Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 – 11:00 pm GMT

PDB ID	:	6Y01
Title	:	The structure of the molybdenum cofactor binding protein from the phototrophic bacterium Rippkaea orientalis
Authors	:	Krausze, J.
Deposited on	:	2020-02-05
Resolution	:	1.23 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

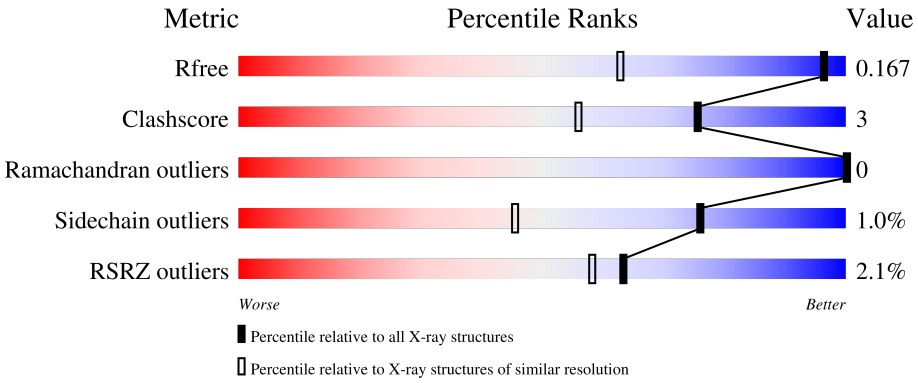
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.23 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	2024 (1.28-1.20)
Clashscore	141614	1007 (1.26-1.22)
Ramachandran outliers	138981	2053 (1.28-1.20)
Sidechain outliers	138945	2051 (1.28-1.20)
RSRZ outliers	127900	1987 (1.28-1.20)

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 of 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	AAA	178	3% 89% · 8%
1	BBB	178	% 88% 5% 7%
1	CCC	178	2% 86% 6% 8%
1	DDD	178	2% 87% 5% · 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5248 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 p450 cytochrome, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	164	Total	C	N	O	S	0	1	0
			1202	760	207	230	5			
1	BBB	165	Total	C	N	O	S	0	2	0
			1217	764	211	238	4			
1	CCC	163	Total	C	N	O	S	0	2	0
			1206	758	206	237	5			
1	DDD	166	Total	C	N	O	S	0	2	0
			1210	763	207	235	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-11	MET	-	initiating methionine	UNP B7K4Z0
AAA	-10	ARG	-	expression tag	UNP B7K4Z0
AAA	-9	GLY	-	expression tag	UNP B7K4Z0
AAA	-8	SER	-	expression tag	UNP B7K4Z0
AAA	-7	HIS	-	expression tag	UNP B7K4Z0
AAA	-6	HIS	-	expression tag	UNP B7K4Z0
AAA	-5	HIS	-	expression tag	UNP B7K4Z0
AAA	-4	HIS	-	expression tag	UNP B7K4Z0
AAA	-3	HIS	-	expression tag	UNP B7K4Z0
AAA	-2	HIS	-	expression tag	UNP B7K4Z0
AAA	-1	GLY	-	expression tag	UNP B7K4Z0
AAA	0	SER	-	expression tag	UNP B7K4Z0
AAA	164	LYS	-	expression tag	UNP B7K4Z0
AAA	165	LEU	-	expression tag	UNP B7K4Z0
AAA	166	ASN	-	expression tag	UNP B7K4Z0
BBB	-11	MET	-	initiating methionine	UNP B7K4Z0
BBB	-10	ARG	-	expression tag	UNP B7K4Z0
BBB	-9	GLY	-	expression tag	UNP B7K4Z0
BBB	-8	SER	-	expression tag	UNP B7K4Z0
BBB	-7	HIS	-	expression tag	UNP B7K4Z0
BBB	-6	HIS	-	expression tag	UNP B7K4Z0

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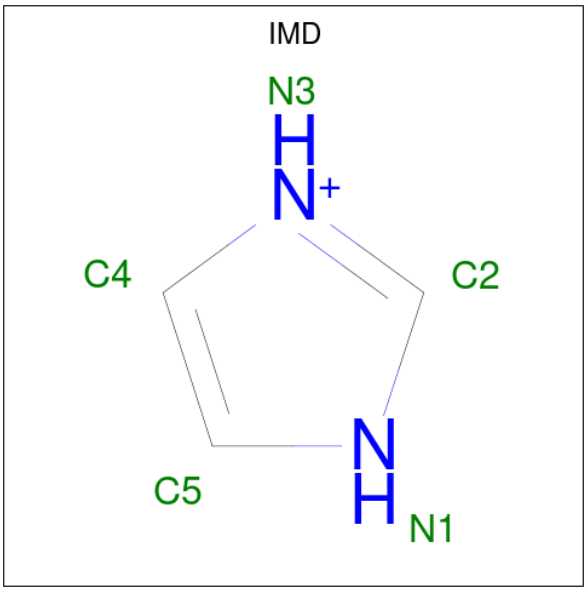
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-5	HIS	-	expression tag	UNP B7K4Z0
BBB	-4	HIS	-	expression tag	UNP B7K4Z0
BBB	-3	HIS	-	expression tag	UNP B7K4Z0
BBB	-2	HIS	-	expression tag	UNP B7K4Z0
BBB	-1	GLY	-	expression tag	UNP B7K4Z0
BBB	0	SER	-	expression tag	UNP B7K4Z0
BBB	164	LYS	-	expression tag	UNP B7K4Z0
BBB	165	LEU	-	expression tag	UNP B7K4Z0
BBB	166	ASN	-	expression tag	UNP B7K4Z0
CCC	-11	MET	-	initiating methionine	UNP B7K4Z0
CCC	-10	ARG	-	expression tag	UNP B7K4Z0
CCC	-9	GLY	-	expression tag	UNP B7K4Z0
CCC	-8	SER	-	expression tag	UNP B7K4Z0
CCC	-7	HIS	-	expression tag	UNP B7K4Z0
CCC	-6	HIS	-	expression tag	UNP B7K4Z0
CCC	-5	HIS	-	expression tag	UNP B7K4Z0
CCC	-4	HIS	-	expression tag	UNP B7K4Z0
CCC	-3	HIS	-	expression tag	UNP B7K4Z0
CCC	-2	HIS	-	expression tag	UNP B7K4Z0
CCC	-1	GLY	-	expression tag	UNP B7K4Z0
CCC	0	SER	-	expression tag	UNP B7K4Z0
CCC	164	LYS	-	expression tag	UNP B7K4Z0
CCC	165	LEU	-	expression tag	UNP B7K4Z0
CCC	166	ASN	-	expression tag	UNP B7K4Z0
DDD	-11	MET	-	initiating methionine	UNP B7K4Z0
DDD	-10	ARG	-	expression tag	UNP B7K4Z0
DDD	-9	GLY	-	expression tag	UNP B7K4Z0
DDD	-8	SER	-	expression tag	UNP B7K4Z0
DDD	-7	HIS	-	expression tag	UNP B7K4Z0
DDD	-6	HIS	-	expression tag	UNP B7K4Z0
DDD	-5	HIS	-	expression tag	UNP B7K4Z0
DDD	-4	HIS	-	expression tag	UNP B7K4Z0
DDD	-3	HIS	-	expression tag	UNP B7K4Z0
DDD	-2	HIS	-	expression tag	UNP B7K4Z0
DDD	-1	GLY	-	expression tag	UNP B7K4Z0
DDD	0	SER	-	expression tag	UNP B7K4Z0
DDD	164	LYS	-	expression tag	UNP B7K4Z0
DDD	165	LEU	-	expression tag	UNP B7K4Z0
DDD	166	ASN	-	expression tag	UNP B7K4Z0

- Molecule 2 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C N 5 3 2	0	0
2	BBB	1	Total C N 5 3 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	3	Total Cl 3 3	0	0
3	BBB	3	Total Cl 3 3	0	0
3	CCC	3	Total Cl 3 3	0	0
3	DDD	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	100	Total O 100 100	0	0
4	BBB	96	Total O 96 96	0	0
4	CCC	105	Total O 105 105	0	0

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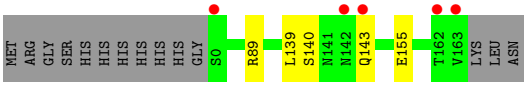
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	DDD	92	Total O 92 92	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

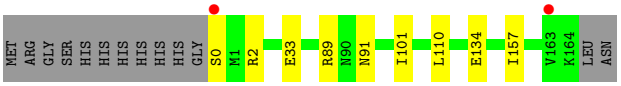
• Molecule 1: p450 cytochrome, putative

Chain AAA:



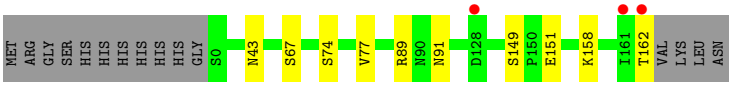
• Molecule 1: p450 cytochrome, putative

Chain BBB:



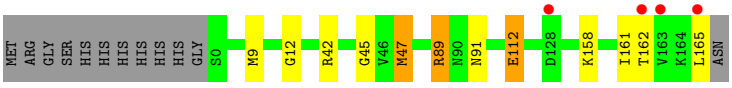
• Molecule 1: p450 cytochrome, putative

Chain CCC:



• Molecule 1: p450 cytochrome, putative

Chain DDD:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.58Å 72.04Å 70.26Å 90.00° 113.33° 90.00°	Depositor
Resolution (Å)	64.52 – 1.23 64.52 – 1.23	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.52-1.23) 100.0 (64.52-1.23)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 1.23Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.142 , 0.163 0.147 , 0.167	Depositor DCC
R_{free} test set	8868 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	15.7	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	5248	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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: IMD, CL

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	AAA	0.85	1/1217 (0.1%)	0.85	0/1658
1	BBB	0.83	2/1230 (0.2%)	0.86	0/1676
1	CCC	0.83	1/1219 (0.1%)	0.84	0/1658
1	DDD	0.81	1/1223 (0.1%)	0.84	2/1667 (0.1%)
All	All	0.83	5/4889 (0.1%)	0.85	2/6659 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	134	GLU	CD-OE1	-9.09	1.15	1.25
1	BBB	33	GLU	CD-OE2	-6.52	1.18	1.25
1	CCC	67	SER	CB-OG	-5.60	1.34	1.42
1	AAA	155	GLU	CD-OE2	5.14	1.31	1.25
1	DDD	112	GLU	CD-OE1	5.11	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	DDD	47	MET	CG-SD-CE	8.18	113.29	100.20
1	DDD	89	ARG	NE-CZ-NH1	6.87	123.74	120.30

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	AAA	1202	0	1231	2	0
1	BBB	1217	0	1237	6	0
1	CCC	1206	0	1237	5	0
1	DDD	1210	0	1234	18	0
2	AAA	5	0	5	0	0
2	BBB	5	0	5	0	0
3	AAA	3	0	0	0	0
3	BBB	3	0	0	0	0
3	CCC	3	0	0	0	0
3	DDD	1	0	0	0	0
4	AAA	100	0	0	0	0
4	BBB	96	0	0	1	0
4	CCC	105	0	0	2	0
4	DDD	92	0	0	1	0
All	All	5248	0	4949	30	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 3.

All (30) 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:DDD:9:MET:SD	1:DDD:112:GLU:OE1	1.96	1.24
1:DDD:42:ARG:H	1:DDD:47:MET:CE	1.54	1.20
1:DDD:42:ARG:HB2	1:DDD:47:MET:CE	1.79	1.12
1:DDD:42:ARG:HB2	1:DDD:47:MET:HE2	1.12	1.11
1:DDD:42:ARG:CB	1:DDD:47:MET:HE2	1.84	1.08
1:DDD:42:ARG:H	1:DDD:47:MET:HE3	0.99	1.07
1:DDD:42:ARG:N	1:DDD:47:MET:HE3	1.69	1.07
1:DDD:42:ARG:CB	1:DDD:47:MET:CE	2.37	1.02
1:BBB:0:SER:OG	1:BBB:2[B]:ARG:HG2	1.58	1.01
1:DDD:42:ARG:N	1:DDD:47:MET:CE	2.31	0.86
1:BBB:91:ASN:OD1	4:BBB:301:HOH:O	1.94	0.84
1:BBB:0:SER:HG	1:BBB:2[B]:ARG:HG2	1.44	0.82
1:CCC:91:ASN:HB2	4:CCC:316:HOH:O	1.82	0.79
1:DDD:158:LYS:O	1:DDD:162:THR:HG23	1.85	0.76
1:AAA:140:SER:O	1:AAA:143:GLN:HG2	1.86	0.76
1:CCC:158:LYS:O	1:CCC:162:THR:HG23	1.89	0.73
1:DDD:42:ARG:H	1:DDD:47:MET:HE1	1.53	0.70
1:DDD:91:ASN:HB2	4:DDD:302:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:42:ARG:CB	1:DDD:47:MET:HE3	2.21	0.69
1:CCC:91:ASN:OD1	4:CCC:301:HOH:O	2.10	0.68
1:DDD:42:ARG:CA	1:DDD:47:MET:HE3	2.31	0.59
1:BBB:0:SER:OG	1:BBB:2[B]:ARG:CG	2.42	0.57
1:DDD:42:ARG:CA	1:DDD:47:MET:CE	2.83	0.56
1:DDD:42:ARG:HB3	1:DDD:47:MET:CE	2.34	0.55
1:AAA:139:LEU:CD1	1:BBB:110:LEU:HD11	2.40	0.51
1:CCC:149:SER:OG	1:CCC:151[B]:GLU:HG2	2.13	0.47
1:DDD:161:ILE:O	1:DDD:165:LEU:HD13	2.16	0.45
1:CCC:74:SER:HB3	1:CCC:77:VAL:HG23	2.00	0.43
1:DDD:12:GLY:HA2	1:DDD:45:GLY:HA3	2.00	0.42
1:BBB:101:ILE:HD11	1:BBB:157:ILE:HD11	2.02	0.41

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	AAA	163/178 (92%)	161 (99%)	2 (1%)	0	100	100
1	BBB	165/178 (93%)	163 (99%)	2 (1%)	0	100	100
1	CCC	163/178 (92%)	161 (99%)	2 (1%)	0	100	100
1	DDD	166/178 (93%)	166 (100%)	0	0	100	100
All	All	657/712 (92%)	651 (99%)	6 (1%)	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	AAA	129/146 (88%)	128 (99%)	1 (1%)	81	55
1	BBB	131/146 (90%)	130 (99%)	1 (1%)	81	55
1	CCC	132/146 (90%)	130 (98%)	2 (2%)	65	29
1	DDD	130/146 (89%)	129 (99%)	1 (1%)	81	55
All	All	522/584 (89%)	517 (99%)	5 (1%)	76	45

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	89	ARG
1	BBB	89	ARG
1	CCC	43	ASN
1	CCC	89	ARG
1	DDD	89	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	IMD	BBB	201	-	3,5,5	5.03	2 (66%)	4,5,5	2.55	1 (25%)
2	IMD	AAA	201	-	3,5,5	0.26	0	4,5,5	0.77	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	IMD	BBB	201	-	-	-	0/1/1/1
2	IMD	AAA	201	-	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	201	IMD	C5-C4	6.53	1.67	1.37
2	BBB	201	IMD	C4-N3	5.43	1.63	1.37

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	201	IMD	C5-C4-N3	-4.84	88.47	108.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	AAA	164/178 (92%)	-0.11	5 (3%)	50	45	19, 25, 50, 79	0
1	BBB	165/178 (92%)	-0.16	2 (1%)	79	74	20, 28, 47, 70	0
1	CCC	163/178 (91%)	-0.13	3 (1%)	68	63	20, 24, 42, 79	0
1	DDD	166/178 (93%)	-0.15	4 (2%)	59	53	21, 29, 50, 81	0
All	All	658/712 (92%)	-0.14	14 (2%)	63	58	19, 26, 50, 81	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	163	VAL	5.3
1	BBB	0	SER	5.2
1	DDD	165	LEU	4.7
1	AAA	142	ASN	4.0
1	AAA	162	THR	3.3
1	BBB	163	VAL	2.8
1	AAA	0	SER	2.8
1	CCC	162	THR	2.8
1	DDD	128	ASP	2.7
1	DDD	163	VAL	2.5
1	AAA	143	GLN	2.2
1	DDD	162	THR	2.1
1	CCC	161	ILE	2.1
1	CCC	128	ASP	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 (i)

There are no monosaccharides 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^{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
2	IMD	AAA	201	5/5	0.82	0.16	61,63,70,75	0
2	IMD	BBB	201	5/5	0.87	0.23	85,100,110,111	0
3	CL	BBB	202	1/1	0.99	0.05	36,36,36,36	0
3	CL	BBB	204	1/1	0.99	0.04	37,37,37,37	0
3	CL	AAA	204	1/1	1.00	0.04	35,35,35,35	0
3	CL	AAA	202	1/1	1.00	0.04	34,34,34,34	0
3	CL	BBB	203	1/1	1.00	0.06	28,28,28,28	0
3	CL	AAA	203	1/1	1.00	0.06	28,28,28,28	0
3	CL	CCC	201	1/1	1.00	0.07	37,37,37,37	0
3	CL	CCC	202	1/1	1.00	0.06	28,28,28,28	0
3	CL	CCC	203	1/1	1.00	0.06	33,33,33,33	0
3	CL	DDD	201	1/1	1.00	0.04	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.