wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 06:29 PM GMT

PDB ID	:	1B12
Title	:	CRYSTAL STRUCTURE OF TYPE 1 SIGNAL PEPTIDASE FROM ESCHERICHIA COLI IN COMPLEX WITH A BETA-LACTAM INHIBITOR
Authors	:	Paetzel, M.; Dalbey, R.; Strynadka, N.C.J.
Deposited on	:	1999-11-24
Resolution	:	1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

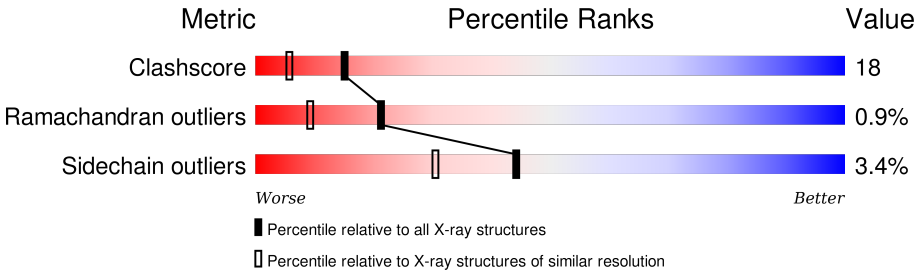
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.95 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))
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	248	78% 15%
1	B	248	69% 15% 15%
1	C	248	68% 19% 9%
1	D	248	69% 17% 10%

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	1PN	A	1001	-	-	X	-
3	1PN	C	1001	-	-	X	-
3	1PN	D	1001	-	-	X	-

2 Entry composition

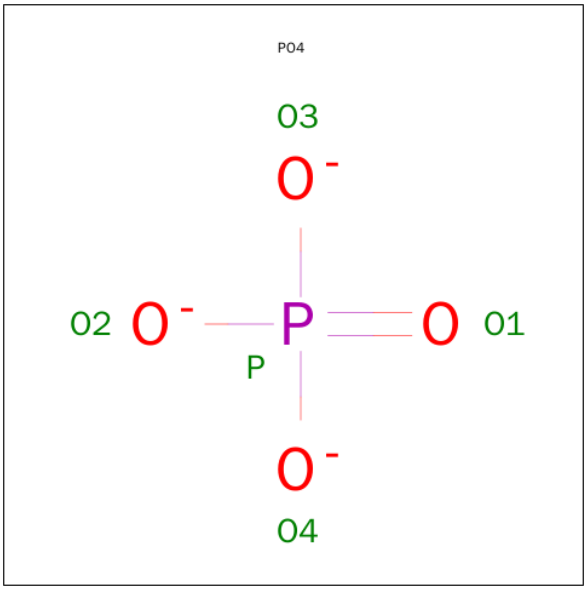
There are 4 unique types of molecules in this entry. The entry contains 7646 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SIGNAL PEPTIDASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1887	1204	319	356	8			
1	B	211	Total	C	N	O	S	0	0	0
			1679	1077	280	314	8			
1	C	226	Total	C	N	O	S	0	0	0
			1775	1135	295	337	8			
1	D	222	Total	C	N	O	S	0	0	0
			1772	1143	293	330	6			

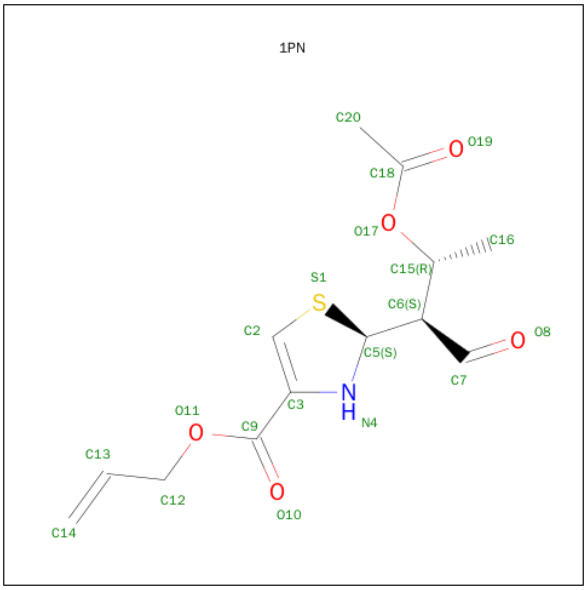
- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is PROP-2-EN-1-YL (2S)-2-[(2S,3R)-3-(ACETYLOXY)-1-OXOBUTAN-2-YL]-2,3-DIHYDRO-1,3-THIAZOLE-4-CARBOXYLATE (three-letter code: 1PN) (formula:

$C_{13}H_{17}NO_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O S 20 13 1 5 1	0	0
3	C	1	Total C N O S 20 13 1 5 1	0	0
3	A	1	Total C N O S 20 13 1 5 1	0	0
3	D	1	Total C N O S 20 13 1 5 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	129	Total O 129 129	0	0
4	B	111	Total O 111 111	0	0
4	C	122	Total O 122 122	0	0
4	D	86	Total O 86 86	0	0

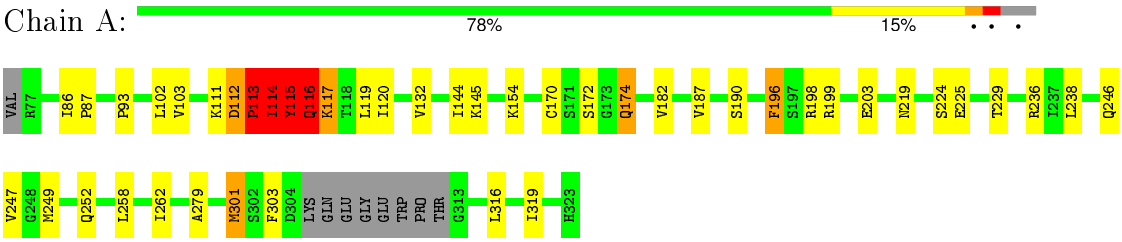
3 Residue-property plots (i)

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.

Note EDS was not executed.

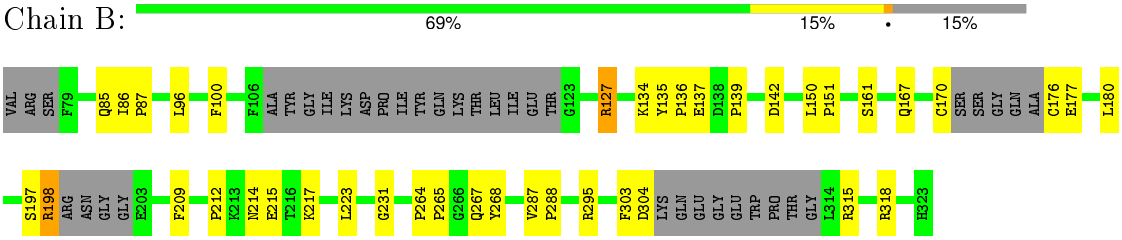
- Molecule 1: SIGNAL PEPTIDASE I

Chain A:



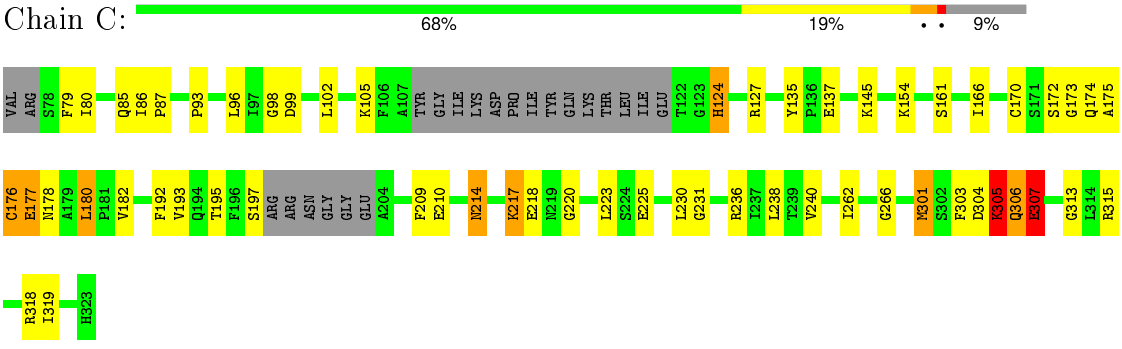
- Molecule 1: SIGNAL PEPTIDASE I

Chain B:



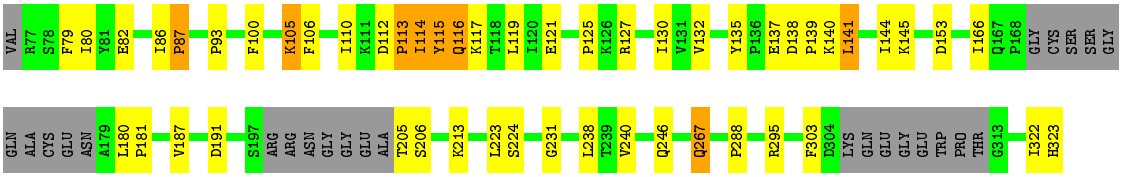
- Molecule 1: SIGNAL PEPTIDASE I

Chain C:



- Molecule 1: SIGNAL PEPTIDASE I

Chain D:


VAL R77 S78 F79 I80 Y81 E82 I86 P87 P93 F100 K105 F106 I110 K111 D112 P113 I114 Y115 Q116 K117 T118 L119 I120 E121 P125 K126 R127 I130 Y131 Y132 Y135 P136 E137 D138 P139 K140 L141 I144 K145 D153 I166 Q167 P168 GLY CYS SER SER GLY
GLN ALA CYS GLU ASN A179 L180 P181 V187 D191 S197 ARG ARG ASN GLY GLY GLU ALA T205 S206 K213 L223 S224 G231 L238 T239 V240 Q246 Q267 P288 R295 F303 D304 LYS GLN GLU GLY GLU TRP PRO THR G313 I322 H323

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	110.70Å 113.20Å 99.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.50 – 1.95	Depositor
% Data completeness (in resolution range)	96.8 (19.50-1.95)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.11	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.220 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7646	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 1PN

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	0.81	5/1935 (0.3%)	1.06	13/2622 (0.5%)
1	B	0.48	0/1721	0.77	0/2330
1	C	0.65	1/1822 (0.1%)	0.90	8/2472 (0.3%)
1	D	0.54	1/1818 (0.1%)	0.76	1/2464 (0.0%)
All	All	0.63	7/7296 (0.1%)	0.88	22/9888 (0.2%)

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	3
1	D	0	2
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	ILE	C-N	-17.71	0.93	1.34
1	C	307	GLU	N-CA	16.00	1.78	1.46
1	A	115	TYR	C-N	-13.86	1.02	1.34
1	D	116	GLN	N-CA	10.98	1.68	1.46
1	A	114	ILE	CA-C	-9.01	1.29	1.52

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	115	TYR	N-CA-C	16.08	154.41	111.00
1	A	114	ILE	O-C-N	-15.77	97.46	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	115	TYR	N-CA-CB	-12.23	88.58	110.60
1	A	117	LYS	N-CA-CB	11.77	131.79	110.60
1	A	114	ILE	CA-C-N	10.58	140.47	117.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	PRO	Peptide
1	A	114	ILE	Mainchain
1	A	116	GLN	Peptide
1	D	115	TYR	Sidechain,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	1887	0	1843	62	0
1	B	1679	0	1635	47	1
1	C	1775	0	1718	82	6
1	D	1772	0	1745	54	8
2	B	5	0	0	0	0
3	A	20	0	16	8	0
3	B	20	0	16	6	0
3	C	20	0	16	8	0
3	D	20	0	16	8	0
4	A	129	0	0	2	1
4	B	111	0	0	2	0
4	C	122	0	0	4	2
4	D	86	0	0	3	0
All	All	7646	0	7005	249	9

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 18.

The worst 5 of 249 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:D:116:GLN:N	1:D:116:GLN:CA	1.68	1.53
1:C:307:GLU:N	1:C:307:GLU:CA	1.78	1.44
1:A:114:ILE:HD12	1:A:115:TYR:CB	1.63	1.27
1:C:177:GLU:HG3	1:C:178:ASN:H	1.11	1.11
1:A:87:PRO:HD2	3:A:1001:1PN:H20	1.37	1.05

The worst 5 of 9 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)
1:C:266:GLY:CA	1:D:115:TYR:OH[4_455]	1.34	0.86
1:D:115:TYR:CD1	4:C:1045:HOH:O[4_555]	1.52	0.68
1:C:266:GLY:N	1:D:115:TYR:CE1[4_455]	1.74	0.46
1:D:115:TYR:CE1	4:C:1045:HOH:O[4_555]	1.76	0.44
1:C:266:GLY:CA	1:D:115:TYR:CZ[4_455]	1.97	0.23

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	235/248 (95%)	221 (94%)	13 (6%)	1 (0%)	39 27
1	B	201/248 (81%)	197 (98%)	3 (2%)	1 (0%)	34 21
1	C	220/248 (89%)	209 (95%)	7 (3%)	4 (2%)	11 2
1	D	214/248 (86%)	207 (97%)	5 (2%)	2 (1%)	21 9
All	All	870/992 (88%)	834 (96%)	28 (3%)	8 (1%)	21 9

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	173	GLY
1	C	177	GLU

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Mol	Chain	Res	Type
1	C	305	LYS
1	D	113	PRO
1	C	218	GLU

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	205/213 (96%)	198 (97%)	7 (3%)	44	30
1	B	184/213 (86%)	179 (97%)	5 (3%)	52	41
1	C	193/213 (91%)	186 (96%)	7 (4%)	42	28
1	D	194/213 (91%)	187 (96%)	7 (4%)	42	28
All	All	776/852 (91%)	750 (97%)	26 (3%)	44	30

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	223	LEU
1	C	214	ASN
1	D	246	GLN
1	C	124	HIS
1	C	197	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	214	ASN
1	C	85	GLN
1	D	167	GLN
1	B	167	GLN
1	C	214	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

5 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	$\#\|Z\| > 2$
3	1PN	A	1001	1	16,20,20	1.81	3 (18%)	18,26,26	2.15	5 (27%)
3	1PN	B	1001	1	16,20,20	1.86	2 (12%)	18,26,26	1.90	4 (22%)
2	PO4	B	1002	-	4,4,4	0.89	0	6,6,6	0.27	0
3	1PN	C	1001	1	16,20,20	1.73	2 (12%)	18,26,26	2.08	5 (27%)
3	1PN	D	1001	1	16,20,20	1.69	3 (18%)	18,26,26	2.09	4 (22%)

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	1PN	A	1001	1	-	0/18/31/31	0/1/1/1
3	1PN	B	1001	1	-	0/18/31/31	0/1/1/1
2	PO4	B	1002	-	-	0/0/0/0	0/0/0/0
3	1PN	C	1001	1	-	0/18/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PN	D	1001	1	-	0/18/31/31	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	1PN	C6-C15	-5.41	1.45	1.53
3	B	1001	1PN	C6-C15	-5.30	1.45	1.53
3	C	1001	1PN	C6-C15	-4.87	1.46	1.53
3	D	1001	1PN	C6-C15	-4.66	1.46	1.53
3	D	1001	1PN	C6-C7	2.06	1.53	1.49

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	1PN	O11-C9-C3	-5.68	106.23	111.91
3	C	1001	1PN	O11-C9-C3	-5.40	106.51	111.91
3	D	1001	1PN	O11-C9-C3	-5.40	106.51	111.91
3	B	1001	1PN	O11-C9-C3	-4.99	106.92	111.91
3	A	1001	1PN	C2-C3-C9	-2.89	124.41	131.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	1PN	8	0
3	B	1001	1PN	6	0
3	C	1001	1PN	8	0
3	D	1001	1PN	8	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.