



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2016 – 06:44 AM EDT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027674  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027674

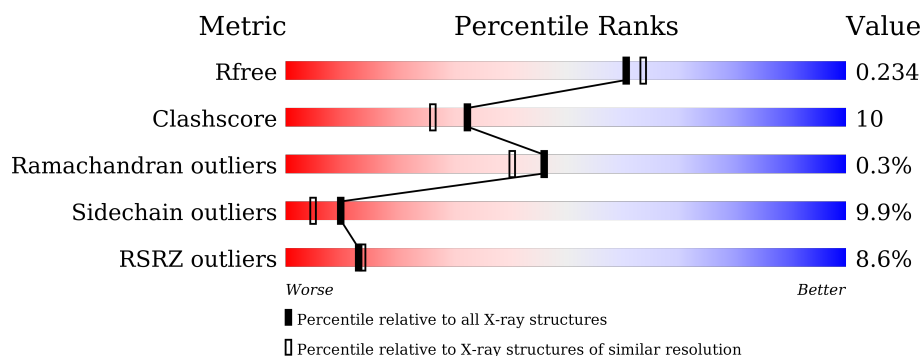
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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))
$R_{free}$	91344	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	275	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>.</div> </div> </div>
1	F	275	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>.</div> </div> </div>
2	B	100	<div> <div></div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>
2	G	100	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>.</div> </div> </div>
3	C	10	<div> <div></div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
3	H	10	<div> <div></div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>

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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	A	303	-	-	-	X
6	EDO	A	305	-	-	-	X
6	EDO	A	306	-	-	-	X
6	EDO	B	302	-	-	-	X
6	EDO	D	305	-	-	-	X
6	EDO	D	306	-	-	-	X
6	EDO	E	303	-	-	-	X
6	EDO	E	304	-	-	-	X
6	EDO	E	310	-	-	-	X
6	EDO	F	301	-	-	-	X
6	EDO	F	304	-	-	-	X
6	EDO	F	306	-	-	-	X
6	EDO	F	307	-	-	-	X
6	EDO	G	104	-	-	-	X
6	EDO	H	101	-	-	-	X
6	EDO	J	301	-	-	-	X
6	EDO	J	305	-	-	X	X
7	GOL	A	310	-	-	-	X
7	GOL	B	306	-	-	-	X
7	GOL	E	311	-	-	X	X
7	GOL	F	308	-	-	-	X
7	GOL	I	308	-	-	-	X
7	GOL	J	307	-	-	-	X
8	SO4	A	311	-	-	-	X
8	SO4	B	307	-	-	-	X
8	SO4	E	312	-	-	X	X
8	SO4	E	313	-	-	-	X
8	SO4	F	309	-	-	-	X
9	PG4	J	308	-	-	X	-

## 2 Entry composition [i](#)

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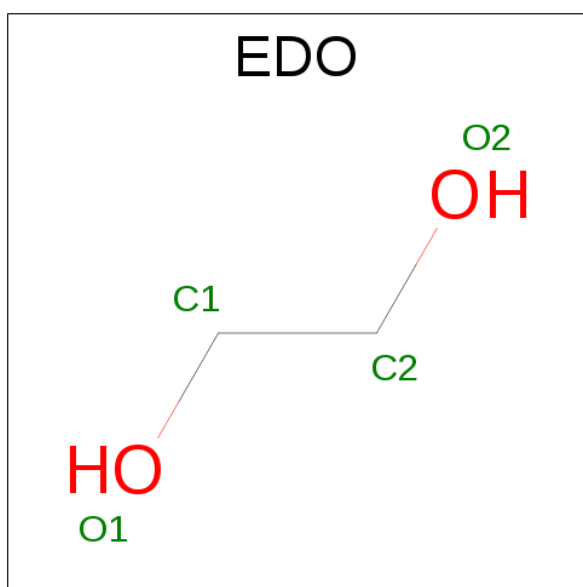
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	199	Total	C	N	O	S	0	0	0
			1570	983	258	319	10			

- 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<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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		

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

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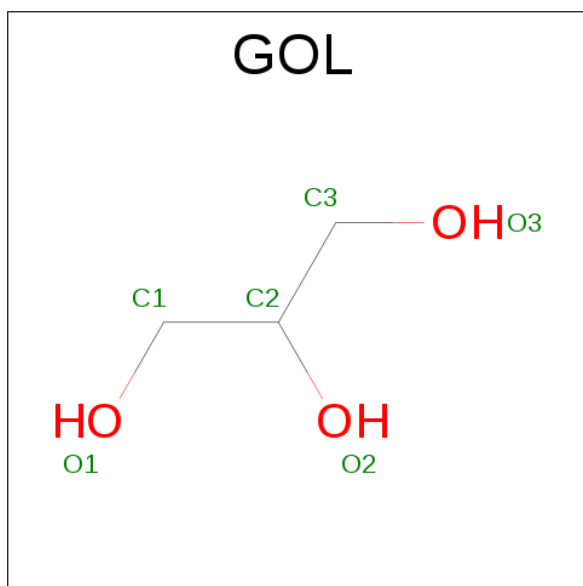
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	H	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
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	I	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 GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

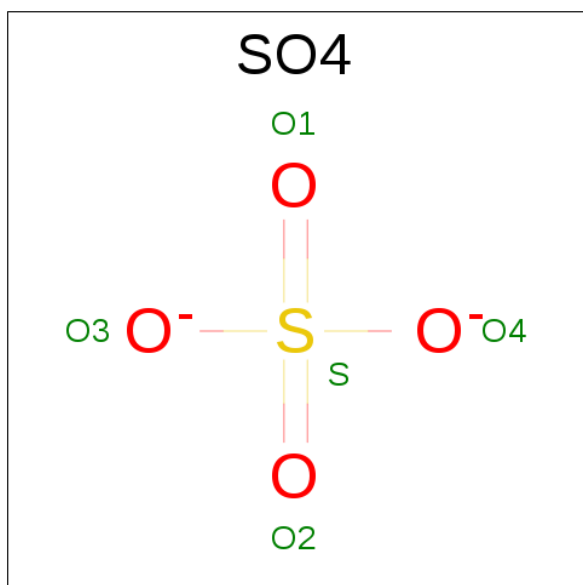
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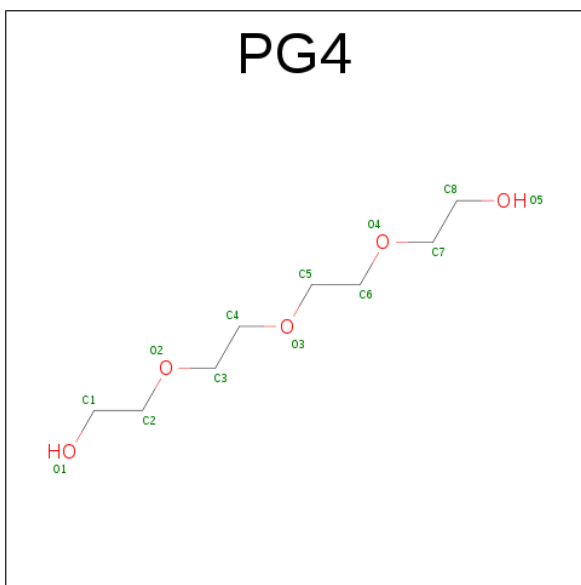
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	I	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



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

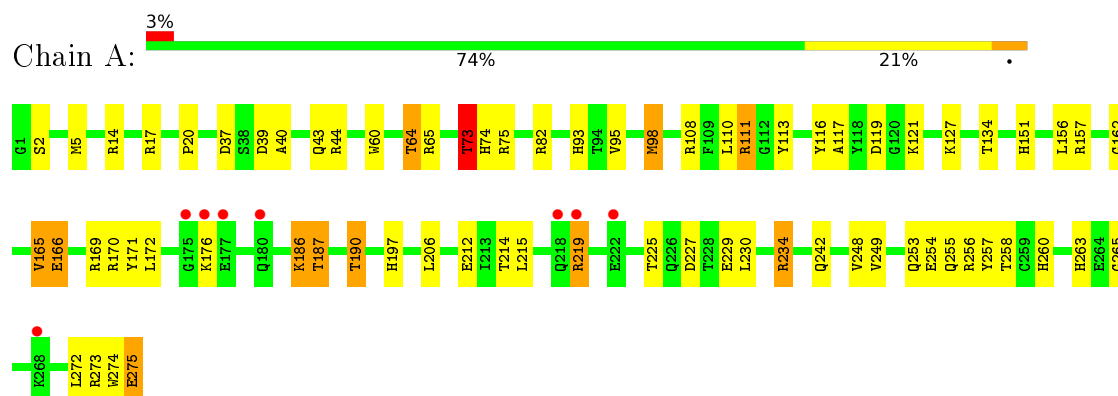
- Molecule 10 is water.

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

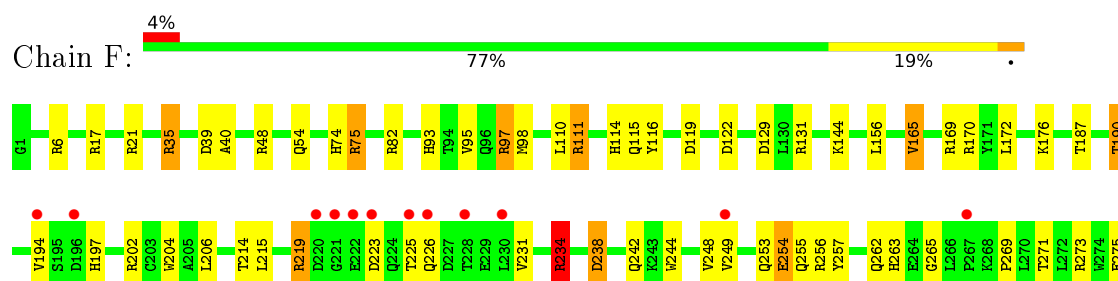
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

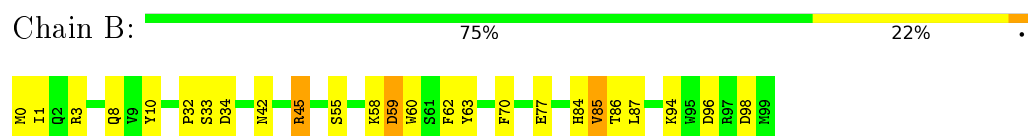
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



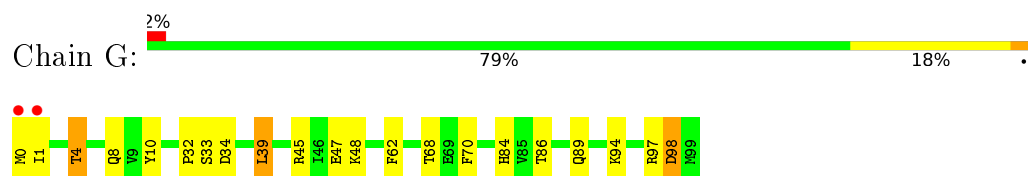
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain




- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin




- Molecule 3: Marker peptide

Chain C:  90% 10%



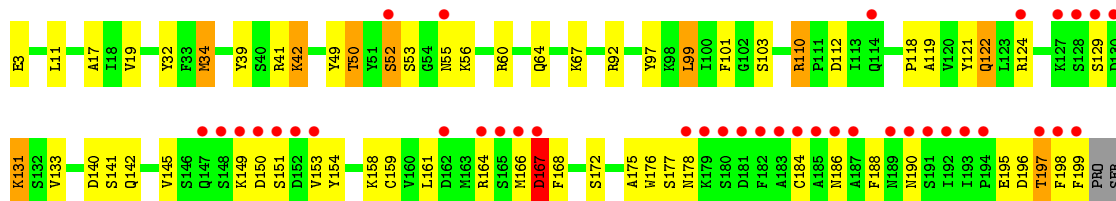
- Molecule 3: Marker peptide

Chain H:  90% 10%



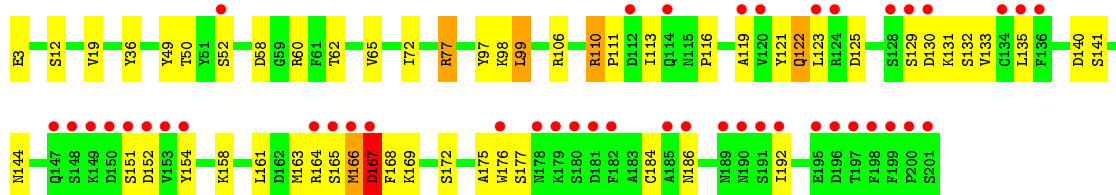
- Molecule 4: 1E6 TCR Alpha Chain

Chain D:  20% 67% 27% 5% ..




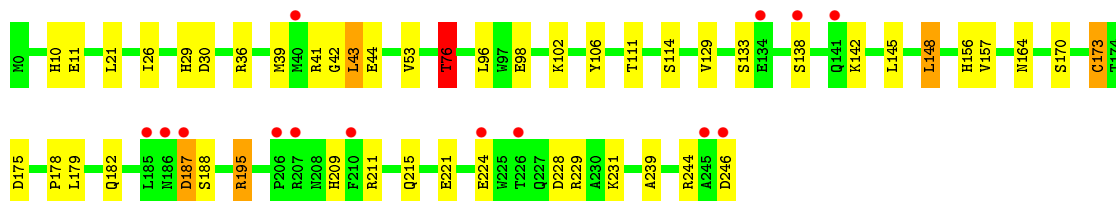
- Molecule 4: 1E6 TCR Alpha Chain

Chain I:  22% 73% 24% ..



- Molecule 5: 1E6 TCR Beta Chain

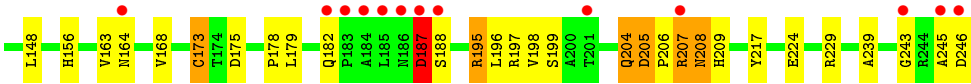
Chain E:  6% 80% 17% ..



- Molecule 5: 1E6 TCR Beta Chain

Chain J:  9% 74% 20% ..





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 93.1 (42.76-2.03)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.03Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.192 , 0.231 0.198 , 0.234	Depositor DCC
$R_{free}$ test set	6446 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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

All (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
4	I	97	TYR	CE1-CZ	-5.39	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	228	ASP	CB-CG	5.34	1.62	1.51
5	J	98	GLU	CD-OE2	5.20	1.31	1.25
5	J	106	TYR	CE1-CZ	-5.14	1.31	1.38

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
5	E	36	ARG	NE-CZ-NH2	-10.26	115.17	120.30
5	J	229	ARG	NE-CZ-NH2	-10.17	115.22	120.30
5	J	36	ARG	NE-CZ-NH2	-9.81	115.40	120.30
5	J	229	ARG	NE-CZ-NH1	9.43	125.02	120.30
4	D	60	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	F	111	ARG	NE-CZ-NH2	-8.58	116.01	120.30
4	D	34	MET	CG-SD-CE	-8.45	86.68	100.20
4	D	60	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	F	35	ARG	NE-CZ-NH2	-8.11	116.24	120.30
5	E	36	ARG	NE-CZ-NH1	8.03	124.31	120.30
5	E	229	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	A	234	ARG	CB-CG-CD	7.92	132.19	111.60
2	G	45	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	F	97	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	F	234	ARG	CB-CG-CD	7.59	131.34	111.60
1	F	75	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	F	111	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	F	170	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	65	ARG	NE-CZ-NH2	7.31	123.95	120.30
4	I	77	ARG	NE-CZ-NH2	-7.26	116.67	120.30
4	I	60	ARG	NE-CZ-NH2	-6.89	116.86	120.30
4	I	60	ARG	NE-CZ-NH1	6.82	123.71	120.30
2	G	45	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	F	35	ARG	NE-CZ-NH1	6.77	123.68	120.30
2	B	59	ASP	CB-CG-OD1	6.67	124.31	118.30
5	J	43	LEU	CB-CG-CD2	6.62	122.26	111.00
2	B	45	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	F	238	ASP	CB-CA-C	-6.55	97.29	110.40
2	B	85	VAL	CB-CA-C	-6.45	99.15	111.40
2	B	45	ARG	NE-CZ-NH2	-6.32	117.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	43	LEU	CB-CG-CD2	6.21	121.56	111.00
4	D	34	MET	CA-CB-CG	6.20	123.84	113.30
1	F	75	ARG	NE-CZ-NH1	-6.18	117.21	120.30
4	I	99	LEU	CB-CG-CD1	6.17	121.50	111.00
4	I	77	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	A	170	ARG	NE-CZ-NH2	-6.11	117.24	120.30
4	D	99	LEU	CB-CG-CD1	6.04	121.27	111.00
1	A	75	ARG	NE-CZ-NH1	6.01	123.31	120.30
5	J	100	LEU	CB-CG-CD2	5.96	121.14	111.00
5	J	208	ASN	N-CA-C	5.94	127.03	111.00
1	A	111	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	F	17	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	F	110	LEU	CA-CB-CG	5.91	128.90	115.30
1	F	82	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	F	122	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	98	MET	CG-SD-CE	-5.75	91.00	100.20
1	A	65	ARG	NE-CZ-NH1	-5.75	117.43	120.30
4	I	77	ARG	CG-CD-NE	-5.74	99.74	111.80
1	F	39	ASP	CB-CG-OD1	5.68	123.42	118.30
1	F	97	ARG	NE-CZ-NH1	-5.65	117.48	120.30
1	A	108	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	82	ARG	NE-CZ-NH2	5.57	123.08	120.30
5	J	36	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	157	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	A	111	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	A	39	ASP	CB-CG-OD1	5.48	123.23	118.30
4	I	58	ASP	CB-CG-OD1	5.45	123.20	118.30
4	I	110	ARG	NE-CZ-NH1	5.45	123.02	120.30
2	G	47	GLU	C-N-CA	-5.42	108.15	121.70
4	D	112	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	73	THR	N-CA-CB	-5.28	100.26	110.30
1	A	110	LEU	CA-CB-CG	5.20	127.26	115.30
5	J	57	ASP	CB-CG-OD1	5.17	122.95	118.30
5	E	76	THR	N-CA-CB	-5.15	100.52	110.30
2	B	96	ASP	CB-CG-OD2	-5.12	113.69	118.30
4	D	110	ARG	NE-CZ-NH1	5.07	122.83	120.30
4	D	92	ARG	NE-CZ-NH1	5.04	122.82	120.30
5	E	30	ASP	CB-CG-OD1	5.04	122.84	118.30

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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:A:5:MET:CE	1:A:171:TYR:HE2	1.75	0.99
5:E:42:GLY:HA2	7:E:311:GOL:C2	1.92	0.99
1:F:40:ALA:HB3	6:F:306:EDO:H22	1.45	0.96
4:D:101:PHE:CD1	5:E:43:LEU:HD12	2.10	0.87
1:F:6:ARG:HD2	7:F:308:GOL:H31	1.56	0.86
5:J:42:GLY:HA2	9:J:308:PG4:H12	1.57	0.86
1:A:5:MET:CE	1:A:171:TYR:CE2	2.55	0.85
1:A:187:THR:CG2	1:A:272:LEU:HD21	2.07	0.84
4:D:101:PHE:CE1	5:E:43:LEU:HD12	2.13	0.83
4:I:133:VAL:HG12	4:I:176:TRP:HB3	1.61	0.83
4:I:62:THR:OG1	4:I:77:ARG:NH2	2.12	0.82
4:D:52:SER:O	4:D:67:LYS:HD2	1.80	0.82
5:J:42:GLY:HA3	9:J:308:PG4:H12	1.60	0.81
6:D:301:EDO:O2	10:D:401:HOH:O	1.98	0.81
5:E:114:SER:OG	5:E:156:HIS:HE1	1.64	0.80
1:A:190:THR:HG21	2:B:98:ASP:OD2	1.82	0.80
5:E:42:GLY:CA	7:E:311:GOL:H2	2.11	0.80
5:J:114:SER:OG	5:J:156:HIS:HE1	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:THR:HG22	10:A:446:HOH:O	1.83	0.79
1:A:60:TRP:O	1:A:64:THR:HG23	1.81	0.78
4:D:133:VAL:HG12	4:D:176:TRP:HB3	1.66	0.78
2:B:45:ARG:HD3	10:B:402:HOH:O	1.83	0.78
4:I:12:SER:O	7:I:308:GOL:O2	2.02	0.77
5:J:164:ASN:HB2	5:J:208:ASN:ND2	1.98	0.75
5:E:221:GLU:HG2	5:E:231:LYS:NZ	2.02	0.75
5:J:198:VAL:HG22	5:J:199:SER:H	1.52	0.73
4:D:50:THR:HG23	4:D:56:LYS:HG3	1.70	0.73
5:E:221:GLU:HA	5:E:231:LYS:HZ3	1.54	0.73
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.72	0.72
1:A:14:ARG:HD3	6:B:302:EDO:H21	1.72	0.71
5:E:43:LEU:C	5:E:43:LEU:HD13	2.11	0.71
4:D:42:LYS:N	6:D:304:EDO:H21	2.05	0.71
1:F:93:HIS:HD2	1:F:119:ASP:OD2	1.74	0.70
1:F:54:GLN:HB3	6:F:307:EDO:H12	1.72	0.70
1:F:40:ALA:HB3	6:F:306:EDO:C2	2.19	0.70
5:J:198:VAL:CG2	5:J:199:SER:H	2.04	0.69
4:D:145:VAL:HA	4:D:190:ASN:HD22	1.59	0.68
1:F:202:ARG:NH2	2:G:98:ASP:O	2.26	0.68
1:A:227:ASP:HB3	1:A:248:VAL:HG12	1.77	0.67
4:I:113:ILE:HD11	4:I:140:ASP:HA	1.77	0.67
1:A:127:LYS:HE3	1:A:134:THR:HG22	1.76	0.66
5:E:42:GLY:HA3	7:E:311:GOL:H31	1.76	0.66
1:A:187:THR:HG23	1:A:272:LEU:HD21	1.77	0.66
5:E:43:LEU:HD13	5:E:44:GLU:N	2.11	0.66
2:B:3:ARG:NH1	2:B:59:ASP:OD2	2.28	0.66
1:A:40:ALA:HB3	6:A:301:EDO:C1	2.27	0.65
4:D:41:ARG:C	6:D:304:EDO:H21	2.17	0.65
5:J:164:ASN:CB	5:J:208:ASN:HD21	2.03	0.65
1:A:73:THR:CG2	10:A:446:HOH:O	2.42	0.65
1:A:40:ALA:HB3	6:A:301:EDO:H11	1.77	0.65
4:I:131:LYS:NZ	4:I:177:SER:O	2.26	0.65
5:J:205:ASP:HB3	5:J:243:GLY:HA3	1.78	0.65
4:D:166:MET:O	4:D:168:PHE:N	2.30	0.64
5:J:76:THR:CG2	10:J:453:HOH:O	2.45	0.64
5:E:42:GLY:CA	7:E:311:GOL:C2	2.72	0.63
1:A:95:VAL:HG11	1:A:116:TYR:OH	1.98	0.63
5:J:208:ASN:HB2	10:J:461:HOH:O	1.98	0.63
5:J:76:THR:HG23	10:J:453:HOH:O	1.98	0.63
4:I:77:ARG:HD2	6:I:302:EDO:H11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:244:ARG:NH2	5:E:246:ASP:O	2.32	0.62
1:A:234:ARG:HD2	1:A:242:GLN:HB2	1.81	0.62
1:A:187:THR:HG22	1:A:272:LEU:HD21	1.77	0.62
5:J:43:LEU:N	9:J:308:PG4:H12	2.14	0.62
5:E:76:THR:CG2	10:E:471:HOH:O	2.47	0.62
5:J:43:LEU:H	9:J:308:PG4:C1	2.13	0.61
1:A:151:HIS:HB2	8:E:312:SO4:O1	1.99	0.61
1:A:17[B]:ARG:N	1:A:17[B]:ARG:HD3	2.16	0.61
4:D:129:SER:O	4:D:131:LYS:O	2.19	0.61
1:A:121:LYS:HE3	2:B:1:ILE:HG13	1.83	0.61
5:J:208:ASN:CB	10:J:461:HOH:O	2.49	0.60
5:J:43:LEU:H	9:J:308:PG4:H12	1.66	0.60
1:A:258:THR:HG23	1:A:260:HIS:NE2	2.16	0.60
1:F:234:ARG:HD3	1:F:242:GLN:OE1	2.01	0.60
4:I:166:MET:O	4:I:168:PHE:N	2.34	0.60
1:A:121:LYS:HE3	2:B:1:ILE:CG1	2.31	0.60
4:I:122:GLN:HG3	4:I:184:CYS:SG	2.42	0.60
5:J:129:VAL:HG23	5:J:239:ALA:HB3	1.83	0.60
4:D:118:PRO:HG2	4:D:195:GLU:HB2	1.84	0.60
1:F:263:HIS:CD2	1:F:265:GLY:H	2.19	0.59
4:D:101:PHE:CE1	5:E:43:LEU:CD1	2.85	0.59
1:F:93:HIS:HE1	10:F:413:HOH:O	1.85	0.59
4:D:17:ALA:HB1	6:D:303:EDO:H11	1.84	0.59
1:A:17[B]:ARG:CD	1:A:17[B]:ARG:N	2.66	0.58
2:B:34:ASP:OD2	6:B:302:EDO:H11	2.03	0.58
5:J:136:GLU:OE1	5:J:140:THR:OG1	2.12	0.58
5:J:42:GLY:HA3	9:J:308:PG4:C1	2.33	0.58
5:E:129:VAL:HG23	5:E:239:ALA:HB3	1.86	0.58
2:B:84:HIS:HD2	2:B:86:THR:OG1	1.87	0.58
5:E:42:GLY:HA2	7:E:311:GOL:C1	2.34	0.58
5:E:26:ILE:HD11	6:E:304:EDO:H11	1.86	0.58
4:D:122:GLN:HG3	4:D:184:CYS:SG	2.43	0.57
5:E:42:GLY:CA	7:E:311:GOL:C3	2.83	0.57
1:A:187:THR:HG21	1:A:272:LEU:HD11	1.87	0.57
1:A:263:HIS:CD2	1:A:265:GLY:H	2.22	0.56
4:D:176:TRP:CD2	5:E:148:LEU:HD21	2.40	0.56
5:E:42:GLY:CA	7:E:311:GOL:H31	2.35	0.56
1:F:234:ARG:HD2	1:F:242:GLN:HB2	1.87	0.56
5:J:126:GLU:HA	5:J:126:GLU:OE1	2.05	0.56
4:D:55:ASN:ND2	4:D:64:GLN:HE21	2.03	0.56
5:E:187:ASP:HB2	10:E:476:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:THR:HG23	10:E:471:HOH:O	2.06	0.56
4:I:163:MET:CE	5:J:198:VAL:HA	2.35	0.56
4:D:154:TYR:O	4:D:175:ALA:HA	2.06	0.56
1:F:54:GLN:HB3	6:F:307:EDO:C1	2.36	0.56
4:I:154:TYR:O	4:I:175:ALA:HA	2.06	0.56
1:A:37:ASP:O	6:A:301:EDO:H11	2.06	0.55
5:J:198:VAL:HG22	5:J:199:SER:N	2.21	0.55
1:F:95:VAL:HG11	1:F:116:TYR:OH	2.07	0.55
5:J:207:ARG:CG	5:J:207:ARG:O	2.55	0.54
1:F:249:VAL:CG2	1:F:257:TYR:CE1	2.91	0.54
2:G:32:PRO:O	2:G:84:HIS:HE1	1.90	0.54
4:I:158:LYS:HA	4:I:172:SER:O	2.08	0.54
5:J:42:GLY:C	9:J:308:PG4:H12	2.28	0.54
1:F:97:ARG:HE	1:F:114:HIS:HE1	1.56	0.53
5:E:221:GLU:HG2	5:E:231:LYS:HZ2	1.70	0.53
4:D:150:ASP:N	4:D:150:ASP:OD1	2.42	0.53
5:J:21:LEU:HD22	5:J:111:THR:HG21	1.91	0.53
1:A:234:ARG:HH21	2:B:8:GLN:NE2	2.07	0.53
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.43	0.53
4:D:158:LYS:HA	4:D:172:SER:O	2.09	0.52
4:D:17:ALA:CB	6:D:303:EDO:H11	2.39	0.52
2:B:32:PRO:O	2:B:84:HIS:HE1	1.92	0.52
4:D:110:ARG:HB3	4:D:141:SER:HB3	1.91	0.52
5:J:30:ASP:HA	6:J:305:EDO:H21	1.91	0.52
5:J:37:GLN:HE21	9:J:308:PG4:H21	1.74	0.52
1:A:186:LYS:N	1:A:186:LYS:HD3	2.25	0.52
4:I:163:MET:HE2	5:J:198:VAL:HA	1.92	0.52
2:G:84:HIS:HD2	2:G:86:THR:OG1	1.92	0.52
5:E:221:GLU:HG2	5:E:231:LYS:HZ3	1.74	0.52
1:F:253:GLN:OE1	1:F:256:ARG:NH1	2.43	0.52
4:I:110:ARG:HB3	4:I:141:SER:HB3	1.92	0.51
4:I:163:MET:HE3	5:J:197:ARG:HB3	1.90	0.51
1:A:95:VAL:CG1	1:A:116:TYR:CZ	2.94	0.51
1:A:249:VAL:CG2	1:A:257:TYR:CE1	2.93	0.51
1:A:253:GLN:OE1	1:A:256:ARG:NH1	2.44	0.51
4:D:161:LEU:HB3	5:E:173:CYS:HB3	1.91	0.51
1:F:6:ARG:HD2	7:F:308:GOL:C3	2.33	0.51
4:I:119:ALA:HB1	4:I:121:TYR:CZ	2.45	0.51
5:E:96:LEU:HB3	6:E:310:EDO:H11	1.91	0.51
1:F:234:ARG:HG3	2:G:10:TYR:CZ	2.45	0.51
1:F:249:VAL:HG23	1:F:257:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:55:ASN:HD21	4:D:64:GLN:NE2	2.10	0.50
2:G:97:ARG:O	2:G:98:ASP:OD2	2.29	0.50
4:I:113:ILE:CD1	4:I:140:ASP:HA	2.42	0.50
1:A:95:VAL:HG13	1:A:116:TYR:CZ	2.46	0.50
4:D:196:ASP:CG	4:D:197:THR:H	2.15	0.50
1:F:234:ARG:CD	1:F:242:GLN:HB2	2.41	0.50
4:I:77:ARG:HD2	6:I:302:EDO:C1	2.41	0.50
1:F:97:ARG:HE	1:F:114:HIS:CE1	2.29	0.50
4:I:123:LEU:HD11	4:I:135:LEU:HB2	1.93	0.50
5:E:106:TYR:HB3	6:E:304:EDO:H12	1.94	0.50
1:F:202:ARG:HD2	1:F:244:TRP:CD2	2.47	0.50
1:F:254:GLU:H	1:F:254:GLU:CD	2.12	0.50
1:A:74:HIS:HD2	10:A:446:HOH:O	1.95	0.50
5:E:21:LEU:HD22	5:E:111:THR:HG21	1.94	0.50
4:I:98:LYS:NZ	10:I:402:HOH:O	2.38	0.49
5:J:163:VAL:HG22	5:J:168:VAL:CG1	2.43	0.49
5:J:198:VAL:CG2	5:J:199:SER:N	2.74	0.49
5:E:114:SER:OG	5:E:156:HIS:CE1	2.55	0.49
5:J:42:GLY:HA2	9:J:308:PG4:C1	2.37	0.49
1:A:249:VAL:HG23	1:A:257:TYR:CE1	2.47	0.49
6:F:301:EDO:O1	6:F:305:EDO:H22	2.12	0.49
5:J:37:GLN:HE21	9:J:308:PG4:C2	2.26	0.49
1:F:95:VAL:HG13	1:F:116:TYR:CZ	2.48	0.49
5:E:43:LEU:CD1	5:E:43:LEU:C	2.81	0.49
4:I:113:ILE:O	4:I:113:ILE:HG13	2.13	0.49
2:G:4:THR:HG22	2:G:86:THR:HB	1.94	0.48
4:I:161:LEU:HB3	5:J:173:CYS:HB3	1.94	0.48
1:F:262:GLN:HG2	1:F:269:PRO:HB3	1.94	0.48
1:F:98:MET:CE	1:F:115:GLN:HE21	2.27	0.48
2:G:34:ASP:OD1	6:G:102:EDO:O1	2.30	0.48
4:D:42:LYS:O	6:D:304:EDO:H22	2.14	0.48
4:I:50:THR:HG21	4:I:65:VAL:HG13	1.96	0.48
1:A:162:GLY:O	1:A:166:GLU:HG2	2.15	0.47
5:J:175:ASP:OD1	5:J:195:ARG:NH1	2.47	0.47
2:B:55[B]:SER:HB2	2:B:63:TYR:CZ	2.49	0.47
4:D:168:PHE:CZ	5:E:142:LYS:HE3	2.50	0.47
1:A:127:LYS:CE	1:A:134:THR:HG22	2.44	0.47
3:H:10:ILE:HD12	3:H:10:ILE:C	2.35	0.47
5:J:42:GLY:CA	9:J:308:PG4:C1	2.71	0.47
4:D:149:LYS:HA	4:D:149:LYS:HE2	1.97	0.47
1:F:190:THR:HG21	1:F:202:ARG:NH2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:152:ASP:OD1	4:I:152:ASP:O	2.33	0.47
4:I:166:MET:O	4:I:166:MET:CG	2.62	0.47
3:C:10:ILE:C	3:C:10:ILE:HD12	2.35	0.47
5:J:10:HIS:ND1	5:J:156:HIS:HD2	2.13	0.47
4:I:125:ASP:OD2	4:I:130:ASP:HB3	2.15	0.47
5:E:221:GLU:HG3	10:E:477:HOH:O	2.15	0.46
4:I:166:MET:O	4:I:166:MET:HG2	2.16	0.46
5:J:41:ARG:HB3	5:J:44:GLU:OE1	2.15	0.46
5:E:10:HIS:ND1	5:E:156:HIS:HD2	2.14	0.46
4:D:196:ASP:O	4:D:197:THR:OG1	2.24	0.46
1:F:165:VAL:HG13	1:F:169:ARG:NH1	2.30	0.46
1:A:5:MET:HE3	1:A:171:TYR:CE2	2.47	0.46
5:J:9:ARG:HG3	6:J:306:EDO:H21	1.97	0.46
4:I:65:VAL:HB	4:I:72:ILE:HG22	1.98	0.46
4:D:52:SER:O	4:D:67:LYS:CD	2.57	0.46
1:F:234:ARG:HH11	2:G:8:GLN:NE2	2.14	0.46
5:J:114:SER:OG	5:J:156:HIS:CE1	2.56	0.46
1:A:5:MET:HE3	1:A:171:TYR:CD2	2.51	0.45
2:B:34:ASP:OD1	7:B:306:GOL:O3	2.34	0.45
1:A:219:ARG:HD3	1:A:256:ARG:HH21	1.81	0.45
4:D:32:TYR:CE2	6:D:305:EDO:C1	3.00	0.45
4:D:39:TYR:HB2	4:D:42:LYS:HG3	1.98	0.45
1:F:249:VAL:HG21	1:F:257:TYR:CE1	2.52	0.45
6:F:301:EDO:O1	6:F:305:EDO:C2	2.64	0.45
1:A:20:PRO:HD2	6:A:303:EDO:H22	1.98	0.45
1:A:40:ALA:HB3	6:A:301:EDO:H12	1.98	0.45
1:A:93:HIS:HE1	10:A:407:HOH:O	1.99	0.45
1:F:129:ASP:O	1:F:131:ARG:NH1	2.49	0.45
5:E:175:ASP:OD1	5:E:195:ARG:NH1	2.50	0.45
4:I:192:ILE:HG13	4:I:192:ILE:O	2.17	0.45
5:E:102:LYS:CG	8:E:312:SO4:O2	2.65	0.44
5:E:42:GLY:HA3	7:E:311:GOL:C3	2.43	0.44
5:J:144:THR:OG1	5:J:197:ARG:HD2	2.17	0.44
4:D:119:ALA:HB1	4:D:121:TYR:CZ	2.51	0.44
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.52	0.44
4:D:166:MET:O	4:D:167:ASP:C	2.54	0.44
1:F:95:VAL:CG1	1:F:116:TYR:CZ	3.00	0.44
1:F:219:ARG:HD3	1:F:256:ARG:HH21	1.83	0.44
5:J:144:THR:HA	5:J:197:ARG:HG3	2.00	0.44
4:D:55:ASN:ND2	4:D:64:GLN:NE2	2.64	0.44
1:A:43:GLN:HA	6:A:301:EDO:O1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:121:TYR:HB3	5:E:133:SER:CB	2.48	0.43
1:F:234:ARG:HH11	2:G:8:GLN:HE21	1.66	0.43
5:J:187:ASP:N	5:J:187:ASP:OD1	2.51	0.43
1:A:165:VAL:HG13	1:A:169:ARG:NH1	2.34	0.43
5:J:163:VAL:HG22	5:J:168:VAL:HG13	2.01	0.43
2:B:42:ASN:ND2	2:B:77:GLU:H	2.17	0.43
1:F:144:LYS:NZ	10:F:404:HOH:O	2.51	0.43
1:F:255:GLN:HA	1:F:255:GLN:NE2	2.33	0.43
5:J:204:GLN:HB3	5:J:245:ALA:HB2	2.01	0.43
1:A:274:TRP:O	1:A:275:GLU:C	2.57	0.43
5:J:224:GLU:HG3	10:J:436:HOH:O	2.19	0.43
2:B:33:SER:HB3	2:B:62:PHE:CE2	2.54	0.43
2:G:39:LEU:HD23	2:G:68:THR:HG22	2.01	0.42
1:A:44:ARG:O	6:A:301:EDO:H21	2.19	0.42
4:I:123:LEU:CD1	4:I:135:LEU:HB2	2.49	0.42
4:I:166:MET:O	4:I:167:ASP:C	2.56	0.42
4:I:77:ARG:CD	6:I:302:EDO:H11	2.49	0.42
5:E:102:LYS:HG2	8:E:312:SO4:O2	2.20	0.42
6:I:305:EDO:H12	10:I:426:HOH:O	2.19	0.42
5:J:156:HIS:HB3	5:J:217:TYR:HB2	2.01	0.42
5:E:42:GLY:C	7:E:311:GOL:H2	2.40	0.42
5:J:129:VAL:CG1	5:J:145:LEU:HD12	2.49	0.42
1:A:249:VAL:HG21	1:A:257:TYR:CE1	2.55	0.42
4:I:113:ILE:HD11	4:I:116:PRO:HB3	2.00	0.42
4:I:131:LYS:CG	4:I:132:SER:N	2.83	0.42
5:J:30:ASP:HA	6:J:305:EDO:H12	2.02	0.42
1:F:187:THR:HA	1:F:204:TRP:O	2.20	0.42
2:G:33:SER:HB3	2:G:62:PHE:CE2	2.54	0.42
4:I:77:ARG:HG2	6:I:306:EDO:H21	2.01	0.42
5:J:30:ASP:HA	6:J:305:EDO:C2	2.49	0.42
4:D:164:ARG:HB2	4:D:164:ARG:HH21	1.83	0.42
4:D:52:SER:O	4:D:67:LYS:HG3	2.20	0.42
5:J:163:VAL:O	5:J:164:ASN:HB3	2.20	0.42
5:E:29:HIS:HE1	10:E:478:HOH:O	2.03	0.41
5:J:208:ASN:HB3	10:J:461:HOH:O	2.16	0.41
1:F:21:ARG:HG2	6:F:304:EDO:H12	2.02	0.41
5:E:157:VAL:HA	5:E:215:GLN:O	2.20	0.41
2:G:39:LEU:N	2:G:39:LEU:CD1	2.84	0.41
1:A:197:HIS:HB3	6:A:308:EDO:C1	2.50	0.41
1:A:121:LYS:HE3	2:B:1:ILE:HG12	2.03	0.41
4:D:56:LYS:HB3	4:D:56:LYS:HE3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4:THR:HG22	2:G:86:THR:CB	2.50	0.41
4:I:163:MET:CE	5:J:197:ARG:HB3	2.49	0.41
5:E:187:ASP:N	5:E:187:ASP:OD1	2.54	0.41
4:D:103:SER:HA	7:E:311:GOL:C3	2.50	0.41
5:J:72:ALA:HB1	6:J:305:EDO:H11	2.03	0.41
1:A:234:ARG:HD3	2:B:10:TYR:CD2	2.55	0.41
5:E:164:ASN:OD1	5:E:209:HIS:N	2.48	0.40
2:B:45:ARG:HH22	6:B:304:EDO:H21	1.86	0.40
4:D:32:TYR:CE2	6:D:305:EDO:H12	2.56	0.40
4:D:186:ASN:OD1	4:D:188:PHE:CZ	2.75	0.40
4:I:110:ARG:HA	4:I:111:PRO:HD3	1.89	0.40
5:J:42:GLY:HA2	9:J:308:PG4:H42	2.03	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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	195/199 (98%)	184 (94%)	8 (4%)	3 (2%)	13	5
4	I	197/199 (99%)	184 (93%)	12 (6%)	1 (0%)	34	26
5	E	245/247 (99%)	242 (99%)	3 (1%)	0	100	100
5	J	242/247 (98%)	235 (97%)	6 (2%)	1 (0%)	39	32
All	All	1639/1662 (99%)	1592 (97%)	42 (3%)	5 (0%)	46	40

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 ⓘ

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%)	7	3
1	F	231/231 (100%)	204 (88%)	27 (12%)	7	3
2	B	96/95 (101%)	90 (94%)	6 (6%)	22	15
2	G	95/95 (100%)	87 (92%)	8 (8%)	14	8
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%)	6	3
4	I	180/180 (100%)	165 (92%)	15 (8%)	14	8
5	E	217/217 (100%)	200 (92%)	17 (8%)	16	9
5	J	215/217 (99%)	191 (89%)	24 (11%)	7	3
All	All	1462/1464 (100%)	1317 (90%)	145 (10%)	10	5

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	64	THR
1	A	73	THR
1	A	98	MET
1	A	111	ARG
1	A	113	TYR
1	A	156	LEU
1	A	165	VAL
1	A	166	GLU
1	A	172	LEU
1	A	176	LYS
1	A	186	LYS
1	A	187	THR
1	A	190	THR
1	A	206	LEU
1	A	212	GLU
1	A	214	THR
1	A	215	LEU
1	A	219	ARG
1	A	225	THR
1	A	229	GLU
1	A	230	LEU
1	A	254	GLU
1	A	255	GLN
1	A	273	ARG
1	A	275	GLU
2	B	0	MET
2	B	58	LYS
2	B	70	PHE
2	B	85	VAL
2	B	87	LEU
2	B	94	LYS
4	D	3	GLU
4	D	11	LEU
4	D	19	VAL
4	D	34	MET
4	D	42	LYS
4	D	49	TYR
4	D	50	THR
4	D	53	SER
4	D	99	LEU
4	D	122	GLN

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Mol	Chain	Res	Type
4	D	124	ARG
4	D	131	LYS
4	D	140	ASP
4	D	142	GLN
4	D	151	SER
4	D	153	VAL
4	D	159	CYS
4	D	167	ASP
4	D	177	SER
4	D	178	ASN
4	D	198	PHE
4	D	199	PHE
5	E	11	GLU
5	E	39	MET
5	E	41	ARG
5	E	53	VAL
5	E	76	THR
5	E	138	SER
5	E	145	LEU
5	E	148	LEU
5	E	170	SER
5	E	173	CYS
5	E	178	PRO
5	E	179	LEU
5	E	182	GLN
5	E	187	ASP
5	E	188	SER
5	E	195	ARG
5	E	224	GLU
1	F	35	ARG
1	F	48	ARG
1	F	74	HIS
1	F	75	ARG
1	F	111	ARG
1	F	156	LEU
1	F	165	VAL
1	F	172	LEU
1	F	176	LYS
1	F	190	THR
1	F	194	VAL
1	F	197	HIS
1	F	206	LEU

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Mol	Chain	Res	Type
1	F	214	THR
1	F	215	LEU
1	F	219	ARG
1	F	223	ASP
1	F	225	THR
1	F	226	GLN
1	F	231	VAL
1	F	234	ARG
1	F	238	ASP
1	F	248	VAL
1	F	254	GLU
1	F	271	THR
1	F	273	ARG
1	F	275	GLU
2	G	0	MET
2	G	1	ILE
2	G	4	THR
2	G	39	LEU
2	G	48	LYS
2	G	70	PHE
2	G	94	LYS
2	G	98	ASP
4	I	3	GLU
4	I	19	VAL
4	I	49	TYR
4	I	52	SER
4	I	99	LEU
4	I	106	ARG
4	I	122	GLN
4	I	144	ASN
4	I	151	SER
4	I	164	ARG
4	I	165	SER
4	I	166	MET
4	I	167	ASP
4	I	169	LYS
4	I	186	ASN
5	J	11	GLU
5	J	39	MET
5	J	41	ARG
5	J	43	LEU
5	J	53	VAL

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Mol	Chain	Res	Type
5	J	76	THR
5	J	80	GLN
5	J	100	LEU
5	J	134	GLU
5	J	138	SER
5	J	140	THR
5	J	142	LYS
5	J	148	LEU
5	J	173	CYS
5	J	178	PRO
5	J	179	LEU
5	J	182	GLN
5	J	187	ASP
5	J	188	SER
5	J	195	ARG
5	J	196	LEU
5	J	207	ARG
5	J	209	HIS
5	J	246	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	93	HIS
1	A	151	HIS
1	A	180	GLN
1	A	263	HIS
2	B	8	GLN
2	B	42	ASN
2	B	84	HIS
4	D	31	GLN
4	D	55	ASN
4	D	186	ASN
4	D	189	ASN
5	E	29	HIS
5	E	50	ASN
5	E	51	ASN
5	E	156	HIS
5	E	186	ASN
1	F	93	HIS
1	F	114	HIS

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Mol	Chain	Res	Type
1	F	115	GLN
1	F	180	GLN
1	F	255	GLN
1	F	263	HIS
2	G	8	GLN
2	G	13	HIS
2	G	84	HIS
4	I	142	GLN
4	I	144	ASN
5	J	80	GLN
5	J	156	HIS
5	J	177	GLN
5	J	204	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	A	301	-	3,3,3	0.26	0	2,2,2	0.81	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	A	302	-	3,3,3	0.41	0	2,2,2	0.72	0
6	EDO	A	303	-	3,3,3	0.43	0	2,2,2	0.91	0
6	EDO	A	304	-	3,3,3	0.63	0	2,2,2	0.47	0
6	EDO	A	305	-	3,3,3	0.55	0	2,2,2	0.96	0
6	EDO	A	306	-	3,3,3	0.61	0	2,2,2	0.36	0
6	EDO	A	307	-	3,3,3	0.50	0	2,2,2	0.52	0
6	EDO	A	308	-	3,3,3	0.50	0	2,2,2	0.47	0
6	EDO	A	309	-	3,3,3	0.58	0	2,2,2	0.21	0
7	GOL	A	310	-	5,5,5	0.82	0	5,5,5	0.74	0
8	SO4	A	311	-	4,4,4	1.23	0	6,6,6	0.85	0
8	SO4	A	312	-	4,4,4	0.61	0	6,6,6	0.77	0
6	EDO	B	301	-	3,3,3	0.46	0	2,2,2	0.65	0
6	EDO	B	302	-	3,3,3	0.62	0	2,2,2	0.68	0
6	EDO	B	303	-	3,3,3	0.72	0	2,2,2	0.48	0
6	EDO	B	304	-	3,3,3	0.43	0	2,2,2	0.76	0
6	EDO	B	305	-	3,3,3	0.50	0	2,2,2	0.46	0
7	GOL	B	306	-	5,5,5	1.16	1 (20%)	5,5,5	1.22	0
8	SO4	B	307	-	4,4,4	0.93	0	6,6,6	0.38	0
6	EDO	D	301	-	3,3,3	0.50	0	2,2,2	0.63	0
6	EDO	D	302	-	3,3,3	0.82	0	2,2,2	0.73	0
6	EDO	D	303	-	3,3,3	0.98	0	2,2,2	0.88	0
6	EDO	D	304	-	3,3,3	0.80	0	2,2,2	0.97	0
6	EDO	D	305	-	3,3,3	0.49	0	2,2,2	0.38	0
6	EDO	D	306	-	3,3,3	0.67	0	2,2,2	0.29	0
6	EDO	E	301	-	3,3,3	0.47	0	2,2,2	0.61	0
6	EDO	E	302	-	3,3,3	0.44	0	2,2,2	0.27	0
6	EDO	E	303	-	3,3,3	0.58	0	2,2,2	0.22	0
6	EDO	E	304	-	3,3,3	0.52	0	2,2,2	0.87	0
6	EDO	E	305	-	3,3,3	0.28	0	2,2,2	0.93	0
6	EDO	E	306	-	3,3,3	0.52	0	2,2,2	0.32	0
6	EDO	E	307	-	3,3,3	0.78	0	2,2,2	0.11	0
6	EDO	E	308	-	3,3,3	0.28	0	2,2,2	0.88	0
6	EDO	E	309	-	3,3,3	0.47	0	2,2,2	0.46	0
6	EDO	E	310	-	3,3,3	0.63	0	2,2,2	0.16	0
7	GOL	E	311	-	5,5,5	0.80	0	5,5,5	0.95	0
8	SO4	E	312	-	4,4,4	0.76	0	6,6,6	0.88	0
8	SO4	E	313	-	4,4,4	0.88	0	6,6,6	0.54	0
6	EDO	F	301	-	3,3,3	0.35	0	2,2,2	0.91	0
6	EDO	F	302	-	3,3,3	0.18	0	2,2,2	0.45	0
6	EDO	F	303	-	3,3,3	0.81	0	2,2,2	0.24	0
6	EDO	F	304	-	3,3,3	0.48	0	2,2,2	0.37	0
6	EDO	F	305	-	3,3,3	0.42	0	2,2,2	0.75	0
6	EDO	F	306	-	3,3,3	0.31	0	2,2,2	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	F	307	-	3,3,3	0.50	0	2,2,2	0.64	0
7	GOL	F	308	-	5,5,5	0.94	0	5,5,5	1.81	2 (40%)
8	SO4	F	309	-	4,4,4	1.50	1 (25%)	6,6,6	0.99	0
8	SO4	F	310	-	4,4,4	0.81	0	6,6,6	0.49	0
8	SO4	F	311	-	4,4,4	0.58	0	6,6,6	0.47	0
6	EDO	G	101	-	3,3,3	0.46	0	2,2,2	0.70	0
6	EDO	G	102	-	3,3,3	0.40	0	2,2,2	0.36	0
6	EDO	G	103	-	3,3,3	0.40	0	2,2,2	1.18	0
6	EDO	G	104	-	3,3,3	0.59	0	2,2,2	0.20	0
6	EDO	H	101	-	3,3,3	0.60	0	2,2,2	0.59	0
6	EDO	I	301	-	3,3,3	0.89	0	2,2,2	0.62	0
6	EDO	I	302	-	3,3,3	0.47	0	2,2,2	0.88	0
6	EDO	I	303	-	3,3,3	0.36	0	2,2,2	0.56	0
6	EDO	I	304	-	3,3,3	0.56	0	2,2,2	0.27	0
6	EDO	I	305	-	3,3,3	0.56	0	2,2,2	0.43	0
6	EDO	I	306	-	3,3,3	0.58	0	2,2,2	0.45	0
6	EDO	I	307	-	3,3,3	0.89	0	2,2,2	0.10	0
7	GOL	I	308	-	5,5,5	0.92	0	5,5,5	1.78	2 (40%)
6	EDO	J	301	-	3,3,3	0.52	0	2,2,2	0.72	0
6	EDO	J	302	-	3,3,3	0.30	0	2,2,2	0.70	0
6	EDO	J	303	-	3,3,3	0.46	0	2,2,2	0.41	0
6	EDO	J	304	-	3,3,3	0.71	0	2,2,2	0.21	0
6	EDO	J	305	-	3,3,3	0.50	0	2,2,2	1.65	1 (50%)
6	EDO	J	306	-	3,3,3	0.67	0	2,2,2	0.08	0
7	GOL	J	307	-	5,5,5	0.51	0	5,5,5	0.77	0
9	PG4	J	308	-	9,9,12	0.67	0	8,8,11	1.25	1 (12%)

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	A	301	-	-	0/1/1/1	0/0/0/0
6	EDO	A	302	-	-	0/1/1/1	0/0/0/0
6	EDO	A	303	-	-	0/1/1/1	0/0/0/0
6	EDO	A	304	-	-	0/1/1/1	0/0/0/0
6	EDO	A	305	-	-	0/1/1/1	0/0/0/0
6	EDO	A	306	-	-	0/1/1/1	0/0/0/0
6	EDO	A	307	-	-	0/1/1/1	0/0/0/0
6	EDO	A	308	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	309	-	-	0/1/1/1	0/0/0/0
7	GOL	A	310	-	-	0/4/4/4	0/0/0/0
8	SO4	A	311	-	-	0/0/0/0	0/0/0/0
8	SO4	A	312	-	-	0/0/0/0	0/0/0/0
6	EDO	B	301	-	-	0/1/1/1	0/0/0/0
6	EDO	B	302	-	-	0/1/1/1	0/0/0/0
6	EDO	B	303	-	-	0/1/1/1	0/0/0/0
6	EDO	B	304	-	-	0/1/1/1	0/0/0/0
6	EDO	B	305	-	-	0/1/1/1	0/0/0/0
7	GOL	B	306	-	-	0/4/4/4	0/0/0/0
8	SO4	B	307	-	-	0/0/0/0	0/0/0/0
6	EDO	D	301	-	-	0/1/1/1	0/0/0/0
6	EDO	D	302	-	-	0/1/1/1	0/0/0/0
6	EDO	D	303	-	-	0/1/1/1	0/0/0/0
6	EDO	D	304	-	-	0/1/1/1	0/0/0/0
6	EDO	D	305	-	-	0/1/1/1	0/0/0/0
6	EDO	D	306	-	-	0/1/1/1	0/0/0/0
6	EDO	E	301	-	-	0/1/1/1	0/0/0/0
6	EDO	E	302	-	-	0/1/1/1	0/0/0/0
6	EDO	E	303	-	-	0/1/1/1	0/0/0/0
6	EDO	E	304	-	-	0/1/1/1	0/0/0/0
6	EDO	E	305	-	-	0/1/1/1	0/0/0/0
6	EDO	E	306	-	-	0/1/1/1	0/0/0/0
6	EDO	E	307	-	-	0/1/1/1	0/0/0/0
6	EDO	E	308	-	-	0/1/1/1	0/0/0/0
6	EDO	E	309	-	-	0/1/1/1	0/0/0/0
6	EDO	E	310	-	-	0/1/1/1	0/0/0/0
7	GOL	E	311	-	-	0/4/4/4	0/0/0/0
8	SO4	E	312	-	-	0/0/0/0	0/0/0/0
8	SO4	E	313	-	-	0/0/0/0	0/0/0/0
6	EDO	F	301	-	-	0/1/1/1	0/0/0/0
6	EDO	F	302	-	-	0/1/1/1	0/0/0/0
6	EDO	F	303	-	-	0/1/1/1	0/0/0/0
6	EDO	F	304	-	-	0/1/1/1	0/0/0/0
6	EDO	F	305	-	-	0/1/1/1	0/0/0/0
6	EDO	F	306	-	-	0/1/1/1	0/0/0/0
6	EDO	F	307	-	-	0/1/1/1	0/0/0/0
7	GOL	F	308	-	-	0/4/4/4	0/0/0/0
8	SO4	F	309	-	-	0/0/0/0	0/0/0/0
8	SO4	F	310	-	-	0/0/0/0	0/0/0/0
8	SO4	F	311	-	-	0/0/0/0	0/0/0/0
6	EDO	G	101	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	G	102	-	-	0/1/1/1	0/0/0/0
6	EDO	G	103	-	-	0/1/1/1	0/0/0/0
6	EDO	G	104	-	-	0/1/1/1	0/0/0/0
6	EDO	H	101	-	-	0/1/1/1	0/0/0/0
6	EDO	I	301	-	-	0/1/1/1	0/0/0/0
6	EDO	I	302	-	-	0/1/1/1	0/0/0/0
6	EDO	I	303	-	-	0/1/1/1	0/0/0/0
6	EDO	I	304	-	-	0/1/1/1	0/0/0/0
6	EDO	I	305	-	-	0/1/1/1	0/0/0/0
6	EDO	I	306	-	-	0/1/1/1	0/0/0/0
6	EDO	I	307	-	-	0/1/1/1	0/0/0/0
7	GOL	I	308	-	-	0/4/4/4	0/0/0/0
6	EDO	J	301	-	-	0/1/1/1	0/0/0/0
6	EDO	J	302	-	-	0/1/1/1	0/0/0/0
6	EDO	J	303	-	-	0/1/1/1	0/0/0/0
6	EDO	J	304	-	-	0/1/1/1	0/0/0/0
6	EDO	J	305	-	-	0/1/1/1	0/0/0/0
6	EDO	J	306	-	-	0/1/1/1	0/0/0/0
7	GOL	J	307	-	-	0/4/4/4	0/0/0/0
9	PG4	J	308	-	-	0/7/7/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	306	GOL	O2-C2	-2.41	1.36	1.43
8	F	309	SO4	O1-S	2.47	1.55	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	308	PG4	O2-C2-C1	-3.08	97.37	110.25
7	I	308	GOL	O2-C2-C1	-2.71	95.44	108.47
7	F	308	GOL	O2-C2-C1	-2.33	97.29	108.47
6	J	305	EDO	O1-C1-C2	-2.31	96.44	112.23
7	I	308	GOL	O3-C3-C2	2.49	122.60	109.97
7	F	308	GOL	O3-C3-C2	2.57	122.99	109.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

28 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	301	EDO	6	0
6	A	303	EDO	1	0
6	A	308	EDO	1	0
6	B	302	EDO	2	0
6	B	304	EDO	1	0
7	B	306	GOL	1	0
6	D	301	EDO	1	0
6	D	303	EDO	2	0
6	D	304	EDO	3	0
6	D	305	EDO	2	0
6	E	304	EDO	2	0
6	E	310	EDO	1	0
7	E	311	GOL	11	0
8	E	312	SO4	3	0
6	F	301	EDO	2	0
6	F	304	EDO	1	0
6	F	305	EDO	2	0
6	F	306	EDO	2	0
6	F	307	EDO	2	0
7	F	308	GOL	2	0
6	G	102	EDO	1	0
6	I	302	EDO	3	0
6	I	305	EDO	1	0
6	I	306	EDO	1	0
7	I	308	GOL	1	0
6	J	305	EDO	4	0
6	J	306	EDO	1	0
9	J	308	PG4	13	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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	275/275 (100%)	0.18	8 (2%) 55 57	25, 50, 82, 95	0
1	F	275/275 (100%)	0.13	12 (4%) 38 40	22, 45, 86, 108	0
2	B	100/100 (100%)	-0.13	0 100 100	30, 42, 62, 78	0
2	G	100/100 (100%)	-0.12	2 (2%) 68 69	28, 41, 69, 83	0
3	C	10/10 (100%)	0.22	0 100 100	32, 35, 42, 43	0
3	H	10/10 (100%)	0.51	0 100 100	25, 28, 32, 35	0
4	D	197/199 (98%)	0.92	39 (19%) 1 1	29, 59, 113, 128	0
4	I	199/199 (100%)	1.05	44 (22%) 1 1	26, 56, 113, 131	0
5	E	247/247 (100%)	0.14	14 (5%) 27 29	22, 44, 87, 118	0
5	J	244/247 (98%)	0.41	23 (9%) 11 11	22, 49, 100, 124	0
All	All	1657/1662 (99%)	0.36	142 (8%) 13 14	22, 47, 99, 131	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	201	SER	10.8
4	I	151	SER	10.1
4	D	199	PHE	7.9
4	D	166	MET	7.4
4	I	130	ASP	7.2
4	D	198	PHE	6.2
5	J	245	ALA	6.0
5	E	246	ASP	5.9
4	I	119	ALA	5.8
4	D	182	PHE	5.7
4	D	164	ARG	5.5
4	D	180	SER	5.4
5	J	246	ASP	5.4

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Mol	Chain	Res	Type	RSRZ
4	I	199	PHE	5.3
4	I	150	ASP	5.1
4	I	198	PHE	5.1
4	I	189	ASN	5.1
4	I	166	MET	5.1
4	I	128	SER	5.0
4	D	130	ASP	5.0
4	D	127	LYS	5.0
4	D	184	CYS	5.0
4	D	185	ALA	4.9
4	I	134	CYS	4.9
4	I	192	ILE	4.9
5	J	40	MET	4.9
4	I	136	PHE	4.9
4	D	187	ALA	4.9
4	I	190	ASN	4.9
4	I	165	SER	4.8
4	D	167	ASP	4.8
4	I	182	PHE	4.5
4	D	194	PRO	4.5
4	D	178	ASN	4.4
4	I	147	GLN	4.4
4	I	148	SER	4.4
4	I	120	VAL	4.3
4	I	149	LYS	4.1
5	E	138	SER	4.1
4	I	197	THR	4.1
4	I	191	SER	4.0
5	E	40	MET	4.0
4	D	151	SER	3.9
4	I	52	SER	3.9
5	J	201	THR	3.9
4	D	190	ASN	3.9
4	I	180	SER	3.9
2	G	0	MET	3.8
4	D	189	ASN	3.8
1	F	223	ASP	3.8
4	I	178	ASN	3.8
4	I	114	GLN	3.8
5	J	135	ALA	3.7
1	A	219	ARG	3.6
4	D	52	SER	3.6

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Mol	Chain	Res	Type	RSRZ
4	I	181	ASP	3.6
1	F	225	THR	3.5
4	I	200	PRO	3.5
5	J	207	ARG	3.5
4	I	154	TYR	3.5
4	D	128	SER	3.5
4	I	129	SER	3.5
4	I	164	ARG	3.5
4	I	176	TRP	3.5
4	D	152	ASP	3.4
4	I	179	LYS	3.4
1	F	249	VAL	3.4
4	D	149	LYS	3.4
4	D	181	ASP	3.4
4	I	123	LEU	3.3
4	D	148	SER	3.3
4	D	191	SER	3.3
4	D	153	VAL	3.3
5	J	138	SER	3.2
5	E	187	ASP	3.2
1	A	176	LYS	3.2
4	I	124	ARG	3.1
1	A	222	GLU	3.1
5	J	185	LEU	3.1
5	E	134	GLU	3.1
5	J	184	ALA	3.1
4	D	192	ILE	3.1
5	J	129	VAL	2.9
4	D	186	ASN	2.8
4	I	167	ASP	2.8
5	E	245	ALA	2.8
4	I	135	LEU	2.8
4	D	150	ASP	2.8
5	J	187	ASP	2.8
1	F	222	GLU	2.8
1	F	221	GLY	2.8
1	F	226	GLN	2.8
4	D	147	GLN	2.8
1	F	196	ASP	2.8
4	D	129	SER	2.8
5	E	226	THR	2.8
5	J	186	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
4	D	193	ILE	2.7
5	J	142	LYS	2.7
5	J	41	ARG	2.7
5	E	224	GLU	2.7
4	I	195	GLU	2.6
4	D	114	GLN	2.6
4	I	186	ASN	2.6
5	J	183	PRO	2.6
4	D	197	THR	2.5
4	D	55	ASN	2.5
1	F	230	LEU	2.5
4	I	152	ASP	2.5
4	D	179	LYS	2.5
1	A	177	GLU	2.4
4	D	183	ALA	2.4
4	I	153	VAL	2.4
4	D	165	SER	2.4
4	D	162	ASP	2.4
5	E	207	ARG	2.4
5	J	144	THR	2.4
5	J	137	ILE	2.3
5	E	186	ASN	2.3
4	D	124	ARG	2.3
5	E	185	LEU	2.3
5	J	188	SER	2.3
2	G	1	ILE	2.3
5	J	182	GLN	2.3
5	J	134	GLU	2.3
1	A	268	LYS	2.2
4	I	112	ASP	2.2
5	J	164	ASN	2.2
1	A	175	GLY	2.1
1	A	180	GLN	2.1
4	I	185	ALA	2.1
4	I	196	ASP	2.1
1	F	228	THR	2.1
5	J	243	GLY	2.1
1	F	194	VAL	2.1
5	E	206	PRO	2.1
5	J	140	THR	2.1
1	A	218	GLN	2.1
1	F	267	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
5	E	141	GLN	2.0
5	E	210	PHE	2.0
1	F	220	ASP	2.0

## 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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	SO4	A	311	5/5	0.54	0.43	11.90	65,77,112,119	0
6	EDO	A	306	4/4	0.70	0.35	11.86	63,67,67,69	0
6	EDO	E	310	4/4	0.89	0.26	8.55	33,35,43,46	0
8	SO4	F	309	5/5	0.68	0.34	8.15	51,56,94,101	0
8	SO4	E	312	5/5	0.76	0.36	7.97	83,84,92,112	0
6	EDO	D	306	4/4	0.89	0.15	7.90	42,48,52,54	0
6	EDO	F	307	4/4	0.89	0.31	7.02	59,59,63,65	0
7	GOL	J	307	6/6	0.87	0.37	6.41	54,57,61,63	0
6	EDO	E	304	4/4	0.88	0.23	6.37	35,48,50,58	0
6	EDO	J	305	4/4	0.97	0.22	6.34	41,42,42,45	0
6	EDO	G	104	4/4	0.75	0.26	6.19	58,60,64,67	0
7	GOL	I	308	6/6	0.77	0.18	5.54	46,47,49,62	0
6	EDO	J	301	4/4	0.79	0.24	5.08	62,71,73,74	0
7	GOL	F	308	6/6	0.77	0.30	5.04	44,58,67,70	0
6	EDO	F	304	4/4	0.95	0.17	4.45	39,41,46,57	0
6	EDO	H	101	4/4	0.89	0.20	4.41	37,44,46,47	0
6	EDO	F	301	4/4	0.93	0.17	4.24	49,52,56,65	0
8	SO4	B	307	5/5	0.92	0.35	4.12	63,73,83,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	EDO	A	305	4/4	0.84	0.27	4.04	57,73,85,86	0
6	EDO	B	302	4/4	0.83	0.19	3.75	47,53,54,62	0
8	SO4	E	313	5/5	0.93	0.16	3.72	54,65,73,84	0
6	EDO	E	303	4/4	0.79	0.25	3.52	56,72,75,79	0
6	EDO	F	306	4/4	0.97	0.23	3.09	30,41,42,46	0
7	GOL	A	310	6/6	0.60	0.28	3.05	58,69,70,75	0
7	GOL	B	306	6/6	0.76	0.23	2.74	50,52,54,62	0
6	EDO	D	305	4/4	0.91	0.22	2.68	52,59,61,65	0
6	EDO	A	303	4/4	0.93	0.22	2.42	49,50,53,56	0
7	GOL	E	311	6/6	0.78	0.23	2.05	48,54,63,66	0
6	EDO	G	101	4/4	0.93	0.15	1.78	41,42,45,46	0
6	EDO	D	302	4/4	0.90	0.14	1.65	39,41,41,46	0
6	EDO	E	301	4/4	0.98	0.19	1.63	28,34,39,42	0
6	EDO	A	302	4/4	0.87	0.20	1.58	61,62,64,73	0
6	EDO	F	305	4/4	0.92	0.25	1.43	55,59,62,63	0
6	EDO	E	307	4/4	0.73	0.16	1.32	59,63,69,70	0
6	EDO	D	303	4/4	0.86	0.15	1.24	44,48,49,49	0
6	EDO	I	307	4/4	0.77	0.21	1.24	48,49,56,58	0
6	EDO	I	306	4/4	0.89	0.22	1.19	44,46,49,52	0
6	EDO	A	307	4/4	0.91	0.16	1.11	49,53,58,66	0
6	EDO	I	301	4/4	0.97	0.15	0.96	29,31,37,42	0
6	EDO	B	303	4/4	0.86	0.15	0.96	44,52,54,65	0
6	EDO	E	308	4/4	0.90	0.12	0.93	57,58,59,59	0
6	EDO	A	301	4/4	0.97	0.14	0.70	38,38,41,42	0
6	EDO	G	102	4/4	0.92	0.18	0.68	44,51,56,59	0
6	EDO	F	302	4/4	0.98	0.17	0.60	44,46,47,48	0
6	EDO	A	304	4/4	0.80	0.17	0.53	52,56,56,62	0
6	EDO	B	301	4/4	0.96	0.12	0.48	40,42,44,50	0
6	EDO	D	301	4/4	0.94	0.11	0.44	49,51,51,55	0
6	EDO	D	304	4/4	0.85	0.15	0.28	47,57,63,64	0
6	EDO	J	302	4/4	0.88	0.14	0.27	63,65,74,78	0
6	EDO	J	304	4/4	0.89	0.16	0.24	47,47,48,51	0
9	PG4	J	308	10/13	0.85	0.18	0.19	45,65,83,84	0
6	EDO	E	302	4/4	0.93	0.13	-0.04	54,54,56,57	0
6	EDO	F	303	4/4	0.90	0.11	-0.34	51,60,65,67	0
6	EDO	B	304	4/4	0.85	0.11	-0.36	53,55,56,63	0
6	EDO	I	303	4/4	0.84	0.15	-0.78	69,71,77,82	0
6	EDO	J	303	4/4	0.80	0.16	-0.79	70,73,81,83	0
6	EDO	I	304	4/4	0.63	0.22	-1.25	74,84,88,92	0
8	SO4	F	310	5/5	0.89	0.27	-	65,82,86,90	0
8	SO4	A	312	5/5	0.85	0.34	-	73,94,103,106	0
6	EDO	E	309	4/4	0.90	0.16	-	60,62,64,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	A	309	4/4	0.80	0.14	-	67,67,71,71	0
8	SO4	F	311	5/5	0.89	0.40	-	72,97,102,105	0
6	EDO	A	308	4/4	0.75	0.24	-	71,73,73,78	0
6	EDO	G	103	4/4	0.91	0.26	-	53,65,72,75	0
6	EDO	J	306	4/4	0.74	0.25	-	53,61,62,66	0
6	EDO	E	306	4/4	0.87	0.15	-	58,62,71,71	0
6	EDO	E	305	4/4	0.93	0.09	-	64,65,68,70	0
6	EDO	B	305	4/4	0.68	0.37	-	55,60,65,69	0
6	EDO	I	305	4/4	0.80	0.24	-	60,62,69,71	0
6	EDO	I	302	4/4	0.84	0.32	-	53,58,60,68	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.