Full wwPDB X-ray Structure Validation Report (i)

Feb 23, 2023 – 06:33 pm GMT

PDB ID	:	6Y8G
Title	:	selenomethionine derivative of ferulic acid esterase (FAE)
Authors	:	von Stetten, D.; Mueller-Dieckmann, C.; Carpentier, P.; Flot, D.
Deposited on	:	2020-03-04
Resolution	:	1.80 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:

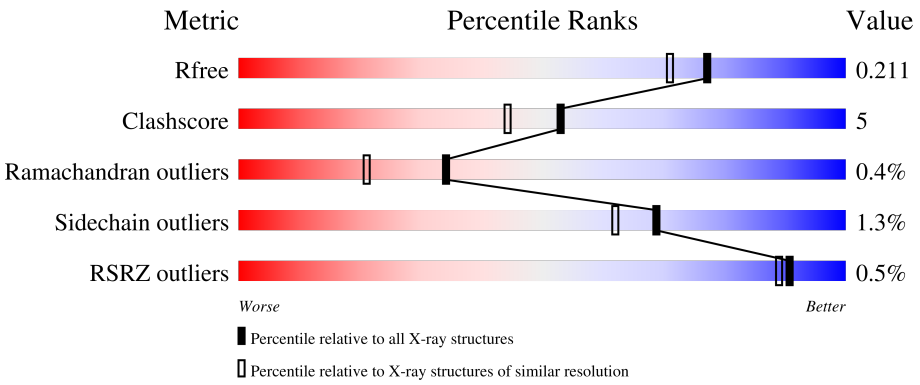
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	297	85% 9% • 5%
1	BBB	297	% 85% 9% • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5040 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 Endo-1,4-beta-xylanase Y.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S	Se			
1	AAA	282	2294	1477	378	426	1	3	9	0	2	0
1	BBB	282	2294	1477	378	426	1	3	9	0	2	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	MSE	-	initiating methionine	UNP P51584
AAA	2	ALA	-	expression tag	UNP P51584
AAA	3	SER	-	expression tag	UNP P51584
AAA	229	GLU	ASP	conflict	UNP P51584
AAA	230	ASP	HIS	conflict	UNP P51584
AAA	290	LEU	-	expression tag	UNP P51584
AAA	291	GLU	-	expression tag	UNP P51584
AAA	292	HIS	-	expression tag	UNP P51584
AAA	293	HIS	-	expression tag	UNP P51584
AAA	294	HIS	-	expression tag	UNP P51584
AAA	295	HIS	-	expression tag	UNP P51584
AAA	296	HIS	-	expression tag	UNP P51584
AAA	297	HIS	-	expression tag	UNP P51584
BBB	1	MSE	-	initiating methionine	UNP P51584
BBB	2	ALA	-	expression tag	UNP P51584
BBB	3	SER	-	expression tag	UNP P51584
BBB	229	GLU	ASP	conflict	UNP P51584
BBB	230	ASP	HIS	conflict	UNP P51584
BBB	290	LEU	-	expression tag	UNP P51584
BBB	291	GLU	-	expression tag	UNP P51584
BBB	292	HIS	-	expression tag	UNP P51584
BBB	293	HIS	-	expression tag	UNP P51584
BBB	294	HIS	-	expression tag	UNP P51584
BBB	295	HIS	-	expression tag	UNP P51584
BBB	296	HIS	-	expression tag	UNP P51584

Continued on next page...

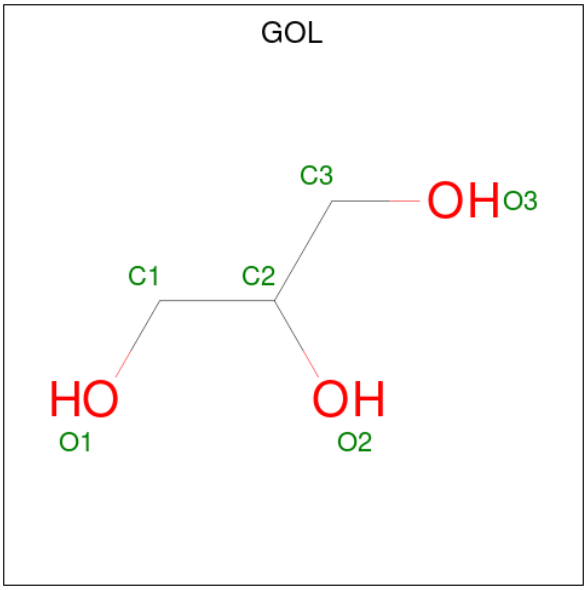
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	297	HIS	-	expression tag	UNP P51584

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
2	AAA	3	3	3	0	0
			Total	Cd		
2	BBB	5	5	5	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	BBB	1	6	3	3	0	0

- Molecule 4 is water.

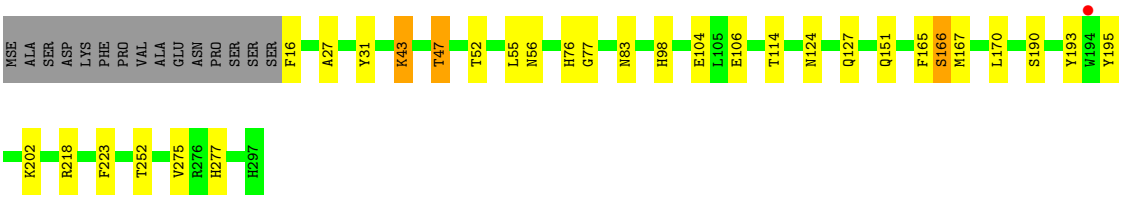
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	AAA	224	224	224	0	0
			Total	O		
4	BBB	214	214	214	0	0

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: Endo-1,4-beta-xylanase Y

Chain AAA:



• Molecule 1: Endo-1,4-beta-xylanase Y

Chain BBB:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.52Å 108.37Å 112.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.90 – 1.80 48.86 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.90-1.80) 98.3 (48.86-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.175 , 0.200 0.189 , 0.211	Depositor DCC
R_{free} test set	3709 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	20.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 39.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5040	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, GOL, CD

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	1/2361 (0.0%)	0.87	1/3198 (0.0%)
1	BBB	0.77	0/2361	0.85	0/3198
All	All	0.79	1/4722 (0.0%)	0.86	1/6396 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	106	GLU	CD-OE2	-5.13	1.20	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	47	THR	CA-CB-OG1	-5.52	97.41	109.00

There are no chirality outliers.

There are no planarity outliers.

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	AAA	2294	0	2128	26	0
1	BBB	2294	0	2127	26	0
2	AAA	3	0	0	0	0
2	BBB	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BBB	6	0	8	0	0
4	AAA	224	0	0	6	0
4	BBB	214	0	0	6	0
All	All	5040	0	4263	48	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 5.

All (48) 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:47:THR:HG22	1:AAA:52:THR:OG1	1.85	0.75
1:AAA:27:ALA:H	1:AAA:277:HIS:HD2	1.38	0.71
1:BBB:31:TYR:OH	1:BBB:104:GLU:OE2	2.08	0.69
1:AAA:27:ALA:H	1:AAA:277:HIS:CD2	2.11	0.68
1:BBB:246:LEU:O	4:BBB:401:HOH:O	2.13	0.67
1:BBB:277:HIS:HE1	4:BBB:566:HOH:O	1.88	0.57
1:AAA:167[B]:MSE:CE	4:AAA:526:HOH:O	2.53	0.57
1:AAA:43:LYS:NZ	1:AAA:83:ASN:HD21	2.02	0.57
1:AAA:76:HIS:HD2	1:AAA:77:GLY:O	1.87	0.56
1:AAA:76:HIS:HE1	1:AAA:114:THR:OG1	1.88	0.56
1:BBB:193:TYR:CZ	1:BBB:195:TYR:HB3	2.41	0.56
1:AAA:16:PHE:N	4:AAA:404:HOH:O	2.39	0.55
1:AAA:202:LYS:NZ	1:BBB:197:ASN:HD21	2.05	0.54
1:BBB:167[B]:MSE:HE2	4:BBB:549:HOH:O	2.08	0.54
1:BBB:167[B]:MSE:CE	4:BBB:549:HOH:O	2.56	0.54
1:AAA:165:PHE:CE1	1:AAA:275:VAL:HG21	2.45	0.51
1:BBB:49:ILE:H	1:BBB:132:ASN:ND2	2.08	0.51
1:AAA:277:HIS:HE1	4:AAA:574:HOH:O	1.94	0.50
1:AAA:193:TYR:CZ	1:AAA:195:TYR:HB3	2.47	0.50
1:BBB:27:ALA:H	1:BBB:277:HIS:CD2	2.30	0.50
1:AAA:76:HIS:CE1	1:AAA:114:THR:HA	2.46	0.50
1:BBB:166:SEP:HA	1:BBB:190:SER:O	2.12	0.50
1:AAA:31:TYR:OH	1:AAA:104:GLU:OE2	2.15	0.49
1:BBB:165:PHE:CE1	1:BBB:275:VAL:HG21	2.48	0.48
1:AAA:43:LYS:HE3	1:AAA:56:ASN:HD21	1.79	0.47
1:BBB:49:ILE:HG23	1:BBB:132:ASN:HD21	1.79	0.47
1:AAA:166:SEP:HA	1:AAA:190:SER:O	2.15	0.47
1:AAA:127:GLN:NE2	1:BBB:127:GLN:HB2	2.30	0.47
1:AAA:124:ASN:HD22	1:BBB:178:ASN:ND2	2.13	0.46
1:BBB:122:ALA:HB3	1:BBB:167[A]:MSE:HE3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:31:TYR:HA	1:AAA:98:HIS:CD2	2.51	0.46
1:BBB:121:THR:HA	4:BBB:491:HOH:O	2.17	0.45
1:AAA:27:ALA:N	1:AAA:277:HIS:CD2	2.84	0.44
1:BBB:27:ALA:H	1:BBB:277:HIS:HD2	1.64	0.44
1:BBB:134:ILE:HB	1:BBB:135:PRO:HD3	1.98	0.44
1:BBB:43:LYS:HE3	1:BBB:56:ASN:ND2	2.33	0.43
1:AAA:55:LEU:HD12	1:AAA:55:LEU:C	2.39	0.43
1:AAA:202:LYS:HZ3	1:BBB:197:ASN:HD21	1.65	0.43
1:BBB:31:TYR:HA	1:BBB:98:HIS:CD2	2.53	0.43
1:AAA:76:HIS:HE1	1:AAA:114:THR:HA	1.83	0.42
1:BBB:43:LYS:HE3	1:BBB:56:ASN:HD21	1.84	0.42
4:AAA:539:HOH:O	1:BBB:119:ASN:HB3	2.19	0.42
1:AAA:170:LEU:HD23	1:AAA:170:LEU:C	2.41	0.41
1:AAA:218:ARG:CZ	4:AAA:431:HOH:O	2.68	0.41
1:AAA:167[B]:MSE:HE2	4:AAA:526:HOH:O	2.20	0.41
1:BBB:144:TYR:CE2	1:BBB:292:HIS:HD2	2.38	0.41
1:BBB:49:ILE:H	1:BBB:132:ASN:HD21	1.68	0.40
1:BBB:123:GLN:HB3	4:BBB:559:HOH:O	2.22	0.40

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	281/297 (95%)	274 (98%)	6 (2%)	1 (0%)	34 21
1	BBB	281/297 (95%)	272 (97%)	8 (3%)	1 (0%)	34 21
All	All	562/594 (95%)	546 (97%)	14 (2%)	2 (0%)	34 21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	252	THR
1	BBB	252	THR

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	239/241 (99%)	236 (99%)	3 (1%)	69	62
1	BBB	239/241 (99%)	236 (99%)	3 (1%)	69	62
All	All	478/482 (99%)	472 (99%)	6 (1%)	69	62

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	43	LYS
1	AAA	151	GLN
1	AAA	223	PHE
1	BBB	43	LYS
1	BBB	123	GLN
1	BBB	223	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)

2 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	SEP	AAA	166	1	8,9,10	0.68	0	8,12,14	1.30	1 (12%)
1	SEP	BBB	166	1	8,9,10	0.62	0	8,12,14	1.62	2 (25%)

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	SEP	AAA	166	1	-	1/5/8/10	-
1	SEP	BBB	166	1	-	1/5/8/10	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	166	SEP	O3P-P-OG	-3.38	97.74	106.73
1	AAA	166	SEP	O3P-P-OG	-2.80	99.29	106.73
1	BBB	166	SEP	OG-P-O1P	2.12	112.42	106.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	166	SEP	N-CA-CB-OG
1	BBB	166	SEP	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AAA	166	SEP	1	0
1	BBB	166	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
3	GOL	BBB	306	-	5,5,5	0.19	0	5,5,5	0.20	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
3	GOL	BBB	306	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	273/297 (91%)	-0.03	1 (0%)	92	90	12, 20, 33, 52	0
1	BBB	273/297 (91%)	-0.07	2 (0%)	87	86	12, 19, 34, 48	0
All	All	546/594 (91%)	-0.05	3 (0%)	91	89	12, 20, 34, 52	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	196	GLY	2.7
1	AAA	194	TRP	2.6
1	BBB	194	TRP	2.3

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95th 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	SEP	AAA	166	10/11	0.97	0.07	14,16,18,18	0
1	SEP	BBB	166	10/11	0.98	0.08	13,16,19,20	0

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, 95th 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
3	GOL	BBB	306	6/6	0.90	0.13	28,31,33,35	0
2	CD	AAA	302	1/1	0.97	0.05	26,26,26,26	0
2	CD	BBB	301	1/1	0.98	0.05	26,26,26,26	0
2	CD	BBB	302	1/1	0.99	0.06	18,18,18,18	0
2	CD	BBB	303	1/1	0.99	0.07	19,19,19,19	0
2	CD	BBB	304	1/1	0.99	0.05	22,22,22,22	0
2	CD	AAA	303	1/1	0.99	0.06	22,22,22,22	0
2	CD	BBB	305	1/1	1.00	0.04	19,19,19,19	0
2	CD	AAA	301	1/1	1.00	0.07	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.