



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 11:01 AM EDT

PDB ID : 3KXF  
Title : Crystal Structure of SB27 TCR in complex with the 'restriction triad' mutant HLA-B\*3508-13mer  
Authors : Archbold, J.K.; Tynan, F.E.; Gras, S.; Rossjohn, J.  
Deposited on : 2009-12-03  
Resolution : 3.10 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

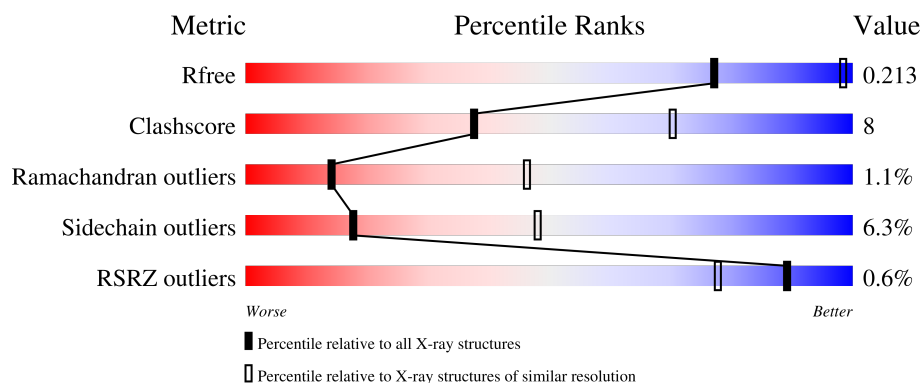
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	276	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 81%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>80%</span> <span>18%</span> </div> </div>
1	C	276	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 16%, green 84%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>82%</span> <span>16%</span> </div> </div>
1	I	276	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 81%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>81%</span> <span>18%</span> </div> </div>
1	K	276	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 18%, green 82%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>80%</span> <span>18%</span> </div> </div>
2	B	99	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 13%, green 87%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>87%</span> <span>13%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	99	 89% 11%
2	J	99	 76% 24%
2	L	99	 86% 13%
3	D	204	 77% 20% .
3	G	204	 75% 22% .
3	M	204	 81% 17% .
3	N	204	 77% 20% .
4	E	241	 78% 21%
4	H	241	 76% 22% .
4	O	241	 76% 22% .
4	P	241	 71% 25% .
5	Q	13	 85% 15%
5	R	13	 92% 8%
5	S	13	 85% 15%
5	T	13	 69% 31%

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	IOD	I	280	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26991 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, B-35 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2246	1400	412	427	7			
1	C	276	Total	C	N	O	S	0	0	0
			2246	1400	412	427	7			
1	K	276	Total	C	N	O	S	0	0	0
			2246	1400	412	427	7			
1	I	276	Total	C	N	O	S	0	1	0
			2254	1405	415	427	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	ALA	GLN	ENGINEERED MUTATION	UNP P30685
A	69	ALA	THR	ENGINEERED MUTATION	UNP P30685
A	155	ALA	GLN	ENGINEERED MUTATION	UNP P30685
A	156	ARG	LEU	SEE REMARK 999	UNP P30685
C	65	ALA	GLN	ENGINEERED MUTATION	UNP P30685
C	69	ALA	THR	ENGINEERED MUTATION	UNP P30685
C	155	ALA	GLN	ENGINEERED MUTATION	UNP P30685
C	156	ARG	LEU	SEE REMARK 999	UNP P30685
K	65	ALA	GLN	ENGINEERED MUTATION	UNP P30685
K	69	ALA	THR	ENGINEERED MUTATION	UNP P30685
K	155	ALA	GLN	ENGINEERED MUTATION	UNP P30685
K	156	ARG	LEU	SEE REMARK 999	UNP P30685
I	65	ALA	GLN	ENGINEERED MUTATION	UNP P30685
I	69	ALA	THR	ENGINEERED MUTATION	UNP P30685
I	155	ALA	GLN	ENGINEERED MUTATION	UNP P30685
I	156	ARG	LEU	SEE REMARK 999	UNP P30685

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	F	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	L	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	J	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

- Molecule 3 is a protein called SB27 T cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	204	Total	C	N	O	S	0	0	0
			1637	1033	263	334	7			
3	G	204	Total	C	N	O	S	0	1	0
			1640	1035	263	335	7			
3	N	204	Total	C	N	O	S	0	0	0
			1637	1033	263	334	7			
3	M	204	Total	C	N	O	S	0	0	0
			1637	1033	263	334	7			

- Molecule 4 is a protein called SB27 T cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	241	Total	C	N	O	S	0	0	0
			1915	1203	331	372	9			
4	H	241	Total	C	N	O	S	0	0	0
			1915	1203	331	372	9			
4	P	241	Total	C	N	O	S	0	1	0
			1919	1206	331	373	9			
4	O	241	Total	C	N	O	S	0	0	0
			1914	1203	331	371	9			

- Molecule 5 is a protein called peptide from Trans-activator protein BZLF1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Q	13	Total	C	N	O	0	0	0
			101	66	15	20			
5	R	13	Total	C	N	O	0	0	0
			101	66	15	20			
5	T	13	Total	C	N	O	0	0	0
			101	66	15	20			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	S	13	Total	C	N	O	0	0	0
			101	66	15	20			

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	I	0	0
			3	3		
6	B	1	Total	I	0	0
			1	1		
6	C	4	Total	I	0	0
			4	4		
6	D	1	Total	I	0	0
			1	1		
6	E	2	Total	I	0	0
			2	2		
6	F	1	Total	I	0	0
			1	1		
6	G	1	Total	I	0	0
			1	1		
6	H	1	Total	I	0	0
			1	1		
6	K	3	Total	I	0	0
			3	3		
6	L	1	Total	I	0	0
			1	1		
6	P	1	Total	I	0	0
			1	1		
6	I	4	Total	I	0	0
			4	4		
6	J	1	Total	I	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	O	0	0
			2	2		
7	B	2	Total	O	0	0
			2	2		
7	D	3	Total	O	0	0
			3	3		

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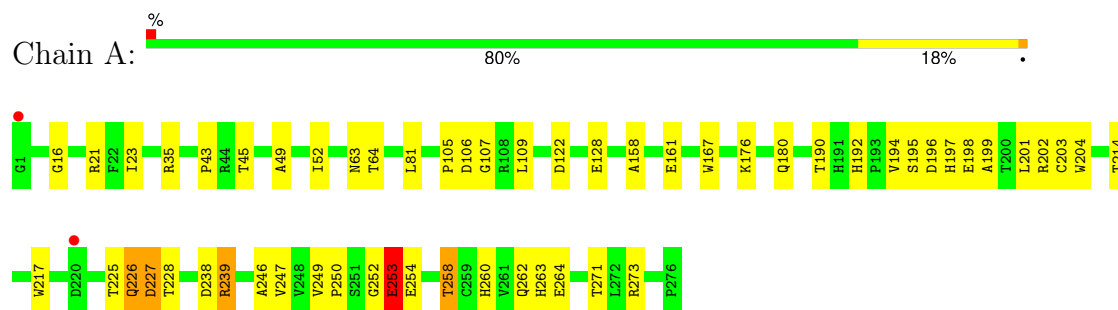
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	3	Total 3	O 3	0	0
7	G	3	Total 3	O 3	0	0
7	H	7	Total 7	O 7	0	0
7	K	3	Total 3	O 3	0	0
7	L	1	Total 1	O 1	0	0
7	N	2	Total 2	O 2	0	0
7	P	6	Total 6	O 6	0	0
7	I	1	Total 1	O 1	0	0
7	J	3	Total 3	O 3	0	0
7	M	2	Total 2	O 2	0	0
7	O	3	Total 3	O 3	0	0

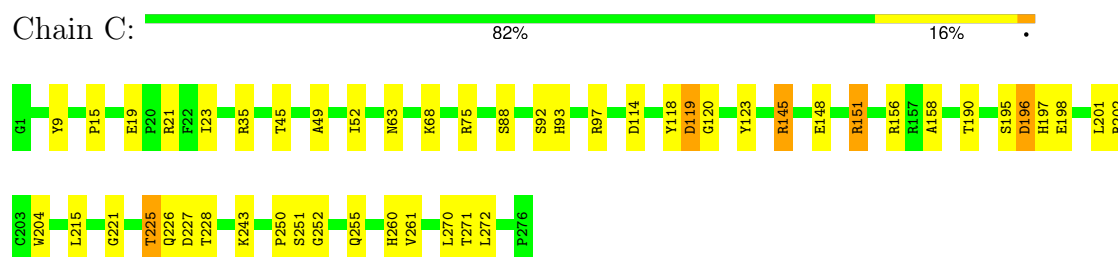
### 3 Residue-property plots

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

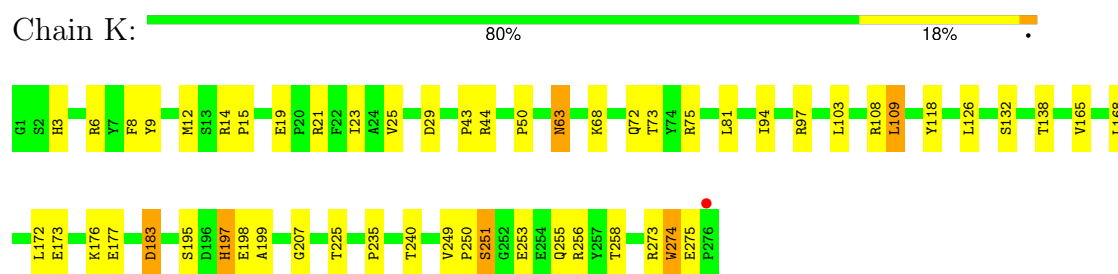
- Molecule 1: HLA class I histocompatibility antigen, B-35 alpha chain



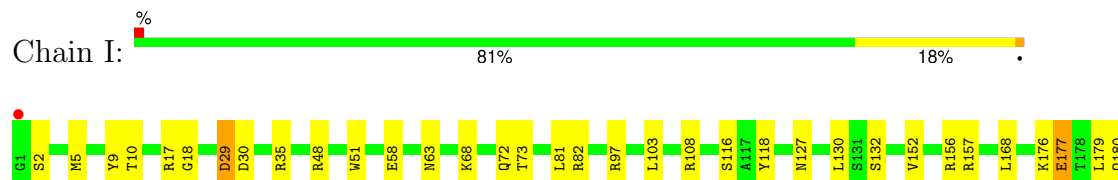
- Molecule 1: HLA class I histocompatibility antigen, B-35 alpha chain



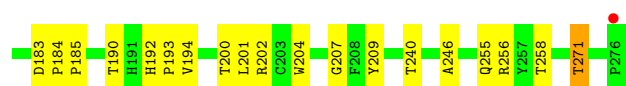
- Molecule 1: HLA class I histocompatibility antigen, B-35 alpha chain



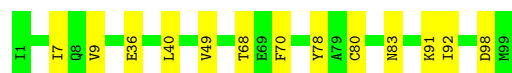
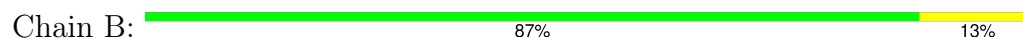
- Molecule 1: HLA class I histocompatibility antigen, B-35 alpha chain







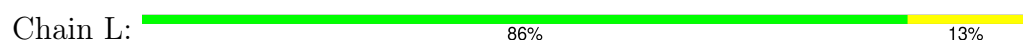
• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin



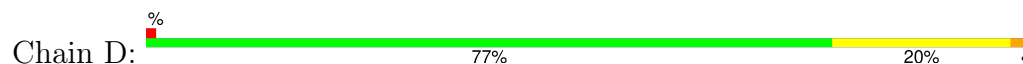
• Molecule 2: Beta-2-microglobulin



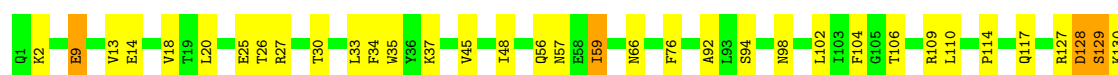
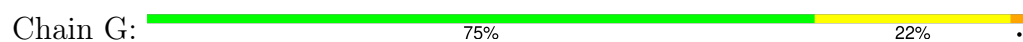
• Molecule 2: Beta-2-microglobulin



• Molecule 3: SB27 T cell receptor alpha chain

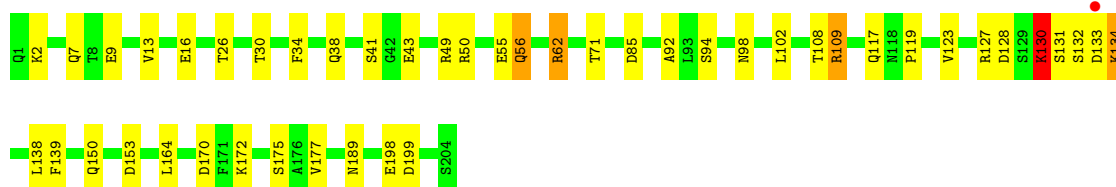
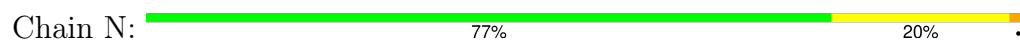


• Molecule 3: SB27 T cell receptor alpha chain

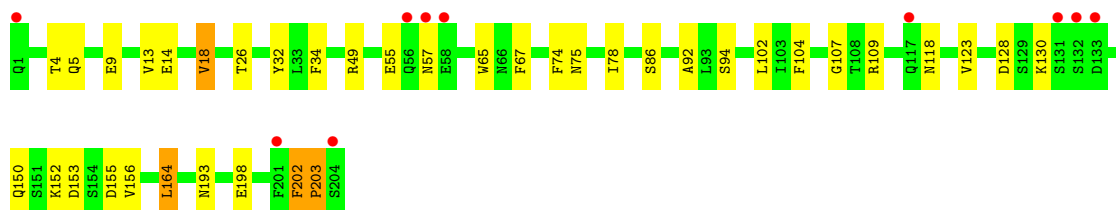
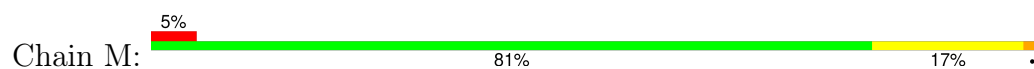




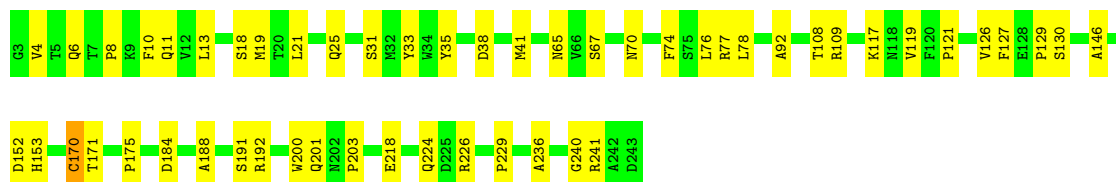
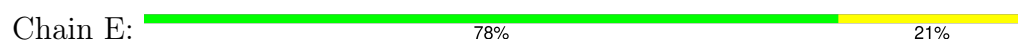
- Molecule 3: SB27 T cell receptor alpha chain



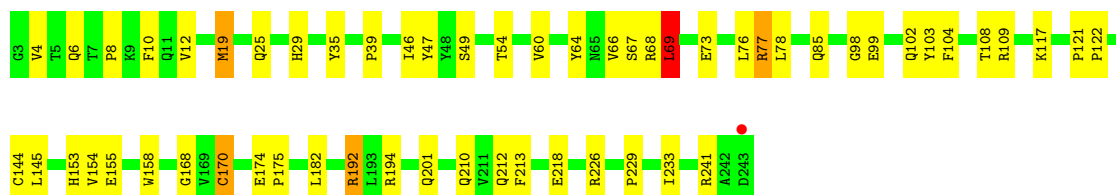
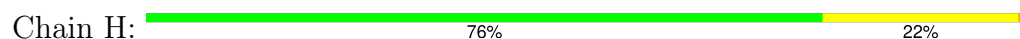
- Molecule 3: SB27 T cell receptor alpha chain



- Molecule 4: SB27 T cell receptor beta chain

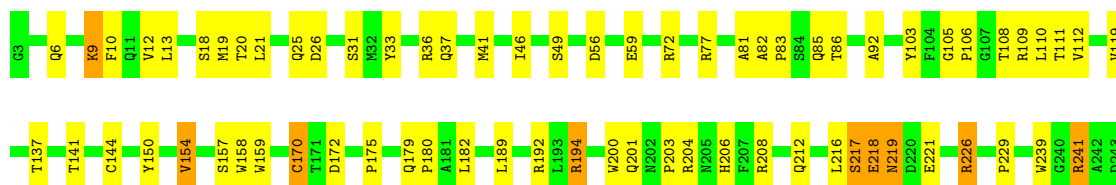


- Molecule 4: SB27 T cell receptor beta chain

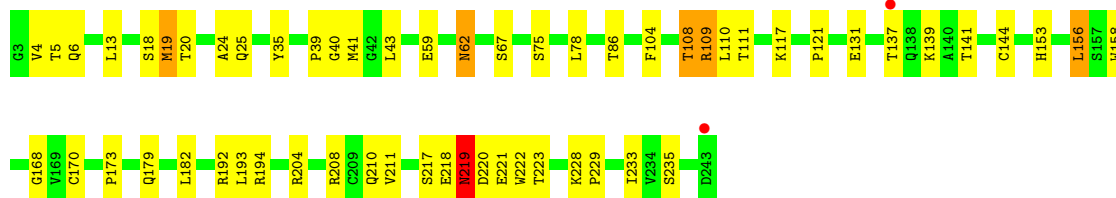
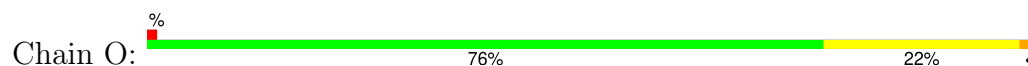


- Molecule 4: SB27 T cell receptor beta chain

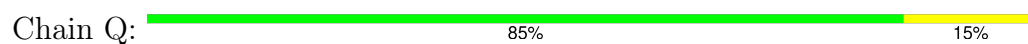




- Molecule 4: SB27 T cell receptor beta chain



- Molecule 5: peptide from Trans-activator protein BZLF1



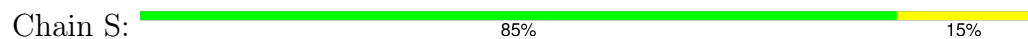
- Molecule 5: peptide from Trans-activator protein BZLF1



- Molecule 5: peptide from Trans-activator protein BZLF1



- Molecule 5: peptide from Trans-activator protein BZLF1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.69Å 207.08Å 123.51Å 90.00° 90.19° 90.00°	Depositor
Resolution (Å)	80.00 – 3.10 79.35 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (80.00-3.10) 98.6 (79.35-3.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.213 , 0.291 0.184 , 0.213	Depositor DCC
$R_{free}$ test set	3612 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.2	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , -7.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.265 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	26991	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: IOD

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	0.34	0/2309	0.54	0/3140
1	C	0.35	0/2309	0.55	0/3140
1	I	0.34	0/2320	0.53	0/3154
1	K	0.34	0/2309	0.54	0/3140
2	B	0.36	0/852	0.49	0/1152
2	F	0.35	0/852	0.52	0/1152
2	J	0.34	0/852	0.48	0/1152
2	L	0.35	0/852	0.48	0/1152
3	D	0.37	0/1675	0.56	0/2276
3	G	0.39	0/1681	0.56	1/2284 (0.0%)
3	M	0.38	0/1675	0.52	0/2276
3	N	0.38	0/1675	0.53	0/2276
4	E	0.36	0/1967	0.53	0/2676
4	H	0.36	0/1967	0.54	0/2676
4	O	0.38	0/1966	0.54	0/2676
4	P	0.36	0/1974	0.53	0/2687
5	Q	0.39	0/104	0.52	0/142
5	R	0.36	0/104	0.51	0/142
5	S	0.31	0/104	0.49	0/142
5	T	0.37	0/104	0.48	0/142
All	All	0.36	0/27651	0.53	1/37577 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	164	LEU	CA-CB-CG	5.71	128.42	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2246	0	2111	48	0
1	C	2246	0	2111	43	0
1	I	2254	0	2124	33	0
1	K	2246	0	2111	32	0
2	B	829	0	794	8	0
2	F	829	0	794	4	0
2	J	829	0	794	13	0
2	L	829	0	794	5	0
3	D	1637	0	1532	33	0
3	G	1640	0	1537	28	0
3	M	1637	0	1532	21	0
3	N	1637	0	1532	24	0
4	E	1915	0	1809	27	0
4	H	1915	0	1809	33	0
4	O	1914	0	1809	37	0
4	P	1919	0	1813	40	0
5	Q	101	0	102	2	0
5	R	101	0	102	1	0
5	S	101	0	102	1	0
5	T	101	0	102	3	0
6	A	3	0	0	1	0
6	B	1	0	0	0	0
6	C	4	0	0	1	0
6	D	1	0	0	0	0
6	E	2	0	0	1	0
6	F	1	0	0	0	0
6	G	1	0	0	1	0
6	H	1	0	0	0	0
6	I	4	0	0	3	0
6	J	1	0	0	0	0
6	K	3	0	0	1	0
6	L	1	0	0	1	0
6	P	1	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	D	3	0	0	0	0
7	E	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	3	0	0	0	0
7	H	7	0	0	0	0
7	I	1	0	0	1	0
7	J	3	0	0	0	0
7	K	3	0	0	0	0
7	L	1	0	0	0	0
7	M	2	0	0	0	0
7	N	2	0	0	0	0
7	O	3	0	0	0	0
7	P	6	0	0	0	0
All	All	26991	0	25414	404	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 8.

All (404) 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:190:THR:CG2	1:A:202:ARG:HB3	1.55	1.36
1:C:195:SER:HB3	1:C:196:ASP:CB	1.65	1.26
1:A:252:GLY:CA	1:A:253:GLU:HB2	1.64	1.25
1:A:252:GLY:HA3	1:A:253:GLU:CB	1.79	1.11
3:M:202:PHE:H	3:M:203:PRO:HD2	1.07	1.11
1:A:190:THR:HG21	1:A:202:ARG:HB3	1.36	1.06
1:C:195:SER:CB	1:C:196:ASP:HB2	1.84	1.06
1:A:195:SER:HB3	1:A:196:ASP:HB3	1.11	1.05
4:H:68:ARG:CA	4:H:69:LEU:HB2	1.88	1.04
3:D:132:SER:HB2	3:D:134:LYS:HA	1.37	1.04
3:G:128:ASP:HB3	3:G:129:SER:C	1.80	1.00
4:H:68:ARG:HA	4:H:69:LEU:CB	1.91	1.00
1:C:195:SER:HB3	1:C:196:ASP:HB2	1.00	0.99
3:M:202:PHE:N	3:M:203:PRO:HD2	1.74	0.96
4:H:68:ARG:HA	4:H:69:LEU:HB2	0.97	0.96
1:A:195:SER:HB2	1:A:197:HIS:H	1.32	0.95
1:A:190:THR:HG22	1:A:202:ARG:O	1.67	0.94
1:A:190:THR:CG2	1:A:202:ARG:CB	2.46	0.93
1:A:195:SER:CB	1:A:196:ASP:HB3	2.00	0.92
3:M:202:PHE:H	3:M:203:PRO:CD	1.83	0.92
4:E:67:SER:HB2	4:E:77:ARG:HH12	1.33	0.92
1:A:195:SER:HB3	1:A:196:ASP:CB	2.00	0.89
4:H:8:PRO:O	4:H:108:THR:HG22	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:38:GLN:HE22	4:P:37:GLN:HE22	1.19	0.88
3:N:133:ASP:O	3:N:134:LYS:HB2	1.71	0.88
3:M:202:PHE:O	3:M:203:PRO:O	1.90	0.88
3:N:55:GLU:N	3:N:56:GLN:HB2	1.90	0.87
4:H:6:GLN:HE21	4:H:108:THR:HG23	1.39	0.87
1:C:195:SER:HB2	1:C:198:GLU:H	1.44	0.83
1:A:190:THR:HG23	1:A:202:ARG:HB3	1.59	0.82
1:A:252:GLY:HA3	1:A:253:GLU:HB2	0.85	0.80
3:G:128:ASP:HB3	3:G:129:SER:O	1.81	0.80
4:H:121:PRO:HD3	4:H:229:PRO:HB3	1.63	0.79
1:C:190:THR:CG2	1:C:202:ARG:HB3	2.13	0.79
1:A:190:THR:HG22	1:A:202:ARG:HB3	1.63	0.78
4:H:6:GLN:NE2	4:H:108:THR:HG23	1.99	0.78
4:O:218:GLU:HB2	4:O:219:ASN:HB2	1.65	0.76
1:C:190:THR:HG21	1:C:204:TRP:HE1	1.50	0.75
1:C:151:ARG:HH11	1:C:151:ARG:CG	2.00	0.75
4:H:201:GLN:HA	4:H:241:ARG:O	1.87	0.74
1:C:19:GLU:HG2	1:C:75:ARG:CZ	2.18	0.74
4:E:8:PRO:O	4:E:108:THR:HG22	1.88	0.73
1:A:195:SER:CB	1:A:197:HIS:H	2.03	0.71
4:P:6:GLN:HE21	4:P:108:THR:HG22	1.56	0.70
4:O:218:GLU:CB	4:O:219:ASN:HB2	2.21	0.69
1:C:190:THR:HG23	1:C:202:ARG:HB3	1.74	0.68
4:O:6:GLN:HE21	4:O:108:THR:HG23	1.60	0.67
3:N:38:GLN:HE22	4:P:37:GLN:NE2	1.91	0.66
4:H:46:ILE:HG22	4:H:47:TYR:HD1	1.60	0.66
3:D:132:SER:CB	3:D:134:LYS:HA	2.21	0.66
4:E:226:ARG:HD3	6:E:244:IOD:I	2.66	0.65
1:K:103:LEU:HD11	1:K:165:VAL:HG13	1.79	0.65
1:A:252:GLY:CA	1:A:253:GLU:CB	2.51	0.65
3:G:135:SER:OG	3:G:136:VAL:N	2.29	0.64
3:D:94:SER:HB2	3:D:102:LEU:HD12	1.78	0.64
4:P:6:GLN:NE2	4:P:108:THR:HG22	2.12	0.63
1:K:195:SER:HB2	1:K:198:GLU:H	1.63	0.63
4:O:218:GLU:CA	4:O:219:ASN:HB2	2.29	0.63
3:G:18:VAL:HG11	3:G:110:LEU:HD13	1.80	0.62
4:O:86:THR:HG23	4:O:111:THR:HA	1.82	0.62
4:H:69:LEU:HD13	4:H:73:GLU:HB2	1.81	0.61
3:G:37:LYS:HB3	3:G:45:VAL:HG13	1.82	0.61
4:P:26:ASP:HB3	4:P:72:ARG:NH1	2.15	0.61
3:N:164:LEU:HD23	4:P:170:CYS:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:THR:O	1:C:228:THR:HG22	2.01	0.61
3:G:34:PHE:HB2	3:G:92:ALA:HB3	1.82	0.60
1:C:151:ARG:HH11	1:C:151:ARG:HG2	1.65	0.60
1:K:81:LEU:HD23	1:K:118:TYR:CD1	2.36	0.60
1:A:238:ASP:O	1:A:239:ARG:HB2	2.01	0.60
1:C:195:SER:CB	1:C:196:ASP:CB	2.58	0.60
3:D:39:PRO:C	3:D:41:SER:H	2.04	0.60
3:N:38:GLN:NE2	4:P:37:GLN:HE22	1.94	0.60
3:N:13:VAL:O	3:N:16:GLU:HB2	2.02	0.59
4:E:8:PRO:O	4:E:108:THR:CG2	2.49	0.59
4:O:156:LEU:HG	4:O:211:VAL:HG22	1.83	0.59
4:H:170:CYS:HB3	4:H:192:ARG:HD3	1.84	0.59
4:P:141:THR:OG1	4:P:194:ARG:HD3	2.02	0.59
1:I:2:SER:HB2	1:I:103:LEU:O	2.02	0.59
3:N:128:ASP:HB2	3:N:134:LYS:O	2.02	0.59
1:A:43:PRO:HG2	6:A:277:IOD:I	2.73	0.59
1:C:45:THR:HG21	1:C:63:ASN:HB2	1.84	0.59
4:E:146:ALA:O	4:E:188:ALA:HA	2.03	0.59
2:J:1:ILE:HG21	2:J:3:ARG:HH21	1.68	0.59
4:P:21:LEU:HD23	4:P:108:THR:HG21	1.85	0.58
1:A:258:THR:HG23	1:A:273:ARG:HE	1.67	0.58
3:D:175:SER:OG	4:E:192:ARG:HD3	2.01	0.58
3:N:34:PHE:HB2	3:N:92:ALA:HB3	1.84	0.58
4:P:6:GLN:OE1	4:P:105:GLY:HA3	2.03	0.58
1:K:108:ARG:HG2	1:K:109:LEU:H	1.67	0.58
3:N:9:GLU:HG3	3:N:109:ARG:HB3	1.84	0.58
1:K:255:GLN:NE2	1:K:274:TRP:HB3	2.19	0.58
1:A:176:LYS:HB2	1:A:180:GLN:HG3	1.84	0.58
1:A:195:SER:HB2	1:A:197:HIS:N	2.13	0.58
2:B:49:VAL:HG12	2:B:68:THR:HB	1.85	0.58
1:K:255:GLN:HE22	1:K:274:TRP:HB3	1.69	0.58
1:C:215:LEU:HD13	1:C:243:LYS:HD3	1.85	0.57
4:E:38:ASP:O	4:E:41:MET:HB2	2.04	0.57
3:N:7:GLN:O	3:N:108:THR:HG23	2.05	0.57
3:D:117:GLN:HG3	4:O:18:SER:HB2	1.86	0.57
1:A:190:THR:HG23	1:A:202:ARG:CB	2.26	0.57
4:P:83:PRO:HA	4:P:112:VAL:HB	1.87	0.56
3:D:34:PHE:HB2	3:D:92:ALA:HB3	1.86	0.56
3:N:117:GLN:O	3:N:119:PRO:HD3	2.06	0.56
4:E:21:LEU:HD12	4:E:76:LEU:HD23	1.85	0.56
4:P:26:ASP:HB3	4:P:72:ARG:HH11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:37:VAL:HG22	2:F:82:VAL:HG22	1.86	0.56
4:O:35:TYR:HB3	4:O:43:LEU:HD22	1.88	0.56
1:C:93:HIS:HB3	1:C:119:ASP:OD1	2.06	0.56
1:K:6:ARG:HB3	1:K:8:PHE:CE1	2.41	0.56
1:I:190:THR:HG21	1:I:204:TRP:HE1	1.69	0.56
1:K:9:TYR:HB2	1:K:97:ARG:HB3	1.87	0.56
1:K:43:PRO:HG2	6:K:279:IOD:I	2.76	0.55
1:A:45:THR:HG21	1:A:63:ASN:HB2	1.88	0.55
4:H:122:PRO:HD3	4:H:213:PHE:CD1	2.40	0.55
3:M:202:PHE:CD2	3:M:203:PRO:HD3	2.41	0.55
4:P:6:GLN:HE21	4:P:108:THR:CG2	2.20	0.55
1:I:258:THR:HB	1:I:271:THR:HG22	1.89	0.55
4:O:117:LYS:HG3	4:O:222:TRP:CH2	2.42	0.54
1:C:197:HIS:O	1:C:250:PRO:HA	2.07	0.54
4:P:33:TYR:OH	5:T:7:GLN:NE2	2.40	0.54
4:P:217:SER:OG	4:P:218:GLU:N	2.40	0.54
1:I:183:ASP:HB2	1:I:209:TYR:H	1.72	0.54
1:A:190:THR:HG21	1:A:204:TRP:HE1	1.73	0.54
2:L:30:PHE:HZ	2:L:64:LEU:HD12	1.72	0.54
3:N:62:ARG:NH2	3:N:85:ASP:OD2	2.37	0.54
1:C:45:THR:HG21	1:C:63:ASN:CB	2.37	0.54
1:K:8:PHE:HB2	1:K:25:VAL:HG23	1.89	0.54
4:H:46:ILE:HD13	4:H:60:VAL:HG23	1.88	0.54
1:I:130:LEU:O	1:I:157:ARG:HD2	2.08	0.54
4:O:218:GLU:N	4:O:219:ASN:HB2	2.21	0.54
1:C:195:SER:HB3	1:C:196:ASP:CA	2.37	0.54
1:C:145:ARG:HA	1:C:148:GLU:HG3	1.89	0.53
3:G:164:LEU:HD11	4:H:194:ARG:HB3	1.90	0.53
3:M:202:PHE:N	3:M:203:PRO:CD	2.48	0.53
4:O:144:CYS:HB2	4:O:158:TRP:CZ2	2.43	0.53
4:P:201:GLN:O	4:P:203:PRO:HD3	2.08	0.53
3:G:128:ASP:CB	3:G:129:SER:C	2.67	0.53
3:M:153:ASP:HB3	3:M:156:VAL:HG23	1.91	0.53
4:O:168:GLY:O	4:O:193:LEU:HA	2.08	0.53
3:D:49:ARG:NH1	3:D:51:ASN:OD1	2.41	0.53
4:P:36:ARG:HB3	4:P:46:ILE:HD11	1.91	0.53
4:O:6:GLN:HE21	4:O:108:THR:CG2	2.22	0.53
3:D:129:SER:N	3:D:130:LYS:O	2.41	0.53
1:K:68:LYS:O	1:K:72:GLN:HG2	2.09	0.53
1:C:195:SER:CA	1:C:196:ASP:HB2	2.39	0.52
1:A:49:ALA:O	1:A:52:ILE:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:63:ASN:HD21	5:T:1:LEU:HD12	1.75	0.52
1:C:195:SER:HB2	1:C:198:GLU:N	2.20	0.52
1:C:9:TYR:HB2	1:C:97:ARG:HB3	1.92	0.52
1:K:235:PRO:HG2	2:L:65:LEU:HD13	1.92	0.52
4:O:217:SER:H	4:O:220:ASP:HB2	1.75	0.52
3:N:94:SER:HB2	3:N:102:LEU:HD12	1.91	0.52
1:C:49:ALA:O	1:C:52:ILE:HG22	2.10	0.52
1:C:260:HIS:CD2	1:C:271:THR:HG22	2.45	0.52
1:K:258:THR:HG22	1:K:273:ARG:HG2	1.91	0.52
3:M:67:PHE:HB2	3:M:74:PHE:CD1	2.44	0.52
3:D:37:LYS:HB3	3:D:45:VAL:HG13	1.92	0.51
3:M:32:TYR:HE1	3:M:34:PHE:CE1	2.28	0.51
3:D:127:ARG:O	3:D:128:ASP:O	2.28	0.51
4:O:121:PRO:HD3	4:O:229:PRO:HB3	1.93	0.51
4:P:110:LEU:HD23	4:P:111:THR:N	2.26	0.51
2:B:36:GLU:HB2	2:B:83:ASN:HB3	1.93	0.51
1:A:190:THR:HG22	1:A:202:ARG:C	2.31	0.51
2:B:9:VAL:CG2	2:B:80:CYS:HB3	2.40	0.51
4:E:10:PHE:CD1	4:E:153:HIS:HB3	2.45	0.51
3:M:5:GLN:NE2	3:M:107:GLY:HA2	2.25	0.51
3:M:18:VAL:HG23	3:M:78:ILE:HB	1.93	0.51
1:C:261:VAL:HG22	1:C:270:LEU:HB2	1.92	0.51
3:M:65:TRP:HA	3:M:75:ASN:O	2.10	0.51
4:O:222:TRP:HB3	4:O:228:LYS:HG3	1.92	0.51
2:B:9:VAL:HG21	2:B:80:CYS:HB3	1.93	0.50
4:H:210:GLN:HG3	4:H:233:ILE:HG23	1.93	0.50
1:K:255:GLN:O	1:K:256:ARG:HB2	2.11	0.50
1:A:201:LEU:O	1:A:246:ALA:HA	2.11	0.50
4:E:171:THR:HG23	4:E:191:SER:HB2	1.94	0.50
3:G:189:ASN:C	3:G:189:ASN:HD22	2.15	0.50
3:G:164:LEU:HD13	4:H:168:GLY:HA2	1.93	0.50
2:J:1:ILE:HG21	2:J:3:ARG:NH2	2.26	0.50
3:D:18:VAL:HG11	3:D:110:LEU:HD13	1.94	0.50
4:E:31:SER:HB3	4:E:33:TYR:CE1	2.47	0.50
1:K:19:GLU:HB3	1:K:75:ARG:HH21	1.77	0.50
1:I:68:LYS:O	1:I:72:GLN:HG2	2.12	0.50
1:K:255:GLN:HE21	1:K:274:TRP:HE3	1.60	0.49
3:D:35:TRP:HD1	3:D:74:PHE:CE2	2.31	0.49
1:I:190:THR:CG2	1:I:202:ARG:HB3	2.42	0.49
3:D:12:VAL:HG21	3:D:18:VAL:HG22	1.93	0.49
4:E:33:TYR:HB2	4:E:92:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:206:HIS:CE1	4:P:208:ARG:HB2	2.47	0.49
4:H:64:TYR:HB3	4:H:76:LEU:HD11	1.95	0.49
4:O:141:THR:OG1	4:O:194:ARG:HD3	2.12	0.49
1:A:214:THR:HB	1:A:262:GLN:HB2	1.94	0.49
1:C:68:LYS:HG2	6:C:278:IOD:I	2.82	0.49
4:E:201:GLN:HA	4:E:241:ARG:O	2.13	0.49
4:E:67:SER:HB2	4:E:77:ARG:NH1	2.15	0.49
4:P:216:LEU:HD13	4:P:229:PRO:HG2	1.94	0.49
2:J:29:GLY:HA2	2:J:61:SER:HB2	1.93	0.49
1:A:109:LEU:HD22	1:A:161:GLU:HG2	1.95	0.49
1:C:151:ARG:CG	1:C:151:ARG:NH1	2.67	0.49
1:I:127:ASN:ND2	1:I:132:SER:OG	2.46	0.49
4:P:157:SER:HG	4:P:159:TRP:HE1	1.61	0.49
4:E:121:PRO:HD3	4:E:229:PRO:HB3	1.95	0.48
4:H:46:ILE:HG22	4:H:47:TYR:CD1	2.43	0.48
1:A:16:GLY:HA2	1:K:50:PRO:HG2	1.93	0.48
4:H:10:PHE:CD1	4:H:153:HIS:HB3	2.48	0.48
1:I:58:GLU:HB3	7:I:281:HOH:O	2.12	0.48
1:C:118:TYR:O	1:C:120:GLY:N	2.46	0.48
3:M:164:LEU:HD11	4:O:194:ARG:HB3	1.94	0.48
4:E:6:GLN:NE2	4:E:108:THR:HG23	2.28	0.48
2:J:9:VAL:HG21	2:J:80:CYS:HB3	1.95	0.48
1:C:15:PRO:HD3	1:C:92:SER:HB2	1.96	0.48
3:G:98:ASN:HB3	5:R:6:PRO:O	2.14	0.48
1:K:8:PHE:HB2	1:K:25:VAL:CG2	2.43	0.48
3:N:133:ASP:O	3:N:134:LYS:CB	2.51	0.48
1:I:73:THR:OG1	5:S:10:LEU:HD23	2.14	0.48
4:P:6:GLN:HB3	4:P:106:PRO:HD2	1.96	0.47
1:C:145:ARG:HA	1:C:148:GLU:CG	2.43	0.47
3:G:20:LEU:HD12	3:G:76:PHE:HD2	1.78	0.47
1:K:108:ARG:CG	1:K:109:LEU:H	2.27	0.47
1:A:252:GLY:N	1:A:253:GLU:HB2	2.25	0.47
1:A:225:THR:HA	1:A:228:THR:HG22	1.96	0.47
4:P:206:HIS:HD2	4:P:239:TRP:CE2	2.33	0.47
1:C:251:SER:HB2	3:D:167:ARG:HD2	1.96	0.47
3:G:127:ARG:HG2	3:G:128:ASP:H	1.80	0.47
1:I:190:THR:CG2	1:I:204:TRP:HE1	2.28	0.47
1:A:194:VAL:H	1:A:199:ALA:HA	1.79	0.47
2:L:43:GLY:N	6:L:100:IOD:I	3.10	0.47
1:K:168:LEU:O	1:K:172:LEU:HG	2.15	0.47
3:D:129:SER:H	3:D:130:LYS:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:210:GLN:HG3	4:O:233:ILE:HG23	1.96	0.47
1:C:19:GLU:HG2	1:C:75:ARG:NH1	2.30	0.46
1:I:190:THR:HG23	1:I:202:ARG:HB3	1.96	0.46
1:A:195:SER:CB	1:A:197:HIS:N	2.76	0.46
1:I:18:GLY:O	6:I:280:IOD:I	3.02	0.46
2:J:81:ARG:HG3	2:J:92:ILE:HG12	1.97	0.46
2:J:96:ASP:C	2:J:98:ASP:H	2.18	0.46
1:A:250:PRO:HG2	1:A:253:GLU:OE1	2.15	0.46
1:K:173:GLU:O	1:K:176:LYS:HG3	2.15	0.46
4:P:19:MET:HE1	4:P:21:LEU:HG	1.96	0.46
4:P:154:VAL:HA	4:P:212:GLN:O	2.16	0.46
2:F:51:HIS:HA	2:F:65:LEU:O	2.15	0.46
3:G:35:TRP:HB2	3:G:48:ILE:HG22	1.97	0.46
3:G:94:SER:HB2	3:G:102:LEU:CD1	2.46	0.46
3:D:117:GLN:HG3	4:O:18:SER:CB	2.46	0.46
3:D:127:ARG:HH11	3:D:128:ASP:HB2	1.80	0.46
4:E:170:CYS:SG	4:E:192:ARG:HD2	2.56	0.46
4:O:13:LEU:HD21	4:O:19:MET:HB2	1.98	0.46
2:B:7:ILE:HD12	2:B:91:LYS:HD3	1.98	0.45
4:O:179:GLN:O	4:O:179:GLN:HG2	2.15	0.45
4:E:126:VAL:HG23	4:E:236:ALA:HB3	1.97	0.45
4:H:144:CYS:HB2	4:H:158:TRP:CZ2	2.52	0.45
1:K:21:ARG:NE	1:K:23:ILE:HD11	2.32	0.45
4:E:152:ASP:HB2	4:E:175:PRO:HG2	1.98	0.45
3:N:123:VAL:HA	3:N:138:LEU:O	2.16	0.45
3:G:94:SER:HB2	3:G:102:LEU:HD12	1.99	0.45
3:D:128:ASP:HB3	3:D:130:LYS:O	2.16	0.45
1:I:207:GLY:HA2	1:I:240:THR:HB	1.99	0.45
1:C:195:SER:HB3	1:C:196:ASP:HB3	1.82	0.45
4:H:98:GLY:HA2	4:H:103:TYR:CE1	2.52	0.45
1:I:255:GLN:HA	1:I:256:ARG:HA	1.71	0.45
4:H:78:LEU:HD23	4:H:85:GLN:NE2	2.32	0.45
2:J:40:LEU:HD23	2:J:45:ARG:HA	1.97	0.45
4:O:217:SER:N	4:O:220:ASP:HB2	2.31	0.45
1:A:158:ALA:HA	3:D:30:THR:HG21	1.99	0.45
4:P:13:LEU:HD11	4:P:19:MET:HB3	1.97	0.45
4:O:210:GLN:HG3	4:O:233:ILE:CG2	2.46	0.45
3:N:55:GLU:HB2	3:N:56:GLN:OE1	2.17	0.45
3:N:177:VAL:HG23	4:P:192:ARG:HE	1.82	0.44
1:I:176:LYS:HG2	1:I:180:GLN:HG3	1.98	0.44
3:M:94:SER:HB2	3:M:102:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:5:THR:OG1	4:O:24:ALA:HB3	2.17	0.44
1:C:215:LEU:HG	1:C:261:VAL:HG12	2.00	0.44
1:K:207:GLY:HA2	1:K:240:THR:HB	2.00	0.44
3:N:98:ASN:HA	4:P:31:SER:OG	2.18	0.44
1:I:5:MET:HB2	1:I:168:LEU:HD13	2.00	0.44
4:H:154:VAL:HA	4:H:212:GLN:O	2.17	0.44
3:N:164:LEU:O	3:N:172:LYS:HA	2.17	0.44
3:G:104:PHE:HZ	4:H:104:PHE:CZ	2.36	0.44
3:G:161:LYS:HA	3:G:175:SER:O	2.18	0.44
3:N:130:LYS:HA	3:N:131:SER:HA	1.67	0.44
3:M:123:VAL:HB	3:M:202:PHE:CB	2.48	0.44
4:O:218:GLU:HB2	4:O:219:ASN:CB	2.43	0.44
3:D:35:TRP:CD1	3:D:74:PHE:CE2	3.05	0.44
1:I:9:TYR:HB2	1:I:97:ARG:HB3	2.00	0.44
1:I:68:LYS:HG2	6:I:277:IOD:I	2.88	0.44
4:O:218:GLU:H	4:O:219:ASN:HB2	1.82	0.44
3:D:39:PRO:C	3:D:41:SER:N	2.70	0.44
1:I:48:ARG:NE	2:J:53:ASP:OD2	2.51	0.44
3:M:94:SER:HB2	3:M:102:LEU:HD13	1.98	0.44
1:C:21:ARG:HE	1:C:23:ILE:HD11	1.82	0.43
4:P:82:ALA:H	4:P:85:GLN:HE21	1.66	0.43
2:J:49:VAL:HG12	2:J:68:THR:HB	2.00	0.43
1:A:226:GLN:HA	1:A:227:ASP:HA	1.63	0.43
4:P:9:LYS:HE2	4:P:10:PHE:CE2	2.53	0.43
1:A:21:ARG:CZ	1:A:23:ILE:HD11	2.48	0.43
1:A:192:HIS:NE2	2:B:98:ASP:HB3	2.33	0.43
1:A:263:HIS:CG	1:A:264:GLU:H	2.36	0.43
3:N:139:PHE:O	3:N:175:SER:HA	2.18	0.43
1:I:10:THR:HG21	2:J:62:PHE:HE1	1.83	0.43
1:I:29:ASP:HB2	1:I:30:ASP:H	1.64	0.43
3:G:59:ILE:H	3:G:59:ILE:HG13	1.68	0.43
3:N:94:SER:HB2	3:N:102:LEU:CD1	2.49	0.43
3:D:20:LEU:HD12	3:D:76:PHE:HD2	1.84	0.43
1:K:183:ASP:N	1:K:183:ASP:OD2	2.52	0.43
4:P:81:ALA:HA	4:P:85:GLN:NE2	2.34	0.43
4:O:137:THR:O	4:O:139:LYS:HG2	2.19	0.43
1:A:105:PRO:C	1:A:107:GLY:H	2.22	0.43
1:A:260:HIS:HD2	1:A:271:THR:HG22	1.83	0.43
3:D:162:CYS:O	3:D:174:ASN:HA	2.19	0.43
4:H:19:MET:HE2	4:H:19:MET:HB3	1.93	0.43
3:D:102:LEU:HB3	4:E:35:TYR:OH	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:36:GLU:O	2:F:82:VAL:HA	2.19	0.43
1:I:81:LEU:HD23	1:I:118:TYR:CG	2.54	0.43
1:I:152:VAL:O	1:I:156:ARG:HG2	2.18	0.43
2:J:9:VAL:CG2	2:J:80:CYS:HB3	2.49	0.43
3:M:67:PHE:HB2	3:M:74:PHE:CE1	2.54	0.43
4:O:39:PRO:C	4:O:41:MET:H	2.23	0.43
4:H:8:PRO:O	4:H:108:THR:CG2	2.54	0.43
3:N:117:GLN:HA	3:N:117:GLN:OE1	2.19	0.43
1:I:51:TRP:CZ2	1:I:179:LEU:HD11	2.54	0.43
3:M:9:GLU:HG3	3:M:109:ARG:HB3	2.00	0.43
4:O:170:CYS:HB3	4:O:192:ARG:HD2	2.01	0.43
4:H:49:SER:OG	4:H:68:ARG:HD3	2.19	0.43
1:K:199:ALA:O	1:K:249:VAL:HG22	2.17	0.43
4:P:119:VAL:HG13	4:P:150:TYR:O	2.19	0.43
4:O:62:ASN:N	4:O:62:ASN:HD22	2.16	0.43
4:H:67:SER:HB2	4:H:77:ARG:HH12	1.84	0.42
4:P:86:THR:HG23	4:P:111:THR:HA	2.01	0.42
4:O:18:SER:HA	4:O:78:LEU:O	2.19	0.42
1:A:195:SER:HB2	1:A:198:GLU:H	1.84	0.42
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.55	0.42
3:D:129:SER:H	3:D:130:LYS:CA	2.32	0.42
3:G:130:LYS:HA	3:G:130:LYS:HD2	1.85	0.42
4:P:172:ASP:HB2	4:P:189:LEU:HD12	2.01	0.42
3:M:104:PHE:HZ	4:O:104:PHE:HZ	1.68	0.42
1:A:81:LEU:HD11	5:Q:13:TYR:HB3	2.02	0.42
4:P:200:TRP:CZ2	4:P:241:ARG:HB2	2.54	0.42
1:I:17:ARG:HA	6:I:280:IOD:I	2.89	0.42
1:I:183:ASP:HA	1:I:184:PRO:HD2	1.90	0.42
4:E:13:LEU:HD11	4:E:19:MET:HB2	2.02	0.42
1:K:126:LEU:HD12	1:K:132:SER:O	2.19	0.42
2:J:2:GLN:HB3	2:J:86:THR:HG22	2.02	0.42
4:O:109:ARG:HB3	4:O:153:HIS:CE1	2.55	0.42
1:C:151:ARG:HH11	1:C:151:ARG:HG3	1.79	0.42
3:G:143:ASP:HB2	6:G:205:IOD:I	2.89	0.42
4:H:4:VAL:HG12	4:H:102:GLN:O	2.20	0.42
3:M:34:PHE:HB2	3:M:92:ALA:HB3	2.01	0.42
3:G:14:GLU:HG3	3:G:114:PRO:HA	2.01	0.42
1:C:195:SER:CB	1:C:196:ASP:CA	2.98	0.42
1:K:12:MET:HG3	1:K:94:ILE:HG12	2.01	0.42
1:I:81:LEU:HD23	1:I:118:TYR:CD1	2.55	0.42
1:I:177:GLU:H	1:I:177:GLU:HG3	1.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:190:THR:HG22	1:I:202:ARG:O	2.20	0.42
1:I:192:HIS:HA	1:I:193:PRO:HD3	1.84	0.42
3:D:88:VAL:HG22	3:D:109:ARG:HB2	2.01	0.41
3:G:2:LYS:HB3	3:G:25:GLU:HB2	2.01	0.41
3:G:9:GLU:HG3	3:G:109:ARG:HB3	2.02	0.41
1:C:190:THR:HG22	1:C:202:ARG:HB3	1.99	0.41
3:D:123:VAL:O	3:D:203:PRO:HD2	2.20	0.41
3:D:126:LEU:HB3	4:E:127:PHE:HB3	2.02	0.41
4:E:119:VAL:O	4:E:226:ARG:NH2	2.39	0.41
1:C:250:PRO:O	1:C:252:GLY:O	2.37	0.41
1:A:167:TRP:NE1	5:Q:1:LEU:HD22	2.36	0.41
3:G:128:ASP:HB3	3:G:129:SER:CA	2.48	0.41
4:P:119:VAL:O	4:P:226:ARG:NH2	2.50	0.41
1:I:201:LEU:O	1:I:246:ALA:HA	2.20	0.41
3:M:13:VAL:HG12	3:M:14:GLU:N	2.36	0.41
1:C:118:TYR:HB2	1:C:123:TYR:CD1	2.55	0.41
3:G:102:LEU:HB3	4:H:35:TYR:OH	2.21	0.41
1:K:250:PRO:HB2	1:K:253:GLU:HB2	2.03	0.41
2:J:16:GLU:HB3	2:J:19:LYS:HG3	2.01	0.41
1:C:158:ALA:HA	3:G:30:THR:HG21	2.03	0.41
1:K:3:HIS:HD2	1:K:29:ASP:OD2	2.03	0.41
4:P:144:CYS:HB2	4:P:158:TRP:CZ2	2.56	0.41
1:A:249:VAL:HG21	1:A:254:GLU:HG3	2.03	0.41
2:B:40:LEU:O	2:B:78:TYR:HA	2.21	0.41
1:C:190:THR:HG21	1:C:204:TRP:NE1	2.27	0.41
3:D:136:VAL:HG22	3:D:179:TRP:HB3	2.03	0.41
4:E:119:VAL:HG12	4:E:229:PRO:HB2	2.02	0.41
2:F:27:VAL:O	2:F:63:TYR:HA	2.20	0.41
3:G:56:GLN:H	3:G:56:GLN:NE2	2.19	0.41
4:P:31:SER:HA	4:P:49:SER:O	2.21	0.41
4:H:155:GLU:HB2	4:H:212:GLN:HB3	2.03	0.41
1:I:184:PRO:HA	1:I:185:PRO:HD3	1.89	0.41
4:O:13:LEU:HD12	4:O:110:LEU:HD21	2.03	0.41
4:O:208:ARG:NH2	4:O:235:SER:OG	2.53	0.41
3:D:117:GLN:O	4:O:18:SER:HB2	2.21	0.41
3:D:128:ASP:HB3	3:D:129:SER:H	1.73	0.41
1:K:14:ARG:HA	1:K:15:PRO:HD2	1.84	0.41
4:E:18:SER:HA	4:E:78:LEU:O	2.20	0.40
1:A:45:THR:HG21	1:A:63:ASN:CB	2.51	0.40
3:D:133:ASP:HA	3:D:134:LYS:HA	1.77	0.40
4:E:203:PRO:HA	4:E:240:GLY:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:THR:HG22	1:A:64:THR:OG1	2.21	0.40
4:H:66:VAL:HG12	4:H:76:LEU:HA	2.03	0.40
4:H:210:GLN:HG3	4:H:233:ILE:CG2	2.52	0.40
1:K:197:HIS:O	1:K:251:SER:N	2.55	0.40
2:L:11:SER:HB2	2:L:21:ASN:ND2	2.36	0.40
2:L:49:VAL:HG12	2:L:68:THR:HB	2.02	0.40
4:P:92:ALA:HA	4:P:103:TYR:O	2.21	0.40
5:T:3:GLU:HA	5:T:4:PRO:HD3	1.88	0.40
2:B:49:VAL:O	2:B:49:VAL:HG23	2.22	0.40
1:C:114:ASP:OD2	1:C:156:ARG:HD2	2.22	0.40
4:E:129:PRO:HD2	4:E:200:TRP:CZ2	2.57	0.40
4:P:219:ASN:HD22	4:P:219:ASN:HA	1.71	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	244 (89%)	27 (10%)	3 (1%)	14	46
1	C	274/276 (99%)	248 (90%)	22 (8%)	4 (2%)	10	39
1	I	275/276 (100%)	252 (92%)	23 (8%)	0	100	100
1	K	274/276 (99%)	255 (93%)	18 (7%)	1 (0%)	34	69
2	B	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
2	F	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
2	J	97/99 (98%)	85 (88%)	11 (11%)	1 (1%)	15	49
2	L	97/99 (98%)	93 (96%)	2 (2%)	2 (2%)	7	30
3	D	202/204 (99%)	179 (89%)	18 (9%)	5 (2%)	5	27
3	G	203/204 (100%)	185 (91%)	16 (8%)	2 (1%)	15	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	202/204 (99%)	181 (90%)	17 (8%)	4 (2%)	7	31
3	N	202/204 (99%)	182 (90%)	17 (8%)	3 (2%)	10	39
4	E	239/241 (99%)	225 (94%)	14 (6%)	0	100	100
4	H	239/241 (99%)	218 (91%)	18 (8%)	3 (1%)	12	42
4	O	239/241 (99%)	219 (92%)	16 (7%)	4 (2%)	9	36
4	P	240/241 (100%)	224 (93%)	13 (5%)	3 (1%)	12	42
5	Q	11/13 (85%)	9 (82%)	2 (18%)	0	100	100
5	R	11/13 (85%)	9 (82%)	2 (18%)	0	100	100
5	S	11/13 (85%)	10 (91%)	0	1 (9%)	1	4
5	T	11/13 (85%)	11 (100%)	0	0	100	100
All	All	3295/3332 (99%)	3013 (91%)	246 (8%)	36 (1%)	14	46

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	GLU
1	C	119	ASP
3	D	128	ASP
3	G	131	SER
4	H	69	LEU
3	N	130	LYS
3	N	134	LYS
3	M	203	PRO
1	C	196	ASP
3	D	14	GLU
3	D	116	ILE
3	D	130	LYS
3	G	57	ASN
1	K	274	TRP
2	L	48	LYS
3	M	128	ASP
1	C	221	GLY
4	H	175	PRO
3	N	56	GLN
4	P	218	GLU
3	M	86	SER
4	O	40	GLY
4	O	219	ASN

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Mol	Chain	Res	Type
4	O	221	GLU
1	C	88	SER
4	H	39	PRO
2	J	97	ARG
1	A	239	ARG
4	P	175	PRO
4	P	180	PRO
3	M	202	PHE
4	O	173	PRO
1	A	106	ASP
3	D	40	PRO
2	L	14	PRO
5	S	8	GLY

### 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	231/231 (100%)	223 (96%)	8 (4%)	36	68
1	C	231/231 (100%)	222 (96%)	9 (4%)	32	65
1	I	232/231 (100%)	222 (96%)	10 (4%)	29	62
1	K	231/231 (100%)	220 (95%)	11 (5%)	25	58
2	B	94/94 (100%)	92 (98%)	2 (2%)	53	79
2	F	94/94 (100%)	90 (96%)	4 (4%)	29	62
2	J	94/94 (100%)	91 (97%)	3 (3%)	39	69
2	L	94/94 (100%)	89 (95%)	5 (5%)	22	54
3	D	189/189 (100%)	176 (93%)	13 (7%)	15	45
3	G	190/189 (100%)	170 (90%)	20 (10%)	7	26
3	M	189/189 (100%)	175 (93%)	14 (7%)	13	42
3	N	189/189 (100%)	170 (90%)	19 (10%)	7	28
4	E	208/208 (100%)	195 (94%)	13 (6%)	18	48
4	H	208/208 (100%)	191 (92%)	17 (8%)	11	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	O	208/208 (100%)	192 (92%)	16 (8%)	13	41
4	P	209/208 (100%)	187 (90%)	22 (10%)	7	26
5	Q	11/11 (100%)	11 (100%)	0	100	100
5	R	11/11 (100%)	11 (100%)	0	100	100
5	S	11/11 (100%)	11 (100%)	0	100	100
5	T	11/11 (100%)	11 (100%)	0	100	100
All	All	2935/2932 (100%)	2749 (94%)	186 (6%)	18	48

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	122	ASP
1	A	128	GLU
1	A	226	GLN
1	A	227	ASP
1	A	247	VAL
1	A	253	GLU
1	A	258	THR
2	B	70	PHE
2	B	92	ILE
1	C	35	ARG
1	C	145	ARG
1	C	151	ARG
1	C	201	LEU
1	C	225	THR
1	C	226	GLN
1	C	227	ASP
1	C	255	GLN
1	C	272	LEU
3	D	10	ILE
3	D	18	VAL
3	D	26	THR
3	D	34	PHE
3	D	41	SER
3	D	84	VAL
3	D	99	THR
3	D	106	THR
3	D	127	ARG
3	D	130	LYS

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Mol	Chain	Res	Type
3	D	134	LYS
3	D	164	LEU
3	D	182	LYS
4	E	4	VAL
4	E	11	GLN
4	E	25	GLN
4	E	65	ASN
4	E	70	ASN
4	E	74	PHE
4	E	109	ARG
4	E	117	LYS
4	E	130	SER
4	E	170	CYS
4	E	184	ASP
4	E	218	GLU
4	E	224	GLN
2	F	68	THR
2	F	69	GLU
2	F	70	PHE
2	F	92	ILE
3	G	9	GLU
3	G	13	VAL
3	G	26	THR
3	G	27	ARG
3	G	33	LEU
3	G	59	ILE
3	G	66	ASN
3	G	106	THR
3	G	117	GLN
3	G	128	ASP
3	G	129	SER
3	G	133	ASP
3	G	146	THR
3	G	150	GLN
3	G	155	ASP
3	G	164	LEU
3	G	170	ASP
3	G	182	LYS
3	G	189	ASN
3	G	193	ASN
4	H	12	VAL
4	H	19	MET

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Mol	Chain	Res	Type
4	H	25	GLN
4	H	29	HIS
4	H	54	THR
4	H	69	LEU
4	H	77	ARG
4	H	99	GLU
4	H	109	ARG
4	H	117	LYS
4	H	145	LEU
4	H	170	CYS
4	H	174	GLU
4	H	182	LEU
4	H	192	ARG
4	H	218	GLU
4	H	226	ARG
1	K	44	ARG
1	K	63	ASN
1	K	73	THR
1	K	109	LEU
1	K	138	THR
1	K	177	GLU
1	K	183	ASP
1	K	197	HIS
1	K	225	THR
1	K	251	SER
1	K	275	GLU
2	L	27	VAL
2	L	34	ASP
2	L	64	LEU
2	L	70	PHE
2	L	85	VAL
3	N	2	LYS
3	N	26	THR
3	N	30	THR
3	N	41	SER
3	N	43	GLU
3	N	49	ARG
3	N	50	ARG
3	N	62	ARG
3	N	71	THR
3	N	109	ARG
3	N	127	ARG

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Mol	Chain	Res	Type
3	N	130	LYS
3	N	132	SER
3	N	150	GLN
3	N	153	ASP
3	N	170	ASP
3	N	189	ASN
3	N	198	GLU
3	N	199	ASP
4	P	9	LYS
4	P	12	VAL
4	P	18	SER
4	P	20	THR
4	P	25	GLN
4	P	41	MET
4	P	56	ASP
4	P	59	GLU
4	P	77	ARG
4	P	109	ARG
4	P	137	THR
4	P	154	VAL
4	P	170	CYS
4	P	179	GLN
4	P	182	LEU
4	P	194	ARG
4	P	204	ARG
4	P	217	SER
4	P	219	ASN
4	P	221	GLU
4	P	226	ARG
4	P	241	ARG
1	I	29	ASP
1	I	35	ARG
1	I	63	ASN
1	I	82	ARG
1	I	108	ARG
1	I	116	SER
1	I	177	GLU
1	I	194	VAL
1	I	200	THR
1	I	271	THR
2	J	38	ASP
2	J	70	PHE

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Mol	Chain	Res	Type
2	J	89	GLN
3	M	4	THR
3	M	18	VAL
3	M	26	THR
3	M	49	ARG
3	M	55	GLU
3	M	57	ASN
3	M	118	ASN
3	M	130	LYS
3	M	150	GLN
3	M	152	LYS
3	M	155	ASP
3	M	164	LEU
3	M	193	ASN
3	M	198	GLU
4	O	4	VAL
4	O	19	MET
4	O	20	THR
4	O	25	GLN
4	O	59	GLU
4	O	62	ASN
4	O	67	SER
4	O	75	SER
4	O	108	THR
4	O	109	ARG
4	O	131	GLU
4	O	156	LEU
4	O	182	LEU
4	O	204	ARG
4	O	219	ASN
4	O	223	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	HIS
1	A	191	HIS
1	A	260	HIS
2	B	51	HIS
1	C	63	ASN
1	C	80	ASN
1	C	86	ASN

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Mol	Chain	Res	Type
1	C	191	HIS
1	C	226	GLN
1	C	255	GLN
3	D	66	ASN
3	D	68	GLN
3	D	111	GLN
3	D	117	GLN
3	D	193	ASN
4	E	118	ASN
4	E	224	GLN
3	G	56	GLN
3	G	66	ASN
3	G	68	GLN
3	G	181	ASN
3	G	189	ASN
4	H	29	HIS
4	H	65	ASN
4	H	85	GLN
4	H	118	ASN
1	K	3	HIS
1	K	63	ASN
1	K	255	GLN
1	K	260	HIS
3	N	66	ASN
3	N	145	GLN
4	P	11	GLN
4	P	37	GLN
4	P	62	ASN
4	P	85	GLN
4	P	153	HIS
4	P	206	HIS
4	P	219	ASN
4	P	232	GLN
5	T	7	GLN
1	I	70	ASN
1	I	80	ASN
3	M	57	ASN
3	M	115	ASN
4	O	11	GLN
4	O	30	ASN
4	O	62	ASN
4	O	85	GLN

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Mol	Chain	Res	Type
4	O	118	ASN
4	O	138	GLN
4	O	153	HIS
4	O	206	HIS

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	276/276 (100%)	0.08	2 (0%) 87 75	12, 26, 37, 43	6 (2%)
1	C	276/276 (100%)	0.09	0 100 100	11, 24, 35, 42	7 (2%)
1	I	276/276 (100%)	0.22	2 (0%) 87 75	12, 26, 37, 43	8 (2%)
1	K	276/276 (100%)	0.06	1 (0%) 92 84	11, 24, 35, 42	7 (2%)
2	B	99/99 (100%)	-0.04	0 100 100	14, 24, 31, 41	8 (8%)
2	F	99/99 (100%)	-0.13	0 100 100	12, 24, 37, 42	5 (5%)
2	J	99/99 (100%)	-0.04	0 100 100	17, 27, 38, 45	5 (5%)
2	L	99/99 (100%)	-0.09	0 100 100	13, 24, 35, 37	7 (7%)
3	D	204/204 (100%)	0.13	2 (0%) 82 67	15, 27, 38, 44	4 (1%)
3	G	204/204 (100%)	0.07	0 100 100	14, 24, 38, 45	4 (1%)
3	M	204/204 (100%)	0.44	10 (4%) 29 14	15, 27, 38, 43	6 (2%)
3	N	204/204 (100%)	0.11	1 (0%) 91 81	14, 24, 38, 45	8 (3%)
4	E	241/241 (100%)	0.11	0 100 100	11, 24, 34, 41	4 (1%)
4	H	241/241 (100%)	0.10	1 (0%) 92 84	11, 22, 35, 43	2 (0%)
4	O	241/241 (100%)	0.12	2 (0%) 86 72	12, 24, 33, 38	2 (0%)
4	P	241/241 (100%)	0.00	0 100 100	11, 23, 34, 43	4 (1%)
5	Q	13/13 (100%)	-0.11	0 100 100	2, 4, 7, 11	0
5	R	13/13 (100%)	0.41	0 100 100	2, 10, 24, 25	0
5	S	13/13 (100%)	0.19	0 100 100	12, 17, 22, 23	0
5	T	13/13 (100%)	0.05	0 100 100	5, 8, 17, 19	0
All	All	3332/3332 (100%)	0.10	21 (0%) 89 78	2, 25, 36, 45	87 (2%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	276	PRO	4.6
3	M	204	SER	4.1
3	N	133	ASP	4.0
3	M	131	SER	3.6
3	D	132	SER	3.3
1	I	276	PRO	3.1
3	D	131	SER	3.0
3	M	57	ASN	3.0
3	M	58	GLU	2.8
4	H	243	ASP	2.7
3	M	1	GLN	2.7
1	I	1	GLY	2.7
1	A	220	ASP	2.7
3	M	132	SER	2.5
4	O	243	ASP	2.2
3	M	133	ASP	2.2
3	M	201	PHE	2.1
4	O	137	THR	2.1
1	A	1	GLY	2.0
3	M	117	GLN	2.0
3	M	56	GLN	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	IOD	H	244	1/1	0.75	0.13	151,151,151,151	0
6	IOD	E	245	1/1	0.81	0.14	149,149,149,149	0
6	IOD	I	280	1/1	0.85	0.09	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	IOD	P	1	1/1	0.91	0.10	86,86,86,86	0
6	IOD	G	205	1/1	0.91	0.11	73,73,73,73	0
6	IOD	C	279	1/1	0.92	0.17	154,154,154,154	0
6	IOD	L	100	1/1	0.93	0.08	69,69,69,69	0
6	IOD	B	100	1/1	0.95	0.10	74,74,74,74	0
6	IOD	F	100	1/1	0.96	0.13	93,93,93,93	0
6	IOD	I	278	1/1	0.97	0.11	40,40,40,40	0
6	IOD	D	205	1/1	0.97	0.11	89,89,89,89	0
6	IOD	J	100	1/1	0.97	0.10	115,115,115,115	0
6	IOD	K	279	1/1	0.98	0.10	32,32,32,32	0
6	IOD	I	279	1/1	0.98	0.13	28,28,28,28	0
6	IOD	A	277	1/1	0.98	0.11	31,31,31,31	0
6	IOD	E	244	1/1	0.98	0.07	50,50,50,50	0
6	IOD	C	278	1/1	0.99	0.10	39,39,39,39	0
6	IOD	I	277	1/1	0.99	0.09	37,37,37,37	0
6	IOD	A	279	1/1	0.99	0.12	21,21,21,21	0
6	IOD	K	277	1/1	1.00	0.12	18,18,18,18	0
6	IOD	K	278	1/1	1.00	0.12	10,10,10,10	0
6	IOD	A	278	1/1	1.00	0.10	14,14,14,14	0
6	IOD	C	277	1/1	1.00	0.09	13,13,13,13	0
6	IOD	C	280	1/1	1.00	0.10	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.