



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2025 – 12:13 PM JST

PDB ID : 9WBD / pdb\_00009wbd  
Title : Crystal structure of HLA-B\*07:02 in complex with SPR epitope and Q04 TCR  
Authors : Ping, Y.; Daichao, W.  
Deposited on : 2025-08-13  
Resolution : 2.75 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

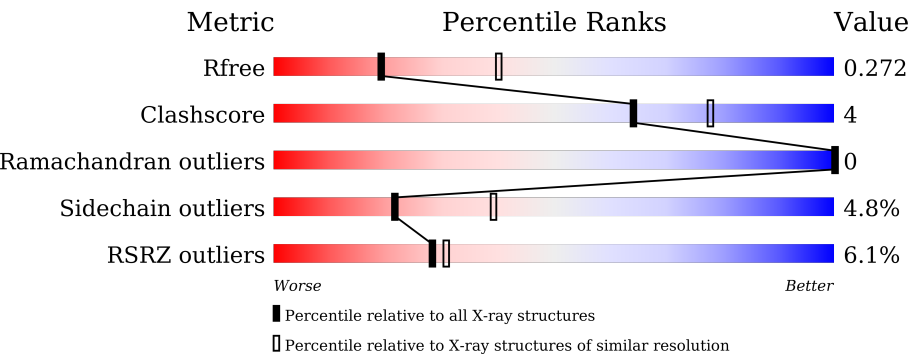
MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	206	<div><div>13%</div><div><div></div><div>78%</div><div>15%</div><div>7%</div></div></div>
1	F	206	<div><div>2%</div><div><div></div><div>83%</div><div>12%</div><div>3%</div></div></div>
1	K	206	<div><div>16%</div><div><div></div><div>80%</div><div>11%</div><div>7%</div></div></div>
1	P	206	<div><div></div><div><div></div><div>83%</div><div>15%</div><div>2%</div></div></div>
2	B	243	<div><div>2%</div><div><div></div><div>88%</div><div>11%</div><div>1%</div></div></div>
2	G	243	<div><div>4%</div><div><div></div><div>84%</div><div>13%</div><div>3%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	L	243	
2	Q	243	
3	C	276	
3	H	276	
3	M	276	
3	R	276	
4	D	100	
4	I	100	
4	N	100	
4	S	100	
5	E	9	
5	J	9	
5	O	9	
5	T	9	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25365 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 T cell receptor alpha variable 25,T cell receptor alpha chain constant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1447	918	238	284	7			
1	F	198	Total	C	N	O	S	0	0	0
			1515	959	248	300	8			
1	K	192	Total	C	N	O	S	0	0	0
			1453	916	241	288	8			
1	P	204	Total	C	N	O	S	0	0	0
			1582	993	261	320	8			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A0B4J276
A	93	TYR	-	linker	UNP A0A0B4J276
A	94	THR	-	linker	UNP A0A0B4J276
A	95	SER	-	linker	UNP A0A0B4J276
A	96	GLY	-	linker	UNP A0A0B4J276
A	97	THR	-	linker	UNP A0A0B4J276
A	98	TYR	-	linker	UNP A0A0B4J276
A	99	LYS	-	linker	UNP A0A0B4J276
A	100	TYR	-	linker	UNP A0A0B4J276
A	101	ILE	-	linker	UNP A0A0B4J276
A	102	PHE	-	linker	UNP A0A0B4J276
A	103	GLY	-	linker	UNP A0A0B4J276
A	104	THR	-	linker	UNP A0A0B4J276
A	105	GLY	-	linker	UNP A0A0B4J276
A	106	THR	-	linker	UNP A0A0B4J276
A	107	ARG	-	linker	UNP A0A0B4J276
A	108	LEU	-	linker	UNP A0A0B4J276
A	109	LYS	-	linker	UNP A0A0B4J276
A	110	VAL	-	linker	UNP A0A0B4J276
A	111	LEU	-	linker	UNP A0A0B4J276

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Chain	Residue	Modelled	Actual	Comment	Reference
A	112	ALA	-	linker	UNP A0A0B4J276
A	113	ASN	-	linker	UNP A0A0B4J276
A	160	CYS	THR	conflict	UNP P01848
F	1	MET	-	initiating methionine	UNP A0A0B4J276
F	93	TYR	-	linker	UNP A0A0B4J276
F	94	THR	-	linker	UNP A0A0B4J276
F	95	SER	-	linker	UNP A0A0B4J276
F	96	GLY	-	linker	UNP A0A0B4J276
F	97	THR	-	linker	UNP A0A0B4J276
F	98	TYR	-	linker	UNP A0A0B4J276
F	99	LYS	-	linker	UNP A0A0B4J276
F	100	TYR	-	linker	UNP A0A0B4J276
F	101	ILE	-	linker	UNP A0A0B4J276
F	102	PHE	-	linker	UNP A0A0B4J276
F	103	GLY	-	linker	UNP A0A0B4J276
F	104	THR	-	linker	UNP A0A0B4J276
F	105	GLY	-	linker	UNP A0A0B4J276
F	106	THR	-	linker	UNP A0A0B4J276
F	107	ARG	-	linker	UNP A0A0B4J276
F	108	LEU	-	linker	UNP A0A0B4J276
F	109	LYS	-	linker	UNP A0A0B4J276
F	110	VAL	-	linker	UNP A0A0B4J276
F	111	LEU	-	linker	UNP A0A0B4J276
F	112	ALA	-	linker	UNP A0A0B4J276
F	113	ASN	-	linker	UNP A0A0B4J276
F	160	CYS	THR	conflict	UNP P01848
K	1	MET	-	initiating methionine	UNP A0A0B4J276
K	93	TYR	-	linker	UNP A0A0B4J276
K	94	THR	-	linker	UNP A0A0B4J276
K	95	SER	-	linker	UNP A0A0B4J276
K	96	GLY	-	linker	UNP A0A0B4J276
K	97	THR	-	linker	UNP A0A0B4J276
K	98	TYR	-	linker	UNP A0A0B4J276
K	99	LYS	-	linker	UNP A0A0B4J276
K	100	TYR	-	linker	UNP A0A0B4J276
K	101	ILE	-	linker	UNP A0A0B4J276
K	102	PHE	-	linker	UNP A0A0B4J276
K	103	GLY	-	linker	UNP A0A0B4J276
K	104	THR	-	linker	UNP A0A0B4J276
K	105	GLY	-	linker	UNP A0A0B4J276
K	106	THR	-	linker	UNP A0A0B4J276
K	107	ARG	-	linker	UNP A0A0B4J276

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Chain	Residue	Modelled	Actual	Comment	Reference
K	108	LEU	-	linker	UNP A0A0B4J276
K	109	LYS	-	linker	UNP A0A0B4J276
K	110	VAL	-	linker	UNP A0A0B4J276
K	111	LEU	-	linker	UNP A0A0B4J276
K	112	ALA	-	linker	UNP A0A0B4J276
K	113	ASN	-	linker	UNP A0A0B4J276
K	160	CYS	THR	conflict	UNP P01848
P	1	MET	-	initiating methionine	UNP A0A0B4J276
P	93	TYR	-	linker	UNP A0A0B4J276
P	94	THR	-	linker	UNP A0A0B4J276
P	95	SER	-	linker	UNP A0A0B4J276
P	96	GLY	-	linker	UNP A0A0B4J276
P	97	THR	-	linker	UNP A0A0B4J276
P	98	TYR	-	linker	UNP A0A0B4J276
P	99	LYS	-	linker	UNP A0A0B4J276
P	100	TYR	-	linker	UNP A0A0B4J276
P	101	ILE	-	linker	UNP A0A0B4J276
P	102	PHE	-	linker	UNP A0A0B4J276
P	103	GLY	-	linker	UNP A0A0B4J276
P	104	THR	-	linker	UNP A0A0B4J276
P	105	GLY	-	linker	UNP A0A0B4J276
P	106	THR	-	linker	UNP A0A0B4J276
P	107	ARG	-	linker	UNP A0A0B4J276
P	108	LEU	-	linker	UNP A0A0B4J276
P	109	LYS	-	linker	UNP A0A0B4J276
P	110	VAL	-	linker	UNP A0A0B4J276
P	111	LEU	-	linker	UNP A0A0B4J276
P	112	ALA	-	linker	UNP A0A0B4J276
P	113	ASN	-	linker	UNP A0A0B4J276
P	160	CYS	THR	conflict	UNP P01848

- Molecule 2 is a protein called TCR beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1877	1183	329	360	5			
2	G	241	Total	C	N	O	S	0	0	0
			1851	1170	323	353	5			
2	L	241	Total	C	N	O	S	0	0	0
			1860	1172	329	354	5			
2	Q	242	Total	C	N	O	S	0	0	0
			1867	1177	328	357	5			

- Molecule 3 is a protein called HLA class I histocompatibility antigen, B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	271	Total	C	N	O	S	0	0	0
			2106	1320	377	403	6			
3	H	273	Total	C	N	O	S	0	0	0
			2160	1351	386	417	6			
3	M	240	Total	C	N	O	S	0	0	0
			1917	1201	342	368	6			
3	R	267	Total	C	N	O	S	0	0	0
			2067	1294	367	400	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP P01889
H	0	MET	-	initiating methionine	UNP P01889
M	0	MET	-	initiating methionine	UNP P01889
R	0	MET	-	initiating methionine	UNP P01889

- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	100	Total	C	N	O	S	0	0	0
			813	518	138	153	4			
4	I	100	Total	C	N	O	S	0	0	0
			813	517	136	156	4			
4	N	100	Total	C	N	O	S	0	0	0
			809	515	137	153	4			
4	S	100	Total	C	N	O	S	0	0	0
			813	515	135	159	4			

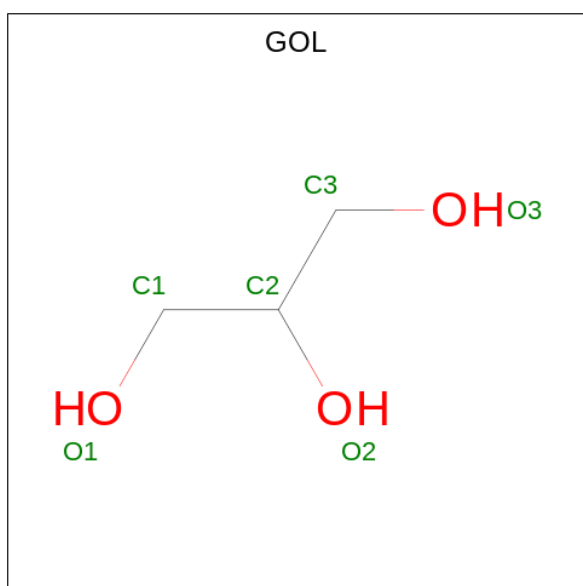
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP P61769
I	0	MET	-	initiating methionine	UNP P61769
N	0	MET	-	initiating methionine	UNP P61769
S	0	MET	-	initiating methionine	UNP P61769

- Molecule 5 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	9	Total	C	N	O	0	0	0
			94	67	13	14			
5	J	9	Total	C	N	O	0	0	0
			94	67	13	14			
5	O	9	Total	C	N	O	0	0	0
			94	67	13	14			
5	T	9	Total	C	N	O	0	0	0
			94	67	13	14			

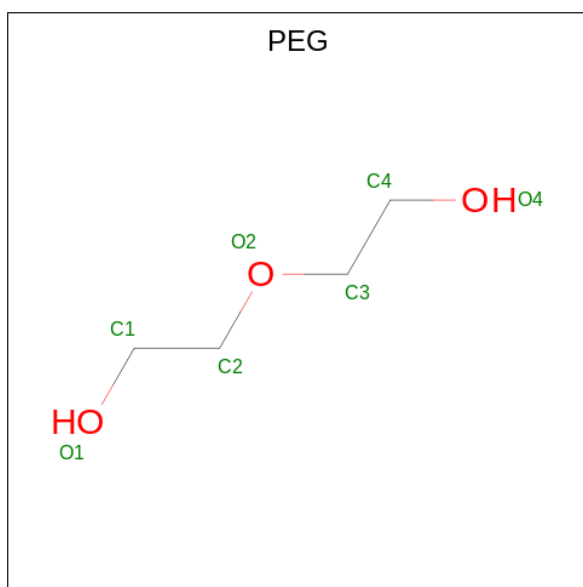
- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	L	1	Total	C	O	0	0
			6	3	3		
6	Q	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	C	O	0	0
			7	4	3		

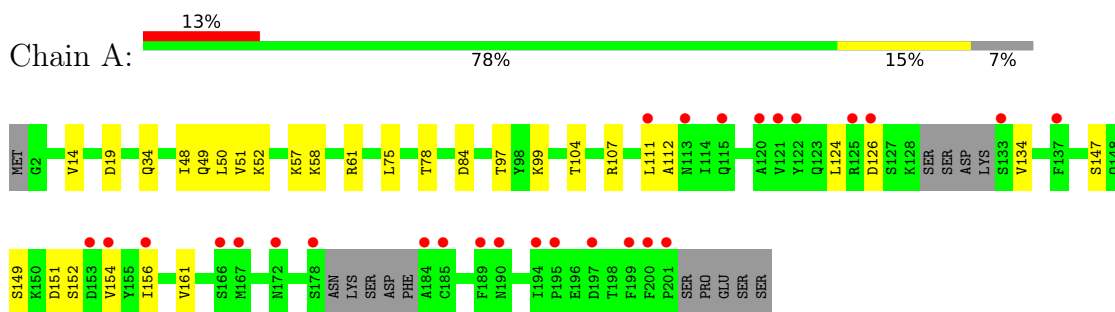
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	4	Total	O	0	0
			4	4		
8	H	4	Total	O	0	0
			4	4		
8	M	2	Total	O	0	0
			2	2		
8	R	4	Total	O	0	0
			4	4		

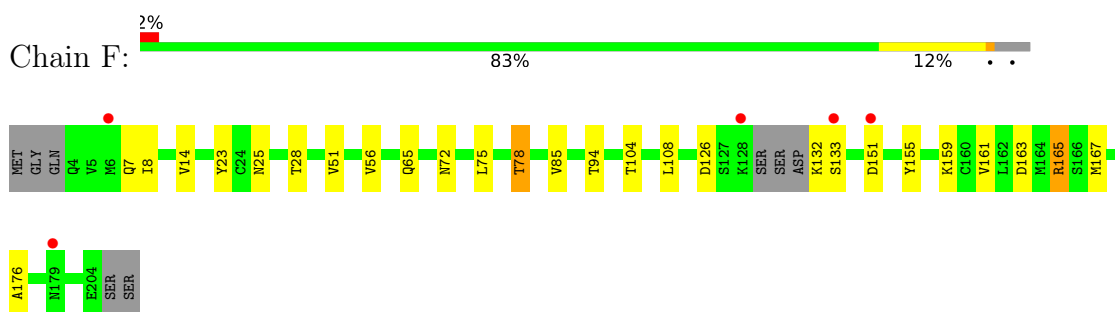
### 3 Residue-property plots [i](#)

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

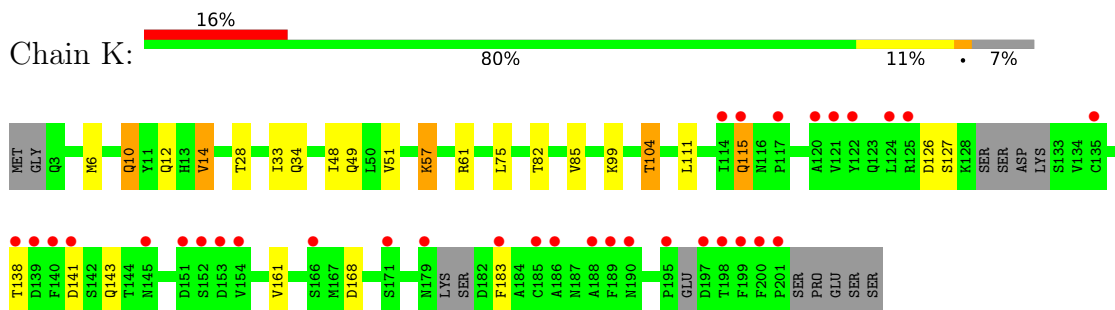
- Molecule 1: T cell receptor alpha variable 25,T cell receptor alpha chain constant



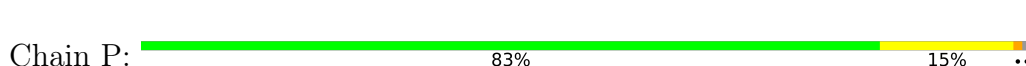
- Molecule 1: T cell receptor alpha variable 25,T cell receptor alpha chain constant

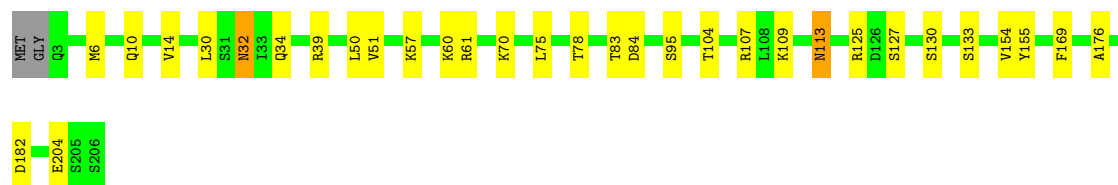


- Molecule 1: T cell receptor alpha variable 25,T cell receptor alpha chain constant

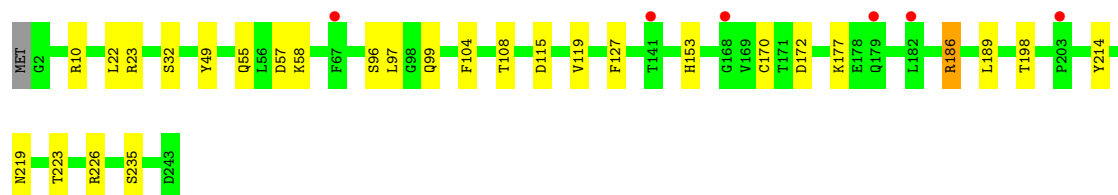
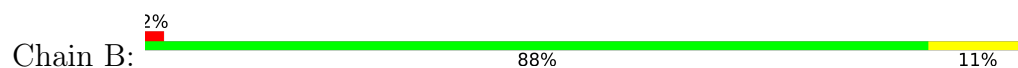


- Molecule 1: T cell receptor alpha variable 25,T cell receptor alpha chain constant

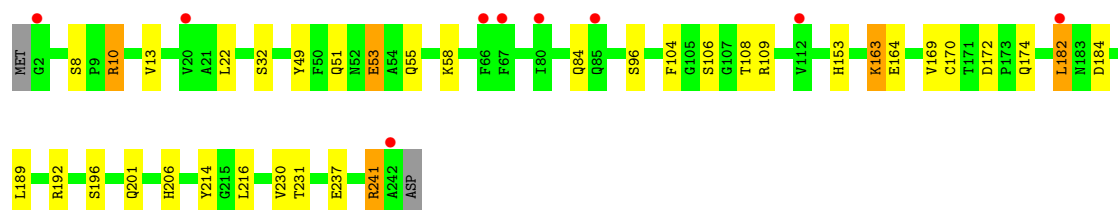
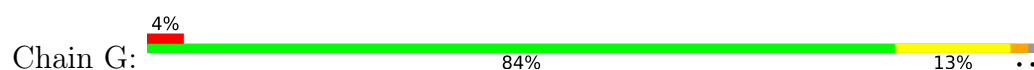




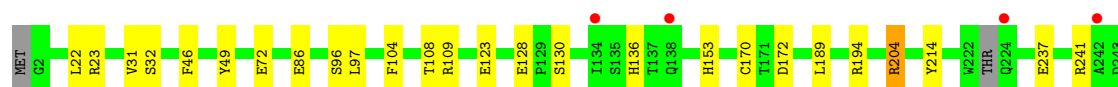
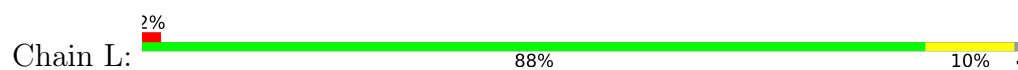
• Molecule 2: TCR beta



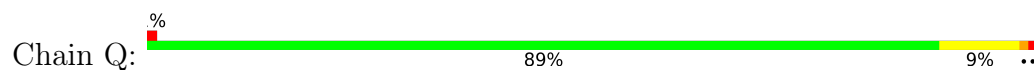
• Molecule 2: TCR beta



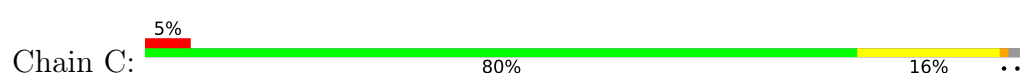
• Molecule 2: TCR beta

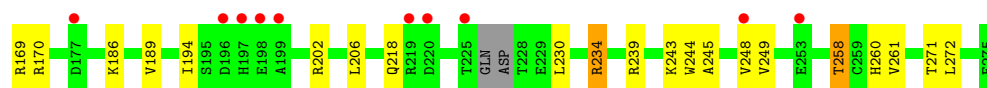


• Molecule 2: TCR beta

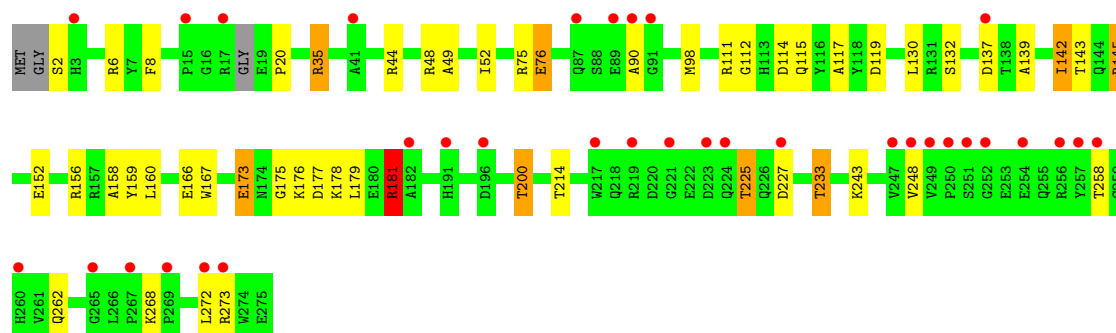
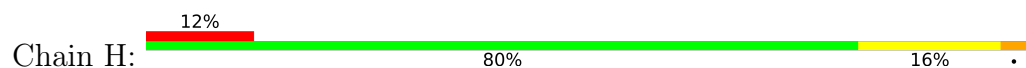


• Molecule 3: HLA class I histocompatibility antigen, B alpha chain

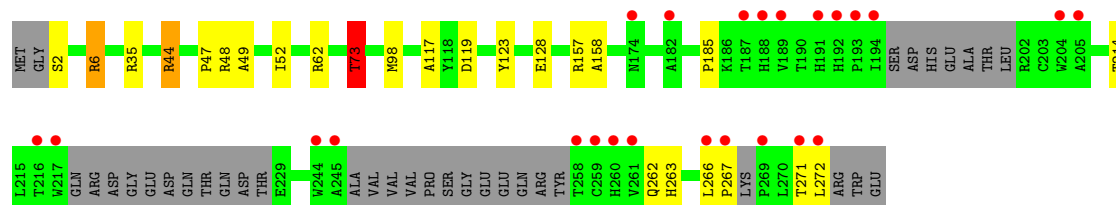
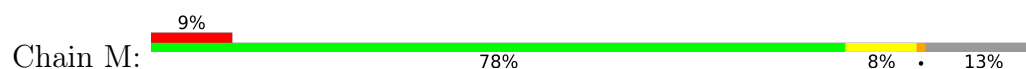




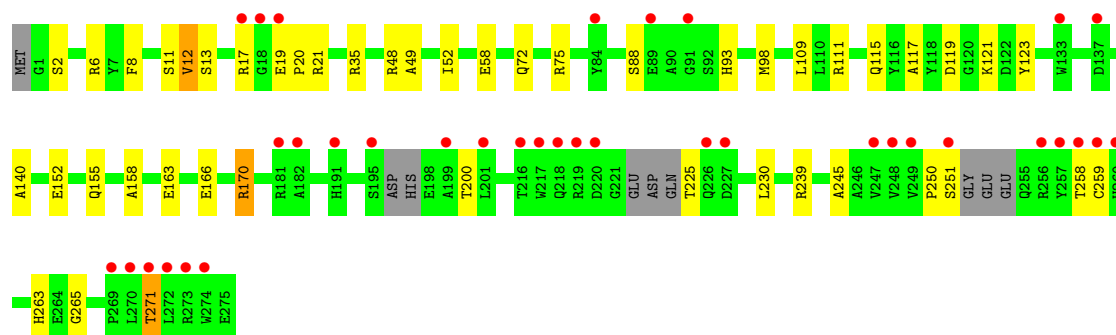
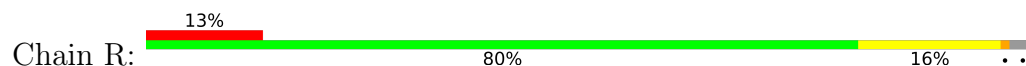
- Molecule 3: HLA class I histocompatibility antigen, B alpha chain



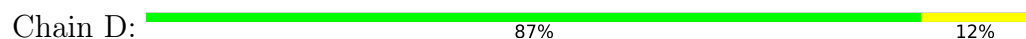
- Molecule 3: HLA class I histocompatibility antigen, B alpha chain



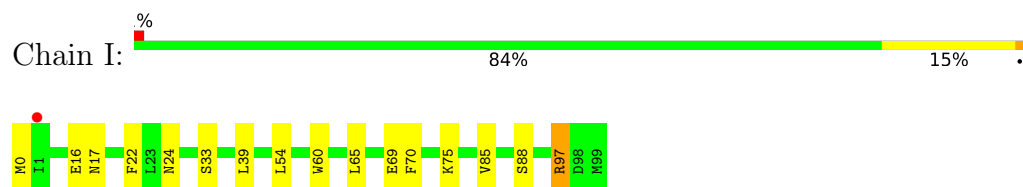
- Molecule 3: HLA class I histocompatibility antigen, B alpha chain



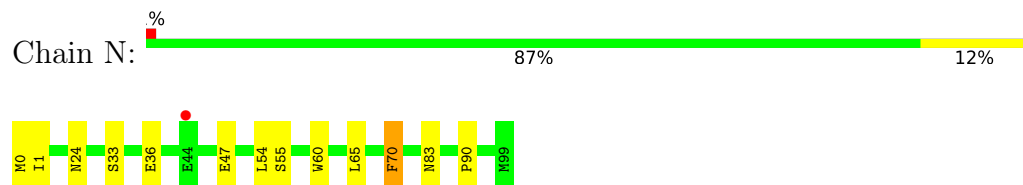
- Molecule 4: Beta-2-microglobulin



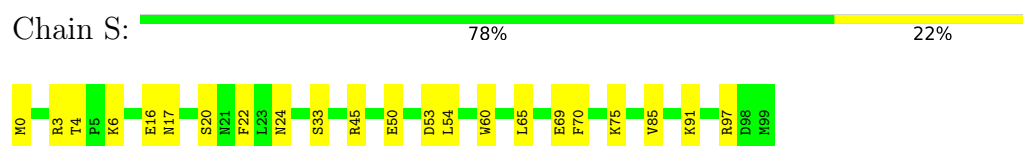
## • Molecule 4: Beta-2-microglobulin



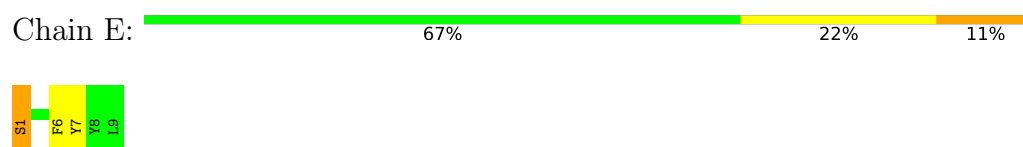
## • Molecule 4: Beta-2-microglobulin



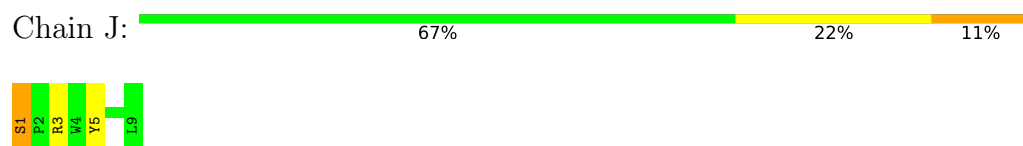
## • Molecule 4: Beta-2-microglobulin



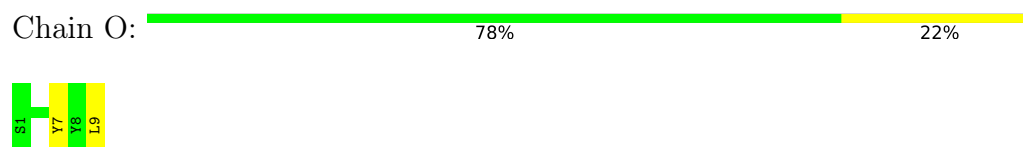
## • Molecule 5: Nucleoprotein



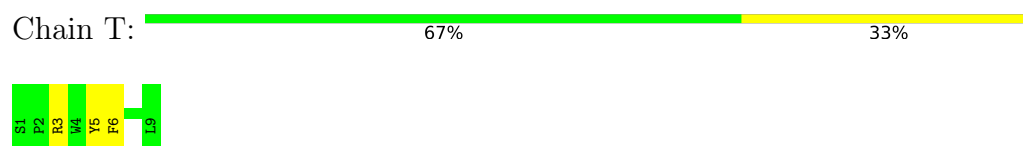
## • Molecule 5: Nucleoprotein



## • Molecule 5: Nucleoprotein



## • Molecule 5: Nucleoprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.79Å 102.56Å 120.70Å 84.14° 68.60° 81.10°	Depositor
Resolution (Å)	48.52 – 2.75 48.52 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.52-2.75) 98.8 (48.52-2.75)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.218 , 0.270 0.220 , 0.272	Depositor DCC
$R_{free}$ test set	5025 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.0	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,-h+l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	25365	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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, PEG

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	0.58	0/1479	1.14	4/2011 (0.2%)
1	F	0.60	0/1550	1.15	6/2109 (0.3%)
1	K	0.57	0/1483	1.11	7/2016 (0.3%)
1	P	0.61	0/1618	1.19	6/2197 (0.3%)
2	B	0.57	0/1928	1.06	5/2626 (0.2%)
2	G	0.58	0/1902	1.10	3/2595 (0.1%)
2	L	0.57	0/1910	1.09	7/2602 (0.3%)
2	Q	0.60	0/1918	1.10	5/2615 (0.2%)
3	C	0.58	0/2165	1.12	5/2956 (0.2%)
3	H	0.56	0/2220	1.11	9/3026 (0.3%)
3	M	0.56	0/1968	1.13	5/2674 (0.2%)
3	R	0.58	0/2124	1.12	5/2898 (0.2%)
4	D	0.60	0/836	1.12	3/1135 (0.3%)
4	I	0.58	0/836	1.04	2/1136 (0.2%)
4	N	0.56	0/832	0.99	1/1131 (0.1%)
4	S	0.58	0/836	1.15	5/1138 (0.4%)
5	E	0.57	0/100	0.96	0/135
5	J	0.54	0/100	1.06	0/135
5	O	0.67	0/100	1.08	0/135
5	T	0.67	0/100	1.15	1/135 (0.7%)
All	All	0.58	0/26005	1.11	79/35405 (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	1
1	F	0	1
1	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	G	0	5
2	L	0	1
2	Q	0	4
3	C	0	5
3	H	0	4
3	M	0	2
3	R	0	2
4	I	0	1
4	S	0	1
All	All	0	30

There are no bond length outliers.

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	123	GLU	CB-CG-CD	9.13	128.12	112.60
3	M	73	THR	CA-CB-OG1	-8.74	96.49	109.60
1	P	204	GLU	CB-CA-C	-8.00	97.25	110.85
3	M	44	ARG	CA-CB-CG	7.82	129.73	114.10
4	S	75	LYS	CB-CA-C	7.77	122.12	109.07
2	L	237	GLU	N-CA-CB	-7.42	98.77	111.69
4	S	91	LYS	N-CA-CB	7.33	122.38	110.43
1	F	126	ASP	CA-CB-CG	7.19	119.79	112.60
4	I	75	LYS	CB-CA-C	6.96	120.77	109.07
3	C	58	GLU	CB-CG-CD	6.93	124.38	112.60
2	B	170	CYS	CB-CA-C	6.86	120.70	110.14
3	H	76	GLU	CB-CG-CD	6.81	124.18	112.60
2	Q	123	GLU	CB-CG-CD	6.71	124.00	112.60
2	Q	99	GLN	N-CA-CB	-6.62	100.02	110.22
1	A	78	THR	CA-CB-OG1	-6.58	99.73	109.60
2	B	115	ASP	CA-CB-CG	6.37	118.97	112.60
2	Q	218	GLU	CB-CG-CD	6.27	123.26	112.60
4	S	6	LYS	CB-CA-C	6.11	119.61	109.53
3	H	176	LYS	CB-CA-C	-6.06	109.57	116.54
1	K	183	PHE	CA-CB-CG	6.04	119.84	113.80
4	S	50	GLU	CB-CG-CD	-6.01	102.38	112.60
1	K	126	ASP	CA-CB-CG	6.01	118.61	112.60
3	R	48	ARG	CG-CD-NE	6.00	125.21	112.00
1	P	182	ASP	CA-CB-CG	6.00	118.60	112.60
3	C	239	ARG	CG-CD-NE	-5.94	98.94	112.00
2	L	136	HIS	CA-CB-CG	5.93	119.73	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	94	THR	CA-CB-OG1	-5.89	100.77	109.60
3	R	6	ARG	CG-CD-NE	-5.88	99.07	112.00
2	B	99	GLN	CB-CA-C	-5.86	99.09	110.46
3	H	268	LYS	CA-CB-CG	5.85	125.81	114.10
3	H	115	GLN	CB-CA-C	-5.77	97.39	110.07
1	F	14	VAL	N-CA-CB	-5.75	102.01	111.44
1	A	19	ASP	CB-CA-C	5.74	119.21	109.50
1	K	183	PHE	N-CA-CB	-5.72	101.08	110.41
2	L	104	PHE	CA-CB-CG	5.68	119.48	113.80
1	K	168	ASP	CA-CB-CG	5.65	118.25	112.60
2	G	53	GLU	CB-CA-C	-5.61	98.27	109.99
4	D	70	PHE	CA-CB-CG	5.58	119.39	113.80
1	A	126	ASP	CA-CB-CG	5.58	118.18	112.60
3	C	115	GLN	CB-CA-C	-5.56	97.84	110.07
3	H	173	GLU	CB-CA-C	5.54	119.66	110.90
3	M	157	ARG	CA-CB-CG	5.50	125.11	114.10
2	L	136	HIS	CB-CG-CD2	5.49	138.33	131.20
2	B	104	PHE	CA-CB-CG	5.47	119.27	113.80
3	H	178	LYS	N-CA-C	-5.46	106.75	113.41
1	F	78	THR	CA-CB-OG1	-5.44	101.44	109.60
3	M	128	GLU	CB-CG-CD	5.42	121.81	112.60
2	Q	13	VAL	N-CA-CB	5.40	118.60	111.25
3	H	145	ARG	CB-CG-CD	5.38	123.68	111.30
4	I	16	GLU	CB-CA-C	5.37	118.41	110.14
2	L	170	CYS	CB-CA-C	5.36	118.92	109.80
2	L	123	GLU	CB-CA-C	5.36	118.68	109.51
3	R	115	GLN	CB-CA-C	-5.32	98.36	110.07
2	Q	77	THR	OG1-CB-CG2	-5.27	98.76	109.30
1	F	163	ASP	CA-CB-CG	5.26	117.86	112.60
3	R	17	ARG	N-CA-C	-5.24	105.10	112.12
1	P	60	LYS	CB-CA-C	5.22	120.80	110.42
2	B	186	ARG	NE-CZ-NH1	-5.21	116.29	121.50
1	F	151	ASP	CA-CB-CG	5.18	117.78	112.60
3	H	166	GLU	CB-CA-C	5.18	120.18	110.70
1	K	10	GLN	N-CA-CB	-5.17	102.50	110.16
2	G	170	CYS	CB-CA-C	5.17	118.59	109.80
1	P	10	GLN	CB-CA-C	5.17	119.64	110.85
4	D	31	HIS	O-C-N	-5.17	117.81	121.84
1	F	159	LYS	CB-CG-CD	5.16	123.18	111.30
4	N	70	PHE	CA-CB-CG	5.16	118.96	113.80
3	M	6	ARG	CG-CD-NE	-5.16	100.66	112.00
2	G	104	PHE	CA-CB-CG	5.15	118.95	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	39	ARG	CB-CG-CD	5.14	123.13	111.30
1	A	97	THR	CA-CB-OG1	-5.14	101.89	109.60
1	P	113	ASN	CA-CB-CG	-5.14	107.46	112.60
1	K	104	THR	OG1-CB-CG2	-5.10	99.10	109.30
4	S	16	GLU	CB-CA-C	5.10	117.99	110.14
3	H	114	ASP	CA-CB-CG	5.08	117.68	112.60
5	T	6	PHE	CA-CB-CG	-5.06	108.74	113.80
1	K	57	LYS	CG-CD-CE	5.03	122.87	111.30
4	D	45	ARG	CG-CD-NE	-5.02	100.95	112.00
3	C	6	ARG	CG-CD-NE	-5.02	100.95	112.00
3	R	58	GLU	CB-CG-CD	5.01	121.12	112.60

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ARG	Sidechain
2	B	186	ARG	Sidechain
2	B	23	ARG	Sidechain
3	C	169	ARG	Sidechain
3	C	17	ARG	Sidechain
3	C	21	ARG	Sidechain
3	C	234	ARG	Sidechain
3	C	6	ARG	Sidechain
1	F	165	ARG	Sidechain
2	G	10	ARG	Sidechain
2	G	109	ARG	Sidechain
2	G	169	VAL	Peptide
2	G	192	ARG	Sidechain
2	G	241	ARG	Sidechain
3	H	156	ARG	Sidechain
3	H	181	ARG	Sidechain
3	H	35	ARG	Sidechain
3	H	48	ARG	Sidechain
4	I	97	ARG	Sidechain
1	K	61	ARG	Sidechain
2	L	109	ARG	Sidechain
3	M	6	ARG	Sidechain
3	M	62	ARG	Sidechain
2	Q	10	ARG	Sidechain
2	Q	109	ARG	Sidechain
2	Q	169	VAL	Peptide

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Mol	Chain	Res	Type	Group
2	Q	241	ARG	Sidechain
3	R	170	ARG	Sidechain
3	R	239	ARG	Sidechain
4	S	45	ARG	Sidechain

## 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	1447	0	1337	13	0
1	F	1515	0	1403	13	0
1	K	1453	0	1325	11	0
1	P	1582	0	1476	14	0
2	B	1877	0	1756	13	0
2	G	1851	0	1722	21	0
2	L	1860	0	1725	15	0
2	Q	1867	0	1736	14	0
3	C	2106	0	1882	17	0
3	H	2160	0	1955	23	0
3	M	1917	0	1743	11	0
3	R	2067	0	1836	20	0
4	D	813	0	758	4	0
4	I	813	0	749	7	0
4	N	809	0	747	6	0
4	S	813	0	737	6	0
5	E	94	0	84	3	0
5	J	94	0	84	3	0
5	O	94	0	84	2	0
5	T	94	0	84	2	0
6	B	6	0	8	0	0
6	L	6	0	8	0	0
6	Q	6	0	8	0	0
7	G	7	0	10	0	0
8	C	4	0	0	0	0
8	H	4	0	0	0	0
8	M	2	0	0	0	0
8	R	4	0	0	0	0
All	All	25365	0	23257	184	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 4.

All (184) 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:F:25:ASN:HD22	1:F:72:ASN:ND2	1.72	0.88
2:Q:10:ARG:HH11	2:Q:10:ARG:HG3	1.39	0.87
1:F:25:ASN:HD22	1:F:72:ASN:HD21	1.24	0.85
3:R:119:ASP:HB3	4:S:0:MET:HB3	1.64	0.77
2:Q:10:ARG:HG3	2:Q:10:ARG:NH1	2.01	0.73
3:M:185:PRO:HD3	3:M:263:HIS:CD2	2.25	0.71
2:G:206:HIS:HE1	2:G:237:GLU:OE1	1.74	0.71
1:A:34:GLN:HE21	1:A:49:GLN:HE21	1.38	0.70
3:R:250:PRO:O	3:R:251:SER:C	2.35	0.69
3:H:119:ASP:HB3	4:I:0:MET:HB3	1.76	0.68
3:M:47:PRO:O	3:M:48:ARG:HD2	1.93	0.67
1:A:50:LEU:HD23	1:A:57:LYS:HD2	1.77	0.65
3:R:258:THR:HB	3:R:271:THR:HG22	1.78	0.64
4:S:17:ASN:HD21	4:S:97:ARG:HH22	1.48	0.62
3:H:200:THR:HG23	3:H:248:VAL:HG12	1.82	0.61
3:H:8:PHE:HE2	3:H:98:MET:HE2	1.64	0.61
1:P:50:LEU:HD23	1:P:57:LYS:HD2	1.84	0.60
3:R:117:ALA:HB2	4:S:60:TRP:CE2	2.36	0.59
3:H:20:PRO:HD2	3:H:75:ARG:HD2	1.84	0.59
1:F:25:ASN:ND2	1:F:72:ASN:HD21	1.97	0.59
2:G:172:ASP:HB2	2:G:189:LEU:HD12	1.85	0.58
3:R:259:CYS:O	3:R:271:THR:HA	2.01	0.58
3:C:167:TRP:CE2	5:E:1:SER:HB2	2.38	0.58
3:H:167:TRP:CE2	5:J:1:SER:HB2	2.39	0.57
2:B:235:SER:O	4:I:88:SER:HB3	2.04	0.57
1:P:61:ARG:NH2	1:P:84:ASP:OD2	2.38	0.56
4:S:22:PHE:CE2	4:S:69:GLU:HG2	2.40	0.56
4:I:17:ASN:OD1	4:I:97:ARG:NH2	2.36	0.56
2:B:22:LEU:HD22	2:B:108:THR:HG21	1.87	0.56
2:L:172:ASP:HB2	2:L:189:LEU:HD12	1.87	0.56
1:A:34:GLN:HE21	1:A:49:GLN:NE2	2.04	0.56
2:G:55:GLN:HE21	2:G:58:LYS:HB3	1.70	0.56
2:G:182:LEU:HD13	2:G:184:ASP:H	1.69	0.56
1:F:165:ARG:HG2	1:F:165:ARG:NH1	2.21	0.55
2:G:22:LEU:HD22	2:G:108:THR:HG21	1.88	0.55
1:A:48:ILE:HD11	1:A:57:LYS:HD3	1.88	0.55
2:B:10:ARG:HD2	3:H:90:ALA:CB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:1:ILE:HG12	2:Q:163:LYS:HG3	1.89	0.54
3:C:93:HIS:HD2	3:C:119:ASP:OD2	1.91	0.54
3:C:117:ALA:HB2	4:D:60:TRP:CE2	2.43	0.54
3:M:117:ALA:HB2	4:N:60:TRP:CE2	2.43	0.54
2:Q:22:LEU:HD22	2:Q:108:THR:HG21	1.90	0.54
2:G:153:HIS:HB3	2:G:214:TYR:HB2	1.90	0.54
2:Q:10:ARG:NH1	2:Q:10:ARG:CG	2.70	0.54
1:A:151:ASP:HB2	1:A:154:VAL:HB	1.89	0.54
2:Q:153:HIS:HB3	2:Q:214:TYR:HB2	1.91	0.53
2:L:153:HIS:HB3	2:L:214:TYR:HB2	1.90	0.53
2:B:55:GLN:HG2	2:B:58:LYS:HG2	1.91	0.53
3:R:12:VAL:HG23	3:R:21:ARG:HB3	1.89	0.53
2:L:241:ARG:HB3	2:L:241:ARG:CZ	2.38	0.53
2:B:10:ARG:HD2	3:H:90:ALA:HB2	1.91	0.53
4:N:83:ASN:HD21	4:N:90:PRO:HG3	1.73	0.53
2:B:153:HIS:HB3	2:B:214:TYR:HB2	1.91	0.52
1:K:48:ILE:HD11	1:K:57:LYS:HD2	1.92	0.52
3:H:8:PHE:CE2	3:H:98:MET:HE2	2.44	0.52
2:G:182:LEU:HD11	2:G:184:ASP:HB3	1.92	0.51
1:K:99:LYS:HE3	2:L:46:PHE:CD2	2.45	0.51
3:H:233:THR:HB	3:H:243:LYS:HE2	1.93	0.51
4:D:17:ASN:OD1	4:D:97:ARG:NH2	2.40	0.51
1:F:165:ARG:HG2	1:F:165:ARG:HH11	1.75	0.51
2:L:22:LEU:HD22	2:L:108:THR:HG21	1.92	0.51
4:I:22:PHE:CE2	4:I:69:GLU:HG3	2.46	0.50
3:H:214:THR:HB	3:H:262:GLN:HB3	1.94	0.50
2:L:32:SER:HB3	2:L:49:TYR:HE1	1.76	0.50
1:P:169:PHE:CD1	2:Q:139:LYS:HE2	2.47	0.49
1:K:12:GLN:HG2	1:K:14:VAL:CG1	2.42	0.49
3:C:55:GLU:OE2	3:C:170:ARG:NH1	2.45	0.49
3:H:111:ARG:HG2	3:H:112:GLY:N	2.26	0.49
3:H:152:GLU:OE2	5:J:5:TYR:OH	2.22	0.49
1:F:56:VAL:HG22	1:F:65:GLN:HG3	1.93	0.49
1:A:51:VAL:HG11	3:C:158:ALA:HA	1.93	0.49
3:C:202:ARG:NH1	3:C:244:TRP:CH2	2.81	0.49
1:A:61:ARG:NH2	1:A:84:ASP:OD2	2.46	0.48
4:I:33:SER:HB2	4:I:54:LEU:HD21	1.94	0.48
4:N:33:SER:HB2	4:N:54:LEU:HD21	1.94	0.48
1:P:107:ARG:HE	1:P:109:LYS:NZ	2.12	0.47
1:P:125:ARG:HD2	2:Q:128:GLU:HB2	1.96	0.47
2:B:32:SER:HB3	2:B:49:TYR:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:MET:CE	2:G:196:SER:HB3	2.45	0.47
3:M:73:THR:HG23	5:O:7:TYR:O	2.14	0.47
2:B:172:ASP:HB2	2:B:189:LEU:HD12	1.95	0.47
1:F:75:LEU:C	1:F:75:LEU:HD23	2.39	0.47
3:H:177:ASP:O	3:H:181:ARG:HB3	2.14	0.47
3:M:119:ASP:HB3	4:N:0:MET:HB3	1.96	0.47
3:R:152:GLU:OE1	5:T:5:TYR:OH	2.31	0.47
4:S:33:SER:HB2	4:S:54:LEU:HD21	1.96	0.47
1:K:82:THR:O	1:K:85:VAL:HG22	2.15	0.47
3:H:139:ALA:O	3:H:142:ILE:HG23	2.14	0.47
2:Q:58:LYS:HB2	2:Q:61:LEU:HD12	1.97	0.47
3:R:230:LEU:CD2	3:R:245:ALA:HB2	2.45	0.47
3:R:230:LEU:HD23	3:R:245:ALA:HB2	1.96	0.46
1:P:32:ASN:ND2	1:P:34:GLN:OE1	2.48	0.46
3:H:111:ARG:HG2	3:H:112:GLY:H	1.80	0.46
3:H:175:GLY:HA3	3:H:179:LEU:HD12	1.98	0.46
3:C:260:HIS:ND1	3:C:271:THR:HG22	2.31	0.46
1:P:95:SER:HB2	3:R:163:GLU:OE2	2.16	0.46
2:G:206:HIS:CE1	2:G:237:GLU:OE1	2.61	0.45
3:H:117:ALA:HB2	4:I:60:TRP:CE2	2.51	0.45
5:E:7:TYR:C	5:E:7:TYR:CD1	2.95	0.45
1:P:127:SER:HB3	1:P:130:SER:HB3	1.98	0.45
1:F:51:VAL:HG11	3:H:158:ALA:HA	1.99	0.45
2:G:49:TYR:HE1	2:G:51:GLN:HB2	1.80	0.45
1:A:112:ALA:HB2	1:A:161:VAL:HG11	1.98	0.45
2:G:216:LEU:O	2:G:230:VAL:HG23	2.16	0.45
3:C:123:TYR:CZ	3:C:140:ALA:HA	2.51	0.45
1:P:75:LEU:HD23	1:P:75:LEU:C	2.42	0.45
1:P:51:VAL:HG11	3:R:158:ALA:HA	1.98	0.45
3:R:123:TYR:CZ	3:R:140:ALA:HA	2.51	0.45
4:D:33:SER:HB2	4:D:54:LEU:HD21	1.99	0.45
2:G:49:TYR:CD1	2:G:49:TYR:C	2.95	0.45
2:G:201:GLN:HA	2:G:241:ARG:O	2.17	0.45
2:L:241:ARG:HB2	2:L:241:ARG:NH1	2.32	0.44
1:P:107:ARG:HE	1:P:109:LYS:HZ2	1.64	0.44
3:R:13:SER:HG	3:R:93:HIS:H	1.64	0.44
1:A:99:LYS:HE3	2:B:57:ASP:OD2	2.17	0.44
1:F:167:MET:HE1	2:G:196:SER:HB3	1.99	0.44
2:B:119:VAL:O	2:B:226:ARG:NH2	2.49	0.44
3:M:214:THR:HB	3:M:262:GLN:HB2	1.99	0.44
1:A:134:VAL:HG13	2:B:127:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:ALA:O	3:C:52:ILE:HG22	2.18	0.44
1:A:149:SER:H	1:A:156:ILE:HD12	1.82	0.44
2:G:13:VAL:CG2	2:G:216:LEU:HD23	2.48	0.44
2:G:163:LYS:HD3	2:G:164:GLU:O	2.18	0.44
1:K:75:LEU:C	1:K:75:LEU:HD23	2.43	0.44
3:C:230:LEU:HD12	3:C:245:ALA:HB2	1.99	0.43
4:D:24:ASN:HB3	4:D:65:LEU:HD11	2.00	0.43
1:F:85:VAL:HG23	1:F:108:LEU:O	2.18	0.43
2:G:230:VAL:HG22	2:G:231:THR:N	2.32	0.43
3:H:225:THR:HG22	3:H:227:ASP:H	1.83	0.43
2:B:97:LEU:HB3	5:E:6:PHE:O	2.18	0.43
2:Q:200:TRP:CZ2	2:Q:241:ARG:HG3	2.53	0.43
3:R:72:GLN:HG3	3:R:75:ARG:HH21	1.83	0.43
3:M:123:TYR:CE2	5:O:9:LEU:HD23	2.53	0.43
3:H:142:ILE:HG13	3:H:143:THR:N	2.32	0.43
2:Q:32:SER:HB3	2:Q:49:TYR:HE1	1.82	0.43
3:H:159:TYR:CG	5:J:3:ARG:HB3	2.54	0.43
3:M:266:LEU:HA	3:M:267:PRO:HD2	1.88	0.43
2:G:13:VAL:HG21	2:G:216:LEU:HD23	2.01	0.43
2:G:32:SER:HB2	2:G:96:SER:OG	2.19	0.43
3:C:111:ARG:NE	3:C:112:GLY:O	2.44	0.43
3:R:263:HIS:HD1	3:R:265:GLY:H	1.67	0.43
1:K:138:THR:OG1	2:L:194:ARG:NH2	2.52	0.42
2:L:241:ARG:NH1	2:L:241:ARG:CB	2.82	0.42
2:B:32:SER:HB2	2:B:96:SER:OG	2.20	0.42
2:Q:101:HIS:HE1	3:R:152:GLU:OE2	2.03	0.42
2:G:182:LEU:HD13	2:G:184:ASP:N	2.35	0.42
2:L:204:ARG:HG3	2:L:204:ARG:HH11	1.84	0.42
1:F:7:GLN:HA	1:F:23:TYR:O	2.19	0.42
2:G:53:GLU:H	2:G:53:GLU:CD	2.27	0.42
2:L:31:VAL:H	2:L:97:LEU:HD23	1.83	0.42
2:L:241:ARG:CZ	2:L:241:ARG:CB	2.98	0.42
1:F:155:TYR:O	1:F:176:ALA:HA	2.20	0.42
1:K:127:SER:HB3	2:L:128:GLU:HG3	2.02	0.42
3:C:109:LEU:HD22	3:C:161:GLU:HA	2.01	0.42
3:C:186:LYS:H	3:C:186:LYS:HD2	1.85	0.42
4:N:24:ASN:HB3	4:N:65:LEU:HD11	2.02	0.41
4:S:24:ASN:HB3	4:S:65:LEU:HD11	2.02	0.41
2:L:32:SER:HB2	2:L:96:SER:OG	2.21	0.41
1:A:75:LEU:HD23	1:A:75:LEU:C	2.46	0.41
3:C:218:GLN:HB2	3:C:258:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:49:ALA:O	3:M:52:ILE:HG22	2.20	0.41
3:R:121:LYS:HB3	3:R:121:LYS:HE2	1.93	0.41
1:A:112:ALA:CB	1:A:161:VAL:HG11	2.50	0.41
1:P:61:ARG:HH22	1:P:84:ASP:CG	2.28	0.41
3:C:98:MET:HE2	3:C:98:MET:HB3	1.97	0.41
3:H:49:ALA:O	3:H:52:ILE:HG22	2.20	0.41
4:I:24:ASN:HB3	4:I:65:LEU:HD11	2.03	0.41
1:K:141:ASP:OD2	1:K:143:GLN:NE2	2.54	0.41
1:P:155:TYR:O	1:P:176:ALA:HA	2.21	0.41
2:L:23:ARG:HH11	2:L:23:ARG:HG2	1.86	0.41
3:M:185:PRO:HD3	3:M:263:HIS:HD2	1.79	0.41
2:Q:10:ARG:HD3	2:Q:11:TYR:HE1	1.86	0.41
3:C:194:ILE:HD11	3:C:248:VAL:HG12	2.02	0.41
3:H:258:THR:HG22	3:H:273:ARG:HG2	2.03	0.41
2:Q:10:ARG:HD3	2:Q:11:TYR:CE1	2.55	0.41
1:P:30:LEU:O	1:P:70:LYS:HE2	2.20	0.41
3:R:49:ALA:O	3:R:52:ILE:HG22	2.21	0.40
3:C:8:PHE:CE2	3:C:98:MET:HG3	2.56	0.40
1:K:51:VAL:HG21	3:M:158:ALA:HA	2.03	0.40
3:R:8:PHE:CE1	3:R:98:MET:HG3	2.56	0.40
5:T:3:ARG:HD2	5:T:5:TYR:HB3	2.03	0.40
1:K:34:GLN:OE1	1:K:49:GLN:HG3	2.22	0.40
1:K:115:GLN:HE21	1:K:115:GLN:HB3	1.72	0.40
3:R:19:GLU:HA	3:R:20:PRO:HD3	1.94	0.40

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	185/206 (90%)	178 (96%)	7 (4%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	194/206 (94%)	189 (97%)	5 (3%)	0	100	100
1	K	184/206 (89%)	179 (97%)	5 (3%)	0	100	100
1	P	202/206 (98%)	194 (96%)	8 (4%)	0	100	100
2	B	240/243 (99%)	235 (98%)	5 (2%)	0	100	100
2	G	239/243 (98%)	233 (98%)	6 (2%)	0	100	100
2	L	237/243 (98%)	231 (98%)	6 (2%)	0	100	100
2	Q	240/243 (99%)	234 (98%)	6 (2%)	0	100	100
3	C	265/276 (96%)	257 (97%)	8 (3%)	0	100	100
3	H	269/276 (98%)	260 (97%)	9 (3%)	0	100	100
3	M	230/276 (83%)	225 (98%)	5 (2%)	0	100	100
3	R	259/276 (94%)	247 (95%)	12 (5%)	0	100	100
4	D	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
4	I	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
4	N	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
4	S	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
5	E	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
5	J	7/9 (78%)	7 (100%)	0	0	100	100
5	O	7/9 (78%)	7 (100%)	0	0	100	100
5	T	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
All	All	3164/3336 (95%)	3074 (97%)	90 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	154/185 (83%)	146 (95%)	8 (5%)	19	35
1	F	165/185 (89%)	157 (95%)	8 (5%)	21	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	154/185 (83%)	145 (94%)	9 (6%)	17	31
1	P	177/185 (96%)	168 (95%)	9 (5%)	20	36
2	B	198/207 (96%)	194 (98%)	4 (2%)	50	70
2	G	193/207 (93%)	186 (96%)	7 (4%)	30	51
2	L	193/207 (93%)	189 (98%)	4 (2%)	48	69
2	Q	195/207 (94%)	189 (97%)	6 (3%)	35	56
3	C	203/234 (87%)	188 (93%)	15 (7%)	11	20
3	H	213/234 (91%)	196 (92%)	17 (8%)	10	18
3	M	190/234 (81%)	183 (96%)	7 (4%)	29	50
3	R	198/234 (85%)	185 (93%)	13 (7%)	14	25
4	D	89/95 (94%)	85 (96%)	4 (4%)	23	42
4	I	89/95 (94%)	86 (97%)	3 (3%)	32	54
4	N	88/95 (93%)	84 (96%)	4 (4%)	23	42
4	S	89/95 (94%)	83 (93%)	6 (7%)	13	25
5	E	9/9 (100%)	8 (89%)	1 (11%)	5	8
5	J	9/9 (100%)	8 (89%)	1 (11%)	5	8
5	O	9/9 (100%)	9 (100%)	0	100	100
5	T	9/9 (100%)	9 (100%)	0	100	100
All	All	2624/2920 (90%)	2498 (95%)	126 (5%)	21	39

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	52	LYS
1	A	58	LYS
1	A	104	THR
1	A	111	LEU
1	A	124	LEU
1	A	147	SER
1	A	152	SER
2	B	177	LYS
2	B	198	THR
2	B	219	ASN
2	B	223	THR
3	C	2	SER

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Mol	Chain	Res	Type
3	C	35	ARG
3	C	76	GLU
3	C	94	THR
3	C	97	SER
3	C	110	LEU
3	C	166	GLU
3	C	189	VAL
3	C	206	LEU
3	C	234	ARG
3	C	243	LYS
3	C	249	VAL
3	C	258	THR
3	C	261	VAL
3	C	272	LEU
4	D	53	ASP
4	D	70	PHE
4	D	71	THR
4	D	75	LYS
5	E	1	SER
1	F	8	ILE
1	F	28	THR
1	F	78	THR
1	F	94	THR
1	F	104	THR
1	F	132	LYS
1	F	133	SER
1	F	161	VAL
2	G	8	SER
2	G	10	ARG
2	G	84	GLN
2	G	106	SER
2	G	163	LYS
2	G	174	GLN
2	G	182	LEU
3	H	2	SER
3	H	6	ARG
3	H	35	ARG
3	H	44	ARG
3	H	76	GLU
3	H	130	LEU
3	H	132	SER
3	H	137	ASP

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Mol	Chain	Res	Type
3	H	142	ILE
3	H	145	ARG
3	H	160	LEU
3	H	173	GLU
3	H	181	ARG
3	H	200	THR
3	H	225	THR
3	H	233	THR
3	H	272	LEU
4	I	39	LEU
4	I	70	PHE
4	I	85	VAL
5	J	1	SER
1	K	6	MET
1	K	10	GLN
1	K	14	VAL
1	K	28	THR
1	K	33	ILE
1	K	104	THR
1	K	111	LEU
1	K	115	GLN
1	K	161	VAL
2	L	72	GLU
2	L	86	GLU
2	L	130	SER
2	L	204	ARG
3	M	2	SER
3	M	35	ARG
3	M	44	ARG
3	M	73	THR
3	M	98	MET
3	M	271	THR
3	M	272	LEU
4	N	36	GLU
4	N	47	GLU
4	N	55	SER
4	N	70	PHE
1	P	6	MET
1	P	14	VAL
1	P	32	ASN
1	P	78	THR
1	P	83	THR

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Mol	Chain	Res	Type
1	P	104	THR
1	P	113	ASN
1	P	133	SER
1	P	154	VAL
2	Q	10	ARG
2	Q	13	VAL
2	Q	53	GLU
2	Q	177	LYS
2	Q	218	GLU
2	Q	241	ARG
3	R	2	SER
3	R	11	SER
3	R	12	VAL
3	R	35	ARG
3	R	88	SER
3	R	109	LEU
3	R	111	ARG
3	R	155	GLN
3	R	166	GLU
3	R	170	ARG
3	R	200	THR
3	R	225	THR
3	R	271	THR
4	S	3	ARG
4	S	4	THR
4	S	20	SER
4	S	53	ASP
4	S	70	PHE
4	S	85	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	13	HIS
1	A	15	GLN
1	A	34	GLN
1	A	143	GLN
2	B	42	GLN
2	B	136	HIS
3	C	87	GLN
3	C	93	HIS

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Mol	Chain	Res	Type
3	C	127	ASN
3	C	174	ASN
3	C	188	HIS
3	C	242	GLN
4	D	13	HIS
1	F	72	ASN
1	F	81	GLN
1	F	191	ASN
2	G	37	GLN
2	G	42	GLN
2	G	51	GLN
2	G	55	GLN
2	G	84	GLN
2	G	138	GLN
2	G	206	HIS
2	G	212	GLN
3	H	87	GLN
3	H	96	GLN
3	H	127	ASN
3	H	141	GLN
3	H	188	HIS
3	H	191	HIS
3	H	192	HIS
4	I	13	HIS
4	I	83	ASN
1	K	25	ASN
1	K	115	GLN
1	K	123	GLN
1	K	143	GLN
1	K	172	ASN
1	K	191	ASN
3	M	63	ASN
3	M	96	GLN
3	M	115	GLN
3	M	127	ASN
3	M	263	HIS
4	N	8	GLN
4	N	13	HIS
4	N	83	ASN
1	P	12	GLN
1	P	15	GLN
1	P	25	ASN

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Mol	Chain	Res	Type
1	P	32	ASN
1	P	34	GLN
1	P	43	HIS
1	P	49	GLN
1	P	59	GLN
1	P	113	ASN
1	P	116	ASN
1	P	143	GLN
2	Q	101	HIS
2	Q	138	GLN
2	Q	166	HIS
2	Q	174	GLN
2	Q	201	GLN
2	Q	224	GLN
3	R	70	GLN
3	R	127	ASN
3	R	144	GLN
3	R	188	HIS
3	R	191	HIS
4	S	2	GLN
4	S	13	HIS
4	S	17	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	GOL	L	301	-	5,5,5	0.26	0	5,5,5	0.39	0
6	GOL	B	301	-	5,5,5	0.15	0	5,5,5	0.38	0
6	GOL	Q	301	-	5,5,5	0.18	0	5,5,5	0.40	0
7	PEG	G	301	-	6,6,6	0.48	0	5,5,5	0.33	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	GOL	L	301	-	-	2/4/4/4	-
6	GOL	B	301	-	-	4/4/4/4	-
6	GOL	Q	301	-	-	4/4/4/4	-
7	PEG	G	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	301	GOL	C1-C2-C3-O3
6	L	301	GOL	O1-C1-C2-C3
6	Q	301	GOL	C1-C2-C3-O3
6	B	301	GOL	O1-C1-C2-O2
7	G	301	PEG	O2-C3-C4-O4
6	B	301	GOL	O1-C1-C2-C3
7	G	301	PEG	O1-C1-C2-O2
6	B	301	GOL	O2-C2-C3-O3
6	L	301	GOL	O1-C1-C2-O2
6	Q	301	GOL	O1-C1-C2-C3
6	Q	301	GOL	O1-C1-C2-O2
6	Q	301	GOL	O2-C2-C3-O3



There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [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	191/206 (92%)	0.57	27 (14%) 7 9	22, 48, 94, 114	0
1	F	198/206 (96%)	0.05	5 (2%) 58 59	20, 37, 70, 82	0
1	K	192/206 (93%)	0.55	33 (17%) 5 6	18, 46, 91, 110	0
1	P	204/206 (99%)	-0.24	0 100 100	19, 34, 57, 76	0
2	B	242/243 (99%)	0.19	6 (2%) 58 59	20, 45, 84, 106	0
2	G	241/243 (99%)	0.06	9 (3%) 45 47	16, 37, 75, 89	0
2	L	241/243 (99%)	0.00	4 (1%) 69 70	16, 38, 76, 128	0
2	Q	242/243 (99%)	-0.12	3 (1%) 76 78	18, 34, 67, 106	0
3	C	271/276 (98%)	0.35	14 (5%) 34 35	22, 45, 89, 115	0
3	H	273/276 (98%)	0.70	34 (12%) 9 12	26, 53, 95, 115	0
3	M	240/276 (86%)	0.42	24 (10%) 14 16	23, 46, 91, 125	0
3	R	267/276 (96%)	0.74	36 (13%) 8 10	21, 51, 94, 112	0
4	D	100/100 (100%)	-0.28	0 100 100	19, 33, 47, 65	0
4	I	100/100 (100%)	0.04	1 (1%) 79 82	27, 40, 66, 83	0
4	N	100/100 (100%)	0.22	1 (1%) 79 82	27, 47, 72, 87	0
4	S	100/100 (100%)	-0.28	0 100 100	22, 34, 56, 63	0
5	E	9/9 (100%)	-0.54	0 100 100	19, 30, 35, 40	0
5	J	9/9 (100%)	-0.33	0 100 100	29, 34, 38, 49	0
5	O	9/9 (100%)	-0.52	0 100 100	19, 24, 35, 35	0
5	T	9/9 (100%)	-0.23	0 100 100	26, 31, 39, 40	0
All	All	3238/3336 (97%)	0.23	197 (6%) 28 31	16, 41, 85, 128	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	120	ALA	4.9
3	C	220	ASP	4.8
3	R	220	ASP	4.6
3	R	227	ASP	4.4
3	R	272	LEU	4.4
3	R	84	TYR	4.3
3	R	248	VAL	4.2
3	R	217	TRP	4.1
1	A	172	ASN	4.1
3	M	204	TRP	4.1
3	H	196	ASP	4.0
1	K	201	PRO	4.0
3	R	201	LEU	4.0
3	M	182	ALA	4.0
3	R	273	ARG	3.9
1	K	200	PHE	3.9
3	C	197	HIS	3.8
1	K	199	PHE	3.8
3	C	198	GLU	3.8
3	C	196	ASP	3.8
1	K	195	PRO	3.8
1	K	185	CYS	3.7
2	B	182	LEU	3.6
3	R	249	VAL	3.6
3	R	259	CYS	3.4
1	A	178	SER	3.4
1	K	153	ASP	3.3
3	H	258	THR	3.3
2	B	179	GLN	3.3
1	K	198	THR	3.3
1	A	199	PHE	3.3
3	M	216	THR	3.2
1	K	186	ALA	3.2
3	R	247	VAL	3.2
3	R	260	HIS	3.2
3	H	91	GLY	3.2
3	R	19	GLU	3.2
3	R	17	ARG	3.2
1	A	153	ASP	3.2
3	M	267	PRO	3.2
3	H	249	VAL	3.2
1	F	133	SER	3.1
3	H	17	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	121	VAL	3.1
3	H	41	ALA	3.1
3	C	253	GLU	3.1
1	A	133	SER	3.1
3	R	133	TRP	3.1
1	K	117	PRO	3.1
3	H	89	GLU	3.1
3	H	254	GLU	3.1
2	G	67	PHE	3.1
3	H	267	PRO	3.1
1	K	151	ASP	3.0
3	R	271	THR	3.0
1	A	200	PHE	3.0
1	K	183	PHE	3.0
3	M	260	HIS	3.0
3	R	18	GLY	3.0
1	A	113	ASN	2.9
1	A	166	SER	2.9
1	A	201	PRO	2.9
3	H	248	VAL	2.9
2	Q	67	PHE	2.9
3	C	199	ALA	2.8
3	H	252	GLY	2.8
2	G	182	LEU	2.8
3	M	266	LEU	2.8
1	K	152	SER	2.8
3	M	217	TRP	2.8
2	G	20	VAL	2.8
3	R	258	THR	2.8
3	R	91	GLY	2.8
1	A	167	MET	2.7
1	A	194	ILE	2.7
1	K	190	ASN	2.7
3	M	174	ASN	2.7
3	H	182	ALA	2.7
3	M	194	ILE	2.7
2	B	141	THR	2.7
1	A	120	ALA	2.7
1	A	189	PHE	2.7
2	G	66	PHE	2.7
3	M	245	ALA	2.7
1	K	125	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	L	134	ILE	2.7
1	K	189	PHE	2.6
3	H	219	ARG	2.6
3	H	260	HIS	2.6
3	M	188	HIS	2.6
3	H	224	GLN	2.6
3	R	226	GLN	2.6
2	B	67	PHE	2.6
3	R	195	SER	2.6
1	K	140	PHE	2.6
3	H	90	ALA	2.6
1	F	128	LYS	2.6
1	A	184	ALA	2.6
3	H	251	SER	2.5
1	K	122	TYR	2.5
1	A	197	ASP	2.5
2	Q	184	ASP	2.5
3	R	218	GLN	2.5
1	A	121	VAL	2.5
3	H	137	ASP	2.5
3	C	225	THR	2.5
3	M	258	THR	2.5
3	R	216	THR	2.5
2	B	203	PRO	2.5
3	H	15	PRO	2.5
3	H	247	VAL	2.5
3	R	219	ARG	2.5
1	K	139	ASP	2.5
1	A	156	ILE	2.5
4	N	44	GLU	2.4
3	R	274	TRP	2.4
3	R	256	ARG	2.4
3	M	191	HIS	2.4
3	R	199	ALA	2.4
3	H	265	GLY	2.4
3	R	270	LEU	2.4
2	Q	85	GLN	2.4
1	A	122	TYR	2.4
3	R	181	ARG	2.4
4	I	1	ILE	2.4
3	C	16	GLY	2.4
1	A	125	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	219	ARG	2.4
3	R	257	TYR	2.4
1	K	141	ASP	2.4
3	H	273	ARG	2.3
1	A	115	GLN	2.3
1	A	154	VAL	2.3
2	L	224	GLN	2.3
3	M	205	ALA	2.3
3	M	187	THR	2.3
1	A	195	PRO	2.3
3	H	250	PRO	2.3
1	A	137	PHE	2.3
1	A	111	LEU	2.3
1	A	185	CYS	2.3
1	K	135	CYS	2.3
3	R	269	PRO	2.3
3	H	191	HIS	2.3
2	G	80	ILE	2.3
1	K	188	ALA	2.3
1	K	124	LEU	2.3
3	C	88	SER	2.3
3	H	256	ARG	2.2
3	R	89	GLU	2.2
2	G	112	VAL	2.2
3	C	248	VAL	2.2
3	M	261	VAL	2.2
1	F	6	MET	2.2
3	M	269	PRO	2.2
1	K	197	ASP	2.2
2	L	138	GLN	2.2
1	F	179	ASN	2.2
1	K	179	ASN	2.2
3	H	223	ASP	2.2
3	R	137	ASP	2.2
1	K	166	SER	2.2
3	C	42	SER	2.2
3	M	271	THR	2.2
1	K	154	VAL	2.2
2	B	168	GLY	2.2
3	H	221	GLY	2.2
1	K	115	GLN	2.1
2	G	242	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	M	259	CYS	2.1
3	R	251	SER	2.1
3	H	87	GLN	2.1
3	M	272	LEU	2.1
3	M	193	PRO	2.1
1	K	114	ILE	2.1
3	M	189	VAL	2.1
1	A	126	ASP	2.1
1	F	151	ASP	2.1
3	H	272	LEU	2.1
2	L	242	ALA	2.1
3	H	217	TRP	2.1
3	M	192	HIS	2.1
1	K	138	THR	2.1
1	A	190	ASN	2.1
3	H	227	ASP	2.1
3	H	269	PRO	2.0
3	C	89	GLU	2.0
3	R	191	HIS	2.0
2	G	85	GLN	2.0
1	K	145	ASN	2.0
3	C	177	ASP	2.0
3	R	182	ALA	2.0
2	G	2	GLY	2.0
3	H	3	HIS	2.0
3	M	244	TRP	2.0
1	K	171	SER	2.0
3	H	257	TYR	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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
6	GOL	Q	301	6/6	0.73	0.21	39,52,53,54	0
6	GOL	L	301	6/6	0.75	0.19	38,40,44,47	0
6	GOL	B	301	6/6	0.79	0.19	40,45,47,50	0
7	PEG	G	301	7/7	0.89	0.13	37,46,46,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.