



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 10:56 AM UTC

PDB ID : 5C0C / pdb_00005c0c
Title : 1E6 TCR in complex with HLA-A02 carrying RQFGPDWIVA
Authors : Rizkallah, P.J.; Bulek, A.M.; Cole, D.K.; Sewell, A.K.
Deposited on : 2015-06-12
Resolution : 1.97 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 ⓘ 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

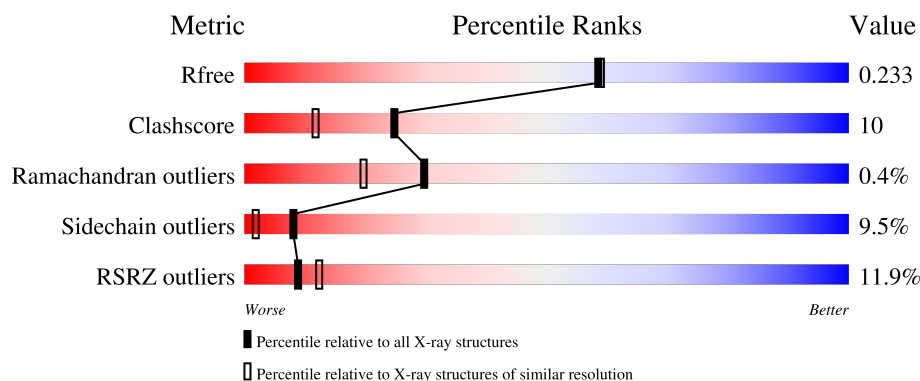
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	277	5% 72% 24% ..
1	F	277	6% 73% 23% ..
2	B	100	2% 79% 17% ..
2	G	100	4% 81% 14% 5%
3	C	10	70% 20% 10%

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Mol	Chain	Length	Quality of chain
3	H	10	 80% 20%
4	D	200	 26% 70% 22% 6%
4	I	200	 20% 74% 20% 6%
5	E	247	 24% 81% 16% ..
5	J	247	 4% 81% 18% .

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
6	EDO	A	301	-	-	X	-
9	GOL	F	308	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14235 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 I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	F	277	Total	C	N	O	S	0	0	0
			2262	1413	411	428	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01892
F	0	MET	-	initiating methionine	UNP P01892

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	G	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Marker peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			85	56	15	14			
3	H	10	Total	C	N	O	0	0	0
			85	56	15	14			

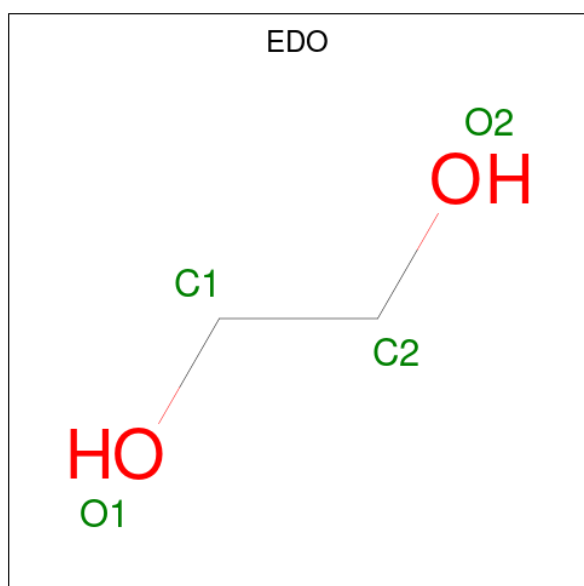
- Molecule 4 is a protein called 1E6 TCR Alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	200	Total	C	N	O	S	0	0	0
			1579	989	260	320	10			
4	I	199	Total	C	N	O	S	0	0	0
			1570	983	258	319	10			

- Molecule 5 is a protein called 1E6 TCR Beta Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	247	Total	C	N	O	S	0	0	0
			1982	1254	342	375	11			
5	J	247	Total	C	N	O	S	0	0	0
			1982	1254	342	375	11			

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

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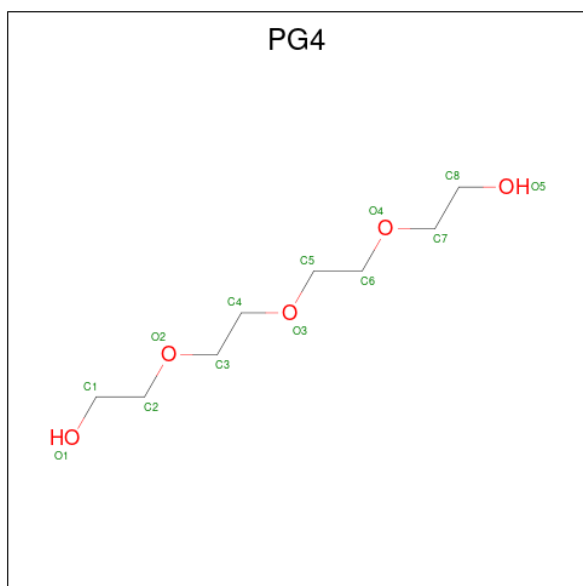
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	I	1	Total 4	C 2	O 2	0	0
6	I	1	Total 4	C 2	O 2	0	0
6	I	1	Total 4	C 2	O 2	0	0

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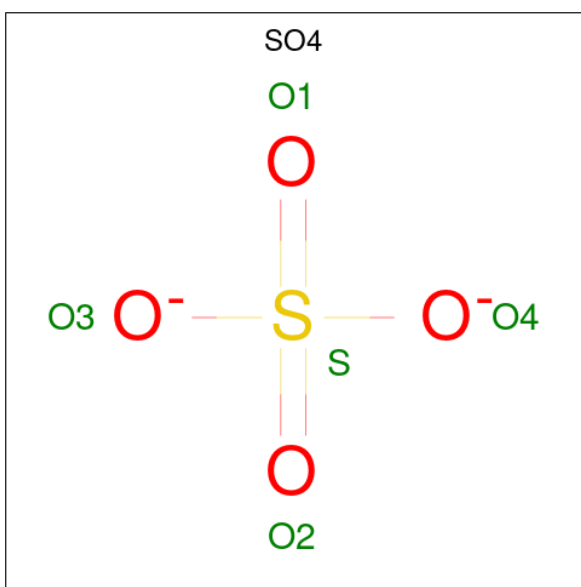
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	J	1	Total	C	O	0	0
			4	2	2		
6	J	1	Total	C	O	0	0
			4	2	2		
6	J	1	Total	C	O	0	0
			4	2	2		
6	J	1	Total	C	O	0	0
			4	2	2		
6	J	1	Total	C	O	0	0
			4	2	2		
6	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



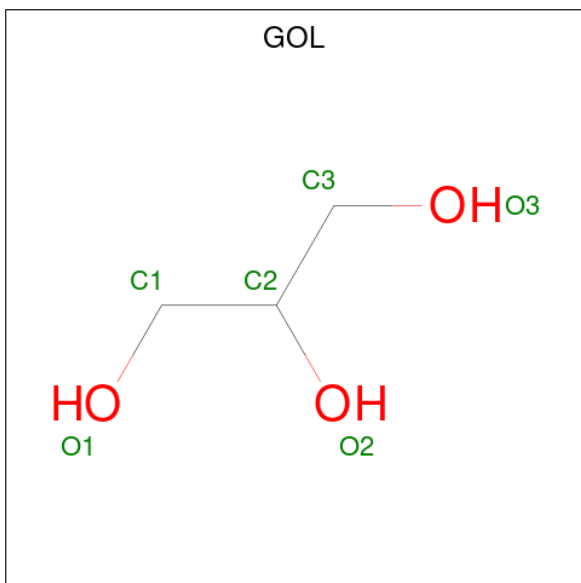
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		
7	I	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	J	1	Total	O	S	0	0
			5	4	1		
8	J	1	Total	O	S	0	0
			5	4	1		
8	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			6	3	3		
9	F	1	Total	C	O	0	0
			6	3	3		
9	F	1	Total	C	O	0	0
			6	3	3		

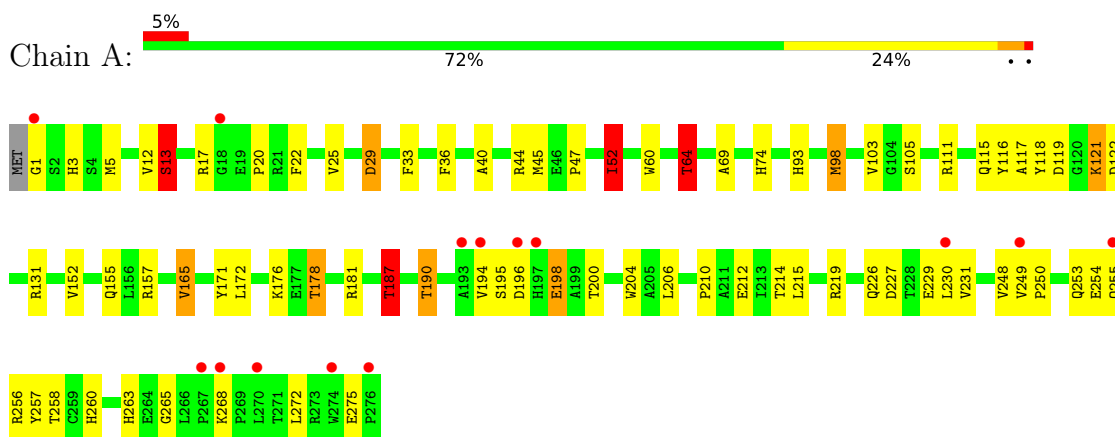
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	85	Total	O	0	0
			85	85		
10	B	45	Total	O	0	0
			45	45		
10	C	7	Total	O	0	0
			7	7		
10	D	43	Total	O	0	0
			43	43		
10	E	84	Total	O	0	0
			84	84		
10	F	113	Total	O	0	0
			113	113		
10	G	39	Total	O	0	0
			39	39		
10	H	6	Total	O	0	0
			6	6		
10	I	46	Total	O	0	0
			46	46		
10	J	101	Total	O	0	0
			101	101		

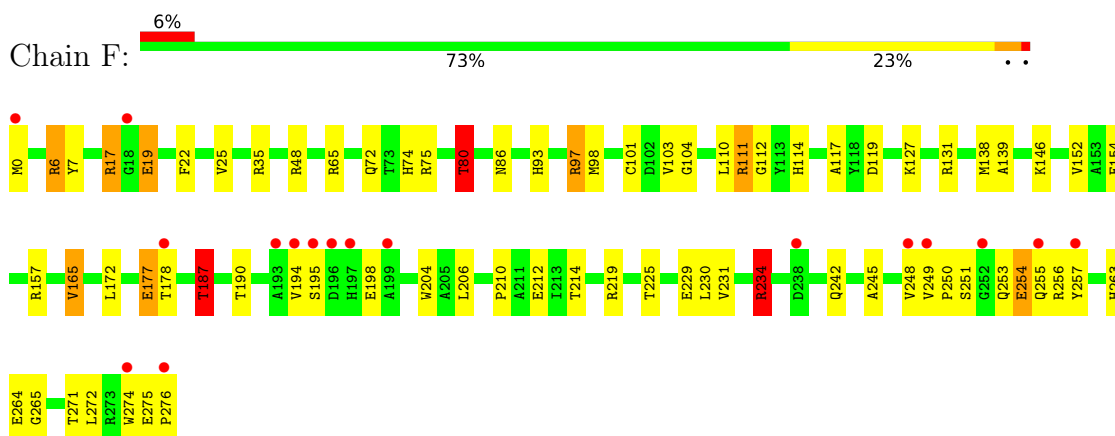
3 Residue-property plots [i](#)

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.

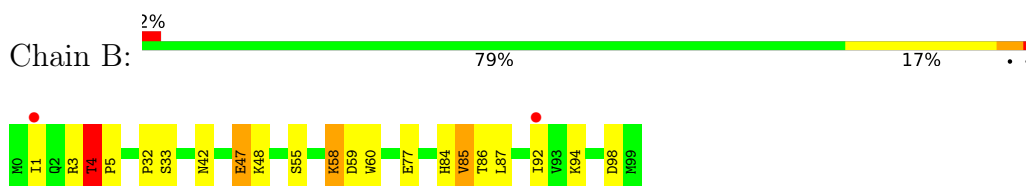
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



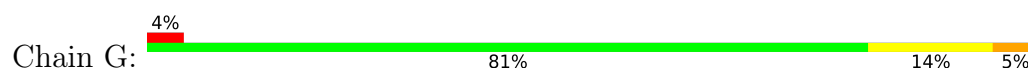
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin



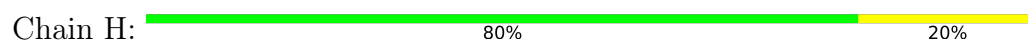
- Molecule 2: Beta-2-microglobulin



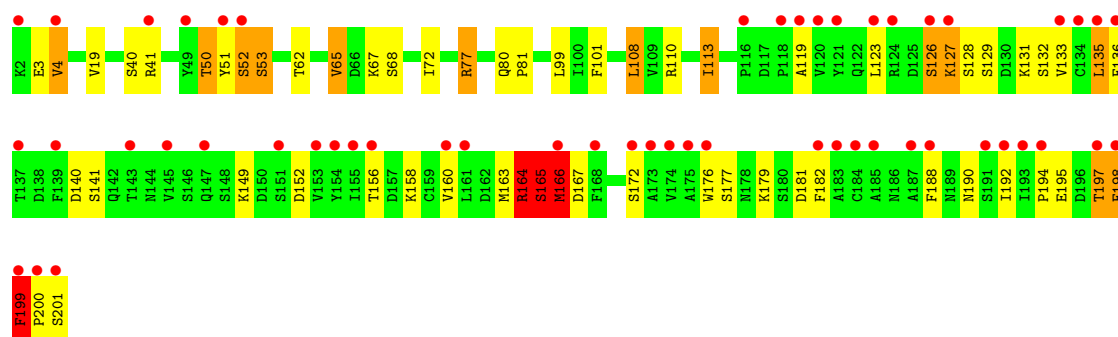
- Molecule 3: Marker peptide



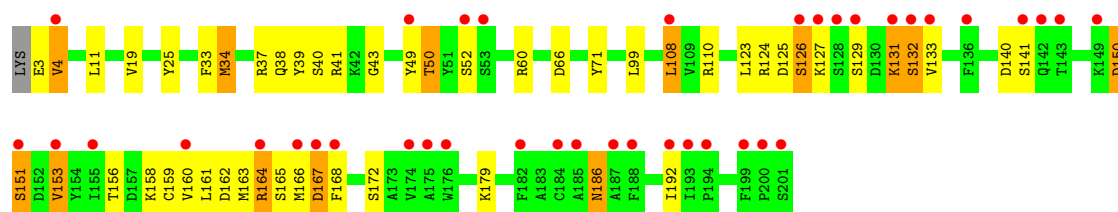
- Molecule 3: Marker peptide



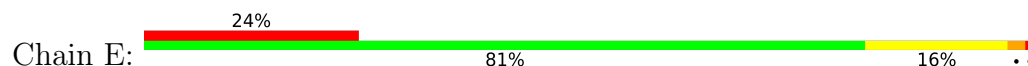
- Molecule 4: 1E6 TCR Alpha Chain

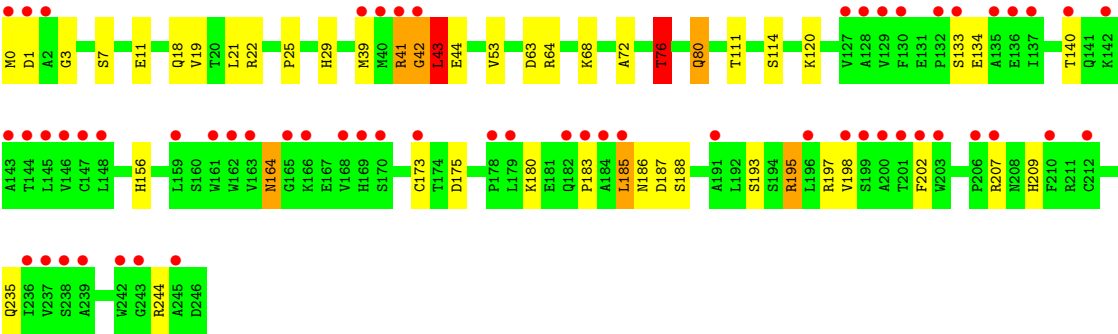


- Molecule 4: 1E6 TCR Alpha Chain

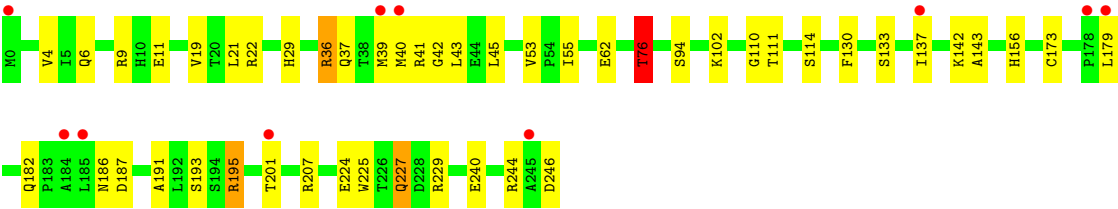
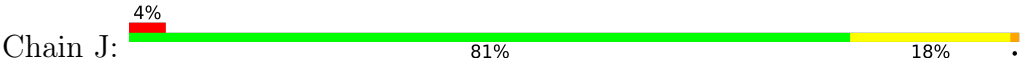


- Molecule 5: 1E6 TCR Beta Chain





● Molecule 5: 1E6 TCR Beta Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.92Å 100.37Å 122.73Å 96.90° 98.02° 96.07°	Depositor
Resolution (Å)	120.38 – 1.97 120.38 – 1.97	Depositor EDS
% Data completeness (in resolution range)	97.4 (120.38-1.97) 97.4 (120.38-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.189 , 0.227 0.196 , 0.233	Depositor DCC
R_{free} test set	7029 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14235	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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: PG4, SO4, EDO, GOL

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	1.19	5/2320 (0.2%)	1.14	11/3149 (0.3%)
1	F	1.28	9/2328 (0.4%)	1.24	17/3159 (0.5%)
2	B	1.22	2/860 (0.2%)	1.20	7/1162 (0.6%)
2	G	1.32	3/860 (0.3%)	1.33	7/1162 (0.6%)
3	C	1.51	1/88 (1.1%)	1.32	1/118 (0.8%)
3	H	1.56	0/88	1.08	0/118
4	D	1.18	2/1615 (0.1%)	1.20	5/2185 (0.2%)
4	I	1.14	0/1606	1.16	9/2174 (0.4%)
5	E	1.20	4/2037 (0.2%)	1.19	6/2769 (0.2%)
5	J	1.19	7/2037 (0.3%)	1.13	8/2769 (0.3%)
All	All	1.22	33/13839 (0.2%)	1.19	71/18765 (0.4%)

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
4	D	0	3
4	I	0	2
All	All	0	5

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	60	TRP	N-CA	14.57	1.63	1.46
1	F	80	THR	CB-CG2	-7.83	1.26	1.52
1	A	116	TYR	C-O	7.50	1.32	1.23
2	G	48	LYS	N-CA	7.41	1.55	1.46
2	G	59	ASP	C-N	-7.07	1.24	1.33

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	59	ASP	CA-C-N	-15.71	97.44	122.73
2	G	59	ASP	C-N-CA	-15.71	97.44	122.73
2	B	85	VAL	CB-CA-C	-11.58	96.87	112.04
1	F	97	ARG	NE-CZ-NH1	11.35	132.85	121.50
1	F	97	ARG	NE-CZ-NH2	-11.15	109.17	119.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	164	ARG	Peptide
4	D	166	MET	Peptide
4	D	198	PHE	Peptide
4	I	131	LYS	Peptide
4	I	151	SER	Peptide

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	2254	0	2103	51	0
1	F	2262	0	2112	58	0
2	B	837	0	803	13	0
2	G	837	0	803	10	0
3	C	85	0	81	3	0
3	H	85	0	81	3	0
4	D	1579	0	1496	47	0
4	I	1570	0	1481	36	0
5	E	1982	0	1896	35	0
5	J	1982	0	1896	29	0
6	A	12	0	17	6	0
6	B	8	0	12	0	0
6	D	12	0	18	3	0
6	E	24	0	36	3	0
6	F	28	0	42	6	0
6	G	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	12	0	18	1	0
6	J	28	0	42	2	0
7	A	10	0	13	1	0
7	I	13	0	18	3	0
8	A	5	0	0	1	0
8	J	15	0	0	2	0
9	B	6	0	8	1	0
9	F	12	0	16	9	0
10	A	85	0	0	6	0
10	B	45	0	0	0	0
10	C	7	0	0	0	0
10	D	43	0	0	4	0
10	E	84	0	0	6	0
10	F	113	0	0	13	0
10	G	39	0	0	0	0
10	H	6	0	0	0	0
10	I	46	0	0	3	0
10	J	101	0	0	4	0
All	All	14235	0	13004	261	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 10.

The worst 5 of 261 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:5:MET:HE1	1:A:171:TYR:HE2	1.22	1.03
1:F:97:ARG:HD3	1:F:114:HIS:HE1	1.30	0.97
4:D:62:THR:OG1	4:D:77:ARG:NH2	1.97	0.97
1:A:5:MET:CE	1:A:171:TYR:HE2	1.79	0.95
4:I:38:GLN:HE22	5:J:37:GLN:HE22	1.20	0.90

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	274/277 (99%)	271 (99%)	3 (1%)	0	100	100
1	F	275/277 (99%)	269 (98%)	6 (2%)	0	100	100
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	G	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	H	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
4	D	198/200 (99%)	181 (91%)	12 (6%)	5 (2%)	4	0
4	I	197/200 (98%)	181 (92%)	14 (7%)	2 (1%)	12	5
5	E	245/247 (99%)	238 (97%)	7 (3%)	0	100	100
5	J	245/247 (99%)	242 (99%)	3 (1%)	0	100	100
All	All	1646/1668 (99%)	1589 (96%)	50 (3%)	7 (0%)	30	20

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	197	THR
4	I	167	ASP
4	D	166	MET
4	D	126	SER
4	I	124	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	232/233 (100%)	207 (89%)	25 (11%)	6	1
1	F	233/233 (100%)	209 (90%)	24 (10%)	7	1
2	B	95/95 (100%)	87 (92%)	8 (8%)	10	3
2	G	95/95 (100%)	88 (93%)	7 (7%)	13	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	8/8 (100%)	7 (88%)	1 (12%)	4	1
3	H	8/8 (100%)	8 (100%)	0	100	100
4	D	181/181 (100%)	161 (89%)	20 (11%)	6	1
4	I	180/181 (99%)	158 (88%)	22 (12%)	5	1
5	E	217/217 (100%)	198 (91%)	19 (9%)	9	2
5	J	217/217 (100%)	203 (94%)	14 (6%)	15	6
All	All	1466/1468 (100%)	1326 (90%)	140 (10%)	8	2

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	I	127	LYS
4	I	153	VAL
5	J	53	VAL
4	D	164	ARG
4	D	160	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	43	GLN
1	F	224	GLN
5	J	209	HIS
1	F	54	GLN
1	F	180	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

42 ligands are modelled in this entry.

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	$\# Z > 2$
6	EDO	J	303	-	3,3,3	0.60	0	2,2,2	0.86	0
6	EDO	A	303	-	3,3,3	0.26	0	2,2,2	0.63	0
6	EDO	F	305	-	3,3,3	0.45	0	2,2,2	0.32	0
6	EDO	F	307	-	3,3,3	0.41	0	2,2,2	0.60	0
6	EDO	A	301	-	3,3,3	0.93	0	2,2,2	0.95	0
6	EDO	J	306	-	3,3,3	0.46	0	2,2,2	0.80	0
6	EDO	D	303	-	3,3,3	0.84	0	2,2,2	0.60	0
6	EDO	E	302	-	3,3,3	0.82	0	2,2,2	0.33	0
6	EDO	F	303	-	3,3,3	0.28	0	2,2,2	1.08	0
6	EDO	A	302	-	3,3,3	0.54	0	2,2,2	1.74	1 (50%)
6	EDO	D	301	-	3,3,3	0.36	0	2,2,2	0.65	0
6	EDO	J	305	-	3,3,3	0.30	0	2,2,2	0.49	0
6	EDO	B	301	-	3,3,3	0.23	0	2,2,2	0.85	0
6	EDO	E	306	-	3,3,3	0.59	0	2,2,2	0.81	0
6	EDO	J	304	-	3,3,3	0.62	0	2,2,2	0.33	0
6	EDO	G	102	-	3,3,3	1.67	0	2,2,2	1.42	0
8	SO4	J	309	-	4,4,4	0.86	0	6,6,6	0.55	0
6	EDO	G	101	-	3,3,3	0.62	0	2,2,2	0.26	0
6	EDO	E	301	-	3,3,3	0.85	0	2,2,2	0.39	0
6	EDO	F	304	-	3,3,3	0.50	0	2,2,2	0.88	0
6	EDO	E	305	-	3,3,3	0.47	0	2,2,2	0.19	0
6	EDO	I	303	-	3,3,3	0.52	0	2,2,2	0.42	0
8	SO4	J	308	-	4,4,4	0.66	0	6,6,6	0.62	0
6	EDO	F	301	-	3,3,3	0.58	0	2,2,2	0.25	0
7	PG4	A	304	-	9,9,12	0.72	0	8,8,11	0.97	0
8	SO4	J	310	-	4,4,4	1.10	0	6,6,6	0.65	0
6	EDO	E	303	-	3,3,3	0.38	0	2,2,2	0.46	0
8	SO4	A	305	-	4,4,4	0.65	0	6,6,6	0.48	0
6	EDO	J	302	-	3,3,3	0.35	0	2,2,2	0.65	0
7	PG4	I	304	-	12,12,12	0.74	0	11,11,11	1.63	3 (27%)
6	EDO	E	304	-	3,3,3	0.73	0	2,2,2	0.38	0
6	EDO	I	302	-	3,3,3	0.72	0	2,2,2	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	B	302	-	3,3,3	0.99	0	2,2,2	0.28	0
6	EDO	J	301	-	3,3,3	0.65	0	2,2,2	0.40	0
6	EDO	F	302	-	3,3,3	0.51	0	2,2,2	0.53	0
9	GOL	F	309	-	5,5,5	0.99	0	5,5,5	1.97	2 (40%)
9	GOL	F	308	-	5,5,5	0.86	0	5,5,5	1.56	1 (20%)
6	EDO	D	302	-	3,3,3	0.39	0	2,2,2	0.63	0
6	EDO	F	306	-	3,3,3	0.29	0	2,2,2	0.55	0
9	GOL	B	303	-	5,5,5	0.75	0	5,5,5	0.93	0
6	EDO	I	301	-	3,3,3	0.87	0	2,2,2	0.28	0
6	EDO	J	307	-	3,3,3	0.85	0	2,2,2	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	J	303	-	-	1/1/1/1	-
6	EDO	A	303	-	-	1/1/1/1	-
6	EDO	F	305	-	-	1/1/1/1	-
6	EDO	F	307	-	-	1/1/1/1	-
6	EDO	A	301	-	-	1/1/1/1	-
6	EDO	J	306	-	-	0/1/1/1	-
6	EDO	D	303	-	-	0/1/1/1	-
6	EDO	E	302	-	-	0/1/1/1	-
6	EDO	F	303	-	-	0/1/1/1	-
6	EDO	A	302	-	-	1/1/1/1	-
6	EDO	D	301	-	-	1/1/1/1	-
6	EDO	J	305	-	-	1/1/1/1	-
6	EDO	B	301	-	-	1/1/1/1	-
6	EDO	E	306	-	-	0/1/1/1	-
6	EDO	J	304	-	-	1/1/1/1	-
6	EDO	G	102	-	-	1/1/1/1	-
6	EDO	G	101	-	-	1/1/1/1	-
6	EDO	E	301	-	-	0/1/1/1	-
6	EDO	F	304	-	-	0/1/1/1	-
6	EDO	E	305	-	-	0/1/1/1	-
6	EDO	I	303	-	-	0/1/1/1	-
6	EDO	F	301	-	-	0/1/1/1	-
7	PG4	A	304	-	-	2/7/7/10	-
6	EDO	E	303	-	-	1/1/1/1	-
6	EDO	J	302	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PG4	I	304	-	-	7/10/10/10	-
6	EDO	E	304	-	-	1/1/1/1	-
6	EDO	I	302	-	-	1/1/1/1	-
6	EDO	B	302	-	-	1/1/1/1	-
6	EDO	J	301	-	-	0/1/1/1	-
6	EDO	F	302	-	-	0/1/1/1	-
9	GOL	F	309	-	-	3/4/4/4	-
9	GOL	F	308	-	-	2/4/4/4	-
6	EDO	D	302	-	-	0/1/1/1	-
6	EDO	F	306	-	-	0/1/1/1	-
9	GOL	B	303	-	-	0/4/4/4	-
6	EDO	I	301	-	-	1/1/1/1	-
6	EDO	J	307	-	-	1/1/1/1	-

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	304	PG4	O4-C6-C5	3.17	124.82	110.35
9	F	309	GOL	O3-C3-C2	2.99	123.82	110.38
7	I	304	PG4	C5-O3-C4	2.75	125.28	113.26
9	F	309	GOL	O2-C2-C1	-2.60	98.42	109.18
6	A	302	EDO	O1-C1-C2	-2.46	93.63	112.39

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	F	309	GOL	C1-C2-C3-O3
9	F	309	GOL	O2-C2-C3-O3
7	I	304	PG4	C6-C5-O3-C4
7	I	304	PG4	O3-C5-C6-O4
7	I	304	PG4	O2-C3-C4-O3

There are no ring outliers.

22 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	303	EDO	1	0
6	F	305	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	301	EDO	4	0
6	J	306	EDO	1	0
6	E	302	EDO	1	0
6	A	302	EDO	2	0
6	D	301	EDO	1	0
6	E	306	EDO	1	0
6	G	102	EDO	1	0
8	J	309	SO4	1	0
6	I	303	EDO	1	0
8	J	308	SO4	1	0
6	F	301	EDO	3	0
7	A	304	PG4	1	0
6	E	303	EDO	1	0
8	A	305	SO4	1	0
7	I	304	PG4	3	0
9	F	309	GOL	2	0
9	F	308	GOL	7	0
6	D	302	EDO	2	0
6	F	306	EDO	1	0
9	B	303	GOL	1	0

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	276/277 (99%)	0.44	14 (5%)	33 43	25, 49, 77, 103	0
1	F	277/277 (100%)	0.36	17 (6%)	27 35	24, 44, 90, 113	0
2	B	100/100 (100%)	0.21	2 (2%)	65 74	30, 43, 63, 75	0
2	G	100/100 (100%)	0.31	4 (4%)	42 52	28, 44, 67, 83	0
3	C	10/10 (100%)	-0.30	0	100 100	31, 32, 38, 48	0
3	H	10/10 (100%)	-0.46	0	100 100	27, 27, 32, 34	0
4	D	200/200 (100%)	1.23	53 (26%)	1 1	26, 56, 117, 147	0
4	I	199/200 (99%)	0.99	39 (19%)	3 3	30, 58, 110, 123	0
5	E	247/247 (100%)	0.96	59 (23%)	2 2	23, 51, 94, 119	0
5	J	247/247 (100%)	0.26	10 (4%)	42 52	24, 43, 81, 107	0
All	All	1666/1668 (99%)	0.61	198 (11%)	9 12	23, 47, 98, 147	0

The worst 5 of 198 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	192	ILE	5.7
4	D	145	VAL	5.7
5	E	2	ALA	5.7
4	D	119	ALA	5.4
4	D	199	PHE	5.3

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($\text{\AA}^2$)	Q<0.9
8	SO4	J	309	5/5	0.71	0.20	55,74,82,114	0
6	EDO	D	302	4/4	0.76	0.14	69,69,71,78	0
6	EDO	D	303	4/4	0.77	0.19	52,65,67,72	0
6	EDO	J	303	4/4	0.78	0.16	50,62,64,67	0
9	GOL	F	308	6/6	0.78	0.16	51,58,66,66	0
8	SO4	J	310	5/5	0.79	0.13	50,56,67,71	0
7	PG4	A	304	10/13	0.79	0.16	52,64,73,75	0
6	EDO	E	306	4/4	0.81	0.19	51,53,53,54	0
6	EDO	F	303	4/4	0.82	0.17	66,67,71,75	0
6	EDO	G	102	4/4	0.82	0.21	43,49,54,56	0
8	SO4	A	305	5/5	0.82	0.12	65,66,73,80	0
8	SO4	J	308	5/5	0.83	0.12	60,75,81,85	0
6	EDO	J	306	4/4	0.84	0.15	54,60,62,67	0
6	EDO	A	303	4/4	0.85	0.19	62,67,70,79	0
7	PG4	I	304	13/13	0.87	0.15	47,56,71,72	0
9	GOL	B	303	6/6	0.87	0.16	49,56,60,65	0
6	EDO	E	304	4/4	0.87	0.12	60,61,61,62	0
6	EDO	J	304	4/4	0.88	0.28	36,51,53,59	0
6	EDO	B	302	4/4	0.89	0.14	43,45,49,58	0
6	EDO	F	301	4/4	0.89	0.15	54,57,61,66	0
6	EDO	E	305	4/4	0.89	0.12	50,55,56,56	0
9	GOL	F	309	6/6	0.89	0.16	42,62,65,70	0
6	EDO	F	305	4/4	0.90	0.13	54,59,62,67	0
6	EDO	F	307	4/4	0.90	0.14	40,50,53,53	0
6	EDO	E	303	4/4	0.90	0.12	56,60,61,67	0
6	EDO	I	301	4/4	0.91	0.12	42,43,47,53	0
6	EDO	I	302	4/4	0.92	0.10	47,47,48,53	0
6	EDO	I	303	4/4	0.92	0.09	55,59,64,64	0
6	EDO	F	302	4/4	0.92	0.13	46,54,57,62	0
6	EDO	A	302	4/4	0.92	0.12	34,37,47,51	0
6	EDO	J	305	4/4	0.92	0.12	60,61,61,69	0
6	EDO	B	301	4/4	0.93	0.10	45,46,47,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	F	304	4/4	0.93	0.11	43,49,50,60	0
6	EDO	D	301	4/4	0.93	0.09	54,61,61,66	0
6	EDO	G	101	4/4	0.94	0.10	39,42,43,46	0
6	EDO	J	302	4/4	0.94	0.10	50,52,52,55	0
6	EDO	A	301	4/4	0.94	0.24	34,39,40,42	0
6	EDO	E	302	4/4	0.95	0.10	32,35,41,46	0
6	EDO	J	301	4/4	0.96	0.07	29,29,34,36	0
6	EDO	F	306	4/4	0.96	0.12	43,50,51,55	0
6	EDO	J	307	4/4	0.96	0.08	27,34,36,42	0
6	EDO	E	301	4/4	0.97	0.06	27,31,34,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.