WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jul 3, 2017 – 03:42 PM EDT

PDB ID	:	2Y4N
Title	:	PaaK1 in complex with phenylacetyl adenylate
Authors	:	Law, A.; Boulanger, M.J.
Deposited on	:	unknown
Resolution	:	1.92 Å(reported)

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

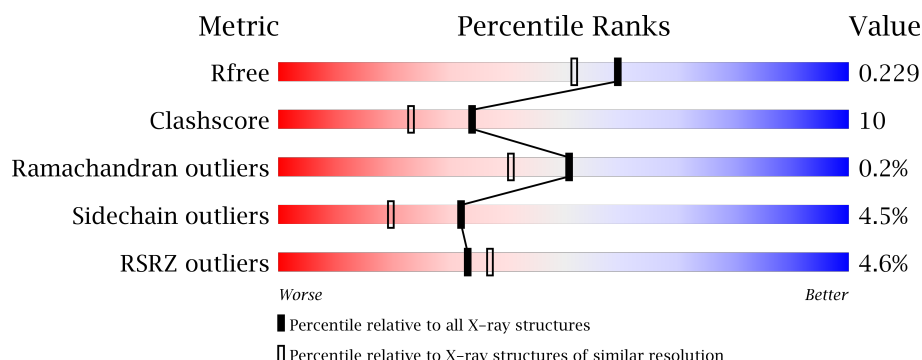|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.92 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	Percentile Ranks	Value
Rfree		0.229
Clashscore		10
Ramachandran outliers		0.2%
Sidechain outliers		4.5%
RSRZ outliers		4.6%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	6276 (1.94-1.90)
Clashscore	112137	7025 (1.94-1.90)
Ramachandran outliers	110173	6947 (1.94-1.90)
Sidechain outliers	110143	6948 (1.94-1.90)
RSRZ outliers	101464	6332 (1.94-1.90)

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	437	3% / 81% / 14% · ·
1	B	437	6% / 81% / 15% · ·

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	PEG	A	503	-	-	X	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7400 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 PHENYLACETATE-COENZYME A LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total 3317	C 2097	N 582	O 626	S 12	0	1	0
1	B	423	Total 3312	C 2094	N 581	O 624	S 13	0	3	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP B4E7B5
A	-3	SER	-	expression tag	UNP B4E7B5
A	-2	HIS	-	expression tag	UNP B4E7B5
A	-1	MET	-	expression tag	UNP B4E7B5
A	0	ALA	-	expression tag	UNP B4E7B5
A	1	SER	-	expression tag	UNP B4E7B5
B	-4	GLY	-	expression tag	UNP B4E7B5
B	-3	SER	-	expression tag	UNP B4E7B5
B	-2	HIS	-	expression tag	UNP B4E7B5
B	-1	MET	-	expression tag	UNP B4E7B5
B	0	ALA	-	expression tag	UNP B4E7B5
B	1	SER	-	expression tag	UNP B4E7B5

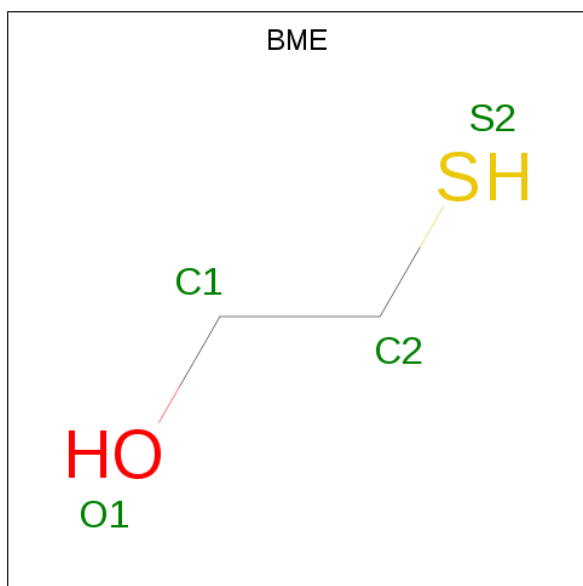- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Mg 2	0	0
2	A	2	Total 2	Mg 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG

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

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).

BME

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

- Molecule 5 is 5'-O-[HYDROXY(PHENYLACETYL)PHOSPHORYL]ADENOSINE (three-letter code: DLL) (formula: $C_{18}H_{20}N_5O_8P$).
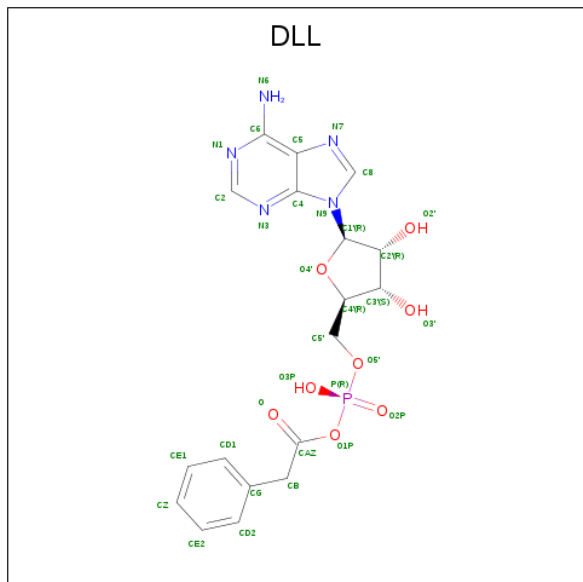
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	18	5	8	1		
5	B	1	Total	C	N	O	P	0	0
			32	18	5	8	1		

- Molecule 6 is 2-PHENYLACETIC ACID (three-letter code: PAC) (formula: $C_8H_8O_2$).
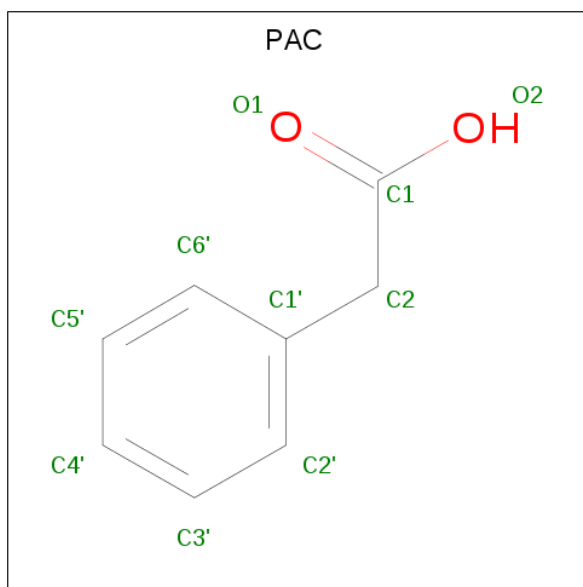
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 10	C 8	O 2	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

PGE
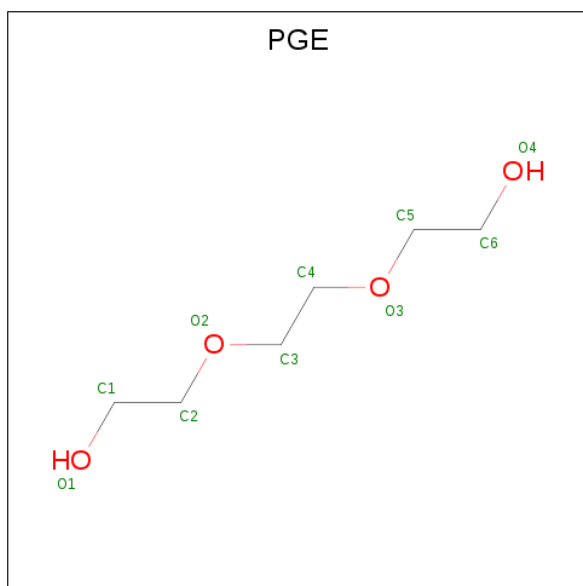
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 10	C 6	O 4	0	0

- Molecule 8 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	394	Total 394	O 394	0	0
8	B	270	Total 270	O 270	0	0

3 Residue-property plots (i)

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

- Molecule 1: PHENYLACETATE-COENZYME A LIGASE
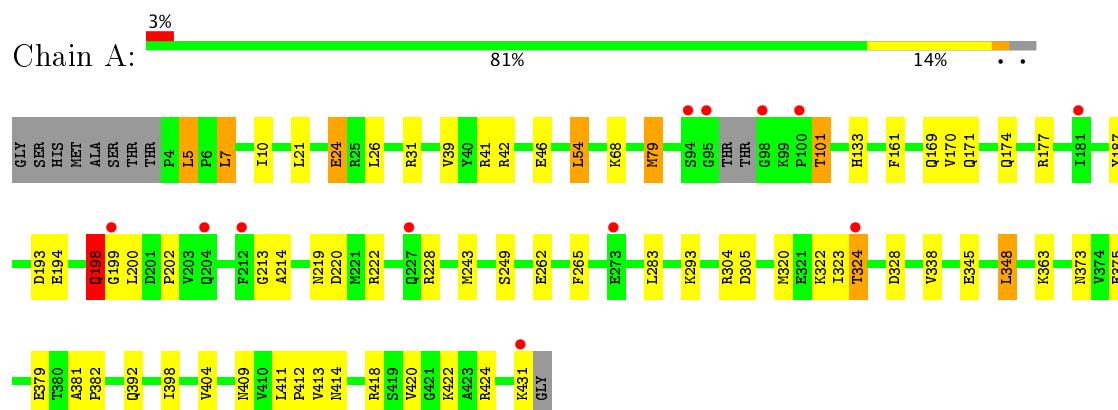
- Molecule 1: PHENYLACETATE-COENZYME A LIGASE
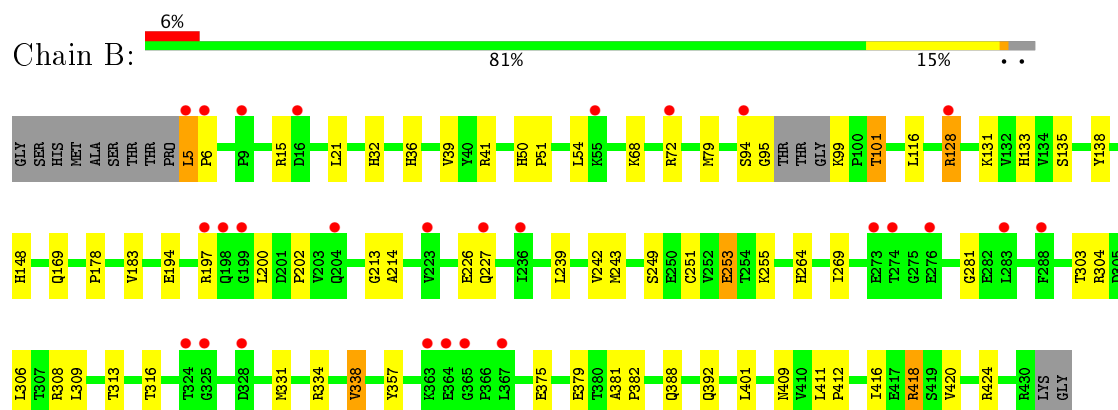
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	57.26Å 62.39Å 76.59Å 91.16° 108.33° 106.27°	Depositor
Resolution (Å)	27.01 – 1.92 27.01 – 1.92	Depositor EDS
% Data completeness (in resolution range)	93.8 (27.01-1.92) 90.8 (27.01-1.92)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.27 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.181 , 0.232 0.180 , 0.229	Depositor DCC
R_{free} test set	3457 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.6	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7400	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PGE, BME, DLL, PAC, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z|>5	RMSZ	#|Z|>5
1	A	0.31	0/3386	0.45	0/4594
1	B	0.28	0/3388	0.43	0/4600
All	All	0.30	0/6774	0.44	0/9194

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	GLN	Peptide
1	A	7	LEU	Peptide

5.2   Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3317	0	3337	61	0
1	B	3312	0	3331	63	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	7	0	10	10	0
4	A	4	0	5	1	0
4	B	8	0	11	2	0
5	A	32	0	18	0	0
5	B	32	0	18	0	0
6	B	10	0	7	3	0
7	B	10	0	14	0	0
8	A	394	0	0	17	1
8	B	270	0	0	13	1
All	All	7400	0	6751	129	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 129 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:251:CYS:HB3	1:B:253:GLU:OE2	1.42	1.17
1:A:198:GLN:HG3	1:A:198:GLN:O	1.61	0.97
1:A:219:ASN:HD21	3:A:503:PEG:H42	1.30	0.96
1:A:379:GLU:HG2	8:A:977:HOH:O	1.65	0.95
1:A:424:ARG:HH11	1:A:424:ARG:HG3	1.29	0.93

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:876:HOH:O	8:B:697:HOH:O[1_565]	2.11	0.09

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	423/437 (97%)	413 (98%)	9 (2%)	1 (0%)	51	41
1	B	422/437 (97%)	406 (96%)	14 (3%)	2 (0%)	32	20
All	All	845/874 (97%)	819 (97%)	23 (3%)	3 (0%)	51	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	243[A]	MET
1	B	243[B]	MET
1	A	243	MET

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	356/364 (98%)	339 (95%)	17 (5%)	30	17
1	B	357/364 (98%)	342 (96%)	15 (4%)	34	22
All	All	713/728 (98%)	681 (96%)	32 (4%)	32	20

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	338	VAL
1	B	5	LEU
1	B	418	ARG
1	A	431	LYS
1	B	21	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	36	HIS
1	B	84	GLN
1	B	165	GLN
1	A	373	ASN
1	B	148	HIS

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 ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	PEG	A	503	-	6,6,6	0.50	0	5,5,5	0.26	0
4	BME	A	504	1	3,3,3	0.33	0	2,2,2	0.60	0
5	DLL	A	505	-	31,35,35	1.61	4 (12%)	34,51,51	1.94	5 (14%)
6	PAC	B	503	-	7,10,10	0.47	0	9,12,12	0.45	0
7	PGE	B	504	-	9,9,9	0.44	0	8,8,8	0.34	0
4	BME	B	505	-	3,3,3	0.46	0	2,2,2	0.23	0
4	BME	B	506	1	3,3,3	0.36	0	2,2,2	0.51	0
5	DLL	B	507	-	31,35,35	1.59	3 (9%)	34,51,51	1.77	3 (8%)

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
3	PEG	A	503	-	-	0/4/4/4	0/0/0/0
4	BME	A	504	1	-	0/1/1/1	0/0/0/0
5	DLL	A	505	-	-	0/13/35/35	0/4/4/4
6	PAC	B	503	-	-	0/2/4/4	0/1/1/1
7	PGE	B	504	-	-	0/7/7/7	0/0/0/0
4	BME	B	505	-	-	0/1/1/1	0/0/0/0
4	BME	B	506	1	-	0/1/1/1	0/0/0/0
5	DLL	B	507	-	-	0/13/35/35	0/4/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	505	DLL	O4'-C4'	-3.45	1.37	1.45
5	B	507	DLL	O4'-C4'	-3.00	1.38	1.45
5	B	507	DLL	O5'-C5'	-2.34	1.35	1.44
5	A	505	DLL	O5'-C5'	-2.11	1.36	1.44
5	A	505	DLL	O4'-C1'	2.34	1.44	1.41

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	505	DLL	N3-C2-N1	-9.12	120.92	128.86
5	B	507	DLL	N3-C2-N1	-8.47	121.48	128.86
5	A	505	DLL	O5'-C5'-C4'	2.18	116.74	109.00
5	A	505	DLL	C5'-C4'-C3'	2.20	123.68	115.29
5	B	507	DLL	O4'-C4'-C3'	2.38	109.90	105.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	PEG	10	0
4	A	504	BME	1	0
6	B	503	PAC	3	0
4	B	505	BME	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	426/437 (97%)	-0.07	12 (2%)	53	58	13, 25, 43, 57	1 (0%)
1	B	423/437 (96%)	0.20	27 (6%)	20	23	14, 31, 52, 65	0
All	All	849/874 (97%)	0.06	39 (4%)	33	37	13, 27, 49, 65	1 (0%)

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	GLY	6.0
1	B	199	GLY	4.6
1	B	367	LEU	4.4
1	A	94	SER	4.3
1	A	431	LYS	4.1

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, 95th 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(Å²)	Q<0.9
3	PEG	A	503	7/7	0.84	0.29	9.51	28,38,39,41	0
4	BME	A	504	4/4	0.97	0.14	1.16	35,38,39,43	2
4	BME	B	505	4/4	0.87	0.18	0.98	51,56,56,59	0
6	PAC	B	503	10/10	0.65	0.21	0.92	56,61,70,74	0
4	BME	B	506	4/4	0.98	0.12	0.43	45,46,46,48	2
2	MG	B	502	1/1	0.99	0.17	0.31	45,45,45,45	0
2	MG	B	501	1/1	0.96	0.10	0.30	34,34,34,34	0
7	PGE	B	504	10/10	0.82	0.16	0.22	53,61,66,67	0
5	DLL	A	505	32/32	0.96	0.09	-0.63	14,20,26,27	0
5	DLL	B	507	32/32	0.96	0.08	-0.99	18,21,28,29	0
2	MG	A	502	1/1	0.97	0.06	-1.32	43,43,43,43	0
2	MG	A	501	1/1	0.97	0.04	-1.73	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.