wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2020 – 06:47 PM BST

PDB ID	:	5C0B
Title	:	1E6 TCR in complex with HLA-A02 carrying RQFGPDFPTI
Authors	:	Rizkallah, P.J.; Bulek, A.M.; Cole, D.K.; Sewell, A.K.
Deposited on	:	2015-06-12
Resolution	:	2.03 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:

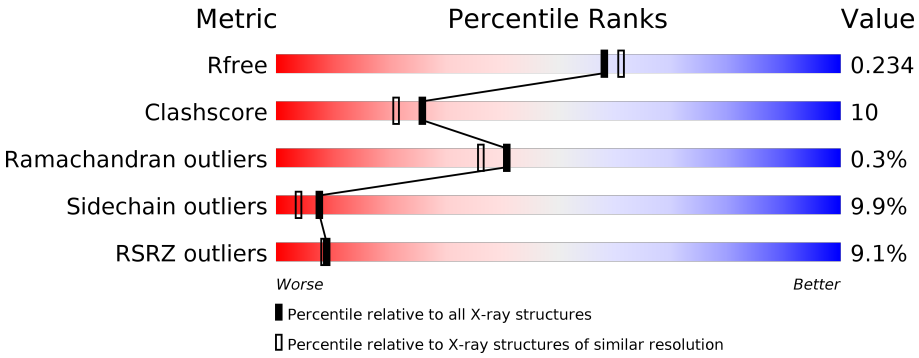
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	275	3% 74% 21% ·
1	F	275	5% 77% 19% ·
2	B	100	% 75% 22% ·
2	G	100	2% 79% 18% ·
3	C	10	90% 10%
3	H	10	90% 10%

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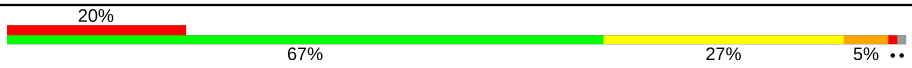
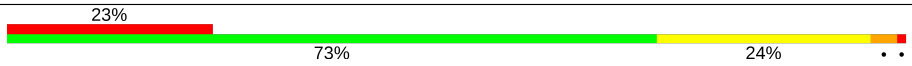
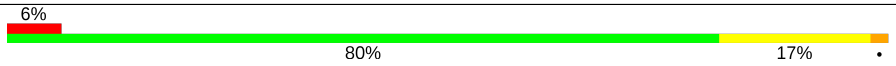
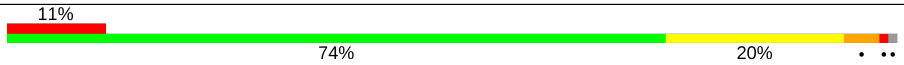
Mol	Chain	Length	Quality of chain
4	D	199	
4	I	199	
5	E	247	
5	J	247	

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	-
6	EDO	J	305	-	-	X	-
7	GOL	B	306	-	X	-	-
7	GOL	E	311	-	-	X	-
8	SO4	A	311	-	-	-	X
8	SO4	E	312	-	-	X	-
9	PG4	J	308	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14197 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	275	Total	C	N	O	S	0	1	0
			2257	1409	413	426	9			
1	F	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			

- 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	1	0
			842	536	142	160	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
			84	55	14	15			
3	H	10	Total	C	N	O	0	0	0
			84	55	14	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	197	Total	C	N	O	S	0	0	0
			1557	975	256	316	10			

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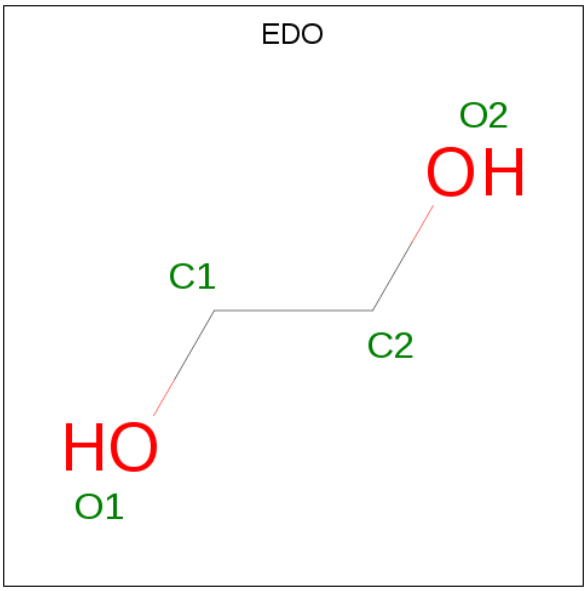
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	199	Total	C	N	O	S	0	0	0
			1570	983	258	319	10			

- 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
			1981	1254	342	374	11			
5	J	244	Total	C	N	O	S	0	0	0
			1961	1242	339	370	10			

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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	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		

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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		
6	B	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		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		

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

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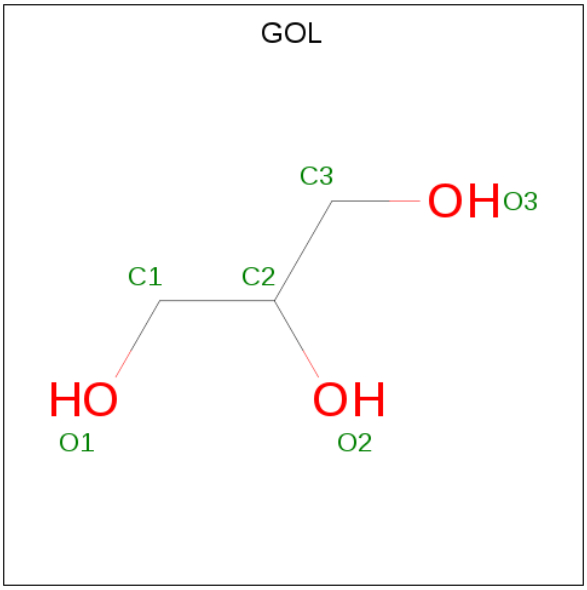
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	E	1	Total C O 6 3 3	0	0
7	F	1	Total C O 6 3 3	0	0

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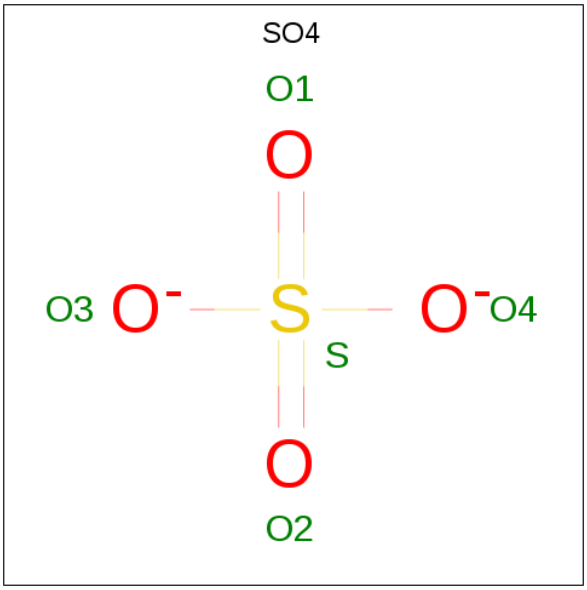
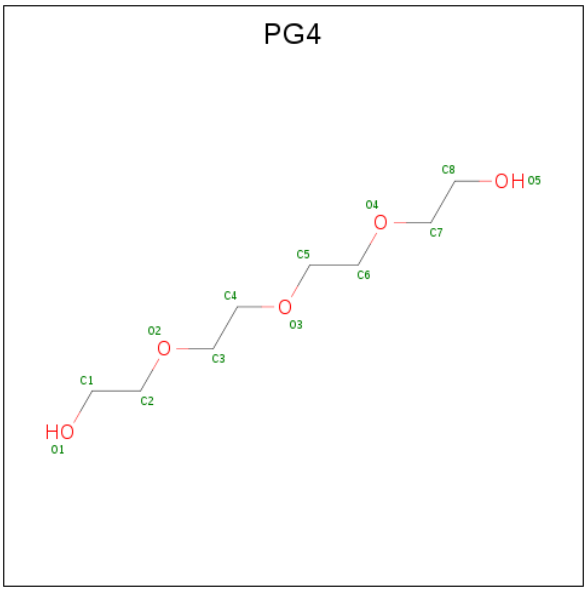
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	1	Total C O 6 3 3	0	0
7	J	1	Total C O 6 3 3	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	E	1	Total O S 5 4 1	0	0
8	E	1	Total O S 5 4 1	0	0
8	F	1	Total O S 5 4 1	0	0
8	F	1	Total O S 5 4 1	0	0
8	F	1	Total O S 5 4 1	0	0

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	J	1	Total C O 10 6 4	0	0

- Molecule 10 is water.

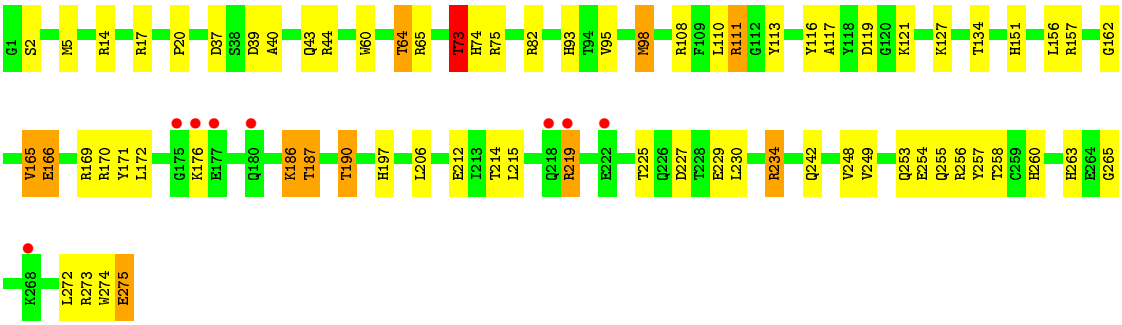
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	61	Total O 61 61	0	0
10	B	52	Total O 52 52	0	0
10	C	6	Total O 6 6	0	0
10	D	39	Total O 39 39	0	0
10	E	79	Total O 79 79	0	0
10	F	100	Total O 100 100	0	0
10	G	31	Total O 31 31	0	0
10	H	8	Total O 8 8	0	0
10	I	32	Total O 32 32	0	0
10	J	64	Total O 64 64	0	0

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.

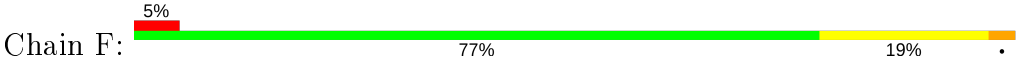
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

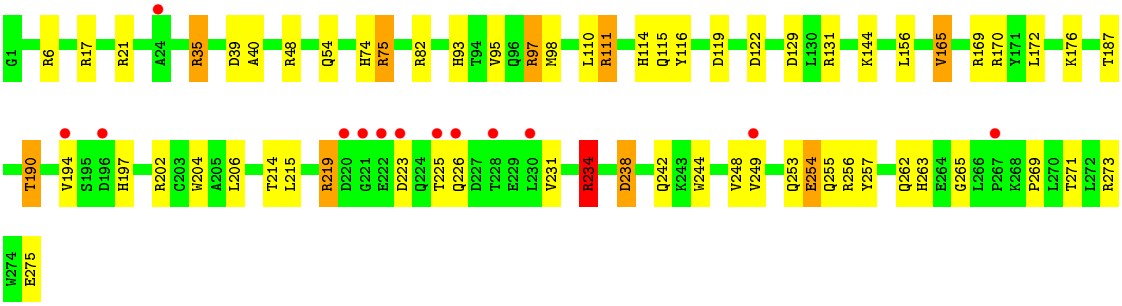
Chain A:



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

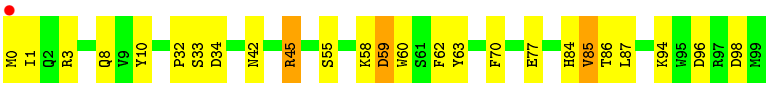
Chain F:





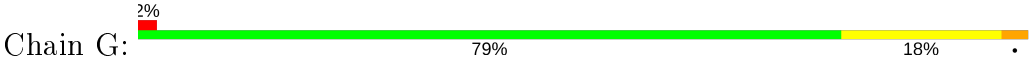
- Molecule 2: Beta-2-microglobulin

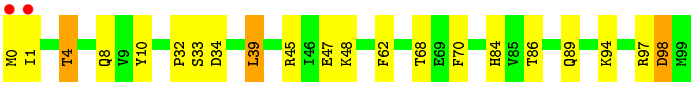
Chain B:



- Molecule 2: Beta-2-microglobulin

Chain G:





- Molecule 3: Marker peptide

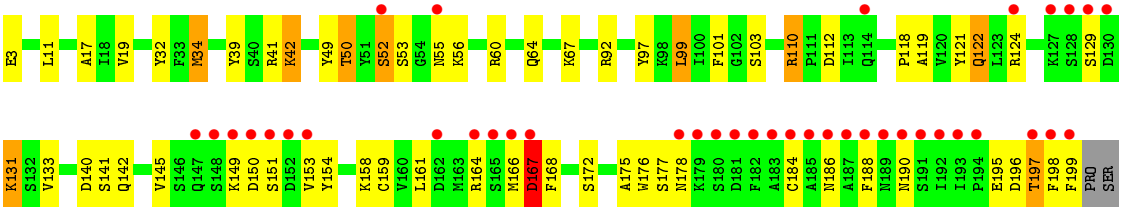
Chain C:

- Molecule 3: Marker peptide

Chain H:

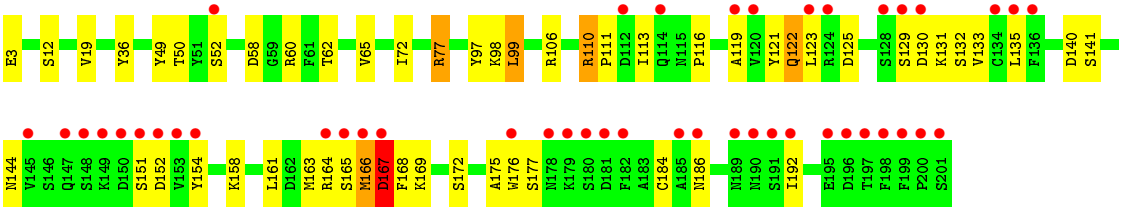
- Molecule 4: 1E6 TCR Alpha Chain

Chain D:



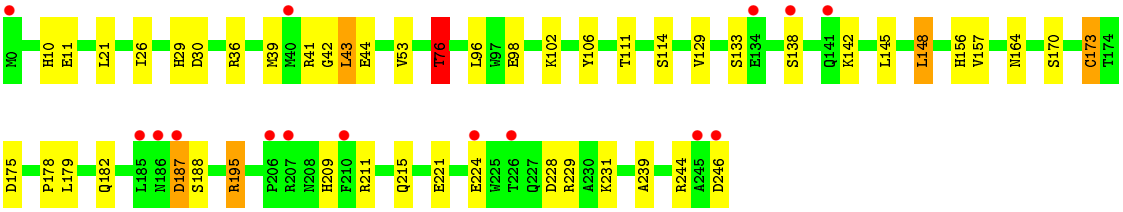
- Molecule 4: 1E6 TCR Alpha Chain

Chain I:



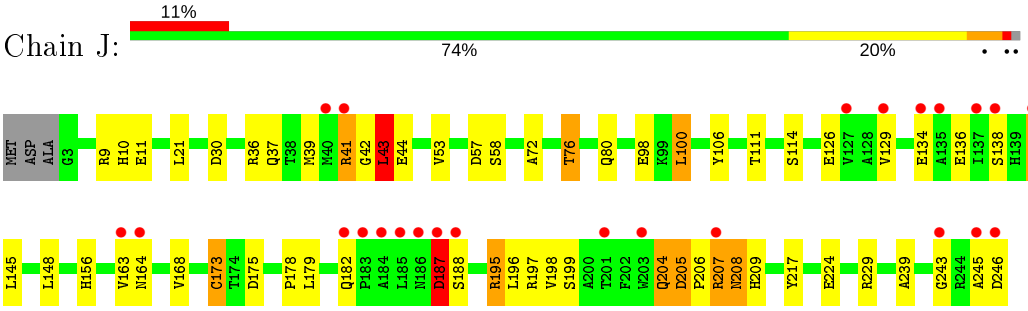
- Molecule 5: 1E6 TCR Beta Chain

Chain E:



• Molecule 5: 1E6 TCR Beta Chain

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	43.94Å 100.28Å 122.44Å 96.98° 98.05° 96.53°	Depositor
Resolution (Å)	42.76 – 2.03 42.76 – 2.03	Depositor EDS
% Data completeness (in resolution range)	97.5 (42.76-2.03) 97.6 (42.76-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.192 , 0.231 0.198 , 0.234	Depositor DCC
R_{free} test set	6446 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14197	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PG4, SO4, EDO

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	0.90	1/2322 (0.0%)	1.06	16/3151 (0.5%)
1	F	0.88	0/2311	1.10	18/3137 (0.6%)
2	B	0.86	0/865	0.99	5/1170 (0.4%)
2	G	0.87	0/860	0.97	3/1162 (0.3%)
3	C	0.87	0/87	0.92	0/116
3	H	0.95	0/87	0.96	0/116
4	D	0.90	1/1592 (0.1%)	1.02	8/2154 (0.4%)
4	I	0.93	2/1606 (0.1%)	1.05	8/2174 (0.4%)
5	E	0.91	2/2036 (0.1%)	0.99	7/2769 (0.3%)
5	J	0.93	3/2016 (0.1%)	1.02	8/2741 (0.3%)
All	All	0.90	9/13782 (0.1%)	1.03	73/18690 (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	I	0	1
5	J	0	3
All	All	0	4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	THR	CB-CG2	-9.42	1.21	1.52
4	D	97	TYR	CE1-CZ	-7.61	1.28	1.38
5	J	58	SER	CB-OG	6.26	1.50	1.42
4	I	36	TYR	CE1-CZ	-6.24	1.30	1.38
5	E	98	GLU	CD-OE2	6.05	1.32	1.25

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	234	ARG	NE-CZ-NH2	14.69	127.64	120.30
1	A	234	ARG	NE-CZ-NH1	13.74	127.17	120.30
1	A	234	ARG	NE-CZ-NH2	-12.55	114.02	120.30
1	F	234	ARG	NE-CZ-NH1	-10.94	114.83	120.30
5	E	229	ARG	NE-CZ-NH2	-10.54	115.03	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	I	129	SER	Peptide
5	J	187	ASP	Peptide
5	J	204	GLN	Peptide
5	J	205	ASP	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	2257	0	2108	54	0
1	F	2246	0	2096	37	0
2	B	842	0	807	18	0
2	G	837	0	803	13	1
3	C	84	0	80	1	0
3	H	84	0	80	1	0
4	D	1557	0	1469	41	0
4	I	1570	0	1481	36	0
5	E	1981	0	1896	44	1
5	J	1961	0	1875	56	0
6	A	36	0	54	8	0
6	B	20	0	30	3	0
6	D	24	0	36	8	0
6	E	40	0	60	3	0
6	F	28	0	42	7	0
6	G	16	0	24	1	0
6	H	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	28	0	42	5	0
6	J	24	0	36	5	0
7	A	6	0	8	0	0
7	B	6	0	7	1	0
7	E	6	0	8	11	0
7	F	6	0	8	2	0
7	I	6	0	8	1	0
7	J	6	0	8	0	0
8	A	10	0	0	0	0
8	B	5	0	0	0	0
8	E	10	0	0	3	0
8	F	15	0	0	0	0
9	J	10	0	13	13	0
10	A	61	0	0	4	0
10	B	52	0	0	1	1
10	C	6	0	0	0	0
10	D	39	0	0	1	0
10	E	79	0	0	5	0
10	F	100	0	0	2	0
10	G	31	0	0	0	0
10	H	8	0	0	0	0
10	I	32	0	0	2	0
10	J	64	0	0	6	1
All	All	14197	0	13085	281	2

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 281 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	1.11	1.11
5:J:42:GLY:CA	9:J:308:PG4:H12	1.80	1.10
5:J:164:ASN:HB2	5:J:208:ASN:HD21	1.20	1.06
5:E:42:GLY:HA2	7:E:311:GOL:H2	1.37	1.04
1:A:5:MET:HE1	1:A:171:TYR:CE2	1.92	1.03

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	Interatomic distance (Å)	Clash overlap (Å)
10:B:402:HOH:O	10:J:402:HOH:O[1_556]	1.48	0.72
5:E:211:ARG:NH1	2:G:89:GLN:OE1[1_556]	2.17	0.03

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	274/275 (100%)	272 (99%)	2 (1%)	0	100	100
1	F	273/275 (99%)	268 (98%)	5 (2%)	0	100	100
2	B	99/100 (99%)	96 (97%)	3 (3%)	0	100	100
2	G	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
3	H	8/10 (80%)	8 (100%)	0	0	100	100
4	D	195/199 (98%)	184 (94%)	8 (4%)	3 (2%)	10	4
4	I	197/199 (99%)	184 (93%)	12 (6%)	1 (0%)	29	22
5	E	245/247 (99%)	242 (99%)	3 (1%)	0	100	100
5	J	242/247 (98%)	235 (97%)	6 (2%)	1 (0%)	34	28
All	All	1639/1662 (99%)	1592 (97%)	42 (3%)	5 (0%)	41	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	167	ASP
4	I	167	ASP
5	J	206	PRO
4	D	197	THR
4	D	52	SER

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	232/231 (100%)	206 (89%)	26 (11%)	6 3
1	F	231/231 (100%)	204 (88%)	27 (12%)	5 2
2	B	96/95 (101%)	90 (94%)	6 (6%)	18 12
2	G	95/95 (100%)	87 (92%)	8 (8%)	11 6
3	C	9/9 (100%)	9 (100%)	0	100 100
3	H	9/9 (100%)	9 (100%)	0	100 100
4	D	178/180 (99%)	156 (88%)	22 (12%)	4 2
4	I	180/180 (100%)	165 (92%)	15 (8%)	11 6
5	E	217/217 (100%)	200 (92%)	17 (8%)	12 7
5	J	215/217 (99%)	191 (89%)	24 (11%)	6 3
All	All	1462/1464 (100%)	1317 (90%)	145 (10%)	8 4

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	179	LEU
1	F	194	VAL
5	J	173	CYS
5	E	187	ASP
1	F	74	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	51	ASN
1	F	93	HIS
5	J	156	HIS
5	E	186	ASN
1	F	114	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

70 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	305	-	3,3,3	0.52	0	2,2,2	1.53	1 (50%)
8	SO4	A	312	-	4,4,4	0.40	0	6,6,6	0.67	0
6	EDO	E	310	-	3,3,3	0.65	0	2,2,2	0.12	0
6	EDO	F	301	-	3,3,3	0.36	0	2,2,2	0.82	0
6	EDO	E	307	-	3,3,3	0.82	0	2,2,2	0.14	0
6	EDO	A	308	-	3,3,3	0.52	0	2,2,2	0.41	0
7	GOL	E	311	-	5,5,5	0.82	0	5,5,5	0.99	0
6	EDO	I	305	-	3,3,3	0.58	0	2,2,2	0.38	0
6	EDO	G	101	-	3,3,3	0.47	0	2,2,2	0.64	0
6	EDO	G	104	-	3,3,3	0.61	0	2,2,2	0.22	0
6	EDO	E	308	-	3,3,3	0.28	0	2,2,2	0.80	0
6	EDO	I	301	-	3,3,3	0.93	0	2,2,2	0.57	0
6	EDO	A	302	-	3,3,3	0.42	0	2,2,2	0.64	0
6	EDO	B	303	-	3,3,3	0.75	0	2,2,2	0.47	0
8	SO4	F	309	-	4,4,4	1.01	0	6,6,6	1.28	1 (16%)
7	GOL	I	308	-	5,5,5	0.94	0	5,5,5	1.93	2 (40%)
6	EDO	E	305	-	3,3,3	0.28	0	2,2,2	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	F	302	-	3,3,3	0.18	0	2,2,2	0.38	0
6	EDO	I	303	-	3,3,3	0.37	0	2,2,2	0.49	0
6	EDO	D	304	-	3,3,3	0.84	0	2,2,2	0.97	0
6	EDO	J	301	-	3,3,3	0.54	0	2,2,2	0.65	0
6	EDO	D	305	-	3,3,3	0.51	0	2,2,2	0.31	0
6	EDO	B	305	-	3,3,3	0.51	0	2,2,2	0.40	0
6	EDO	A	303	-	3,3,3	0.45	0	2,2,2	0.83	0
6	EDO	I	302	-	3,3,3	0.48	0	2,2,2	0.82	0
7	GOL	J	307	-	5,5,5	0.54	0	5,5,5	0.80	0
6	EDO	E	309	-	3,3,3	0.49	0	2,2,2	0.39	0
8	SO4	F	311	-	4,4,4	0.44	0	6,6,6	0.47	0
8	SO4	E	313	-	4,4,4	0.67	0	6,6,6	0.55	0
6	EDO	F	306	-	3,3,3	0.32	0	2,2,2	0.42	0
6	EDO	J	304	-	3,3,3	0.73	0	2,2,2	0.25	0
6	EDO	I	304	-	3,3,3	0.58	0	2,2,2	0.24	0
6	EDO	D	303	-	3,3,3	1.02	0	2,2,2	0.88	0
6	EDO	A	304	-	3,3,3	0.66	0	2,2,2	0.46	0
6	EDO	A	301	-	3,3,3	0.26	0	2,2,2	0.73	0
8	SO4	A	311	-	4,4,4	0.90	0	6,6,6	0.86	0
6	EDO	B	304	-	3,3,3	0.44	0	2,2,2	0.68	0
6	EDO	F	304	-	3,3,3	0.50	0	2,2,2	0.31	0
6	EDO	D	301	-	3,3,3	0.51	0	2,2,2	0.56	0
6	EDO	G	103	-	3,3,3	0.41	0	2,2,2	1.07	0
6	EDO	J	306	-	3,3,3	0.70	0	2,2,2	0.10	0
6	EDO	J	302	-	3,3,3	0.30	0	2,2,2	0.63	0
6	EDO	F	305	-	3,3,3	0.44	0	2,2,2	0.68	0
6	EDO	D	302	-	3,3,3	0.86	0	2,2,2	0.65	0
6	EDO	J	303	-	3,3,3	0.48	0	2,2,2	0.35	0
6	EDO	E	302	-	3,3,3	0.46	0	2,2,2	0.21	0
7	GOL	B	306	-	5,5,5	1.14	1 (20%)	5,5,5	1.30	1 (20%)
6	EDO	A	309	-	3,3,3	0.60	0	2,2,2	0.20	0
6	EDO	E	303	-	3,3,3	0.60	0	2,2,2	0.17	0
6	EDO	E	301	-	3,3,3	0.48	0	2,2,2	0.54	0
8	SO4	B	307	-	4,4,4	0.61	0	6,6,6	0.40	0
7	GOL	A	310	-	5,5,5	0.85	0	5,5,5	0.77	0
6	EDO	H	101	-	3,3,3	0.63	0	2,2,2	0.52	0
8	SO4	E	312	-	4,4,4	0.36	0	6,6,6	0.65	0
9	PG4	J	308	-	9,9,12	0.64	0	8,8,11	1.19	1 (12%)
7	GOL	F	308	-	5,5,5	0.97	0	5,5,5	1.94	2 (40%)
8	SO4	F	310	-	4,4,4	0.56	0	6,6,6	0.64	0
6	EDO	A	307	-	3,3,3	0.51	0	2,2,2	0.50	0
6	EDO	G	102	-	3,3,3	0.41	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	I	306	-	3,3,3	0.60	0	2,2,2	0.46	0
6	EDO	E	304	-	3,3,3	0.53	0	2,2,2	0.82	0
6	EDO	B	301	-	3,3,3	0.47	0	2,2,2	0.58	0
6	EDO	A	306	-	3,3,3	0.63	0	2,2,2	0.31	0
6	EDO	D	306	-	3,3,3	0.70	0	2,2,2	0.29	0
6	EDO	F	303	-	3,3,3	0.84	0	2,2,2	0.23	0
6	EDO	E	306	-	3,3,3	0.54	0	2,2,2	0.27	0
6	EDO	F	307	-	3,3,3	0.52	0	2,2,2	0.56	0
6	EDO	A	305	-	3,3,3	0.57	0	2,2,2	0.87	0
6	EDO	B	302	-	3,3,3	0.64	0	2,2,2	0.67	0
6	EDO	I	307	-	3,3,3	0.92	0	2,2,2	0.06	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	305	-	-	1/1/1/1	-
6	EDO	E	310	-	-	0/1/1/1	-
6	EDO	F	301	-	-	1/1/1/1	-
6	EDO	E	307	-	-	0/1/1/1	-
6	EDO	A	308	-	-	1/1/1/1	-
7	GOL	E	311	-	-	0/4/4/4	-
6	EDO	I	305	-	-	1/1/1/1	-
6	EDO	G	101	-	-	1/1/1/1	-
6	EDO	G	104	-	-	1/1/1/1	-
6	EDO	E	308	-	-	1/1/1/1	-
6	EDO	I	301	-	-	0/1/1/1	-
6	EDO	A	302	-	-	1/1/1/1	-
6	EDO	B	303	-	-	1/1/1/1	-
7	GOL	I	308	-	-	2/4/4/4	-
6	EDO	E	305	-	-	0/1/1/1	-
6	EDO	F	302	-	-	0/1/1/1	-
6	EDO	I	303	-	-	0/1/1/1	-
6	EDO	D	304	-	-	0/1/1/1	-
6	EDO	J	301	-	-	1/1/1/1	-
6	EDO	D	305	-	-	1/1/1/1	-
6	EDO	B	305	-	-	0/1/1/1	-
6	EDO	A	303	-	-	1/1/1/1	-
6	EDO	I	302	-	-	1/1/1/1	-
7	GOL	J	307	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	E	309	-	-	1/1/1/1	-
6	EDO	I	304	-	-	1/1/1/1	-
6	EDO	F	306	-	-	0/1/1/1	-
6	EDO	J	304	-	-	0/1/1/1	-
6	EDO	D	303	-	-	1/1/1/1	-
6	EDO	A	304	-	-	0/1/1/1	-
6	EDO	A	301	-	-	1/1/1/1	-
6	EDO	B	304	-	-	1/1/1/1	-
6	EDO	F	304	-	-	0/1/1/1	-
6	EDO	D	301	-	-	1/1/1/1	-
6	EDO	G	103	-	-	1/1/1/1	-
6	EDO	J	306	-	-	1/1/1/1	-
6	EDO	J	302	-	-	1/1/1/1	-
6	EDO	F	305	-	-	1/1/1/1	-
6	EDO	D	302	-	-	1/1/1/1	-
6	EDO	J	303	-	-	1/1/1/1	-
6	EDO	E	302	-	-	1/1/1/1	-
7	GOL	B	306	-	-	4/4/4/4	-
6	EDO	A	309	-	-	1/1/1/1	-
6	EDO	E	301	-	-	0/1/1/1	-
7	GOL	A	310	-	-	4/4/4/4	-
6	EDO	H	101	-	-	1/1/1/1	-
6	EDO	E	303	-	-	0/1/1/1	-
9	PG4	J	308	-	-	7/7/7/10	-
7	GOL	F	308	-	-	3/4/4/4	-
6	EDO	A	307	-	-	1/1/1/1	-
6	EDO	G	102	-	-	1/1/1/1	-
6	EDO	I	306	-	-	1/1/1/1	-
6	EDO	E	304	-	-	0/1/1/1	-
6	EDO	B	301	-	-	1/1/1/1	-
6	EDO	A	306	-	-	1/1/1/1	-
6	EDO	D	306	-	-	0/1/1/1	-
6	EDO	F	303	-	-	1/1/1/1	-
6	EDO	E	306	-	-	0/1/1/1	-
6	EDO	F	307	-	-	1/1/1/1	-
6	EDO	A	305	-	-	1/1/1/1	-
6	EDO	B	302	-	-	1/1/1/1	-
6	EDO	I	307	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	306	GOL	O2-C2	-2.33	1.36	1.43

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	308	GOL	O2-C2-C1	-3.11	95.44	109.12
9	J	308	PG4	O2-C2-C1	-2.89	97.37	110.07
7	F	308	GOL	O2-C2-C1	-2.69	97.29	109.12
7	F	308	GOL	O3-C3-C2	2.67	122.99	110.20
8	F	309	SO4	O4-S-O1	2.60	122.86	109.31

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	308	GOL	O1-C1-C2-C3
7	B	306	GOL	O1-C1-C2-O2
7	B	306	GOL	O1-C1-C2-C3
7	A	310	GOL	C1-C2-C3-O3
7	F	308	GOL	C1-C2-C3-O3

There are no ring outliers.

28 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	305	EDO	4	0
6	E	310	EDO	1	0
6	F	301	EDO	2	0
6	A	308	EDO	1	0
7	E	311	GOL	11	0
6	I	305	EDO	1	0
7	I	308	GOL	1	0
6	D	304	EDO	3	0
6	D	305	EDO	2	0
6	A	303	EDO	1	0
6	I	302	EDO	3	0
6	F	306	EDO	2	0
6	D	303	EDO	2	0
6	A	301	EDO	6	0
6	B	304	EDO	1	0
6	F	304	EDO	1	0
6	D	301	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	306	EDO	1	0
6	F	305	EDO	2	0
7	B	306	GOL	1	0
8	E	312	SO4	3	0
9	J	308	PG4	13	0
7	F	308	GOL	2	0
6	G	102	EDO	1	0
6	I	306	EDO	1	0
6	E	304	EDO	2	0
6	F	307	EDO	2	0
6	B	302	EDO	2	0

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, 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	275/275 (100%)	0.22	8 (2%) 51 51	25, 50, 82, 95	0
1	F	275/275 (100%)	0.16	13 (4%) 31 31	22, 45, 86, 108	0
2	B	100/100 (100%)	-0.10	1 (1%) 82 82	30, 42, 62, 78	0
2	G	100/100 (100%)	-0.09	2 (2%) 65 64	28, 41, 69, 83	0
3	C	10/10 (100%)	0.23	0 100 100	32, 35, 42, 43	0
3	H	10/10 (100%)	0.53	0 100 100	25, 28, 32, 35	0
4	D	197/199 (98%)	0.96	40 (20%) 1 0	29, 59, 113, 128	0
4	I	199/199 (100%)	1.10	45 (22%) 0 0	26, 56, 113, 131	0
5	E	247/247 (100%)	0.17	15 (6%) 21 20	22, 44, 87, 118	0
5	J	244/247 (98%)	0.46	26 (10%) 6 5	22, 49, 100, 124	0
All	All	1657/1662 (99%)	0.39	150 (9%) 9 8	22, 47, 99, 131	0

The worst 5 of 150 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	201	SER	10.8
4	I	151	SER	10.5
4	D	199	PHE	8.0
4	D	166	MET	7.6
4	I	130	ASP	7.3

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 (i)

There are no monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
8	SO4	A	311	5/5	0.52	0.45	65,77,112,119	0
7	GOL	A	310	6/6	0.57	0.28	58,69,70,75	0
6	EDO	I	304	4/4	0.65	0.21	74,84,88,92	0
8	SO4	F	309	5/5	0.68	0.35	51,56,94,101	0
6	EDO	B	305	4/4	0.69	0.36	55,60,65,69	0
6	EDO	E	307	4/4	0.70	0.16	59,63,69,70	0
6	EDO	A	306	4/4	0.71	0.35	63,67,67,69	0
7	GOL	B	306	6/6	0.74	0.24	50,52,54,62	0
6	EDO	A	308	4/4	0.75	0.23	71,73,73,78	0
6	EDO	G	104	4/4	0.75	0.25	58,60,64,67	0
8	SO4	E	312	5/5	0.75	0.37	83,84,92,112	0
6	EDO	J	306	4/4	0.75	0.24	53,61,62,66	0
7	GOL	F	308	6/6	0.76	0.31	44,58,67,70	0
7	GOL	I	308	6/6	0.76	0.19	46,47,49,62	0
6	EDO	I	307	4/4	0.76	0.22	48,49,56,58	0
6	EDO	J	301	4/4	0.77	0.24	62,71,73,74	0
7	GOL	E	311	6/6	0.78	0.23	48,54,63,66	0
6	EDO	A	304	4/4	0.79	0.17	52,56,56,62	0
6	EDO	J	303	4/4	0.80	0.16	70,73,81,83	0
6	EDO	E	303	4/4	0.80	0.25	56,72,75,79	0
6	EDO	A	309	4/4	0.80	0.14	67,67,71,71	0
6	EDO	I	305	4/4	0.80	0.25	60,62,69,71	0
6	EDO	B	302	4/4	0.83	0.18	47,53,54,62	0
6	EDO	I	302	4/4	0.83	0.32	53,58,60,68	0
8	SO4	A	312	5/5	0.84	0.36	73,94,103,106	0
6	EDO	A	305	4/4	0.84	0.26	57,73,85,86	0
6	EDO	B	304	4/4	0.85	0.12	53,55,56,63	0
6	EDO	D	304	4/4	0.85	0.15	47,57,63,64	0
6	EDO	B	303	4/4	0.85	0.16	44,52,54,65	0
6	EDO	I	303	4/4	0.85	0.15	69,71,77,82	0
9	PG4	J	308	10/13	0.85	0.18	45,65,83,84	0
6	EDO	A	302	4/4	0.86	0.19	61,62,64,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	D	303	4/4	0.86	0.15	44,48,49,49	0
7	GOL	J	307	6/6	0.87	0.37	54,57,61,63	0
6	EDO	J	302	4/4	0.87	0.15	63,65,74,78	0
6	EDO	E	306	4/4	0.87	0.14	58,62,71,71	0
6	EDO	E	304	4/4	0.88	0.23	35,48,50,58	0
6	EDO	E	310	4/4	0.88	0.27	33,35,43,46	0
8	SO4	F	311	5/5	0.88	0.41	72,97,102,105	0
6	EDO	D	302	4/4	0.89	0.13	39,41,41,46	0
6	EDO	D	306	4/4	0.89	0.15	42,48,52,54	0
6	EDO	F	303	4/4	0.89	0.12	51,60,65,67	0
6	EDO	J	304	4/4	0.89	0.16	47,47,48,51	0
6	EDO	H	101	4/4	0.89	0.21	37,44,46,47	0
8	SO4	F	310	5/5	0.89	0.28	65,82,86,90	0
6	EDO	I	306	4/4	0.89	0.21	44,46,49,52	0
6	EDO	E	309	4/4	0.90	0.16	60,62,64,69	0
6	EDO	E	308	4/4	0.90	0.12	57,58,59,59	0
6	EDO	F	307	4/4	0.90	0.29	59,59,63,65	0
6	EDO	G	103	4/4	0.91	0.26	53,65,72,75	0
6	EDO	D	305	4/4	0.91	0.23	52,59,61,65	0
6	EDO	A	307	4/4	0.91	0.15	49,53,58,66	0
8	SO4	B	307	5/5	0.92	0.35	63,73,83,86	0
6	EDO	G	101	4/4	0.92	0.15	41,42,45,46	0
6	EDO	G	102	4/4	0.92	0.18	44,51,56,59	0
6	EDO	F	305	4/4	0.92	0.24	55,59,62,63	0
6	EDO	A	303	4/4	0.93	0.23	49,50,53,56	0
8	SO4	E	313	5/5	0.93	0.16	54,65,73,84	0
6	EDO	E	305	4/4	0.93	0.09	64,65,68,70	0
6	EDO	E	302	4/4	0.93	0.13	54,54,56,57	0
6	EDO	F	301	4/4	0.93	0.17	49,52,56,65	0
6	EDO	D	301	4/4	0.94	0.11	49,51,51,55	0
6	EDO	F	304	4/4	0.95	0.18	39,41,46,57	0
6	EDO	B	301	4/4	0.95	0.12	40,42,44,50	0
6	EDO	I	301	4/4	0.96	0.16	29,31,37,42	0
6	EDO	E	301	4/4	0.97	0.20	28,34,39,42	0
6	EDO	A	301	4/4	0.97	0.14	38,38,41,42	0
6	EDO	F	306	4/4	0.97	0.22	30,41,42,46	0
6	EDO	J	305	4/4	0.97	0.22	41,42,42,45	0
6	EDO	F	302	4/4	0.98	0.17	44,46,47,48	0

6.5 Other polymers (i)

There are no such residues in this entry.