



# Full wwPDB X-ray Structure Validation Report ⓘ

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 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (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

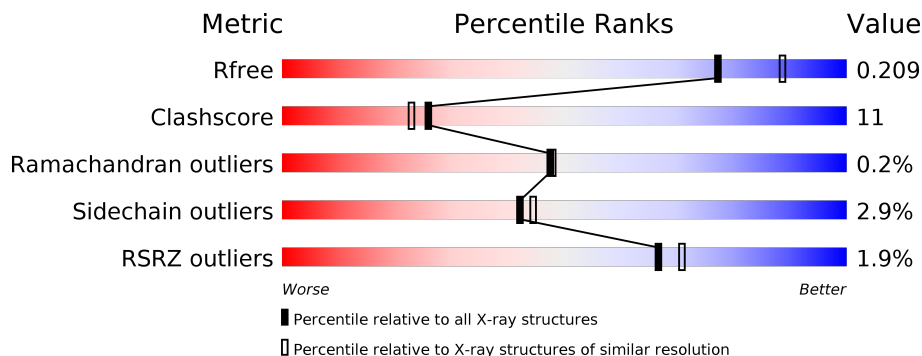
# 1 Overall quality at a glance

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  $\geq 3$ , 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  $\leq 5\%$ . 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	327	 2% 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 [i](#)

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
			Total	C	N	O	S			
1	A	327	2615	1674	439	490	12	0	0	0
1	B	327	2615	1674	439	490	12	0	0	0
1	C	327	2615	1674	439	490	12	0	0	0
1	D	327	2615	1674	439	490	12	0	0	0

- 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		

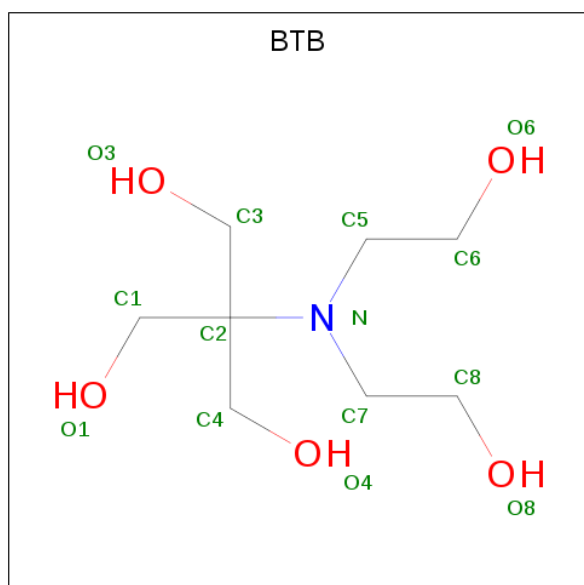
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



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

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

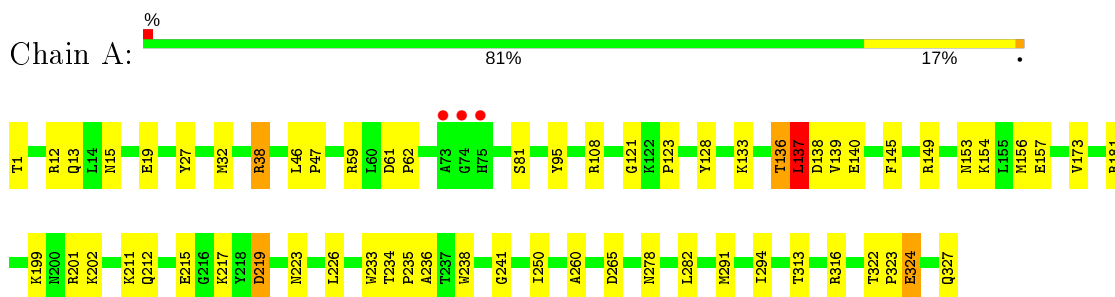
- Molecule 6 is water.

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

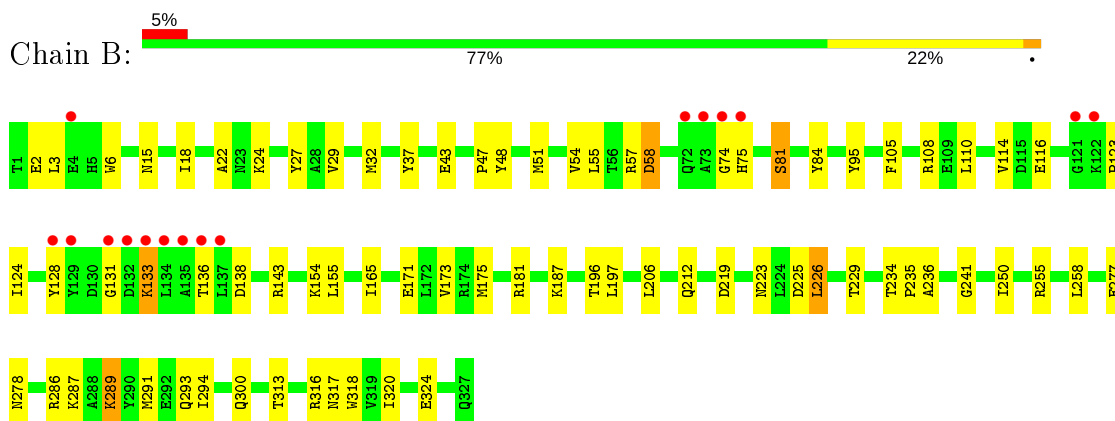
### 3 Residue-property plots

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.

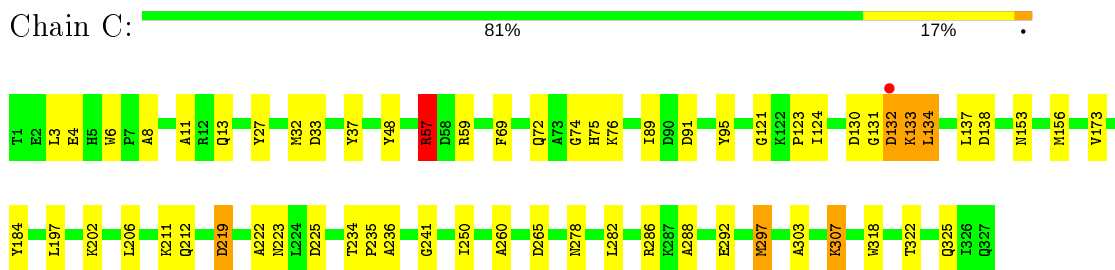
- Molecule 1: PHOSPHORYLCHOLINE PHOSPHATASE



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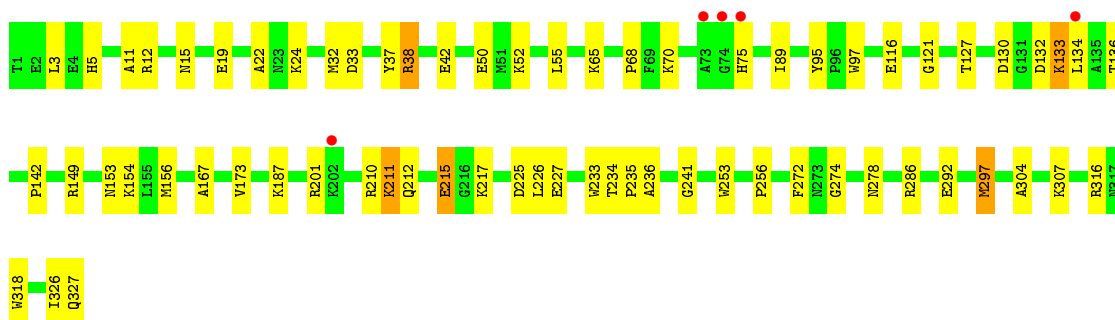


- Molecule 1: PHOSPHORYLCHOLINE PHOSPHATASE



- Molecule 1: PHOSPHORYLCHOLINE PHOSPHATASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 2.12Å)	Xtrriage
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 <sup>2</sup> )	19.6	Xtrriage
Anisotropy	0.034	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 58.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11407	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage'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.*

<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, 0.333 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, 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

All (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
1	D	215	GLU	CG-CD	5.55	1.60	1.51
1	A	233	TRP	CD2-CE2	5.52	1.48	1.41
1	D	233	TRP	CD2-CE2	5.35	1.47	1.41
1	D	318	TRP	CD2-CE2	5.14	1.47	1.41
1	B	6	TRP	CD2-CE2	5.11	1.47	1.41
1	B	318	TRP	CD2-CE2	5.00	1.47	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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
1	C	134	LEU	CB-CG-CD1	-7.28	98.63	111.00
1	D	286	ARG	NE-CZ-NH1	-6.85	116.88	120.30
1	D	12	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	A	265	ASP	CB-CG-OD1	6.48	124.13	118.30
1	D	38	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	59	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	D	316	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	219	ASP	CB-CG-OD1	5.92	123.63	118.30
1	D	12	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	38	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	B	255	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	D	297	MET	CG-SD-CE	5.79	109.47	100.20
1	C	297	MET	CG-SD-CE	5.76	109.41	100.20
1	B	219	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	C	219	ASP	CB-CG-OD1	5.65	123.39	118.30
1	C	225	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	137	LEU	CA-CB-CG	5.33	127.56	115.30
1	A	108	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	D	116	GLU	CB-CA-C	-5.13	100.15	110.40

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

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
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.

All (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
5:C:1335:BTB:H81	5:C:1335:BTB:H41	1.15	1.12
5:A:1335:BTB:H42	5:A:1335:BTB:C6	1.64	1.11
5:C:1335:BTB:H12	5:C:1335:BTB:H62	1.30	1.08
5:A:1335:BTB:H62	5:A:1335:BTB:H42	1.13	1.08
5:A:1336:BTB:H72	5:A:1336:BTB:O4	1.30	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:MET:HG2	6:D:2190:HOH:O	1.55	1.04
5:C:1335:BTB:C8	5:C:1335:BTB:C4	2.36	1.02
1:C:219:ASP:HB3	6:C:2171:HOH:O	1.58	1.01
1:A:140:GLU:OE1	5:A:1335:BTB:H12	1.61	1.01
1:A:316:ARG:HD3	6:A:2217:HOH:O	1.59	1.01
1:D:215:GLU:HG3	1:D:217:LYS:HG2	1.43	1.00
5:C:1335:BTB:C6	5:C:1335:BTB:H12	1.93	0.98
5:A:1335:BTB:H62	5:A:1335:BTB:C4	1.94	0.98
5:A:1336:BTB:H72	5:A:1336:BTB:HO4	1.30	0.97
1:C:211:LYS:HE2	6:C:2166:HOH:O	1.63	0.96
1:C:121:GLY:HA2	6:C:2117:HOH:O	1.64	0.94
1:A:212:GLN:HE22	1:A:223:ASN:HD21	1.12	0.94
1:D:297:MET:SD	6:D:2186:HOH:O	2.25	0.92
1:A:199:LYS:HD2	6:A:2147:HOH:O	1.73	0.87
1:A:219:ASP:HB2	6:A:2165:HOH:O	1.76	0.86
1:C:8:ALA:HB2	5:C:1335:BTB:H71	1.60	0.83
1:B:15:ASN:OD1	1:B:154:LYS:HE2	1.80	0.80
1:D:11:ALA:HB1	6:D:2017:HOH:O	1.80	0.80
1:A:15:ASN:OD1	1:A:154:LYS:HE2	1.82	0.80
1:D:15:ASN:OD1	1:D:154:LYS:HE2	1.81	0.80
1:A:121:GLY:O	5:A:1335:BTB:O1	2.01	0.79
5:A:1336:BTB:O6	5:A:1336:BTB:H12	1.82	0.79
1:B:316:ARG:NH1	1:B:317:ASN:HD21	1.82	0.78
1:B:48:TYR:HB2	1:B:124:ILE:HD13	1.65	0.78
1:D:38:ARG:HH11	1:D:327:GLN:HE21	1.30	0.78
1:D:215:GLU:HG3	1:D:217:LYS:CG	2.15	0.77
1:C:212:GLN:HE22	1:C:223:ASN:HD21	1.34	0.75
1:B:278:ASN:HD22	1:B:316:ARG:NH1	1.86	0.73
1:C:3:LEU:O	5:C:1335:BTB:H11	1.88	0.73
5:C:1335:BTB:H62	5:C:1335:BTB:C1	2.15	0.73
1:C:57:ARG:HD3	6:C:2055:HOH:O	1.88	0.71
1:C:132:ASP:OD2	1:C:133:LYS:HE2	1.89	0.71
1:A:327:GLN:HB3	5:A:1336:BTB:H82	1.72	0.71
1:C:288:ALA:O	1:C:292:GLU:HG3	1.91	0.70
1:B:123:PRO:HB3	1:B:138:ASP:HB3	1.74	0.69
1:B:181:ARG:HD3	6:B:2081:HOH:O	1.91	0.69
1:B:81:SER:HB2	1:B:128:TYR:HA	1.76	0.68
1:B:57:ARG:HB2	6:B:2030:HOH:O	1.92	0.68
1:C:265:ASP:OD2	6:C:2097:HOH:O	2.10	0.68
1:B:212:GLN:HE22	1:B:223:ASN:HD21	1.41	0.68
1:B:75:HIS:HE1	6:B:2043:HOH:O	1.77	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1336:BTB:H42	5:A:1336:BTB:H81	1.76	0.67
1:B:291:MET:HE1	1:B:320:ILE:HG21	1.76	0.67
1:A:153:ASN:HA	1:A:156:MET:HE2	1.77	0.66
1:B:181:ARG:O	1:B:181:ARG:HG2	1.95	0.65
1:D:149:ARG:HG2	6:D:2114:HOH:O	1.95	0.65
1:A:149:ARG:HG2	1:A:149:ARG:HH11	1.63	0.64
5:C:1335:BTB:O1	5:C:1335:BTB:H72	1.98	0.63
1:D:3:LEU:HD12	6:D:2017:HOH:O	1.97	0.63
6:C:2205:HOH:O	1:D:253:TRP:HZ3	1.82	0.62
1:B:29:VAL:HG11	1:B:165:ILE:HD12	1.81	0.62
1:A:211:LYS:O	1:A:215:GLU:HG2	2.01	0.61
1:B:278:ASN:HA	1:B:316:ARG:NH1	2.15	0.61
1:C:8:ALA:CB	5:C:1335:BTB:H71	2.29	0.61
1:A:313:THR:HG22	1:A:316:ARG:CZ	2.30	0.61
1:C:297:MET:HG3	6:C:2207:HOH:O	1.99	0.60
5:A:1336:BTB:C7	5:A:1336:BTB:O4	2.24	0.60
1:B:27:TYR:CE2	1:B:250:ILE:HG21	2.36	0.60
1:D:3:LEU:HB2	6:D:2017:HOH:O	2.02	0.60
1:C:303:ALA:O	1:C:307:LYS:HG2	2.02	0.60
1:A:38:ARG:HH11	1:A:327:GLN:HE21	1.49	0.60
1:C:278:ASN:HB2	6:C:2217:HOH:O	2.02	0.60
1:A:137:LEU:HD21	1:A:139:VAL:HG22	1.83	0.59
1:C:222:ALA:CB	6:C:2171:HOH:O	2.50	0.59
1:D:22:ALA:O	1:D:24:LYS:HG3	2.02	0.59
1:A:236:ALA:O	1:A:241:GLY:HA3	2.03	0.59
1:A:95:TYR:CZ	5:A:1333:BTB:H52	2.38	0.58
1:C:297:MET:HE3	6:C:2227:HOH:O	2.03	0.58
1:C:211:LYS:HE3	1:D:89:ILE:O	2.03	0.58
1:C:75:HIS:HE1	6:C:2076:HOH:O	1.87	0.58
1:A:140:GLU:OE1	5:A:1335:BTB:C1	2.43	0.58
1:D:272:PHE:HE2	1:D:297:MET:HE2	1.69	0.58
1:C:59:ARG:HD3	6:C:2022:HOH:O	2.04	0.58
1:B:289:LYS:O	1:B:293:GLN:HG3	2.03	0.57
1:B:58:ASP:HB3	6:B:2028:HOH:O	2.04	0.57
1:B:95:TYR:CZ	5:B:1331:BTB:H72	2.39	0.57
6:C:2197:HOH:O	1:D:297:MET:CE	2.51	0.57
1:D:70:LYS:HG3	6:D:2032:HOH:O	2.04	0.57
1:B:291:MET:CE	1:B:320:ILE:HG21	2.35	0.56
5:A:1336:BTB:H51	5:A:1336:BTB:O1	2.04	0.56
1:C:211:LYS:CE	6:C:2166:HOH:O	2.34	0.56
1:D:15:ASN:ND2	6:D:2017:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:PHE:HE2	1:D:297:MET:CE	2.20	0.55
5:C:1335:BTB:C8	5:C:1335:BTB:H42	2.32	0.55
1:D:127:THR:HG22	1:D:136:THR:HG22	1.89	0.55
1:A:13:GLN:NE2	6:A:2020:HOH:O	2.40	0.54
1:D:292:GLU:HA	4:D:1332:IOD:I	2.78	0.54
1:D:75:HIS:HE1	6:D:2073:HOH:O	1.89	0.54
1:D:167:ALA:HB3	3:D:1329:CL:CL	2.45	0.54
1:A:137:LEU:CD2	1:A:139:VAL:HG22	2.39	0.53
1:B:108:ARG:NH2	1:B:225:ASP:OD2	2.41	0.53
1:D:149:ARG:HH11	1:D:149:ARG:HG2	1.73	0.53
1:A:133:LYS:NZ	6:A:2112:HOH:O	2.41	0.53
6:C:2197:HOH:O	1:D:297:MET:HE1	2.06	0.53
1:A:202:LYS:HD2	6:A:2148:HOH:O	2.09	0.53
1:C:197:LEU:HD13	1:C:206:LEU:HD13	1.90	0.52
1:B:187:LYS:HE2	6:B:2071:HOH:O	2.09	0.52
1:D:153:ASN:HA	1:D:156:MET:HE2	1.91	0.52
1:A:217:LYS:HE3	1:C:13:GLN:HE22	1.74	0.52
1:B:22:ALA:O	1:B:24:LYS:HG3	2.10	0.52
1:A:137:LEU:HD21	1:A:139:VAL:CG2	2.40	0.51
5:C:1335:BTB:O8	5:C:1335:BTB:H42	2.09	0.51
1:A:15:ASN:OD1	1:A:154:LYS:CE	2.57	0.51
1:C:212:GLN:HE22	1:C:223:ASN:ND2	2.06	0.51
1:D:236:ALA:O	1:D:241:GLY:HA3	2.11	0.51
1:A:201:ARG:NH2	6:A:2153:HOH:O	2.43	0.51
1:C:48:TYR:HB2	1:C:124:ILE:HD13	1.93	0.51
1:D:38:ARG:HD2	1:D:327:GLN:NE2	2.26	0.51
1:C:222:ALA:HB2	6:C:2171:HOH:O	2.09	0.51
1:C:234:THR:HA	1:C:235:PRO:C	2.30	0.51
1:D:32:MET:HG3	1:D:37:TYR:CE2	2.46	0.51
1:D:65:LYS:NZ	6:D:2068:HOH:O	2.44	0.51
1:C:95:TYR:CZ	5:C:1334:BTB:H72	2.46	0.51
1:C:6:TRP:O	5:C:1335:BTB:O1	2.29	0.50
1:A:324:GLU:O	5:A:1336:BTB:C8	2.59	0.50
1:C:11:ALA:HB3	5:C:1335:BTB:H62	1.94	0.50
1:D:212:GLN:HA	1:D:215:GLU:HG2	1.93	0.50
1:A:1:THR:CA	6:A:2002:HOH:O	2.46	0.49
1:C:123:PRO:HB3	1:C:138:ASP:HB3	1.93	0.49
5:A:1336:BTB:C8	5:A:1336:BTB:H42	2.38	0.49
1:A:27:TYR:CE2	1:A:250:ILE:HG21	2.47	0.49
1:B:18:ILE:HG12	1:B:155:LEU:HD23	1.94	0.49
1:A:123:PRO:HB2	1:A:138:ASP:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:MET:HG2	1:D:173:VAL:HG13	1.94	0.49
1:C:260:ALA:HA	1:C:282:LEU:O	2.12	0.49
1:D:95:TYR:CZ	5:D:1333:BTB:H52	2.46	0.49
1:A:327:GLN:O	5:A:1336:BTB:H62	2.12	0.49
1:C:322:THR:OG1	1:C:325:GLN:HG3	2.13	0.48
1:B:223:ASN:HA	1:B:226:LEU:HD22	1.95	0.48
1:B:324:GLU:CD	1:B:324:GLU:H	2.17	0.48
1:C:57:ARG:CD	6:C:2055:HOH:O	2.53	0.48
1:C:95:TYR:OH	6:C:2096:HOH:O	2.17	0.47
1:D:234:THR:HA	1:D:235:PRO:C	2.35	0.47
1:C:222:ALA:HB3	6:C:2171:HOH:O	2.12	0.47
6:A:2227:HOH:O	1:B:300:GLN:NE2	2.43	0.47
1:C:286:ARG:HB3	6:C:2038:HOH:O	2.14	0.47
1:B:110:LEU:O	1:B:114:VAL:HG23	2.13	0.47
1:A:137:LEU:CD2	1:A:139:VAL:CG2	2.94	0.46
1:A:236:ALA:HB1	1:A:238:TRP:CZ2	2.51	0.46
1:A:260:ALA:HA	1:A:282:LEU:O	2.15	0.46
1:A:215:GLU:HG3	6:A:2077:HOH:O	2.15	0.46
1:C:27:TYR:CE2	1:C:250:ILE:HG21	2.50	0.46
1:A:32:MET:HG2	1:A:173:VAL:HG13	1.97	0.46
1:B:108:ARG:HH21	1:B:225:ASP:CG	2.19	0.46
5:C:1335:BTB:O8	5:C:1335:BTB:C4	2.62	0.46
1:B:236:ALA:O	1:B:241:GLY:HA3	2.15	0.45
5:D:1333:BTB:H32	5:D:1333:BTB:H72	1.61	0.45
1:B:196:THR:HB	1:B:229:THR:O	2.16	0.45
1:A:95:TYR:CE1	5:A:1333:BTB:H71	2.52	0.45
5:A:1334:BTB:H72	6:A:2181:HOH:O	2.17	0.45
1:B:2:GLU:CD	1:B:3:LEU:H	2.20	0.45
1:B:48:TYR:HB2	1:B:124:ILE:CD1	2.42	0.45
1:A:322:THR:HB	1:A:324:GLU:OE1	2.17	0.45
1:C:153:ASN:HA	1:C:156:MET:HE2	1.98	0.45
1:D:201:ARG:NE	1:D:227:GLU:OE1	2.46	0.45
5:C:1334:BTB:C5	5:C:1334:BTB:O4	2.65	0.44
1:D:256:PRO:HD2	1:D:274:GLY:O	2.16	0.44
1:A:327:GLN:C	5:A:1336:BTB:H62	2.38	0.44
1:D:304:ALA:HA	1:D:307:LYS:HE3	2.00	0.44
1:A:1:THR:N	6:A:2002:HOH:O	1.77	0.44
1:B:258:LEU:HD23	1:B:258:LEU:C	2.38	0.44
1:B:32:MET:HG2	1:B:173:VAL:HG13	2.00	0.44
1:C:33:ASP:HA	1:C:37:TYR:CE1	2.53	0.44
1:C:89:ILE:O	1:D:211:LYS:HE3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LYS:HE2	6:C:2237:HOH:O	2.17	0.44
1:D:225:ASP:OD2	6:D:2141:HOH:O	2.21	0.44
1:A:38:ARG:HD2	1:A:327:GLN:NE2	2.33	0.43
1:C:72:GLN:HG2	1:C:75:HIS:HB3	2.00	0.43
1:B:133:LYS:HE2	1:B:133:LYS:HB3	1.77	0.43
1:B:32:MET:HG3	1:B:37:TYR:CE2	2.53	0.43
1:C:130:ASP:O	1:C:133:LYS:HE3	2.18	0.43
1:D:75:HIS:CE1	1:D:134:LEU:HD11	2.54	0.43
1:A:324:GLU:O	5:A:1336:BTB:H82	2.19	0.43
1:B:48:TYR:OH	1:B:116:GLU:HG2	2.19	0.43
5:C:1334:BTB:H52	5:C:1334:BTB:H32	1.38	0.43
1:D:37:TYR:CD1	1:D:142:PRO:HB3	2.53	0.43
1:A:234:THR:HA	1:A:235:PRO:C	2.39	0.42
1:B:277:GLU:HA	1:B:313:THR:HG21	2.00	0.42
1:C:32:MET:HG2	1:C:173:VAL:HG13	2.01	0.42
1:D:5:HIS:O	1:D:326:ILE:HA	2.19	0.42
1:A:38:ARG:HB2	1:A:145:PHE:CE1	2.54	0.42
1:D:210:ARG:HG2	6:D:2121:HOH:O	2.18	0.42
6:C:2197:HOH:O	1:D:297:MET:HE3	2.15	0.42
1:B:197:LEU:HD13	1:B:206:LEU:HD13	2.02	0.42
1:A:1:THR:OG1	1:A:157:GLU:OE2	2.31	0.42
1:A:217:LYS:HE3	1:C:13:GLN:NE2	2.34	0.42
1:C:278:ASN:ND2	6:C:2218:HOH:O	2.44	0.42
1:C:91:ASP:OD2	6:C:2097:HOH:O	2.21	0.42
1:A:136:THR:CG2	6:A:2116:HOH:O	2.68	0.42
1:D:38:ARG:HD2	1:D:327:GLN:HE22	1.84	0.42
1:B:234:THR:HA	1:B:235:PRO:C	2.40	0.41
1:C:57:ARG:HD2	1:C:69:PHE:CE1	2.55	0.41
1:D:201:ARG:NH2	6:D:2090:HOH:O	2.23	0.41
1:D:33:ASP:HA	1:D:37:TYR:CE1	2.55	0.41
1:A:15:ASN:O	1:A:19:GLU:HG2	2.20	0.41
1:A:46:LEU:HB3	1:A:47:PRO:CD	2.51	0.41
1:C:292:GLU:HB3	6:C:2226:HOH:O	2.19	0.41
5:A:1336:BTB:HO6	5:A:1336:BTB:H12	1.81	0.41
1:A:291:MET:HE1	1:A:294:ILE:CG2	2.50	0.41
1:A:61:ASP:HA	1:A:62:PRO:HD3	1.94	0.41
1:B:43:GLU:O	1:B:47:PRO:CD	2.69	0.41
1:D:52:LYS:HG2	6:D:2055:HOH:O	2.21	0.41
1:A:140:GLU:CD	5:A:1335:BTB:H12	2.35	0.41
1:B:54:VAL:HG12	1:B:105:PHE:CZ	2.55	0.41
5:A:1335:BTB:H71	5:A:1335:BTB:H31	1.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ASP:N	1:D:133:LYS:O	2.50	0.41
1:A:81:SER:HB2	1:A:128:TYR:HA	2.02	0.40
1:C:222:ALA:O	6:C:2173:HOH:O	2.22	0.40
1:C:236:ALA:O	1:C:241:GLY:HA3	2.21	0.40
1:B:171:GLU:O	1:B:175:MET:HG3	2.21	0.40
1:B:278:ASN:HD22	1:B:316:ARG:CZ	2.35	0.40
1:D:50:GLU:HA	1:D:55:LEU:O	2.22	0.40

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
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

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	THR
1	A	137	LEU
1	A	181	ARG
1	A	226	LEU
1	A	278	ASN
1	A	323	PRO
1	B	51	MET
1	B	55	LEU
1	B	58	ASP
1	B	81	SER
1	B	84	TYR
1	B	133	LYS
1	B	136	THR
1	B	226	LEU
1	B	286	ARG
1	B	287	LYS
1	B	289	LYS
1	B	294	ILE
1	C	4	GLU
1	C	57	ARG
1	C	76	LYS
1	C	132	ASP
1	C	133	LYS
1	C	134	LEU

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Mol	Chain	Res	Type
1	C	137	LEU
1	C	202	LYS
1	C	307	LYS
1	D	19	GLU
1	D	68	PRO
1	D	132	ASP
1	D	133	LYS
1	D	226	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	185	ASN
1	A	223	ASN
1	A	295	ASN
1	A	327	GLN
1	B	23	ASN
1	B	75	HIS
1	B	185	ASN
1	B	223	ASN
1	B	278	ASN
1	B	300	GLN
1	B	317	ASN
1	C	13	GLN
1	C	75	HIS
1	C	185	ASN
1	C	223	ASN
1	C	278	ASN
1	D	75	HIS
1	D	185	ASN
1	D	223	ASN
1	D	327	GLN

### 5.3.3 RNA

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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-

All (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
5	A	1334	BTB	C5-N	2.75	1.51	1.48
5	A	1335	BTB	C7-C8	2.65	1.61	1.51
5	C	1335	BTB	C2-N	-2.48	1.43	1.48
5	A	1334	BTB	C1-C2	2.40	1.56	1.53
5	A	1333	BTB	C4-C2	2.25	1.56	1.53
5	C	1334	BTB	C2-N	-2.17	1.44	1.48
5	A	1335	BTB	C4-C2	-2.06	1.50	1.53
5	C	1335	BTB	C5-N	2.05	1.50	1.48
5	A	1336	BTB	C5-C6	2.03	1.59	1.51
5	A	1336	BTB	C3-C2	-2.03	1.50	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
5	A	1333	BTB	O1-C1-C2	-2.77	103.87	111.44
5	A	1335	BTB	O4-C4-C2	2.59	118.54	111.44
5	C	1334	BTB	O4-C4-C2	2.42	118.08	111.44
5	C	1335	BTB	C6-C5-N	2.41	120.99	111.59
5	C	1334	BTB	O1-C1-C2	-2.40	104.87	111.44
5	C	1335	BTB	O3-C3-C2	-2.38	104.94	111.44
5	C	1334	BTB	C8-C7-N	2.15	119.99	111.59
5	C	1335	BTB	O6-C6-C5	2.13	120.03	111.19

There are no chirality outliers.

All (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
5	C	1334	BTB	N-C2-C4-O4
5	C	1335	BTB	O1-C1-C2-C3
5	C	1335	BTB	O1-C1-C2-C4
5	C	1335	BTB	C1-C2-C3-O3
5	C	1335	BTB	C4-C2-C3-O3
5	C	1335	BTB	N-C2-C3-O3
5	C	1335	BTB	C1-C2-C4-O4
5	C	1335	BTB	C3-C2-C4-O4
5	C	1335	BTB	N-C2-C4-O4
5	C	1335	BTB	C6-C5-N-C2
5	C	1335	BTB	N-C7-C8-O8
5	D	1333	BTB	C1-C2-C4-O4
5	A	1335	BTB	C1-C2-C4-O4
5	A	1335	BTB	C3-C2-C4-O4
5	A	1335	BTB	N-C2-C4-O4
5	A	1335	BTB	C1-C2-N-C5
5	A	1335	BTB	C1-C2-N-C7
5	A	1335	BTB	C3-C2-N-C5
5	A	1335	BTB	C3-C2-N-C7
5	A	1335	BTB	C4-C2-N-C5
5	A	1335	BTB	C4-C2-N-C7
5	A	1335	BTB	C6-C5-N-C2
5	A	1335	BTB	C8-C7-N-C5
5	A	1335	BTB	N-C5-C6-O6
5	A	1336	BTB	C1-C2-C3-O3
5	A	1336	BTB	C4-C2-C3-O3
5	A	1336	BTB	N-C2-C3-O3
5	A	1336	BTB	C1-C2-N-C5
5	A	1336	BTB	C1-C2-N-C7
5	A	1336	BTB	C3-C2-N-C5
5	A	1336	BTB	C3-C2-N-C7
5	A	1336	BTB	C4-C2-N-C5
5	A	1336	BTB	C4-C2-N-C7
5	C	1335	BTB	N-C5-C6-O6
5	A	1333	BTB	N-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	D	1333	BTB	N-C5-C6-O6
5	C	1334	BTB	N-C7-C8-O8
5	C	1334	BTB	N-C5-C6-O6
5	B	1331	BTB	N-C7-C8-O8
5	B	1331	BTB	O1-C1-C2-C4
5	D	1333	BTB	C3-C2-C4-O4
5	B	1331	BTB	N-C2-C3-O3
5	B	1331	BTB	C3-C2-N-C5
5	B	1331	BTB	C4-C2-N-C5
5	A	1335	BTB	N-C2-C3-O3
5	B	1331	BTB	N-C5-C6-O6
5	A	1336	BTB	N-C7-C8-O8

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<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	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

All (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
1	B	134	LEU	3.5
1	D	74	GLY	3.5
1	A	74	GLY	3.4
1	D	73	ALA	3.4
1	B	133	LYS	3.2
1	D	202	LYS	3.2
1	B	135	ALA	3.2
1	B	131	GLY	2.9
1	B	136	THR	2.9
1	D	75	HIS	2.8
1	A	75	HIS	2.7
1	B	121	GLY	2.7
1	B	137	LEU	2.7
1	B	128	TYR	2.6
1	B	75	HIS	2.4
1	B	122	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	134	LEU	2.3
1	B	129	TYR	2.2
1	C	132	ASP	2.2
1	B	4	GLU	2.2

## 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. 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	B-factors(Å <sup>2</sup> )	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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.