wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2020 – 09:12 am BST

PDB ID	:	1ZGL
Title	:	Crystal structure of 3A6 TCR bound to MBP/HLA-DR2a
Authors	:	Li, Y.; Huang, Y.; Lue, J.; Quandt, J.A.; Martin, R.; Mariuzza, R.A.
Deposited on	:	2005-04-21
Resolution	:	2.80 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

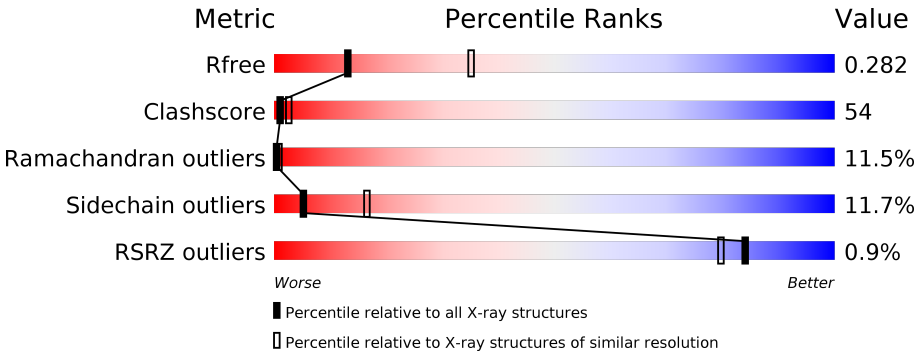
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	181	35% 55% 9% ·
1	D	181	45% 44% 9% · ·
1	G	181	% 41% 48% 9% · ·
1	J	181	39% 51% 9% ·
2	B	192	% 39% 43% 5% · 9%
2	E	192	40% 43% 8% · 9%

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Mol	Chain	Length	Quality of chain
2	H	192	5% 33% 46% 8% 13%
2	K	192	40% 44% 9% 6%
3	C	15	13% 60% 20% 7%
3	F	15	13% 60% 27%
3	I	15	27% 20% 33% 7% 13%
3	L	15	20% 40% 27% 7% 7%
4	M	209	% 28% 39% 17% 15%
4	Q	209	% 23% 43% 20% 11%
4	S	209	2% 25% 41% 17% 16%
4	U	209	34% 41% 17% 7%
5	P	249	29% 53% 13%
5	R	249	32% 49% 12%
5	T	249	3% 31% 47% 11% 9%
5	V	249	33% 50% 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23456 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 HLA class II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1362	887	224	246	5			
1	D	178	Total	C	N	O	S	0	0	0
			1366	889	224	248	5			
1	G	178	Total	C	N	O	S	0	0	0
			1362	887	224	246	5			
1	J	178	Total	C	N	O	S	0	0	0
			1366	889	224	248	5			

- Molecule 2 is a protein called major histocompatibility complex, class II, DR beta 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	8	0	0
			1319	831	234	250	4			
2	E	175	Total	C	N	O	S	0	0	0
			1307	823	230	250	4			
2	H	168	Total	C	N	O	S	0	0	0
			1284	811	226	243	4			
2	K	180	Total	C	N	O	S	5	0	0
			1347	851	235	257	4			

- Molecule 3 is a protein called Myelin basic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	14	Total	C	N	O	0	0	0
			114	76	21	17			
3	F	15	Total	C	N	O	0	0	0
			119	78	22	19			
3	I	13	Total	C	N	O	0	0	0
			107	71	20	16			
3	L	14	Total	C	N	O	0	0	0
			114	76	21	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	14	GLY	-	cloning artifact	UNP Q6AI64
C	15	GLY	-	cloning artifact	UNP Q6AI64
F	14	GLY	-	cloning artifact	UNP Q6AI64
F	15	GLY	-	cloning artifact	UNP Q6AI64
I	14	GLY	-	cloning artifact	UNP Q6AI64
I	15	GLY	-	cloning artifact	UNP Q6AI64
L	14	GLY	-	cloning artifact	UNP Q6AI64
L	15	GLY	-	cloning artifact	UNP Q6AI64

- Molecule 4 is a protein called T cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	178	Total	C	N	O	S	0	0	0
			1268	800	206	258	4			
4	Q	187	Total	C	N	O	S	0	0	0
			1331	835	218	271	7			
4	S	176	Total	C	N	O	S	0	0	0
			1231	770	204	253	4			
4	U	195	Total	C	N	O	S	0	0	0
			1356	850	224	276	6			

- Molecule 5 is a protein called T cell receptor beta chain.

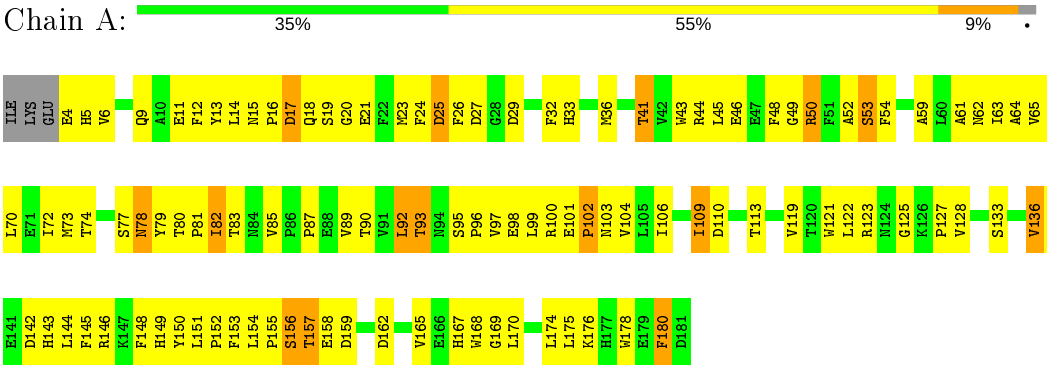
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	242	Total	C	N	O	S	0	0	0
			1813	1135	322	351	5			
5	R	238	Total	C	N	O	S	0	0	0
			1790	1118	321	346	5			
5	T	226	Total	C	N	O	S	0	0	0
			1657	1037	294	321	5			
5	V	242	Total	C	N	O	S	0	0	0
			1843	1156	324	358	5			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

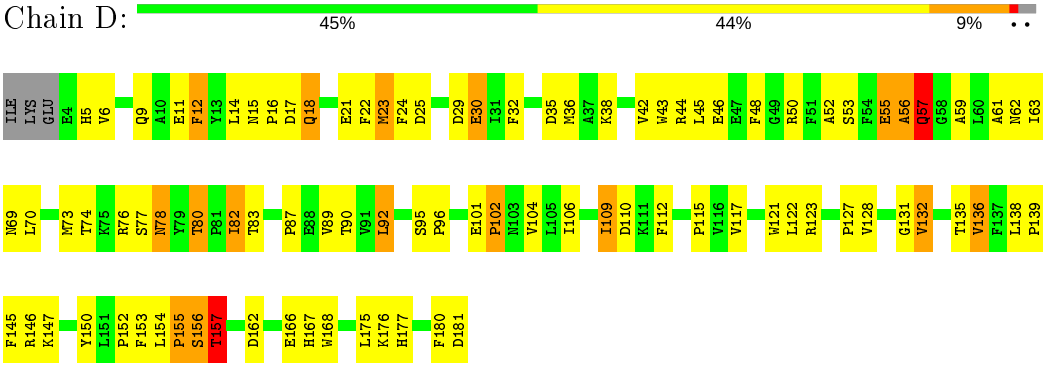
• Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain A:



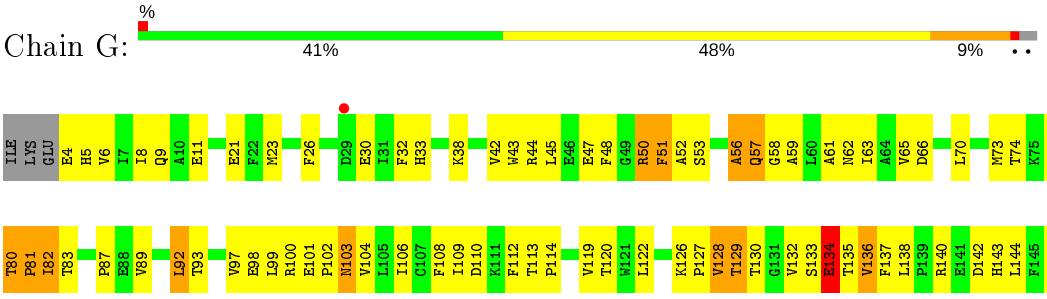
• Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

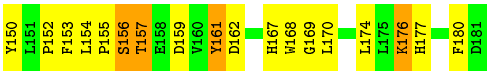
Chain D:



• Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain G:



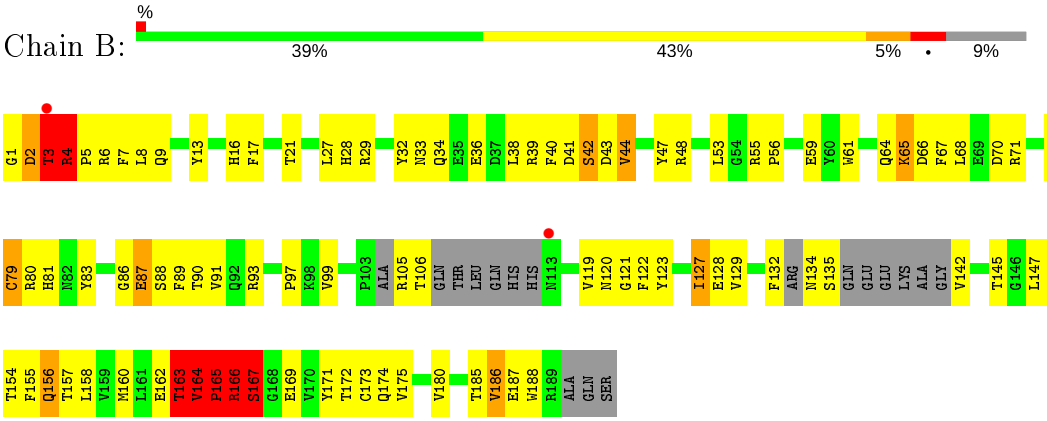


• Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain J:

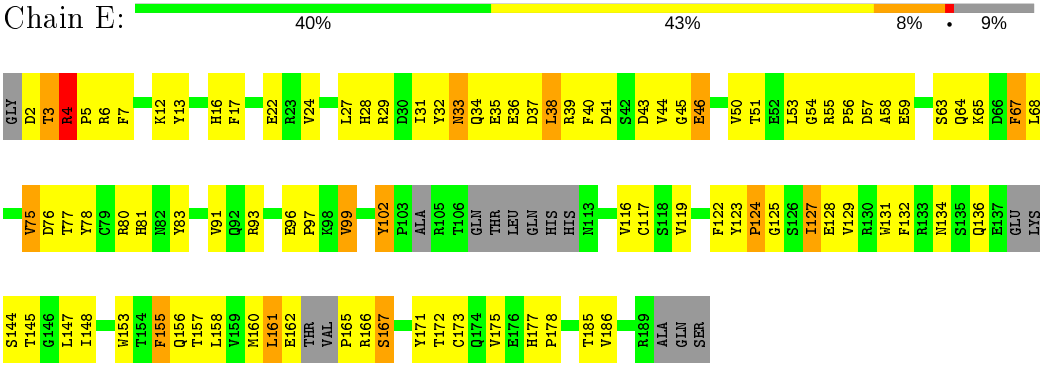
• Molecule 2: major histocompatibility complex, class II, DR beta 5

Chain B:



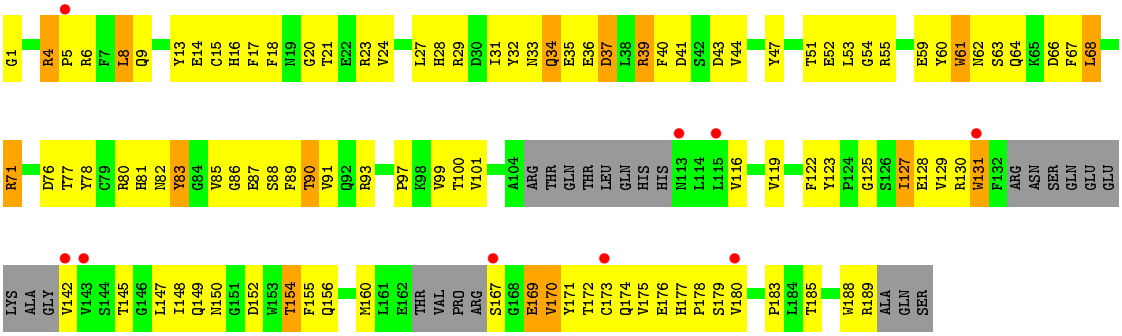
• Molecule 2: major histocompatibility complex, class II, DR beta 5

Chain E:



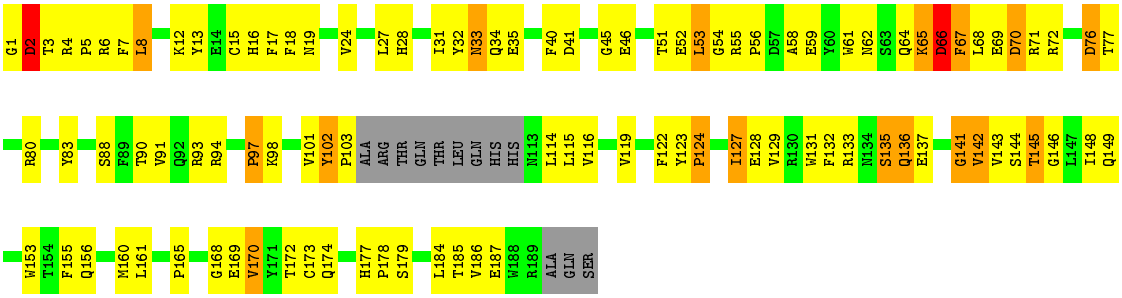
• Molecule 2: major histocompatibility complex, class II, DR beta 5

Chain H:



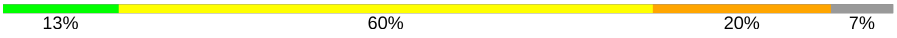
- Molecule 2: major histocompatibility complex, class II, DR beta 5

Chain K:



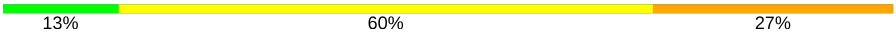
- Molecule 3: Myelin basic protein

Chain C:



- Molecule 3: Myelin basic protein

Chain F:

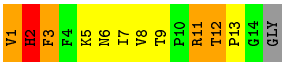


- Molecule 3: Myelin basic protein

Chain I:

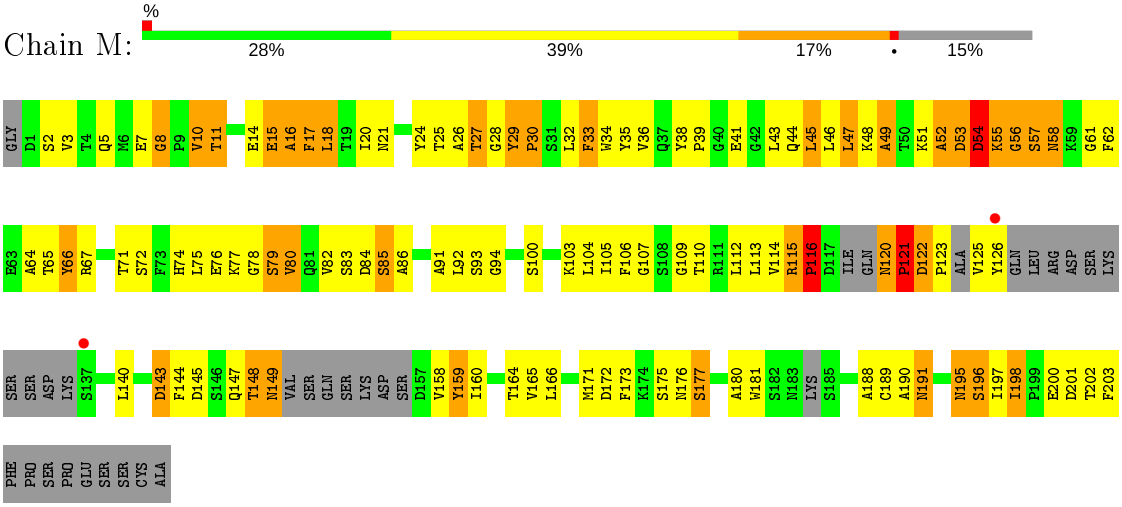
- Molecule 3: Myelin basic protein

Chain L:



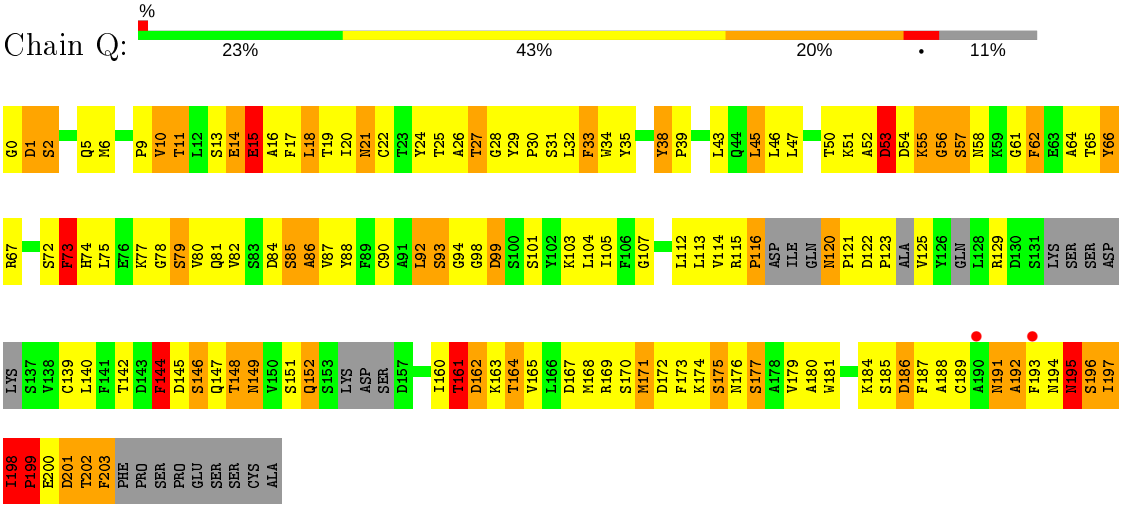
- Molecule 4: T cell receptor alpha chain

Chain M:



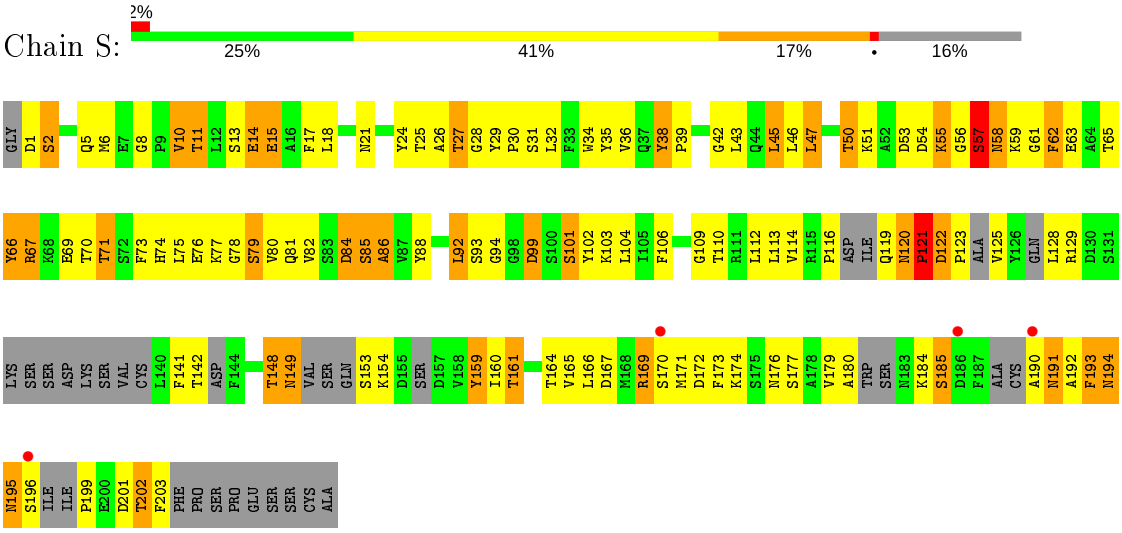
• Molecule 4: T cell receptor alpha chain

Chain Q:



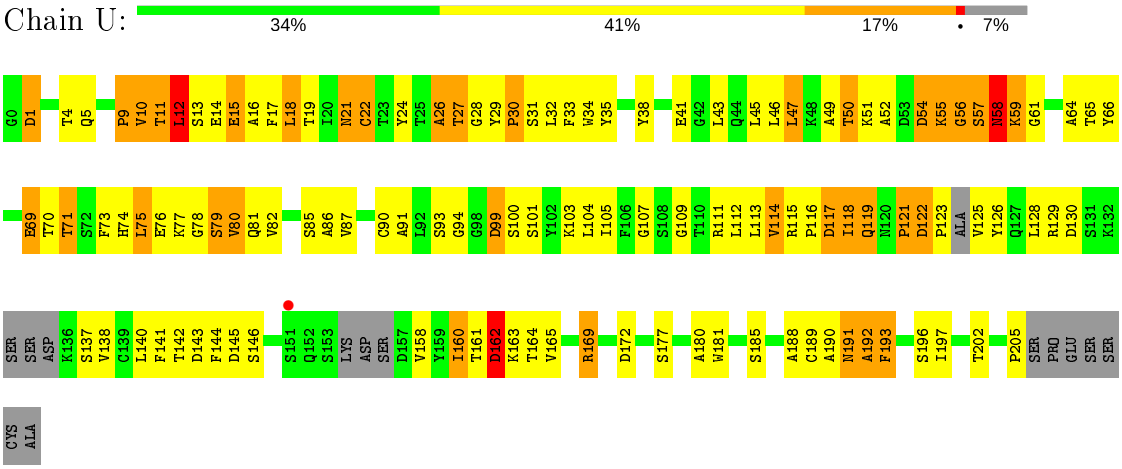
• Molecule 4: T cell receptor alpha chain

Chain S:



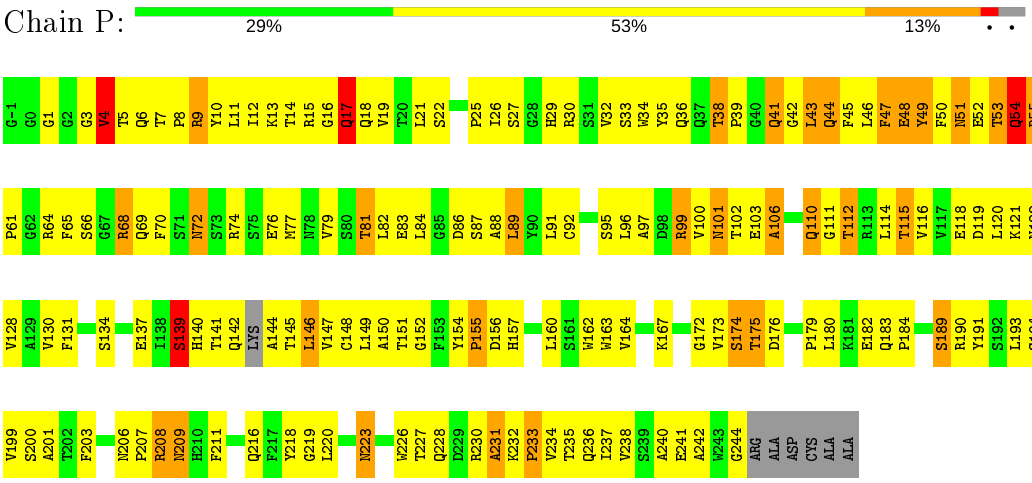
• Molecule 4: T cell receptor alpha chain

Chain U:



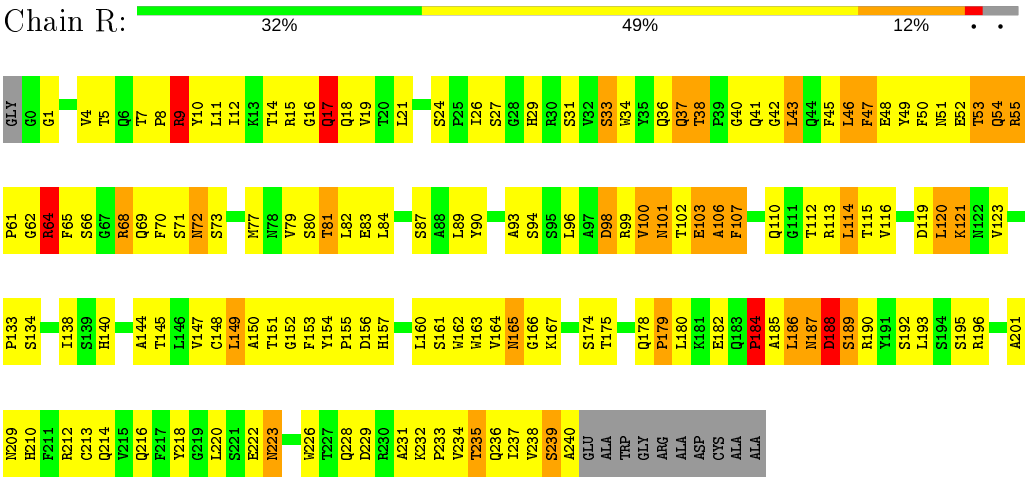
• Molecule 5: T cell receptor beta chain

Chain P:



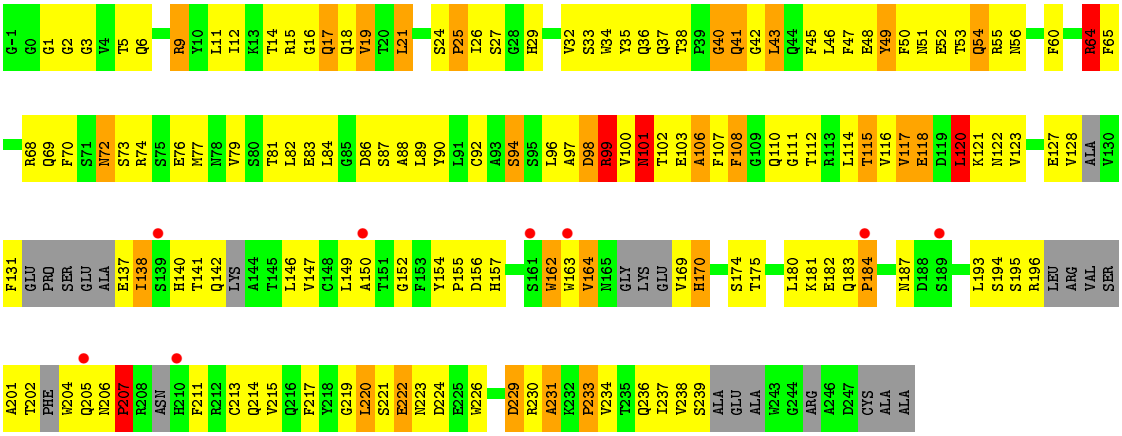
• Molecule 5: T cell receptor beta chain

Chain R:



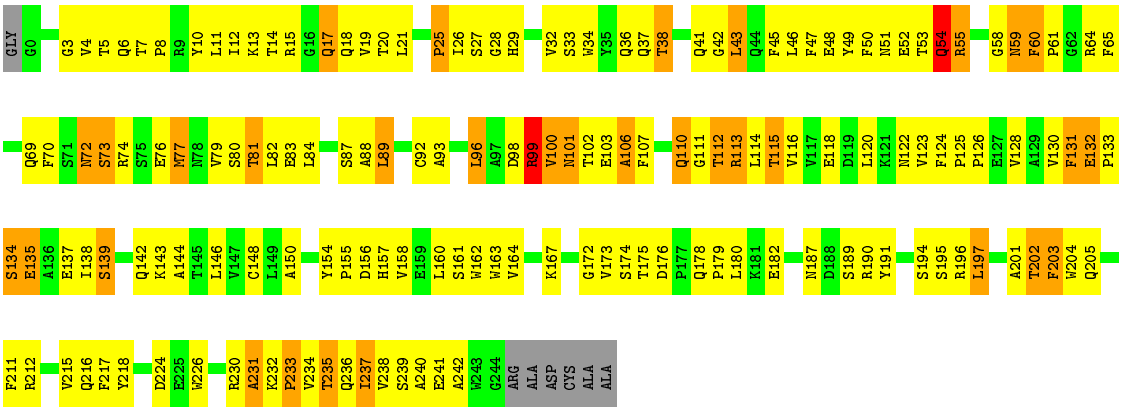
• Molecule 5: T cell receptor beta chain

Chain T:



- Molecule 5: T cell receptor beta chain

Chain V:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	96.48Å 97.69Å 124.02Å 74.39° 83.19° 61.55°	Depositor
Resolution (Å)	30.00 – 2.80 29.86 – 2.59	Depositor EDS
% Data completeness (in resolution range)	86.4 (30.00-2.80) 85.9 (29.86-2.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.280 , 0.329 0.287 , 0.282	Depositor DCC
R_{free} test set	5144 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	44.4	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 85.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h-k,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	23456	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0.45	0/1406	0.74	0/1930
1	D	0.45	0/1410	0.73	1/1935 (0.1%)
1	G	0.46	0/1406	0.73	0/1930
1	J	0.41	0/1410	0.71	0/1935
2	B	0.48	0/1350	0.81	5/1843 (0.3%)
2	E	0.44	0/1337	0.76	2/1827 (0.1%)
2	H	0.46	0/1316	0.72	0/1796
2	K	0.44	0/1382	0.76	3/1891 (0.2%)
3	C	0.47	0/118	0.85	0/160
3	F	0.52	0/123	0.94	0/165
3	I	0.56	0/111	0.82	0/150
3	L	0.58	0/118	0.88	0/160
4	M	0.47	0/1291	0.78	1/1759 (0.1%)
4	Q	0.52	0/1355	0.87	5/1844 (0.3%)
4	S	0.45	0/1244	0.78	2/1684 (0.1%)
4	U	0.51	0/1380	0.83	3/1885 (0.2%)
5	P	0.53	1/1860 (0.1%)	0.77	1/2538 (0.0%)
5	R	0.50	1/1835 (0.1%)	0.73	2/2505 (0.1%)
5	T	0.51	1/1691 (0.1%)	0.76	0/2297
5	V	2.79	3/1892 (0.2%)	1.71	3/2580 (0.1%)
All	All	0.91	6/24035 (0.0%)	0.88	28/32814 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	P	0	1
5	T	0	1
5	V	0	1
All	All	0	3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	V	132	GLU	CD-OE2	116.11	2.53	1.25
5	V	132	GLU	CD-OE1	25.49	1.53	1.25
5	V	33	SER	CB-OG	8.87	1.53	1.42
5	T	33	SER	CB-OG	8.73	1.53	1.42
5	R	33	SER	CB-OG	8.61	1.53	1.42

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	V	132	GLU	OE1-CD-OE2	-75.19	33.07	123.30
5	V	132	GLU	CG-CD-OE2	-13.42	91.46	118.30
5	P	41	GLN	N-CA-C	-7.76	90.05	111.00
1	D	157	THR	N-CA-C	-6.71	92.88	111.00
2	B	165	PRO	N-CA-CB	6.67	111.30	103.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	P	49	TYR	Sidechain
5	T	49	TYR	Sidechain
5	V	132	GLU	Sidechain

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	1362	0	1227	122	0
1	D	1366	0	1231	101	0
1	G	1362	0	1227	121	0
1	J	1366	0	1231	121	0
2	B	1319	0	1134	140	0
2	E	1307	0	1111	117	0
2	H	1284	0	1119	127	0
2	K	1347	0	1154	135	0
3	C	114	0	119	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	119	0	122	46	0
3	I	107	0	107	27	0
3	L	114	0	119	25	0
4	M	1268	0	1072	168	0
4	Q	1331	0	1116	183	0
4	S	1231	0	1037	166	0
4	U	1356	0	1112	145	0
5	P	1813	0	1629	214	0
5	R	1790	0	1629	215	0
5	T	1657	0	1440	217	0
5	V	1843	0	1674	199	0
All	All	23456	0	20610	2362	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 54.

The worst 5 of 2362 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)
4:M:82:VAL:HA	4:M:114:VAL:HG11	1.24	1.20
4:M:26:ALA:HB1	4:M:30:PRO:HG2	1.18	1.17
4:S:26:ALA:HB1	4:S:30:PRO:HG2	1.21	1.16
2:B:71:ARG:HH12	3:C:9:THR:HB	1.12	1.14
4:Q:120:ASN:HB3	4:Q:121:PRO:HD2	1.25	1.14

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	176/181 (97%)	143 (81%)	24 (14%)	9 (5%)	2 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	176/181 (97%)	148 (84%)	18 (10%)	10 (6%)	1 5
1	G	176/181 (97%)	141 (80%)	24 (14%)	11 (6%)	1 3
1	J	176/181 (97%)	141 (80%)	23 (13%)	12 (7%)	1 3
2	B	165/192 (86%)	120 (73%)	29 (18%)	16 (10%)	0 1
2	E	165/192 (86%)	121 (73%)	31 (19%)	13 (8%)	1 2
2	H	160/192 (83%)	122 (76%)	30 (19%)	8 (5%)	2 6
2	K	176/192 (92%)	133 (76%)	23 (13%)	20 (11%)	0 1
3	C	12/15 (80%)	7 (58%)	1 (8%)	4 (33%)	0 0
3	F	13/15 (87%)	7 (54%)	5 (38%)	1 (8%)	1 2
3	I	11/15 (73%)	5 (46%)	2 (18%)	4 (36%)	0 0
3	L	12/15 (80%)	7 (58%)	2 (17%)	3 (25%)	0 0
4	M	166/209 (79%)	99 (60%)	37 (22%)	30 (18%)	0 0
4	Q	175/209 (84%)	97 (55%)	32 (18%)	46 (26%)	0 0
4	S	154/209 (74%)	92 (60%)	31 (20%)	31 (20%)	0 0
4	U	185/209 (88%)	112 (60%)	35 (19%)	38 (20%)	0 0
5	P	238/249 (96%)	176 (74%)	42 (18%)	20 (8%)	1 2
5	R	236/249 (95%)	161 (68%)	56 (24%)	19 (8%)	1 2
5	T	206/249 (83%)	140 (68%)	37 (18%)	29 (14%)	0 0
5	V	240/249 (96%)	185 (77%)	33 (14%)	22 (9%)	1 1
All	All	3018/3384 (89%)	2157 (72%)	515 (17%)	346 (12%)	0 1

5 of 346 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	PRO
1	A	156	SER
1	A	158	GLU
2	B	2	ASP
2	B	65	LYS

5.3.2 Protein sidechains (i)

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	136/166 (82%)	122 (90%)	14 (10%)	7 21
1	D	137/166 (82%)	123 (90%)	14 (10%)	7 22
1	G	136/166 (82%)	122 (90%)	14 (10%)	7 21
1	J	137/166 (82%)	127 (93%)	10 (7%)	14 38
2	B	126/173 (73%)	116 (92%)	10 (8%)	12 34
2	E	124/173 (72%)	115 (93%)	9 (7%)	14 38
2	H	125/173 (72%)	111 (89%)	14 (11%)	6 18
2	K	128/173 (74%)	123 (96%)	5 (4%)	32 66
3	C	13/13 (100%)	12 (92%)	1 (8%)	13 35
3	F	13/13 (100%)	10 (77%)	3 (23%)	1 2
3	I	12/13 (92%)	8 (67%)	4 (33%)	0 0
3	L	13/13 (100%)	9 (69%)	4 (31%)	0 0
4	M	117/183 (64%)	101 (86%)	16 (14%)	3 11
4	Q	124/183 (68%)	107 (86%)	17 (14%)	3 11
4	S	112/183 (61%)	97 (87%)	15 (13%)	4 12
4	U	120/183 (66%)	103 (86%)	17 (14%)	3 10
5	P	183/213 (86%)	154 (84%)	29 (16%)	2 8
5	R	184/213 (86%)	156 (85%)	28 (15%)	3 8
5	T	160/213 (75%)	140 (88%)	20 (12%)	4 14
5	V	190/213 (89%)	167 (88%)	23 (12%)	5 15
All	All	2290/2992 (76%)	2023 (88%)	267 (12%)	5 16

5 of 267 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	R	53	THR
1	G	128	VAL
5	V	21	LEU
5	R	64	ARG
5	R	184	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
5	R	140	HIS
1	G	167	HIS
5	V	37	GLN
5	R	209	ASN
5	R	228	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 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	U	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	149:ASN	C	150:VAL	N	6.07

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, 95^{th} 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	178/181 (98%)	-0.48	0 100 100	32, 54, 80, 90	1 (0%)
1	D	178/181 (98%)	-0.54	0 100 100	35, 56, 79, 87	1 (0%)
1	G	178/181 (98%)	-0.44	1 (0%) 89 86	14, 56, 70, 80	1 (0%)
1	J	178/181 (98%)	-0.42	0 100 100	30, 61, 87, 94	1 (0%)
2	B	175/192 (91%)	-0.50	2 (1%) 80 75	23, 59, 88, 96	2 (1%)
2	E	175/192 (91%)	-0.61	0 100 100	30, 58, 87, 92	0
2	H	168/192 (87%)	-0.13	9 (5%) 25 17	35, 60, 102, 106	0
2	K	179/192 (93%)	-0.34	0 100 100	37, 63, 91, 97	0
3	C	14/15 (93%)	-0.05	0 100 100	31, 54, 59, 59	0
3	F	15/15 (100%)	-0.39	0 100 100	32, 46, 55, 56	0
3	I	13/15 (86%)	-0.14	0 100 100	41, 48, 53, 53	0
3	L	14/15 (93%)	0.10	0 100 100	46, 53, 58, 60	0
4	M	178/209 (85%)	-0.38	2 (1%) 80 75	39, 63, 89, 103	0
4	Q	187/209 (89%)	-0.45	2 (1%) 80 75	16, 60, 96, 99	0
4	S	176/209 (84%)	-0.25	4 (2%) 60 51	35, 64, 99, 103	0
4	U	195/209 (93%)	-0.49	1 (0%) 91 88	14, 59, 83, 90	0
5	P	242/249 (97%)	-0.44	0 100 100	9, 63, 82, 97	0
5	R	238/249 (95%)	-0.46	0 100 100	26, 59, 86, 91	0
5	T	226/249 (90%)	-0.22	8 (3%) 44 34	20, 63, 98, 102	0
5	V	242/249 (97%)	-0.57	0 100 100	23, 50, 68, 80	0
All	All	3149/3384 (93%)	-0.42	29 (0%) 84 80	9, 59, 90, 106	6 (0%)

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	S	190	ALA	4.7
5	T	161	SER	3.6
4	U	151	SER	3.4
2	H	142	VAL	3.3
2	H	131	TRP	3.2

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.