

wwPDB X-ray Structure Validation Summary Report (i)

Jan 3, 2023 – 06:12 am GMT

:	7PWX
:	dUTPase from M. tuberculosis in complex with Stl
:	Marina, A.; Sanz-Frasquet, C.
:	2021-10-07
:	2.75 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
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)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.75 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.



Motric	Whole archive	Similar resolution		
Wiethic	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R _{free}	130704	$1235\ (2.78-2.74)$		
Clashscore	141614	1277 (2.78-2.74)		
Ramachandran outliers	138981	1257 (2.78-2.74)		
Sidechain outliers	138945	1257 (2.78-2.74)		
RSRZ outliers	127900	1207 (2.78-2.74)		

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	HHH	136	85%	12% ••
1	III	136	74%	20% • •
1	JJJ	136	83%	12% • •
1	KKK	136	% • 79%	18% ••
1	LLL	136	87%	12% •

Continued on next page...



Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	MMM	136	77%	17% • •
2	AAA	147	4% 72% 7% •	20%
2	CCC	147	82%	16% ••
2	DDD	147	% 	14% •••
2	EEE	147	% 	10% •
2	FFF	147	% 81%	17% ••
2	GGG	147	71% 14%	• 13%



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12287 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	ипп	124	Total	С	Ν	0	S	0	0	0
	111111	104	946	602	167	176	1	0	0	0
1	TIT	121	Total	С	Ν	0	S	0	0	0
	111	131	950	606	167	176	1	0	0	0
1	TTT	121	Total	С	Ν	0	S	0	0	0
	1 111	101	952	604	168	179	1	0		0
1	UUU	V 195	Total	С	Ν	0	S	0	0	0
	IXIXIX	155	946	604	172	169	1			U
1	ттт	126	Total	С	Ν	0	S	0	0	0
		150	977	620	178	177	2	0	0	0
1	1 MMM	131	Total	С	Ν	0	S	0	0	0
			950	603	172	174	1	0	U	U

• Molecule 1 is a protein called Deoxyuridine 5'-triphosphate nucleotidohydrolase.

• Molecule 2 is a protein called Orf20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CCC	146	Total	С	Ν	0	S	0	0	0
		140	1174	757	186	229	2	0	0	0
2	מחמ	145	Total	С	Ν	0	S	0	0	0
	עעע	140	1167	757	180	228	2	0	0	0
2	FFF	146	Total	С	Ν	0	S	0	0	0
		140	1148	742	178	226	2	0		0
2	FFF	146	Total	С	Ν	0	S	0	ე	0
	I, I, I,	140	1184	768	186	228	2	0		0
9	CCC	198	Total	С	Ν	0	S	0	0	0
	GGG	128	919	588	145	184	2	0	0	0
9	2 AAA	110	Total	С	Ν	0	S	0	0	0
		118	787	499	130	156	2		0	0

• Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	HHH	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 8 & 4 & 1 & 3 \end{array}$	0	0
3	JJJ	1	Total C N O 8 4 1 3	0	0
3	LLL	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 8 & 4 & 1 & 3 \end{array}$	0	0
3	LLL	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 8 & 4 & 1 & 3 \end{array}$	0	0

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





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	III	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	JJJ	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	JJJ	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	JJJ	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	DDD	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	DDD	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	FFF	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	GGG	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	JJJ	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
5	KKK	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
5	MMM	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
5	FFF	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0



• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	HHH	7	Total O 7 7	0	0
6	III	8	Total O 8 8	0	0
6	JJJ	9	Total O 9 9	0	0
6	KKK	2	Total O 2 2	0	0
6	LLL	8	Total O 8 8	0	0
6	MMM	7	Total O 7 7	0	0
6	CCC	7	Total O 7 7	0	0
6	DDD	12	Total O 12 12	0	0
6	EEE	4	Total O 4 4	0	0
6	FFF	17	Total O 17 17	0	0
6	GGG	8	Total O 8 8	0	0
6	AAA	6	Total O 6 6	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: Deoxyuridine 5'-triphosphate nucleotidohydrolase



• Molecule 2: Orf20









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	79.41Å 150.43Å 107.37Å	Depositor
a, b, c, α , β , γ	90.00° 98.85° 90.00°	Depositor
Bosolution(A)	75.33 - 2.75	Depositor
Resolution (A)	75.21 - 2.75	EDS
% Data completeness	95.1 (75.33-2.75)	Depositor
(in resolution range)	95.1 (75.21-2.75)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.88 (at 2.73 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
P. P.	0.201 , 0.259	Depositor
n, n_{free}	0.203 , 0.256	DCC
R_{free} test set	3102 reflections $(5.04%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	63.7	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29 , 40.6	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12287	wwPDB-VP
Average B, all atoms $(Å^2)$	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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, EDO, TRS

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		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	HHH	0.70	0/960	0.83	0/1311	
1	III	0.65	0/964	0.86	0/1314	
1	JJJ	0.65	0/967	0.85	0/1322	
1	KKK	0.69	0/960	0.86	0/1312	
1	LLL	0.68	0/992	0.87	0/1354	
1	MMM	0.68	0/965	0.87	0/1319	
2	AAA	0.78	0/795	0.82	0/1076	
2	CCC	0.68	0/1199	0.78	0/1622	
2	DDD	0.68	0/1192	0.78	0/1611	
2	EEE	0.69	0/1173	0.76	0/1590	
2	FFF	0.67	0/1214	0.84	2/1640~(0.1%)	
2	GGG	0.79	0/937	0.81	0/1273	
All	All	0.69	0/12318	0.83	2/16744~(0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	FFF	48[A]	ASN	CB-CA-C	-8.13	94.14	110.40
2	FFF	48[B]	ASN	CB-CA-C	-8.13	94.14	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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	HHH	946	0	934	13	0
1	III	950	0	964	17	0
1	JJJ	952	0	968	13	0
1	KKK	946	0	960	14	0
1	LLL	977	0	1002	17	0
1	MMM	950	0	979	18	0
2	AAA	787	0	572	3	0
2	CCC	1174	0	1112	13	0
2	DDD	1167	0	1088	12	0
2	EEE	1148	0	1046	7	0
2	FFF	1184	0	1119	12	0
2	GGG	919	0	735	15	0
3	HHH	8	0	12	5	0
3	JJJ	8	0	12	0	0
3	LLL	16	0	24	5	0
4	DDD	8	0	12	0	0
4	\mathbf{FFF}	4	0	6	0	0
4	GGG	4	0	6	0	0
4	III	4	0	6	0	0
4	JJJ	12	0	18	0	0
5	FFF	7	0	10	0	0
5	JJJ	7	0	10	0	0
5	KKK	7	0	10	0	0
5	MMM	7	0	10	2	0
6	AAA	6	0	0	0	0
6	CCC	7	0	0	0	0
6	DDD	12	0	0	0	0
6	EEE	4	0	0	0	0
6	\mathbf{FFF}	17	0	0	0	0
6	GGG	8	0	0	1	0
6	HHH	7	0	0	0	0
6	III	8	0	0	0	0
6	JJJ	9	0	0	0	0
6	KKK	2	0	0	0	0
6	LLL	8	0	0	0	0
6	MMM	7	0	0	0	0
All	All	12287	0	11615	134	0

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.

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 6.

The worst 5 of 134 close contacts within the same asymmetric unit are listed below, sorted by



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LLL:122:VAL:HG12	1:MMM:3:THR:HG22	1.30	1.08
1:LLL:122:VAL:CG1	1:MMM:3:THR:HG22	1.99	0.92
2:FFF:10:LEU:HD21	2:FFF:55:VAL:HA	1.61	0.82
2:GGG:27:LEU:HD13	2:GGG:27:LEU:O	1.87	0.74
3:LLL:202:TRS:H12	1:MMM:60:LEU:HD13	1.70	0.73

their clash magnitude.

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	Perce	entiles
1	HHH	132/136~(97%)	127 (96%)	5 (4%)	0	100	100
1	III	129/136~(95%)	122 (95%)	7 (5%)	0	100	100
1	JJJ	129/136~(95%)	125~(97%)	4 (3%)	0	100	100
1	KKK	133/136~(98%)	131 (98%)	2 (2%)	0	100	100
1	LLL	134/136~(98%)	128 (96%)	6 (4%)	0	100	100
1	MMM	129/136~(95%)	116 (90%)	13 (10%)	0	100	100
2	AAA	102/147~(69%)	90~(88%)	11 (11%)	1 (1%)	15	27
2	CCC	144/147~(98%)	138 (96%)	6 (4%)	0	100	100
2	DDD	143/147~(97%)	136 (95%)	7 (5%)	0	100	100
2	EEE	144/147~(98%)	138 (96%)	6 (4%)	0	100	100
2	FFF	146/147~(99%)	142 (97%)	4 (3%)	0	100	100
2	GGG	122/147~(83%)	110 (90%)	12 (10%)	0	100	100
All	All	1587/1698~(94%)	1503 (95%)	83 (5%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
2	AAA	68	PRO

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	HHH	92/106~(87%)	87~(95%)	5(5%)	22 38
1	III	98/106~(92%)	84 (86%)	14 (14%)	3 4
1	JJJ	98/106~(92%)	93~(95%)	5(5%)	24 41
1	KKK	90/106~(85%)	81 (90%)	9 (10%)	7 13
1	LLL	98/106~(92%)	94~(96%)	4 (4%)	30 50
1	MMM	99/106~(93%)	90~(91%)	9~(9%)	9 16
2	AAA	51/135~(38%)	43 (84%)	8 (16%)	2 3
2	CCC	122/135~(90%)	109~(89%)	13 (11%)	6 11
2	DDD	117/135~(87%)	110 (94%)	7~(6%)	19 33
2	EEE	111/135~(82%)	107~(96%)	4 (4%)	35 55
2	\mathbf{FFF}	121/135~(90%)	110 (91%)	11 (9%)	9 16
2	GGG	75/135~(56%)	67~(89%)	8 (11%)	6 11
All	All	1172/1446 (81%)	1075 (92%)	97~(8%)	11 20

5 of 97 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
2	CCC	150	GLN
2	FFF	57	GLU
2	DDD	12	THR
2	DDD	147	LEU
2	\mathbf{FFF}	115	SER

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains 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)

16 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	Bos	Link	B	ond leng	gths	E	Bond ang	gles
	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	TRS	HHH	201	-	7,7,7	0.16	0	$9,\!9,\!9$	0.34	0
4	EDO	III	201	-	3,3,3	0.10	0	2,2,2	0.27	0
4	EDO	JJJ	204	-	3,3,3	0.13	0	$2,\!2,\!2$	0.14	0
4	EDO	FFF	202	-	3,3,3	0.11	0	2,2,2	0.26	0
3	TRS	LLL	202	-	7,7,7	0.19	0	$9,\!9,\!9$	0.27	0
5	PEG	FFF	201	-	6,6,6	0.17	0	$5,\!5,\!5$	0.08	0
4	EDO	JJJ	203	-	3,3,3	0.20	0	2,2,2	0.33	0
4	EDO	DDD	201	-	3,3,3	0.09	0	2,2,2	0.31	0
5	PEG	JJJ	202	-	6,6,6	0.20	0	$5,\!5,\!5$	0.14	0
4	EDO	JJJ	205	-	3,3,3	0.11	0	2,2,2	0.32	0
5	PEG	KKK	201	-	6,6,6	0.15	0	$5,\!5,\!5$	0.12	0
5	PEG	MMM	201	-	6,6,6	0.22	0	$5,\!5,\!5$	0.19	0
3	TRS	LLL	201	-	7,7,7	0.18	0	$9,\!9,\!9$	0.28	0
4	EDO	DDD	202	-	3,3,3	0.16	0	2,2,2	0.38	0
3	TRS	JJJ	201	-	7,7,7	0.24	0	$9,\!9,\!9$	0.32	0
4	EDO	GGG	201	-	3,3,3	0.12	0	2,2,2	0.30	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	TRS	HHH	201	-	-	4/9/9/9	-
4	EDO	III	201	-	-	1/1/1/1	-
4	EDO	JJJ	204	-	-	0/1/1/1	-
4	EDO	FFF	202	-	-	1/1/1/1	-
3	TRS	LLL	202	-	-	3/9/9/9	-
5	PEG	FFF	201	-	-	1/4/4/4	-
4	EDO	JJJ	203	-	-	1/1/1/1	-
4	EDO	DDD	201	-	-	1/1/1/1	-
5	PEG	JJJ	202	-	-	1/4/4/4	-
4	EDO	JJJ	205	-	-	1/1/1/1	-
5	PEG	KKK	201	-	-	2/4/4/4	-
5	PEG	MMM	201	-	-	3/4/4/4	-
3	TRS	LLL	201	-	-	1/9/9/9	-
4	EDO	DDD	202	-	-	1/1/1/1	-
3	TRS	JJJ	201	-	-	6/9/9/9	-
4	EDO	GGG	201	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	LLL	201	TRS	N-C-C2-O2
5	MMM	201	PEG	C4-C3-O2-C2
5	KKK	201	PEG	O1-C1-C2-O2
5	KKK	201	PEG	O2-C3-C4-O4
4	III	201	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	HHH	201	TRS	5	0
3	LLL	202	TRS	4	0
5	MMM	201	PEG	2	0

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	LLL	201	TRS	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 (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, 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	HHH	134/136~(98%)	0.06	0 100 100	39, 52, 70, 118	0
1	III	131/136~(96%)	0.04	0 100 100	37, 52, 90, 115	0
1	JJJ	131/136~(96%)	0.03	0 100 100	40, 58, 80, 113	0
1	KKK	135/136~(99%)	0.05	1 (0%) 87 91	41, 68, 94, 106	0
1	LLL	136/136~(100%)	-0.11	0 100 100	32, 51, 77, 123	0
1	MMM	131/136~(96%)	-0.09	0 100 100	34, 56, 86, 110	0
2	AAA	118/147~(80%)	0.19	6 (5%) 28 34	58, 94, 136, 160	1 (0%)
2	CCC	146/147~(99%)	-0.17	0 100 100	35, 51, 81, 104	0
2	DDD	145/147~(98%)	-0.14	1 (0%) 87 91	40, 61, 91, 105	0
2	EEE	146/147~(99%)	-0.11	1 (0%) 87 91	44, 63, 98, 116	0
2	\mathbf{FFF}	146/147~(99%)	0.00	1 (0%) 87 91	38, 54, 90, 116	0
2	GGG	128/147~(87%)	-0.13	0 100 100	50, 81, 124, 140	0
All	All	$162\overline{7/1698}~(95\%)$	-0.04	10 (0%) 89 92	32, 59, 103, 160	1 (0%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	AAA	139	ILE	4.5
2	AAA	75	ILE	3.7
2	FFF	12	THR	3.2
2	AAA	10	LEU	3.1
2	AAA	30	SER	3.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.



$7 \mathrm{PWX}$

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
4	EDO	DDD	202	4/4	0.57	0.25	93,96,96,96	0
4	EDO	JJJ	203	4/4	0.69	0.25	75,85,88,89	0
4	EDO	GGG	201	4/4	0.76	0.18	94,95,96,98	0
5	PEG	MMM	201	7/7	0.80	0.28	98,108,115,119	0
5	PEG	KKK	201	7/7	0.82	0.19	76,87,104,105	0
4	EDO	JJJ	205	4/4	0.82	0.11	93,98,99,100	0
5	PEG	FFF	201	7/7	0.87	0.26	86,97,101,103	0
5	PEG	JJJ	202	7/7	0.89	0.10	98,104,108,111	0
4	EDO	JJJ	204	4/4	0.89	0.12	95,102,104,106	0
4	EDO	FFF	202	4/4	0.92	0.13	71,76,79,82	0
4	EDO	III	201	4/4	0.92	0.24	76,80,82,82	0
3	TRS	HHH	201	8/8	0.95	0.25	$63,\!65,\!68,\!73$	0
4	EDO	DDD	201	4/4	0.96	0.22	65,68,71,72	0
3	TRS	LLL	201	8/8	0.96	0.25	70,76,81,85	0
3	TRS	LLL	202	8/8	0.96	0.25	$55,\!59,\!61,\!62$	0
3	TRS	JJJ	201	8/8	0.96	0.28	62,70,78,78	0

6.5 Other polymers (i)

There are no such residues in this entry.

