



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 11:49 PM BST

PDB ID : 6UAX
Title : Crystal structure of a GH128 (subgroup II) endo-beta-1,3-glucanase from *Sorangium cellulosum* (ScGH128_II)
Authors : Santos, C.R.; Costa, P.A.C.R.; Domingues, M.N.; Lima, E.A.; Mandelli, F.; Vieira, P.S.; Murakami, M.T.
Deposited on : 2019-09-11
Resolution : 1.30 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	:	2.13.1
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)	:	2.13.1

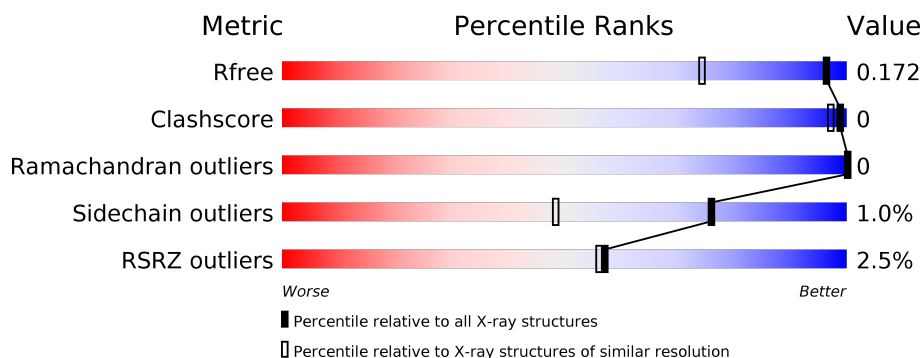
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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	A	355	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 1%; height: 10px; background-color: red;"></div> <div style="width: 69%, height: 10px; background-color: green;"></div> <div style="width: 1%, height: 10px; background-color: yellow;"></div> <div style="width: 29%, height: 10px; background-color: grey;"></div> </div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%;"></div> </div> <div> <div style="width: 1%; text-align: center;">%</div> <div style="width: 69%; text-align: center;">70%</div> <div style="width: 1%; text-align: center;">•</div> <div style="width: 29%; text-align: right;">27%</div> </div> </div>
1	B	355	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 3%, height: 10px; background-color: red;"></div> <div style="width: 67%, height: 10px; background-color: green;"></div> <div style="width: 1%, height: 10px; background-color: yellow;"></div> <div style="width: 29%, height: 10px; background-color: grey;"></div> </div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%;"></div> </div> <div> <div style="width: 3%; text-align: center;">3%</div> <div style="width: 67%; text-align: center;">70%</div> <div style="width: 1%; text-align: center;">•</div> <div style="width: 29%; text-align: right;">28%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4875 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 Hypothetical serine rich protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	13	0
			2065	1307	351	397	10			
1	B	256	Total	C	N	O	S	0	3	0
			2003	1271	339	384	9			

There are 42 discrepancies between the modelled and reference sequences:

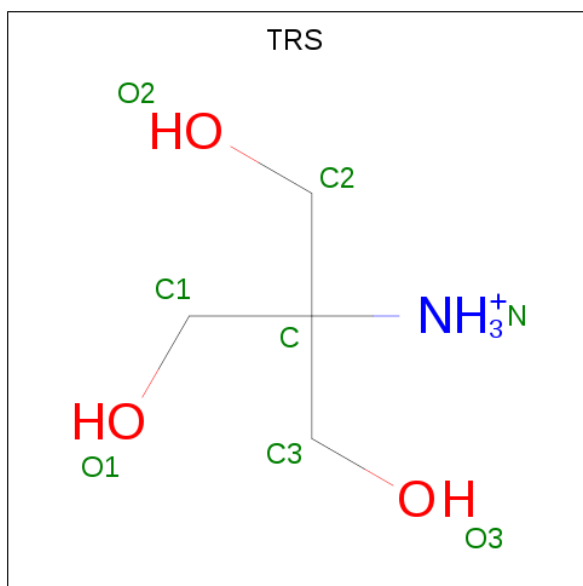
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	initiating methionine	UNP A9GMG4
A	8	GLY	-	expression tag	UNP A9GMG4
A	9	SER	-	expression tag	UNP A9GMG4
A	10	SER	-	expression tag	UNP A9GMG4
A	11	HIS	-	expression tag	UNP A9GMG4
A	12	HIS	-	expression tag	UNP A9GMG4
A	13	HIS	-	expression tag	UNP A9GMG4
A	14	HIS	-	expression tag	UNP A9GMG4
A	15	HIS	-	expression tag	UNP A9GMG4
A	16	HIS	-	expression tag	UNP A9GMG4
A	17	SER	-	expression tag	UNP A9GMG4
A	18	SER	-	expression tag	UNP A9GMG4
A	19	GLY	-	expression tag	UNP A9GMG4
A	20	LEU	-	expression tag	UNP A9GMG4
A	21	VAL	-	expression tag	UNP A9GMG4
A	22	PRO	-	expression tag	UNP A9GMG4
A	23	ARG	-	expression tag	UNP A9GMG4
A	24	GLY	-	expression tag	UNP A9GMG4
A	25	SER	-	expression tag	UNP A9GMG4
A	26	HIS	-	expression tag	UNP A9GMG4
A	27	MET	-	expression tag	UNP A9GMG4
B	7	MET	-	initiating methionine	UNP A9GMG4
B	8	GLY	-	expression tag	UNP A9GMG4
B	9	SER	-	expression tag	UNP A9GMG4
B	10	SER	-	expression tag	UNP A9GMG4

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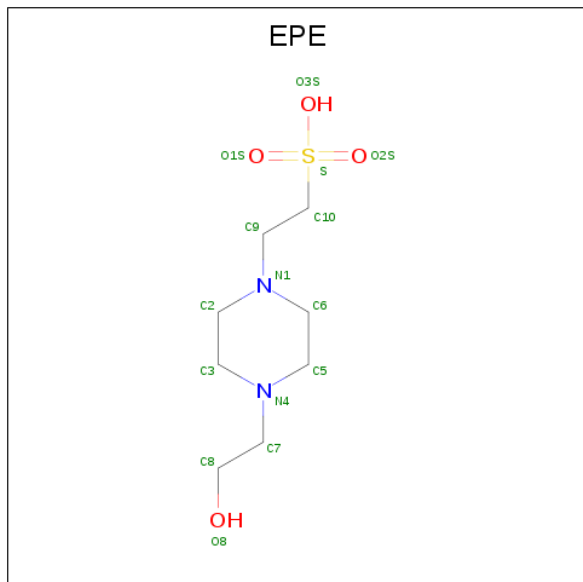
Chain	Residue	Modelled	Actual	Comment	Reference
B	11	HIS	-	expression tag	UNP A9GMG4
B	12	HIS	-	expression tag	UNP A9GMG4
B	13	HIS	-	expression tag	UNP A9GMG4
B	14	HIS	-	expression tag	UNP A9GMG4
B	15	HIS	-	expression tag	UNP A9GMG4
B	16	HIS	-	expression tag	UNP A9GMG4
B	17	SER	-	expression tag	UNP A9GMG4
B	18	SER	-	expression tag	UNP A9GMG4
B	19	GLY	-	expression tag	UNP A9GMG4
B	20	LEU	-	expression tag	UNP A9GMG4
B	21	VAL	-	expression tag	UNP A9GMG4
B	22	PRO	-	expression tag	UNP A9GMG4
B	23	ARG	-	expression tag	UNP A9GMG4
B	24	GLY	-	expression tag	UNP A9GMG4
B	25	SER	-	expression tag	UNP A9GMG4
B	26	HIS	-	expression tag	UNP A9GMG4
B	27	MET	-	expression tag	UNP A9GMG4

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	2	Total	Ca	0	0
			2	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	420	Total	O	0	0
			420	420		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	351	Total	O	0	0
			351	351		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.76Å 65.63Å 86.55Å 90.00° 95.96° 90.00°	Depositor
Resolution (Å)	46.55 – 1.30 46.50 – 1.21	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.55-1.30) 97.6 (46.50-1.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.21Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.129 , 0.167 0.138 , 0.172	Depositor DCC
R_{free} test set	7780 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	11.9	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4875	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: CA, EPE, TRS, CL

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	A	0.99	2/2133 (0.1%)	1.05	2/2906 (0.1%)
1	B	0.91	2/2061 (0.1%)	1.05	4/2809 (0.1%)
All	All	0.95	4/4194 (0.1%)	1.05	6/5715 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	GLU	CD-OE1	6.59	1.32	1.25
1	A	301	GLU	CD-OE1	6.39	1.32	1.25
1	B	203	GLU	CD-OE2	-6.26	1.18	1.25
1	A	99	GLY	C-O	-5.01	1.15	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	348	TYR	CG-CD1-CE1	6.33	126.36	121.30
1	B	136	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	A	247	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	A	330	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	348	TYR	CB-CG-CD2	5.03	124.02	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118[B]	SER	Peptide

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	A	2065	0	1913	1	0
1	B	2003	0	1851	1	0
2	A	8	0	12	1	0
2	B	8	0	12	0	0
3	A	15	0	18	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	420	0	0	2	0
6	B	351	0	0	0	0
All	All	4875	0	3806	3	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 0.

All (3) 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:A:119[A]:PRO:HG3	6:A:505:HOH:O	2.08	0.53
2:A:401:TRS:H32	6:A:709:HOH:O	2.09	0.52
1:B:296:LEU:HD23	1:B:296:LEU:C	2.38	0.44

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	A	269/355 (76%)	254 (94%)	15 (6%)	0	100	100
1	B	257/355 (72%)	252 (98%)	5 (2%)	0	100	100
All	All	526/710 (74%)	506 (96%)	20 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	A	208/257 (81%)	206 (99%)	2 (1%)	76	48
1	B	200/257 (78%)	198 (99%)	2 (1%)	76	48
All	All	408/514 (79%)	404 (99%)	4 (1%)	76	48

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	TRP
1	A	241	CYS
1	B	124	TRP
1	B	132	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](#)

Of 8 ligands modelled in this entry, 5 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$
2	TRS	A	401	-	7,7,7	0.81	0	9,9,9	1.02	0
3	EPE	A	402	-	15,15,15	2.10	3 (20%)	18,20,20	2.06	6 (33%)
2	TRS	B	401	-	7,7,7	0.52	0	9,9,9	1.10	2 (22%)

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	TRS	A	401	-	-	8/9/9/9	-
3	EPE	A	402	-	-	2/9/19/19	0/1/1/1
2	TRS	B	401	-	-	0/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	EPE	C10-S	-6.94	1.67	1.77
3	A	402	EPE	C5-N4	2.25	1.53	1.46
3	A	402	EPE	O1S-S	2.22	1.51	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	EPE	O1S-S-C10	4.03	111.76	106.92
3	A	402	EPE	C5-C6-N1	-3.72	103.00	110.64
3	A	402	EPE	C9-N1-C6	3.15	119.28	111.23
3	A	402	EPE	O3S-S-C10	2.95	110.53	105.77
3	A	402	EPE	C5-N4-C3	2.74	115.00	108.83
2	B	401	TRS	O1-C1-C	2.18	117.90	111.00
3	A	402	EPE	C7-N4-C3	-2.12	105.82	111.23
2	B	401	TRS	C2-C-C1	-2.05	104.47	110.81

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	EPE	C10-C9-N1-C6
2	A	401	TRS	C2-C-C1-O1
2	A	401	TRS	C3-C-C1-O1
2	A	401	TRS	N-C-C1-O1
2	A	401	TRS	C3-C-C2-O2
2	A	401	TRS	C2-C-C3-O3
3	A	402	EPE	C10-C9-N1-C2
2	A	401	TRS	C1-C-C2-O2
2	A	401	TRS	N-C-C3-O3
2	A	401	TRS	N-C-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	TRS	1	0

5.7 Other polymers [i](#)

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 [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	A	258/355 (72%)	0.44	2 (0%) 86 86	7, 9, 16, 62	0
1	B	256/355 (72%)	0.44	11 (4%) 35 32	8, 12, 27, 47	0
All	All	514/710 (72%)	0.44	13 (2%) 57 56	7, 10, 23, 62	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	356	CYS	5.6
1	B	355	ALA	5.4
1	B	139	TYR	3.4
1	B	119	PRO	2.7
1	B	248	TYR	2.5
1	B	156	ASN	2.3
1	B	244	CYS	2.3
1	B	142	THR	2.3
1	B	241	CYS	2.2
1	B	100	CYS	2.2
1	B	354	HIS	2.1
1	A	99	GLY	2.0
1	B	154	GLY	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, 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
3	EPE	A	402	15/15	0.76	0.16	31,38,81,123	0
2	TRS	B	401	8/8	0.88	0.15	14,17,20,21	0
2	TRS	A	401	8/8	0.90	0.12	11,20,26,34	0
4	CA	A	404	1/1	0.98	0.10	28,28,28,28	0
4	CA	B	402	1/1	1.00	0.05	15,15,15,15	0
4	CA	A	403	1/1	1.00	0.05	13,13,13,13	0
5	CL	A	405	1/1	1.00	0.04	16,16,16,16	0
5	CL	B	403	1/1	1.00	0.06	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.