



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2020 – 09:04 AM GMT

PDB ID : 6ZS0
Title : Crystal structure of 5-dimethylallyltryptophan synthase from *Streptomyces coelicolor*
Authors : Ostertag, E.; Broger, K.; Stehle, T.; Zocher, G.
Deposited on : 2020-07-15
Resolution : 1.50 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 ⓘ symbol.

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 : 2.14.6
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) : 2.14.6

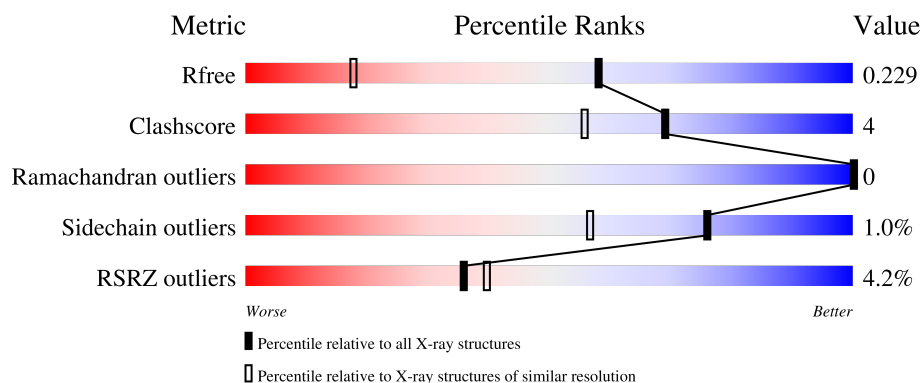
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	AAA	370	<div> <div>5%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	BBB	370	<div> <div>3%</div> <div>87%</div> <div>7%</div> <div>5%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5967 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 DMATS type aromatic prenyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	359	Total	C	N	O	S	0	14	0
			2753	1729	509	506	9			
1	BBB	350	Total	C	N	O	S	0	15	0
			2676	1680	492	496	8			

There are 30 discrepancies between the modelled and reference sequences:

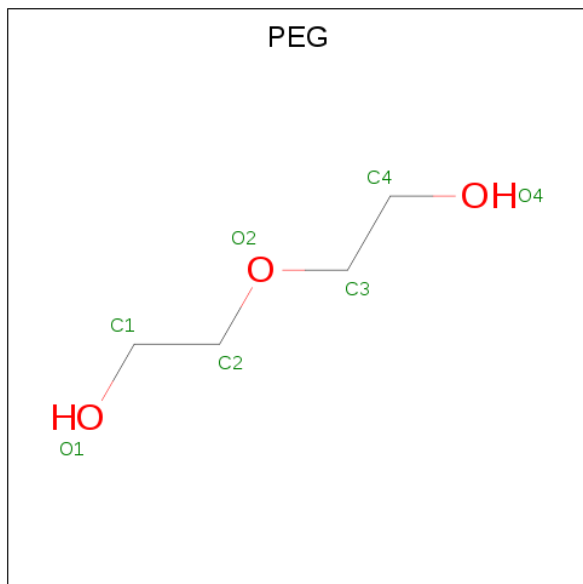
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	MET	-	initiating methionine	UNP A0A4R8NF71
AAA	357	LEU	-	expression tag	UNP A0A4R8NF71
AAA	358	VAL	-	expression tag	UNP A0A4R8NF71
AAA	359	PRO	-	expression tag	UNP A0A4R8NF71
AAA	360	ARG	-	expression tag	UNP A0A4R8NF71
AAA	361	GLY	-	expression tag	UNP A0A4R8NF71
AAA	362	SER	-	expression tag	UNP A0A4R8NF71
AAA	363	HIS	-	expression tag	UNP A0A4R8NF71
AAA	364	HIS	-	expression tag	UNP A0A4R8NF71
AAA	365	HIS	-	expression tag	UNP A0A4R8NF71
AAA	366	HIS	-	expression tag	UNP A0A4R8NF71
AAA	367	HIS	-	expression tag	UNP A0A4R8NF71
AAA	368	HIS	-	expression tag	UNP A0A4R8NF71
AAA	369	HIS	-	expression tag	UNP A0A4R8NF71
AAA	370	HIS	-	expression tag	UNP A0A4R8NF71
BBB	1	MET	-	initiating methionine	UNP A0A4R8NF71
BBB	357	LEU	-	expression tag	UNP A0A4R8NF71
BBB	358	VAL	-	expression tag	UNP A0A4R8NF71
BBB	359	PRO	-	expression tag	UNP A0A4R8NF71
BBB	360	ARG	-	expression tag	UNP A0A4R8NF71
BBB	361	GLY	-	expression tag	UNP A0A4R8NF71
BBB	362	SER	-	expression tag	UNP A0A4R8NF71
BBB	363	HIS	-	expression tag	UNP A0A4R8NF71
BBB	364	HIS	-	expression tag	UNP A0A4R8NF71
BBB	365	HIS	-	expression tag	UNP A0A4R8NF71

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	366	HIS	-	expression tag	UNP A0A4R8NF71
BBB	367	HIS	-	expression tag	UNP A0A4R8NF71
BBB	368	HIS	-	expression tag	UNP A0A4R8NF71
BBB	369	HIS	-	expression tag	UNP A0A4R8NF71
BBB	370	HIS	-	expression tag	UNP A0A4R8NF71

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	BBB	1	Total C O 7 4 3	0	0
2	BBB	1	Total C O 7 4 3	0	0

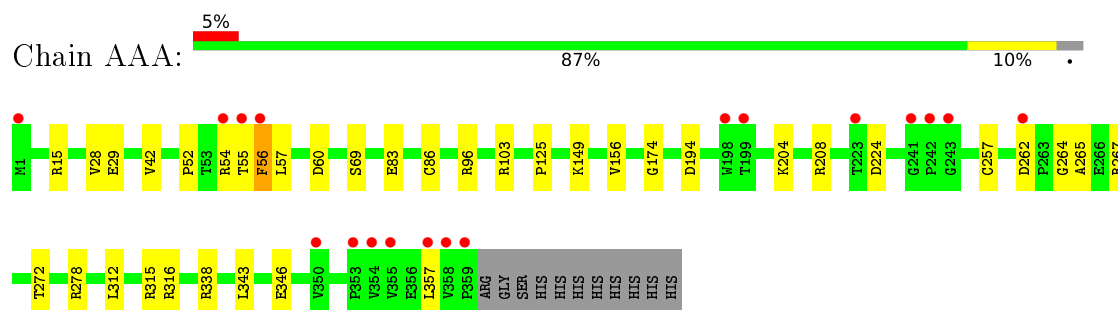
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	276	Total O 276 276	0	0
3	BBB	248	Total O 248 248	0	0

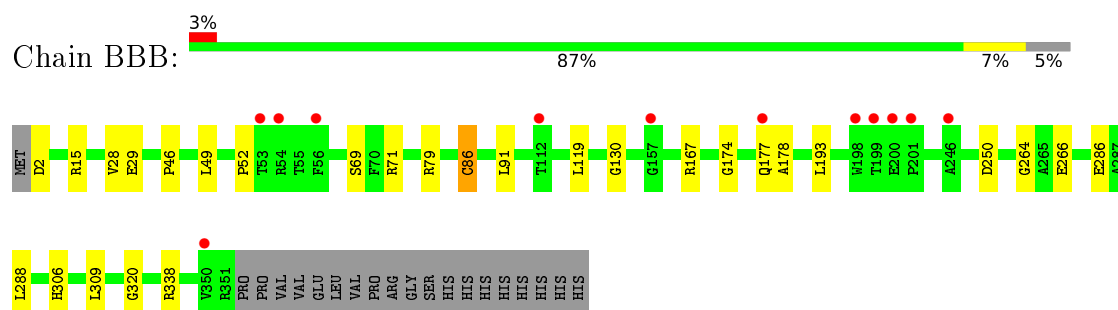
3 Residue-property plots [i](#)

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: DMATS type aromatic prenyltransferase



- Molecule 1: DMATS type aromatic prenyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.88Å 70.45Å 91.14Å 90.00° 92.95° 90.00°	Depositor
Resolution (Å)	41.05 – 1.50 41.06 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (41.05-1.50) 97.7 (41.06-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.189 , 0.220 0.199 , 0.229	Depositor DCC
R_{free} test set	1773 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5967	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PEG

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	0.70	1/2830 (0.0%)	0.78	1/3863 (0.0%)
1	BBB	0.71	1/2762 (0.0%)	0.79	0/3769
All	All	0.71	2/5592 (0.0%)	0.78	1/7632 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	83	GLU	CD-OE2	-5.78	1.19	1.25
1	BBB	286	GLU	CD-OE2	5.21	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	56	PHE	CB-CA-C	6.66	123.72	110.40

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	2753	0	2693	24	0
1	BBB	2676	0	2606	16	0
2	BBB	14	0	20	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AAA	276	0	0	6	0
3	BBB	248	0	0	1	0
All	All	5967	0	5319	40	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 4.

All (40) 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:42[B]:VAL:HG11	1:AAA:86[B]:CYS:SG	2.32	0.69
1:AAA:312:LEU:HD11	1:AAA:343:LEU:HB3	1.78	0.66
1:AAA:42[B]:VAL:HG21	1:AAA:52:PRO:HG3	1.81	0.62
1:AAA:224:ASP:OD1	1:AAA:267:ARG:NH2	2.30	0.61
1:BBB:52:PRO:HG2	1:BBB:86[A]:CYS:SG	2.42	0.59
1:AAA:257[B]:CYS:SG	1:AAA:272:THR:HB	2.43	0.58
1:AAA:55[A]:THR:HG22	1:AAA:57:LEU:H	1.69	0.57
1:BBB:15:ARG:HH22	1:BBB:29:GLU:CD	2.07	0.57
1:BBB:15:ARG:HG2	1:BBB:28[B]:VAL:HG13	1.86	0.56
1:BBB:174:GLY:O	1:BBB:264:GLY:HA2	2.07	0.55
1:BBB:46:PRO:HB2	1:BBB:49:LEU:HD13	1.88	0.55
1:AAA:96[B]:ARG:NH1	3:AAA:506:HOH:O	2.40	0.55
1:BBB:320:GLY:HA3	3:BBB:591:HOH:O	2.09	0.52
1:AAA:54:ARG:O	1:AAA:56:PHE:CZ	2.64	0.51
1:AAA:55[B]:THR:HG23	3:AAA:593:HOH:O	2.12	0.49
1:AAA:208[A]:ARG:NH1	3:AAA:511:HOH:O	2.47	0.47
1:AAA:208[B]:ARG:NH1	3:AAA:513:HOH:O	2.48	0.47
1:BBB:15:ARG:HG2	1:BBB:28[B]:VAL:CG1	2.45	0.46
1:BBB:71:ARG:HB2	1:BBB:338:ARG:HG2	1.97	0.46
1:BBB:69[B]:SER:OG	1:BBB:338:ARG:NH2	2.40	0.46
1:AAA:54:ARG:O	1:AAA:56:PHE:CE1	2.69	0.46
1:AAA:262:ASP:HB2	1:AAA:265:ALA:HB2	1.98	0.46
1:BBB:2:ASP:HA	2:BBB:402:PEG:O4	2.16	0.45
1:AAA:15:ARG:HH22	1:AAA:29:GLU:CD	2.19	0.45
1:AAA:52:PRO:HG2	1:AAA:86[A]:CYS:SG	2.56	0.45
1:AAA:174:GLY:O	1:AAA:264:GLY:HA2	2.18	0.44
1:AAA:69[B]:SER:OG	1:AAA:338:ARG:HG2	2.18	0.44
1:AAA:103[A]:ARG:HD3	3:AAA:630:HOH:O	2.17	0.43
1:AAA:125:PRO:HD2	1:AAA:156:VAL:HG21	2.01	0.43
1:AAA:149:LYS:HD3	1:AAA:204[B]:LYS:HE2	2.01	0.43
1:BBB:309[B]:LEU:HD13	1:BBB:309[B]:LEU:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:60:ASP:OD2	1:AAA:346:GLU:HA	2.20	0.42
1:BBB:288:LEU:HD21	1:BBB:306:HIS:CD2	2.55	0.42
1:BBB:119:LEU:HD12	1:BBB:193:LEU:HD21	2.01	0.41
1:BBB:167:ARG:NH2	1:BBB:177:GLN:OE1	2.53	0.41
1:BBB:91:LEU:HD21	1:BBB:130:GLY:HA2	2.02	0.41
1:AAA:315:ARG:HD2	1:AAA:316:ARG:O	2.22	0.40
1:AAA:278:ARG:NH2	3:AAA:509:HOH:O	2.42	0.40
1:BBB:178:ALA:HA	1:BBB:266:GLU:O	2.22	0.40
1:AAA:15:ARG:HA	1:AAA:28:VAL:HG13	2.03	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	371/370 (100%)	365 (98%)	6 (2%)	0	100	100
1	BBB	363/370 (98%)	356 (98%)	7 (2%)	0	100	100
All	All	734/740 (99%)	721 (98%)	13 (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	278/286 (97%)	276 (99%)	2 (1%)	84	69
1	BBB	269/286 (94%)	264 (98%)	5 (2%)	57	27
All	All	547/572 (96%)	540 (99%)	7 (1%)	76	44

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	194	ASP
1	AAA	357	LEU
1	BBB	79[A]	ARG
1	BBB	79[B]	ARG
1	BBB	86[A]	CYS
1	BBB	86[B]	CYS
1	BBB	250	ASP

Some 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](#)

2 ligands 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	$\# Z > 2$
2	PEG	BBB	402	-	6,6,6	0.15	0	5,5,5	0.07	0
2	PEG	BBB	401	-	6,6,6	0.17	0	5,5,5	0.14	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	PEG	BBB	402	-	-	2/4/4/4	-
2	PEG	BBB	401	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	401	PEG	O2-C3-C4-O4
2	BBB	401	PEG	O1-C1-C2-O2
2	BBB	402	PEG	C4-C3-O2-C2
2	BBB	402	PEG	O2-C3-C4-O4
2	BBB	401	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	402	PEG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	359/370 (97%)	0.19	18 (5%)	28 31	12, 24, 45, 71	0
1	BBB	350/370 (94%)	0.23	12 (3%)	45 49	11, 24, 42, 58	0
All	All	709/740 (95%)	0.21	30 (4%)	36 40	11, 24, 44, 71	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	359	PRO	5.7
1	BBB	199	THR	4.3
1	BBB	198	TRP	4.2
1	AAA	199	THR	4.0
1	BBB	200	GLU	4.0
1	AAA	198	TRP	3.8
1	BBB	350	VAL	3.8
1	AAA	358	VAL	3.6
1	AAA	355	VAL	3.5
1	BBB	56	PHE	3.4
1	BBB	53	THR	3.3
1	AAA	354	VAL	3.1
1	AAA	243	GLY	3.0
1	AAA	1	MET	2.6
1	BBB	201	PRO	2.5
1	AAA	56	PHE	2.5
1	BBB	112	THR	2.4
1	AAA	262	ASP	2.4
1	AAA	54	ARG	2.4
1	BBB	54	ARG	2.4
1	AAA	223	THR	2.4
1	BBB	177	GLN	2.4
1	BBB	246	ALA	2.3
1	AAA	350	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	AAA	357	LEU	2.2
1	AAA	55[A]	THR	2.1
1	BBB	157	GLY	2.1
1	AAA	242	PRO	2.1
1	AAA	353	PRO	2.1
1	AAA	241	GLY	2.1

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 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(\AA^2)	Q<0.9
2	PEG	BBB	402	7/7	0.86	0.10	46,48,49,50	0
2	PEG	BBB	401	7/7	0.90	0.10	44,47,51,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.