



Full wwPDB X-ray Structure Validation Report

Sep 16, 2014 – 01:27 PM EDT

PDB ID : 4MS8
Title : 42F3 TCR pCPB9/H-2Ld Complex
Authors : Birnbaum, M.E.; Adams, J.J.; Garcia, K.C.
Deposited on : 2013-09-18
Resolution : 1.92 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

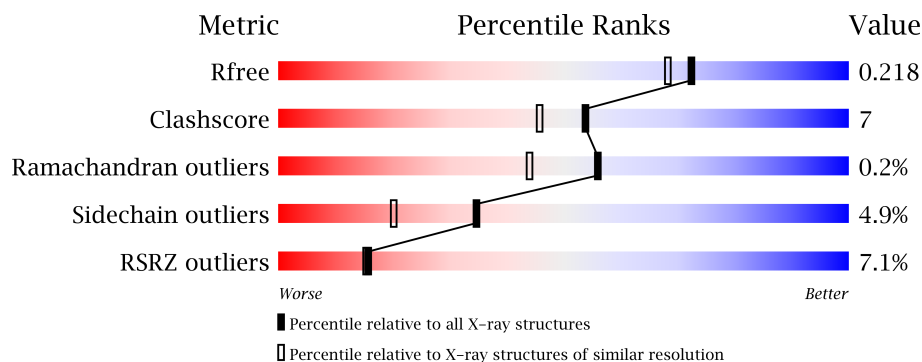
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 1.92 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}	66092	4387 (1.94-1.90)
Clashscore	79885	5258 (1.94-1.90)
Ramachandran outliers	78287	5193 (1.94-1.90)
Sidechain outliers	78261	5194 (1.94-1.90)
RSRZ outliers	66119	4389 (1.94-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	C	212	
2	D	243	
3	A	180	
4	B	9	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5275 atoms, of which 0 are hydrogen and 0 are deuterium.

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 42F3 alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	196	Total	C	N	O	S	0	0	0
			1517	961	249	299	8			

- Molecule 2 is a protein called 42F3 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	239	Total	C	N	O	S	0	0	0
			1895	1194	329	366	6			

- Molecule 3 is a protein called H-2 class I histocompatibility antigen, L-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	162	Total	C	N	O	S	0	0	0
			1335	846	230	252	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP P01897
A	8	TYR	PHE	ENGINEERED MUTATION	UNP P01897
A	12	THR	VAL	ENGINEERED MUTATION	UNP P01897
A	15	ARG	PRO	ENGINEERED MUTATION	UNP P01897
A	23	THR	ILE	ENGINEERED MUTATION	UNP P01897
A	30	ASP	ASN	ENGINEERED MUTATION	UNP P01897
A	49	VAL	ALA	ENGINEERED MUTATION	UNP P01897
A	131	ARG	LYS	ENGINEERED MUTATION	UNP P01897

- Molecule 4 is a protein called pCPB9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	9	Total	C	N	O	0	1	0
			72	49	9	14			

- Molecule 5 is water.

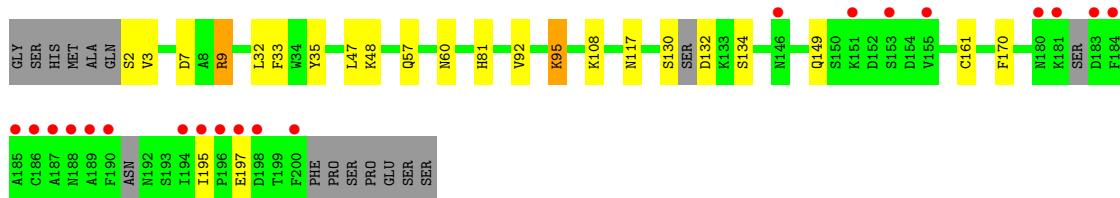
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	164	Total 164	O 164	0	0
5	D	213	Total 213	O 213	0	0
5	A	74	Total 74	O 74	0	0
5	B	5	Total 5	O 5	0	0

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.

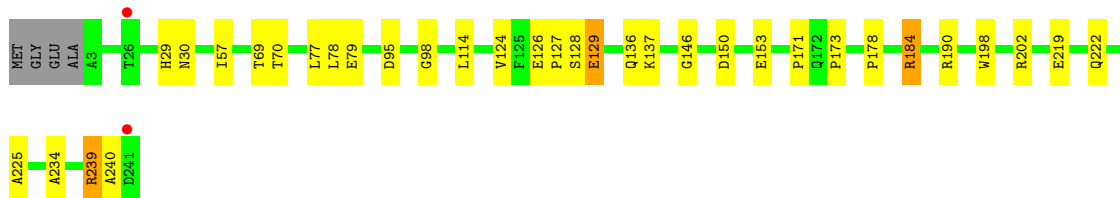
- Molecule 1: 42F3 alpha

Chain C: 



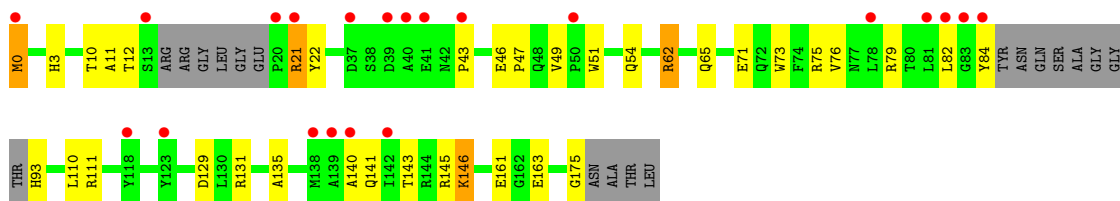
- Molecule 2: 42F3 beta

Chain D: 



- Molecule 3: H-2 class I histocompatibility antigen, L-D alpha chain

Chain A: 



- Molecule 4: pCPB9

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.26Å 60.62Å 70.10Å 90.00° 96.06° 90.00°	Depositor
Resolution (Å)	34.85 – 1.92 43.57 – 1.92	Depositor EDS
% Data completeness (in resolution range)	93.1 (34.85-1.92) 93.1 (43.57-1.92)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 1.92Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.180 , 0.219 0.179 , 0.218	Depositor DCC
R_{free} test set	2653 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 52107 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5275	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	C	0.81	1/1551 (0.1%)	0.81	0/2098
2	D	0.77	0/1947	0.80	1/2655 (0.0%)
3	A	0.64	0/1373	0.69	0/1861
4	B	0.62	0/77	0.56	0/103
All	All	0.75	1/4948 (0.0%)	0.77	1/6717 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	35	TYR	CD1-CE1	5.67	1.47	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	184	ARG	NE-CZ-NH2	-5.86	117.37	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1517	0	1439	14	0
2	D	1895	0	1791	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1335	0	1216	26	0
4	B	72	0	68	4	0
5	A	74	0	0	12	0
5	B	5	0	0	0	0
5	C	164	0	0	9	1
5	D	213	0	0	13	2
All	All	5275	0	4514	64	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (64) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:130:SER:HG	1:C:132:ASP:N	1.62	0.96
1:C:9:ARG:NH2	5:C:435:HOH:O	2.00	0.93
2:D:136:GLN:O	5:D:374:HOH:O	1.95	0.84
3:A:84:TYR:O	5:A:241:HOH:O	2.00	0.80
3:A:111:ARG:NH1	5:A:237:HOH:O	2.16	0.78
5:C:464:HOH:O	4:B:4[A]:GLU:HG2	1.84	0.78
3:A:146:LYS:NZ	5:A:247:HOH:O	2.25	0.70
2:D:240:ALA:O	5:D:483:HOH:O	2.08	0.70
2:D:219:GLU:OE2	5:D:356:HOH:O	2.09	0.69
2:D:129:GLU:HG3	5:D:479:HOH:O	1.93	0.69
2:D:153:GLU:OE2	5:D:493:HOH:O	2.12	0.67
1:C:108:LYS:NZ	5:C:414:HOH:O	2.27	0.65
2:D:95:ASP:OD2	5:D:477:HOH:O	2.14	0.65
3:A:129:ASP:O	3:A:131:ARG:NH1	2.30	0.64
1:C:7:ASP:HB2	5:C:390:HOH:O	1.96	0.64
2:D:222:GLN:NE2	5:D:449:HOH:O	2.27	0.62
2:D:150:ASP:OD1	2:D:173:PRO:HG2	2.00	0.62
1:C:60:ASN:OD1	5:C:455:HOH:O	2.17	0.60
2:D:225:ALA:O	5:D:395:HOH:O	2.17	0.57
2:D:77:LEU:HG	2:D:79:GLU:HG3	1.86	0.57
2:D:222:GLN:O	5:D:464:HOH:O	2.17	0.57
3:A:12:THR:HA	3:A:93:HIS:O	2.04	0.57
1:C:95:LYS:HE3	5:C:400:HOH:O	2.04	0.57
2:D:146:GLY:O	2:D:184:ARG:HD3	2.05	0.57
3:A:161:GLU:OE1	5:A:257:HOH:O	2.17	0.56
3:A:79:ARG:HA	3:A:82:LEU:HD12	1.86	0.56
3:A:143:THR:HG21	4:B:9:LEU:HD23	1.89	0.54
1:C:57:GLN:HG2	5:C:356:HOH:O	2.08	0.53
3:A:141:GLN:O	5:A:245:HOH:O	2.19	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:69:THR:HG23	2:D:70:THR:HG23	1.92	0.51
1:C:60:ASN:ND2	5:C:459:HOH:O	2.27	0.51
1:C:32:LEU:HD23	1:C:92:VAL:HG12	1.93	0.51
3:A:65:GLN:HG3	5:A:258:HOH:O	2.11	0.50
3:A:46:GLU:HG3	3:A:47:PRO:HD2	1.92	0.50
3:A:145:ARG:HA	5:A:265:HOH:O	2.11	0.49
1:C:33:PHE:CZ	2:D:98:GLY:HA3	2.48	0.48
3:A:0:MET:SD	3:A:3:HIS:NE2	2.87	0.48
3:A:21:ARG:O	3:A:21:ARG:HG3	2.12	0.48
3:A:11:ALA:HA	3:A:22:TYR:HA	1.95	0.48
3:A:62:ARG:NH2	5:A:234:HOH:O	2.46	0.47
3:A:73:TRP:NE1	4:B:7:PHE:O	2.35	0.47
4:B:4[A]:GLU:HG3	4:B:6:GLY:N	2.30	0.47
1:C:195:ILE:H	1:C:195:ILE:HD12	1.80	0.47
2:D:126:GLU:OE1	2:D:239:ARG:NH1	2.47	0.47
2:D:129:GLU:HB2	5:D:463:HOH:O	2.13	0.47
3:A:163:GLU:HG3	5:A:224:HOH:O	2.15	0.46
3:A:62:ARG:CZ	5:A:234:HOH:O	2.62	0.46
3:A:71:GLU:O	3:A:75:ARG:HG3	2.16	0.45
1:C:57:GLN:CG	5:C:356:HOH:O	2.65	0.45
2:D:30:ASN:OD1	3:A:76:VAL:HG21	2.16	0.44
3:A:175:GLY:O	5:A:244:HOH:O	2.21	0.43
3:A:49:VAL:HG21	3:A:51:TRP:CE2	2.53	0.43
3:A:10:THR:OG1	5:A:208:HOH:O	2.21	0.43
3:A:135:ALA:HB1	3:A:140:ALA:CB	2.49	0.43
2:D:178:PRO:HG3	5:D:468:HOH:O	2.19	0.43
2:D:29:HIS:CD2	2:D:95:ASP:HB3	2.52	0.43
2:D:202:ARG:NH1	5:D:465:HOH:O	2.41	0.43
2:D:78:LEU:HD12	2:D:78:LEU:N	2.35	0.41
2:D:171:PRO:HA	5:D:510:HOH:O	2.21	0.41
2:D:124:VAL:HG23	2:D:234:ALA:HB3	2.02	0.41
1:C:170:PHE:CE2	2:D:137:LYS:HE2	2.55	0.41
3:A:135:ALA:HB1	3:A:140:ALA:HB1	2.01	0.41
2:D:127:PRO:HD2	2:D:198:TRP:CZ2	2.55	0.40
1:C:170:PHE:CD2	2:D:137:LYS:HE2	2.56	0.40

All (2) 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	Distance(Å)	Clash(Å)
5:D:504:HOH:O	5:D:507:HOH:O[4_546]	1.83	0.37
5:C:455:HOH:O	5:D:446:HOH:O[4_546]	1.98	0.22

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	C	188/212 (89%)	184 (98%)	4 (2%)	0	100	100
2	D	237/243 (98%)	233 (98%)	4 (2%)	0	100	100
3	A	156/180 (87%)	149 (96%)	6 (4%)	1 (1%)	33	18
4	B	8/9 (89%)	8 (100%)	0	0	100	100
All	All	589/644 (92%)	574 (98%)	14 (2%)	1 (0%)	56	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	43	PRO

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	C	169/186 (91%)	157 (93%)	12 (7%)	21	9
2	D	206/208 (99%)	200 (97%)	6 (3%)	55	43
3	A	131/148 (88%)	125 (95%)	6 (5%)	37	22
4	B	7/6 (117%)	6 (86%)	1 (14%)	5	1
All	All	513/548 (94%)	488 (95%)	25 (5%)	35	20

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

Mol	Chain	Res	Type
1	C	2	SER

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Mol	Chain	Res	Type
1	C	3	VAL
1	C	9	ARG
1	C	47	LEU
1	C	48	LYS
1	C	81	HIS
1	C	95	LYS
1	C	117	ASN
1	C	134	SER
1	C	149	GLN
1	C	161	CYS
1	C	197	GLU
2	D	57	ILE
2	D	114	LEU
2	D	128	SER
2	D	129	GLU
2	D	190	ARG
2	D	239	ARG
3	A	0	MET
3	A	21	ARG
3	A	54	GLN
3	A	62	ARG
3	A	110	LEU
3	A	146	LYS
4	B	9	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	124	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	C	196/212 (92%)	0.10	20 (10%) 7 6	23, 40, 73, 96	0
2	D	239/243 (98%)	-0.09	2 (0%) 83 85	24, 36, 63, 88	0
3	A	162/180 (90%)	0.66	21 (12%) 4 4	31, 59, 94, 117	0
4	B	9/9 (100%)	0.33	0 100 100	42, 47, 58, 61	0
All	All	606/644 (94%)	0.18	43 (7%) 16 15	23, 42, 80, 117	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	81	LEU	5.8
3	A	142	ILE	5.3
1	C	194	ILE	4.9
3	A	138	MET	4.9
2	D	26	THR	4.5
1	C	196	PRO	4.3
3	A	83	GLY	4.1
3	A	82	LEU	3.9
3	A	84	TYR	3.9
3	A	43	PRO	3.7
1	C	184	PHE	3.7
1	C	200	PHE	3.5
1	C	183	ASP	3.4
3	A	13	SER	3.4
2	D	241	ASP	3.3
1	C	185	ALA	3.2
3	A	37	ASP	3.2
1	C	189	ALA	3.1
1	C	151	LYS	3.0
3	A	40	ALA	2.9
3	A	0	MET	2.8

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Mol	Chain	Res	Type	RSRZ
3	A	20	PRO	2.8
1	C	186	CYS	2.7
1	C	155	VAL	2.6
1	C	195	ILE	2.6
1	C	190	PHE	2.6
1	C	181	LYS	2.6
3	A	41	GLU	2.6
3	A	118	TYR	2.5
1	C	153	SER	2.4
3	A	140	ALA	2.4
1	C	197	GLU	2.4
1	C	188	ASN	2.3
1	C	198	ASP	2.2
3	A	139	ALA	2.2
3	A	21	ARG	2.2
3	A	123	TYR	2.2
3	A	39	ASP	2.1
3	A	50	PRO	2.1
1	C	180	ASN	2.1
1	C	146	ASN	2.1
1	C	187	ALA	2.1
3	A	78	LEU	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 carbohydrates 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.