wwPDB X-ray Structure Validation Summary Report (i)

Nov 27, 2023 – 12:31 pm GMT

PDB ID	:	7QNT
Title	:	TarM(Se) native
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Deposited on	:	2021-12-22
Resolution	:	3.21 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:

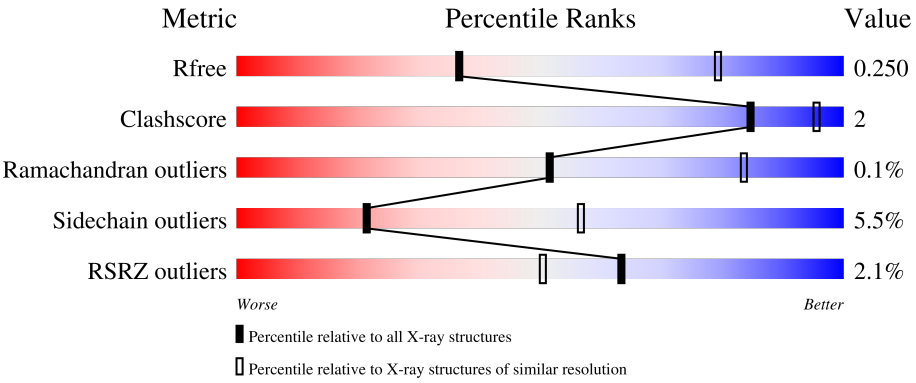
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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-RAY DIFFRACTION

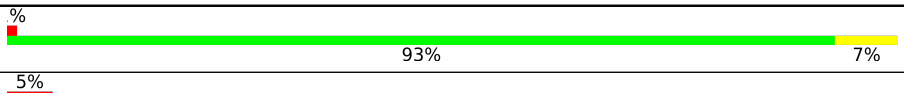
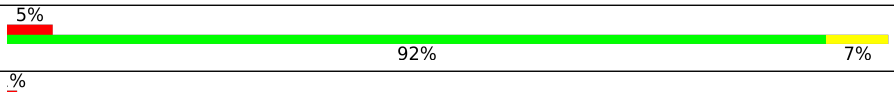
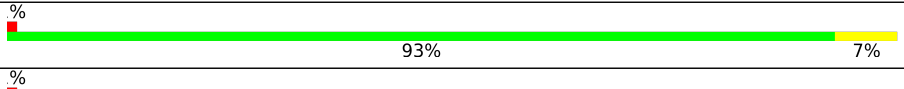
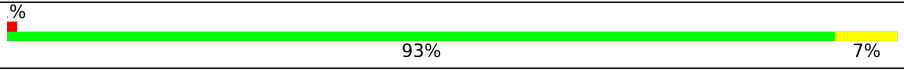
The reported resolution of this entry is 3.21 Å.

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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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	
1	BBB	492	
1	CCC	492	
1	DDD	492	

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.

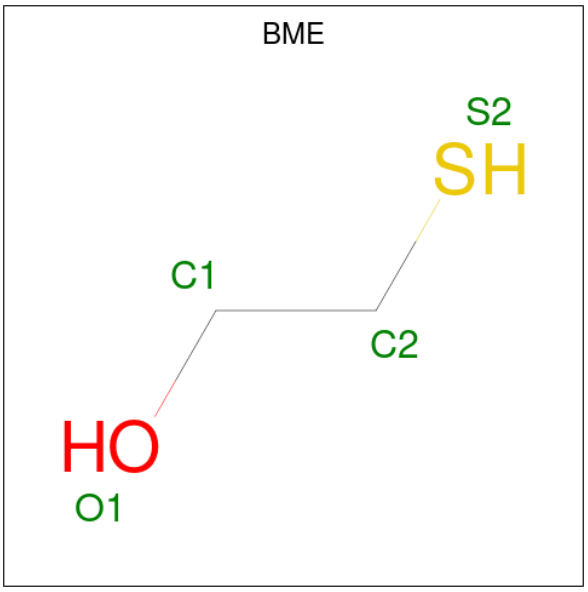
- Molecule 1 is a protein called TarM(Se).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	492	Total	C	N	O	S	0	0	0
			3410	2150	581	667	12			
1	BBB	491	Total	C	N	O	S	0	0	0
			3298	2077	573	637	11			
1	CCC	492	Total	C	N	O	S	0	0	0
			3369	2128	577	650	14			
1	DDD	492	Total	C	N	O	S	0	0	0
			3312	2092	573	636	11			

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

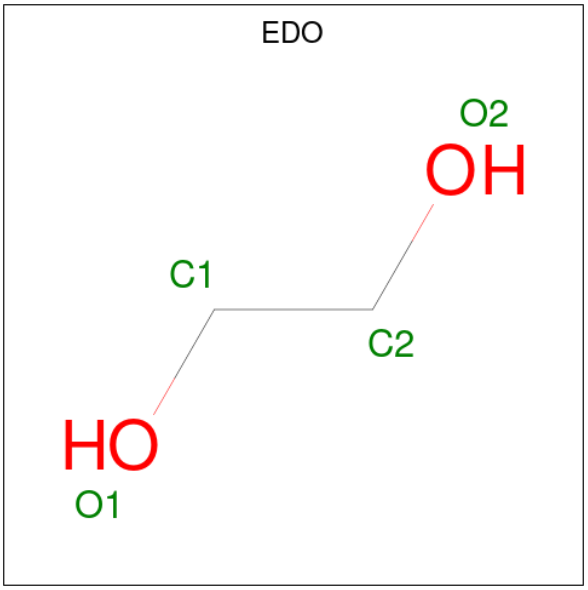
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	3	Total	Cl	0	0
			3	3		
2	BBB	5	Total	Cl	0	0
			5	5		
2	CCC	2	Total	Cl	0	0
			2	2		
2	DDD	6	Total	Cl	0	0
			6	6		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O S 4 2 1 1	0	0
3	CCC	1	Total C O S 4 2 1 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	Total C O 4 2 2	0	0

- Molecule 5 is water.

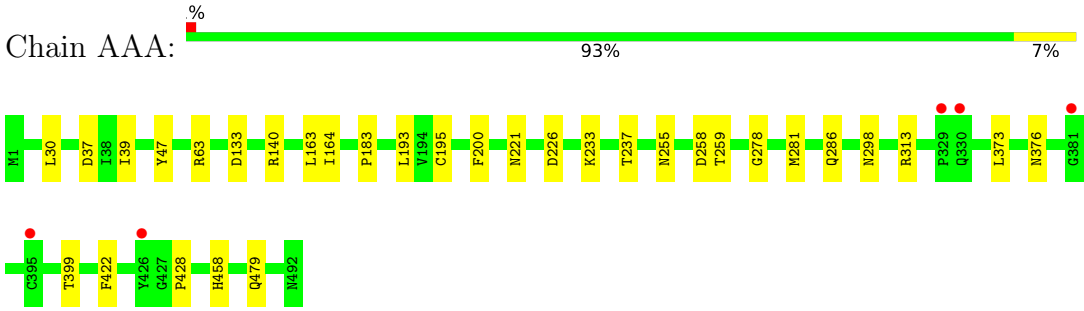
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	67	Total O 67 67	0	0
5	BBB	58	Total O 58 58	0	0
5	CCC	70	Total O 70 70	0	0
5	DDD	69	Total O 69 69	0	0

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.

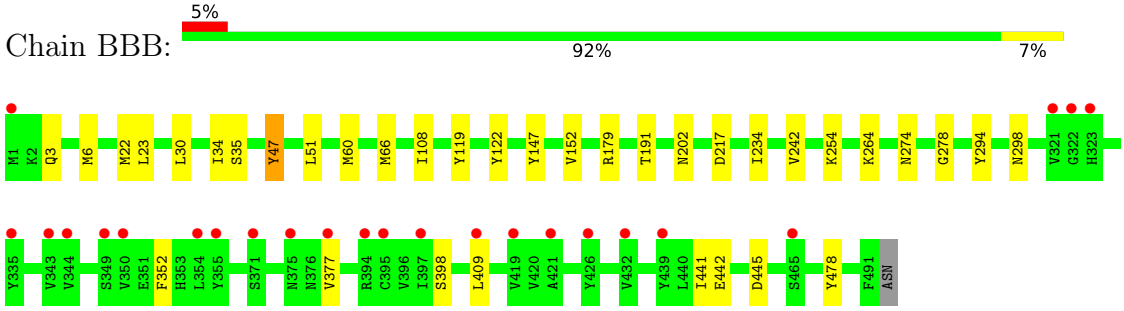
- Molecule 1: TarM(Se)

Chain AAA:



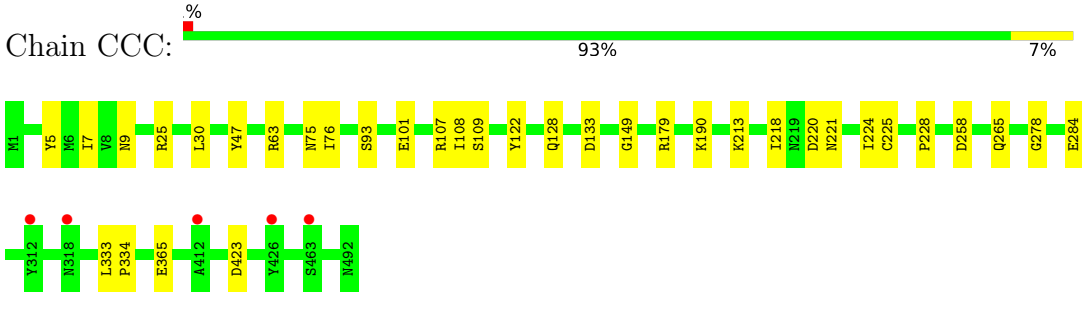
- Molecule 1: TarM(Se)

Chain BBB:



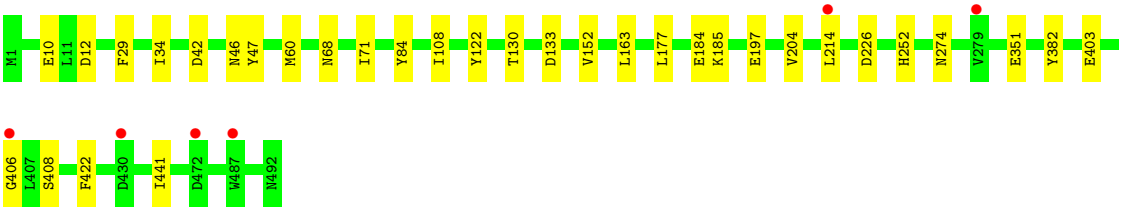
- Molecule 1: TarM(Se)

Chain CCC:



- Molecule 1: TarM(Se)

Chain DDD:


M1
E10
L11
D12
F29
I34
D42
N46
Y47
M60
N68
I71
Y84
I108
Y122
T130
D133
V152
L163
L177
E184
K185
E197
V204
L214
D226
H252
N274
V279
E351
Y382
E403

G406
L407
S408
F422
D430
I441
D472
W487
M492

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	154.01Å 154.01Å 207.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.99 – 3.21 48.99 – 3.21	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.99-3.21) 100.0 (48.99-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.228 , 0.257 0.230 , 0.250	Depositor 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 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.*

[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: 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).

Mol	Chain	Bond lengths		Bond angles	
		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

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

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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.

The worst 5 of 53 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: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

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	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 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	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

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	284	GLU
1	DDD	130	THR
1	CCC	365	GLU
1	DDD	46	ASN
1	DDD	152	VAL

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					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

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	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

The worst 5 of 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

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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
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.