



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 10:57 pm GMT

PDB ID : 5C08  
Title : 1E6 TCR in Complex with HLA-A0e carrying RQWGPDPAAV  
Authors : Rizkallah, P.J.; Bulek, A.M.; Cole, D.K.; Sewell, A.K.  
Deposited on : 2015-06-12  
Resolution : 2.33 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

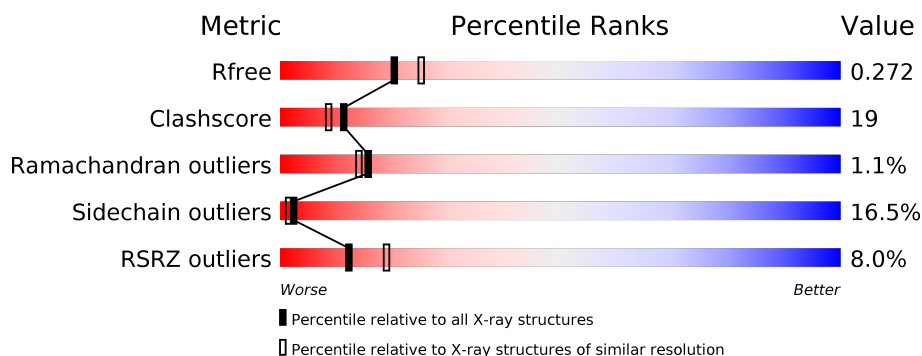
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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))
$R_{free}$	111664	1763 (2.36-2.32)
Clashscore	122126	1858 (2.36-2.32)
Ramachandran outliers	120053	1834 (2.36-2.32)
Sidechain outliers	120020	1835 (2.36-2.32)
RSRZ outliers	108989	1737 (2.36-2.32)

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	276	<div> <div>4%</div> <div> <div>64%</div> <div>26%</div> <div>8%</div> </div> </div>
1	F	276	<div> <div>3%</div> <div> <div>57%</div> <div>32%</div> <div>9%</div> </div> </div>
2	B	100	<div> <div>%</div> <div> <div>62%</div> <div>32%</div> <div>5%</div> </div> </div>
2	G	100	<div> <div>69%</div> <div>25%</div> <div>6%</div> </div>
3	C	10	<div> <div>80%</div> <div>20%</div> </div>
3	H	10	<div> <div>80%</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	191	
4	I	191	
5	E	245	
5	J	245	

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	F	301	-	-	X	-
6	EDO	F	303	-	-	X	-
8	SO4	J	305	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13627 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	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	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	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
			78	49	15	14			
3	H	10	Total	C	N	O	0	0	0
			78	49	15	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	189	Total	C	N	O	S	0	0	0
			1488	927	248	303	10			

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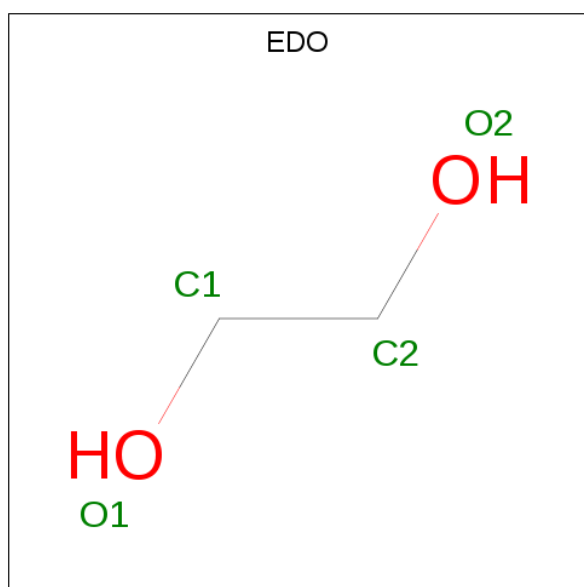
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	191	Total	C	N	O	S	0	0	0
			1501	936	250	305	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	244	Total	C	N	O	S	0	0	0
			1961	1242	339	370	10			
5	J	245	Total	C	N	O	S	0	0	0
			1966	1245	340	371	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	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	C	1	Total	C	O	0	0
			4	2	2		

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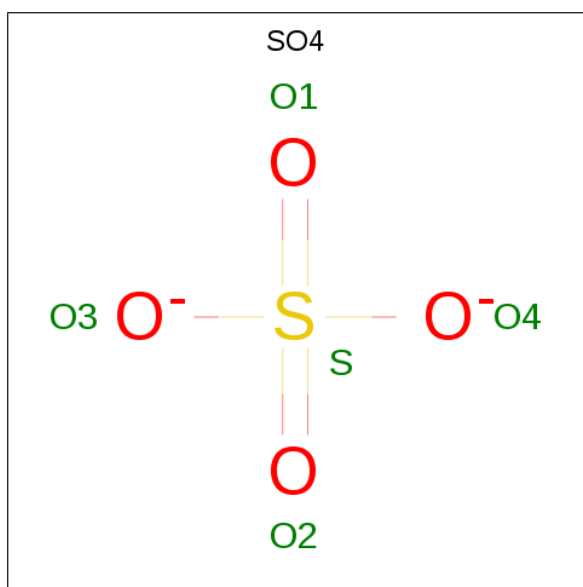
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total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

- 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	D	1	Total	C	O	0	0
			6	3	3		
7	E	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	D	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 9 is water.

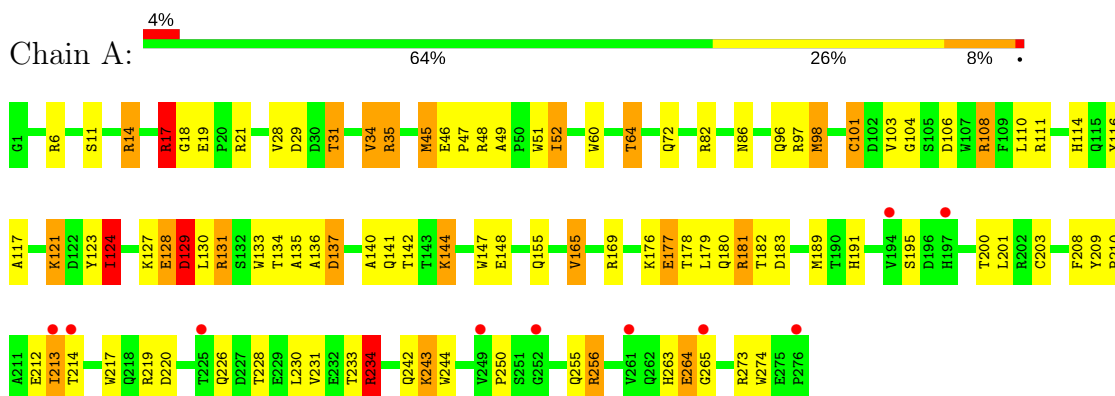
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	35	Total	O	0	0
			35	35		
9	B	18	Total	O	0	0
			18	18		
9	C	6	Total	O	0	0
			6	6		
9	D	21	Total	O	0	0
			21	21		
9	E	32	Total	O	0	0
			32	32		
9	F	33	Total	O	0	0
			33	33		
9	G	15	Total	O	0	0
			15	15		
9	H	5	Total	O	0	0
			5	5		
9	I	16	Total	O	0	0
			16	16		
9	J	39	Total	O	0	0
			39	39		



### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

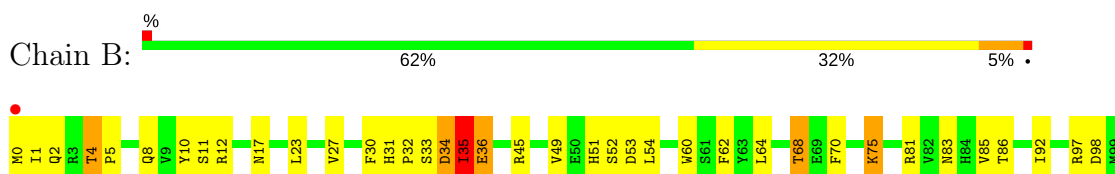
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



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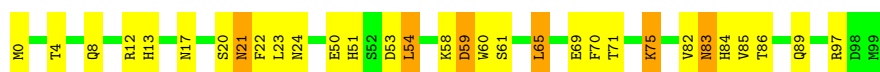


- Molecule 2: Beta-2-microglobulin

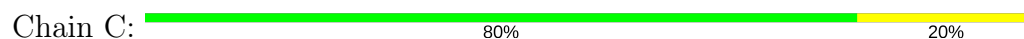


- Molecule 2: Beta-2-microglobulin





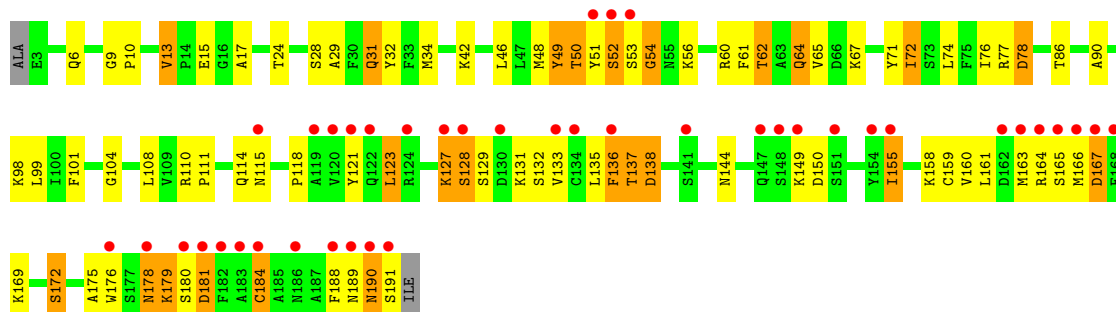
- Molecule 3: Marker peptide



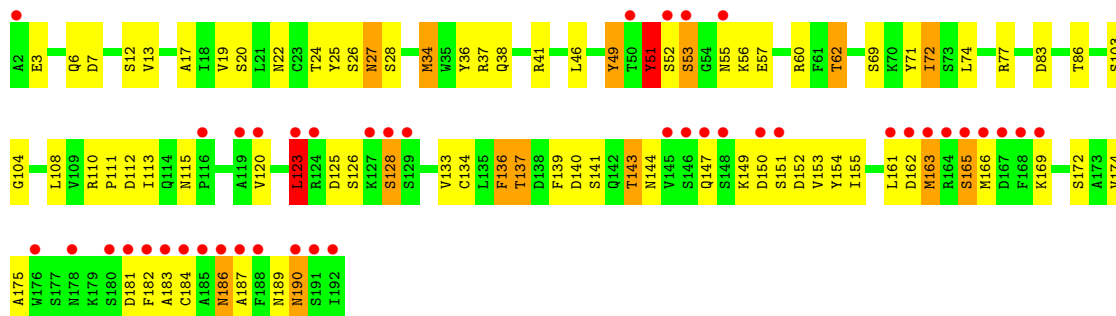
- Molecule 3: Marker peptide



- Molecule 4: 1E6 TCR Alpha Chain

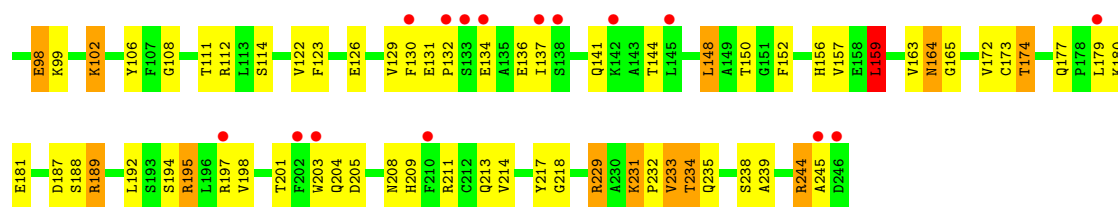


- Molecule 4: 1E6 TCR Alpha Chain

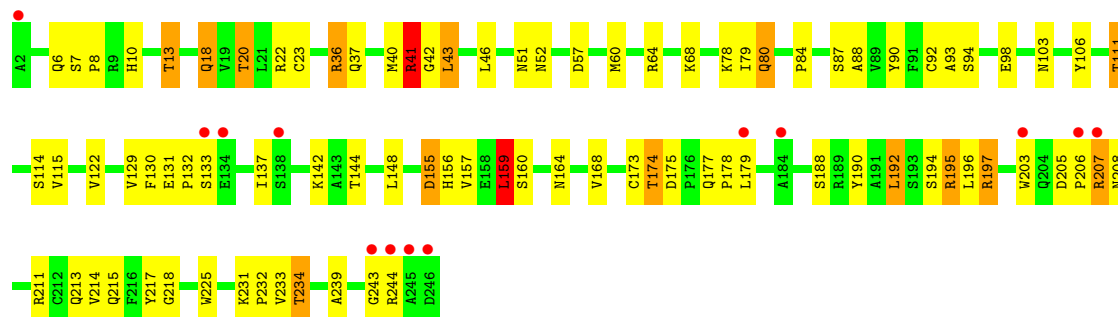


- Molecule 5: 1E6 TCR Beta Chain





### • Molecule 5: 1E6 TCR Beta Chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.80Å 99.26Å 122.15Å 96.33° 98.07° 96.42°	Depositor
Resolution (Å)	48.91 – 2.33 48.91 – 2.33	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.91-2.33) 97.4 (48.91-2.33)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.206 , 0.272 0.206 , 0.272	Depositor DCC
$R_{free}$ test set	4159 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.5	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.1	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	0.95	EDS
Total number of atoms	13627	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.75	0/2320	0.98	9/3149 (0.3%)
1	F	0.76	0/2320	0.97	11/3149 (0.3%)
2	B	0.75	0/860	0.93	1/1162 (0.1%)
2	G	0.77	0/860	0.99	1/1162 (0.1%)
3	C	0.98	0/81	1.05	0/110
3	H	0.74	0/81	0.95	1/110 (0.9%)
4	D	0.74	0/1520	0.97	3/2055 (0.1%)
4	I	0.80	1/1533 (0.1%)	0.97	3/2073 (0.1%)
5	E	0.74	1/2016 (0.0%)	0.94	5/2741 (0.2%)
5	J	0.80	1/2021 (0.0%)	1.00	10/2748 (0.4%)
All	All	0.76	3/13612 (0.0%)	0.97	44/18459 (0.2%)

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
1	A	0	2
1	F	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	94	SER	CB-OG	-8.10	1.31	1.42
4	I	36	TYR	CG-CD2	5.37	1.46	1.39
5	E	58	SER	CB-OG	-5.12	1.35	1.42

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	21	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	F	110	LEU	CA-CB-CG	8.20	134.17	115.30
1	A	230	LEU	CA-CB-CG	7.45	132.44	115.30
5	J	36	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	F	101	CYS	CB-CA-C	-7.32	95.76	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	ARG	Peptide
1	A	136	ALA	Peptide
1	F	100	GLY	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	82	0
1	F	2254	0	2103	101	0
2	B	837	0	803	35	0
2	G	837	0	803	27	0
3	C	78	0	73	0	0
3	H	78	0	73	1	0
4	D	1488	0	1405	75	0
4	I	1501	0	1421	68	0
5	E	1961	0	1875	78	0
5	J	1966	0	1880	60	0
6	A	8	0	12	3	0
6	B	12	0	18	8	0
6	C	4	0	6	0	0
6	D	4	0	6	0	0
6	E	20	0	30	4	0
6	F	16	0	24	9	0
6	G	4	0	6	2	0
6	I	20	0	30	8	0
6	J	12	0	18	2	0
7	A	6	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	6	0	8	3	0
7	E	6	0	8	2	0
8	D	10	0	0	0	0
8	E	10	0	0	1	0
8	F	5	0	0	0	0
8	J	10	0	0	0	0
9	A	35	0	0	0	0
9	B	18	0	0	0	0
9	C	6	0	0	0	0
9	D	21	0	0	0	0
9	E	32	0	0	0	0
9	F	33	0	0	4	0
9	G	15	0	0	1	0
9	H	5	0	0	0	0
9	I	16	0	0	1	0
9	J	39	0	0	3	0
All	All	13627	0	12713	495	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 19.

The worst 5 of 495 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)
5:E:40:MET:CE	5:E:41:ARG:HH21	1.56	1.17
5:E:218:GLY:H	5:E:234:THR:HG22	1.04	1.16
5:E:40:MET:HE2	5:E:41:ARG:HH21	1.03	1.10
2:G:75:LYS:H	2:G:75:LYS:HE3	1.12	1.10
4:I:60:ARG:HD3	6:I:203:EDO:H21	1.14	1.06

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	274/276 (99%)	267 (97%)	4 (2%)	3 (1%)	16	14
1	F	274/276 (99%)	265 (97%)	9 (3%)	0	100	100
2	B	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	G	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
3	H	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
4	D	187/191 (98%)	168 (90%)	12 (6%)	7 (4%)	4	1
4	I	189/191 (99%)	172 (91%)	11 (6%)	6 (3%)	4	2
5	E	242/245 (99%)	225 (93%)	15 (6%)	2 (1%)	21	22
5	J	243/245 (99%)	236 (97%)	7 (3%)	0	100	100
All	All	1621/1644 (99%)	1533 (95%)	70 (4%)	18 (1%)	16	14

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	128	SER
4	D	167	ASP
4	D	181	ASP
4	I	51	TYR
4	I	152	ASP

### 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	232/232 (100%)	191 (82%)	41 (18%)	2	1
1	F	232/232 (100%)	186 (80%)	46 (20%)	1	1
2	B	95/95 (100%)	82 (86%)	13 (14%)	4	3
2	G	95/95 (100%)	79 (83%)	16 (17%)	2	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	7/7 (100%)	5 (71%)	2 (29%)	0	0
3	H	7/7 (100%)	7 (100%)	0	100	100
4	D	170/171 (99%)	137 (81%)	33 (19%)	1	1
4	I	171/171 (100%)	142 (83%)	29 (17%)	2	1
5	E	215/215 (100%)	185 (86%)	30 (14%)	4	3
5	J	215/215 (100%)	187 (87%)	28 (13%)	4	4
All	All	1439/1440 (100%)	1201 (84%)	238 (16%)	2	1

5 of 238 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	189	ARG
1	F	101	CYS
5	J	68	LYS
5	E	198	VAL
1	F	25	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	164	ASN
1	F	86	ASN
5	J	139	HIS
5	E	209	HIS
1	F	70	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

35 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	0.57	0	2,2,2	0.66	0
6	EDO	A	302	-	3,3,3	0.53	0	2,2,2	0.42	0
7	GOL	A	303	-	5,5,5	0.78	0	5,5,5	1.31	0
6	EDO	B	301	-	3,3,3	0.35	0	2,2,2	0.46	0
6	EDO	B	302	-	3,3,3	0.64	0	2,2,2	0.18	0
6	EDO	B	303	-	3,3,3	0.40	0	2,2,2	0.57	0
6	EDO	C	101	-	3,3,3	0.52	0	2,2,2	0.39	0
6	EDO	D	201	-	3,3,3	0.43	0	2,2,2	1.05	0
7	GOL	D	202	-	5,5,5	0.40	0	5,5,5	0.55	0
8	SO4	D	203	-	4,4,4	0.52	0	6,6,6	0.13	0
8	SO4	D	204	-	4,4,4	0.61	0	6,6,6	0.55	0
6	EDO	E	301	-	3,3,3	0.62	0	2,2,2	0.26	0
6	EDO	E	302	-	3,3,3	0.45	0	2,2,2	0.50	0
6	EDO	E	303	-	3,3,3	0.46	0	2,2,2	0.54	0
6	EDO	E	304	-	3,3,3	0.65	0	2,2,2	0.76	0
6	EDO	E	305	-	3,3,3	0.72	0	2,2,2	0.06	0
7	GOL	E	306	-	5,5,5	0.46	0	5,5,5	0.65	0
8	SO4	E	307	-	4,4,4	0.57	0	6,6,6	0.43	0
8	SO4	E	308	-	4,4,4	0.47	0	6,6,6	0.43	0
6	EDO	F	301	-	3,3,3	0.72	0	2,2,2	0.50	0
6	EDO	F	302	-	3,3,3	0.53	0	2,2,2	0.65	0
6	EDO	F	303	-	3,3,3	0.73	0	2,2,2	0.74	0
6	EDO	F	304	-	3,3,3	0.69	0	2,2,2	0.17	0
8	SO4	F	305	-	4,4,4	0.55	0	6,6,6	0.28	0
6	EDO	G	101	-	3,3,3	0.53	0	2,2,2	0.31	0
6	EDO	I	201	-	3,3,3	0.43	0	2,2,2	0.77	0
6	EDO	I	202	-	3,3,3	0.65	0	2,2,2	0.24	0
6	EDO	I	203	-	3,3,3	0.75	0	2,2,2	0.34	0
6	EDO	I	204	-	3,3,3	0.60	0	2,2,2	0.26	0
6	EDO	I	205	-	3,3,3	0.72	0	2,2,2	0.42	0
6	EDO	J	301	-	3,3,3	0.50	0	2,2,2	0.34	0
6	EDO	J	302	-	3,3,3	0.53	0	2,2,2	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	J	303	-	3,3,3	0.72	0	2,2,2	0.58	0
8	SO4	J	304	-	4,4,4	0.58	0	6,6,6	0.33	0
8	SO4	J	305	-	4,4,4	0.67	0	6,6,6	0.28	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
7	GOL	A	303	-	-	0/4/4/4	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	C	101	-	-	0/1/1/1	0/0/0/0
6	EDO	D	201	-	-	0/1/1/1	0/0/0/0
7	GOL	D	202	-	-	0/4/4/4	0/0/0/0
8	SO4	D	203	-	-	0/0/0/0	0/0/0/0
8	SO4	D	204	-	-	0/0/0/0	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
7	GOL	E	306	-	-	0/4/4/4	0/0/0/0
8	SO4	E	307	-	-	0/0/0/0	0/0/0/0
8	SO4	E	308	-	-	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
8	SO4	F	305	-	-	0/0/0/0	0/0/0/0
6	EDO	G	101	-	-	0/1/1/1	0/0/0/0
6	EDO	I	201	-	-	0/1/1/1	0/0/0/0
6	EDO	I	202	-	-	0/1/1/1	0/0/0/0
6	EDO	I	203	-	-	0/1/1/1	0/0/0/0
6	EDO	I	204	-	-	0/1/1/1	0/0/0/0
6	EDO	I	205	-	-	0/1/1/1	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SO4	J	304	-	-	0/0/0/0	0/0/0/0
8	SO4	J	305	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	302	EDO	3	0
7	A	303	GOL	3	0
6	B	301	EDO	2	0
6	B	302	EDO	3	0
6	B	303	EDO	3	0
7	D	202	GOL	3	0
6	E	301	EDO	1	0
6	E	303	EDO	3	0
7	E	306	GOL	2	0
8	E	308	SO4	1	0
6	F	301	EDO	4	0
6	F	302	EDO	1	0
6	F	303	EDO	4	0
6	G	101	EDO	2	0
6	I	201	EDO	2	0
6	I	203	EDO	3	0
6	I	204	EDO	1	0
6	I	205	EDO	2	0
6	J	303	EDO	2	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	276/276 (100%)	0.36	10 (3%) 42 53	24, 48, 97, 125	0
1	F	276/276 (100%)	0.34	9 (3%) 46 57	24, 52, 88, 101	0
2	B	100/100 (100%)	-0.02	1 (1%) 82 88	31, 46, 65, 98	0
2	G	100/100 (100%)	0.04	0 100 100	32, 45, 66, 74	0
3	C	10/10 (100%)	0.18	0 100 100	27, 29, 33, 45	0
3	H	10/10 (100%)	0.06	0 100 100	29, 32, 33, 44	0
4	D	189/191 (98%)	1.09	41 (21%) 0 1	29, 55, 124, 140	0
4	I	191/191 (100%)	0.98	42 (21%) 0 1	28, 55, 119, 141	0
5	E	244/245 (99%)	0.46	15 (6%) 21 30	21, 52, 107, 128	0
5	J	245/245 (100%)	0.28	13 (5%) 26 37	22, 46, 85, 111	0
All	All	1641/1644 (99%)	0.47	131 (7%) 12 19	21, 49, 105, 141	0

The worst 5 of 131 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	191	SER	12.0
4	D	190	ASN	11.2
4	I	191	SER	8.8
5	E	138	SER	8.1
4	I	128	SER	7.8

### 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
8	SO4	J	305	5/5	0.66	0.41	75,79,97,97	0
6	EDO	F	304	4/4	0.67	0.26	62,63,72,75	0
6	EDO	F	301	4/4	0.77	0.21	55,56,57,60	0
6	EDO	I	203	4/4	0.77	0.16	39,48,50,51	0
6	EDO	J	301	4/4	0.79	0.21	65,76,76,79	0
7	GOL	D	202	6/6	0.81	0.18	49,68,70,73	0
6	EDO	G	101	4/4	0.81	0.17	52,52,54,57	0
6	EDO	E	301	4/4	0.82	0.25	59,67,69,71	0
6	EDO	E	305	4/4	0.82	0.21	48,55,56,62	0
8	SO4	F	305	5/5	0.82	0.25	96,97,104,113	0
7	GOL	A	303	6/6	0.83	0.31	38,55,56,65	0
6	EDO	F	303	4/4	0.84	0.26	43,48,51,55	0
6	EDO	I	202	4/4	0.85	0.21	53,54,60,61	0
6	EDO	E	302	4/4	0.86	0.22	50,54,55,65	0
6	EDO	E	303	4/4	0.87	0.19	61,61,64,67	0
8	SO4	E	307	5/5	0.87	0.23	62,70,80,84	0
6	EDO	B	302	4/4	0.88	0.14	58,62,63,69	0
8	SO4	E	308	5/5	0.88	0.24	74,83,92,94	0
6	EDO	I	204	4/4	0.90	0.13	43,44,45,48	0
6	EDO	I	205	4/4	0.90	0.20	34,36,39,64	0
8	SO4	J	304	5/5	0.90	0.24	77,80,82,87	0
6	EDO	A	302	4/4	0.91	0.26	46,58,64,68	0
6	EDO	A	301	4/4	0.91	0.15	49,53,65,65	0
6	EDO	F	302	4/4	0.91	0.22	39,45,45,51	0
6	EDO	B	301	4/4	0.92	0.19	43,48,51,55	0
8	SO4	D	203	5/5	0.92	0.16	84,85,91,92	0
6	EDO	C	101	4/4	0.92	0.17	37,40,42,45	0
8	SO4	D	204	5/5	0.92	0.25	72,73,82,88	0
6	EDO	E	304	4/4	0.93	0.16	35,41,44,45	0
6	EDO	B	303	4/4	0.93	0.17	48,49,53,58	0
6	EDO	J	303	4/4	0.94	0.14	35,40,41,46	0
6	EDO	I	201	4/4	0.95	0.13	40,46,47,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	D	201	4/4	0.96	0.14	41,43,47,48	0
6	EDO	J	302	4/4	0.96	0.16	34,39,45,49	0
7	GOL	E	306	6/6	0.97	0.14	39,42,43,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.