



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:01 PM UTC

PDB ID : 9CM4 / pdb_00009cm4
Title : HCV2 Fab bound to selected RNA loop
Authors : Disare, M.T.; Lewicka, A.; Piccirilli, J.A.
Deposited on : 2024-07-12
Resolution : 1.82 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

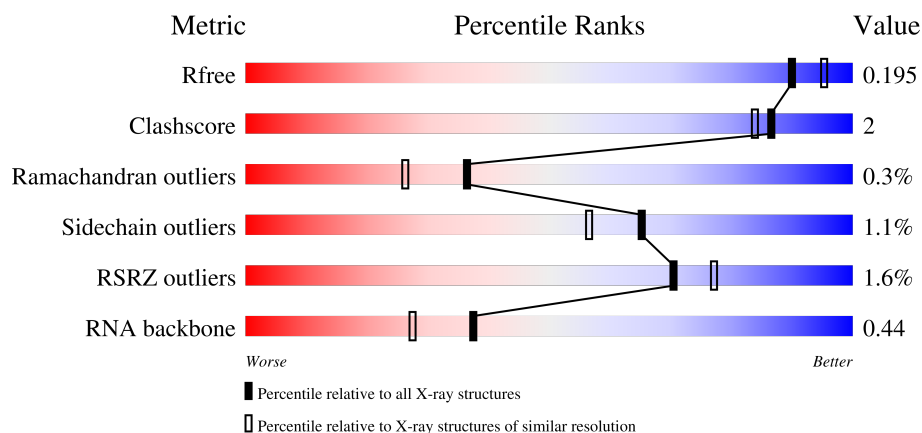
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

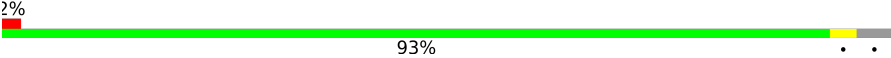

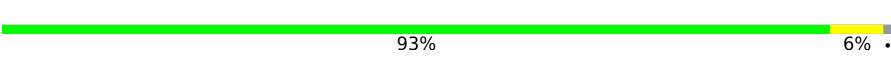
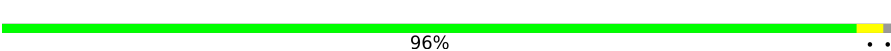
The reported resolution of this entry is 1.82 Å.

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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)
RNA backbone	3983	1006 (2.22-1.42)

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	233	 2% 93% 5% 2%
1	H	233	 3% 88% 7% 2%
2	B	215	 93% 6% 1%
2	L	215	 96% 4% 1%

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Mol	Chain	Length	Quality of chain
3	G	20	
3	J	20	

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	SO4	B	302	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9006 atoms, of which 154 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 HCV2 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	224	Total	C	N	O	S	0	0	0
			1692	1073	282	332	5			
1	A	224	Total	C	N	O	S	0	0	0
			1692	1073	282	332	5			

- Molecule 2 is a protein called HCV2 fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1629	1017	273	334	5			
2	B	213	Total	C	N	O	S	0	0	0
			1629	1017	273	334	5			

- Molecule 3 is a RNA chain called HCV2 RNA loop.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	20	Total	C	H	N	O	P	0	0	0
			502	190	77	76	139	20			
3	J	20	Total	C	H	N	O	P	0	0	0
			502	190	77	76	139	20			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

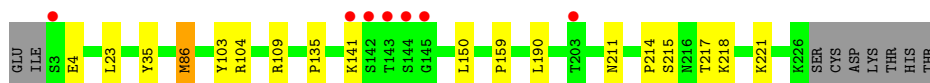
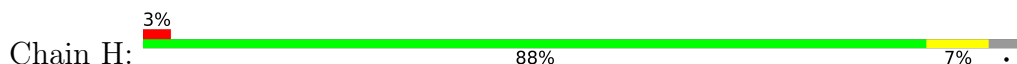
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	277	Total	O	0	0
			277	277		
6	L	293	Total	O	0	0
			293	293		
6	A	294	Total	O	0	0
			294	294		
6	B	343	Total	O	0	0
			343	343		
6	G	69	Total	O	0	0
			69	69		
6	J	57	Total	O	0	0
			57	57		

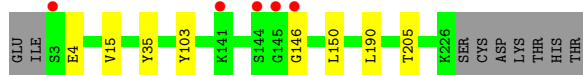
3 Residue-property plots

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.

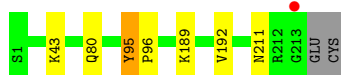
- Molecule 1: HCV2 Fab heavy chain



- Molecule 1: HCV2 Fab heavy chain



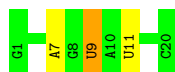
- Molecule 2: HCV2 fab light chain



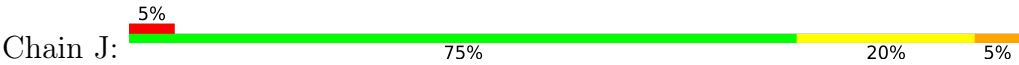
- Molecule 2: HCV2 fab light chain



- Molecule 3: HCV2 RNA loop



- Molecule 3: HCV2 RNA loop



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.23Å 52.21Å 133.34Å 90.00° 124.92° 90.00°	Depositor
Resolution (Å)	54.67 – 1.82 54.67 – 1.82	Depositor EDS
% Data completeness (in resolution range)	98.2 (54.67-1.82) 98.1 (54.67-1.82)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.160 , 0.198 (Not available) , 0.195	Depositor DCC
R_{free} test set	1987 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9006	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.79% 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, 0.333 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: SO4, MG

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	0.71	0/1737	0.79	0/2367
1	H	0.73	1/1737 (0.1%)	0.79	0/2367
2	B	0.72	0/1664	0.81	0/2259
2	L	0.70	0/1664	0.78	0/2259
3	G	0.53	0/474	0.77	0/736
3	J	0.54	0/474	0.76	0/736
All	All	0.70	1/7750 (0.0%)	0.79	0/10724

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	86	MET	SD-CE	-5.76	1.65	1.79

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	1692	0	1642	4	0
1	H	1692	0	1642	9	0
2	B	1629	0	1584	7	0
2	L	1629	0	1584	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	425	77	217	1	0
3	J	425	77	217	2	0
4	B	1	0	0	0	0
4	L	1	0	0	0	0
5	B	15	0	0	1	1
5	L	10	0	0	0	0
6	A	294	0	0	4	1
6	B	343	0	0	0	0
6	G	69	0	0	0	0
6	H	277	0	0	1	0
6	J	57	0	0	1	0
6	L	293	0	0	3	0
All	All	8852	154	6886	30	1

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 2.

All (30) 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)
6:A:341:HOH:O	3:G:9:U:H1'	1.76	0.85
3:J:9:U:H1'	6:J:101:HOH:O	1.85	0.77
1:A:4:GLU:HG2	6:A:469:HOH:O	1.88	0.73
2:B:185:ALA:O	2:B:189:LYS:HG2	1.96	0.65
2:L:95:TYR:HB3	2:L:96:PRO:HD3	1.80	0.63
1:H:215:SER:OG	1:H:217:THR:HG23	1.99	0.63
1:H:109:ARG:HB3	6:H:506:HOH:O	1.99	0.62
2:B:95:TYR:HB3	2:B:96:PRO:HD3	1.83	0.60
1:H:141:LYS:HG2	1:H:141:LYS:O	2.01	0.60
2:B:95:TYR:HB3	2:B:96:PRO:CD	2.31	0.60
2:L:95:TYR:HB3	2:L:96:PRO:CD	2.33	0.58
1:H:23:LEU:HG	1:H:86:MET:HE2	1.87	0.55
2:L:189:LYS:HG3	6:L:462:HOH:O	2.08	0.53
1:H:135:PRO:HD3	1:H:221:LYS:HE2	1.94	0.50
2:B:7:GLN:HB2	2:B:24:CYS:SG	2.53	0.48
2:B:71:ASP:OD2	5:B:302:SO4:O2	2.32	0.47
1:A:205:THR:HG23	6:A:470:HOH:O	2.14	0.47
2:L:192:VAL:HG22	2:L:211:ASN:OD1	2.14	0.47
2:L:80:GLN:OE1	6:L:401:HOH:O	2.21	0.45
1:A:35:TYR:CD2	1:A:103:TYR:HA	2.52	0.44
2:L:43:LYS:HD3	6:L:647:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:43:LYS:HB3	2:L:43:LYS:HE2	1.49	0.43
1:H:211:ASN:ND2	1:H:218:LYS:HG2	2.33	0.43
1:H:35:TYR:CD2	1:H:103:TYR:HA	2.54	0.42
2:B:34:VAL:HA	2:B:90:GLN:O	2.19	0.42
1:H:159:PRO:HD2	1:H:214:PRO:CB	2.50	0.42
1:A:146:GLY:HA2	6:A:490:HOH:O	2.20	0.42
3:J:8:G:C2	3:J:10:A:O4'	2.73	0.41
2:B:167:GLN:HG3	2:B:174:TYR:CZ	2.56	0.41
1:H:215:SER:O	1:H:217:THR:HG23	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:302:SO4:O4	6:A:496:HOH:O[4_446]	2.18	0.02

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	222/233 (95%)	218 (98%)	4 (2%)	0	100	100
1	H	222/233 (95%)	217 (98%)	4 (2%)	1 (0%)	24	14
2	B	211/215 (98%)	206 (98%)	4 (2%)	1 (0%)	24	14
2	L	211/215 (98%)	205 (97%)	5 (2%)	1 (0%)	24	14
All	All	866/896 (97%)	846 (98%)	17 (2%)	3 (0%)	36	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	95	TYR

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Mol	Chain	Res	Type
2	L	95	TYR
1	H	104	ARG

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	187/196 (95%)	184 (98%)	3 (2%)	55	44
1	H	187/196 (95%)	184 (98%)	3 (2%)	55	44
2	B	188/190 (99%)	186 (99%)	2 (1%)	65	56
2	L	188/190 (99%)	188 (100%)	0	100	100
All	All	750/772 (97%)	742 (99%)	8 (1%)	65	56

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	4	GLU
1	H	150	LEU
1	H	190	LEU
1	A	15	VAL
1	A	150	LEU
1	A	190	LEU
2	B	4	GLN
2	B	5	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	211	ASN
2	L	80	GLN
2	L	161	GLN
1	A	6	GLN
1	A	42	GLN
1	A	211	ASN

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Mol	Chain	Res	Type
2	B	39	GLN
2	B	80	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	G	19/20 (95%)	3 (15%)	0
3	J	19/20 (95%)	3 (15%)	0
All	All	38/40 (95%)	6 (15%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	G	7	A
3	G	9	U
3	G	11	U
3	J	2	G
3	J	8	G
3	J	11	U

There are no RNA pucker outliers to report.

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](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z > 2$
5	SO4	L	303	-	4,4,4	0.38	0	6,6,6	0.22	0
5	SO4	B	303	-	4,4,4	0.26	0	6,6,6	0.14	0
5	SO4	B	302	-	4,4,4	0.60	0	6,6,6	0.33	0
5	SO4	L	302	-	4,4,4	0.21	0	6,6,6	0.37	0
5	SO4	B	304	-	4,4,4	0.26	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	302	SO4	1	1

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	224/233 (96%)	-0.35	5 (2%) 62 69	17, 22, 49, 119	0
1	H	224/233 (96%)	-0.38	7 (3%) 51 58	16, 22, 51, 94	0
2	B	213/215 (99%)	-0.45	1 (0%) 87 90	17, 23, 39, 49	0
2	L	213/215 (99%)	-0.35	1 (0%) 87 90	16, 24, 41, 59	0
3	G	20/20 (100%)	-0.29	0 100 100	25, 36, 65, 65	0
3	J	20/20 (100%)	-0.29	1 (5%) 34 40	23, 34, 56, 72	0
All	All	914/936 (97%)	-0.38	15 (1%) 70 77	16, 23, 46, 119	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	143	THR	3.6
1	H	203	THR	3.4
1	A	144	SER	3.0
1	H	145	GLY	2.8
2	B	213	GLY	2.6
1	A	3	SER	2.5
2	L	213	GLY	2.4
3	J	1	G	2.4
1	H	142	SER	2.4
1	H	144	SER	2.2
1	H	141	LYS	2.2
1	A	145	GLY	2.1
1	A	146	GLY	2.0
1	A	141	LYS	2.0
1	H	3	SER	2.0

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
5	SO4	B	304	5/5	0.80	0.08	85,86,106,106	0
5	SO4	B	303	5/5	0.82	0.10	56,62,88,94	0
5	SO4	L	302	5/5	0.83	0.10	70,78,99,102	0
5	SO4	L	303	5/5	0.84	0.12	58,64,82,83	0
4	MG	B	301	1/1	0.88	0.12	50,50,50,50	0
4	MG	L	301	1/1	0.91	0.09	49,49,49,49	0
5	SO4	B	302	5/5	0.94	0.09	38,38,47,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.