



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:41 AM UTC

PDB ID : 2W3C / pdb_00002w3c
Title : Globular head region of the human general vesicular transport factor p115
Authors : Striegl, H.; Roske, Y.; Kummel, D.; Heinemann, U.
Deposited on : 2008-11-11
Resolution : 2.22 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 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

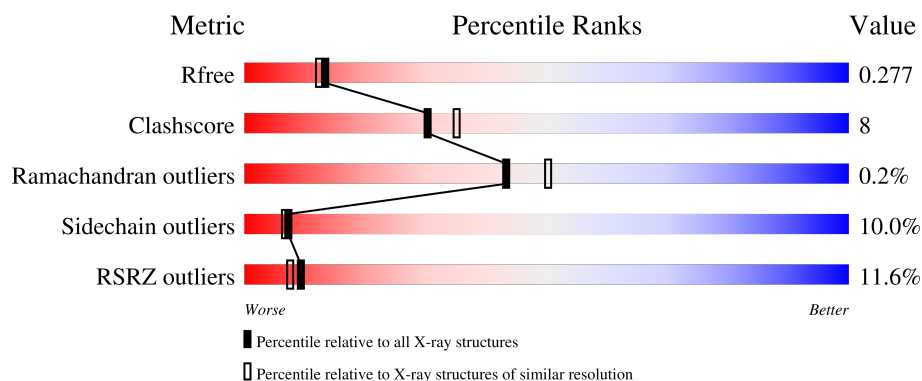
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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 $\leq 5\%$. 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	577	11% 73% 20% • 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4439 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 GENERAL VESICULAR TRANSPORT FACTOR P115.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	551	4295	2737	727	805	26	0	2	0

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total 123	O 123	0	0

- Molecule 1: GENERAL VESICULAR TRANSPORT FACTOR P115



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.55Å 68.89Å 85.75Å 90.00° 108.74° 90.00°	Depositor
Resolution (Å)	19.85 – 2.22 19.85 – 2.22	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.85-2.22) 97.7 (19.85-2.22)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.269 0.230 , 0.277	Depositor DCC
R_{free} test set	2352 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4439	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEG

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	0.74	0/4366	1.07	12/5917 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	601	PHE	CA-C-N	6.44	126.02	119.19
1	A	601	PHE	C-N-CA	6.44	126.02	119.19
1	A	58	GLY	N-CA-C	-6.25	107.80	114.67
1	A	263	PHE	N-CA-C	6.08	120.01	112.59
1	A	412	ILE	CA-C-N	-5.26	115.77	122.77
1	A	412	ILE	C-N-CA	-5.26	115.77	122.77
1	A	362	ARG	CA-C-N	5.11	125.10	119.89
1	A	362	ARG	C-N-CA	5.11	125.10	119.89
1	A	469	ASN	N-CA-C	5.09	117.18	110.36
1	A	600	ASN	N-CA-C	5.09	119.49	113.28
1	A	439	CYS	N-CA-C	5.05	117.17	111.11
1	A	518	ASN	N-CA-C	5.02	117.72	111.24

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	A	4295	0	4352	73	0
2	A	21	0	30	0	0
3	A	123	0	0	4	0
All	All	4439	0	4382	73	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 8.

All (73) 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:362:ARG:HG3	1:A:362:ARG:HH11	1.16	1.09
1:A:406:THR:HG21	1:A:422:GLY:H	1.26	0.97
1:A:307:MET:HG2	1:A:312:LEU:HD23	1.48	0.92
1:A:507:ILE:H	1:A:507:ILE:HD12	1.45	0.82
1:A:406:THR:CG2	1:A:422:GLY:H	1.92	0.81
1:A:435:LEU:HG	1:A:607:MET:HE1	1.70	0.73
1:A:358:SER:HB2	1:A:360:PRO:O	1.87	0.73
1:A:212:ARG:HG3	1:A:212:ARG:HH11	1.53	0.71
1:A:362:ARG:HH11	1:A:362:ARG:CG	1.95	0.71
1:A:362:ARG:HG3	1:A:362:ARG:NH1	1.96	0.69
1:A:435:LEU:HG	1:A:607:MET:CE	2.26	0.66
1:A:212:ARG:HG3	1:A:212:ARG:NH1	2.11	0.64
1:A:624:ILE:O	1:A:628:ILE:HG12	1.98	0.62
1:A:263:PHE:HE1	1:A:284:LEU:HD13	1.64	0.61
1:A:477:GLN:O	1:A:481:ILE:HD12	2.00	0.60
1:A:263:PHE:CE1	1:A:284:LEU:HD13	2.37	0.59
1:A:115:GLU:HG2	1:A:153:LEU:HD11	1.84	0.59
1:A:406:THR:HG21	1:A:422:GLY:N	2.08	0.58
1:A:492:VAL:O	1:A:496:MET:HG3	2.06	0.55
1:A:415:THR:C	1:A:417:ASN:H	2.14	0.55
1:A:263:PHE:CE1	1:A:284:LEU:CD1	2.89	0.55
1:A:406:THR:HG22	1:A:422:GLY:HA3	1.90	0.53
1:A:362:ARG:CG	1:A:362:ARG:NH1	2.59	0.53
1:A:77:GLU:HG2	3:A:2004:HOH:O	2.10	0.52
1:A:114:THR:HG23	1:A:149:LEU:HD23	1.92	0.52
1:A:139:ARG:O	1:A:143:VAL:HG23	2.10	0.52
1:A:87:TYR:O	1:A:91:SER:HB3	2.10	0.52
1:A:532:GLU:HA	1:A:535:GLN:HG3	1.91	0.52
1:A:406:THR:CG2	1:A:422:GLY:N	2.69	0.51
1:A:148:SER:O	1:A:152:GLN:HG3	2.11	0.51
1:A:435:LEU:HD11	1:A:604:PRO:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLU:CG	3:A:2004:HOH:O	2.60	0.50
1:A:457:GLN:HE22	1:A:460:ARG:HH11	1.60	0.49
1:A:197:ASN:OD1	1:A:200:ILE:HG13	2.12	0.49
1:A:600:ASN:C	1:A:600:ASN:ND2	2.70	0.49
1:A:545:LEU:O	1:A:548:SER:HB2	2.13	0.49
1:A:139:ARG:NH1	1:A:177:ASP:OD2	2.46	0.48
1:A:549:ILE:HG12	1:A:564:LEU:HB3	1.95	0.48
1:A:183:ARG:O	1:A:187:VAL:HG23	2.12	0.48
1:A:212:ARG:HH11	1:A:212:ARG:CG	2.24	0.48
1:A:62:MET:C	1:A:64:HIS:H	2.21	0.47
1:A:600:ASN:O	1:A:600:ASN:CG	2.55	0.47
1:A:150:LEU:HB3	1:A:192:ALA:HB1	1.96	0.47
1:A:213:LEU:HD21	1:A:235:LEU:HD23	1.97	0.47
1:A:403:ILE:O	1:A:406:THR:HB	2.16	0.46
1:A:507:ILE:H	1:A:507:ILE:CD1	2.21	0.46
1:A:221:GLY:O	1:A:224:ASP:HB2	2.15	0.46
1:A:423:GLN:HG3	3:A:2083:HOH:O	2.16	0.46
1:A:375:GLU:HG2	1:A:433:ASP:OD1	2.16	0.45
1:A:488:ILE:HG13	1:A:489:GLN:N	2.31	0.45
1:A:62:MET:C	1:A:64:HIS:N	2.74	0.45
1:A:186:GLY:O	1:A:189:LEU:HB3	2.15	0.45
1:A:395:LYS:HA	1:A:395:LYS:HD3	1.68	0.44
1:A:358:SER:HB2	1:A:360:PRO:C	2.43	0.44
1:A:364:ALA:HA	1:A:367:VAL:HG12	1.99	0.43
1:A:527:ALA:HB2	1:A:572:ILE:HG12	1.99	0.43
1:A:292:SER:OG	1:A:294:THR:HB	2.18	0.43
1:A:352:ALA:HB2	1:A:392:PHE:CE2	2.54	0.43
1:A:210:PHE:HB2	3:A:2035:HOH:O	2.18	0.43
1:A:260:LYS:HD2	1:A:311:GLY:O	2.18	0.43
1:A:127:LEU:O	1:A:131:LEU:HG	2.19	0.42
1:A:490:THR:O	1:A:494:LEU:HG	2.19	0.42
1:A:169:SER:O	1:A:172:MET:HB2	2.19	0.42
1:A:122:GLU:H	1:A:122:GLU:CD	2.28	0.42
1:A:75:ASP:O	1:A:78:ILE:HG22	2.20	0.41
1:A:386:LEU:O	1:A:390:GLN:HG3	2.20	0.41
1:A:507:ILE:HD12	1:A:507:ILE:N	2.25	0.41
1:A:575:GLU:H	1:A:575:GLU:CD	2.29	0.41
1:A:602:PRO:HD2	1:A:606:TYR:CG	2.55	0.41
1:A:548:SER:O	1:A:552:ASN:HB2	2.20	0.40
1:A:415:THR:C	1:A:417:ASN:N	2.80	0.40
1:A:259:MET:HE2	1:A:262:TRP:CZ3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ASN:O	1:A:400:GLN:HG3	2.22	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	Percentiles
1	A	545/577 (94%)	516 (95%)	28 (5%)	1 (0%)	43 50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	VAL

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	483/512 (94%)	435 (90%)	48 (10%)	7 7

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	VAL
1	A	72	ASP

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Mol	Chain	Res	Type
1	A	111	SER
1	A	148	SER
1	A	150	LEU
1	A	163	VAL
1	A	164	SER
1	A	183	ARG
1	A	189	LEU
1	A	195	ARG
1	A	212	ARG
1	A	229	VAL
1	A	237	GLN
1	A	264	GLU
1	A	265	VAL
1	A	272	TRP
1	A	280	LEU
1	A	284	LEU
1	A	294	THR
1	A	325	VAL
1	A	362	ARG
1	A	369	LEU
1	A	382	ARG
1	A	386	LEU
1	A	413	ASP
1	A	423	GLN
1	A	449	GLN
1	A	450	GLU
1	A	459	LEU
1	A	481	ILE
1	A	484	GLN
1	A	488	ILE
1	A	490	THR
1	A	491	ARG
1	A	507	ILE
1	A	513	LEU
1	A	523	THR
1	A	533	GLU
1	A	564	LEU
1	A	567	LEU
1	A	569	GLU
1	A	578	ILE
1	A	580	LYS
1	A	591	SER

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Mol	Chain	Res	Type
1	A	600	ASN
1	A	608	ILE
1	A	616	LEU
1	A	626	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	159	GLN
1	A	208	ASN
1	A	423	GLN
1	A	457	GLN
1	A	462	GLN
1	A	476	GLN
1	A	518	ASN
1	A	529	ASN
1	A	538	GLN
1	A	576	ASN
1	A	600	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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	PEG	A	1632	-	6,6,6	0.48	0	5,5,5	0.32	0
2	PEG	A	1631	-	6,6,6	0.52	0	5,5,5	0.17	0
2	PEG	A	1630	-	6,6,6	0.56	0	5,5,5	0.21	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
2	PEG	A	1632	-	-	3/4/4/4	-
2	PEG	A	1631	-	-	0/4/4/4	-
2	PEG	A	1630	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1630	PEG	O2-C3-C4-O4
2	A	1632	PEG	O1-C1-C2-O2
2	A	1632	PEG	O2-C3-C4-O4
2	A	1630	PEG	O1-C1-C2-O2
2	A	1630	PEG	C1-C2-O2-C3
2	A	1632	PEG	C4-C3-O2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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 ⓘ

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	551/577 (95%)	0.82	64 (11%) 9 7	12, 41, 69, 84	2 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	VAL	4.4
1	A	600	ASN	4.3
1	A	203	ILE	4.2
1	A	598	GLN	3.9
1	A	160	ILE	3.9
1	A	227	ILE	3.9
1	A	197	ASN	3.6
1	A	61	ALA	3.6
1	A	174	LEU	3.3
1	A	187	VAL	3.2
1	A	182	ILE	3.2
1	A	56	GLU	3.2
1	A	467	ILE	3.0
1	A	530	LEU	3.0
1	A	162	LEU	2.9
1	A	228	VAL	2.9
1	A	471	PRO	2.9
1	A	296	PRO	2.8
1	A	252	GLU	2.8
1	A	245	SER	2.7
1	A	189	LEU	2.7
1	A	168	VAL	2.7
1	A	555	SER	2.7
1	A	297	PRO	2.7
1	A	235	LEU	2.7
1	A	170	ARG	2.6
1	A	234	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	199	ALA	2.6
1	A	265	VAL	2.6
1	A	629	TYR	2.6
1	A	200	ILE	2.6
1	A	578	ILE	2.6
1	A	238	ASN	2.5
1	A	116	ILE	2.4
1	A	176	ALA	2.4
1	A	171	LEU	2.4
1	A	246	ASN	2.4
1	A	172	MET	2.4
1	A	232	CYS	2.4
1	A	198	GLY	2.3
1	A	190	LEU	2.3
1	A	272	TRP	2.3
1	A	188	LEU	2.3
1	A	240	LEU	2.3
1	A	274	ALA	2.3
1	A	206	PHE	2.2
1	A	583	PHE	2.2
1	A	384	ALA	2.2
1	A	231	ASP	2.2
1	A	166	MET	2.2
1	A	169	SER	2.2
1	A	294	THR	2.2
1	A	577	PHE	2.2
1	A	410	SER	2.2
1	A	309	GLN	2.1
1	A	90	ILE	2.1
1	A	185	ASP	2.1
1	A	164	SER	2.1
1	A	589	LEU	2.1
1	A	223	SER	2.1
1	A	192	ALA	2.1
1	A	557	GLU	2.0
1	A	181	VAL	2.0
1	A	239	LEU	2.0

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 [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	PEG	A	1630	7/7	0.80	0.12	55,66,80,82	0
2	PEG	A	1632	7/7	0.83	0.11	61,67,92,94	0
2	PEG	A	1631	7/7	0.91	0.11	32,45,55,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.