



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2017 – 11:45 AM EDT

PDB ID : 5GXX
Title : Crystal structure of endoglucanase CelQ from *Clostridium thermocellum* complexed with Tris
Authors : Jeng, W.Y.; Liu, C.I.; Wang, A.H.J.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

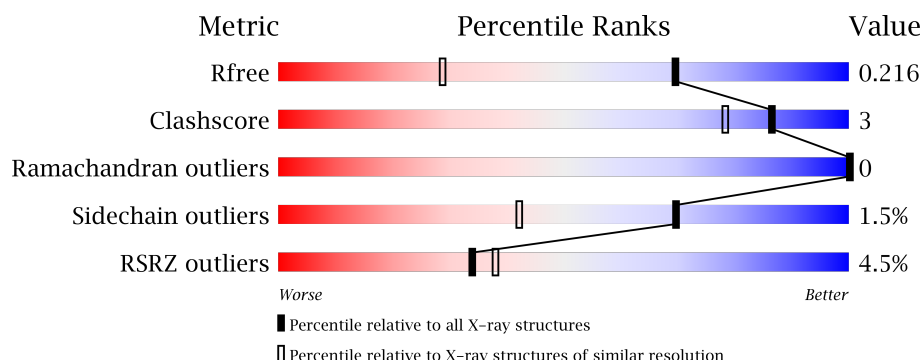
1 Overall quality at a glance

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}	100719	2279 (1.50-1.50)
Clashscore	112137	2503 (1.50-1.50)
Ramachandran outliers	110173	2445 (1.50-1.50)
Sidechain outliers	110143	2443 (1.50-1.50)
RSRZ outliers	101464	2305 (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. 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	610	<div> <div>2%</div> <div>94%</div> <div>6%</div> <div>• •</div> </div>
1	B	610	<div> <div>7%</div> <div>91%</div> <div>6%</div> <div>•</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11398 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 Glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	600	Total	C	N	O	S	0	2	0
			4813	3076	800	919	18			
1	B	599	Total	C	N	O	S	0	3	0
			4811	3075	799	919	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	initiating methionine	UNP Q9AJF8
A	251	THR	ILE	engineered mutation	UNP Q9AJF8
A	629	LEU	-	expression tag	UNP Q9AJF8
A	630	GLU	-	expression tag	UNP Q9AJF8
A	631	HIS	-	expression tag	UNP Q9AJF8
A	632	HIS	-	expression tag	UNP Q9AJF8
A	633	HIS	-	expression tag	UNP Q9AJF8
A	634	HIS	-	expression tag	UNP Q9AJF8
A	635	HIS	-	expression tag	UNP Q9AJF8
A	636	HIS	-	expression tag	UNP Q9AJF8
B	27	MET	-	initiating methionine	UNP Q9AJF8
B	251	THR	ILE	engineered mutation	UNP Q9AJF8
B	629	LEU	-	expression tag	UNP Q9AJF8
B	630	GLU	-	expression tag	UNP Q9AJF8
B	631	HIS	-	expression tag	UNP Q9AJF8
B	632	HIS	-	expression tag	UNP Q9AJF8
B	633	HIS	-	expression tag	UNP Q9AJF8
B	634	HIS	-	expression tag	UNP Q9AJF8
B	635	HIS	-	expression tag	UNP Q9AJF8
B	636	HIS	-	expression tag	UNP Q9AJF8

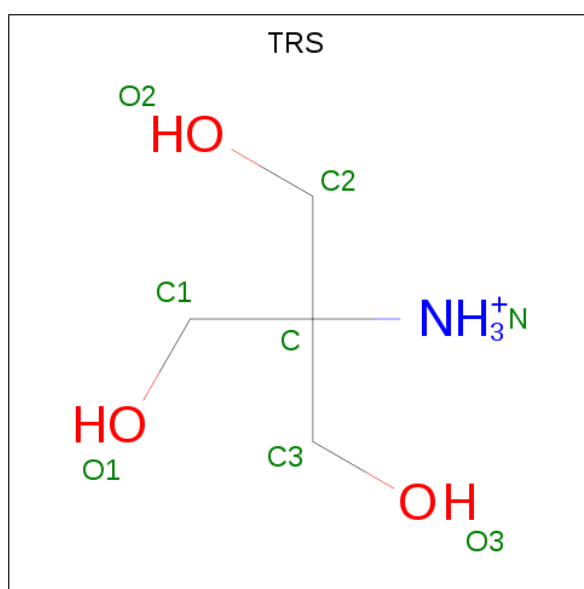
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	4	Total Cl 4 4	0	0
3	A	4	Total Cl 4 4	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	832	Total O 832 832	0	0

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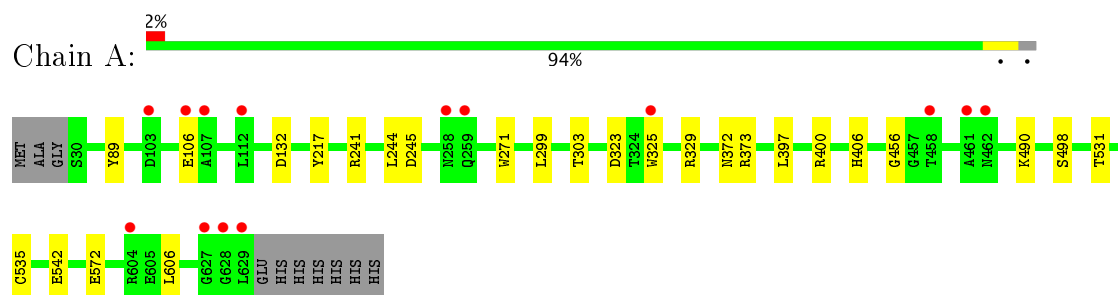
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	914	Total	O	0	0
			914	914		

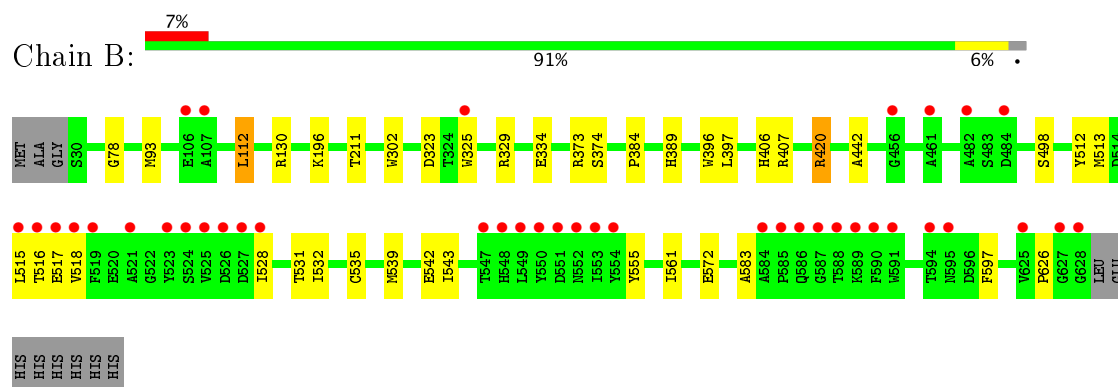
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Glucanase



• Molecule 1: Glucanase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.59Å 109.09Å 140.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.74 – 1.50 29.71 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.74-1.50) 99.8 (29.71-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.188 , 0.217 0.187 , 0.216	Depositor DCC
R_{free} test set	13315 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	14.1	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.044 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11398	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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, 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	0.37	0/4964	0.69	0/6759
1	B	0.41	0/4965	0.74	2/6761 (0.0%)
All	All	0.39	0/9929	0.72	2/13520 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	407	ARG	NE-CZ-NH2	-5.44	117.58	120.30

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	A	4813	0	4500	19	0
1	B	4811	0	4497	33	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	8	0	12	0	0
5	A	832	0	0	5	1
5	B	914	0	0	9	1
All	All	11398	0	9021	47	1

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 3.

All (47) 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:B:532:ILE:HG21	1:B:535:CYS:SG	1.88	1.12
1:A:241:ARG:NH1	1:A:244:LEU:HD23	1.82	0.95
1:B:211:THR:OG1	5:B:801:HOH:O	1.82	0.94
1:A:456:GLY:O	5:A:801:HOH:O	1.85	0.94
1:B:532:ILE:HD11	1:B:543:ILE:HD11	1.53	0.90
1:B:323:ASP:OD2	1:B:325:TRP:HE3	1.55	0.88
1:A:241:ARG:HB3	5:A:1102:HOH:O	1.76	0.84
1:B:532:ILE:HD11	1:B:543:ILE:CD1	2.09	0.83
1:B:112:LEU:HD22	5:B:1469:HOH:O	1.83	0.79
1:A:400:ARG:NH1	5:A:802:HOH:O	2.07	0.79
1:B:516:THR:HA	5:B:806:HOH:O	1.88	0.74
1:B:323:ASP:OD2	1:B:325:TRP:CE3	2.41	0.72
1:B:532:ILE:CG2	1:B:535:CYS:SG	2.78	0.65
1:A:241:ARG:HH12	1:A:244:LEU:HD23	1.60	0.65
1:A:490:LYS:HE2	1:A:606:LEU:HD11	1.80	0.64
1:B:515:LEU:O	1:B:518:VAL:HG22	2.01	0.59
1:B:528:ILE:HA	1:B:583:ALA:O	2.03	0.58
1:B:211:THR:HG21	5:B:1429:HOH:O	2.07	0.55
1:B:572:GLU:O	5:B:802:HOH:O	2.18	0.55
1:A:106:GLU:HA	5:A:1170:HOH:O	2.07	0.55
1:A:535:CYS:SG	1:B:532:ILE:HG22	2.48	0.54
1:A:535:CYS:SG	1:B:532:ILE:CG2	2.96	0.54
1:B:396:TRP:CD1	1:B:397:LEU:HG	2.45	0.52
1:A:323:ASP:OD2	1:A:325:TRP:HE3	1.93	0.51
1:A:542:GLU:HB3	1:B:531:THR:HG22	1.93	0.51
1:B:420:ARG:NH1	5:B:809:HOH:O	2.45	0.48
1:B:512:TYR:CD1	1:B:555:TYR:HB3	2.50	0.45
1:B:93:MET:HB2	1:B:442:ALA:HB1	1.99	0.45
1:A:299:LEU:O	1:A:303:THR:HG23	2.17	0.45
1:A:241:ARG:NH2	1:A:245:ASP:OD1	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:ILE:HD11	1:B:543:ILE:HD12	1.95	0.44
1:B:542:GLU:HG2	1:B:561:ILE:HD11	1.99	0.44
1:B:211:THR:CG2	5:B:1429:HOH:O	2.65	0.44
1:B:539:MET:HA	1:B:539:MET:HE3	2.00	0.44
1:A:241:ARG:HH12	1:A:244:LEU:CD2	2.28	0.44
1:B:517:GLU:HB3	5:B:1356:HOH:O	2.18	0.43
1:A:217:TYR:CE2	4:A:707:TRS:H21	2.54	0.43
1:B:302:TRP:CE2	1:B:334:GLU:HG3	2.54	0.42
1:B:374:SER:O	1:B:384:PRO:HD3	2.20	0.42
1:A:572:GLU:O	5:A:803:HOH:O	2.22	0.41
1:A:531:THR:HG22	1:B:542:GLU:HB3	2.03	0.41
1:B:112:LEU:HG	5:B:1334:HOH:O	2.20	0.41
1:A:89:TYR:CG	1:A:271:TRP:HA	2.56	0.41
1:A:535:CYS:SG	1:B:532:ILE:HG21	2.58	0.41
1:B:78:GLY:HA3	1:B:389:HIS:HA	2.03	0.40
1:B:597:PHE:CG	1:B:626:PRO:HG3	2.56	0.40
1:B:512:TYR:HB2	1:B:597:PHE:HB3	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1363:HOH:O	5:B:1325:HOH:O[3_555]	2.19	0.01

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	A	600/610 (98%)	583 (97%)	17 (3%)	0	100	100
1	B	600/610 (98%)	583 (97%)	17 (3%)	0	100	100
All	All	1200/1220 (98%)	1166 (97%)	34 (3%)	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	490/496 (99%)	483 (99%)	7 (1%)	71	45
1	B	490/496 (99%)	482 (98%)	8 (2%)	68	39
All	All	980/992 (99%)	965 (98%)	15 (2%)	70	42

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	ASP
1	A	329	ARG
1	A	372	ASN
1	A	373	ARG
1	A	397	LEU
1	A	406	HIS
1	A	498	SER
1	B	112	LEU
1	B	196	LYS
1	B	329	ARG
1	B	373	ARG
1	B	406	HIS
1	B	420	ARG
1	B	498	SER
1	B	513	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	ASN
1	A	565	ASN
1	B	346	ASN
1	B	352	GLN

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Mol	Chain	Res	Type
1	B	385	GLN
1	B	600	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 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	$\# Z > 2$
4	TRS	A	707	-	7,7,7	0.35	0	9,9,9	0.81	0
4	TRS	B	707	-	7,7,7	0.28	0	9,9,9	0.93	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
4	TRS	A	707	-	-	0/9/9/9	0/0/0/0
4	TRS	B	707	-	-	0/9/9/9	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	707	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 ⓘ

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	A	600/610 (98%)	-0.04	14 (2%) 61 66	9, 18, 31, 42	0
1	B	599/610 (98%)	0.00	40 (6%) 19 21	7, 13, 37, 47	0
All	All	1199/1220 (98%)	-0.02	54 (4%) 34 38	7, 16, 33, 47	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	525	VAL	5.7
1	A	629	LEU	5.2
1	B	519	PHE	4.9
1	B	587	GLY	4.5
1	B	523	TYR	4.5
1	B	107	ALA	4.4
1	B	521	ALA	4.3
1	B	554	TYR	4.0
1	B	550	TYR	4.0
1	B	516	THR	3.9
1	B	553	ILE	3.8
1	A	627	GLY	3.7
1	B	594	THR	3.5
1	B	549	LEU	3.5
1	B	526	ASP	3.4
1	B	547	THR	3.4
1	B	527	ASP	3.3
1	A	259	GLN	3.3
1	A	628	GLY	3.2
1	B	524	SER	3.2
1	B	627	GLY	3.1
1	B	628	GLY	3.1
1	B	586	GLN	3.0
1	B	484	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	515	LEU	3.0
1	B	482	ALA	2.9
1	B	517	GLU	2.9
1	B	591	TRP	2.8
1	B	625	VAL	2.8
1	B	589	LYS	2.7
1	B	588	THR	2.7
1	B	595	ASN	2.7
1	B	106	GLU	2.6
1	A	106	GLU	2.6
1	B	528	ILE	2.6
1	A	462	ASN	2.5
1	B	548	HIS	2.5
1	A	325	TRP	2.5
1	B	584	ALA	2.5
1	A	103	ASP	2.4
1	B	518	VAL	2.4
1	B	325	TRP	2.4
1	B	551	ASP	2.3
1	B	456	GLY	2.3
1	B	552	ASN	2.3
1	B	461	ALA	2.3
1	B	585	PRO	2.2
1	A	458	THR	2.2
1	A	258	ASN	2.2
1	A	107	ALA	2.1
1	A	461	ALA	2.1
1	A	112	LEU	2.1
1	A	604	ARG	2.1
1	B	590	PHE	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	TRS	B	707	8/8	0.94	0.08	1.55	13,15,16,17	0
4	TRS	A	707	8/8	0.92	0.10	1.44	16,24,25,26	0
2	CA	B	701	1/1	1.00	0.06	-0.43	11,11,11,11	0
3	CL	A	705	1/1	0.98	0.06	-1.42	29,29,29,29	0
2	CA	A	702	1/1	0.98	0.06	-2.23	30,30,30,30	0
2	CA	A	701	1/1	0.99	0.04	-2.34	17,17,17,17	0
3	CL	B	703	1/1	0.99	0.04	-2.64	21,21,21,21	0
2	CA	B	702	1/1	0.97	0.07	-3.18	33,33,33,33	0
3	CL	A	706	1/1	0.99	0.04	-4.16	27,27,27,27	0
3	CL	B	704	1/1	0.99	0.04	-	19,19,19,19	0
3	CL	B	705	1/1	0.97	0.08	-	28,28,28,28	0
3	CL	A	703	1/1	1.00	0.03	-	13,13,13,13	0
3	CL	B	706	1/1	0.92	0.16	-	41,41,41,41	0
3	CL	A	704	1/1	0.93	0.07	-	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.