

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	7QNT
Title	:	TarM(Se) native
Authors	:	Guo, Y.; Stehle, T.
Deposited on	:	2021-12-22
Resolution	:	3.21 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 (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	:	2.36
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: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.21 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.



Matria	Whole archive	Similar resolution		
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R_{free}	130704	1335 (3.24-3.20)		
Clashscore	141614	1460 (3.24-3.20)		
Ramachandran outliers	138981	1437 (3.24-3.20)		
Sidechain outliers	138945	1436 (3.24-3.20)		
RSRZ outliers	127900	1291 (3.24-3.20)		

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	492	% • • 93%	7%
1	BBB	492	5% 92%	7%
1	CCC	492	% • 93%	7%
1	DDD	492	% • • 93%	7%



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2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13681 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	Atoms				ZeroOcc	AltConf	Trace	
1	A A A	402	Total	С	Ν	0	\mathbf{S}	0	0	0
	AAA	492	3410	2150	581	667	12	0	0	
1	DDD	401	Total	С	Ν	0	S	0	0	0
	I BBB	491	3298	2077	573	637	11	0	0	0
1	CCC	CCC 492	Total	С	Ν	0	S	0	0	0
			3369	2128	577	650	14	0	0	
1	מממ	402	Total	С	Ν	0	S	0	0	0
I DDD	492	3312	2092	573	636	11	U	0	0	

• Molecule 1 is a protein called TarM(Se).

• Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	3	Total Cl 3 3	0	0
2	BBB	5	Total Cl 5 5	0	0
2	CCC	2	Total Cl 2 2	0	0
2	DDD	6	Total Cl 6 6	0	0

• Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	0 1	S 1	0	0
3	CCC	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	0 1	S 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	CCC	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 5 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	67	$\begin{array}{cc} \text{Total} & \text{O} \\ 67 & 67 \end{array}$	0	0
5	BBB	58	Total O 58 58	0	0
5	CCC	70	Total O 70 70	0	0
5	DDD	69	Total O 69 69	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: TarM(Se)



G406 M1 L407 E10 L407 E10 L407 D12 L41 L34 L41 L34 L41 L34 L42 D42 L41 L34 L41 L34 L41 L34 L48 Y34 Y84 Y122 H60 Y133 L17 L17 L163 Y122 H60 Y133 L163 Y122 L163 Y122 L163 Y122 L163 Y122 L163 Y133 L163 Y134 L163 Y132 L163 Y132 L164 Y134 L163 Y134 L163 Y134 L164 Y134 L163 Y134 L164 Y134 L164 Y134 L174 Y134



4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 63	Depositor	
Cell constants	154.01Å 154.01Å 207.72Å	Deperitor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	48.99 - 3.21	Depositor	
Resolution (A)	48.99 - 3.21	EDS	
% Data completeness	100.0 (48.99-3.21)	Depositor	
(in resolution range)	$100.0 \ (48.99-3.21)$	EDS	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$1.68 (at 3.19 \text{\AA})$	Xtriage	
Refinement program	REFMAC 5.8.0258	Depositor	
D D	0.228 , 0.257	Depositor	
n, n_{free}	0.230 , 0.250	DCC	
R_{free} test set	2277 reflections $(5.00%)$	wwPDB-VP	
Wilson B-factor $(Å^2)$	93.0	Xtriage	
Anisotropy	0.030	Xtriage	
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.21 , 87.6	EDS	
L-test for $twinning^2$	$< L >=0.43, < L^2>=0.25$	Xtriage	
Estimated twinning fraction	0.407 for h,-h-k,-l	Xtriage	
Reported twinning fraction	0.563 for H, K, L	Dopositor	
Reported twinning fraction	0.437 for -K, -H, -L	Depositor	
Outliers	0 of 45535 reflections	Xtriage	
F_o, F_c correlation	0.91	EDS	
Total number of atoms	13681	wwPDB-VP	
Average B, all atoms $(Å^2)$	93.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.51% 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: BME, CL, EDO

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).

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	AAA	0.66	0/3469	0.66	0/4737	
1	BBB	0.67	0/3351	0.66	0/4587	
1	CCC	0.66	0/3424	0.66	0/4670	
1	DDD	0.67	0/3367	0.67	0/4603	
All	All	0.66	0/13611	0.66	0/18597	

There are no bond length outliers.

There are no bond angle outliers.

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	3410	0	2641	12	0
1	BBB	3298	0	2435	18	0
1	CCC	3369	0	2592	14	0
1	DDD	3312	0	2439	10	0
2	AAA	3	0	0	0	0
2	BBB	5	0	0	0	0
2	CCC	2	0	0	0	0
2	DDD	6	0	0	0	0
3	AAA	4	0	6	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CCC	4	0	6	0	0
4	CCC	4	0	6	0	0
5	AAA	67	0	0	0	0
5	BBB	58	0	0	0	0
5	CCC	70	0	0	0	0
5	DDD	69	0	0	0	0
All	All	13681	0	10125	53	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 2.

All (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:DDD:84:TYR:CE1	1:DDD:84:TYR:CE2	2.61	0.82
1:BBB:398:SER:OG	1:BBB:409:LEU:HD11	1.81	0.81
1:CCC:218:ILE:HG22	1:CCC:220:ASP:H	1.52	0.73
1:BBB:3:GLN:HA	1:BBB:35:SER:HB3	1.75	0.69
1:AAA:278:GLY:HA2	1:AAA:298:ASN:HB2	1.82	0.62
1:DDD:29:PHE:HB3	1:DDD:34:ILE:HB	1.80	0.62
1:CCC:25:ARG:NH1	1:CCC:224:ILE:HG21	2.16	0.60
1:BBB:23:LEU:HD22	1:BBB:60:MET:HG3	1.86	0.57
1:CCC:7:ILE:HB	1:CCC:225:CYS:HA	1.88	0.55
1:DDD:422:PHE:HA	1:DDD:441:ILE:O	2.07	0.55
1:CCC:278:GLY:HA2	1:CCC:298:ASN:HB2	1.89	0.53
1:BBB:377:VAL:HG23	1:BBB:377:VAL:O	2.07	0.53
1:AAA:373:LEU:HA	1:AAA:376:ASN:HB2	1.92	0.52
1:AAA:399:THR:HA	1:AAA:422:PHE:CG	2.45	0.51
1:DDD:108:ILE:HG23	1:DDD:122:TYR:HE1	1.76	0.51
1:BBB:278:GLY:HA2	1:BBB:298:ASN:HB3	1.93	0.49
1:BBB:352:PHE:HB2	1:BBB:377:VAL:HA	1.95	0.48
1:CCC:25:ARG:HH12	1:CCC:224:ILE:HG21	1.77	0.48
1:BBB:147:TYR:HB3	1:BBB:152:VAL:HG11	1.96	0.48
1:BBB:217:ASP:HA	1:BBB:242:VAL:HG23	1.96	0.47
1:AAA:458:HIS:HB3	1:CCC:149:GLY:HA3	1.96	0.47
1:CCC:30:LEU:HD13	1:CCC:63:ARG:HB2	1.96	0.47
1:BBB:108:ILE:HG23	1:BBB:122:TYR:HE1	1.79	0.47
1:CCC:333:LEU:HB2	1:CCC:334:PRO:HD3	1.98	0.46
1:AAA:193:LEU:HB2	1:AAA:200:PHE:HE2	1.82	0.45
1:CCC:228:PRO:HB2	1:CCC:265:GLN:HB3	1.98	0.45
1:BBB:398:SER:CB	1:BBB:409:LEU:HD11	2.47	0.44



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A. 1		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:CCC:108:ILE:HG23	1:CCC:122:TYR:HE1	1.83	0.44
1:AAA:163:LEU:HD12	1:AAA:163:LEU:HA	1.86	0.44
1:CCC:75:ASN:OD1	1:CCC:76:ILE:N	2.51	0.44
1:CCC:101:GLU:HG3	1:CCC:109:SER:OG	2.18	0.44
1:DDD:403:GLU:HG2	1:DDD:406:GLY:HA2	2.00	0.43
1:DDD:403:GLU:HG3	1:DDD:406:GLY:H	1.82	0.43
1:BBB:51:LEU:HD11	1:BBB:66:MET:HE3	2.00	0.43
1:DDD:10:GLU:HB3	1:DDD:42:ASP:HB2	2.01	0.43
1:BBB:30:LEU:HA	1:BBB:34:ILE:O	2.19	0.43
1:AAA:193:LEU:HG	1:AAA:195:CYS:SG	2.58	0.42
1:BBB:51:LEU:HD11	1:BBB:66:MET:CE	2.49	0.42
1:CCC:5:TYR:HE2	1:CCC:221:ASN:HD22	1.68	0.42
1:DDD:163:LEU:HD12	1:DDD:163:LEU:HA	1.85	0.42
1:AAA:164:ILE:HG22	1:AAA:183:PRO:HG3	2.01	0.42
1:CCC:190:LYS:HB3	1:CCC:190:LYS:HE3	1.85	0.42
1:AAA:133:ASP:HB3	1:AAA:140:ARG:HD2	2.00	0.42
1:BBB:179:ARG:HG2	1:BBB:191:THR:HG23	2.01	0.42
1:DDD:177:LEU:HD12	1:DDD:177:LEU:HA	1.92	0.42
1:BBB:6:MET:SD	1:BBB:22:MET:O	2.78	0.42
1:BBB:441:ILE:HG22	1:BBB:442:GLU:N	2.34	0.41
1:AAA:233:LYS:O	1:AAA:237:THR:HG23	2.19	0.41
1:DDD:68:ASN:HB3	1:DDD:71:ILE:HG23	2.03	0.41
1:AAA:258:ASP:OD1	1:AAA:259:THR:N	2.54	0.41
1:BBB:254:LYS:HA	1:BBB:254:LYS:HD2	1.70	0.40
1:AAA:30:LEU:HD22	1:AAA:63:ARG:HD2	2.04	0.40
1:BBB:47:TYR:O	1:BBB:51:LEU:HD13	2.21	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	Perce	ntiles
1	AAA	490/492~(100%)	443 (90%)	46 (9%)	1 (0%)	47	79
1	BBB	489/492~(99%)	441 (90%)	48 (10%)	0	100	100
1	CCC	490/492~(100%)	445 (91%)	45~(9%)	0	100	100
1	DDD	490/492~(100%)	450 (92%)	40 (8%)	0	100	100
All	All	1959/1968~(100%)	1779 (91%)	179~(9%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	428	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	241/455~(53%)	231~(96%)	10 (4%)	30	65	
1	BBB	207/455~(46%)	198~(96%)	9 (4%)	29	63	
1	CCC	230/455~(50%)	218~(95%)	12 (5%)	23	58	
1	DDD	209/455~(46%)	191 (91%)	18 (9%)	10	37	
All	All	887/1820 (49%)	838 (94%)	49 (6%)	21	57	

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	37	ASP
1	AAA	39	ILE
1	AAA	47	TYR
1	AAA	221	ASN
1	AAA	226	ASP
1	AAA	255	ASN
1	AAA	281	MET
1	AAA	286	GLN
1	AAA	313	ARG
1	AAA	479	GLN



Mol	Chain	Res	Type
1	BBB	47	TYR
1	BBB	119	TYR
1	BBB	202	ASN
1	BBB	234	ILE
1	BBB	264	LYS
1	BBB	274	ASN
1	BBB	294	TYR
1	BBB	445	ASP
1	BBB	478	TYR
1	CCC	9	ASN
1	CCC	47	TYR
1	CCC	93	SER
1	CCC	107	ARG
1	CCC	128	GLN
1	CCC	133	ASP
1	CCC	179	ARG
1	CCC	213	LYS
1	CCC	258	ASP
1	CCC	284	GLU
1	CCC	365	GLU
1	CCC	423	ASP
1	DDD	12	ASP
1	DDD	46	ASN
1	DDD	47	TYR
1	DDD	60	MET
1	DDD	130	THR
1	DDD	133	ASP
1	DDD	152	VAL
1	DDD	184	GLU
1	DDD	185	LYS
1	DDD	197	GLU
1	DDD	204	VAL
1	DDD	214	LEU
1	DDD	226	ASP
1	DDD	252	HIS
1	DDD	274	ASN
1	DDD	351	GLU
1	DDD	382	TYR
1	DDD	408	SER

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 19 ligands modelled in this entry, 16 are monoatomic - leaving 3 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).

Mal	Type	Chain	Dog	Link	B	ond leng	gths	E	Bond ang	gles
		Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BME	CCC	503	-	3,3,3	0.13	0	$1,\!2,\!2$	0.08	0
4	EDO	CCC	504	-	3,3,3	0.06	0	2,2,2	0.19	0
3	BME	AAA	504	-	3,3,3	0.13	0	1,2,2	0.04	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	BME	CCC	503	-	-	0/1/1/1	-
4	EDO	CCC	504	-	-	1/1/1/1	-
3	BME	AAA	504	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.



There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	CCC	504	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 (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	< RSRZ >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	AAA	492/492~(100%)	-0.35	6 (1%) 79 68	41, 85, 153, 167	0
1	BBB	491/492~(99%)	-0.14	24 (4%) 29 18	63, 96, 160, 200	0
1	CCC	492/492~(100%)	-0.41	5 (1%) 82 73	54, 82, 147, 163	0
1	DDD	492/492~(100%)	-0.37	6 (1%) 79 68	63, 96, 138, 148	0
All	All	1967/1968~(99%)	-0.32	41 (2%) 63 50	41, 90, 150, 200	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	349	SER	6.5
1	CCC	426	TYR	6.4
1	BBB	395	CYS	6.1
1	BBB	344	VAL	5.9
1	BBB	426	TYR	5.7
1	BBB	397	ILE	5.2
1	BBB	322	GLY	4.9
1	BBB	350	VAL	4.4
1	CCC	318	ASN	4.2
1	AAA	395	CYS	3.6
1	CCC	463	SER	3.5
1	BBB	323	HIS	3.3
1	BBB	377	VAL	3.2
1	BBB	421	ALA	3.1
1	DDD	430	ASP	2.9
1	BBB	343	VAL	2.7
1	BBB	439	TYR	2.6
1	BBB	419	VAL	2.6
1	AAA	426	TYR	2.6
1	BBB	465	SER	2.5
1	DDD	406	GLY	2.4



Mol	Chain	Res	Type	RSRZ
1	BBB	394	ARG	2.4
1	BBB	432	VAL	2.4
1	AAA	330	GLN	2.4
1	DDD	487	TRP	2.3
1	DDD	214	LEU	2.3
1	DDD	279	VAL	2.3
1	BBB	371	SER	2.2
1	BBB	409	LEU	2.2
1	BBB	354	LEU	2.2
1	BBB	375	ASN	2.2
1	AAA	329	PRO	2.1
1	BBB	321	VAL	2.1
1	BBB	335	TYR	2.1
1	BBB	355	TYR	2.1
1	AAA	392	ASP	2.1
1	AAA	381	GLY	2.0
1	CCC	412	ALA	2.0
1	BBB	1	MET	2.0
1	CCC	312	TYR	2.0
1	DDD	472	ASP	2.0

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, 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	CL	DDD	503	1/1	0.73	0.33	$95,\!95,\!95,\!95$	0
3	BME	AAA	504	4/4	0.76	0.18	109,113,113,115	0
3	BME	CCC	503	4/4	0.79	0.33	65,68,70,72	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors ($Å^2$)	Q<0.9
4	EDO	CCC	504	4/4	0.79	0.22	90,91,91,93	0
2	CL	AAA	503	1/1	0.84	0.27	72,72,72,72	0
2	CL	BBB	505	1/1	0.84	0.19	81,81,81,81	0
2	CL	DDD	505	1/1	0.85	0.21	78,78,78,78	0
2	CL	DDD	501	1/1	0.86	0.12	100,100,100,100	0
2	CL	BBB	504	1/1	0.86	0.21	82,82,82,82	0
2	CL	AAA	502	1/1	0.92	0.22	92,92,92,92	0
2	CL	CCC	501	1/1	0.92	0.14	$58,\!58,\!58,\!58$	0
2	CL	BBB	501	1/1	0.93	0.11	81,81,81,81	0
2	CL	BBB	503	1/1	0.94	0.28	71,71,71,71	0
2	CL	BBB	502	1/1	0.94	0.16	$68,\!68,\!68,\!68$	0
2	CL	DDD	504	1/1	0.95	0.06	85,85,85,85	0
2	CL	DDD	506	1/1	0.97	0.13	$65,\!65,\!65,\!65$	0
2	CL	CCC	502	1/1	0.97	0.06	87,87,87,87	0
2	CL	AAA	501	1/1	0.97	0.15	49,49,49,49	0
2	CL	DDD	502	1/1	0.97	0.08	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.

