Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:49 PM GMT

PDB ID	:	4MUU
Title	:	Structure of ThiT with pyrithiamine bound
Authors	:	Swier, L.J.Y.M.; Guskov, A.; Slotboom, D.J.
Deposited on	:	2013-09-23
Resolution	:	2.10 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 ⓘ symbol.

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

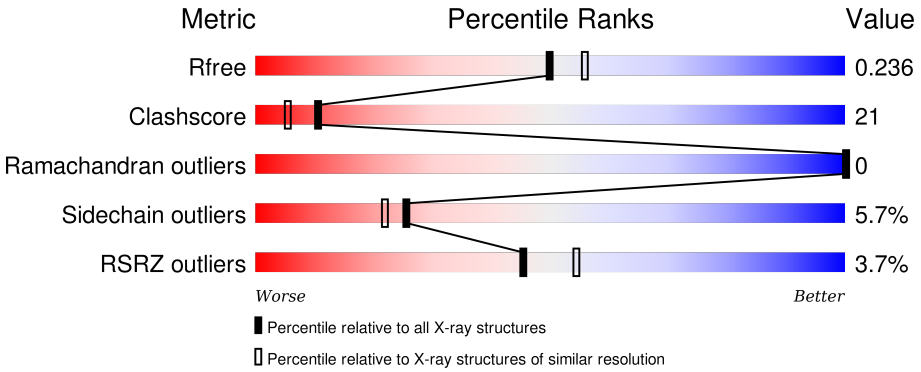
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	192	3% 74% 17% • 7%
1	B	192	4% 77% 15% • 8%

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
3	BNG	B	203	-	-	X	X
4	PEG	A	203	-	-	X	X
4	PEG	A	206	-	-	X	X
4	PEG	A	208	-	-	-	X
4	PEG	B	205	-	-	X	X
4	PEG	B	206	-	-	-	X
5	PG0	A	213	-	-	-	X
5	PG0	A	214	-	-	-	X
5	PG0	A	215	-	-	-	X
6	PG4	A	216	-	-	-	X
6	PG4	A	218	-	-	X	X
6	PG4	A	219	-	-	-	X
6	PG4	A	220	-	-	-	X
6	PG4	B	214	-	-	-	X
6	PG4	B	215	-	-	X	X
6	PG4	B	216	-	-	-	X
7	1PE	A	221	-	-	X	-
8	PGE	A	222	-	-	X	-
9	P6G	B	207	-	-	-	X
9	P6G	B	208	-	-	X	X
9	P6G	B	209	-	-	X	-
9	P6G	B	210	-	-	X	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 3380 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.

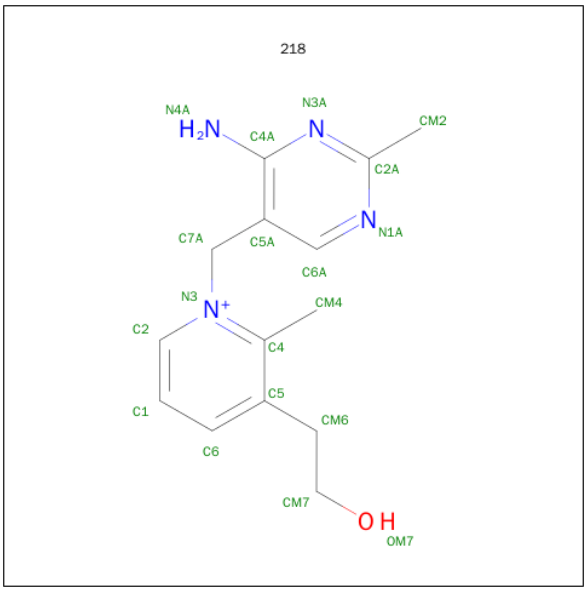
- Molecule 1 is a protein called Thiamine transporter ThiT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1382	948	215	216	3			
1	B	177	Total	C	N	O	S	0	1	0
			1381	948	214	216	3			

There are 20 discrepancies between the modelled and reference sequences:

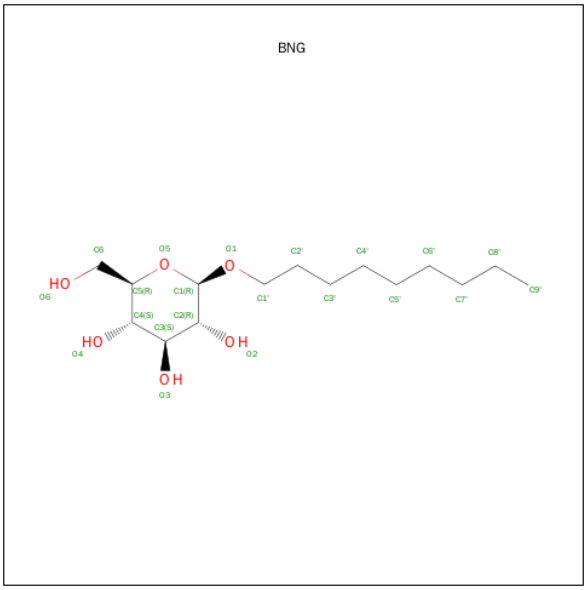
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP D8KFM5
A	2	HIS	-	EXPRESSION TAG	UNP D8KFM5
A	3	HIS	-	EXPRESSION TAG	UNP D8KFM5
A	4	HIS	-	EXPRESSION TAG	UNP D8KFM5
A	5	HIS	-	EXPRESSION TAG	UNP D8KFM5
A	6	HIS	-	EXPRESSION TAG	UNP D8KFM5
A	7	HIS	-	EXPRESSION TAG	UNP D8KFM5
A	8	HIS	-	EXPRESSION TAG	UNP D8KFM5
A	9	HIS	-	EXPRESSION TAG	UNP D8KFM5
A	10	ALA	-	EXPRESSION TAG	UNP D8KFM5
B	1	MET	-	EXPRESSION TAG	UNP D8KFM5
B	2	HIS	-	EXPRESSION TAG	UNP D8KFM5
B	3	HIS	-	EXPRESSION TAG	UNP D8KFM5
B	4	HIS	-	EXPRESSION TAG	UNP D8KFM5
B	5	HIS	-	EXPRESSION TAG	UNP D8KFM5
B	6	HIS	-	EXPRESSION TAG	UNP D8KFM5
B	7	HIS	-	EXPRESSION TAG	UNP D8KFM5
B	8	HIS	-	EXPRESSION TAG	UNP D8KFM5
B	9	HIS	-	EXPRESSION TAG	UNP D8KFM5
B	10	ALA	-	EXPRESSION TAG	UNP D8KFM5

- Molecule 2 is 1-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-3-(2-HYDROXYETHYL)-2-METHYLPYRIDINIUM (three-letter code: 218) (formula: $C_{14}H_{19}N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	14	4	1		
2	B	1	Total	C	N	O	0	0
			19	14	4	1		

- Molecule 3 is SUGAR (B-NONYLGLUCOSIDE) (three-letter code: BNG) (formula: $C_{15}H_{30}O_6$).



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

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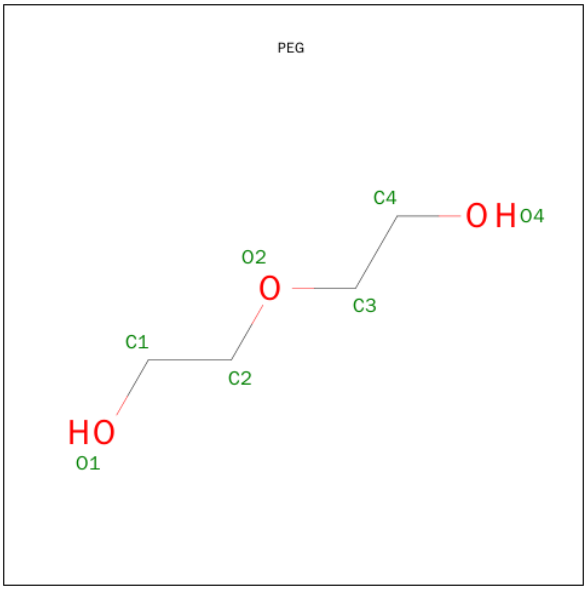
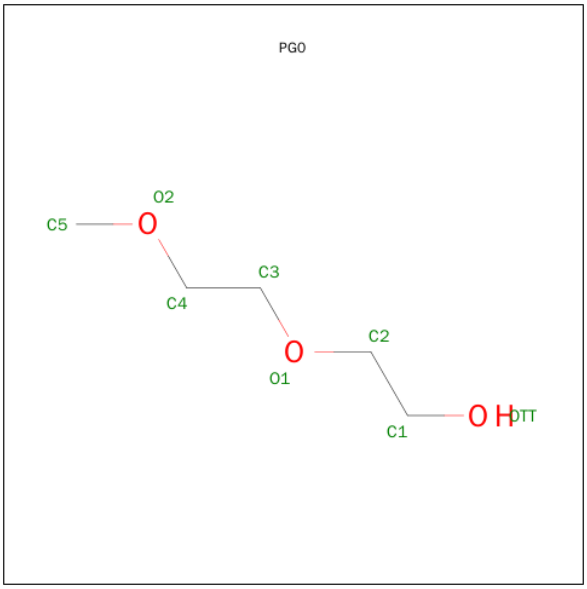
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 21 15 6	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



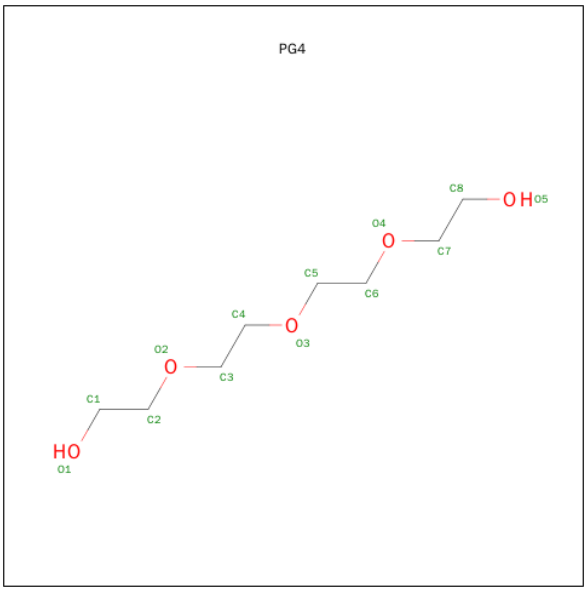
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0

- Molecule 5 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



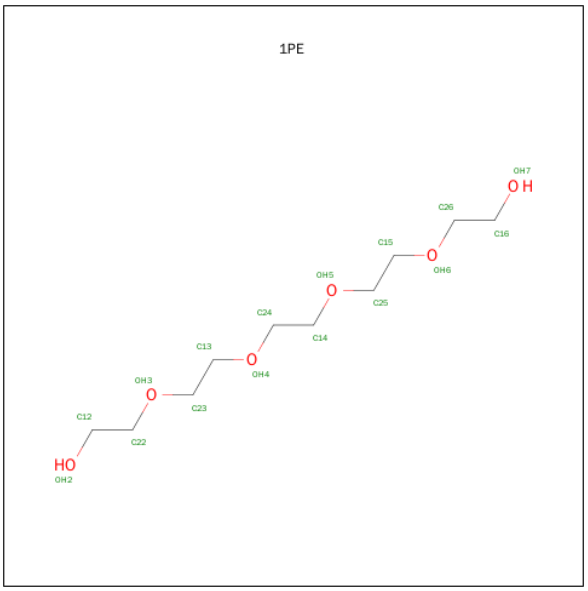
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 5 3	0	0
5	A	1	Total C O 8 5 3	0	0
5	A	1	Total C O 8 5 3	0	0
5	A	1	Total C O 8 5 3	0	0
5	A	1	Total C O 8 5 3	0	0
5	A	1	Total C O 8 5 3	0	0
5	B	1	Total C O 8 5 3	0	0
5	B	1	Total C O 8 5 3	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



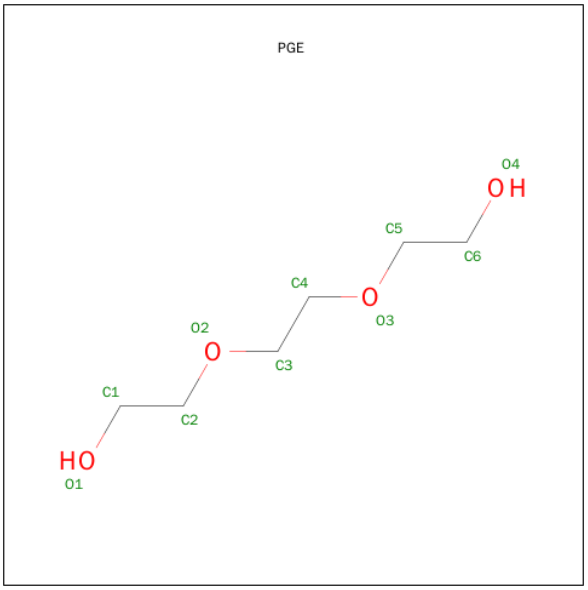
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 13 8 5	0	0
6	A	1	Total C O 13 8 5	0	0
6	A	1	Total C O 13 8 5	0	0
6	A	1	Total C O 13 8 5	0	0
6	A	1	Total C O 13 8 5	0	0
6	B	1	Total C O 13 8 5	0	0
6	B	1	Total C O 13 8 5	0	0
6	B	1	Total C O 13 8 5	0	0
6	B	1	Total C O 13 8 5	0	0

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



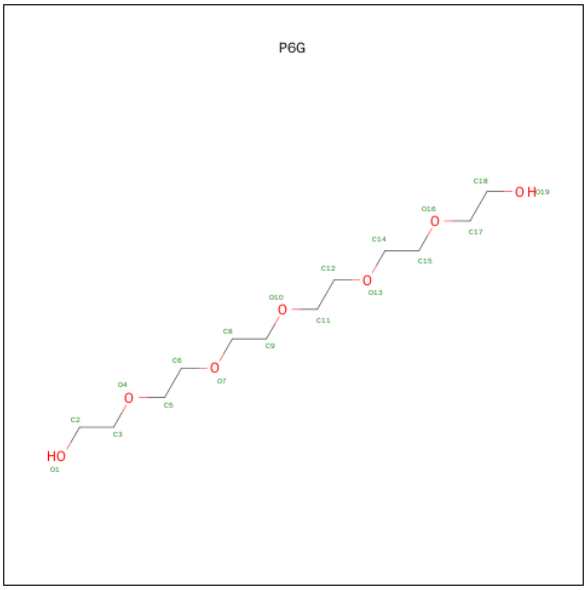
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 16 10 6	0	0

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



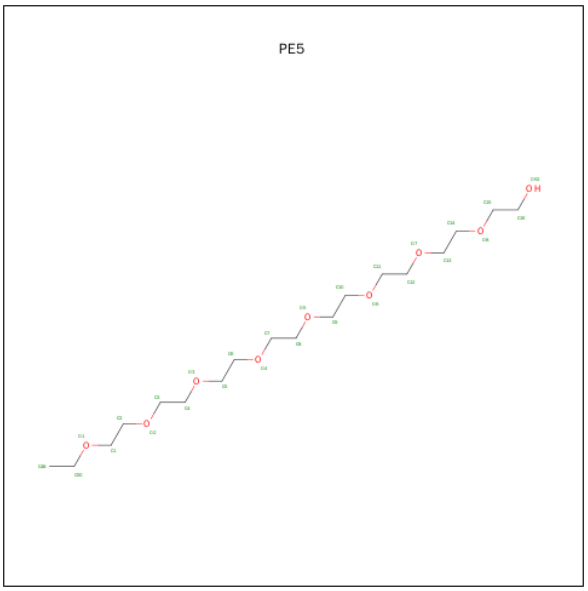
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 10 6 4	0	0
8	B	1	Total C O 10 6 4	0	0
8	B	1	Total C O 10 6 4	0	0

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



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

- Molecule 10 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (three-letter code: PE5) (formula: $C_{18}H_{38}O_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 27 18 9	0	0

- Molecule 11 is water.

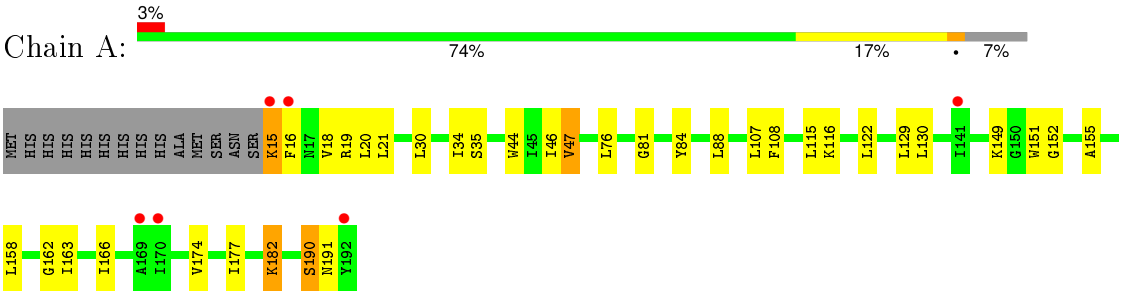
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	57	Total O 61 61	0	4
11	B	53	Total O 55 55	0	2

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.

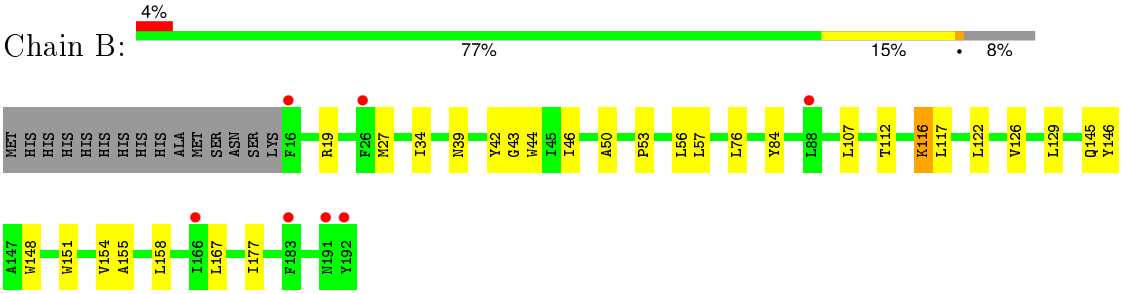
- Molecule 1: Thiamine transporter ThiT

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	61.56Å 84.59Å 127.26Å 90.00° 95.61° 90.00°	Depositor
Resolution (Å)	42.22 – 2.10 47.49 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (42.22-2.10) 98.8 (47.49-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.194 , 0.236 0.205 , 0.236	Depositor DCC
R_{free} test set	1876 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 75.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 37536 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3380	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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: PGE, PG0, PE5, 218, 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	0.58	0/1421	0.66	0/1937
1	B	0.59	0/1420	0.65	0/1937
All	All	0.58	0/2841	0.65	0/3874

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	1382	0	1473	49	0
1	B	1381	0	1470	38	0
2	A	19	0	19	2	0
2	B	19	0	19	1	0
3	A	21	0	30	4	0
3	B	42	0	60	15	0
4	A	49	0	63	13	0
4	B	21	0	27	7	0
5	A	48	0	72	14	0
5	B	16	0	24	1	0
6	A	65	0	90	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	52	0	72	15	0
7	A	16	0	22	22	0
8	A	10	0	14	7	0
8	B	20	0	28	0	0
9	B	76	0	104	35	0
10	B	27	0	38	6	0
11	A	61	0	0	4	0
11	B	55	0	0	3	0
All	All	3380	0	3625	147	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 21.

All (147) 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:42:TYR:HA	6:B:216:PG4:H11	1.51	0.90
4:A:206:PEG:H32	4:A:207:PEG:H21	1.53	0.90
9:B:207:P6G:H22	6:B:213:PG4:H71	1.54	0.88
4:A:206:PEG:H42	4:B:204:PEG:H31	1.60	0.84
1:A:122:LEU:HD22	4:A:203:PEG:H42	1.60	0.83
1:A:152:GLY:H	6:A:217:PG4:H12	1.45	0.82
1:A:116:LYS:HG2	6:B:216:PG4:H71	1.60	0.81
3:A:202:BNG:H3'1	3:A:202:BNG:H7'1	1.63	0.80
1:B:42:TYR:CE2	4:B:205:PEG:H42	2.19	0.77
1:A:81:GLY:CA	6:A:218:PG4:H22	2.15	0.77
1:B:46:ILE:HD13	9:B:208:P6G:H22	1.67	0.76
1:A:46:ILE:HG21	7:A:221:1PE:H141	1.68	0.76
6:A:220:PG4:H22	9:B:210:P6G:H171	1.68	0.76
5:A:213:PG0:H31	3:B:203:BNG:H2'1	1.68	0.74
9:B:207:P6G:C2	6:B:213:PG4:H71	2.18	0.74
1:B:39:ASN:OD1	9:B:208:P6G:H31	1.88	0.73
10:B:217:PE5:H61	10:B:217:PE5:H12	1.72	0.72
1:B:19:ARG:HG2	5:B:212:PG0:H31	1.70	0.72
1:A:35:SER:HB2	7:A:221:1PE:H161	1.73	0.71
7:A:221:1PE:H131	8:A:222:PGE:H52	1.72	0.70
1:A:47:VAL:HG13	5:A:210:PG0:H41	1.72	0.69
9:B:208:P6G:H92	9:B:209:P6G:C18	2.22	0.69
1:B:117:LEU:H	6:B:215:PG4:H51	1.57	0.69
9:B:208:P6G:H151	11:B:312:HOH:O	1.91	0.69
1:A:84:TYR:CE2	7:A:221:1PE:H122	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:N	6:B:215:PG4:H51	2.07	0.69
7:A:221:1PE:H131	8:A:222:PGE:H12	1.75	0.68
1:B:126:VAL:CG1	3:B:202:BNG:H9'3	2.25	0.67
1:B:129[A]:LEU:HD21	3:B:203:BNG:H9'1	1.75	0.66
7:A:221:1PE:C13	8:A:222:PGE:H52	2.25	0.66
1:A:84:TYR:HE2	7:A:221:1PE:H122	1.60	0.65
4:A:206:PEG:H32	4:A:207:PEG:C2	2.25	0.65
9:B:210:P6G:H81	9:B:210:P6G:H122	1.78	0.65
1:A:115:LEU:O	6:B:216:PG4:H82	1.99	0.63
1:A:151:TRP:CE2	6:A:217:PG4:H51	2.34	0.63
1:A:190:SER:OG	1:A:191:ASN:O	2.16	0.62
9:B:209:P6G:H82	9:B:209:P6G:O4	2.01	0.61
5:A:213:PG0:H52	3:B:203:BNG:H4'2	1.82	0.61
1:A:34:ILE:HD13	6:A:219:PG4:H61	1.83	0.61
6:B:215:PG4:H52	6:B:215:PG4:O2	1.99	0.60
1:A:81:GLY:HA3	6:A:218:PG4:H22	1.83	0.60
1:B:34:ILE:HD13	9:B:207:P6G:H92	1.83	0.59
4:B:205:PEG:H11	4:B:205:PEG:H41	1.84	0.59
1:B:43:GLY:O	9:B:208:P6G:H91	2.03	0.59
1:B:129[A]:LEU:CD2	3:B:203:BNG:H9'1	2.33	0.59
1:B:116:LYS:HA	6:B:215:PG4:H62	1.84	0.58
6:A:216:PG4:C4	6:A:216:PG4:H12	2.32	0.58
1:B:46:ILE:CD1	9:B:208:P6G:H22	2.33	0.58
1:B:151:TRP:NE1	9:B:210:P6G:H172	2.19	0.57
1:B:126:VAL:HG11	3:B:202:BNG:H9'3	1.86	0.57
1:A:163:ILE:HG21	4:A:207:PEG:H42	1.86	0.57
1:A:88:LEU:CD2	4:A:204:PEG:H22	2.34	0.57
1:B:43:GLY:HA3	4:B:205:PEG:H31	1.86	0.57
9:B:208:P6G:H92	9:B:209:P6G:H182	1.86	0.56
1:A:122:LEU:CD2	4:A:203:PEG:H21	2.35	0.56
7:A:221:1PE:C13	8:A:222:PGE:H12	2.34	0.56
1:A:129:LEU:HD22	5:A:212:PG0:H21	1.86	0.56
3:B:203:BNG:H2'2	3:B:203:BNG:O5	2.06	0.56
1:B:146:TYR:CG	9:B:208:P6G:H152	2.41	0.56
9:B:209:P6G:H51	9:B:209:P6G:H111	1.88	0.56
1:A:116:LYS:CG	6:B:216:PG4:H71	2.33	0.56
5:A:213:PG0:H31	3:B:203:BNG:C2'	2.35	0.55
1:A:130:LEU:HD13	5:A:212:PG0:H11	1.88	0.55
1:B:84:TYR:CE1	9:B:209:P6G:H142	2.41	0.54
1:A:122:LEU:CD2	4:A:203:PEG:H42	2.34	0.54
1:A:35:SER:CA	7:A:221:1PE:H161	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:VAL:HG13	3:B:202:BNG:H9'3	1.90	0.54
1:B:56:LEU:HD23	9:B:207:P6G:H151	1.90	0.54
7:A:221:1PE:H262	11:A:317:HOH:O	2.08	0.53
1:B:27:MET:SD	9:B:207:P6G:H152	2.47	0.53
9:B:208:P6G:H81	9:B:209:P6G:H151	1.89	0.53
1:A:35:SER:CB	7:A:221:1PE:H161	2.39	0.52
9:B:209:P6G:O1	9:B:209:P6G:H52	2.09	0.52
5:A:211:PG0:H22	6:A:218:PG4:H42	1.92	0.52
1:A:129:LEU:CD2	5:A:212:PG0:H21	2.39	0.52
6:B:215:PG4:C6	6:B:215:PG4:H31	2.39	0.52
4:A:209:PEG:H31	1:B:167:LEU:HD22	1.91	0.51
1:B:151:TRP:CE2	9:B:210:P6G:H172	2.45	0.51
1:A:44:TRP:CG	2:A:201:218:H6A	2.47	0.50
1:A:35:SER:HB2	7:A:221:1PE:C16	2.42	0.50
1:A:155:ALA:CB	6:A:217:PG4:H11	2.42	0.50
1:B:148:TRP:CD1	4:B:205:PEG:H12	2.48	0.49
1:B:129[A]:LEU:HD11	3:B:203:BNG:H5	1.95	0.49
9:B:209:P6G:H51	9:B:209:P6G:C11	2.43	0.48
5:A:213:PG0:H31	3:B:203:BNG:C3'	2.43	0.48
10:B:217:PE5:H111	10:B:217:PE5:H132	1.47	0.48
1:B:146:TYR:O	4:B:205:PEG:H21	2.13	0.48
3:A:202:BNG:H9'1	6:A:218:PG4:O5	2.13	0.48
1:A:162:GLY:HA3	3:B:203:BNG:H6'2	1.96	0.48
1:B:148:TRP:HD1	4:B:205:PEG:H12	1.78	0.48
1:B:117:LEU:H	6:B:215:PG4:C5	2.25	0.47
11:A:308:HOH:O	6:B:216:PG4:H72	2.14	0.47
1:A:20:LEU:HD21	5:A:214:PG0:H31	1.96	0.47
1:B:117:LEU:H	6:B:215:PG4:H72	1.80	0.47
9:B:210:P6G:H81	9:B:210:P6G:C12	2.44	0.47
1:A:166:ILE:HD11	3:B:203:BNG:H1	1.95	0.47
1:A:174:VAL:HG22	4:A:208:PEG:H42	1.95	0.47
1:A:155:ALA:HB3	6:A:217:PG4:H11	1.98	0.46
1:A:151:TRP:NE1	6:A:217:PG4:H62	2.31	0.46
1:A:151:TRP:HE1	6:A:217:PG4:H62	1.81	0.46
7:A:221:1PE:C13	8:A:222:PGE:C5	2.94	0.46
1:B:44:TRP:HD1	9:B:208:P6G:H141	1.81	0.45
3:A:202:BNG:H3'1	3:A:202:BNG:C7'	2.36	0.45
1:A:182:LYS:NZ	11:A:344:HOH:O	2.44	0.45
1:A:108:PHE:CZ	6:A:220:PG4:H21	2.51	0.45
3:A:202:BNG:H2	3:A:202:BNG:H1'2	1.68	0.45
10:B:217:PE5:H52A	10:B:217:PE5:H32	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:TYR:CD2	9:B:208:P6G:H152	2.52	0.44
10:B:217:PE5:O8	11:B:352:HOH:O	2.21	0.44
7:A:221:1PE:H252	7:A:221:1PE:H262	1.30	0.44
1:A:81:GLY:HA2	6:A:218:PG4:H22	1.96	0.44
1:B:154:VAL:HB	9:B:210:P6G:H31	1.98	0.44
9:B:208:P6G:C8	9:B:209:P6G:H151	2.47	0.44
7:A:221:1PE:H162	11:A:330:HOH:O	2.17	0.43
2:B:201:218:HM41	2:B:201:218:HM62	1.77	0.43
6:B:216:PG4:H61	6:B:216:PG4:H32	2.00	0.43
6:A:218:PG4:H21	6:A:218:PG4:H41	1.49	0.43
1:A:44:TRP:CD1	2:A:201:218:H6A	2.53	0.43
1:B:155:ALA:HB1	9:B:210:P6G:H121	1.98	0.43
1:A:44:TRP:CZ3	7:A:221:1PE:H142	2.54	0.43
7:A:221:1PE:H132	8:A:222:PGE:C5	2.49	0.43
1:B:158:LEU:HD23	9:B:210:P6G:H91	2.00	0.43
1:A:46:ILE:CG2	7:A:221:1PE:H141	2.44	0.42
1:A:177:ILE:HG22	4:A:208:PEG:H12	2.01	0.42
7:A:221:1PE:H241	7:A:221:1PE:H232	1.35	0.42
1:A:30:LEU:CD2	6:A:219:PG4:H31	2.49	0.42
1:A:16:PHE:CE2	1:A:18:VAL:HB	2.54	0.42
1:A:44:TRP:CE2	7:A:221:1PE:H231	2.55	0.42
5:A:212:PG0:H22	9:B:210:P6G:H81	2.02	0.42
1:B:56:LEU:CD2	9:B:207:P6G:H151	2.48	0.42
1:A:15:LYS:N	1:A:15:LYS:CD	2.82	0.42
5:A:215:PG0:H21	1:B:177:ILE:HD11	2.01	0.42
10:B:217:PE5:H11	10:B:217:PE5:H32	1.87	0.42
7:A:221:1PE:H131	8:A:222:PGE:C1	2.47	0.42
1:A:158:LEU:HD11	3:B:203:BNG:H4'1	2.02	0.41
1:A:163:ILE:CD1	4:A:206:PEG:H41	2.51	0.41
4:A:203:PEG:H42	4:A:203:PEG:H21	1.55	0.41
5:A:213:PG0:H11	5:A:213:PG0:H32	1.21	0.41
10:B:217:PE5:H71	10:B:217:PE5:H51	1.67	0.41
9:B:208:P6G:H81	9:B:208:P6G:H111	1.83	0.41
1:A:35:SER:HA	7:A:221:1PE:H161	2.01	0.41
9:B:209:P6G:H31	11:B:318:HOH:O	2.20	0.41
3:B:203:BNG:H9'3	3:B:203:BNG:H6'1	1.60	0.40
5:A:211:PG0:C2	6:A:218:PG4:H42	2.50	0.40
1:A:129:LEU:C	1:A:129:LEU:HD23	2.42	0.40
1:B:50:ALA:O	1:B:53:PRO:HD2	2.22	0.40
9:B:210:P6G:H121	9:B:210:P6G:H92	1.70	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	176/192 (92%)	173 (98%)	3 (2%)	0	100	100
1	B	176/192 (92%)	173 (98%)	3 (2%)	0	100	100
All	All	352/384 (92%)	346 (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	141/155 (91%)	132 (94%)	9 (6%)	22	18
1	B	141/155 (91%)	134 (95%)	7 (5%)	30	27
All	All	282/310 (91%)	266 (94%)	16 (6%)	25	22

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	19	ARG
1	A	21	LEU
1	A	47	VAL
1	A	76	LEU
1	A	107	LEU
1	A	149	LYS
1	A	182	LYS

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Mol	Chain	Res	Type
1	A	190	SER
1	B	57	LEU
1	B	76	LEU
1	B	107	LEU
1	B	112	THR
1	B	116	LYS
1	B	122	LEU
1	B	145	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	ASN
1	B	161	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

41 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	218	A	201	-	19,20,20	1.89	6 (31%)	24,27,27	1.32	4 (16%)
3	BNG	A	202	-	21,21,21	0.83	0	26,26,26	1.47	5 (19%)
4	PEG	A	203	-	6,6,6	0.57	0	5,5,5	0.40	0
4	PEG	A	204	-	6,6,6	0.58	0	5,5,5	0.73	0
4	PEG	A	205	-	6,6,6	0.54	0	5,5,5	0.24	0
4	PEG	A	206	-	6,6,6	0.57	0	5,5,5	0.28	0
4	PEG	A	207	-	6,6,6	0.55	0	5,5,5	0.39	0
4	PEG	A	208	-	6,6,6	0.55	0	5,5,5	0.66	0
4	PEG	A	209	-	6,6,6	0.51	0	5,5,5	0.61	0
5	PG0	A	210	-	7,7,7	0.32	0	6,6,6	0.32	0
5	PG0	A	211	-	7,7,7	0.30	0	6,6,6	0.38	0
5	PG0	A	212	-	7,7,7	0.33	0	6,6,6	0.31	0
5	PG0	A	213	-	7,7,7	0.26	0	6,6,6	0.68	0
5	PG0	A	214	-	7,7,7	0.31	0	6,6,6	0.21	0
5	PG0	A	215	-	7,7,7	0.36	0	6,6,6	0.35	0
6	PG4	A	216	-	12,12,12	0.80	0	11,11,11	0.39	0
6	PG4	A	217	-	12,12,12	0.72	0	11,11,11	0.26	0
6	PG4	A	218	-	12,12,12	0.72	0	11,11,11	0.42	0
6	PG4	A	219	-	12,12,12	0.74	0	11,11,11	0.36	0
6	PG4	A	220	-	12,12,12	0.71	0	11,11,11	0.38	0
7	1PE	A	221	-	15,15,15	0.72	0	14,14,14	0.67	0
8	PGE	A	222	-	9,9,9	0.42	0	8,8,8	0.68	0
2	218	B	201	-	19,20,20	2.01	5 (26%)	24,27,27	1.24	3 (12%)
3	BNG	B	202	-	21,21,21	0.79	0	26,26,26	1.06	2 (7%)
3	BNG	B	203	-	21,21,21	0.92	0	26,26,26	1.21	3 (11%)
4	PEG	B	204	-	6,6,6	0.53	0	5,5,5	0.40	0
4	PEG	B	205	-	6,6,6	0.55	0	5,5,5	0.32	0
4	PEG	B	206	-	6,6,6	0.65	0	5,5,5	0.27	0
9	P6G	B	207	-	18,18,18	0.75	0	17,17,17	0.33	0
9	P6G	B	208	-	18,18,18	0.78	0	17,17,17	0.61	0
9	P6G	B	209	-	18,18,18	0.70	0	17,17,17	0.58	0
9	P6G	B	210	-	18,18,18	0.76	0	17,17,17	0.33	0
5	PG0	B	211	-	7,7,7	0.31	0	6,6,6	0.33	0
5	PG0	B	212	-	7,7,7	0.32	0	6,6,6	0.19	0
6	PG4	B	213	-	12,12,12	0.72	0	11,11,11	0.26	0
6	PG4	B	214	-	12,12,12	0.72	0	11,11,11	0.25	0
6	PG4	B	215	-	12,12,12	0.68	0	11,11,11	0.41	0
6	PG4	B	216	-	12,12,12	0.72	0	11,11,11	0.30	0
10	PE5	B	217	-	26,26,26	0.79	0	25,25,25	0.30	0
8	PGE	B	218	-	9,9,9	0.32	0	8,8,8	0.37	0
8	PGE	B	219	-	9,9,9	0.34	0	8,8,8	0.31	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	218	A	201	-	-	0/7/7/7	0/2/2/2
3	BNG	A	202	-	-	0/12/32/32	0/1/1/1
4	PEG	A	203	-	-	0/4/4/4	0/0/0/0
4	PEG	A	204	-	-	0/4/4/4	0/0/0/0
4	PEG	A	205	-	-	0/4/4/4	0/0/0/0
4	PEG	A	206	-	-	0/4/4/4	0/0/0/0
4	PEG	A	207	-	-	0/4/4/4	0/0/0/0
4	PEG	A	208	-	-	0/4/4/4	0/0/0/0
4	PEG	A	209	-	-	0/4/4/4	0/0/0/0
5	PG0	A	210	-	-	0/5/5/5	0/0/0/0
5	PG0	A	211	-	-	0/5/5/5	0/0/0/0
5	PG0	A	212	-	-	0/5/5/5	0/0/0/0
5	PG0	A	213	-	-	0/5/5/5	0/0/0/0
5	PG0	A	214	-	-	0/5/5/5	0/0/0/0
5	PG0	A	215	-	-	0/5/5/5	0/0/0/0
6	PG4	A	216	-	-	0/10/10/10	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
8	PGE	A	222	-	-	0/7/7/7	0/0/0/0
2	218	B	201	-	-	0/7/7/7	0/2/2/2
3	BNG	B	202	-	-	0/12/32/32	0/1/1/1
3	BNG	B	203	-	-	0/12/32/32	0/1/1/1
4	PEG	B	204	-	-	0/4/4/4	0/0/0/0
4	PEG	B	205	-	-	0/4/4/4	0/0/0/0
4	PEG	B	206	-	-	0/4/4/4	0/0/0/0
9	P6G	B	207	-	-	0/16/16/16	0/0/0/0
9	P6G	B	208	-	-	0/16/16/16	0/0/0/0
9	P6G	B	209	-	-	0/16/16/16	0/0/0/0
9	P6G	B	210	-	-	0/16/16/16	0/0/0/0
5	PG0	B	211	-	-	0/5/5/5	0/0/0/0
5	PG0	B	212	-	-	0/5/5/5	0/0/0/0
6	PG4	B	213	-	-	0/10/10/10	0/0/0/0
6	PG4	B	214	-	-	0/10/10/10	0/0/0/0
6	PG4	B	215	-	-	0/10/10/10	0/0/0/0
6	PG4	B	216	-	-	0/10/10/10	0/0/0/0
10	PE5	B	217	-	-	0/24/24/24	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PGE	B	218	-	-	0/7/7/7	0/0/0/0
8	PGE	B	219	-	-	0/7/7/7	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	218	C7A-N3	-2.32	1.44	1.48
2	A	201	218	CM6-C5	2.12	1.55	1.51
2	B	201	218	C1-C6	2.12	1.43	1.38
2	A	201	218	C6-C5	2.25	1.43	1.39
2	B	201	218	CM6-C5	2.49	1.56	1.51
2	A	201	218	C4-C5	2.60	1.44	1.39
2	A	201	218	CM4-C4	2.96	1.56	1.49
2	B	201	218	C4-C5	3.24	1.45	1.39
2	B	201	218	CM4-C4	3.26	1.56	1.49
2	A	201	218	C4A-N4A	4.39	1.45	1.34
2	B	201	218	C4A-N4A	4.92	1.46	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	202	BNG	O1-C1-C2	-2.91	104.37	108.04
2	A	201	218	C5A-C6A-N1A	-2.81	118.98	123.86
3	A	202	BNG	O5-C1-O1	-2.75	103.42	110.05
2	A	201	218	C1-C6-C5	-2.75	116.64	120.90
3	B	202	BNG	C6-C5-C4	-2.64	106.51	113.02
3	A	202	BNG	C4-C3-C2	-2.51	106.10	110.79
3	A	202	BNG	C3-C4-C5	-2.46	105.92	110.20
2	B	201	218	C5A-C6A-N1A	-2.44	119.62	123.86
2	B	201	218	C1-C6-C5	-2.44	117.12	120.90
3	B	203	BNG	O5-C5-C4	-2.21	105.54	109.68
3	B	202	BNG	C4-C3-C2	-2.08	106.92	110.79
3	B	203	BNG	C1-O5-C5	-2.04	109.79	113.75
3	B	203	BNG	C1-C2-C3	2.10	114.11	109.97
2	B	201	218	C6A-N1A-C2A	2.10	119.45	115.77
2	A	201	218	C6A-N1A-C2A	2.49	120.11	115.77
2	A	201	218	CM2-C2A-N1A	2.50	120.02	117.03
3	A	202	BNG	C1-C2-C3	2.52	114.94	109.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

35 monomers are involved in 141 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	218	2	0
3	A	202	BNG	4	0
4	A	203	PEG	4	0
4	A	204	PEG	1	0
4	A	206	PEG	4	0
4	A	207	PEG	3	0
4	A	208	PEG	2	0
4	A	209	PEG	1	0
5	A	210	PG0	1	0
5	A	211	PG0	2	0
5	A	212	PG0	4	0
5	A	213	PG0	5	0
5	A	214	PG0	1	0
5	A	215	PG0	1	0
6	A	216	PG4	1	0
6	A	217	PG4	6	0
6	A	218	PG4	7	0
6	A	219	PG4	2	0
6	A	220	PG4	2	0
7	A	221	1PE	22	0
8	A	222	PGE	7	0
2	B	201	218	1	0
3	B	202	BNG	3	0
3	B	203	BNG	12	0
4	B	204	PEG	1	0
4	B	205	PEG	6	0
9	B	207	P6G	6	0
9	B	208	P6G	13	0
9	B	209	P6G	10	0
9	B	210	P6G	10	0
5	B	212	PG0	1	0
6	B	213	PG4	2	0
6	B	215	PG4	7	0
6	B	216	PG4	6	0
10	B	217	PE5	6	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	178/192 (92%)	0.03	6 (3%) 49 58	17, 30, 57, 79	0
1	B	177/192 (92%)	0.09	7 (3%) 42 51	19, 32, 56, 87	0
All	All	355/384 (92%)	0.06	13 (3%) 45 54	17, 32, 57, 87	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	TYR	4.5
1	B	192	TYR	3.8
1	B	16	PHE	3.8
1	B	26	PHE	3.3
1	A	141	ILE	2.7
1	A	169	ALA	2.5
1	A	16	PHE	2.2
1	B	166	ILE	2.2
1	B	191	ASN	2.2
1	B	183	PHE	2.1
1	A	15	LYS	2.1
1	B	88	LEU	2.1
1	A	170	ILE	2.0

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 (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^{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	PEG	B	205	7/7	0.74	0.45	19.32	66,73,78,78	0
6	PG4	B	215	13/13	0.88	0.38	9.06	56,62,71,75	0
4	PEG	A	203	7/7	0.90	0.33	7.61	49,52,53,55	0
6	PG4	A	218	13/13	0.75	0.20	6.94	55,68,76,77	0
6	PG4	B	214	13/13	0.90	0.27	6.90	62,72,86,91	0
6	PG4	A	220	13/13	0.88	0.22	6.18	46,56,77,78	0
9	P6G	B	210	19/19	0.76	0.32	6.11	53,63,73,74	0
6	PG4	A	216	13/13	0.80	0.21	5.52	45,59,79,82	0
4	PEG	B	206	7/7	0.87	0.26	4.96	42,51,58,58	0
5	PG0	A	215	8/8	0.76	0.34	4.85	44,62,64,66	0
4	PEG	A	206	7/7	0.89	0.26	4.59	49,54,66,68	0
6	PG4	B	216	13/13	0.79	0.22	4.09	36,67,86,87	0
9	P6G	B	207	19/19	0.91	0.23	3.38	57,68,83,83	0
9	P6G	B	208	19/19	0.79	0.21	3.05	25,45,64,68	0
4	PEG	A	208	7/7	0.89	0.20	2.86	48,54,59,64	0
3	BNG	B	203	21/21	0.81	0.26	2.86	46,67,82,90	0
5	PG0	A	213	8/8	0.89	0.15	2.59	40,69,77,80	0
6	PG4	A	219	13/13	0.84	0.22	2.26	57,64,70,75	0
5	PG0	A	214	8/8	0.76	0.28	2.10	77,83,87,91	0
5	PG0	B	212	8/8	0.79	0.31	1.87	59,72,78,78	0
4	PEG	A	204	7/7	0.94	0.22	1.76	44,48,51,63	0
4	PEG	A	207	7/7	0.92	0.16	1.55	48,57,58,65	0
6	PG4	B	213	13/13	0.82	0.17	1.53	63,66,78,79	0
9	P6G	B	209	19/19	0.86	0.14	1.53	40,46,57,61	0
3	BNG	B	202	21/21	0.87	0.17	1.29	41,51,65,72	0
5	PG0	B	211	8/8	0.85	0.17	1.15	45,55,59,60	0
7	1PE	A	221	16/16	0.91	0.14	0.88	27,46,60,63	0
2	218	B	201	19/19	0.95	0.12	0.45	15,23,33,35	0
3	BNG	A	202	21/21	0.93	0.12	0.45	29,51,60,67	21
4	PEG	A	209	7/7	0.87	0.16	0.44	33,52,62,65	0
5	PG0	A	210	8/8	0.90	0.13	0.05	42,50,57,57	0
2	218	A	201	19/19	0.96	0.10	-0.01	18,24,30,32	0
10	PE5	B	217	27/27	0.91	0.12	-0.31	29,38,43,45	27
6	PG4	A	217	13/13	0.79	0.18	-	54,61,72,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	PEG	A	205	7/7	0.81	0.19	-	61,63,67,73	0
8	PGE	A	222	10/10	0.80	0.19	-	38,50,56,56	0
8	PGE	B	219	10/10	0.92	0.19	-	47,61,70,71	0
8	PGE	B	218	10/10	0.90	0.12	-	48,60,67,68	0
4	PEG	B	204	7/7	0.93	0.18	-	49,53,59,59	0
5	PG0	A	211	8/8	0.85	0.29	-	52,56,62,64	0
5	PG0	A	212	8/8	0.78	0.43	-	44,67,72,73	0

6.5 Other polymers

There are no such residues in this entry.