



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:23 AM GMT

PDB ID : 2GVZ
Title : Crystal Structure of Complex of Gs- with The Catalytic Domains of Mammalian Adenylyl Cyclase: Complex with MANT-ATP and Mn
Authors : Mou, T.-C.; Sprang, S.R.
Deposited on : 2006-05-03
Resolution : 3.27 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

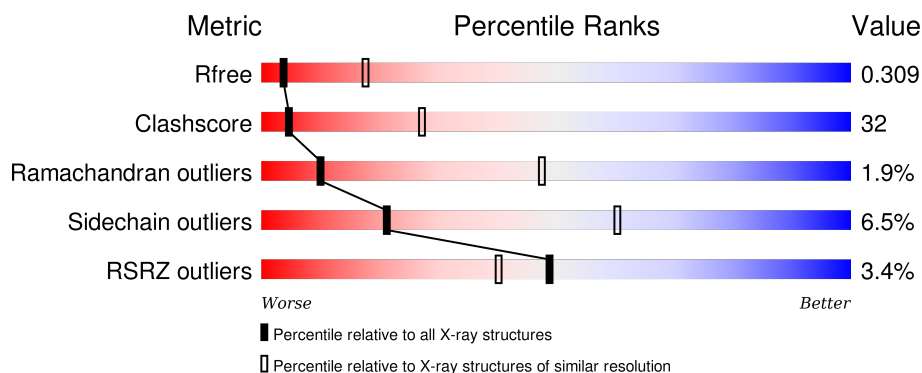
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 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	1756 (3.36-3.20)
Clashscore	102246	1941 (3.36-3.20)
Ramachandran outliers	100387	1905 (3.36-3.20)
Sidechain outliers	100360	1903 (3.36-3.20)
RSRZ outliers	91569	1764 (3.36-3.20)

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 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	225	<div> <div>5%</div> <div>37% 41% 6% 16%</div> </div>
2	B	212	<div> <div>3%</div> <div>41% 45% • 11%</div> </div>
3	C	394	<div> <div>2%</div> <div>37% 44% • 16%</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
5	CL	C	397	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5751 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 Adenylate cyclase type 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1476	929	259	271	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	MET	-	INITIATING METHIONINE	UNP P30803
A	357	HIS	-	EXPRESSION TAG	UNP P30803
A	358	HIS	-	EXPRESSION TAG	UNP P30803
A	359	HIS	-	EXPRESSION TAG	UNP P30803
A	360	HIS	-	EXPRESSION TAG	UNP P30803
A	361	HIS	-	EXPRESSION TAG	UNP P30803
A	362	HIS	-	EXPRESSION TAG	UNP P30803
A	476	MET	VAL	ENGINEERED	UNP P30803

- Molecule 2 is a protein called Adenylate cyclase type 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	188	Total	C	N	O	S	0	0	0
			1457	930	239	278	10			

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(s), alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	330	Total	C	N	O	S	0	0	0
			2702	1714	470	505	13			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

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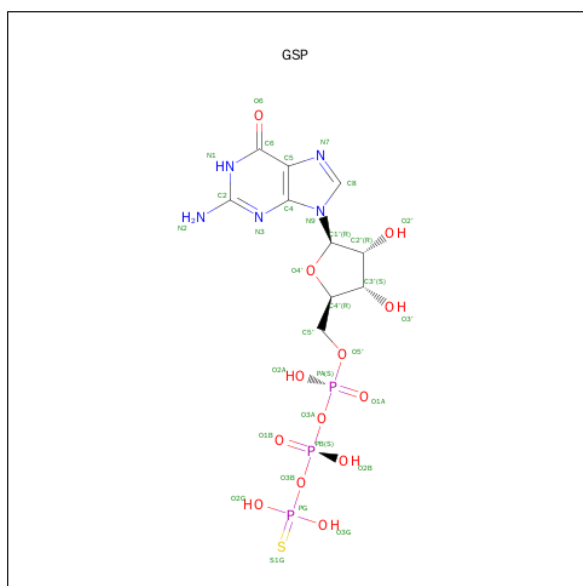
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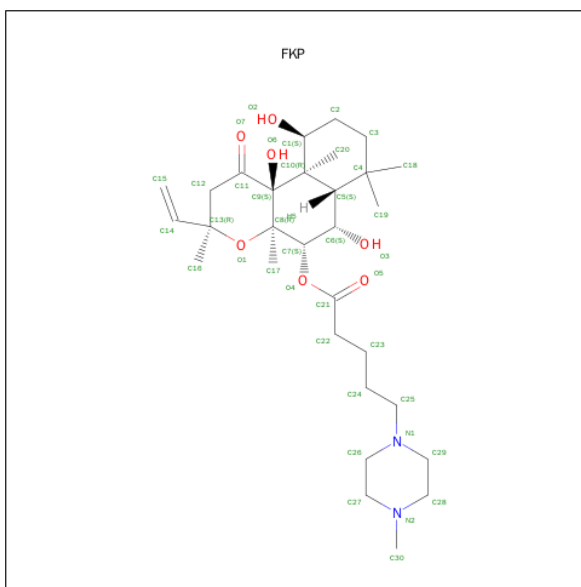
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mn	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Cl	0	0
			1	1		

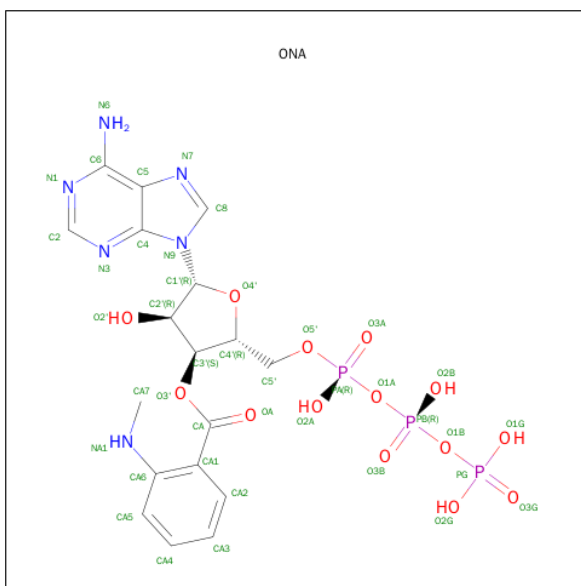
- Molecule 6 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			39	30	2	7		

- Molecule 8 is 3'-O-[2-(METHYLAMINO)BENZOYL]ADENOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE) (three-letter code: ONA) (formula: $C_{18}H_{23}N_6O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			41	18	6	14	3		

G353	G354	G355	R356	R357	Y358	G359	Y360		T364	C365	A366	Y367	D368	T369	E370	N371	I372	R373	R374	V375	F376	N377	D378	C379	R380	D381	I382	I383	Q384	R385	K386	R387	L388	ARG	GLN	TYR	GLU	LEU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
R283	T284		Y287	I288	L289	F290	L291	N292	K293	Q294	D295	L296	L297		V301		G304	K305	S306	V307	I308		F312	R313	E314	F315		Y318	T319	T320	F321		A324	T325	P326	E327	P328		D331	P332	R333	V334	T335	R336	A337		F340	I341	D342	D343	F344	F345	L346	R347	I348	S349	T350	A351	S352																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
H64	V65	ASN	GLY	PHE	ASN	GLY	GLU	GLY	GLY	GLU	GLU	ASP	PRO	GLN	ALA	ALA	ARG	SER	ASN	SER	ASP	G86	E87		T90	K91	V92		I95		N98	L99	K100	E101	A102	I103	E104		T105	I106	V107	A108	A109	M110		L113	V117	E118	L119		N124		R127	V128		I131	L132	S133	V134																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	116.80 Å 132.10 Å 69.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.97 – 3.27 44.74 – 3.27	Depositor EDS
% Data completeness (in resolution range)	85.8 (14.97-3.27) 76.4 (44.74-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 3.25 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.275 , 0.330 0.260 , 0.309	Depositor DCC
R_{free} test set	774 reflections (6.01%)	DCC
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	1.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 14536 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5751	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: FKP, GSP, MN, ONA, CL

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	0.42	0/1504	0.71	2/2027 (0.1%)
2	B	0.56	0/1481	0.67	0/1999
3	C	0.50	0/2759	0.68	0/3733
All	All	0.50	0/5744	0.69	2/7759 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	ARG	N-CA-C	-8.39	88.34	111.00
1	A	388	ASP	N-CA-C	7.44	131.10	111.00

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	1476	0	1450	120	0
2	B	1457	0	1463	96	0
3	C	2702	0	2650	172	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
5	C	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	32	0	12	1	0
7	A	39	0	50	6	0
8	A	41	0	19	2	0
All	All	5751	0	5644	365	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 32.

The worst 5 of 365 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)
2:B:925:LEU:HG	2:B:982:LYS:HZ2	1.23	1.00
3:C:231:ARG:HH21	3:C:272:LEU:HD22	1.26	0.98
3:C:63:LEU:HD13	3:C:373:ARG:HE	1.31	0.94
7:A:1:FKP:H173	7:A:1:FKP:H201	1.51	0.90
3:C:119:LEU:HD12	3:C:119:LEU:H	1.37	0.88

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	187/225 (83%)	153 (82%)	30 (16%)	4 (2%)	9	44
2	B	184/212 (87%)	156 (85%)	26 (14%)	2 (1%)	17	59
3	C	326/394 (83%)	270 (83%)	49 (15%)	7 (2%)	9	44
All	All	697/831 (84%)	579 (83%)	105 (15%)	13 (2%)	10	47

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	351	ALA
1	A	382	ILE
1	A	456	ALA
1	A	479	VAL
1	A	480	ASN

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	158/189 (84%)	145 (92%)	13 (8%)	14	49
2	B	161/184 (88%)	150 (93%)	11 (7%)	20	58
3	C	297/351 (85%)	281 (95%)	16 (5%)	27	67
All	All	616/724 (85%)	576 (94%)	40 (6%)	21	60

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1013	GLN
2	B	1062	ILE
3	C	354	ASP
2	B	1031	ASP
2	B	1077	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1002	HIS
2	B	1013	GLN
3	C	213	GLN
2	B	1001	ASN
3	C	220	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 ⓘ

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\# Z > 2$
7	FKP	A	1	-	37,42,42	2.46	15 (40%)	49,68,68	2.66	18 (36%)
8	ONA	A	100	4	35,44,44	3.97	13 (37%)	47,67,67	3.09	18 (38%)
6	GSP	C	395	4	25,34,34	1.80	8 (32%)	31,54,54	2.79	8 (25%)

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
7	FKP	A	1	-	-	0/14/97/97	0/4/4/4
8	ONA	A	100	4	-	0/28/48/48	0/4/4/4
6	GSP	C	395	4	-	0/15/38/38	0/3/3/3

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	100	ONA	O5'-C5'	-3.91	1.28	1.44
6	C	395	GSP	C8-N7	-2.49	1.29	1.34
6	C	395	GSP	PG-O2G	-2.20	1.47	1.55
7	A	1	FKP	C27-N2	2.02	1.50	1.46
6	C	395	GSP	C2'-C3'	2.04	1.59	1.53

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	100	ONA	N3-C2-N1	-14.29	117.95	128.89
7	A	1	FKP	C19-C4-C18	-10.64	91.89	107.91
6	C	395	GSP	C5-C6-N1	-9.98	109.95	123.59
8	A	100	ONA	PB-O1B-PG	-5.74	113.41	132.67
6	C	395	GSP	PB-O3B-PG	-4.15	118.76	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1	FKP	6	0
8	A	100	ONA	2	0
6	C	395	GSP	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	189/225 (84%)	0.39	11 (5%)	26 20	30, 87, 99, 116	0
2	B	188/212 (88%)	0.17	6 (3%)	51 43	13, 49, 96, 98	0
3	C	330/394 (83%)	0.13	7 (2%)	67 58	19, 55, 93, 100	0
All	All	707/831 (85%)	0.21	24 (3%)	49 40	13, 59, 97, 116	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	477	THR	9.1
1	A	475	GLU	5.3
1	A	476	MET	4.4
2	B	1056	CYS	3.5
3	C	117	VAL	3.3

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
5	CL	C	397	1/1	0.95	0.86	13.48	59,59,59,59	0
7	FKP	A	1	39/39	0.92	0.30	1.74	13,23,87,89	0
8	ONA	A	100	41/41	0.84	0.34	0.70	53,88,97,100	0
6	GSP	C	395	32/32	0.96	0.19	-0.09	31,41,73,76	0
4	MN	A	582	1/1	0.95	0.14	-1.45	31,31,31,31	0
4	MN	C	396	1/1	0.95	0.11	-1.60	17,17,17,17	0
4	MN	A	581	1/1	0.93	0.23	-	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.