/16/16/16	0/0/0/0
2	BNG	B	201	-	-	0/12/32/32	0/1/1/1
2	BNG	B	202	-	-	0/12/32/32	0/1/1/1
2	BNG	B	203	-	-	0/12/32/32	0/1/1/1
2	BNG	B	204	-	-	0/12/32/32	0/1/1/1
2	BNG	B	205	-	-	0/12/32/32	0/1/1/1
3	26G	B	206	-	-	0/7/7/7	0/2/2/2
4	PG4	B	207	-	-	0/10/10/10	0/0/0/0
4	PG4	B	208	-	-	0/10/10/10	0/0/0/0
4	PG4	B	209	-	-	0/10/10/10	0/0/0/0
5	PEG	B	210	-	-	0/4/4/4	0/0/0/0
5	PEG	B	211	-	-	0/4/4/4	0/0/0/0
5	PEG	B	212	-	-	0/4/4/4	0/0/0/0
5	PEG	B	213	-	-	0/4/4/4	0/0/0/0
5	PEG	B	214	-	-	0/4/4/4	0/0/0/0
5	PEG	B	215	-	-	0/4/4/4	0/0/0/0
5	PEG	B	216	-	-	0/4/4/4	0/0/0/0
5	PEG	B	217	-	-	0/4/4/4	0/0/0/0
5	PEG	B	218	-	-	0/4/4/4	0/0/0/0
5	PEG	B	219	-	-	0/4/4/4	0/0/0/0
5	PEG	B	220	-	-	0/4/4/4	0/0/0/0
5	PEG	B	221	-	-	0/4/4/4	0/0/0/0
8	1PE	B	222	-	-	0/13/13/13	0/0/0/0
6	PG0	B	223	-	-	0/5/5/5	0/0/0/0
7	P6G	B	224	-	-	0/16/16/16	0/0/0/0
7	P6G	B	225	-	-	0/16/16/16	0/0/0/0
7	P6G	B	226	-	-	0/16/16/16	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	BNG	O1-C1	2.18	1.44	1.40
3	B	206	26G	C6A-C5A	2.25	1.42	1.37
3	A	203	26G	C6A-C5A	2.38	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	206	26G	C4A-N4A	2.84	1.41	1.34
3	A	203	26G	C4A-N4A	2.97	1.41	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	BNG	C1-O5-C5	-3.80	106.36	113.75
2	B	202	BNG	C1-O5-C5	-3.45	107.05	113.75
2	B	204	BNG	C1-O5-C5	-3.33	107.29	113.75
2	B	203	BNG	C1-O5-C5	-3.23	107.47	113.75
3	A	203	26G	C5A-C6A-N1A	-3.17	118.36	123.86
2	B	201	BNG	C6-C5-C4	-2.56	106.69	113.02
3	B	206	26G	C5A-C6A-N1A	-2.50	119.52	123.86
2	B	205	BNG	C6-C5-C4	-2.30	107.33	113.02
2	B	201	BNG	C6'-C5'-C4'	-2.14	103.50	114.53
2	B	204	BNG	C6-C5-C4	-2.11	107.80	113.02
2	B	202	BNG	O5-C5-C4	-2.03	105.87	109.68
2	A	202	BNG	O5-C5-C6	2.02	111.45	106.36
3	A	203	26G	N4A-C4A-N3A	2.14	120.04	116.95
2	B	202	BNG	O5-C5-C6	2.29	112.14	106.36
2	A	202	BNG	C1-C2-C3	2.37	114.64	109.97
2	A	202	BNG	C1'-O1-C1	2.37	118.09	113.94
2	A	201	BNG	C1'-O1-C1	2.45	118.23	113.94
3	B	206	26G	C6A-N1A-C2A	2.85	120.75	115.77
3	A	203	26G	C6A-N1A-C2A	2.95	120.93	115.77
2	B	202	BNG	O1-C1-C2	3.02	111.86	108.04
2	B	203	BNG	O1-C1-C2	4.53	113.77	108.04
2	A	201	BNG	O1-C1-C2	6.19	115.85	108.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

38 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	BNG	1	0
2	A	202	BNG	4	0
4	A	204	PG4	2	0
4	A	205	PG4	2	0
4	A	206	PG4	2	0
4	A	208	PG4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	209	PG4	3	0
4	A	210	PG4	4	0
4	A	211	PG4	7	0
5	A	213	PEG	6	0
5	A	214	PEG	1	0
5	A	216	PEG	2	0
6	A	217	PG0	3	0
7	A	218	P6G	3	0
7	A	219	P6G	1	0
7	A	220[A]	P6G	3	0
7	A	220[B]	P6G	1	0
7	A	221	P6G	1	0
2	B	201	BNG	5	0
2	B	202	BNG	3	0
2	B	203	BNG	1	0
3	B	206	26G	1	0
4	B	207	PG4	1	0
4	B	209	PG4	10	0
5	B	210	PEG	3	0
5	B	212	PEG	2	0
5	B	213	PEG	2	0
5	B	214	PEG	2	0
5	B	216	PEG	3	0
5	B	217	PEG	4	0
5	B	218	PEG	1	0
5	B	219	PEG	2	0
5	B	220	PEG	2	0
5	B	221	PEG	2	0
8	B	222	1PE	3	0
7	B	224	P6G	2	0
7	B	225	P6G	2	0
7	B	226	P6G	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	176/182 (96%)	-0.40	0	100	100	13, 29, 51, 71	0
1	B	177/182 (97%)	-0.38	0	100	100	15, 29, 54, 73	1 (0%)
All	All	353/364 (96%)	-0.39	0	100	100	13, 29, 52, 73	1 (0%)

There are no RSRZ outliers to report.

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	PG4	B	207	13/13	0.73	0.24	48.92	52,61,69,73	13
5	PEG	A	214	7/7	0.75	0.57	44.09	77,80,83,85	0
5	PEG	B	214	7/7	0.80	0.33	40.21	67,72,73,75	0
7	P6G	B	224	19/19	0.88	0.38	38.11	49,69,79,82	0
7	P6G	A	220[A]	19/19	0.91	0.33	22.65	35,54,60,60	19

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	P6G	B	226	19/19	0.81	0.33	21.14	69,79,92,94	0
7	P6G	A	220[B]	19/19	0.91	0.33	20.06	41,55,60,60	19
7	P6G	A	219	19/19	0.86	0.28	18.82	51,63,74,79	0
5	PEG	B	221	7/7	0.89	0.27	17.66	64,67,71,73	0
4	PG4	B	209	13/13	0.82	0.28	17.55	46,60,68,69	0
4	PG4	A	205	13/13	0.80	0.24	15.35	36,54,74,77	0
5	PEG	A	215	7/7	0.90	0.55	14.36	46,51,60,61	7
4	PG4	A	206	13/13	0.73	0.31	13.11	47,73,82,87	0
2	BNG	A	201	21/21	0.87	0.20	11.86	55,70,79,81	21
4	PG4	A	207	13/13	0.74	0.22	11.52	52,68,74,75	0
4	PG4	A	204	13/13	0.83	0.31	10.33	64,71,78,80	0
7	P6G	B	225	19/19	0.93	0.16	10.17	34,47,78,79	0
4	PG4	A	210	13/13	0.81	0.31	9.33	44,58,83,85	0
6	PG0	A	217	8/8	0.81	0.16	8.99	26,46,54,55	0
4	PG4	B	208	13/13	0.71	0.28	8.14	45,75,85,85	0
4	PG4	A	211	13/13	0.87	0.24	8.14	55,64,75,75	0
2	BNG	B	203	21/21	0.70	0.23	6.85	45,59,78,82	0
7	P6G	A	218	19/19	0.92	0.16	5.41	55,64,70,71	0
2	BNG	A	202	21/21	0.84	0.17	5.10	34,50,88,94	0
5	PEG	A	213	7/7	0.92	0.20	4.96	33,43,48,51	0
5	PEG	B	210	7/7	0.94	0.15	4.14	54,56,58,60	0
7	P6G	A	221	19/19	0.94	0.14	3.95	29,48,72,73	0
2	BNG	B	204	21/21	0.94	0.14	3.90	27,48,63,75	0
8	1PE	B	222	16/16	0.91	0.14	3.70	33,81,86,86	0
5	PEG	B	213	7/7	0.92	0.17	3.04	37,54,63,65	0
2	BNG	B	201	21/21	0.95	0.13	1.51	18,31,42,51	0
2	BNG	B	202	21/21	0.93	0.13	1.48	28,52,63,63	0
5	PEG	B	216	7/7	0.86	0.12	0.87	43,67,82,84	0
4	PG4	A	208	13/13	0.86	0.13	0.87	45,84,90,91	0
2	BNG	B	205	21/21	0.94	0.13	0.60	35,46,67,70	0
3	26G	A	203	18/18	0.97	0.10	-0.09	15,21,38,45	0
3	26G	B	206	18/18	0.98	0.09	-1.02	14,21,39,45	0
5	PEG	B	212	7/7	0.65	0.40	-	69,71,75,75	0
5	PEG	B	215	7/7	0.78	0.20	-	55,62,78,79	0
6	PG0	B	223	8/8	0.57	0.30	-	68,76,77,82	0
5	PEG	A	216	7/7	0.75	0.10	-	59,68,74,74	0
5	PEG	B	219	7/7	0.69	0.29	-	63,71,78,78	0
5	PEG	B	211	7/7	0.82	0.14	-	49,54,75,78	0
5	PEG	A	212	7/7	0.93	0.14	-	37,46,60,72	0
4	PG4	A	209	13/13	0.83	0.10	-	48,71,82,85	0
5	PEG	B	220	7/7	0.74	0.17	-	59,66,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	PEG	B	217	7/7	0.90	0.26	-	66,71,74,75	0
5	PEG	B	218	7/7	0.80	0.27	-	75,78,86,90	0

6.5 Other polymers (i)

There are no such residues in this entry.