



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 31, 2016 – 04:22 PM EDT

PDB ID : 2G97
Title : Crystal Structure of Visfatin/Pre-B Cell Colony Enhancing Factor 1/Nicotinamide Phosphoribosyltransferase In Complex with the Specific Inhibitor FK-866
Authors : Kim, M.-K.; Eom, S.H.
Deposited on : 2006-03-05
Resolution : 2.90 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

<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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20028320

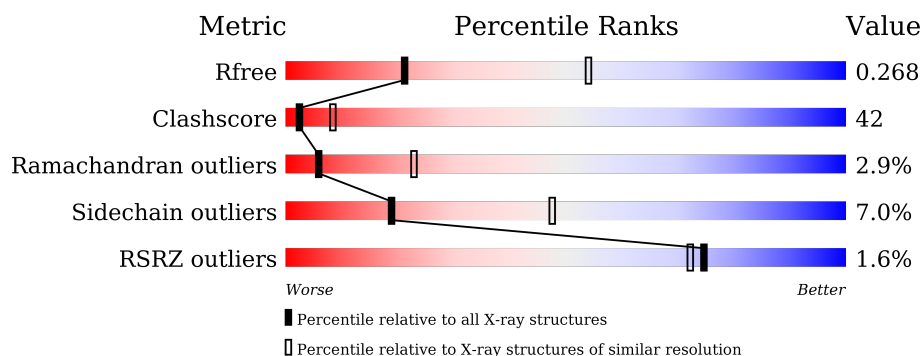
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 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	491	<div> <div>%</div> <div> <div></div> <div>34%</div> <div>55%</div> <div>5%</div> <div>6%</div> </div> </div>
1	B	491	<div> <div>2%</div> <div> <div></div> <div>37%</div> <div>51%</div> <div>7%</div> <div>6%</div> </div> </div>

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	DGB	A	1001	-	-	X	X
2	DGB	B	1002	-	-	X	-

2 Entry composition [i](#)

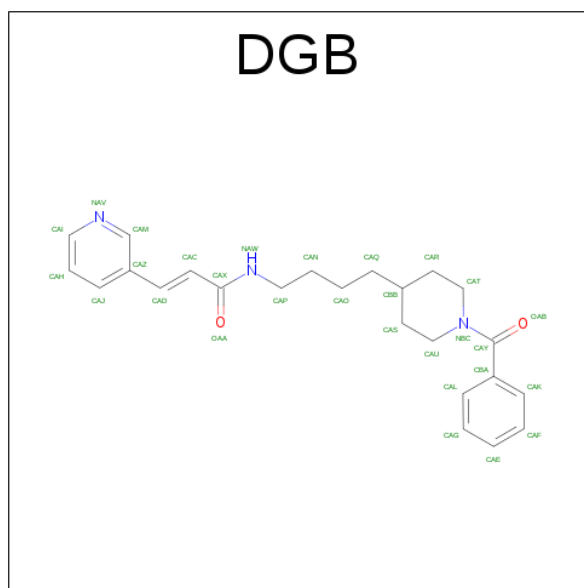
There are 3 unique types of molecules in this entry. The entry contains 7575 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3700	2374	616	704	6			
1	B	463	Total	C	N	O	S	0	0	0
			3700	2374	616	704	6			

- Molecule 2 is (2E)-N-{4-[1-(BENZENECARBONYL)PIPERIDIN-4-YL]BUTYL}-3-(PYRIDIN-3-YL)PROP-2-ENAMIDE (three-letter code: DGB) (formula: C₂₄H₂₉N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	24	3	2		
2	B	1	Total	C	N	O	0	0
			29	24	3	2		

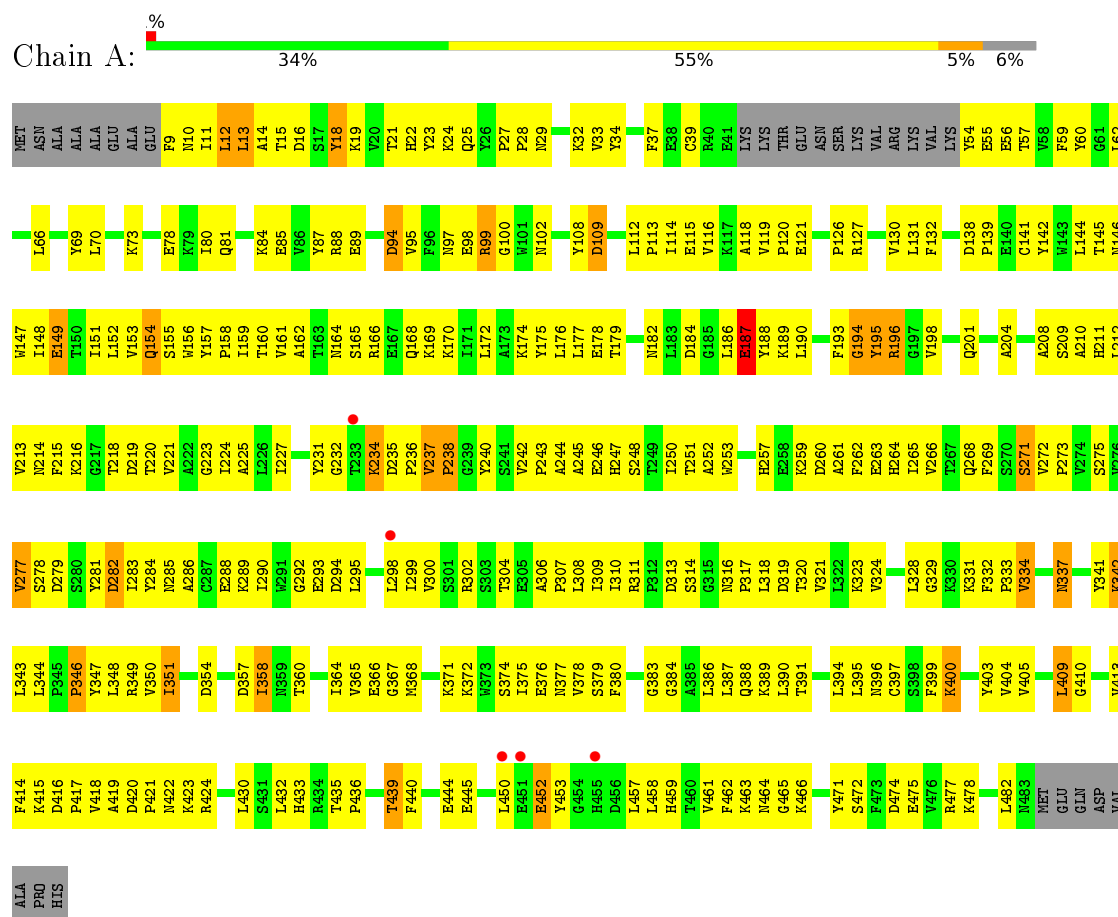
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total 68	O 68	0	0
3	B	49	Total 49	O 49	0	0

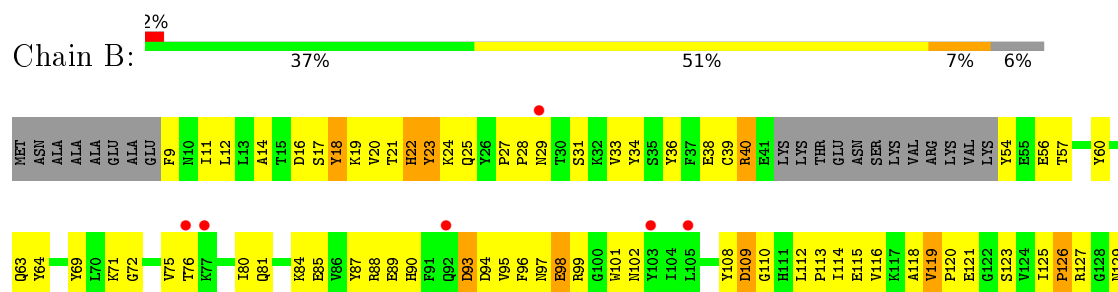
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Nicotinamide phosphoribosyltransferase



• Molecule 1: Nicotinamide phosphoribosyltransferase



M422	K423	R424	S425	K426	K427	G428	R429	L430	S431	L432	H433	R434	T439	F440	V441	T442	L443	E444	E445	G446	K447	G448	D449	L450	E451	L458	H459	T460	V461	F462	K463	M464	G465	K469	S470	Y471	S472	F473	D474	E475	V476	L482	M483	MET	GLU	GLN	ASP	VAL	ALA	PRO	HIS				
R349	V350	I351	D354	D357	Q362	E363	I364	V365	E366	G367	M368	K371	K372	W373	S374	I375	E376	N377	V378	S379	G383	G384	A385	L386	L387	Q388	K389	L390	T391	R392	D393	L394	L395	N396	F399	K400	C401	S402	Y403	V404	L409	G410	V411	M412	V413	F414	K415	V418	A419	D420	P421				
P273	V274	S275	V276	V277	S278	D279	S280	T281	D282	I283	V284	V285	A286	K289	I290	V291	G292	E293	D294	L295	R296	R302	S303	T304	P307	L308	I309	T310	R311	P312	D313	I316	P317	L318	D319	T320	V321	L322	L325	F332	P333	N337	S338	Y341	K342	L343	L344	P345	P346	V347	L348				
G197	V198	S199	A204	A210	R211	L212	V213	N214	P215	K216	G217	T218	D219	T220	V221	I224	A225	L226	T227	K228	K229	Y230	Y231	G232	T233	K234	D235	P236	V237	P238	G239	Y240	S241	V242	P243	E246	H247	S248	T249	I250	T251	A252	W253	A261	P262	E263	H264	I265	Q268	P269	S270	S271	V272		
V130	L131	F132	T133	V134	E135	P139	E140	C141	Y142	H143	L144	T145	M146	W147	I148	E149	T150	L151	L152	V153	Q154	S155	H156	Y157	P158	I159	T160	N164	S165	R166	E167	Q168	K169	K170	I171	Y175	L176	L177	E178	T179	M182	L183	D184	G185	L186	E187	Y188	K189	L190	H191	D192	F193	G194	Y195	R196

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.02Å 106.48Å 118.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 38.74 – 3.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.90) 92.4 (38.74-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.49 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.268 0.239 , 0.268	Depositor DCC
R_{free} test set	1923 reflections (9.86%)	DCC
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7575	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.21 % 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 2.1136e-05. 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: DGB

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	0.39	0/3788	0.64	0/5136
1	B	0.38	0/3788	0.64	0/5136
All	All	0.38	0/7576	0.64	0/10272

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	3700	0	3665	348	0
1	B	3700	0	3665	305	0
2	A	29	0	31	14	0
2	B	29	0	31	18	0
3	A	68	0	0	22	0
3	B	49	0	0	5	0
All	All	7575	0	7392	626	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 42.

The worst 5 of 626 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:160:THR:HG22	1:B:390:LEU:HD23	1.39	1.03
1:A:272:VAL:HB	1:A:273:PRO:HD2	1.42	1.02
1:A:439:THR:HG22	1:A:440:PHE:H	1.27	0.99
1:B:116:VAL:HG22	1:B:134:VAL:HG22	1.46	0.97
1:A:413:VAL:HG21	1:B:252:ALA:HA	1.45	0.94

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	459/491 (94%)	383 (83%)	62 (14%)	14 (3%)	5	21
1	B	459/491 (94%)	397 (86%)	49 (11%)	13 (3%)	6	24
All	All	918/982 (94%)	780 (85%)	111 (12%)	27 (3%)	6	23

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	282	ASP
1	A	154	GLN
1	A	194	GLY
1	A	271	SER
1	A	282	ASP

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	408/431 (95%)	380 (93%)	28 (7%)	19	48
1	B	408/431 (95%)	379 (93%)	29 (7%)	18	47
All	All	816/862 (95%)	759 (93%)	57 (7%)	19	47

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	409	LEU
1	B	94	ASP
1	B	400	LYS
1	A	422	ASN
1	B	18	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	388	GLN
1	B	90	HIS
1	B	388	GLN
1	A	422	ASN
1	B	111	HIS

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

2 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	DGB	A	1001	-	31,31,31	1.06	4 (12%)	39,39,39	1.60	7 (17%)
2	DGB	B	1002	-	31,31,31	1.36	4 (12%)	39,39,39	1.56	9 (23%)

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	DGB	A	1001	-	-	2/21/31/31	0/3/3/3
2	DGB	B	1002	-	-	0/21/31/31	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	DGB	CAC-CAX	-5.22	1.37	1.48
2	A	1001	DGB	CAC-CAX	-3.62	1.41	1.48
2	B	1002	DGB	CAZ-CAD	-3.15	1.38	1.47
2	A	1001	DGB	CAZ-CAD	-2.21	1.40	1.47
2	A	1001	DGB	CAC-CAD	2.17	1.38	1.32

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	DGB	OAA-CAX-CAC	-3.58	116.64	122.92
2	B	1002	DGB	CAZ-CAD-CAC	-3.47	118.95	126.98
2	B	1002	DGB	CAS-CAU-NBC	-3.44	105.97	110.99
2	B	1002	DGB	OAA-CAX-CAC	-3.17	117.35	122.92
2	A	1001	DGB	OAA-CAX-NAW	-2.52	119.39	122.57

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	DGB	OAA-CAX-NAW-CAP
2	A	1001	DGB	CAC-CAX-NAW-CAP

There are no ring outliers.

2 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	DGB	14	0
2	B	1002	DGB	18	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	463/491 (94%)	0.03	5 (1%) 82 80	4, 17, 34, 49	0
1	B	463/491 (94%)	-0.03	10 (2%) 65 60	5, 16, 34, 50	0
All	All	926/982 (94%)	0.00	15 (1%) 74 72	4, 16, 34, 50	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	237	VAL	5.3
1	B	236	PRO	4.7
1	B	92	GLN	3.0
1	A	451	GLU	2.8
1	B	235	ASP	2.7

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 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(\AA^2)	Q<0.9
2	DGB	A	1001	29/29	0.85	0.28	2.52	18,22,28,29	0
2	DGB	B	1002	29/29	0.87	0.25	1.29	12,18,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.