



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:28 PM UTC

PDB ID : 5SWS / pdb_00005sws
Title : Crystal Structure of NP2-B17 TCR-H2Db-NP complex
Authors : Gras, S.; Del Campo, C.M.; Farenc, C.; Josephs, T.M.; Rossjohn, J.
Deposited on : 2016-08-08
Resolution : 2.86 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
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

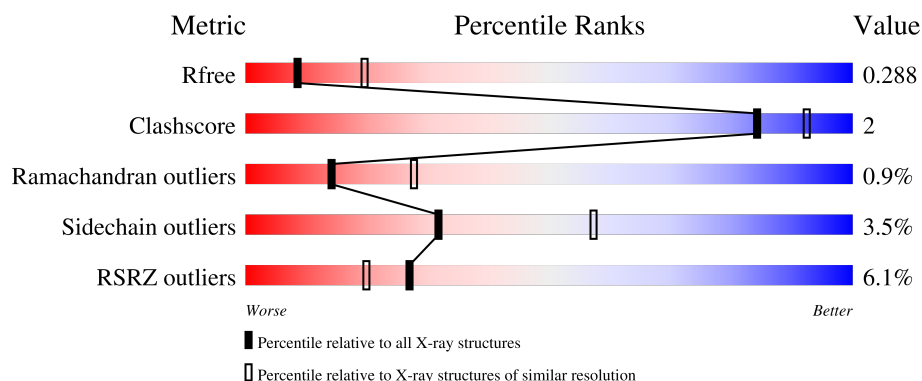
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	280	6% 88% 9% ..
2	B	99	3% 86% 12% .
3	C	9	89% 11%
4	D	207	11% 87% 7% ..
5	E	242	3% 90% 9% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6758 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2240	1417	396	418	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	2	0
			818	523	138	149	8			

- Molecule 3 is a protein called influenza NP366 epitope.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			69	38	11	18	2			

- Molecule 4 is a protein called NP1-B17 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	198	Total	C	N	O	S	0	0	0
			1558	975	258	317	8			

- Molecule 5 is a protein called NP1-B17 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	239	Total	C	N	O	S	0	1	0
			1934	1230	335	360	9			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	46	Total	O	0	0
			46	46		

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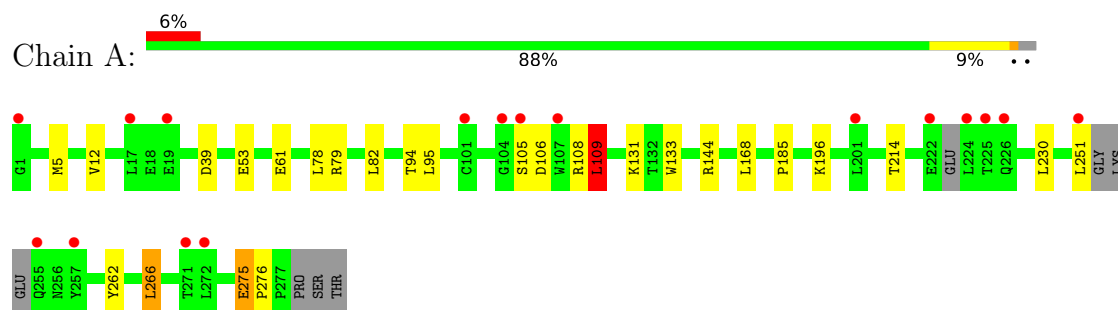
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	15	Total 15	O 15	0	0
6	C	2	Total 2	O 2	0	0
6	D	35	Total 35	O 35	0	0
6	E	41	Total 41	O 41	0	0

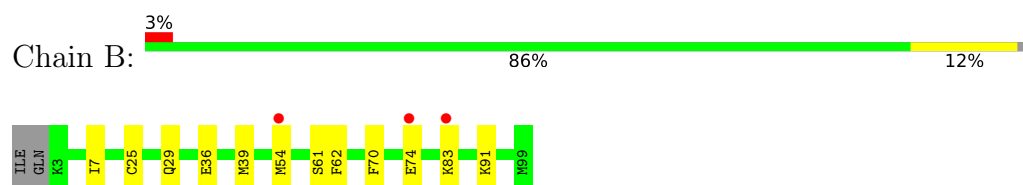
3 Residue-property plots

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.

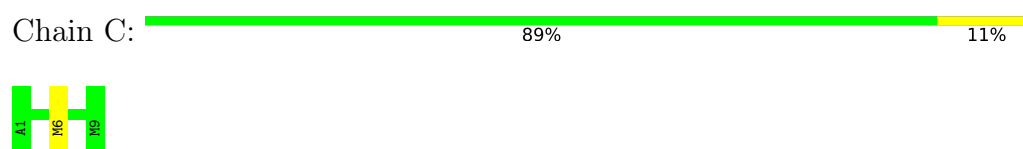
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



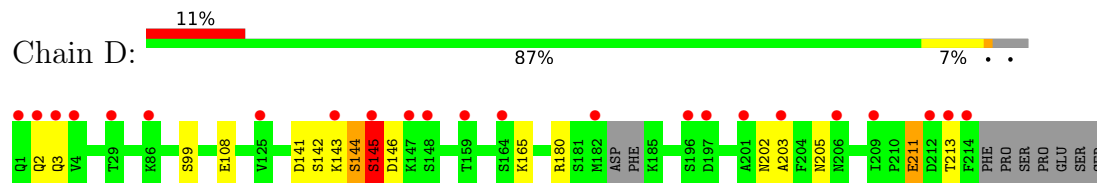
- Molecule 2: Beta-2-microglobulin



- Molecule 3: influenza NP366 epitope



- Molecule 4: NP1-B17 TCR alpha chain



- Molecule 5: NP1-B17 TCR beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.02Å 126.94Å 80.48Å 90.00° 105.66° 90.00°	Depositor
Resolution (Å)	30.48 – 2.86 30.48 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.48-2.86) 99.0 (30.48-2.86)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.86Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.1	Depositor
R, R_{free}	0.231 , 0.274 0.249 , 0.288	Depositor DCC
R_{free} test set	1104 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.041 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6758	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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

5.1 Standard geometry

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	0.67	0/2306	1.16	0/3132
2	B	0.70	0/844	1.06	0/1142
3	C	0.62	0/68	1.06	0/88
4	D	0.76	1/1593 (0.1%)	1.13	10/2158 (0.5%)
5	E	0.67	0/1988	1.05	0/2703
All	All	0.69	1/6799 (0.0%)	1.11	10/9223 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	144	SER	CA-C	5.00	1.58	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	144	SER	CA-C-N	6.56	133.51	121.70
4	D	144	SER	C-N-CA	6.56	133.51	121.70
4	D	211	GLU	CA-C-N	6.33	133.10	121.70
4	D	211	GLU	C-N-CA	6.33	133.10	121.70
4	D	141	ASP	CA-CB-CG	5.79	118.39	112.60
4	D	202	ASN	CA-C-N	5.78	129.06	119.35
4	D	202	ASN	C-N-CA	5.78	129.06	119.35
4	D	203	ALA	N-CA-C	-5.67	105.27	113.21
4	D	145	SER	CA-C-N	5.43	131.48	121.70
4	D	145	SER	C-N-CA	5.43	131.48	121.70

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	2240	0	2115	11	0
2	B	818	0	795	6	0
3	C	69	0	61	0	0
4	D	1558	0	1469	6	0
5	E	1934	0	1863	7	0
6	A	46	0	0	0	0
6	B	15	0	0	0	0
6	C	2	0	0	0	0
6	D	35	0	0	0	0
6	E	41	0	0	0	0
All	All	6758	0	6303	30	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 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)
5:E:40:TYR:HB2	5:E:105:ALA:HB3	1.85	0.59
1:A:79:ARG:HA	1:A:82:LEU:HD12	1.91	0.52
4:D:145:SER:HB3	4:D:146:ASP:HA	1.91	0.52
2:B:29:GLN:HA	2:B:61:SER:HB2	1.93	0.51
2:B:36:GLU:HB2	2:B:83[B]:LYS:HB2	1.92	0.50
2:B:36:GLU:HB2	2:B:83[A]:LYS:HB3	1.94	0.49
4:D:144:SER:H	4:D:145:SER:HA	1.77	0.48
4:D:144:SER:N	4:D:145:SER:HA	2.28	0.47
2:B:54[A]:MET:HE2	2:B:62:PHE:HB3	1.97	0.47
5:E:167:GLU:HB2	5:E:224:GLN:HB3	1.97	0.47
4:D:145:SER:HB3	4:D:146:ASP:CA	2.45	0.47
5:E:154:LEU:HD13	5:E:205:LEU:HD23	1.97	0.46
1:A:275:GLU:CB	1:A:276:PRO:HA	2.44	0.46
1:A:214:THR:HB	1:A:262:TYR:HB2	1.97	0.46
1:A:275:GLU:HB2	1:A:276:PRO:HA	1.97	0.46
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.98	0.45
4:D:2:GLN:H	4:D:3:GLN:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:SER:HA	1:A:106:ASP:HA	1.69	0.45
2:B:7:ILE:HD12	2:B:91:LYS:HD2	1.98	0.45
1:A:133:TRP:HB2	1:A:144:ARG:HG3	1.98	0.44
5:E:12:LEU:HD13	5:E:163:PRO:HG3	2.01	0.42
1:A:108:ARG:O	1:A:109:LEU:HB3	2.20	0.41
4:D:145:SER:CB	4:D:146:ASP:HA	2.50	0.41
1:A:78:LEU:HD13	1:A:95:LEU:HB2	2.02	0.41
5:E:92:GLY:HA2	5:E:93:SER:HA	1.87	0.41
2:B:25:CYS:HB2	2:B:39:MET:HE3	2.02	0.41
1:A:185:PRO:HD2	1:A:266:LEU:HD23	2.03	0.41
5:E:6:GLN:HB2	5:E:118:PRO:HD2	2.02	0.41
1:A:12:VAL:HG22	1:A:94:THR:HG23	2.03	0.40
5:E:16:GLY:HA2	5:E:93:SER:HB2	2.02	0.40

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	267/280 (95%)	247 (92%)	18 (7%)	2 (1%)	18	35
2	B	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
3	C	7/9 (78%)	6 (86%)	0	1 (14%)	0	0
4	D	194/207 (94%)	174 (90%)	17 (9%)	3 (2%)	8	18
5	E	238/242 (98%)	226 (95%)	11 (5%)	1 (0%)	30	48
All	All	803/837 (96%)	747 (93%)	49 (6%)	7 (1%)	14	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	GLU

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Mol	Chain	Res	Type
4	D	165	LYS
1	A	109	LEU
3	C	6	MET
4	D	99	SER
4	D	211	GLU
5	E	58	ASP

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	232/238 (98%)	223 (96%)	9 (4%)	28	54
2	B	93/93 (100%)	91 (98%)	2 (2%)	45	69
3	C	8/8 (100%)	8 (100%)	0	100	100
4	D	178/187 (95%)	171 (96%)	7 (4%)	28	54
5	E	210/212 (99%)	203 (97%)	7 (3%)	33	58
All	All	721/738 (98%)	696 (96%)	25 (4%)	32	57

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	53	GLU
1	A	61	GLU
1	A	109	LEU
1	A	131	LYS
1	A	196	LYS
1	A	230	LEU
1	A	251	LEU
1	A	266	LEU
2	B	70	PHE
2	B	74	GLU
4	D	108	GLU
4	D	142	SER

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Mol	Chain	Res	Type
4	D	143	LYS
4	D	145	SER
4	D	180	ARG
4	D	205	ASN
4	D	213	THR
5	E	19	VAL
5	E	31	THR
5	E	164	ASP
5	E	168	LEU
5	E	194	LEU
5	E	198	ARG
5	E	251	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	54	GLN
1	A	87	GLN
1	A	97	GLN
1	A	174	ASN
1	A	192	HIS
2	B	13	HIS
3	C	3	ASN
3	C	5	ASN
4	D	22	ASN
4	D	43	GLN
4	D	130	GLN
5	E	6	GLN
5	E	48	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	273/280 (97%)	0.64	17 (6%) 26 19	25, 46, 73, 85	8 (2%)
2	B	97/99 (97%)	0.38	3 (3%) 51 43	17, 41, 59, 64	2 (2%)
3	C	9/9 (100%)	-0.00	0 100 100	26, 31, 36, 39	0
4	D	198/207 (95%)	0.91	23 (11%) 9 7	32, 54, 71, 98	2 (1%)
5	E	239/242 (98%)	0.51	7 (2%) 53 45	20, 43, 67, 75	1 (0%)
All	All	816/837 (97%)	0.63	50 (6%) 27 20	17, 46, 70, 98	13 (1%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	GLU	5.5
4	D	4	VAL	4.0
1	A	225	THR	3.9
1	A	104	GLY	3.9
4	D	2	GLN	3.9
4	D	159	THR	3.5
1	A	105	SER	3.3
4	D	182	MET	3.2
1	A	19	GLU	3.1
2	B	54[A]	MET	3.1
4	D	209	ILE	3.0
4	D	164	SER	3.0
1	A	251	LEU	2.9
4	D	203	ALA	2.9
1	A	17	LEU	2.9
1	A	101	CYS	2.9
1	A	257	TYR	2.8
5	E	188	LEU	2.8
4	D	212	ASP	2.7
4	D	201	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
4	D	206	ASN	2.7
4	D	197	ASP	2.6
5	E	111	ASP	2.6
5	E	81	PRO	2.6
1	A	1	GLY	2.5
4	D	3	GLN	2.5
5	E	138	VAL	2.4
4	D	196	SER	2.4
5	E	71	THR	2.3
4	D	214	PHE	2.2
5	E	108	ALA	2.2
4	D	86	LYS	2.2
4	D	143	LYS	2.2
4	D	147	LYS	2.2
1	A	271	THR	2.2
4	D	29	THR	2.2
2	B	83[A]	LYS	2.1
4	D	145	SER	2.1
5	E	254	ALA	2.1
4	D	1	GLN	2.1
4	D	125	VAL	2.1
1	A	201	LEU	2.1
1	A	226	GLN	2.1
1	A	224	LEU	2.1
4	D	213	THR	2.1
1	A	107	TRP	2.1
1	A	272	LEU	2.0
1	A	255	GLN	2.0
4	D	148	SER	2.0
2	B	74	GLU	2.0

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.