



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:40 am GMT

PDB ID : 5C0C  
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](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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

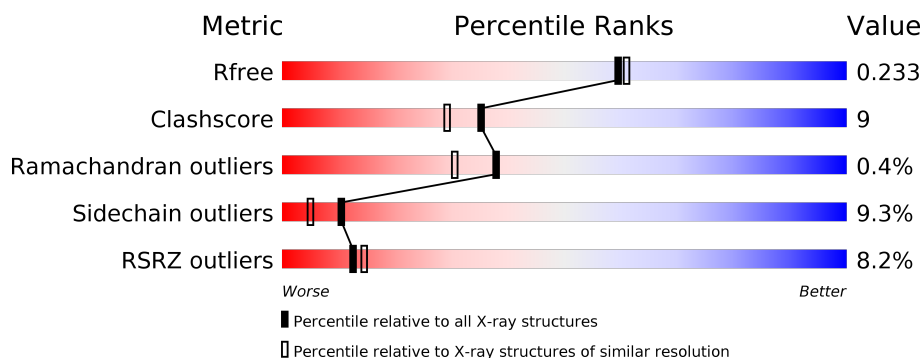
# 1 Overall quality at a glance

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))
$R_{free}$	100719	9293 (2.00-1.96)
Clashscore	112137	10621 (2.00-1.96)
Ramachandran outliers	110173	10502 (2.00-1.96)
Sidechain outliers	110143	10501 (2.00-1.96)
RSRZ outliers	101464	9395 (2.00-1.96)

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	277	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>• •</div> </div> </div>
1	F	277	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>• •</div> </div> </div>
2	B	100	<div> <div></div> <div> <div></div> <div>80%</div> <div>16%</div> <div>• •</div> </div> </div>
2	G	100	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>•</div> </div> </div>
3	C	10	<div> <div></div> <div> <div></div> <div>80%</div> <div>10%</div> <div>10%</div> </div> </div>
3	H	10	<div> <div></div> <div> <div></div> <div>70%</div> <div>30%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	200	
4	I	200	
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	X
6	EDO	A	302	-	-	-	X
6	EDO	A	303	-	-	-	X
6	EDO	E	301	-	-	-	X
6	EDO	E	303	-	-	-	X
6	EDO	F	301	-	-	-	X
6	EDO	F	302	-	-	-	X
6	EDO	F	306	-	-	-	X
6	EDO	G	102	-	-	-	X
6	EDO	I	301	-	-	-	X
6	EDO	I	303	-	-	-	X
6	EDO	J	303	-	-	-	X
6	EDO	J	304	-	-	-	X
7	PG4	A	304	-	-	-	X
7	PG4	I	304	-	-	-	X
8	SO4	J	309	-	-	-	X
9	GOL	B	303	-	-	-	X
9	GOL	F	308	-	-	X	X
9	GOL	F	309	-	-	-	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			

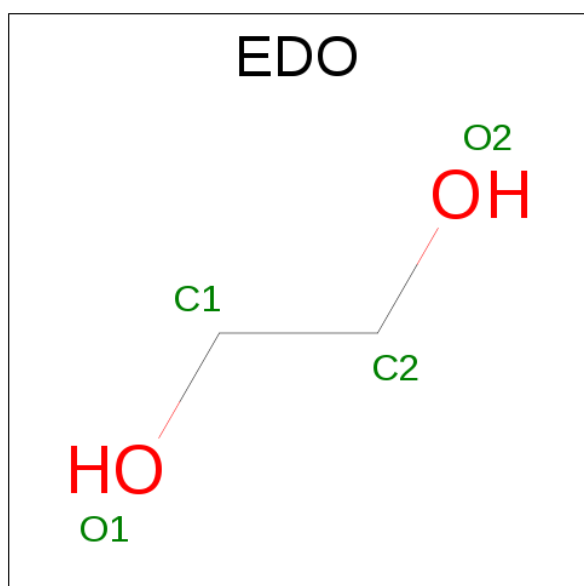
- Molecule 4 is a protein called 1E6 TCR Alpha Chain.

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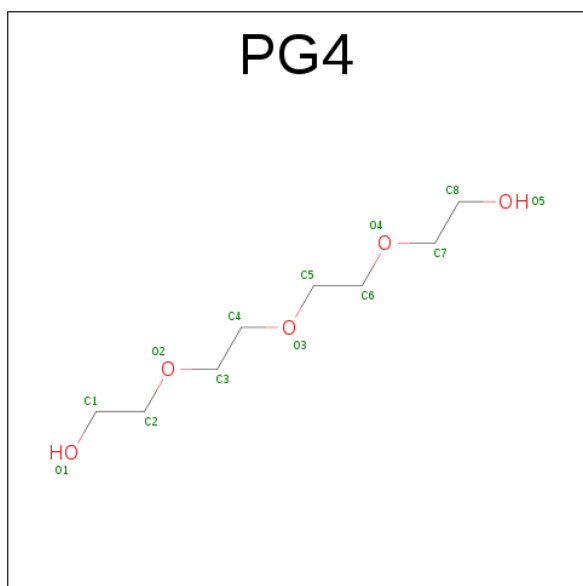
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total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

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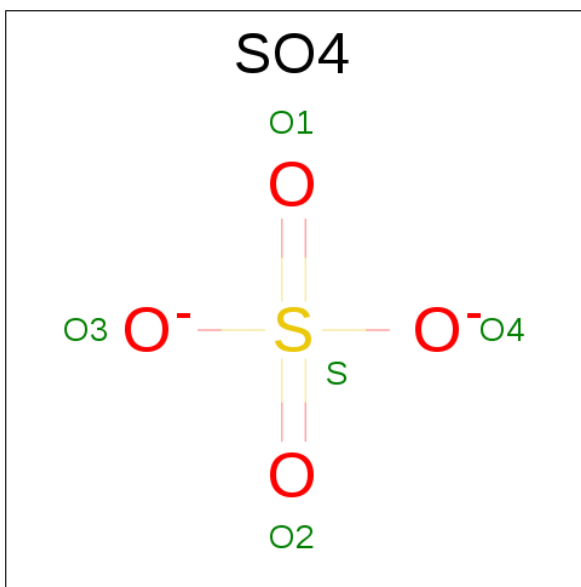
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



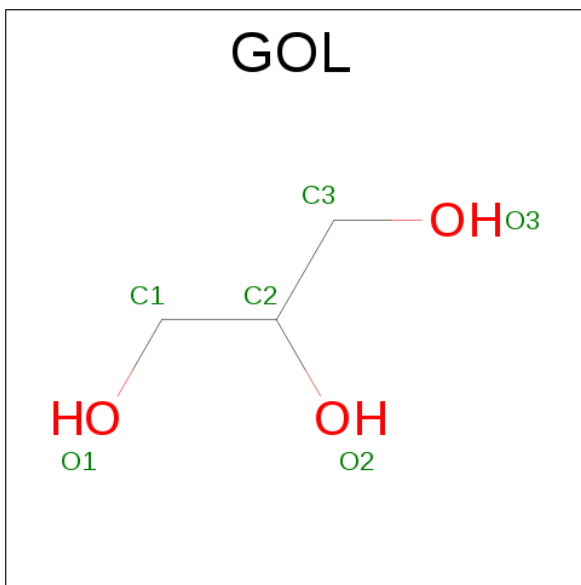
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 10 6 4	0	0
7	I	1	Total C O 13 8 5	0	0

- 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	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 (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





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		

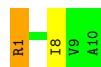
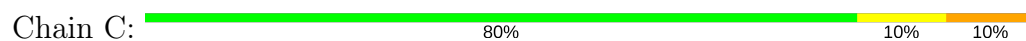


- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain





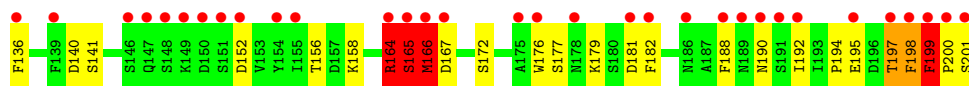
- Molecule 3: Marker peptide



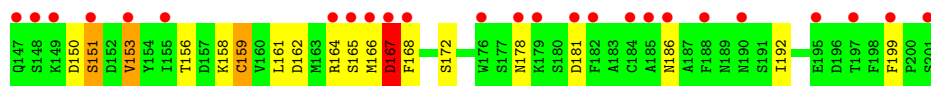
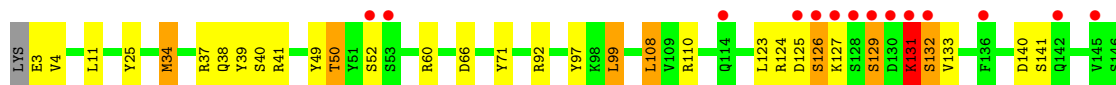
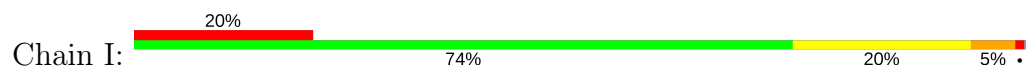
- Molecule 3: Marker peptide



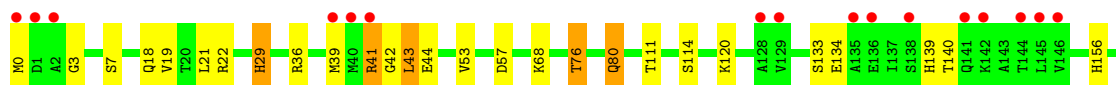
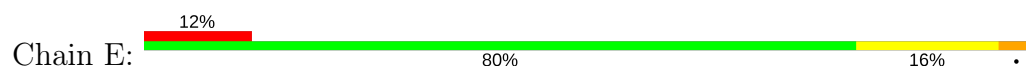
- Molecule 4: 1E6 TCR Alpha Chain



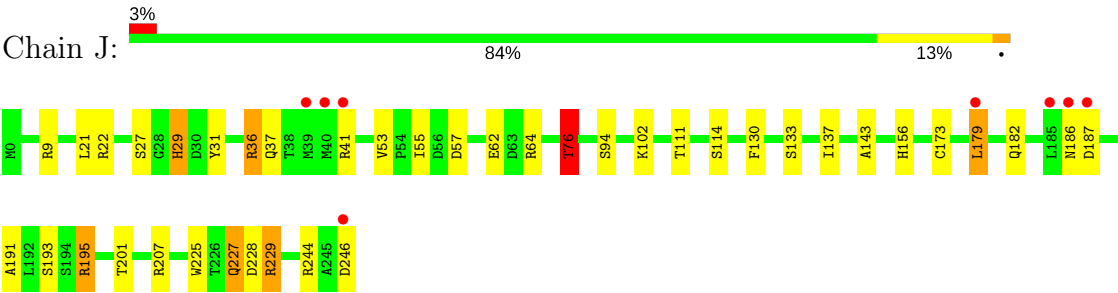
- Molecule 4: 1E6 TCR Alpha Chain



- 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, $\alpha$ , $\beta$ , $\gamma$	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) 93.4 (120.38-1.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 1.97Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.189 , 0.227 0.196 , 0.233	Depositor DCC
$R_{free}$ test set	7029 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<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, 0.333 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	0.94	3/2320 (0.1%)	1.04	14/3149 (0.4%)
1	F	1.02	6/2328 (0.3%)	1.28	23/3159 (0.7%)
2	B	1.00	1/860 (0.1%)	1.07	6/1162 (0.5%)
2	G	1.01	2/860 (0.2%)	1.12	7/1162 (0.6%)
3	C	1.23	0/88	1.97	2/118 (1.7%)
3	H	1.39	0/88	1.18	1/118 (0.8%)
4	D	0.94	0/1615	1.14	10/2185 (0.5%)
4	I	0.94	2/1606 (0.1%)	1.11	8/2174 (0.4%)
5	E	0.96	0/2037	1.06	7/2769 (0.3%)
5	J	0.95	2/2037 (0.1%)	1.02	8/2769 (0.3%)
All	All	0.97	16/13839 (0.1%)	1.12	86/18765 (0.5%)

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 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	55	SER	CB-OG	8.65	1.53	1.42
2	G	60	TRP	N-CA	8.44	1.63	1.46
1	F	80	THR	CB-CG2	-7.77	1.26	1.52
4	I	97	TYR	CE1-CZ	-7.39	1.28	1.38
1	A	13	SER	CB-OG	-6.94	1.33	1.42

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	97	ARG	NE-CZ-NH1	25.09	132.85	120.30
1	F	97	ARG	NE-CZ-NH2	-22.27	109.17	120.30
3	C	1	ARG	NE-CZ-NH1	15.04	127.82	120.30
4	I	34	MET	CG-SD-CE	-13.91	77.94	100.20
4	I	60	ARG	NE-CZ-NH2	-12.82	113.89	120.30

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	50	0
1	F	2262	0	2112	58	0
2	B	837	0	803	12	0
2	G	837	0	803	10	0
3	C	85	0	81	2	0
3	H	85	0	81	3	0
4	D	1579	0	1496	44	0
4	I	1570	0	1481	32	0
5	E	1982	0	1896	32	0
5	J	1982	0	1896	27	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	0	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	14	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	249	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 9.

The worst 5 of 249 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	1.04	1.14
1:A:5:MET:HE1	1:A:171:TYR:CE2	1.95	1.02
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

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.



The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	6	2
4	I	197/200 (98%)	181 (92%)	14 (7%)	2 (1%)	18	10
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%)	38	30

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%)	213 (92%)	19 (8%)	13	7
1	F	233/233 (100%)	211 (91%)	22 (9%)	10	5
2	B	95/95 (100%)	88 (93%)	7 (7%)	16	9
2	G	95/95 (100%)	88 (93%)	7 (7%)	16	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	8/8 (100%)	8 (100%)	0	100	100
3	H	8/8 (100%)	8 (100%)	0	100	100
4	D	181/181 (100%)	164 (91%)	17 (9%)	10	5
4	I	180/181 (99%)	153 (85%)	27 (15%)	3	1
5	E	217/217 (100%)	195 (90%)	22 (10%)	9	4
5	J	217/217 (100%)	201 (93%)	16 (7%)	16	9
All	All	1466/1468 (100%)	1329 (91%)	137 (9%)	10	5

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	224	GLU
1	F	194	VAL
5	J	62	GLU
5	E	244	ARG
1	F	110	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	144	ASN
5	E	235	GLN
5	J	182	GLN
5	E	29	HIS
5	E	156	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 carbohydrates 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	A	301	-	3,3,3	0.90	0	2,2,2	0.97	0
6	EDO	A	302	-	3,3,3	0.56	0	2,2,2	1.82	1 (50%)
6	EDO	A	303	-	3,3,3	0.28	0	2,2,2	0.63	0
7	PG4	A	304	-	9,9,12	0.72	0	8,8,11	0.97	0
8	SO4	A	305	-	4,4,4	0.65	0	6,6,6	0.47	0
6	EDO	B	301	-	3,3,3	0.23	0	2,2,2	0.86	0
6	EDO	B	302	-	3,3,3	0.98	0	2,2,2	0.34	0
9	GOL	B	303	-	5,5,5	0.72	0	5,5,5	0.80	0
6	EDO	D	301	-	3,3,3	0.39	0	2,2,2	0.66	0
6	EDO	D	302	-	3,3,3	0.42	0	2,2,2	0.63	0
6	EDO	D	303	-	3,3,3	0.88	0	2,2,2	0.68	0
6	EDO	E	301	-	3,3,3	0.88	0	2,2,2	0.42	0
6	EDO	E	302	-	3,3,3	0.81	0	2,2,2	0.39	0
6	EDO	E	303	-	3,3,3	0.42	0	2,2,2	0.45	0
6	EDO	E	304	-	3,3,3	0.74	0	2,2,2	0.45	0
6	EDO	E	305	-	3,3,3	0.47	0	2,2,2	0.17	0
6	EDO	E	306	-	3,3,3	0.61	0	2,2,2	0.82	0
6	EDO	F	301	-	3,3,3	0.61	0	2,2,2	0.22	0
6	EDO	F	302	-	3,3,3	0.56	0	2,2,2	0.52	0
6	EDO	F	303	-	3,3,3	0.30	0	2,2,2	1.10	0
6	EDO	F	304	-	3,3,3	0.50	0	2,2,2	0.90	0
6	EDO	F	305	-	3,3,3	0.47	0	2,2,2	0.34	0
6	EDO	F	306	-	3,3,3	0.32	0	2,2,2	0.54	0
6	EDO	F	307	-	3,3,3	0.43	0	2,2,2	0.60	0
9	GOL	F	308	-	5,5,5	0.81	0	5,5,5	1.40	1 (20%)
9	GOL	F	309	-	5,5,5	0.96	0	5,5,5	1.76	2 (40%)
6	EDO	G	101	-	3,3,3	0.60	0	2,2,2	0.26	0
6	EDO	G	102	-	3,3,3	1.67	0	2,2,2	1.55	0
6	EDO	I	301	-	3,3,3	0.86	0	2,2,2	0.34	0
6	EDO	I	302	-	3,3,3	0.74	0	2,2,2	0.81	0
6	EDO	I	303	-	3,3,3	0.56	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	PG4	I	304	-	12,12,12	0.74	0	11,11,11	1.61	3 (27%)
6	EDO	J	301	-	3,3,3	0.67	0	2,2,2	0.39	0
6	EDO	J	302	-	3,3,3	0.37	0	2,2,2	0.65	0
6	EDO	J	303	-	3,3,3	0.61	0	2,2,2	0.91	0
6	EDO	J	304	-	3,3,3	0.65	0	2,2,2	0.31	0
6	EDO	J	305	-	3,3,3	0.32	0	2,2,2	0.48	0
6	EDO	J	306	-	3,3,3	0.48	0	2,2,2	0.80	0
6	EDO	J	307	-	3,3,3	0.85	0	2,2,2	0.48	0
8	SO4	J	308	-	4,4,4	0.65	0	6,6,6	0.73	0
8	SO4	J	309	-	4,4,4	0.89	0	6,6,6	0.53	0
8	SO4	J	310	-	4,4,4	1.13	0	6,6,6	0.60	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	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
7	PG4	A	304	-	-	0/7/7/10	0/0/0/0
8	SO4	A	305	-	-	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
9	GOL	B	303	-	-	0/4/4/4	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	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	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	F	308	-	-	0/4/4/4	0/0/0/0
9	GOL	F	309	-	-	0/4/4/4	0/0/0/0
6	EDO	G	101	-	-	0/1/1/1	0/0/0/0
6	EDO	G	102	-	-	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
7	PG4	I	304	-	-	0/10/10/10	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
6	EDO	J	307	-	-	0/1/1/1	0/0/0/0
8	SO4	J	308	-	-	0/0/0/0	0/0/0/0
8	SO4	J	309	-	-	0/0/0/0	0/0/0/0
8	SO4	J	310	-	-	0/0/0/0	0/0/0/0

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(°)
6	A	302	EDO	O1-C1-C2	-2.57	93.63	112.08
9	F	309	GOL	O2-C2-C1	-2.21	98.42	108.84
9	F	308	GOL	O3-C3-C2	2.08	120.54	110.07
7	I	304	PG4	O2-C3-C4	2.31	121.01	110.41
9	F	309	GOL	O3-C3-C2	2.73	123.82	110.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	301	EDO	4	0
6	A	302	EDO	2	0
7	A	304	PG4	1	0
8	A	305	SO4	1	0
6	D	301	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	302	EDO	2	0
6	E	302	EDO	1	0
6	E	303	EDO	1	0
6	E	306	EDO	1	0
6	F	301	EDO	3	0
6	F	305	EDO	2	0
6	F	306	EDO	1	0
9	F	308	GOL	7	0
9	F	309	GOL	2	0
6	G	102	EDO	1	0
6	I	303	EDO	1	0
7	I	304	PG4	3	0
6	J	303	EDO	1	0
6	J	306	EDO	1	0
8	J	308	SO4	1	0
8	J	309	SO4	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, 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	276/277 (99%)	0.16	5 (1%) 69 71	25, 49, 77, 103	0
1	F	277/277 (100%)	0.23	10 (3%) 43 47	24, 44, 90, 113	0
2	B	100/100 (100%)	-0.03	0 100 100	30, 43, 63, 75	0
2	G	100/100 (100%)	0.01	2 (2%) 65 68	28, 44, 67, 83	0
3	C	10/10 (100%)	-0.16	0 100 100	31, 32, 38, 48	0
3	H	10/10 (100%)	0.01	0 100 100	27, 27, 32, 34	0
4	D	200/200 (100%)	1.19	44 (22%) 1 1	26, 56, 117, 147	0
4	I	199/200 (99%)	0.98	39 (19%) 1 1	30, 58, 110, 123	0
5	E	247/247 (100%)	0.78	29 (11%) 5 6	23, 51, 94, 119	0
5	J	247/247 (100%)	0.18	8 (3%) 48 51	24, 43, 81, 107	0
All	All	1666/1668 (99%)	0.47	137 (8%) 12 14	23, 47, 98, 147	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	200	PRO	12.2
4	D	151	SER	8.2
4	D	199	PHE	8.1
4	I	199	PHE	7.8
4	I	201	SER	7.6

### 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
6	EDO	J	304	4/4	0.80	0.33	16.15	36,51,53,59	0
7	PG4	A	304	10/13	0.74	0.31	15.01	52,64,73,75	0
6	EDO	F	301	4/4	0.88	0.22	11.02	54,57,61,66	0
8	SO4	J	309	5/5	0.74	0.39	10.00	55,74,82,114	0
6	EDO	A	301	4/4	0.98	0.21	9.00	34,39,40,42	0
9	GOL	F	309	6/6	0.79	0.26	8.92	42,62,65,70	0
6	EDO	I	303	4/4	0.91	0.19	7.06	55,59,64,64	0
7	PG4	I	304	13/13	0.83	0.22	7.04	47,56,71,72	0
9	GOL	B	303	6/6	0.82	0.20	6.07	49,56,60,65	0
6	EDO	F	302	4/4	0.90	0.17	4.49	46,54,57,62	0
9	GOL	F	308	6/6	0.81	0.20	4.17	51,58,66,66	0
6	EDO	G	102	4/4	0.70	0.19	2.93	43,49,54,56	0
6	EDO	E	303	4/4	0.84	0.19	2.86	56,60,61,67	0
6	EDO	J	303	4/4	0.80	0.16	2.52	50,62,64,67	0
6	EDO	A	302	4/4	0.92	0.15	2.51	34,37,47,51	0
6	EDO	A	303	4/4	0.94	0.15	2.37	62,67,70,79	0
6	EDO	F	306	4/4	0.98	0.15	2.25	43,50,51,55	0
6	EDO	I	301	4/4	0.87	0.14	2.17	42,43,47,53	0
6	EDO	E	301	4/4	0.96	0.15	2.12	27,31,34,39	0
8	SO4	J	310	5/5	0.91	0.20	1.97	50,56,67,71	0
6	EDO	J	301	4/4	0.96	0.14	1.93	29,29,34,36	0
8	SO4	A	305	5/5	0.90	0.17	1.58	65,66,73,80	0
6	EDO	B	301	4/4	0.93	0.12	1.49	45,46,47,51	0
6	EDO	F	304	4/4	0.89	0.13	1.44	43,49,50,60	0
6	EDO	E	302	4/4	0.95	0.13	1.22	32,35,41,46	0
6	EDO	G	101	4/4	0.95	0.13	0.82	39,42,43,46	0
6	EDO	B	302	4/4	0.84	0.13	0.80	43,45,49,58	0
8	SO4	J	308	5/5	0.93	0.15	0.70	60,75,81,85	0
6	EDO	F	307	4/4	0.92	0.12	0.15	40,50,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	I	302	4/4	0.93	0.12	-0.09	47,47,48,53	0
6	EDO	J	307	4/4	0.96	0.10	-0.14	27,34,36,42	0
6	EDO	E	305	4/4	0.93	0.10	-0.68	50,55,56,56	0
6	EDO	J	302	4/4	0.94	0.10	-0.81	50,52,52,55	0
6	EDO	D	302	4/4	0.78	0.13	-1.14	69,69,71,78	0
6	EDO	F	303	4/4	0.87	0.15	-	66,67,71,75	0
6	EDO	J	306	4/4	0.86	0.14	-	54,60,62,67	0
6	EDO	F	305	4/4	0.88	0.13	-	54,59,62,67	0
6	EDO	J	305	4/4	0.88	0.09	-	60,61,61,69	0
6	EDO	E	304	4/4	0.80	0.12	-	60,61,61,62	0
6	EDO	D	301	4/4	0.90	0.18	-	54,61,61,66	0
6	EDO	D	303	4/4	0.50	0.28	-	52,65,67,72	0
6	EDO	E	306	4/4	0.87	0.14	-	51,53,53,54	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.