wwPDB X-ray Structure Validation Summary Report (i)

Aug 3, 2023 – 01:17 am BST

PDB ID	:	8COL
Title	:	Crystal structure of Rhizobium etli constitutive L-asparaginase ReAIV (orthorombic form R4oP-2)
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Deposited on	:	2023-02-28
Resolution	:	2.00 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 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:

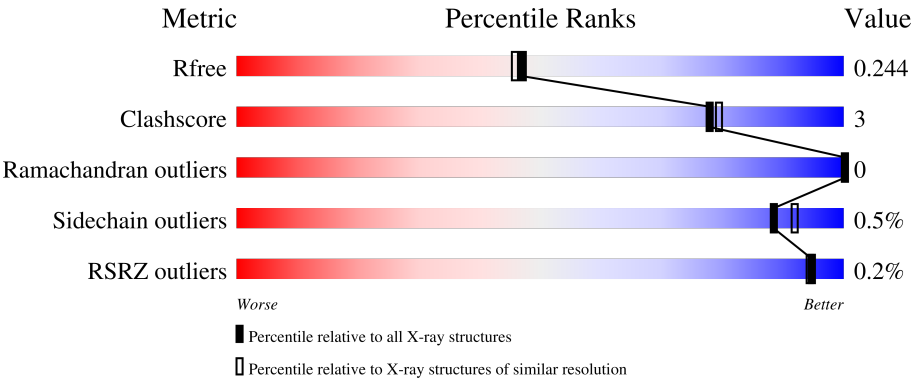
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	341	94%
1	BBB	341	91% 7%
1	CCC	341	91% 7%
1	DDD	341	93% 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10871 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 Putative L-asparaginase II protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	333	Total	C	N	O	S	0	5	0
			2481	1546	447	462	26			
1	BBB	335	Total	C	N	O	S	0	3	0
			2484	1546	448	462	28			
1	CCC	334	Total	C	N	O	S	0	7	0
			2498	1555	450	465	28			
1	DDD	335	Total	C	N	O	S	0	4	0
			2489	1549	448	464	28			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-5	GLY	-	expression tag	UNP Q2KB35
AAA	-4	ILE	-	expression tag	UNP Q2KB35
AAA	-3	ASP	-	expression tag	UNP Q2KB35
AAA	-2	PRO	-	expression tag	UNP Q2KB35
AAA	-1	PHE	-	expression tag	UNP Q2KB35
AAA	0	THR	-	expression tag	UNP Q2KB35
BBB	-5	GLY	-	expression tag	UNP Q2KB35
BBB	-4	ILE	-	expression tag	UNP Q2KB35
BBB	-3	ASP	-	expression tag	UNP Q2KB35
BBB	-2	PRO	-	expression tag	UNP Q2KB35
BBB	-1	PHE	-	expression tag	UNP Q2KB35
BBB	0	THR	-	expression tag	UNP Q2KB35
CCC	-5	GLY	-	expression tag	UNP Q2KB35
CCC	-4	ILE	-	expression tag	UNP Q2KB35
CCC	-3	ASP	-	expression tag	UNP Q2KB35
CCC	-2	PRO	-	expression tag	UNP Q2KB35
CCC	-1	PHE	-	expression tag	UNP Q2KB35
CCC	0	THR	-	expression tag	UNP Q2KB35
DDD	-5	GLY	-	expression tag	UNP Q2KB35
DDD	-4	ILE	-	expression tag	UNP Q2KB35
DDD	-3	ASP	-	expression tag	UNP Q2KB35

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	-2	PRO	-	expression tag	UNP Q2KB35
DDD	-1	PHE	-	expression tag	UNP Q2KB35
DDD	0	THR	-	expression tag	UNP Q2KB35

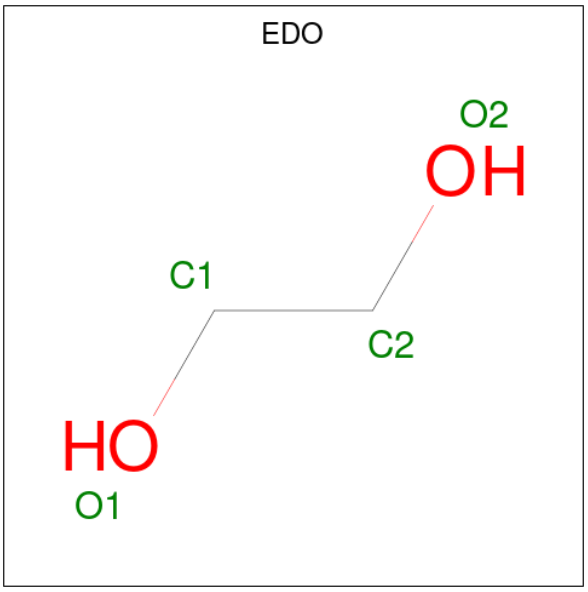
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total Zn 1 1	0	0
2	BBB	1	Total Zn 1 1	0	0
2	CCC	1	Total Zn 1 1	0	0
2	DDD	1	Total Zn 1 1	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	2	Total Cl 2 2	0	0
3	CCC	2	Total Cl 2 2	0	0
3	DDD	2	Total Cl 2 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	DDD	1	Total C O 4 2 2	0	0
4	DDD	1	Total C O 4 2 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	CCC	1	Total Mg 1 1	0	0
5	DDD	1	Total Mg 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	198	Total O 200 200	0	2
6	BBB	222	Total O 224 224	0	2
6	CCC	230	Total O 231 231	0	1

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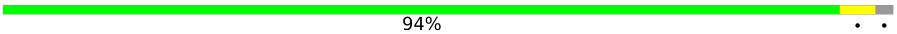
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	DDD	232	Total 233	O 233	0	1

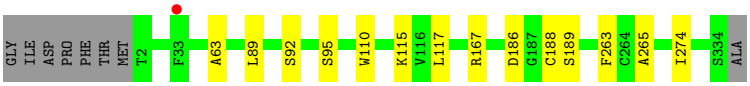
3 Residue-property plots (i)

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: Putative L-asparaginase II protein

Chain AAA:



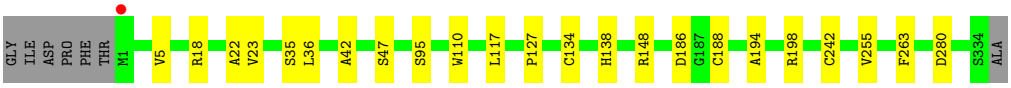


• Molecule 1: Putative L-asparaginase II protein

Chain BBB:

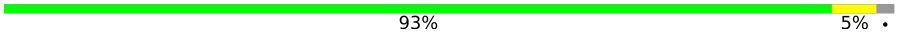
• Molecule 1: Putative L-asparaginase II protein

Chain CCC:



• Molecule 1: Putative L-asparaginase II protein

Chain DDD:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.10Å 89.75Å 169.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.60 – 2.00 84.60 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (84.60-2.00) 99.7 (84.60-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.177 , 0.234 0.190 , 0.244	Depositor DCC
R_{free} test set	1000 reflections (1.16%)	wwPDB-VP
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 56.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10871	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2210e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: CSO, CL, EDO, ZN, MG

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	0.80	0/2533	0.87	0/3422
1	BBB	0.83	0/2523	0.88	0/3409
1	CCC	0.82	1/2549 (0.0%)	0.86	0/3443
1	DDD	0.85	3/2531 (0.1%)	0.91	0/3420
All	All	0.83	4/10136 (0.0%)	0.88	0/13694

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	260	GLU	CD-OE1	6.19	1.32	1.25
1	CCC	255	VAL	C-O	5.36	1.33	1.23
1	DDD	73	LEU	C-O	5.30	1.33	1.23
1	DDD	277	LYS	C-O	5.21	1.33	1.23

There are no bond angle outliers.

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	2481	0	2466	8	0
1	BBB	2484	0	2466	16	0
1	CCC	2498	0	2490	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DDD	2489	0	2472	16	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
2	CCC	1	0	0	0	0
2	DDD	1	0	0	0	0
3	AAA	3	0	0	0	0
3	BBB	2	0	0	0	0
3	CCC	2	0	0	0	0
3	DDD	2	0	0	0	0
4	AAA	8	0	12	0	0
4	DDD	8	0	12	0	0
5	CCC	1	0	0	0	0
5	DDD	1	0	0	0	0
6	AAA	200	0	0	2	0
6	BBB	224	0	0	2	0
6	CCC	231	0	0	5	0
6	DDD	233	0	0	5	0
All	All	10871	0	9918	56	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.

The worst 5 of 56 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:AAA:188[B]:CYS:SG	6:AAA:644:HOH:O	2.08	1.11
1:CCC:47[B]:SER:OG	6:CCC:501:HOH:O	1.71	1.08
1:CCC:186[A]:ASP:OD1	6:CCC:502[A]:HOH:O	1.90	0.89
1:CCC:242[B]:CSO:OD	6:CCC:503:HOH:O	1.90	0.86
1:CCC:134[B]:CYS:HG	1:CCC:188[B]:CYS:HG	1.41	0.65

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	335/341 (98%)	329 (98%)	6 (2%)	0	100	100
1	BBB	334/341 (98%)	331 (99%)	3 (1%)	0	100	100
1	CCC	337/341 (99%)	332 (98%)	5 (2%)	0	100	100
1	DDD	335/341 (98%)	329 (98%)	6 (2%)	0	100	100
All	All	1341/1364 (98%)	1321 (98%)	20 (2%)	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	252/253 (100%)	249 (99%)	3 (1%)	71	76
1	BBB	250/253 (99%)	250 (100%)	0	100	100
1	CCC	254/253 (100%)	252 (99%)	2 (1%)	81	86
1	DDD	251/253 (99%)	251 (100%)	0	100	100
All	All	1007/1012 (100%)	1002 (100%)	5 (0%)	88	92

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

Mol	Chain	Res	Type
1	AAA	95	SER
1	AAA	167	ARG
1	AAA	263	PHE
1	CCC	95	SER
1	CCC	263	PHE

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)

7 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSO	BBB	242[B]	-	3,6,7	0.85	0	0,6,8	-	-
1	CSO	DDD	242[A]	-	3,6,7	0.75	0	0,6,8	-	-
1	CSO	BBB	242[A]	-	3,6,7	0.79	0	0,6,8	-	-
1	CSO	CCC	242[B]	-	3,6,7	0.80	0	0,6,8	-	-
1	CSO	CCC	242[A]	-	3,6,7	0.78	0	0,6,8	-	-
1	CSO	DDD	242[B]	-	3,6,7	0.84	0	0,6,8	-	-
1	CSO	AAA	242	1	3,6,7	0.95	0	0,6,8	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	BBB	242[B]	-	-	0/1/5/7	-
1	CSO	DDD	242[A]	-	-	1/1/5/7	-
1	CSO	BBB	242[A]	-	-	1/1/5/7	-
1	CSO	CCC	242[B]	-	-	0/1/5/7	-
1	CSO	CCC	242[A]	-	-	0/1/5/7	-
1	CSO	DDD	242[B]	-	-	0/1/5/7	-
1	CSO	AAA	242	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	BBB	242[A]	CSO	N-CA-CB-SG
1	DDD	242[A]	CSO	N-CA-CB-SG

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	BBB	242[B]	CSO	1	0
1	DDD	242[A]	CSO	1	0
1	CCC	242[B]	CSO	1	0
1	DDD	242[B]	CSO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 15 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	EDO	AAA	405	-	3,3,3	0.23	0	2,2,2	0.24	0
4	EDO	DDD	406	-	3,3,3	0.07	0	2,2,2	0.26	0
4	EDO	AAA	404	-	3,3,3	0.06	0	2,2,2	0.09	0
4	EDO	DDD	402	-	3,3,3	0.21	0	2,2,2	0.29	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
4	EDO	AAA	405	-	-	1/1/1/1	-
4	EDO	DDD	406	-	-	0/1/1/1	-
4	EDO	AAA	404	-	-	1/1/1/1	-
4	EDO	DDD	402	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	DDD	402	EDO	O1-C1-C2-O2
4	AAA	405	EDO	O1-C1-C2-O2
4	AAA	404	EDO	O1-C1-C2-O2

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	332/341 (97%)	-0.46	1 (0%) 94 93	26, 33, 46, 61	0
1	BBB	334/341 (97%)	-0.46	0 100 100	24, 31, 44, 68	0
1	CCC	333/341 (97%)	-0.50	1 (0%) 94 93	23, 31, 45, 83	0
1	DDD	334/341 (97%)	-0.49	0 100 100	22, 30, 41, 65	0
All	All	1333/1364 (97%)	-0.48	2 (0%) 95 94	22, 31, 44, 83	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	1	MET	2.9
1	AAA	33	PHE	2.3

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

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
1	CSO	AAA	242	7/8	0.94	0.15	27,30,35,41	0
1	CSO	DDD	242[A]	7/8	0.97	0.13	26,29,32,32	4
1	CSO	DDD	242[B]	7/8	0.97	0.13	26,28,30,30	4
1	CSO	CCC	242[A]	7/8	0.98	0.13	27,28,29,30	4
1	CSO	CCC	242[B]	7/8	0.98	0.13	27,28,30,32	4
1	CSO	BBB	242[A]	7/8	0.98	0.11	27,29,30,31	4
1	CSO	BBB	242[B]	7/8	0.98	0.11	27,30,31,32	4

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
5	MG	CCC	403	1/1	0.71	0.08	48,48,48,48	0
4	EDO	AAA	404	4/4	0.83	0.19	64,64,64,65	0
4	EDO	DDD	402	4/4	0.84	0.15	44,45,48,49	0
4	EDO	AAA	405	4/4	0.85	0.14	50,52,52,55	0
5	MG	DDD	405	1/1	0.85	0.18	54,54,54,54	0
3	CL	AAA	406	1/1	0.94	0.07	60,60,60,60	0
4	EDO	DDD	406	4/4	0.94	0.11	48,52,54,56	0
3	CL	AAA	402	1/1	0.95	0.09	62,62,62,62	0
3	CL	AAA	403	1/1	0.96	0.06	45,45,45,45	0
3	CL	CCC	404	1/1	0.98	0.10	57,57,57,57	0
3	CL	DDD	403	1/1	0.98	0.11	49,49,49,49	0
3	CL	BBB	403	1/1	0.98	0.10	40,40,40,40	0
3	CL	CCC	402	1/1	0.98	0.08	41,41,41,41	0
2	ZN	AAA	401	1/1	0.99	0.07	43,43,43,43	1
2	ZN	BBB	401	1/1	0.99	0.04	39,39,39,39	1
2	ZN	CCC	401	1/1	0.99	0.07	39,39,39,39	1
3	CL	DDD	404	1/1	0.99	0.09	30,30,30,30	0
2	ZN	DDD	401	1/1	0.99	0.05	29,29,29,29	1
3	CL	BBB	402	1/1	1.00	0.07	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.