W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 16, 2025 – 12:08 PM JST

|		
PDB ID	:	9KFB / pdb_00009kfb
Title	:	RABV-G-ecto/NM57-scFv complex
Authors	:	Lu, G.; Yang, F.; Lin, S.
Deposited on	:	2024-11-05
Resolution	:	4.30 Å(reported)

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 4.30 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.
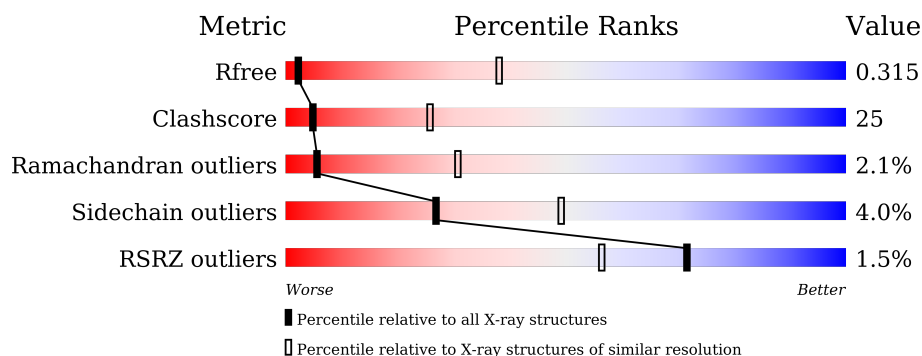
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1028 (4.72-3.86)
Clashscore	180529	1030 (4.70-3.90)
Ramachandran outliers	177936	1014 (4.76-3.84)
Sidechain outliers	177891	1022 (4.76-3.82)
RSRZ outliers	164620	1026 (4.72-3.86)

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	264	2% 51% 30% • 15%
1	M	264	39% 35% • 22%
1	X	264	.% 41% 28% • 28%
2	B	433	2% 41% 35% • • 19%
2	F	433	.% 48% 27% • 23%
2	K	433	.% 38% 35% • • 24%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 12653 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 NM57-scFv light chain, NM57-scFv heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1695	1068	284	335	8			
1	M	207	Total	C	N	O	S	0	0	0
			1562	984	267	303	8			
1	X	190	Total	C	N	O	S	0	0	0
			1438	909	245	276	8			

- Molecule 2 is a protein called RABV-G-ecto.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	349	Total	C	N	O	S	0	0	0
			2749	1741	476	509	23			
2	K	328	Total	C	N	O	S	0	0	0
			2590	1647	447	474	22			
2	F	334	Total	C	N	O	S	0	0	0
			2619	1664	449	482	24			

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: NM57-scFv light chain, NM57-scFv heavy chain

Chain A:

• Molecule 1: NM57-scFv light chain, NM57-scFv heavy chain

Chain M:

• Molecule 1: NM57-scFv light chain, NM57-scFv heavy chain

Chain X:

MET GLN SER A3 L4 T5 Q6 P7 R8 S9 V10 SER GLY SER PRO GLY GLN SER VAL THR ILE S21 G24 T25 S26 S36 W37 Y38 H41 P42 A45 P46 K47 L48 M49 I50 Y51 D52 A53 T54 K55 P61 ASP ARG PHE G66 S67 K68 S69 G70 N71 T72 A73 S74

LEU THR ILE SER GLY LEU GLN ALA GLU GLU ALA ASP GLU TYR TYR C90 C91 S92 Y93 A94 T98 P99 G100 V101 V102 F103 G104 G105 G106 T107 LYS LEU THR VAL LEU GLN PRO LYS GLY GLY GLY GLY SER GLY GLY GLY SER GLY GLY GLY SER GLY GLY GLY SER

GLN V138 Q139 L140 K155 A160 S161 GLY G163 T164 F165 N166 R167 Y168 T169 V170 N171 R174 Q179 G180 L181 E182 W183 M184 G185 I186 I187 I188 P189 T193 A194 N195 F200 R203 L204 T205 I206 T207 ALA ASP GLU SER T212 Y216 M217 E218 L219 S220 S221 V229

A233 R234 E235 N236 L237 D238 N239 SER GLY THR TYR Y244 Y245 F246 S247 G248 W249 F250 D251 P252 W253 G254 GLN G256 T257 V261 SER SER

● Molecule 2: RABV-G-ecto

2%
Chain B: 41% 35% 19%

K1 L11 W14 S15 D18 I19 H20 P25 N26 N27 N37 L38 S39 E40 F41 M44 E45 L46 G49 Y50 I51 S52 A53 I54 K55 V56 N57 G58 F59 T60 C61 T62 G63 V64 V65 THR GLU ALA GLU THR TYR THR GLY SER GLY THR THR PHE LYS ARG LYS

HIS PHE R88 P89 T90 P91 D92 A93 C94 R95 A96 A97 K101 M102 A103 GLY D105 E109 GLU SER LEU HIS ASN PRO TYR GLY SER GLY GLY R126 K129 E130 S131 I134 I135 S136 P137 S138 V139 L142 D143 P144 Y145 L149 H150 S151 R152 V153 F154 P155 G156 G157 K158

C159 S160 G161 I162 T163 V164 S165 C169 Y168 N172 Y175 T176 I177 W178 M179 P180 E181 N182 P183 R184 R186 T187 P188 C189 D190 I191 F192 T193 N194 S195 R196 G197 K198 R199 A200 S201 N202 K205 T206 C207 G208 V209 V210 D211 E212 R213 G214 L219 R224 L225 K226 L227 C228
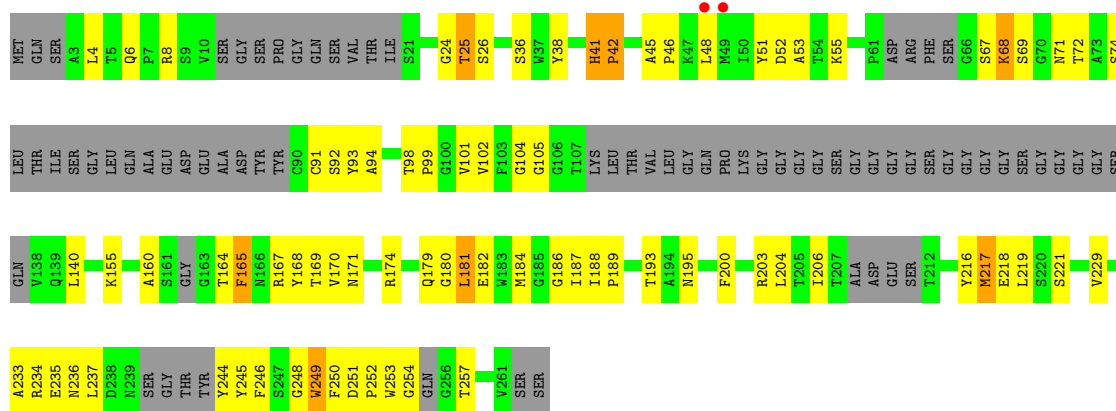
L231 G232 L233 R234 G238 T239 W240 V241 A242 T245 T249 K250 W251 C252 P253 P254 D255 Q256 L257 V258 N259 L260 H261 D262 F263 ARG SER ASP GLU ILE E269 H270 V273 K279 R280 E281 E282 D285 E288 S289 T292 S297 F298 R299 R300 L301 T316 I317 F318

N319 K320 E324 A325 D326 A327 T334 E337 I338 I339 K342 G343 C344 L345 K346 V347 H352 P353 V358 F359 F360 N361 G362 I363 I364 D368 D369 H370 V371 L372 I373 P374 Q377 S378 S379 L380 Q383 H384 M385 E386 L387 L388 K389 S390 I393 PRO LEU MET HIS PRO

LEU ALA ASP PRO SER THR VAL PHE LYS GLY GLU GLY ASP GLU ALA GLU ASP PHE VAL GLU VAL HIS LEU PRO ASP VAL TYR LYS GLN ILE SER ARG VAL ASP GLY LEU LEU PRO ASN TRP GLY LYS

● Molecule 2: RABV-G-ecto

.%
Chain K: 38% 35% 24%

K1 F2 P3 I4 Y5 T6 I7 P8 W14 S15 P16 I17 D18 N26 C35 T36 N37 E40 F41 S42 Y43 M44 E45 L46 K47 V48 G49 Y50 I51 S52 A53 I54 K55 V56 N57 G58 F59 T60 C61 THR GLY VAL VAL THR GLU ALA GLU THR TYR THR GLY SER GLY GLY THR

THR PHE LYS ARG LYS HIS F87 R88 P89 T90 P91 D92 A93 C94 R95 A96 A97 Y98 K101 MET ALA GLY ASP P106 R107 Y108 E109 GLU SER LEU HIS ASN PRO TYR GLY SER GLY ARG THR THR LYS SER LEU ILE I134 I135 S136 P137 D141 L142 D143 P144 Y145 D146 K147

S148 L149 H150 S151 R152 V153 F154 P155 K158 C159 I162 T163 V164 S165 S166 S170 T171 Y175 T176 I177 W178 M179 P180 E181 N182 P183 R184 T187 P188 C189 F192 R196 G197 K198 R199 A200 S201 N202 GLY ASN K205 T206 C207 G208 F209 V210 D211 E212 R213 G214 L215 S218

L219 K220 R224 L227 C228 G229 V230 L231 G232 L233 R234 L235 M236 D237 G238 T239 A242 M243 Q244 T245 S246 D247 E248 T249 K250 P253 P254 D255 Q256 L257 V258 ASN LEU HIS ASP PHE ARG SER ASP GLU ILE GLU H270 L276 V277 K278 K279 R280 E281 L284 D285 E288 S289

I290 M291 T292 T293 K294 R300 L301 S302 R305 K306 L307 K313 A314 Y315 T316 N319 K320 M323 E324 Y329 K330 W335 I338 I339 P340 S341 K342 G343 C344 L345 K346 R350 H354 V355 N356 F359 F360 N361 G362 I363 D369 H370 V371 L372 I373 P374 E375 M376

Q377 S378 L381 Q382 K389 S390 P394 LEU MET HIS PRO LEU ALA ASP PRO SER THR VAL PHE LYS GLU ASP GLU GLU ALA GLU ASP PHE VAL GLU VAL HIS LEU PRO ASP VAL LYS TYR LYS GLN ILE SER GLY VAL ASP GLY LEU ASN TRP GLY LYS

• Molecule 2: RABV-G-ecto

Chain F:

%

48%   27%   •   23%

K1 F2 Y5 T6 I7 P8 S15 P16 I17 D18 I19 H20 H21 P25 N26 N27 L28 C35 F41 S42 Y43 M44 E45 L46 G49 Y50 I51 S52 A53 I54 K55 V56 F59 T62 G63 VAL VAL THR GLU ALA GLU THR TYR THR THR GLY GLY SER GLY GLY THR THR PHE

LYS ARG LYS HIS F87 R88 P89 T90 P91 C94 K101 M102 A103 GLY ASP PRO ARG TYR GLU GLU SER LEU HIS ASN PRO TYR GLY SER GLY GLY ARG THR THR LYS GLU SER LEU ILE I134 P137 S138 V139 T140 D141 L142 D143 P144 S148 L149 H150 S151 R152 V153 F154 P155

G156 G157 K158 C159 S160 G161 I162 T163 T167 Y168 C169 S170 I177 W178 M179 P180 E181 R184 P185 R186 T187 P188 C189 N194 S195 A200 F209 E212 ARG GLY L215 Y216 K217 S218 R224 L227 C228 G229 V230 L231 R234 G238 T239 W240 V241 A242 M243 Q244 T245

T249 L257 V258 N259 LEU HIS ASP PHE ARG SER ASP E267 H270 L271 V272 V273 L276 V277 E281 K294 F298 R299 S302 R305 K306 G312 F318 N319 K320 M323 E324 A327 H328 Y329 V332 R333 T334 W335 N336 E337 I338 L345 K346 V347 G348

G349 R350 V355 N356 F359 F360 I363 L372 I373 P374 E375 M376 Q377 S378 S379 L380 L381 Q382 E386 L387 L388 K389 M396 HIS PRO LEU ALA ASP PRO SER THR VAL PHE LYS GLU ASP GLU GLU ALA GLU ASP PHE VAL GLU VAL HIS LEU PRO ASP VAL TYR LYS GLN ILE

SER GLY VAL ASP LEU GLY LEU PRO ASN TRP GLY LYS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	157.62Å 157.62Å 221.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.64 – 4.30 36.64 – 4.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.64-4.30) 99.5 (36.64-4.30)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 4.27Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.261 , 0.314 0.264 , 0.315	Depositor DCC
R_{free} test set	902 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å^2)	175.9	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 339.9	EDS
L-test for twinning[2]	$< |L| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	12653	wwPDB-VP
Average B, all atoms (Å^2)	212.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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	0.29	0/1733	0.77	6/2348 (0.3%)
1	M	0.39	0/1598	0.97	9/2164 (0.4%)
1	X	0.31	0/1469	0.74	8/1985 (0.4%)
2	B	0.32	0/2813	0.81	16/3808 (0.4%)
2	F	0.31	0/2681	0.80	13/3630 (0.4%)
2	K	0.32	0/2653	0.92	22/3590 (0.6%)
All	All	0.32	0/12947	0.84	74/17525 (0.4%)

There are no bond length outliers.

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	94	ALA	CB-CA-C	-17.24	84.23	110.10
1	M	173	VAL	N-CA-C	12.16	143.83	111.00
2	B	153	VAL	CB-CA-C	11.34	132.94	111.40
1	M	173	VAL	N-CA-CB	-11.30	86.63	111.50
2	B	358	VAL	CB-CA-C	9.89	130.19	111.40

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	1695	0	1610	70	0
1	M	1562	0	1490	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	1438	0	1367	66	0
2	B	2749	0	2720	155	0
2	F	2619	0	2594	106	0
2	K	2590	0	2565	147	0
All	All	12653	0	12346	620	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 25.

The worst 5 of 620 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:A:152:SER:O	1:A:222:LEU:CD1	1.96	1.14
2:K:180:PRO:CG	2:K:180:PRO:O	1.83	1.11
2:K:180:PRO:O	2:K:180:PRO:HG2	1.32	1.07
1:A:152:SER:O	1:A:222:LEU:HD13	1.55	1.03
2:K:201:SER:HB3	2:K:206:THR:HA	1.39	1.02

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	212/264 (80%)	179 (84%)	31 (15%)	2 (1%)	14	50
1	M	195/264 (74%)	158 (81%)	31 (16%)	6 (3%)	3	23
1	X	172/264 (65%)	146 (85%)	23 (13%)	3 (2%)	7	36
2	B	339/433 (78%)	276 (81%)	56 (16%)	7 (2%)	5	31
2	F	324/433 (75%)	267 (82%)	50 (15%)	7 (2%)	5	30
2	K	316/433 (73%)	261 (83%)	47 (15%)	8 (2%)	4	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1558/2091 (74%)	1287 (83%)	238 (15%)	33 (2%)	5 31

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	144	PRO
2	K	153	VAL
2	K	155	PRO
2	F	154	PHE
2	F	187	THR

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	182/202 (90%)	175 (96%)	7 (4%)	28	50
1	M	167/202 (83%)	165 (99%)	2 (1%)	67	79
1	X	153/202 (76%)	148 (97%)	5 (3%)	33	55
2	B	313/381 (82%)	291 (93%)	22 (7%)	12	33
2	F	298/381 (78%)	288 (97%)	10 (3%)	32	54
2	K	295/381 (77%)	284 (96%)	11 (4%)	29	51
All	All	1408/1749 (80%)	1351 (96%)	57 (4%)	27	49

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

Mol	Chain	Res	Type
2	B	344	CYS
1	X	195	ASN
2	K	159	CYS
1	X	181	LEU
2	F	187	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	259	ASN
2	B	370	HIS
1	X	171	ASN
1	M	201	GLN
2	B	256	GLN

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	224/264 (84%)	-0.10	5 (2%)	62	46	152, 209, 248, 262	0
1	M	207/264 (78%)	-0.16	0	100	100	163, 242, 276, 300	0
1	X	190/264 (71%)	-0.07	2 (1%)	77	62	186, 241, 274, 283	0
2	B	349/433 (80%)	-0.07	7 (2%)	64	49	132, 198, 257, 298	0
2	F	334/433 (77%)	-0.15	5 (1%)	71	56	133, 209, 266, 290	0
2	K	328/433 (75%)	-0.03	6 (1%)	67	51	133, 197, 252, 282	0
All	All	1632/2091 (78%)	-0.09	25 (1%)	71	56	132, 213, 266, 300	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	ALA	3.0
2	B	176	THR	2.9
2	F	345	LEU	2.8
2	B	157	GLY	2.8
2	F	273	VAL	2.7

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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.