wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 03:07 am BST

PDB ID	:	4AS2
Title	:	Pseudomonas Aeruginosa Phosphorylcholine Phosphatase. Monoclinic form
Authors	:	Infantes, L.; Otero, L.H.; Albert, A.
Deposited on	:	2012-04-27
Resolution	:	2.12 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

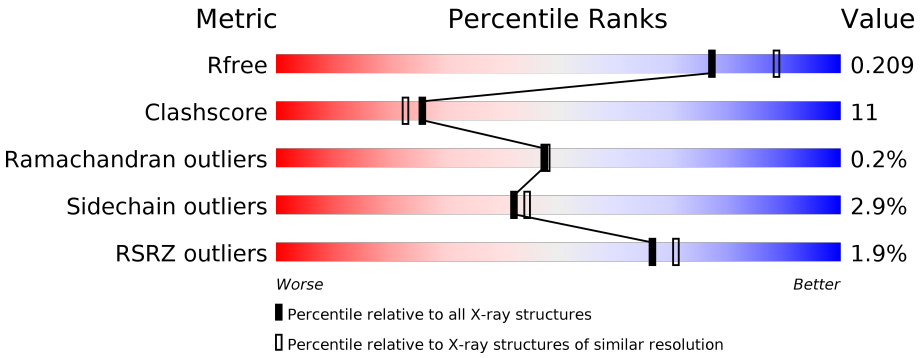
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.12 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}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 respectively. 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	327	81% 17%
1	B	327	5% 77% 22%
1	C	327	81% 17%
1	D	327	2% 80% 19%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IOD	D	1332	-	-	X	-
5	BTB	A	1335	-	X	X	-
5	BTB	A	1336	-	-	X	-
5	BTB	C	1335	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11407 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 PHOSPHORYLCHOLINE PHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2615	1674	439	490	12			
1	B	327	Total	C	N	O	S	0	0	0
			2615	1674	439	490	12			
1	C	327	Total	C	N	O	S	0	0	0
			2615	1674	439	490	12			
1	D	327	Total	C	N	O	S	0	0	0
			2615	1674	439	490	12			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

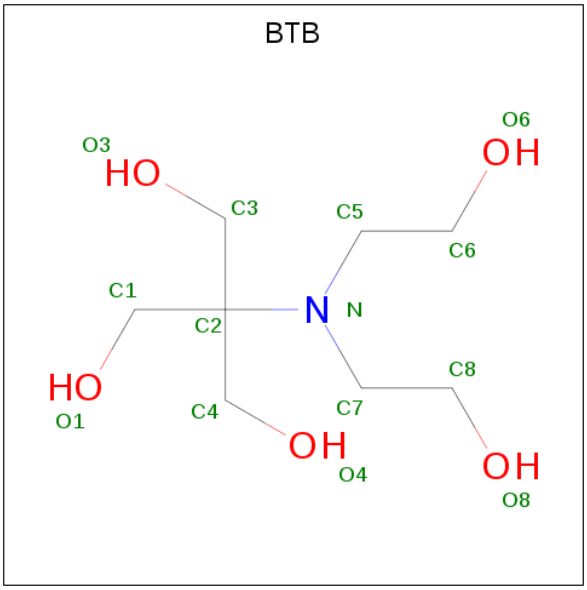
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total I 2 2	0	0
4	A	4	Total I 4 4	0	0
4	D	3	Total I 3 3	0	0
4	C	4	Total I 4 4	0	0

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is water.

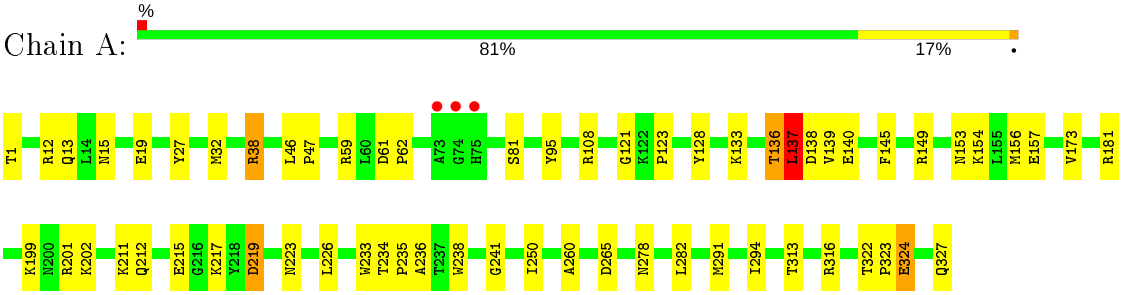
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	229	Total O 229 229	0	0
6	B	133	Total O 133 133	0	0
6	C	243	Total O 243 243	0	0
6	D	209	Total O 209 209	0	0

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.

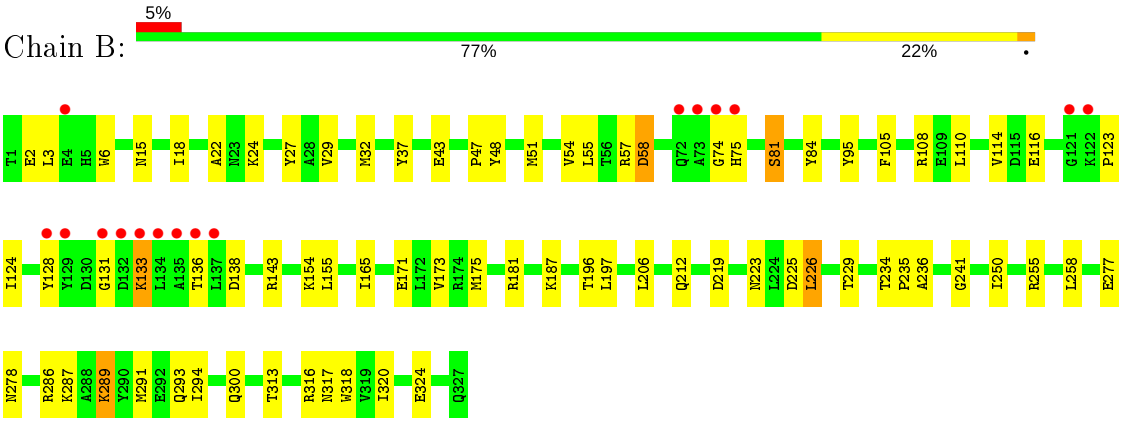
- Molecule 1: PHOSPHORYLCHOLINE PHOSPHATASE

Chain A:



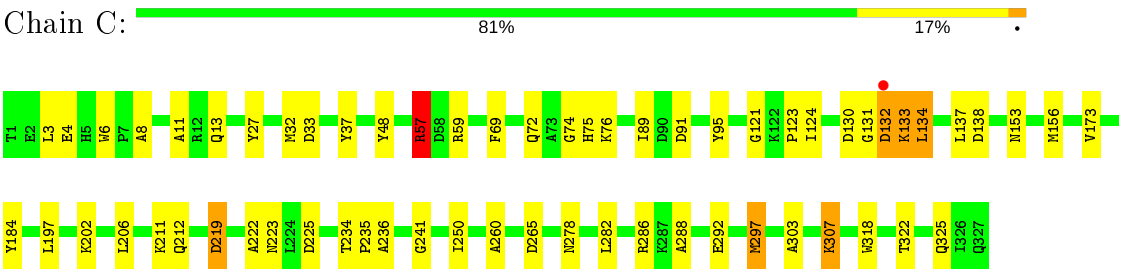
- Molecule 1: PHOSPHORYLCHOLINE PHOSPHATASE

Chain B:



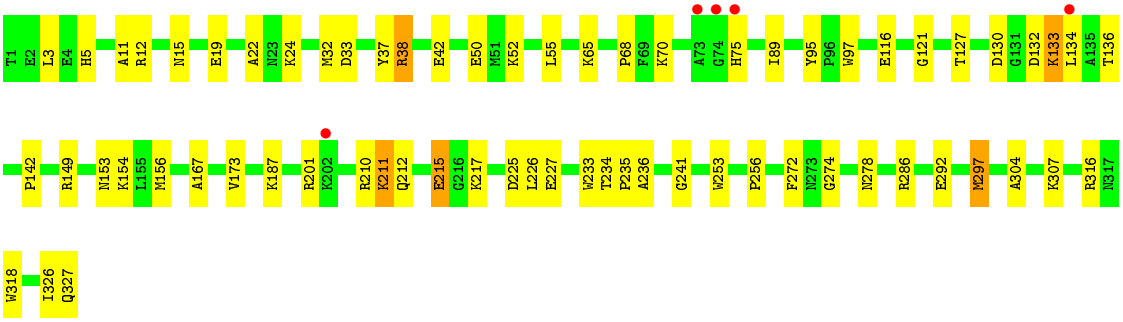
- Molecule 1: PHOSPHORYLCHOLINE PHOSPHATASE

Chain C:



- Molecule 1: PHOSPHORYLCHOLINE PHOSPHATASE

Chain D:


T1 E2 L3 E4 H5 A11 R12 N15 E19 A22 N23 K24 M32 D33 Y37 R38 E42 E50 M51 K52 L55 K65 P68 F69 K70 A73 G74 H75 I89 Y95 P96 W97 E116 G121 T127 D130 G131 D132 K133 L134 A135 T136
P142 R149 N153 K154 L155 M156 A167 V173 K187 R201 H202 R210 K211 Q212 E215 G216 K217 D225 L226 E227 W233 T234 P235 A236 G241 W253 P256 F272 M273 G274 N278 R286 E292 M297 A304 K307 R316 N317
W318 I326 Q327

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	136.01Å 156.63Å 71.82Å 90.00° 118.03° 90.00°	Depositor
Resolution (Å)	95.29 – 2.12 47.88 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.8 (95.29-2.12) 99.9 (47.88-2.12)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.154 , 0.210 0.154 , 0.209	Depositor DCC
R_{free} test set	3788 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	19.6	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 58.5	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	11407	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, IOD, CL, BTB

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	1.00	2/2680 (0.1%)	1.01	8/3643 (0.2%)
1	B	0.89	2/2680 (0.1%)	0.90	3/3643 (0.1%)
1	C	1.01	2/2680 (0.1%)	1.02	5/3643 (0.1%)
1	D	1.04	5/2680 (0.2%)	1.00	8/3643 (0.2%)
All	All	0.99	11/10720 (0.1%)	0.98	24/14572 (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	B	0	1
1	C	0	1
All	All	0	2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	GLU	CG-CD	8.07	1.64	1.51
1	C	318	TRP	CD2-CE2	6.25	1.48	1.41
1	D	97	TRP	CD2-CE2	6.14	1.48	1.41
1	D	42	GLU	CD-OE1	5.93	1.32	1.25
1	C	184	TYR	CG-CD2	5.62	1.46	1.39

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	57	ARG	NE-CZ-NH2	-11.31	114.65	120.30
1	A	324	GLU	OE1-CD-OE2	-7.86	113.87	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	219	ASP	CB-CG-OD1	7.79	125.31	118.30
1	D	211	LYS	CD-CE-NZ	-7.74	93.91	111.70
1	A	12	ARG	NE-CZ-NH2	-7.60	116.50	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	74	GLY	Peptide
1	C	74	GLY	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	2615	0	2581	53	0
1	B	2615	0	2581	45	0
1	C	2615	0	2581	50	0
1	D	2615	0	2581	51	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	1	0
4	A	4	0	0	0	0
4	B	2	0	0	0	0
4	C	4	0	0	0	0
4	D	3	0	0	2	0
5	A	56	0	76	24	1
5	B	14	0	19	1	0
5	C	28	0	38	18	0
5	D	14	0	19	2	0
6	A	229	0	0	13	0
6	B	133	0	0	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	243	0	0	26	0
6	D	209	0	0	17	1
All	All	11407	0	10476	222	2

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 11.

The worst 5 of 222 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)
4:D:1332:IOD:I	6:D:2185:HOH:O	2.21	1.25
1:D:187:LYS:HE3	6:D:2116:HOH:O	1.38	1.22
1:D:278:ASN:HB2	6:D:2170:HOH:O	1.43	1.19
1:B:143:ARG:HB2	6:B:2067:HOH:O	1.40	1.18
5:C:1335:BTB:C8	5:C:1335:BTB:H41	1.66	1.15

All (2) 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:D:121:GLY:O	5:A:1335:BTB:O4[3_444]	1.97	0.23
6:D:2020:HOH:O	6:D:2196:HOH:O[2_555]	2.16	0.04

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	325/327 (99%)	316 (97%)	9 (3%)	0	100 100
1	B	325/327 (99%)	314 (97%)	10 (3%)	1 (0%)	41 40
1	C	325/327 (99%)	316 (97%)	8 (2%)	1 (0%)	41 40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	325/327 (99%)	315 (97%)	10 (3%)	0	100 100
All	All	1300/1308 (99%)	1261 (97%)	37 (3%)	2 (0%)	47 48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	131	GLY
1	C	131	GLY

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	274/274 (100%)	268 (98%)	6 (2%)	52 55
1	B	274/274 (100%)	262 (96%)	12 (4%)	28 27
1	C	274/274 (100%)	265 (97%)	9 (3%)	38 39
1	D	274/274 (100%)	269 (98%)	5 (2%)	59 63
All	All	1096/1096 (100%)	1064 (97%)	32 (3%)	42 44

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

Mol	Chain	Res	Type
1	B	286	ARG
1	B	294	ILE
1	D	132	ASP
1	B	289	LYS
1	C	4	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	278	ASN
1	B	317	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	75	HIS
1	B	223	ASN
1	D	185	ASN

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)

Of 29 ligands modelled in this entry, 21 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	$\#\|Z\| > 2$
5	BTB	A	1334	-	13,13,13	1.32	2 (15%)	7,16,16	1.43	1 (14%)
5	BTB	C	1334	-	13,13,13	1.13	2 (15%)	7,16,16	1.55	3 (42%)
5	BTB	A	1335	-	13,13,13	1.92	5 (38%)	7,16,16	2.30	3 (42%)
5	BTB	C	1335	-	13,13,13	1.50	3 (23%)	7,16,16	1.72	3 (42%)
5	BTB	D	1333	-	13,13,13	1.09	0	7,16,16	1.82	2 (28%)
5	BTB	A	1336	-	13,13,13	1.29	2 (15%)	7,16,16	0.78	0
5	BTB	A	1333	-	13,13,13	0.99	1 (7%)	7,16,16	1.27	1 (14%)
5	BTB	B	1331	-	13,13,13	0.97	0	7,16,16	1.45	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
5	BTB	A	1334	-	-	0/21/21/21	-
5	BTB	C	1334	-	-	5/21/21/21	-
5	BTB	A	1335	-	-	13/21/21/21	-
5	BTB	C	1335	-	-	11/21/21/21	-
5	BTB	D	1333	-	-	3/21/21/21	-
5	BTB	A	1336	-	-	10/21/21/21	-
5	BTB	A	1333	-	-	1/21/21/21	-
5	BTB	B	1331	-	-	9/21/21/21	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1335	BTB	C1-C2	-3.26	1.49	1.53
5	A	1335	BTB	C3-C2	-3.12	1.49	1.53
5	C	1334	BTB	C7-N	-2.91	1.43	1.48
5	C	1335	BTB	C4-C2	-2.82	1.49	1.53
5	A	1335	BTB	C7-N	2.77	1.52	1.48

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1335	BTB	O3-C3-C2	-4.03	100.41	111.44
5	A	1334	BTB	O3-C3-C2	-3.30	102.41	111.44
5	A	1335	BTB	C6-C5-N	3.02	123.39	111.59
5	D	1333	BTB	O1-C1-C2	-3.02	103.18	111.44
5	D	1333	BTB	O3-C3-C2	-2.90	103.49	111.44

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1331	BTB	O1-C1-C2-C3
5	B	1331	BTB	C1-C2-C3-O3
5	B	1331	BTB	C4-C2-C3-O3
5	C	1334	BTB	C1-C2-C4-O4
5	C	1334	BTB	C3-C2-C4-O4

There are no ring outliers.

8 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1334	BTB	1	0
5	C	1334	BTB	3	0
5	A	1335	BTB	8	1
5	C	1335	BTB	15	0
5	D	1333	BTB	2	0
5	A	1336	BTB	13	0
5	A	1333	BTB	2	0
5	B	1331	BTB	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	327/327 (100%)	-0.44	3 (0%) 84 86	10, 17, 37, 54	0
1	B	327/327 (100%)	-0.14	16 (4%) 29 35	13, 26, 47, 68	0
1	C	327/327 (100%)	-0.60	1 (0%) 94 95	9, 17, 34, 51	0
1	D	327/327 (100%)	-0.46	5 (1%) 73 77	9, 16, 35, 60	0
All	All	1308/1308 (100%)	-0.41	25 (1%) 66 71	9, 19, 41, 68	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	73	ALA	3.9
1	B	132	ASP	3.9
1	B	74	GLY	3.7
1	A	73	ALA	3.6
1	B	72	GLN	3.6

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å^2)	Q<0.9
5	BTB	A	1335	14/14	0.86	0.23	14,23,26,26	0
5	BTB	A	1336	14/14	0.89	0.31	24,27,29,30	0
5	BTB	C	1335	14/14	0.91	0.18	25,30,31,32	0
5	BTB	B	1331	14/14	0.93	0.11	26,29,34,38	0
5	BTB	D	1333	14/14	0.94	0.14	20,23,28,29	0
5	BTB	A	1333	14/14	0.95	0.11	21,25,31,31	0
5	BTB	A	1334	14/14	0.95	0.09	17,23,28,29	0
5	BTB	C	1334	14/14	0.95	0.11	19,23,30,31	0
2	MG	D	1328	1/1	0.96	0.11	14,14,14,14	0
2	MG	B	1328	1/1	0.98	0.08	29,29,29,29	0
2	MG	C	1328	1/1	0.98	0.04	17,17,17,17	0
4	IOD	D	1330	1/1	0.98	0.04	30,30,30,30	1
4	IOD	A	1332	1/1	0.99	0.10	25,25,25,25	1
3	CL	B	1329	1/1	0.99	0.09	27,27,27,27	0
3	CL	C	1329	1/1	0.99	0.08	22,22,22,22	0
4	IOD	D	1332	1/1	0.99	0.08	25,25,25,25	1
4	IOD	D	1331	1/1	0.99	0.10	30,30,30,30	1
4	IOD	A	1330	1/1	0.99	0.08	19,19,19,19	1
4	IOD	C	1333	1/1	0.99	0.03	28,28,28,28	1
2	MG	A	1328	1/1	0.99	0.06	15,15,15,15	0
4	IOD	A	1331	1/1	0.99	0.05	28,28,28,28	1
4	IOD	B	1332	1/1	0.99	0.06	28,28,28,28	1
4	IOD	B	1330	1/1	0.99	0.16	22,22,22,22	1
4	IOD	C	1332	1/1	0.99	0.07	19,19,19,19	1
4	IOD	A	1337	1/1	0.99	0.09	28,28,28,28	1
4	IOD	C	1330	1/1	1.00	0.07	18,18,18,18	0
3	CL	D	1329	1/1	1.00	0.10	20,20,20,20	0
3	CL	A	1329	1/1	1.00	0.10	18,18,18,18	0
4	IOD	C	1331	1/1	1.00	0.08	24,24,24,24	1

6.5 Other polymers (i)

There are no such residues in this entry.