wwPDB X-ray Structure Validation Summary Report (i)

Mar 10, 2026 – 01:14 AM UTC

PDB ID	:	2HU8 / pdb_00002hu8
Title	:	Binding of inhibitors by Acylaminoacyl peptidase
Authors	:	Kiss, A.L.; Hornung, B.; Radi, K.; Gengeliczki, Z.; Sztaray, B.; Harmat, V.; Polgar, L.
Deposited on	:	2006-07-26
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

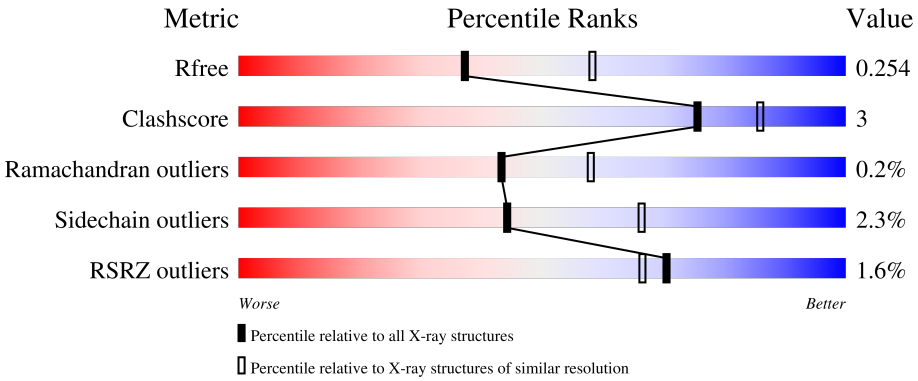
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 <=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	582	92% 7%
1	B	582	3% 89% 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8890 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.

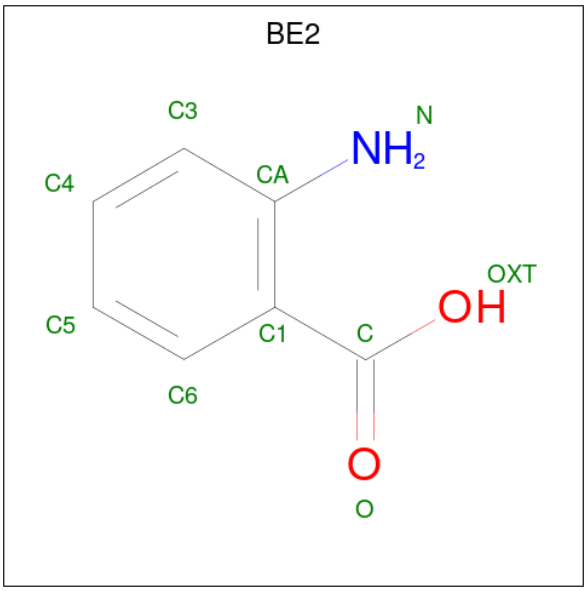
- Molecule 1 is a protein called Acylamino-acid-releasing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total	C	N	O	S	0	4	0
			4363	2763	756	832	12			
1	B	573	Total	C	N	O	S	0	3	0
			4254	2706	732	803	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	ALA	SER	engineered mutation	UNP Q9YBQ2
B	445	ALA	SER	engineered mutation	UNP Q9YBQ2

- Molecule 2 is 2-AMINOBENZOIC ACID (CCD ID: BE2) (formula: $C_7H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	7	1	1		

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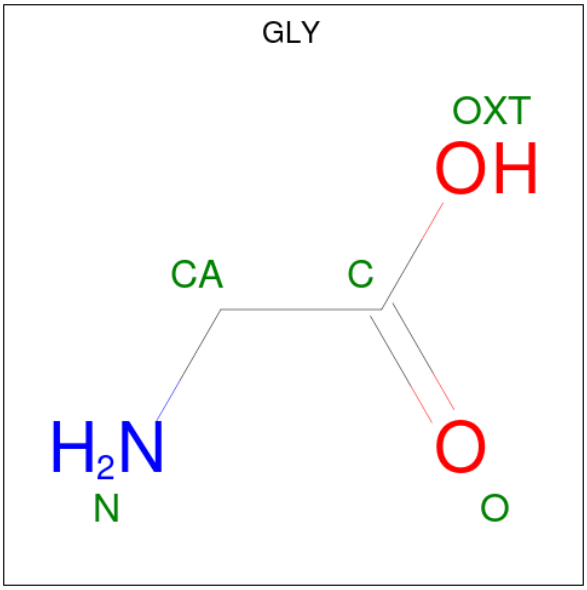
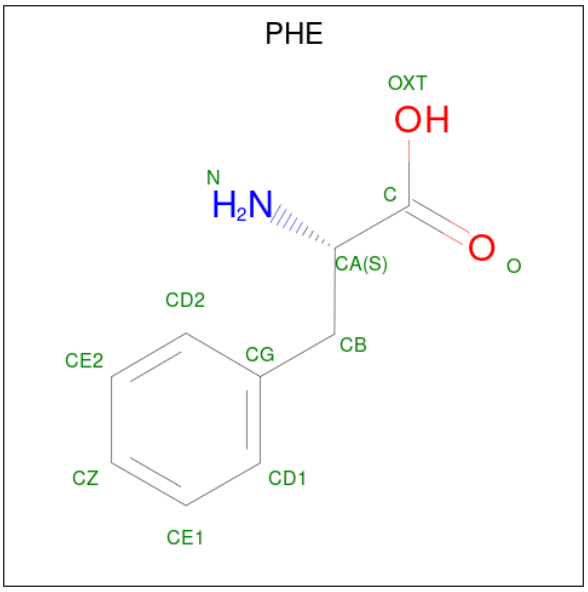
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			9	7	1	1		

- Molecule 3 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



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

- Molecule 4 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 12 9 1 2	0	0
4	B	1	Total C N O 12 9 1 2	0	0

- Molecule 5 is water.

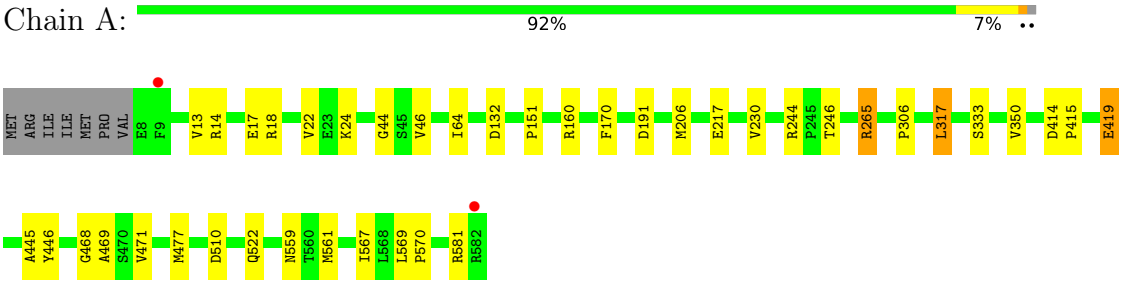
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	159	Total O 159 159	0	0
5	B	64	Total O 64 64	0	0

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.

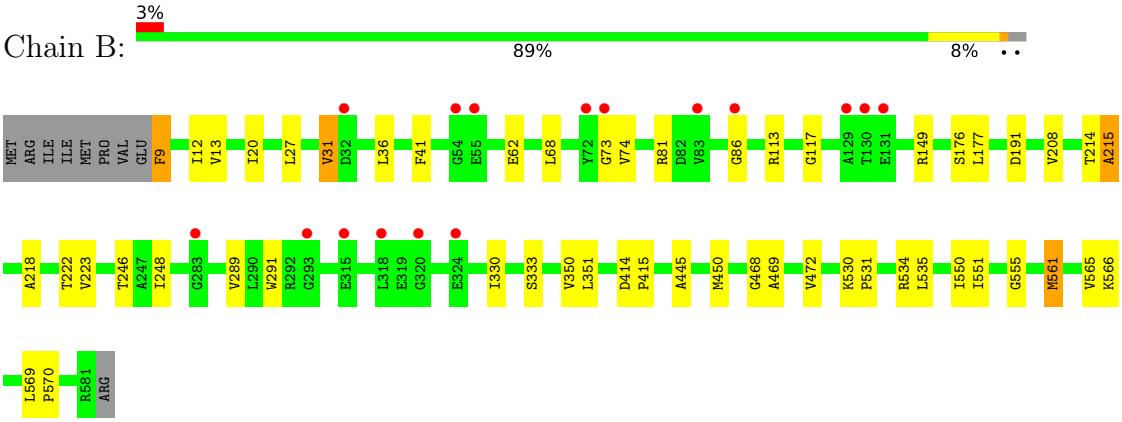
• Molecule 1: Acylamino-acid-releasing enzyme

Chain A:



• Molecule 1: Acylamino-acid-releasing enzyme

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.81Å 103.92Å 169.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.40 19.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.96-2.40) 99.3 (19.96-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.79 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.215 , 0.261 (Not available) , 0.254	Depositor DCC
R_{free} test set	2264 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 26.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8890	wwPDB-VP
Average B, all atoms (Å^2)	6.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BE2

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	0.44	0/4467	0.76	0/6059
1	B	0.39	1/4354 (0.0%)	0.74	0/5922
All	All	0.42	1/8821 (0.0%)	0.75	0/11981

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	566	LYS	CE-NZ	-5.12	1.34	1.49

There are no bond angle outliers.

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	4363	0	4310	23	0
1	B	4254	0	4157	30	0
2	A	9	0	3	0	0
2	B	9	0	3	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	12	0	9	0	0
4	B	12	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	159	0	0	2	0
5	B	64	0	0	2	0
All	All	8890	0	8497	51	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 3.

The worst 5 of 51 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:31:VAL:HG22	1:B:74:VAL:O	1.86	0.75
1:A:132:ASP:HB3	5:A:1162:HOH:O	1.90	0.69
1:A:246:THR:HG21	5:A:1066:HOH:O	2.01	0.59
1:B:9:PHE:O	1:B:13:VAL:HG23	2.03	0.59
1:B:208[B]:VAL:HG23	1:B:223:VAL:HB	1.86	0.57

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	567/582 (97%)	549 (97%)	18 (3%)	0	100	100
1	B	555/582 (95%)	537 (97%)	16 (3%)	2 (0%)	30	43
All	All	1122/1164 (96%)	1086 (97%)	34 (3%)	2 (0%)	43	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	215	ALA
1	B	73	GLY

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	339/468 (72%)	331 (98%)	8 (2%)	43 65
1	B	327/468 (70%)	319 (98%)	8 (2%)	43 65
All	All	666/936 (71%)	650 (98%)	16 (2%)	44 65

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	561[A]	MET
1	B	534	ARG
1	B	9	PHE
1	B	222	THR
1	A	581	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
3	GLY	A	1002	2,4	3,3,4	0.74	0	1,2,4	0.21	0
4	PHE	A	1003	3	11,12,12	0.70	1 (9%)	11,15,15	0.71	1 (9%)
2	BE2	B	2001	3	9,9,10	1.53	1 (11%)	11,11,13	1.32	2 (18%)
4	PHE	B	2003	3	11,12,12	0.69	1 (9%)	11,15,15	0.83	1 (9%)
3	GLY	B	2002	2,4	3,3,4	0.70	0	1,2,4	0.26	0
2	BE2	A	1001	3	9,9,10	1.59	1 (11%)	11,11,13	1.24	1 (9%)

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
3	GLY	A	1002	2,4	-	0/0/1/2	-
4	PHE	A	1003	3	-	4/8/8/8	0/1/1/1
2	BE2	B	2001	3	-	2/2/2/4	0/1/1/1
4	PHE	B	2003	3	-	3/8/8/8	0/1/1/1
3	GLY	B	2002	2,4	-	0/0/1/2	-
2	BE2	A	1001	3	-	2/2/2/4	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	BE2	OXT-C	-4.26	1.23	1.41
2	B	2001	BE2	OXT-C	-4.19	1.23	1.41
4	A	1003	PHE	OXT-C	-2.15	1.23	1.30
4	B	2003	PHE	OXT-C	-2.08	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2001	BE2	OXT-C-C1	3.59	121.95	111.94
2	A	1001	BE2	OXT-C-C1	3.21	120.90	111.94
4	B	2003	PHE	OXT-C-O	-2.70	117.96	124.08
4	A	1003	PHE	OXT-C-O	-2.25	118.99	124.08
2	B	2001	BE2	C6-C1-CA	2.03	120.31	118.63

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	PHE	O-C-CA-N
4	A	1003	PHE	OXT-C-CA-N
2	A	1001	BE2	OXT-C-C1-CA
2	B	2001	BE2	OXT-C-C1-CA
4	B	2003	PHE	OXT-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	575/582 (98%)	-0.49	2 (0%)	90	88	4, 6, 7, 8	4 (0%)
1	B	573/582 (98%)	0.16	16 (2%)	55	51	4, 6, 6, 7	3 (0%)
All	All	1148/1164 (98%)	-0.17	18 (1%)	70	66	4, 6, 6, 8	7 (0%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	PHE	3.2
1	B	131	GLU	2.7
1	B	54	GLY	2.6
1	B	283	GLY	2.5
1	B	320	GLY	2.5

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 oligosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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(Å^2)	Q<0.9
2	BE2	B	2001	9/10	0.82	0.15	25,26,26,26	0
2	BE2	A	1001	9/10	0.85	0.12	25,26,26,27	0
3	GLY	A	1002	4/5	0.91	0.08	24,25,25,25	0
4	PHE	B	2003	12/12	0.91	0.09	24,25,25,25	0
3	GLY	B	2002	4/5	0.92	0.09	25,25,25,25	0
4	PHE	A	1003	12/12	0.93	0.08	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.