



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:42 PM GMT

PDB ID : 4POP  
Title : ThiT with LMG139 bound  
Authors : Swier, L.J.Y.M.; Guskov, A.; Slotboom, D.J.  
Deposited on : 2014-02-26  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (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

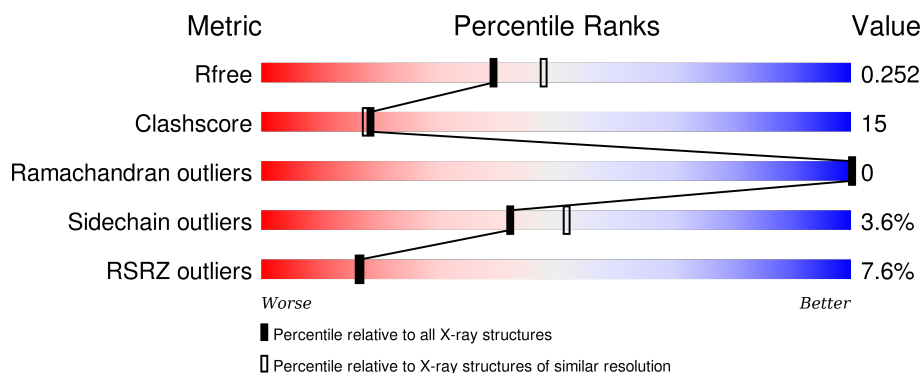
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	192	
1	B	192	

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
10	P33	B	222	-	-	-	X
3	PG0	A	203	-	-	-	X
4	BNG	A	205	-	-	-	X
4	BNG	A	206	-	-	-	X
4	BNG	B	204	-	-	-	X
5	PEG	A	211	-	-	-	X
5	PEG	A	215	-	-	X	-
5	PEG	B	207	-	-	-	X
5	PEG	B	210	-	-	-	X
5	PEG	B	215	-	-	X	-
6	PG4	A	217	-	-	-	X
6	PG4	A	220	-	-	X	X
6	PG4	B	218	-	-	X	-
7	1PE	A	222	-	-	X	-
8	PGE	A	223	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 3367 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.

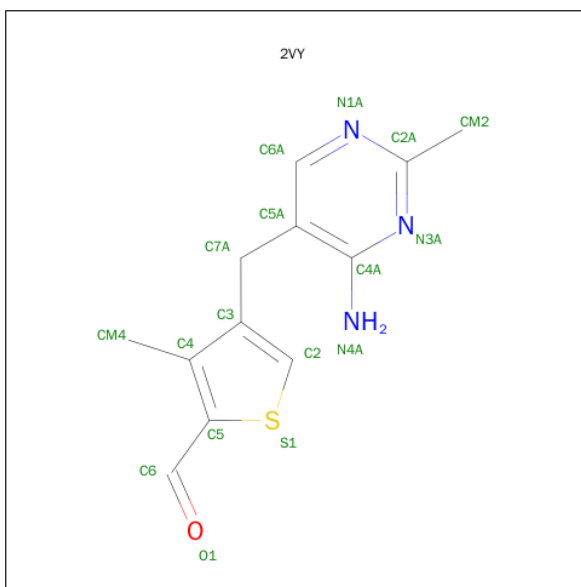
- Molecule 1 is a protein called Thiamine transporter ThiT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	0	0
			1377	945	214	215	3			
1	B	176	Total	C	N	O	S	0	1	0
			1375	941	215	216	3			

There are 20 discrepancies between the modelled and reference sequences:

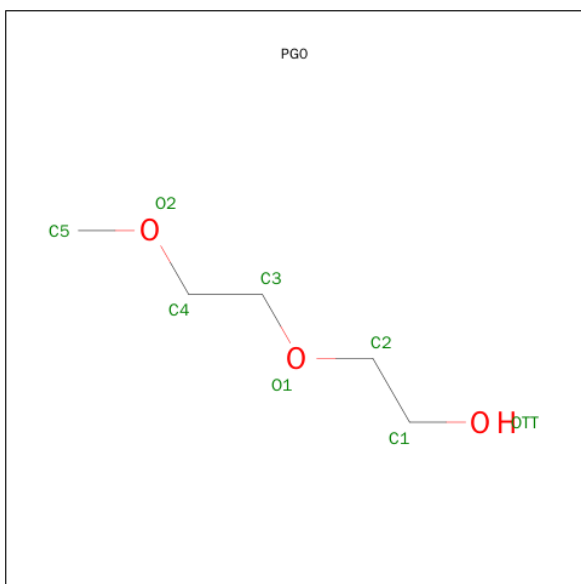
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	INITIATING METHIONINE	UNP A2RI47
A	-8	HIS	-	EXPRESSION TAG	UNP A2RI47
A	-7	HIS	-	EXPRESSION TAG	UNP A2RI47
A	-6	HIS	-	EXPRESSION TAG	UNP A2RI47
A	-5	HIS	-	EXPRESSION TAG	UNP A2RI47
A	-4	HIS	-	EXPRESSION TAG	UNP A2RI47
A	-3	HIS	-	EXPRESSION TAG	UNP A2RI47
A	-2	HIS	-	EXPRESSION TAG	UNP A2RI47
A	-1	HIS	-	EXPRESSION TAG	UNP A2RI47
A	0	ALA	-	EXPRESSION TAG	UNP A2RI47
B	-9	MET	-	INITIATING METHIONINE	UNP A2RI47
B	-8	HIS	-	EXPRESSION TAG	UNP A2RI47
B	-7	HIS	-	EXPRESSION TAG	UNP A2RI47
B	-6	HIS	-	EXPRESSION TAG	UNP A2RI47
B	-5	HIS	-	EXPRESSION TAG	UNP A2RI47
B	-4	HIS	-	EXPRESSION TAG	UNP A2RI47
B	-3	HIS	-	EXPRESSION TAG	UNP A2RI47
B	-2	HIS	-	EXPRESSION TAG	UNP A2RI47
B	-1	HIS	-	EXPRESSION TAG	UNP A2RI47
B	0	ALA	-	EXPRESSION TAG	UNP A2RI47

- Molecule 2 is 4-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-3-METHYLTHIOPHENE-2-CARBALDEHYDE (three-letter code: 2VY) (formula: C<sub>12</sub>H<sub>13</sub>N<sub>3</sub>OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			17	12	3	1	1		
2	B	1	Total	C	N	O	S	0	0
			17	12	3	1	1		

- Molecule 3 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: C<sub>5</sub>H<sub>12</sub>O<sub>3</sub>).



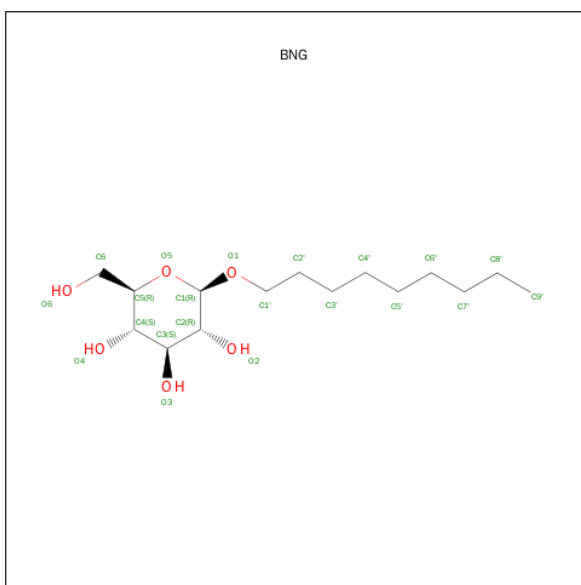
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	5	3		

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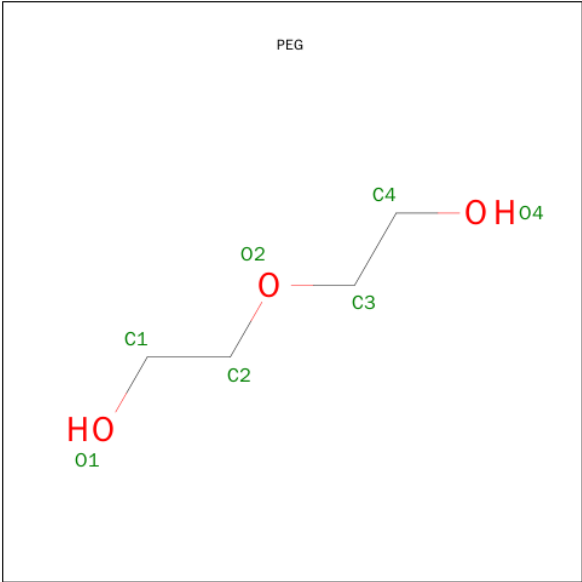
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	5	3		
3	B	1	Total	C	O	0	0
			8	5	3		

- Molecule 4 is SUGAR (B-NONYLGLUCOSIDE) (three-letter code: BNG) (formula: C<sub>15</sub>H<sub>30</sub>O<sub>6</sub>).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



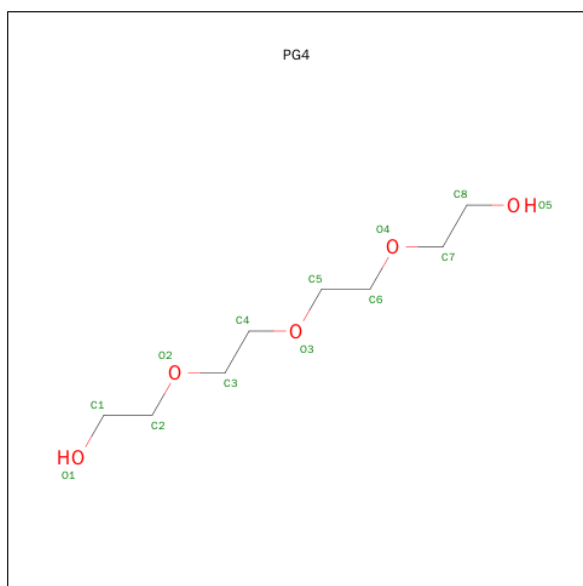
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total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

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

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



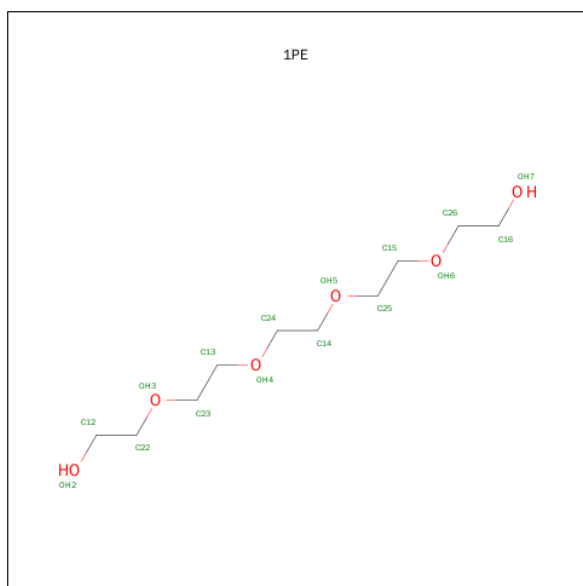
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		

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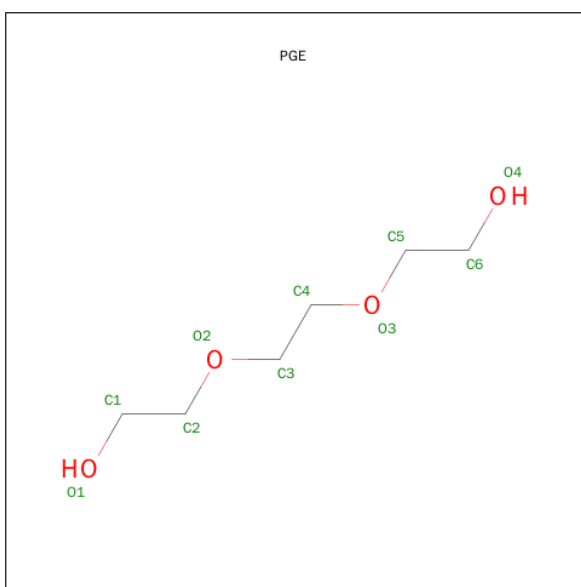
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	8	5		
6	B	1	Total	C	O	0	0
			13	8	5		
6	B	1	Total	C	O	0	0
			13	8	5		
6	B	1	Total	C	O	0	0
			13	8	5		
6	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



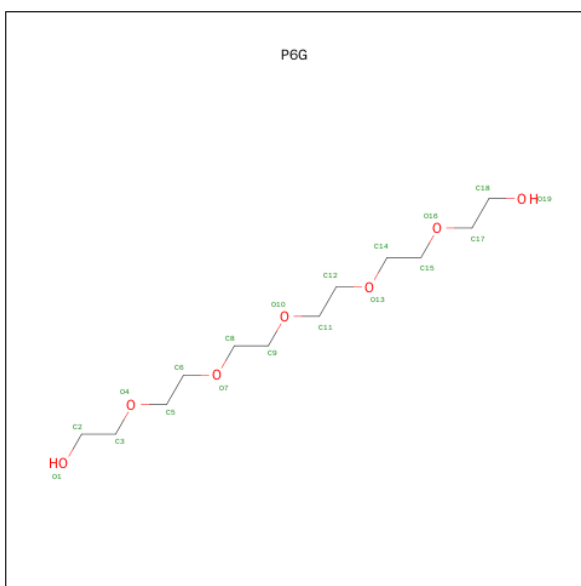
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			16	10	6		
7	A	1	Total	C	O	0	0
			16	10	6		
7	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



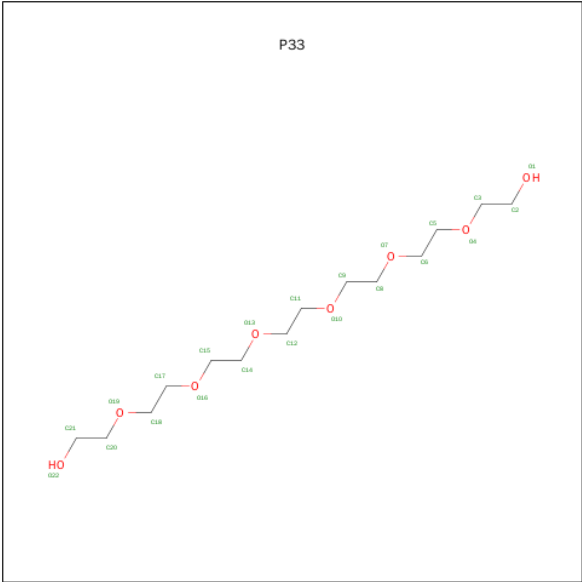
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 10 is 3,6,9,12,15,18-HEXA OXAICOSANE-1,20-DIOL (three-letter code: P33) (formula:  $C_{14}H_{30}O_8$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			22	14	8		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	43	Total	O	0	1
			44	44		
11	B	45	Total	O	0	0
			45	45		



- Molecule 1: Thiamine transporter ThiT



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.61Å 84.12Å 127.15Å 90.00° 95.13° 90.00°	Depositor
Resolution (Å)	47.77 – 2.20 47.77 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.77-2.20) 99.2 (47.77-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.199 , 0.248 0.209 , 0.252	Depositor DCC
$R_{free}$ test set	1660 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.2	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 64.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 33184 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3367	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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: PGE, PG0, 1PE, PG4, P6G, P33, 2VY, 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	0.66	0/1416	0.66	0/1930
1	B	0.62	0/1413	0.63	0/1926
All	All	0.64	0/2829	0.64	0/3856

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	1377	0	1471	38	0
1	B	1375	0	1469	23	0
2	A	17	0	13	0	0
2	B	17	0	13	0	0
3	A	16	0	24	2	0
3	B	8	0	12	0	0
4	A	63	0	90	9	0
4	B	42	0	60	5	0
5	A	70	0	90	26	0
5	B	77	0	100	25	0
6	A	52	0	72	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	65	0	90	21	0
7	A	32	0	44	7	0
7	B	16	0	22	2	0
8	A	10	0	14	1	0
9	A	19	0	26	7	0
10	B	22	0	30	2	0
11	A	44	0	0	3	0
11	B	45	0	0	3	0
All	All	3367	0	3640	107	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 15.

All (107) 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)
5:A:215:PEG:H31	9:A:224:P6G:H121	1.43	0.98
4:A:206:BNG:O3	6:A:220:PG4:H21	1.73	0.87
6:B:218:PG4:H61	6:B:218:PG4:H32	1.54	0.87
5:B:215:PEG:O4	6:B:218:PG4:H52	1.77	0.85
7:A:222:1PE:H141	6:B:216:PG4:H32	1.56	0.85
5:A:215:PEG:H31	9:A:224:P6G:C12	2.11	0.81
4:A:206:BNG:H4	6:A:220:PG4:H51	1.65	0.78
5:B:215:PEG:H31	6:B:218:PG4:O3	1.83	0.78
1:A:171:LYS:HD2	5:A:210:PEG:H21	1.67	0.77
1:B:30:THR:HG21	5:B:215:PEG:H42	1.67	0.74
1:A:145:ALA:CB	6:A:220:PG4:H31	2.19	0.72
5:A:215:PEG:C3	9:A:224:P6G:H121	2.17	0.72
4:A:206:BNG:H62	6:A:220:PG4:H61	1.72	0.72
6:B:218:PG4:C6	6:B:218:PG4:H32	2.21	0.71
1:B:179:HIS:CE1	5:B:214:PEG:H41	2.25	0.71
1:A:142:GLY:H	6:A:220:PG4:H32	1.56	0.70
1:A:120:LEU:HB2	7:A:222:1PE:H122	1.76	0.67
1:B:138:TRP:CD2	5:B:207:PEG:H32	2.30	0.67
1:A:36:ILE:HG21	5:A:215:PEG:H11	1.77	0.67
4:B:204:BNG:H5	11:B:339:HOH:O	1.94	0.67
1:A:171:LYS:NZ	11:A:327:HOH:O	2.27	0.67
1:A:116:VAL:HG13	7:A:222:1PE:H221	1.77	0.66
5:B:215:PEG:H22	6:B:218:PG4:C4	2.25	0.66
5:B:209:PEG:H42	5:B:215:PEG:H32	1.78	0.65
1:B:138:TRP:CG	5:B:207:PEG:H32	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ILE:HG21	5:A:213:PEG:H21	1.78	0.65
5:B:209:PEG:C4	5:B:215:PEG:H32	2.29	0.63
1:A:74:TYR:CZ	5:A:207:PEG:H41	2.36	0.61
1:A:145:ALA:HB2	6:A:220:PG4:H22	1.83	0.61
1:A:142:GLY:N	6:A:220:PG4:H32	2.16	0.60
5:B:215:PEG:H22	6:B:218:PG4:O3	2.01	0.60
1:A:167:ILE:CG2	5:A:209:PEG:H11	2.32	0.60
1:B:119:LEU:HA	6:B:217:PG4:H81	1.84	0.60
4:A:206:BNG:C6	6:A:220:PG4:H61	2.32	0.59
4:B:203:BNG:H9'3	5:B:205:PEG:H11	1.83	0.59
1:A:34:TRP:CE2	5:A:215:PEG:H32	2.38	0.59
5:B:215:PEG:H31	6:B:218:PG4:C5	2.34	0.57
1:B:91:SER:HA	5:B:210:PEG:H22	1.86	0.57
1:A:172:LYS:NZ	5:A:216:PEG:H21	2.19	0.57
5:A:215:PEG:H31	9:A:224:P6G:C11	2.34	0.56
1:A:145:ALA:HB2	6:A:220:PG4:H31	1.87	0.56
1:A:98:PHE:CE2	1:A:112:LEU:HD13	2.41	0.56
1:B:106:LYS:NZ	11:B:318:HOH:O	2.37	0.56
1:A:29:ASN:HA	8:A:223:PGE:H12	1.86	0.56
4:A:206:BNG:H2	6:A:220:PG4:H22	1.87	0.56
7:A:222:1PE:C14	6:B:216:PG4:H32	2.31	0.56
1:B:71:GLY:N	7:B:221:1PE:H261	2.20	0.56
1:A:10:LEU:HD21	5:A:211:PEG:H41	1.87	0.55
1:A:142:GLY:H	6:A:220:PG4:C3	2.19	0.55
5:B:215:PEG:H21	6:B:218:PG4:H71	1.90	0.54
1:A:120:LEU:HD13	7:A:222:1PE:H121	1.90	0.54
1:A:30:THR:OG1	5:A:215:PEG:H12	2.09	0.52
1:A:75:ILE:HG21	4:A:205:BNG:H2'2	1.92	0.52
1:A:36:ILE:CG2	5:A:215:PEG:H11	2.39	0.52
1:B:83:LEU:HD23	1:B:128:ALA:HB2	1.92	0.52
1:A:168:ILE:CG2	5:A:213:PEG:H21	2.39	0.51
4:A:206:BNG:H62	6:A:220:PG4:C6	2.39	0.51
1:A:34:TRP:CZ2	5:A:215:PEG:H32	2.46	0.51
4:B:203:BNG:H61	4:B:204:BNG:H1'2	1.93	0.50
6:B:218:PG4:O4	6:B:218:PG4:H42	2.12	0.50
1:B:30:THR:OG1	6:B:218:PG4:O5	2.28	0.50
1:A:167:ILE:HG22	5:A:209:PEG:H11	1.94	0.49
1:A:116:VAL:CG1	7:A:222:1PE:H221	2.42	0.49
1:A:9:ARG:NH1	1:A:13:GLU:OE2	2.46	0.49
1:B:74:TYR:CZ	6:B:218:PG4:H61	2.49	0.48
5:A:215:PEG:H31	9:A:224:P6G:H112	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:TRP:NE1	6:B:216:PG4:H31	2.28	0.48
4:B:203:BNG:C9'	5:B:205:PEG:H11	2.44	0.48
1:B:7:ASN:N	5:B:214:PEG:H31	2.29	0.47
1:B:91:SER:HB2	5:B:210:PEG:H11	1.97	0.47
1:B:71:GLY:CA	7:B:221:1PE:H261	2.45	0.47
4:A:206:BNG:C4	6:A:220:PG4:H51	2.41	0.46
4:A:206:BNG:H62	6:A:220:PG4:H51	1.97	0.46
5:B:215:PEG:H21	6:B:218:PG4:C7	2.44	0.46
4:B:203:BNG:H9'3	5:B:205:PEG:C1	2.46	0.46
1:A:145:ALA:CB	6:A:220:PG4:C3	2.92	0.46
5:A:216:PEG:H22	5:A:216:PEG:H42	1.37	0.46
1:B:180:SER:OG	1:B:181:ASN:O	2.23	0.46
3:A:202:PG0:OTT	6:A:218:PG4:H12	2.16	0.46
1:A:6:PHE:HD1	1:A:7:ASN:H	1.64	0.45
6:B:220:PG4:H62	6:B:220:PG4:H42	1.71	0.45
10:B:222:P33:H31	10:B:222:P33:H81	1.97	0.45
1:A:145:ALA:HB3	6:A:220:PG4:C3	2.46	0.45
5:A:211:PEG:H21	11:A:341:HOH:O	2.16	0.45
1:B:179:HIS:HE1	5:B:214:PEG:H41	1.81	0.45
1:B:179:HIS:O	11:B:336:HOH:O	2.21	0.45
1:A:141:TRP:HA	6:A:220:PG4:H41	1.98	0.45
5:A:208:PEG:H21	5:A:208:PEG:H42	1.58	0.44
1:A:74:TYR:CE2	5:A:207:PEG:H22	2.52	0.44
1:A:148:LEU:HD13	3:A:203:PG0:H41	2.00	0.43
5:A:215:PEG:C4	9:A:224:P6G:H121	2.49	0.43
1:A:71:GLY:HA2	11:A:336:HOH:O	2.19	0.43
5:A:215:PEG:O4	5:A:215:PEG:C2	2.64	0.43
7:A:222:1PE:H152	7:A:222:1PE:H161	1.03	0.42
1:A:167:ILE:HG21	5:A:209:PEG:H11	2.00	0.42
1:B:33:GLY:HA2	5:B:215:PEG:H11	2.01	0.42
5:B:215:PEG:H31	6:B:218:PG4:H52	2.01	0.42
1:A:120:LEU:HD21	6:A:217:PG4:H41	2.02	0.42
6:A:217:PG4:H42	6:A:217:PG4:H61	1.68	0.42
9:A:224:P6G:H142	9:A:224:P6G:H111	1.65	0.41
1:A:172:LYS:HZ2	5:A:216:PEG:H21	1.83	0.41
10:B:222:P33:H31	10:B:222:P33:C8	2.50	0.41
1:B:30:THR:HG21	5:B:215:PEG:C4	2.44	0.41
1:B:31:VAL:O	6:B:220:PG4:H11	2.19	0.41
1:B:74:TYR:CE1	6:B:218:PG4:H32	2.56	0.41
5:B:215:PEG:H22	6:B:218:PG4:H42	1.99	0.40
1:B:33:GLY:HA2	5:B:215:PEG:C1	2.50	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	175/192 (91%)	174 (99%)	1 (1%)	0	100	100
1	B	175/192 (91%)	172 (98%)	3 (2%)	0	100	100
All	All	350/384 (91%)	346 (99%)	4 (1%)	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	141/155 (91%)	135 (96%)	6 (4%)	35	43
1	B	141/155 (91%)	137 (97%)	4 (3%)	51	63
All	All	282/310 (91%)	272 (96%)	10 (4%)	42	53

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PHE
1	A	9	ARG
1	A	11	LEU
1	A	66	LEU
1	A	102	THR

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Mol	Chain	Res	Type
1	A	112	LEU
1	B	7	ASN
1	B	9	ARG
1	B	66	LEU
1	B	175	LYS

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

Mol	Chain	Res	Type
1	A	72	HIS

### 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](#)

46 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	2VY	A	201	-	16,18,18	3.05	5 (31%)	17,25,25	2.88	6 (35%)
3	PG0	A	202	-	7,7,7	0.32	0	6,6,6	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PG0	A	203	-	7,7,7	0.30	0	6,6,6	0.30	0
4	BNG	A	204	-	21,21,21	0.77	0	26,26,26	1.03	1 (3%)
4	BNG	A	205	-	21,21,21	0.75	0	26,26,26	1.24	4 (15%)
4	BNG	A	206	-	21,21,21	0.91	1 (4%)	26,26,26	1.06	2 (7%)
5	PEG	A	207	-	6,6,6	0.58	0	5,5,5	0.49	0
5	PEG	A	208	-	6,6,6	0.55	0	5,5,5	0.48	0
5	PEG	A	209	-	6,6,6	0.58	0	5,5,5	0.34	0
5	PEG	A	210	-	6,6,6	0.54	0	5,5,5	0.58	0
5	PEG	A	211	-	6,6,6	0.56	0	5,5,5	0.43	0
5	PEG	A	212	-	6,6,6	0.55	0	5,5,5	0.65	0
5	PEG	A	213	-	6,6,6	0.54	0	5,5,5	0.42	0
5	PEG	A	214	-	6,6,6	0.56	0	5,5,5	0.40	0
5	PEG	A	215	-	6,6,6	0.56	0	5,5,5	1.58	1 (20%)
5	PEG	A	216	-	6,6,6	0.56	0	5,5,5	0.28	0
6	PG4	A	217	-	12,12,12	0.68	0	11,11,11	0.48	0
6	PG4	A	218	-	12,12,12	0.73	0	11,11,11	0.21	0
6	PG4	A	219	-	12,12,12	0.72	0	11,11,11	0.28	0
6	PG4	A	220	-	12,12,12	0.72	0	11,11,11	0.64	0
7	1PE	A	221	-	15,15,15	0.77	0	14,14,14	0.27	0
7	1PE	A	222	-	15,15,15	0.74	0	14,14,14	0.52	0
8	PGE	A	223	-	9,9,9	0.40	0	8,8,8	0.31	0
9	P6G	A	224	-	18,18,18	0.77	0	17,17,17	0.43	0
2	2VY	B	201	-	16,18,18	3.39	6 (37%)	17,25,25	2.52	9 (52%)
3	PG0	B	202	-	7,7,7	0.27	0	6,6,6	0.20	0
4	BNG	B	203	-	21,21,21	0.77	0	26,26,26	1.00	2 (7%)
4	BNG	B	204	-	21,21,21	0.84	0	26,26,26	1.22	1 (3%)
5	PEG	B	205	-	6,6,6	0.60	0	5,5,5	0.29	0
5	PEG	B	206	-	6,6,6	0.57	0	5,5,5	0.47	0
5	PEG	B	207	-	6,6,6	0.54	0	5,5,5	0.36	0
5	PEG	B	208	-	6,6,6	0.56	0	5,5,5	0.29	0
5	PEG	B	209	-	6,6,6	0.61	0	5,5,5	0.31	0
5	PEG	B	210	-	6,6,6	0.55	0	5,5,5	0.69	0
5	PEG	B	211	-	6,6,6	0.58	0	5,5,5	0.24	0
5	PEG	B	212	-	6,6,6	0.57	0	5,5,5	0.27	0
5	PEG	B	213	-	6,6,6	0.56	0	5,5,5	0.38	0
5	PEG	B	214	-	6,6,6	0.54	0	5,5,5	0.35	0
5	PEG	B	215	-	6,6,6	0.58	0	5,5,5	0.62	0
6	PG4	B	216	-	12,12,12	0.77	0	11,11,11	0.32	0
6	PG4	B	217	-	12,12,12	0.75	0	11,11,11	0.38	0
6	PG4	B	218	-	12,12,12	0.78	0	11,11,11	0.65	0
6	PG4	B	219	-	12,12,12	0.77	0	11,11,11	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	PG4	B	220	-	12,12,12	0.73	0	11,11,11	0.26	0
7	1PE	B	221	-	15,15,15	0.70	0	14,14,14	0.43	0
10	P33	B	222	-	21,21,21	0.93	0	20,20,20	0.38	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	2VY	A	201	-	-	0/3/6/6	0/2/2/2
3	PG0	A	202	-	-	0/5/5/5	0/0/0/0
3	PG0	A	203	-	-	0/5/5/5	0/0/0/0
4	BNG	A	204	-	-	0/12/32/32	0/1/1/1
4	BNG	A	205	-	-	0/12/32/32	0/1/1/1
4	BNG	A	206	-	-	0/12/32/32	0/1/1/1
5	PEG	A	207	-	-	0/4/4/4	0/0/0/0
5	PEG	A	208	-	-	0/4/4/4	0/0/0/0
5	PEG	A	209	-	-	0/4/4/4	0/0/0/0
5	PEG	A	210	-	-	0/4/4/4	0/0/0/0
5	PEG	A	211	-	-	0/4/4/4	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
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	PG4	A	217	-	-	0/10/10/10	0/0/0/0
6	PG4	A	218	-	-	0/10/10/10	0/0/0/0
6	PG4	A	219	-	-	0/10/10/10	0/0/0/0
6	PG4	A	220	-	-	0/10/10/10	0/0/0/0
7	1PE	A	221	-	-	0/13/13/13	0/0/0/0
7	1PE	A	222	-	-	0/13/13/13	0/0/0/0
8	PGE	A	223	-	-	0/7/7/7	0/0/0/0
9	P6G	A	224	-	-	0/16/16/16	0/0/0/0
2	2VY	B	201	-	-	0/3/6/6	0/2/2/2
3	PG0	B	202	-	-	0/5/5/5	0/0/0/0
4	BNG	B	203	-	-	0/12/32/32	0/1/1/1
4	BNG	B	204	-	-	0/12/32/32	0/1/1/1
5	PEG	B	205	-	-	0/4/4/4	0/0/0/0
5	PEG	B	206	-	-	0/4/4/4	0/0/0/0
5	PEG	B	207	-	-	0/4/4/4	0/0/0/0
5	PEG	B	208	-	-	0/4/4/4	0/0/0/0
5	PEG	B	209	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
6	PG4	B	216	-	-	0/10/10/10	0/0/0/0
6	PG4	B	217	-	-	0/10/10/10	0/0/0/0
6	PG4	B	218	-	-	0/10/10/10	0/0/0/0
6	PG4	B	219	-	-	0/10/10/10	0/0/0/0
6	PG4	B	220	-	-	0/10/10/10	0/0/0/0
7	1PE	B	221	-	-	0/13/13/13	0/0/0/0
10	P33	B	222	-	-	0/19/19/19	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	206	BNG	O1-C1	2.07	1.43	1.40
2	A	201	2VY	C6A-C5A	2.12	1.42	1.37
2	B	201	2VY	C6A-N1A	2.21	1.39	1.34
2	A	201	2VY	C5-C6	2.30	1.51	1.48
2	B	201	2VY	C6A-C5A	2.37	1.42	1.37
2	A	201	2VY	C4A-N4A	3.07	1.41	1.34
2	B	201	2VY	C4A-N4A	3.53	1.42	1.34
2	B	201	2VY	C5-C6	3.93	1.53	1.48
2	A	201	2VY	O1-C6	5.80	1.39	1.21
2	B	201	2VY	O1-C6	6.17	1.41	1.21
2	A	201	2VY	C2-C3	9.50	1.42	1.37
2	B	201	2VY	C2-C3	10.04	1.43	1.37

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	2VY	C3-C2-S1	-6.75	105.07	112.26
2	A	201	2VY	O1-C6-C5	-6.52	111.92	125.13
2	B	201	2VY	O1-C6-C5	-6.38	112.21	125.13
2	B	201	2VY	C3-C2-S1	-3.95	108.05	112.26
4	B	204	BNG	C1-O5-C5	-3.49	106.97	113.75
2	A	201	2VY	C5A-C6A-N1A	-3.42	117.92	123.86
4	A	205	BNG	C1'-O1-C1	-3.01	108.68	113.94
2	B	201	2VY	C5A-C6A-N1A	-2.91	118.80	123.86
4	A	204	BNG	C1-O5-C5	-2.58	108.74	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	2VY	CM4-C4-C3	-2.57	119.87	125.24
5	A	215	PEG	O2-C3-C4	-2.55	98.69	110.43
4	A	205	BNG	C1-O5-C5	-2.42	109.05	113.75
4	B	203	BNG	C4-C3-C2	-2.40	106.31	110.79
4	A	205	BNG	C1-C2-C3	-2.38	105.27	109.97
4	A	206	BNG	C3-C4-C5	-2.34	106.11	110.20
4	A	206	BNG	C1-O5-C5	-2.29	109.29	113.75
4	A	205	BNG	C4-C3-C2	-2.19	106.71	110.79
2	B	201	2VY	C5A-C4A-N3A	-2.15	117.65	121.23
2	A	201	2VY	CM4-C4-C3	-2.11	120.83	125.24
4	B	203	BNG	C1-O5-C5	-2.05	109.77	113.75
2	A	201	2VY	C6A-C5A-C4A	2.02	118.62	115.72
2	B	201	2VY	C6A-C5A-C4A	2.15	118.81	115.72
2	B	201	2VY	C6A-N1A-C2A	2.19	119.61	115.77
2	B	201	2VY	C2A-N3A-C4A	2.37	122.90	118.19
2	B	201	2VY	N4A-C4A-N3A	2.56	120.67	116.95
2	A	201	2VY	C6A-N1A-C2A	3.42	121.75	115.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

32 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202	PG0	1	0
3	A	203	PG0	1	0
4	A	205	BNG	1	0
4	A	206	BNG	8	0
5	A	207	PEG	2	0
5	A	208	PEG	1	0
5	A	209	PEG	3	0
5	A	210	PEG	1	0
5	A	211	PEG	2	0
5	A	213	PEG	2	0
5	A	215	PEG	12	0
5	A	216	PEG	3	0
6	A	217	PG4	2	0
6	A	218	PG4	1	0
6	A	220	PG4	17	0
7	A	222	1PE	7	0
8	A	223	PGE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	224	P6G	7	0
4	B	203	BNG	4	0
4	B	204	BNG	2	0
5	B	205	PEG	3	0
5	B	207	PEG	2	0
5	B	209	PEG	2	0
5	B	210	PEG	2	0
5	B	214	PEG	3	0
5	B	215	PEG	15	0
6	B	216	PG4	3	0
6	B	217	PG4	1	0
6	B	218	PG4	15	0
6	B	220	PG4	2	0
7	B	221	1PE	2	0
10	B	222	P33	2	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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	177/192 (92%)	0.43	9 (5%) 32 31	31, 48, 75, 104	0
1	B	176/192 (91%)	0.55	18 (10%) 9 8	32, 50, 86, 115	0
All	All	353/384 (91%)	0.49	27 (7%) 17 16	31, 49, 80, 115	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	182	TYR	4.3
1	B	79	SER	4.2
1	B	16	PHE	4.0
1	A	131	ILE	3.7
1	A	79	SER	3.7
1	B	9	ARG	3.7
1	A	160	ILE	3.5
1	A	181	ASN	3.4
1	B	35	ILE	3.3
1	A	182	TYR	3.2
1	B	78	LEU	3.0
1	B	156	ILE	2.8
1	B	157	LEU	2.8
1	B	160	ILE	2.7
1	B	132	PHE	2.6
1	A	159	ALA	2.6
1	A	33	GLY	2.5
1	B	159	ALA	2.5
1	B	176	LEU	2.5
1	B	171	LYS	2.4
1	B	36	ILE	2.3
1	B	175	LYS	2.3
1	A	111	LEU	2.2
1	B	77	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	180	SER	2.1
1	B	170	VAL	2.1
1	B	92	LEU	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 carbohydrates 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. 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	PGE	A	223	10/10	0.35	0.36	6.48	80,98,121,162	0
3	PG0	A	203	8/8	0.60	0.27	5.44	74,93,111,113	0
4	BNG	A	205	21/21	0.77	0.35	4.89	50,78,92,100	0
5	PEG	B	210	7/7	0.84	0.28	4.56	70,89,90,91	0
6	PG4	A	217	13/13	0.91	0.21	4.55	73,77,96,97	0
5	PEG	A	211	7/7	0.64	0.20	4.40	76,88,95,98	0
4	BNG	A	206	21/21	0.32	0.33	3.85	46,88,105,109	0
4	BNG	B	204	21/21	0.80	0.32	3.82	45,69,86,88	0
10	P33	B	222	22/22	0.72	0.38	3.51	42,58,92,108	22
5	PEG	B	207	7/7	0.62	0.36	2.78	66,68,76,78	0
6	PG4	A	220	13/13	0.62	0.22	2.25	46,92,136,167	0
7	1PE	A	221	16/16	0.72	0.24	2.00	67,96,107,111	0
5	PEG	B	214	7/7	0.85	0.40	1.83	63,87,103,134	0
6	PG4	B	217	13/13	0.82	0.28	1.75	44,73,102,103	0
7	1PE	A	222	16/16	0.79	0.20	1.53	57,73,107,110	0
6	PG4	B	220	13/13	0.59	0.20	1.50	83,90,120,120	0
7	1PE	B	221	16/16	0.80	0.17	1.40	73,96,111,117	0
4	BNG	B	203	21/21	0.78	0.21	1.40	53,68,81,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PEG	B	205	7/7	0.88	0.20	1.32	57,66,76,84	0
6	PG4	B	216	13/13	0.81	0.19	0.84	60,73,91,97	0
5	PEG	A	215	7/7	0.87	0.21	0.71	46,53,70,80	0
3	PG0	B	202	8/8	0.79	0.21	0.43	78,82,96,107	0
2	2VY	B	201	17/17	0.92	0.16	0.20	27,41,53,63	0
6	PG4	B	218	13/13	0.74	0.17	0.20	58,72,82,91	0
2	2VY	A	201	17/17	0.95	0.14	-0.12	27,37,51,57	0
5	PEG	B	206	7/7	0.88	0.17	-0.72	65,77,82,85	0
3	PG0	A	202	8/8	0.21	0.31	-	85,103,127,162	0
5	PEG	A	210	7/7	0.76	0.23	-	107,110,163,179	0
4	BNG	A	204	21/21	0.63	0.28	-	49,95,118,123	0
9	P6G	A	224	19/19	0.69	0.16	-	44,87,137,195	0
6	PG4	A	219	13/13	0.67	0.18	-	95,105,118,120	13
6	PG4	B	219	13/13	0.65	0.24	-	73,99,111,111	0
5	PEG	B	208	7/7	0.65	0.33	-	90,95,111,119	0
5	PEG	A	216	7/7	0.45	0.17	-	104,111,143,145	0
5	PEG	B	213	7/7	0.89	0.14	-	72,79,95,97	0
5	PEG	A	212	7/7	0.52	0.28	-	82,87,95,113	0
5	PEG	B	215	7/7	0.78	0.19	-	49,63,79,84	0
5	PEG	A	207	7/7	0.78	0.17	-	74,78,85,86	0
6	PG4	A	218	13/13	0.83	0.25	-	62,69,78,80	13
5	PEG	B	211	7/7	0.38	0.26	-	103,107,111,113	0
5	PEG	A	209	7/7	0.83	0.33	-	49,61,90,95	0
5	PEG	A	213	7/7	0.88	0.20	-	79,83,99,101	0
5	PEG	A	214	7/7	0.41	0.20	-	110,124,162,210	0
5	PEG	B	212	7/7	0.49	0.30	-	74,81,105,107	0
5	PEG	B	209	7/7	0.67	0.25	-	85,88,91,92	0
5	PEG	A	208	7/7	0.84	0.20	-	92,108,132,193	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.