



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2026 – 04:20 PM EDT

PDB ID : 9Z0A / pdb_00009z0a
Title : Crystal Structure of the Polycaprolactam (Nylon6) and Poly(Hexamethylene Adipamide) (Nylon66) Hydrolase Nyl12 at Room Temperature
Authors : Capra, N.; Meilleur, F.
Deposited on : 2025-10-31
Resolution : 1.90 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

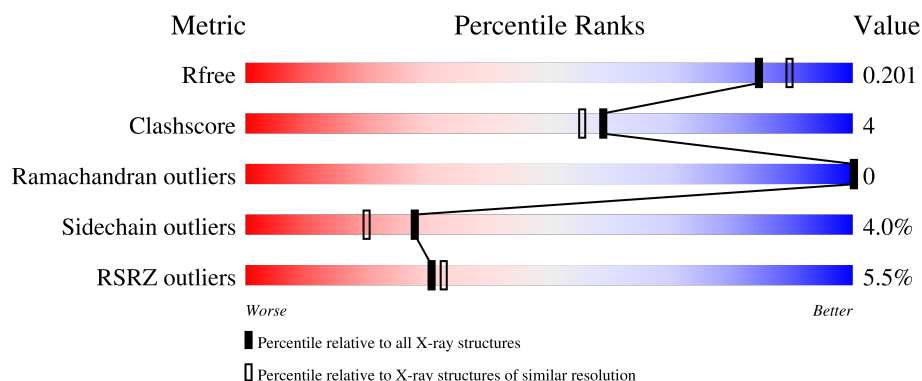
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	328	
1	B	328	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PGE	A	401[B]	-	-	X	-
3	PEG	B	401[B]	-	-	X	-

2 Entry composition [i](#)

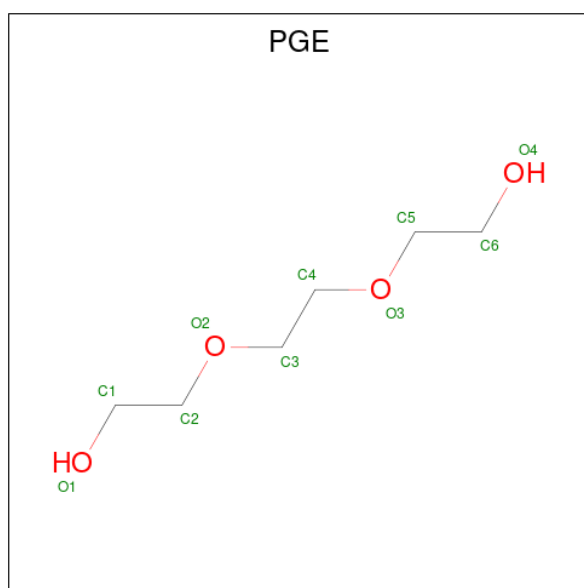
There are 4 unique types of molecules in this entry. The entry contains 4873 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Polycaprolactam (Nylon6) and Poly(Hexamethylene Adipamide) (Nylon66) Hydrolase Nyl12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2313	1486	391	432	4			
1	B	310	Total	C	N	O	S	0	0	0
			2344	1508	397	435	4			

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	1
			20	12	8		

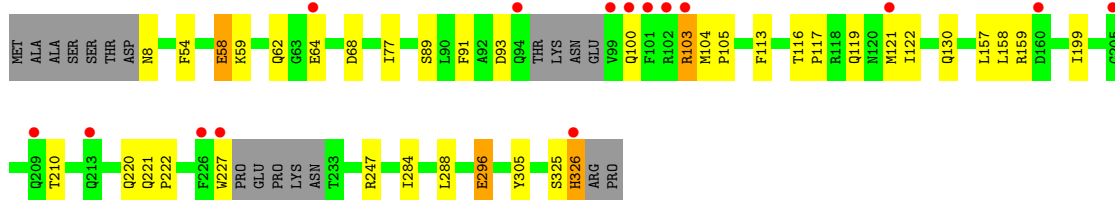
- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	1
			14	8	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	95	Total	O	0	0
			95	95		
4	B	87	Total	O	0	0
			87	87		



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.59Å 79.43Å 108.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.37 – 1.90 29.37 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.37-1.90) 99.3 (29.37-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.151 , 0.196 0.163 , 0.201	Depositor DCC
R_{free} test set	2688 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4873	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: PGE, 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	0.96	2/2358 (0.1%)	1.29	11/3194 (0.3%)
1	B	1.02	1/2392 (0.0%)	1.30	10/3242 (0.3%)
All	All	0.99	3/4750 (0.1%)	1.30	21/6436 (0.3%)

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	4
1	B	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	ILE	CB-CG1	-6.50	1.40	1.53
1	B	284	ILE	CB-CG1	-5.35	1.42	1.53
1	A	65	ALA	CA-CB	-5.01	1.45	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	VAL	N-CA-CB	-6.90	103.36	112.26
1	B	64	GLU	N-CA-C	6.76	119.06	110.61
1	B	54	PHE	CA-CB-CG	6.74	120.54	113.80
1	A	54	PHE	CA-CB-CG	6.53	120.33	113.80
1	A	226	PHE	CA-CB-CG	-6.46	107.34	113.80
1	A	210	THR	CA-CB-OG1	-6.41	99.99	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	LYS	N-CA-CB	-6.29	100.87	110.12
1	B	296	GLU	CB-CG-CD	6.14	123.03	112.60
1	B	59	LYS	CA-CB-CG	5.84	125.79	114.10
1	B	210	THR	CA-CB-OG1	-5.84	100.84	109.60
1	A	220	GLN	N-CA-CB	5.80	118.88	110.47
1	B	59	LYS	N-CA-CB	-5.68	101.77	110.12
1	A	214	GLN	CB-CA-C	-5.59	101.52	110.79
1	B	247	ARG	CD-NE-CZ	-5.59	116.58	124.40
1	B	68	ASP	N-CA-C	-5.48	106.95	113.97
1	A	292	GLY	CA-C-O	-5.39	118.71	122.22
1	B	93	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	68	ASP	N-CA-C	-5.24	107.06	113.50
1	A	298	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	93	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	58	GLU	N-CA-CB	5.06	117.56	110.12

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	A	103	ARG	Sidechain
1	A	159	ARG	Sidechain
1	A	247	ARG	Sidechain
1	B	103	ARG	Sidechain

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	2313	0	2327	19	0
1	B	2344	0	2353	15	0
2	A	20	0	28	11	0
3	B	14	0	20	9	0
4	A	95	0	0	4	0
4	B	87	0	0	1	0
All	All	4873	0	4728	41	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 4.

All (41) 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)
3:B:401[B]:PEG:C1	3:B:401[B]:PEG:H41	2.06	0.84
3:B:401[B]:PEG:H41	3:B:401[B]:PEG:H11	1.63	0.80
1:B:113:PHE:HB2	3:B:401[B]:PEG:H12	1.64	0.79
3:B:401[B]:PEG:C4	3:B:401[B]:PEG:O1	2.36	0.74
1:B:325:SER:O	1:B:326:HIS:C	2.34	0.70
3:B:401[B]:PEG:C1	3:B:401[B]:PEG:C4	2.70	0.69
1:A:233:THR:HB	2:A:401[B]:PGE:H2	1.75	0.68
1:A:233:THR:N	2:A:401[B]:PGE:HO1	1.92	0.66
1:A:324:TYR:O	1:A:325:SER:C	2.40	0.64
1:B:77:ILE:H	3:B:401[A]:PEG:H31	1.67	0.59
2:A:401[A]:PGE:H62	4:A:503:HOH:O	2.03	0.58
3:B:401[B]:PEG:O1	3:B:401[B]:PEG:O4	2.21	0.58
1:A:113:PHE:H	2:A:401[B]:PGE:H22	1.70	0.56
1:A:233:THR:CB	2:A:401[B]:PGE:H2	2.36	0.55
1:B:58:GLU:O	1:B:62:GLN:HG3	2.07	0.55
3:B:401[B]:PEG:H41	3:B:401[B]:PEG:O1	2.03	0.55
1:A:233:THR:OG1	2:A:401[B]:PGE:C2	2.56	0.54
1:B:100:GLN:HB2	1:B:103:ARG:HG3	1.92	0.51
1:A:116:THR:HB	1:A:117:PRO:HD3	1.93	0.50
1:A:157:LEU:H	1:A:157:LEU:HD23	1.77	0.50
1:A:58:GLU:CD	4:A:501:HOH:O	2.54	0.50
1:A:233:THR:OG1	2:A:401[B]:PGE:O2	2.29	0.49
1:A:186:ASN:HD22	2:A:401[B]:PGE:C2	2.26	0.48
1:B:227:TRP:C	4:B:510:HOH:O	2.59	0.46
1:A:215:VAL:HG22	1:B:305:TYR:CD1	2.52	0.45
1:B:116:THR:HB	1:B:117:PRO:HD3	1.98	0.45
1:B:113:PHE:HB2	3:B:401[A]:PEG:H21	1.99	0.44
1:A:248:HIS:HE1	1:A:298:ASP:OD1	2.01	0.44
2:A:401[A]:PGE:C6	4:A:503:HOH:O	2.65	0.44
1:B:104:MET:HA	1:B:104:MET:HE2	2.01	0.43
1:B:157:LEU:H	1:B:157:LEU:HD23	1.84	0.42
1:B:91:PHE:HB2	1:B:105:PRO:HG3	2.01	0.42
1:A:89:SER:OG	1:A:130:GLN:HG2	2.20	0.42
1:B:89:SER:OG	1:B:130:GLN:HG2	2.20	0.42
1:B:221:GLN:HB3	1:B:222:PRO:HD2	2.01	0.41
1:A:186:ASN:HD22	2:A:401[B]:PGE:H2	1.85	0.41
1:A:186:ASN:HD22	2:A:401[A]:PGE:H2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:HIS:HD2	4:A:505:HOH:O	2.04	0.41
1:A:265:HIS:HA	1:A:266:PRO:HA	1.93	0.40
1:A:295:ILE:HD12	1:A:295:ILE:O	2.22	0.40
1:B:158:LEU:HD23	1:B:158:LEU:HA	1.91	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	301/328 (92%)	292 (97%)	9 (3%)	0	100	100
1	B	304/328 (93%)	296 (97%)	8 (3%)	0	100	100
All	All	605/656 (92%)	588 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	239/258 (93%)	230 (96%)	9 (4%)	29	21
1	B	242/258 (94%)	232 (96%)	10 (4%)	27	19
All	All	481/516 (93%)	462 (96%)	19 (4%)	28	20

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	ARG
1	A	103	ARG
1	A	122	ILE
1	A	159	ARG
1	A	199	ILE
1	A	215	VAL
1	A	295	ILE
1	A	296	GLU
1	A	322	VAL
1	B	8	ASN
1	B	119	GLN
1	B	121	MET
1	B	122	ILE
1	B	159	ARG
1	B	199	ILE
1	B	220	GLN
1	B	288	LEU
1	B	296	GLU
1	B	326	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	41	GLN
1	A	100	GLN
1	A	146	HIS
1	A	248	HIS
1	A	251	GLN
1	A	265	HIS
1	B	18	GLN
1	B	119	GLN
1	B	220	GLN
1	B	265	HIS

5.3.3 RNA ⓘ

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](#)

4 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	PGE	A	401[B]	-	9,9,9	0.80	0	8,8,8	0.50	0
2	PGE	A	401[A]	-	9,9,9	0.91	1 (11%)	8,8,8	0.57	0
3	PEG	B	401[A]	-	6,6,6	1.12	0	5,5,5	0.79	0
3	PEG	B	401[B]	-	6,6,6	1.15	0	5,5,5	0.65	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	PGE	A	401[B]	-	-	5/7/7/7	-
2	PGE	A	401[A]	-	-	4/7/7/7	-
3	PEG	B	401[A]	-	-	2/4/4/4	-
3	PEG	B	401[B]	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[A]	PGE	C4-C3	2.04	1.59	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401[A]	PGE	C1-C2-O2-C3
2	A	401[B]	PGE	C1-C2-O2-C3
2	A	401[B]	PGE	O2-C3-C4-O3
3	B	401[B]	PEG	O2-C3-C4-O4
2	A	401[B]	PGE	O1-C1-C2-O2
2	A	401[B]	PGE	O3-C5-C6-O4
2	A	401[A]	PGE	O3-C5-C6-O4
3	B	401[A]	PEG	C1-C2-O2-C3
3	B	401[B]	PEG	C1-C2-O2-C3
2	A	401[A]	PGE	O1-C1-C2-O2
3	B	401[A]	PEG	C4-C3-O2-C2
2	A	401[B]	PGE	C3-C4-O3-C5
2	A	401[A]	PGE	C3-C4-O3-C5

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401[B]	PGE	8	0
2	A	401[A]	PGE	3	0
3	B	401[A]	PEG	2	0
3	B	401[B]	PEG	7	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	307/328 (93%)	0.32	19 (6%) 26 28	15, 27, 62, 113	0
1	B	310/328 (94%)	0.11	15 (4%) 35 38	14, 25, 51, 113	0
All	All	617/656 (94%)	0.22	34 (5%) 30 32	14, 26, 58, 113	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	TRP	4.8
1	B	101	PHE	4.6
1	A	160	ASP	4.2
1	A	226	PHE	4.0
1	B	102	ARG	4.0
1	A	103	ARG	3.9
1	B	326	HIS	3.7
1	A	221	GLN	3.7
1	B	160	ASP	3.5
1	A	100	GLN	3.3
1	A	159	ARG	3.2
1	A	224	LYS	3.1
1	A	204	LYS	3.0
1	B	209	GLN	2.8
1	A	101	PHE	2.8
1	B	100	GLN	2.8
1	B	99	VAL	2.8
1	B	226	PHE	2.8
1	A	325	SER	2.7
1	A	205	GLY	2.7
1	B	64	GLU	2.7
1	B	205	GLY	2.6
1	B	94	GLN	2.5
1	A	322	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	102	ARG	2.4
1	A	94	GLN	2.4
1	A	199	ILE	2.3
1	A	225	PRO	2.3
1	B	213	GLN	2.3
1	B	121	MET	2.2
1	A	213	GLN	2.2
1	B	103	ARG	2.2
1	A	284	ILE	2.1
1	A	157	LEU	2.1

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 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(\AA^2)	Q<0.9
3	PEG	B	401[A]	7/7	0.72	0.19	26,34,40,43	7
3	PEG	B	401[B]	7/7	0.72	0.19	26,30,42,44	7
2	PGE	A	401[A]	10/10	0.81	0.16	22,30,37,39	10
2	PGE	A	401[B]	10/10	0.81	0.16	19,30,54,54	10

6.5 Other polymers [i](#)

There are no such residues in this entry.