



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 19, 2023 – 08:24 AM EDT

PDB ID : 2RA6
Title : Crystal Structure of the Possum Milk Whey Lipocalin Trichosurin at pH 4.6
with Bound 4-ethylphenol
Authors : Watson, R.P.
Deposited on : 2007-09-14
Resolution : 1.50 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 ⓘ 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 ⓘ](#)) 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 : 2.36
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

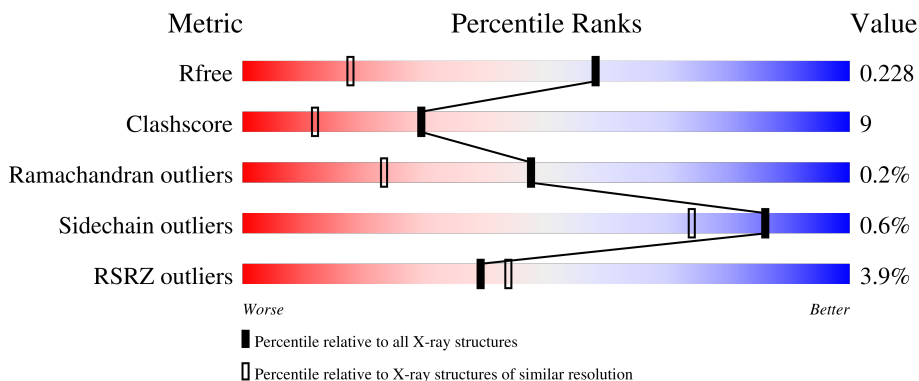
1 Overall quality at a glance

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}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (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 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 $\leq 5\%$. 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	166	
1	B	166	
1	C	166	
1	D	166	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5187 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 Trichosurin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	141	1173	746	203	221	3	0	0	0
1	B	142	1184	752	207	222	3	0	0	0
1	C	143	1180	751	203	223	3	0	0	0
1	D	143	1187	755	205	224	3	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q29147
A	102	GLU	GLY	engineered mutation	UNP Q29147
B	1	MET	-	initiating methionine	UNP Q29147
B	102	GLU	GLY	engineered mutation	UNP Q29147
C	1	MET	-	initiating methionine	UNP Q29147
C	102	GLU	GLY	engineered mutation	UNP Q29147
D	1	MET	-	initiating methionine	UNP Q29147
D	102	GLU	GLY	engineered mutation	UNP Q29147

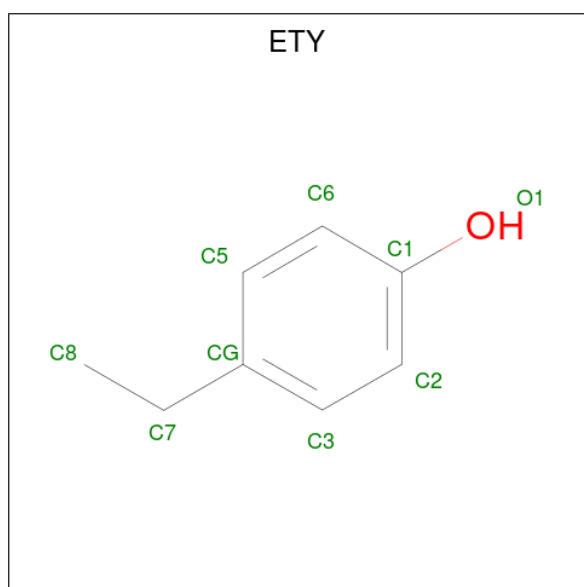
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	2	Total 2	Zn 2	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	2	Total 2	Zn 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	0	0
3	B	3	Total Cl 3 3	0	0
3	C	2	Total Cl 2 2	0	0
3	D	2	Total Cl 2 2	0	0

- Molecule 4 is 4-ethylphenol (three-letter code: ETY) (formula: C₈H₁₀O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 9 8 1	0	0
4	B	1	Total C O 9 8 1	0	0
4	C	1	Total C O 9 8 1	0	0
4	D	1	Total C O 9 8 1	0	0

- Molecule 5 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 3 1	0	0
5	A	1	Total C O 4 3 1	0	0
5	B	1	Total C O 4 3 1	0	0
5	B	1	Total C O 4 3 1	0	0
5	C	1	Total C O 4 3 1	0	0
5	C	1	Total C O 4 3 1	0	0
5	D	1	Total C O 4 3 1	0	0
5	D	1	Total C O 4 3 1	0	0

- Molecule 6 is water.

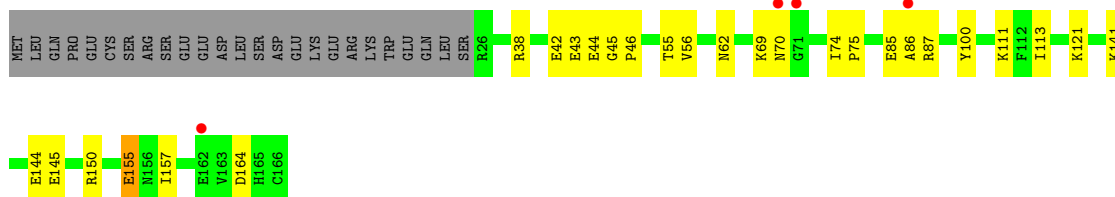
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	93	Total O 93 93	0	0
6	B	92	Total O 92 92	0	0
6	C	97	Total O 97 97	0	0
6	D	98	Total O 98 98	0	0

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.

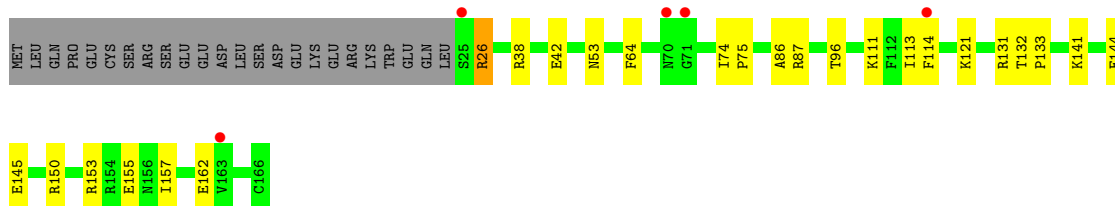
- Molecule 1: Trichosurin

Chain A: 



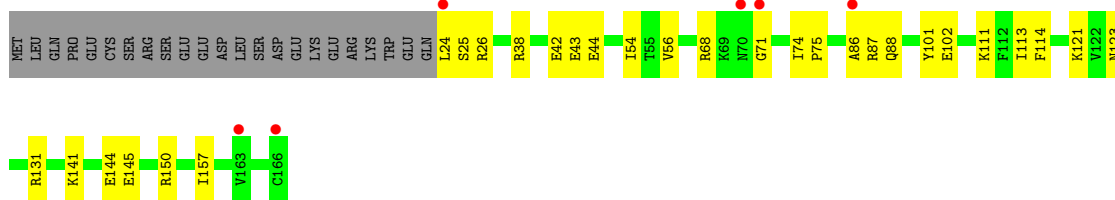
- Molecule 1: Trichosurin

Chain B: 



- Molecule 1: Trichosurin

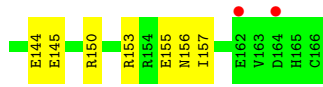
Chain C: 



- Molecule 1: Trichosurin

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.32Å 100.47Å 84.70Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	20.00 – 1.50 29.29 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-1.50) 98.9 (29.29-1.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.50Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.241 0.221 , 0.228	Depositor DCC
R_{free} test set	11762 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtrriage
Anisotropy	0.693	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.477 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5187	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6803e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CL, ZN, IPA, ETY

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	0.35	0/1202	0.58	0/1621
1	B	0.33	0/1213	0.57	0/1635
1	C	0.34	0/1209	0.57	0/1632
1	D	0.33	0/1216	0.59	0/1640
All	All	0.34	0/4840	0.58	0/6528

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	A	1173	0	1109	23	0
1	B	1184	0	1122	23	0
1	C	1180	0	1110	24	0
1	D	1187	0	1125	26	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	1	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	9	0	10	0	0
4	B	9	0	10	1	0
4	C	9	0	10	1	0
4	D	9	0	10	1	0
5	A	8	0	16	0	0
5	B	8	0	16	1	0
5	C	8	0	16	1	0
5	D	8	0	16	2	0
6	A	93	0	0	2	0
6	B	92	0	0	3	0
6	C	97	0	0	0	0
6	D	98	0	0	5	0
All	All	5187	0	4570	89	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 9.

The worst 5 of 89 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:D:54:ILE:HG23	6:D:951:HOH:O	1.76	0.83
1:A:111:LYS:HE2	1:A:113:ILE:HD11	1.62	0.80
1:B:86:ALA:O	1:B:87:ARG:HG2	1.85	0.76
1:A:86:ALA:O	1:A:87:ARG:HG2	1.85	0.76
1:D:86:ALA:O	1:D:87:ARG:HG2	1.85	0.75

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	A	139/166 (84%)	136 (98%)	3 (2%)	0	100	100
1	B	140/166 (84%)	136 (97%)	3 (2%)	1 (1%)	22	6
1	C	141/166 (85%)	136 (96%)	5 (4%)	0	100	100
1	D	141/166 (85%)	136 (96%)	5 (4%)	0	100	100
All	All	561/664 (84%)	544 (97%)	16 (3%)	1 (0%)	47	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	26	ARG

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	A	127/153 (83%)	124 (98%)	3 (2%)	49	19
1	B	128/153 (84%)	128 (100%)	0	100	100
1	C	127/153 (83%)	127 (100%)	0	100	100
1	D	129/153 (84%)	129 (100%)	0	100	100
All	All	511/612 (84%)	508 (99%)	3 (1%)	86	74

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	155	GLU
1	A	164	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	49	ASN

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Mol	Chain	Res	Type
1	D	70	ASN
1	D	137	ASN
1	D	88	GLN
1	B	107	ASN

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 27 ligands modelled in this entry, 15 are monoatomic - leaving 12 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	$\# Z > 2$
5	IPA	C	703	-	3,3,3	0.24	0	3,3,3	1.70	1 (33%)
4	ETY	A	604	-	9,9,9	1.30	0	11,11,11	0.27	0
5	IPA	D	704	-	3,3,3	0.25	0	3,3,3	1.70	1 (33%)
4	ETY	B	601	-	9,9,9	1.36	0	11,11,11	0.27	0
5	IPA	C	707	-	3,3,3	0.28	0	3,3,3	1.72	1 (33%)
5	IPA	B	706	-	3,3,3	0.21	0	3,3,3	1.74	1 (33%)
4	ETY	C	603	-	9,9,9	1.31	0	11,11,11	0.27	0
5	IPA	B	702	-	3,3,3	0.27	0	3,3,3	1.73	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	IPA	A	705	-	3,3,3	0.23	0	3,3,3	1.70	1 (33%)
5	IPA	D	701	-	3,3,3	0.28	0	3,3,3	1.73	1 (33%)
5	IPA	A	708	-	3,3,3	0.26	0	3,3,3	1.73	1 (33%)
4	ETY	D	602	-	9,9,9	1.30	0	11,11,11	0.24	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	ETY	C	603	-	-	0/2/2/2	0/1/1/1
4	ETY	B	601	-	-	0/2/2/2	0/1/1/1
4	ETY	A	604	-	-	0/2/2/2	0/1/1/1
4	ETY	D	602	-	-	0/2/2/2	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	706	IPA	C3-C2-C1	-2.89	91.62	113.47
5	D	701	IPA	C3-C2-C1	-2.87	91.78	113.47
5	B	702	IPA	C3-C2-C1	-2.87	91.78	113.47
5	A	708	IPA	C3-C2-C1	-2.86	91.86	113.47
5	C	707	IPA	C3-C2-C1	-2.85	91.89	113.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	704	IPA	2	0
4	B	601	ETY	1	0
5	C	707	IPA	1	0
4	C	603	ETY	1	0
5	B	702	IPA	1	0
4	D	602	ETY	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, 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	141/166 (84%)	0.31	4 (2%) 53 57	11, 20, 36, 41	0
1	B	142/166 (85%)	0.30	5 (3%) 44 48	12, 20, 36, 41	0
1	C	143/166 (86%)	0.35	6 (4%) 36 40	12, 20, 39, 43	0
1	D	143/166 (86%)	0.31	7 (4%) 29 32	12, 20, 38, 46	0
All	All	569/664 (85%)	0.32	22 (3%) 39 44	11, 20, 38, 46	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	70	ASN	6.6
1	B	70	ASN	5.3
1	C	70	ASN	5.0
1	A	70	ASN	4.4
1	D	162	GLU	3.9

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
5	IPA	D	701	4/4	0.66	0.16	37,38,38,38	0
5	IPA	A	708	4/4	0.68	0.27	36,37,37,37	0
4	ETY	C	603	9/9	0.81	0.30	36,37,38,40	0
4	ETY	A	604	9/9	0.82	0.25	32,33,34,36	0
4	ETY	D	602	9/9	0.82	0.24	31,32,33,33	0
5	IPA	C	703	4/4	0.83	0.22	36,37,37,37	0
5	IPA	B	702	4/4	0.83	0.19	34,34,35,35	0
4	ETY	B	601	9/9	0.84	0.23	30,31,32,34	0
5	IPA	A	705	4/4	0.86	0.22	35,36,36,36	0
5	IPA	C	707	4/4	0.91	0.22	34,35,35,35	0
5	IPA	B	706	4/4	0.94	0.17	34,34,35,35	0
5	IPA	D	704	4/4	0.94	0.17	33,35,35,35	0
3	CL	B	904	1/1	0.95	0.08	20,20,20,20	0
3	CL	C	905	1/1	0.96	0.09	17,17,17,17	0
3	CL	D	907	1/1	0.96	0.09	20,20,20,20	0
3	CL	D	908	1/1	0.96	0.07	19,19,19,19	0
3	CL	A	901	1/1	0.96	0.09	20,20,20,20	0
2	ZN	B	802	1/1	0.96	0.06	25,25,25,25	0
3	CL	C	906	1/1	0.97	0.07	21,21,21,21	0
3	CL	B	903	1/1	0.97	0.08	18,18,18,18	0
2	ZN	D	805	1/1	0.97	0.06	26,26,26,26	0
3	CL	B	909	1/1	0.97	0.10	29,29,29,29	0
3	CL	A	902	1/1	0.97	0.07	18,18,18,18	0
2	ZN	C	804	1/1	0.98	0.08	17,17,17,17	0
2	ZN	D	806	1/1	0.98	0.07	17,17,17,17	0
2	ZN	B	801	1/1	0.98	0.08	17,17,17,17	0
2	ZN	A	803	1/1	0.98	0.08	17,17,17,17	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.