



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 07:52 PM BST

PDB ID : 4P2Q
Title : Crystal structure of the 5cc7 TCR in complex with 5c2/I-Ek
Authors : Birnbaum, M.E.; Ozkan, E.; Garcia, K.C.
Deposited on : 2014-03-04
Resolution : 3.30 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

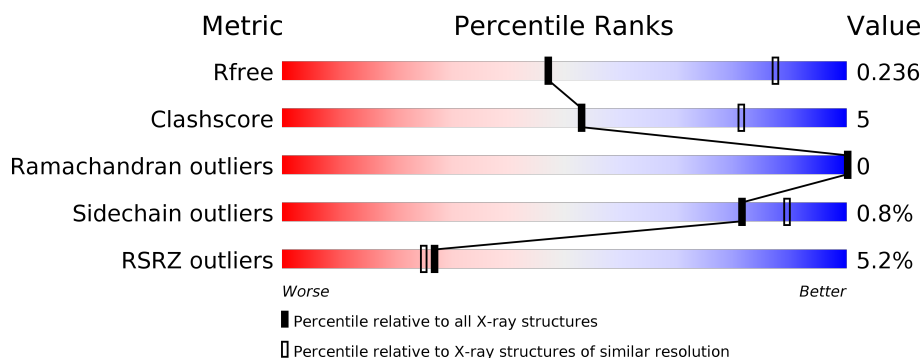
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	204	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 70%; height: 10px; background-color: green;"></div> <div style="width: 18%; height: 10px; background-color: yellow;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 70% 18% 12% </div> </div>
1	F	204	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 74%; height: 10px; background-color: green;"></div> <div style="width: 14%; height: 10px; background-color: yellow;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 74% 14% 12% </div> </div>
1	K	204	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 73%; height: 10px; background-color: green;"></div> <div style="width: 15%; height: 10px; background-color: yellow;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 73% 15% 12% </div> </div>
1	P	204	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red;"></div> <div style="width: 73%; height: 10px; background-color: green;"></div> <div style="width: 15%; height: 10px; background-color: yellow;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 4% 73% 15% 12% </div> </div>
2	B	212	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red;"></div> <div style="width: 67%; height: 10px; background-color: green;"></div> <div style="width: 14%; height: 10px; background-color: yellow;"></div> <div style="width: 19%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 5% 67% 14% 19% </div> </div>
2	G	212	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red;"></div> <div style="width: 66%; height: 10px; background-color: green;"></div> <div style="width: 15%; height: 10px; background-color: yellow;"></div> <div style="width: 19%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 5% 66% 15% 19% </div> </div>

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Mol	Chain	Length	Quality of chain
2	L	212	
2	Q	212	
3	C	14	
3	H	14	
3	M	14	
3	R	14	
4	D	205	
4	I	205	
4	N	205	
4	S	205	
5	E	266	
5	J	266	
5	O	266	
5	T	266	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25667 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 H-2 class II histocompatibility antigen, E-K alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1473	951	243	275	4			
1	F	180	Total	C	N	O	S	0	0	0
			1473	951	243	275	4			
1	K	180	Total	C	N	O	S	0	0	0
			1469	948	242	275	4			
1	P	179	Total	C	N	O	S	0	0	0
			1461	942	241	274	4			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP P04224
A	-1	ASP	-	expression tag	UNP P04224
A	0	PRO	-	expression tag	UNP P04224
A	192	SER	-	expression tag	UNP P04224
A	193	ARG	-	expression tag	UNP P04224
A	194	GLY	-	expression tag	UNP P04224
A	195	GLY	-	expression tag	UNP P04224
A	196	LEU	-	expression tag	UNP P04224
A	197	GLU	-	expression tag	UNP P04224
A	198	VAL	-	expression tag	UNP P04224
A	199	LEU	-	expression tag	UNP P04224
A	200	PHE	-	expression tag	UNP P04224
A	201	GLN	-	expression tag	UNP P04224
F	-2	ALA	-	expression tag	UNP P04224
F	-1	ASP	-	expression tag	UNP P04224
F	0	PRO	-	expression tag	UNP P04224
F	192	SER	-	expression tag	UNP P04224
F	193	ARG	-	expression tag	UNP P04224
F	194	GLY	-	expression tag	UNP P04224
F	195	GLY	-	expression tag	UNP P04224
F	196	LEU	-	expression tag	UNP P04224

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Chain	Residue	Modelled	Actual	Comment	Reference
F	197	GLU	-	expression tag	UNP P04224
F	198	VAL	-	expression tag	UNP P04224
F	199	LEU	-	expression tag	UNP P04224
F	200	PHE	-	expression tag	UNP P04224
F	201	GLN	-	expression tag	UNP P04224
K	-2	ALA	-	expression tag	UNP P04224
K	-1	ASP	-	expression tag	UNP P04224
K	0	PRO	-	expression tag	UNP P04224
K	192	SER	-	expression tag	UNP P04224
K	193	ARG	-	expression tag	UNP P04224
K	194	GLY	-	expression tag	UNP P04224
K	195	GLY	-	expression tag	UNP P04224
K	196	LEU	-	expression tag	UNP P04224
K	197	GLU	-	expression tag	UNP P04224
K	198	VAL	-	expression tag	UNP P04224
K	199	LEU	-	expression tag	UNP P04224
K	200	PHE	-	expression tag	UNP P04224
K	201	GLN	-	expression tag	UNP P04224
P	-2	ALA	-	expression tag	UNP P04224
P	-1	ASP	-	expression tag	UNP P04224
P	0	PRO	-	expression tag	UNP P04224
P	192	SER	-	expression tag	UNP P04224
P	193	ARG	-	expression tag	UNP P04224
P	194	GLY	-	expression tag	UNP P04224
P	195	GLY	-	expression tag	UNP P04224
P	196	LEU	-	expression tag	UNP P04224
P	197	GLU	-	expression tag	UNP P04224
P	198	VAL	-	expression tag	UNP P04224
P	199	LEU	-	expression tag	UNP P04224
P	200	PHE	-	expression tag	UNP P04224
P	201	GLN	-	expression tag	UNP P04224

- Molecule 2 is a protein called MHC class II E-beta-k.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1387	885	237	259	6			
2	G	171	Total	C	N	O	S	0	0	0
			1382	883	237	256	6			
2	L	171	Total	C	N	O	S	0	0	0
			1382	883	237	256	6			
2	Q	171	Total	C	N	O	S	0	0	0
			1382	883	237	256	6			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP Q31163
B	-2	SER	-	expression tag	UNP Q31163
B	-1	GLY	-	expression tag	UNP Q31163
B	0	GLY	-	expression tag	UNP Q31163
B	1	GLY	-	expression tag	UNP Q31163
B	2	GLY	-	expression tag	UNP Q31163
B	199	SER	-	expression tag	UNP Q31163
B	200	ARG	-	expression tag	UNP Q31163
B	201	GLY	-	expression tag	UNP Q31163
B	202	GLY	-	expression tag	UNP Q31163
B	203	LEU	-	expression tag	UNP Q31163
B	204	GLU	-	expression tag	UNP Q31163
B	205	VAL	-	expression tag	UNP Q31163
B	206	LEU	-	expression tag	UNP Q31163
B	207	PHE	-	expression tag	UNP Q31163
B	208	GLN	-	expression tag	UNP Q31163
G	-3	GLY	-	expression tag	UNP Q31163
G	-2	SER	-	expression tag	UNP Q31163
G	-1	GLY	-	expression tag	UNP Q31163
G	0	GLY	-	expression tag	UNP Q31163
G	1	GLY	-	expression tag	UNP Q31163
G	2	GLY	-	expression tag	UNP Q31163
G	199	SER	-	expression tag	UNP Q31163
G	200	ARG	-	expression tag	UNP Q31163
G	201	GLY	-	expression tag	UNP Q31163
G	202	GLY	-	expression tag	UNP Q31163
G	203	LEU	-	expression tag	UNP Q31163
G	204	GLU	-	expression tag	UNP Q31163
G	205	VAL	-	expression tag	UNP Q31163
G	206	LEU	-	expression tag	UNP Q31163
G	207	PHE	-	expression tag	UNP Q31163
G	208	GLN	-	expression tag	UNP Q31163
L	-3	GLY	-	expression tag	UNP Q31163
L	-2	SER	-	expression tag	UNP Q31163
L	-1	GLY	-	expression tag	UNP Q31163
L	0	GLY	-	expression tag	UNP Q31163
L	1	GLY	-	expression tag	UNP Q31163
L	2	GLY	-	expression tag	UNP Q31163
L	199	SER	-	expression tag	UNP Q31163
L	200	ARG	-	expression tag	UNP Q31163
L	201	GLY	-	expression tag	UNP Q31163
L	202	GLY	-	expression tag	UNP Q31163

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Chain	Residue	Modelled	Actual	Comment	Reference
L	203	LEU	-	expression tag	UNP Q31163
L	204	GLU	-	expression tag	UNP Q31163
L	205	VAL	-	expression tag	UNP Q31163
L	206	LEU	-	expression tag	UNP Q31163
L	207	PHE	-	expression tag	UNP Q31163
L	208	GLN	-	expression tag	UNP Q31163
Q	-3	GLY	-	expression tag	UNP Q31163
Q	-2	SER	-	expression tag	UNP Q31163
Q	-1	GLY	-	expression tag	UNP Q31163
Q	0	GLY	-	expression tag	UNP Q31163
Q	1	GLY	-	expression tag	UNP Q31163
Q	2	GLY	-	expression tag	UNP Q31163
Q	199	SER	-	expression tag	UNP Q31163
Q	200	ARG	-	expression tag	UNP Q31163
Q	201	GLY	-	expression tag	UNP Q31163
Q	202	GLY	-	expression tag	UNP Q31163
Q	203	LEU	-	expression tag	UNP Q31163
Q	204	GLU	-	expression tag	UNP Q31163
Q	205	VAL	-	expression tag	UNP Q31163
Q	206	LEU	-	expression tag	UNP Q31163
Q	207	PHE	-	expression tag	UNP Q31163
Q	208	GLN	-	expression tag	UNP Q31163

- Molecule 3 is a protein called 5c2 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	14	Total	C	N	O	0	0	0
			104	67	18	19			
3	H	14	Total	C	N	O	0	0	0
			104	67	18	19			
3	M	13	Total	C	N	O	0	0	0
			100	65	17	18			
3	R	13	Total	C	N	O	0	0	0
			100	65	17	18			

- Molecule 4 is a protein called 5cc7 T-cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	196	Total	C	N	O	S	0	0	0
			1523	942	264	309	8			
4	I	196	Total	C	N	O	S	0	0	0
			1517	939	261	309	8			

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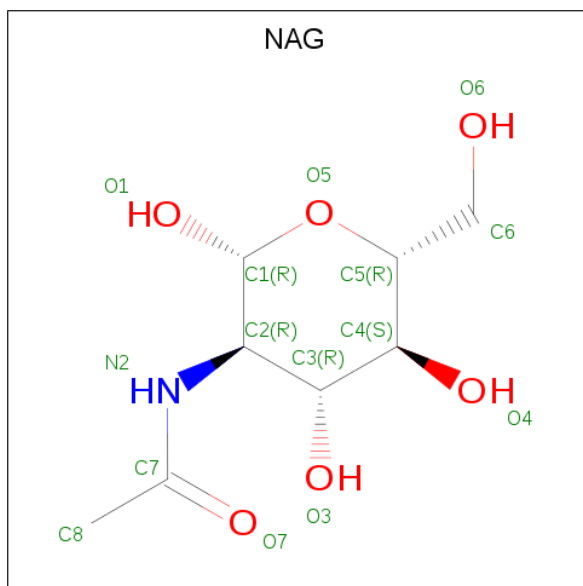
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	196	Total	C	N	O	S	0	0	0
			1523	942	264	309	8			
4	S	196	Total	C	N	O	S	0	0	0
			1523	942	264	309	8			

- Molecule 5 is a protein called 5cc7 T-cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	245	Total	C	N	O	S	0	0	0
			1929	1212	336	372	9			
5	J	245	Total	C	N	O	S	0	0	0
			1929	1212	336	372	9			
5	O	242	Total	C	N	O	S	0	0	0
			1920	1208	334	369	9			
5	T	242	Total	C	N	O	S	0	0	0
			1916	1205	333	369	9			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

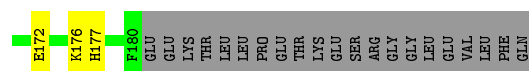


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	K	1	Total	C	N	O	0	0
			14	8	1	5		
6	L	1	Total	C	N	O	0	0
			14	8	1	5		



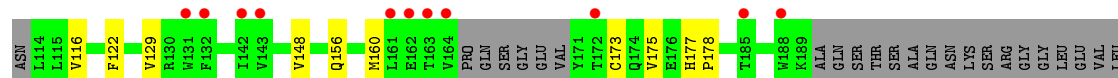
- Molecule 2: MHC class II E-beta-k



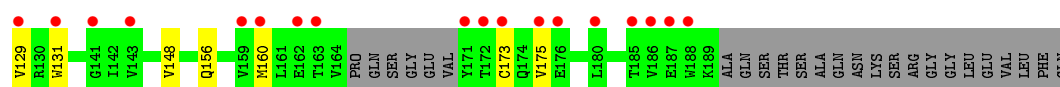
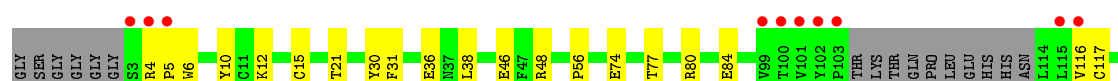
- Molecule 2: MHC class II E-beta-k



- Molecule 2: MHC class II E-beta-k



- Molecule 2: MHC class II E-beta-k



- Molecule 3: 5c2 peptide

Chain C:  93% 7%



- Molecule 3: 5c2 peptide

Chain H:  93% 7%




- Molecule 3: 5c2 peptide

Chain M:  64% 29% 7%




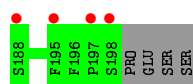
- Molecule 3: 5c2 peptide

Chain R:  7% 86% 7% 7%




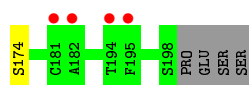
- Molecule 4: 5cc7 T-cell receptor alpha chain

Chain D:  4% 84% 11% .

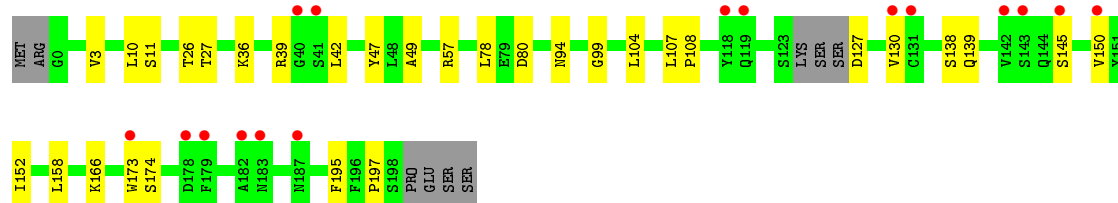
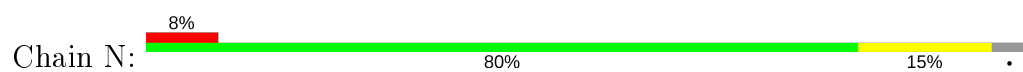


- Molecule 4: 5cc7 T-cell receptor alpha chain

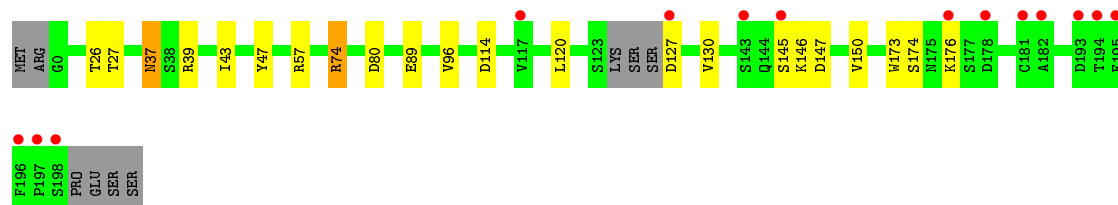
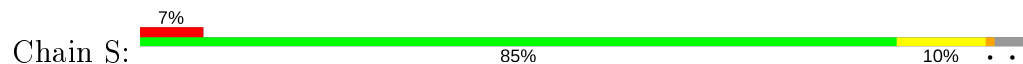
Chain I:  6% 84% 12% .



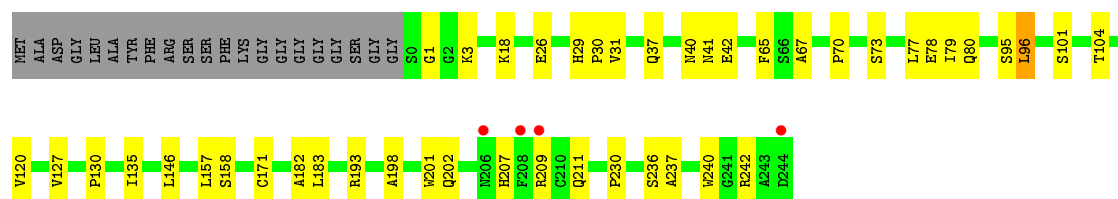
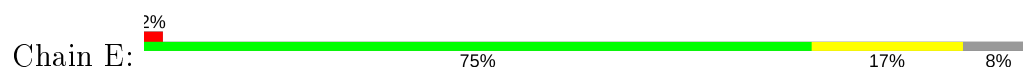
- Molecule 4: 5cc7 T-cell receptor alpha chain



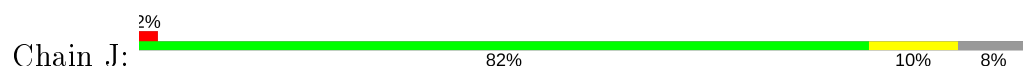
- Molecule 4: 5cc7 T-cell receptor alpha chain



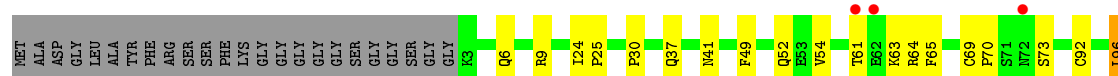
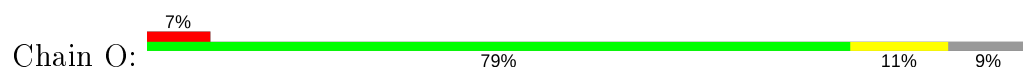
- Molecule 5: 5cc7 T-cell receptor beta chain

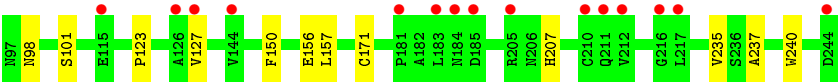


- Molecule 5: 5cc7 T-cell receptor beta chain

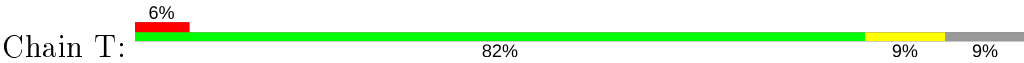


- Molecule 5: 5cc7 T-cell receptor beta chain





● Molecule 5: 5cc7 T-cell receptor beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	262.90Å 102.21Å 214.11Å 90.00° 95.04° 90.00°	Depositor
Resolution (Å)	39.63 – 3.30 39.67 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.63-3.30) 99.3 (39.67-3.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.188 , 0.236 0.189 , 0.236	Depositor DCC
R_{free} test set	4237 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	103.1	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 78.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25667	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NAG

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	0.35	0/1516	0.56	0/2062
1	F	0.31	0/1516	0.50	0/2062
1	K	0.31	0/1512	0.51	0/2058
1	P	0.26	0/1504	0.46	0/2047
2	B	0.38	0/1424	0.51	0/1943
2	G	0.35	0/1419	0.53	0/1937
2	L	0.31	0/1419	0.47	0/1937
2	Q	0.28	0/1419	0.46	0/1937
3	C	0.38	0/106	0.47	0/139
3	H	0.33	0/106	0.45	0/139
3	M	0.38	0/102	0.37	0/134
3	R	0.28	0/102	0.40	0/134
4	D	0.33	0/1551	0.51	0/2098
4	I	0.30	0/1545	0.48	0/2091
4	N	0.32	0/1551	0.50	0/2098
4	S	0.30	0/1551	0.47	0/2098
5	E	0.30	0/1978	0.48	0/2691
5	J	0.28	0/1978	0.46	0/2691
5	O	0.25	0/1969	0.43	0/2678
5	T	0.25	0/1965	0.44	0/2674
All	All	0.30	0/26233	0.48	0/35648

There are no bond length outliers.

There are no bond angle outliers.

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	1473	0	1402	21	0
1	F	1473	0	1403	19	0
1	K	1469	0	1391	21	0
1	P	1461	0	1378	19	0
2	B	1387	0	1279	19	0
2	G	1382	0	1272	20	0
2	L	1382	0	1272	22	0
2	Q	1382	0	1273	17	0
3	C	104	0	99	1	0
3	H	104	0	99	1	0
3	M	100	0	96	4	0
3	R	100	0	96	1	0
4	D	1523	0	1441	17	0
4	I	1517	0	1430	15	0
4	N	1523	0	1441	24	0
4	S	1523	0	1441	16	0
5	E	1929	0	1816	27	0
5	J	1929	0	1816	17	0
5	O	1920	0	1816	20	0
5	T	1916	0	1805	19	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	G	14	0	13	0	0
6	K	14	0	13	0	0
6	L	14	0	13	0	0
All	All	25667	0	24131	269	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 5.

All (269) 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:K:133:SER:HB2	1:K:150:TYR:HB2	1.63	0.79
2:L:10:TYR:HB3	2:L:31:PHE:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:TYR:HB3	2:B:31:PHE:HB2	1.64	0.79
2:L:21:THR:O	2:L:80:ARG:NH1	2.16	0.77
2:L:48:ARG:NH1	1:P:141:ASP:OD2	2.17	0.77
2:B:21:THR:O	2:B:80:ARG:NH1	2.22	0.73
2:Q:10:TYR:HB3	2:Q:31:PHE:HB2	1.72	0.71
1:K:140:ARG:O	2:L:12:LYS:NZ	2.23	0.71
2:G:10:TYR:HB3	2:G:31:PHE:HB2	1.73	0.70
2:G:46:GLU:OE1	2:G:48:ARG:NH2	2.23	0.70
1:A:141:ASP:OD2	2:G:48:ARG:NH1	2.22	0.70
3:R:5:ARG:NH2	5:T:98:ASN:O	2.24	0.70
1:A:123:ARG:NH1	1:A:161:TYR:OH	2.24	0.70
5:T:70:PRO:HB2	5:T:73:SER:HB2	1.72	0.70
1:F:114:PRO:HG3	2:G:6:TRP:CD2	2.28	0.69
5:T:37:GLN:HE21	5:T:41:ASN:HA	1.57	0.69
1:P:133:SER:HB2	1:P:150:TYR:HB2	1.75	0.69
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.75	0.68
5:J:70:PRO:HB2	5:J:73:SER:HB2	1.75	0.68
2:Q:129:VAL:HG22	2:Q:175:VAL:HG22	1.74	0.68
1:A:114:PRO:HG3	2:B:6:TRP:CE2	2.30	0.67
1:P:122:LEU:HB2	1:P:162:ASP:HB2	1.75	0.67
2:B:4:ARG:HD2	2:B:5:PRO:HD2	1.74	0.67
1:K:114:PRO:HG3	2:L:6:TRP:CE2	2.31	0.66
4:I:47:TYR:HE1	5:J:101:SER:HB3	1.59	0.66
2:L:4:ARG:HD2	2:L:5:PRO:HD2	1.79	0.66
2:G:21:THR:O	2:G:80:ARG:NH1	2.28	0.65
4:S:47:TYR:HE1	5:T:101:SER:HB3	1.62	0.65
5:O:70:PRO:HB2	5:O:73:SER:HB2	1.77	0.65
4:D:37:ASN:HD21	4:D:43:ILE:HD13	1.61	0.65
1:F:133:SER:HB2	1:F:150:TYR:HB2	1.79	0.65
1:K:26:PHE:HB2	1:K:31:ILE:HD11	1.79	0.65
1:K:114:PRO:HG3	2:L:6:TRP:CD2	2.32	0.64
5:E:1:GLY:HA2	5:E:3:LYS:H	1.61	0.64
2:B:46:GLU:OE1	2:B:48:ARG:NH2	2.31	0.64
2:G:16:HIS:HB2	2:G:25:ARG:HG2	1.81	0.63
4:N:39:ARG:HH12	5:O:157:LEU:H	1.46	0.63
1:P:114:PRO:HG3	2:Q:6:TRP:CE2	2.33	0.63
1:P:140:ARG:O	2:Q:12:LYS:NZ	2.30	0.63
2:Q:46:GLU:OE1	2:Q:48:ARG:NH2	2.32	0.62
5:O:37:GLN:HE21	5:O:41:ASN:HA	1.62	0.62
5:E:70:PRO:HB2	5:E:73:SER:HB2	1.80	0.62
2:Q:4:ARG:HD2	2:Q:5:PRO:HD2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:VAL:HG22	2:B:175:VAL:HG22	1.83	0.60
2:Q:80:ARG:O	2:Q:84:GLU:HG2	2.02	0.60
5:E:1:GLY:HA2	5:E:3:LYS:N	2.18	0.58
1:K:39:SER:HB2	1:K:60:LEU:HD11	1.86	0.58
3:M:3:TYR:OH	4:N:94:ASN:OD1	2.22	0.58
5:J:219:GLU:OE1	5:J:219:GLU:N	2.34	0.58
4:S:147:ASP:OD2	4:S:176:LYS:NZ	2.37	0.58
4:N:158:LEU:HB3	5:O:171:CYS:HB2	1.86	0.58
1:A:82:ASP:OD2	2:B:3:SER:OG	2.19	0.57
1:P:107:CYS:HB3	1:P:149:HIS:HB2	1.85	0.57
1:A:140:ARG:O	2:B:12:LYS:NZ	2.38	0.57
4:N:47:TYR:HE1	5:O:101:SER:HB3	1.69	0.57
4:S:37:ASN:HD21	4:S:43:ILE:HD13	1.70	0.57
4:I:57:ARG:NH1	4:I:80:ASP:OD2	2.32	0.57
1:F:140:ARG:O	2:G:12:LYS:NZ	2.37	0.56
5:J:209:ARG:NH2	5:J:211:GLN:OE1	2.38	0.56
4:D:145:SER:HB3	4:D:152:ILE:HG13	1.88	0.55
5:E:209:ARG:NH2	5:E:211:GLN:OE1	2.33	0.55
5:J:209:ARG:NH1	5:J:236:SER:OG	2.39	0.55
2:B:25:ARG:HH21	2:B:41:ASP:CG	2.09	0.55
4:I:150:VAL:HG12	4:I:174:SER:HB2	1.89	0.55
4:I:47:TYR:CE1	5:J:101:SER:HB3	2.40	0.55
2:L:80:ARG:O	2:L:84:GLU:HG2	2.07	0.54
2:B:25:ARG:NH2	2:B:41:ASP:OD2	2.41	0.54
4:S:74:ARG:HH11	4:S:74:ARG:HB2	1.73	0.54
5:J:30:PRO:HD2	5:J:96:LEU:HA	1.90	0.54
5:E:209:ARG:NH1	5:E:236:SER:OG	2.41	0.53
4:D:47:TYR:HE1	5:E:101:SER:HB3	1.73	0.53
2:B:74:GLU:HA	2:B:77:THR:OG1	2.09	0.53
5:J:1:GLY:HA2	5:J:3:LYS:H	1.73	0.53
2:Q:116:VAL:HG22	2:Q:160:MET:HG2	1.89	0.53
2:L:148:VAL:HB	2:L:156:GLN:HG3	1.89	0.53
4:D:145:SER:HB2	4:D:150:VAL:HG23	1.90	0.53
1:A:39:SER:HB2	1:A:60:LEU:HD11	1.90	0.52
2:L:85:ILE:HD12	3:M:1:LEU:HD23	1.92	0.52
2:Q:21:THR:O	2:Q:80:ARG:NH1	2.43	0.52
2:G:132:PHE:HB2	2:G:172:THR:HG23	1.92	0.52
1:A:97:VAL:HG21	1:A:178:TRP:HZ2	1.73	0.52
2:B:35:GLU:HG2	2:B:51:THR:HG21	1.91	0.52
5:T:182:ALA:O	5:T:183:LEU:HB3	2.09	0.52
5:E:37:GLN:HE21	5:E:41:ASN:HA	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:GLU:HG2	4:D:49:ALA:HB3	1.92	0.51
2:G:117:CYS:HB2	2:G:131:TRP:CZ2	2.46	0.51
4:D:57:ARG:NH1	4:D:80:ASP:OD2	2.29	0.51
1:F:122:LEU:HB2	1:F:162:ASP:HB2	1.92	0.51
4:N:39:ARG:HG2	5:O:9:ARG:HH21	1.75	0.51
4:N:145:SER:HB3	4:N:152:ILE:HG13	1.92	0.51
4:D:10:LEU:HD23	4:D:104:LEU:HD13	1.93	0.51
4:I:36:LYS:HB2	4:I:42:LEU:HD23	1.93	0.51
1:F:13:TYR:OH	1:F:67:LYS:HE2	2.11	0.51
4:N:78:LEU:HD22	4:N:166:LYS:HD3	1.93	0.51
5:T:130:PRO:HD2	5:T:201:TRP:CZ2	2.46	0.51
4:D:9:ALA:HB3	4:N:11:SER:HB2	1.93	0.51
4:N:10:LEU:HD23	4:N:104:LEU:HD13	1.93	0.50
2:Q:74:GLU:HA	2:Q:77:THR:OG1	2.11	0.50
4:N:145:SER:HB2	4:N:150:VAL:HG23	1.93	0.50
4:N:150:VAL:HG12	4:N:174:SER:HB2	1.93	0.50
2:L:16:HIS:HB2	2:L:25:ARG:HG2	1.93	0.50
5:E:130:PRO:HD2	5:E:201:TRP:CZ2	2.47	0.50
5:J:182:ALA:O	5:J:183:LEU:HB3	2.12	0.50
1:A:114:PRO:HG3	2:B:6:TRP:CD2	2.47	0.50
2:L:46:GLU:OE1	2:L:48:ARG:NH2	2.44	0.50
1:P:116:VAL:O	1:P:167:HIS:HD2	1.95	0.50
5:E:182:ALA:O	5:E:183:LEU:HB3	2.10	0.49
2:Q:117:CYS:HB2	2:Q:131:TRP:CZ2	2.47	0.49
4:S:114:ASP:CG	5:T:137:HIS:HE2	2.16	0.49
1:F:39:SER:HB2	1:F:60:LEU:HD11	1.95	0.49
2:G:25:ARG:NH2	2:G:41:ASP:OD2	2.46	0.49
4:S:39:ARG:HG2	5:T:9:ARG:HH21	1.78	0.48
2:L:129:VAL:HG22	2:L:175:VAL:HG22	1.95	0.48
5:T:31:VAL:HB	5:T:95:SER:HB3	1.95	0.48
1:A:133:SER:HB2	1:A:150:TYR:HB2	1.94	0.48
5:T:207:HIS:HB2	5:T:240:TRP:CZ3	2.48	0.48
2:G:31:PHE:CE2	2:G:36:GLU:HB2	2.49	0.48
2:L:116:VAL:HG22	2:L:160:MET:HG2	1.95	0.48
2:G:80:ARG:O	2:G:84:GLU:HG2	2.13	0.48
1:K:8:ILE:HB	1:K:25:ASP:HB3	1.94	0.48
5:J:130:PRO:HD2	5:J:201:TRP:CZ2	2.49	0.48
1:A:122:LEU:HB2	1:A:162:ASP:HB2	1.96	0.48
1:A:160:PHE:CD2	1:A:177:HIS:HE1	2.32	0.48
1:K:134:GLU:HG3	1:K:149:HIS:CE1	2.49	0.48
1:K:111:LYS:HG2	1:K:140:ARG:CZ	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:211:GLN:HG3	5:T:234:ILE:HG23	1.95	0.47
2:B:30:TYR:HB2	2:B:38:LEU:HB3	1.96	0.47
4:I:148:SER:HA	4:S:146:LYS:HE3	1.95	0.47
4:N:26:THR:OG1	4:N:27:THR:N	2.46	0.47
4:I:110:ILE:HG13	4:I:137:ASP:HA	1.96	0.47
5:O:127:VAL:HG23	5:O:237:ALA:HB3	1.96	0.47
2:G:26:LEU:HB3	2:G:42:SER:HB3	1.96	0.47
2:G:129:VAL:HG22	2:G:175:VAL:HG22	1.96	0.47
1:K:14:LEU:HD22	1:K:115:PRO:HG2	1.97	0.47
4:N:36:LYS:HB2	4:N:42:LEU:HD23	1.97	0.47
4:I:94:ASN:OD1	4:I:95:LYS:HG3	2.15	0.46
5:O:30:PRO:HD2	5:O:96:LEU:HA	1.97	0.46
4:S:89:GLU:HB3	4:S:96:VAL:HG22	1.97	0.46
5:E:31:VAL:HB	5:E:95:SER:HB3	1.97	0.46
4:N:108:PRO:HD2	4:N:138:SER:OG	2.15	0.46
4:D:3:VAL:HB	4:D:99:GLY:HA2	1.97	0.46
2:Q:30:TYR:HB2	2:Q:38:LEU:HB3	1.98	0.46
5:E:135:ILE:HG23	5:E:198:ALA:HB1	1.97	0.46
5:E:157:LEU:HD23	5:E:158:SER:N	2.31	0.46
5:J:1:GLY:HA2	5:J:3:LYS:N	2.31	0.46
1:A:14:LEU:HD22	1:A:115:PRO:HG2	1.96	0.46
4:D:26:THR:OG1	4:D:27:THR:N	2.48	0.46
1:P:121:TRP:O	1:P:127:PRO:HA	2.15	0.46
2:G:4:ARG:HD2	2:G:5:PRO:HD2	1.98	0.46
4:S:39:ARG:HH12	5:T:157:LEU:H	1.63	0.46
4:D:158:LEU:HB3	5:E:171:CYS:HB2	1.96	0.45
5:E:127:VAL:HG23	5:E:237:ALA:HB3	1.97	0.45
2:G:74:GLU:HA	2:G:77:THR:OG1	2.17	0.45
2:L:74:GLU:HA	2:L:77:THR:OG1	2.16	0.45
5:E:202:GLN:HA	5:E:242:ARG:O	2.16	0.45
1:F:26:PHE:HB2	1:F:31:ILE:HD11	1.99	0.45
2:G:35:GLU:HG2	2:G:51:THR:HG21	1.97	0.45
4:S:57:ARG:NH1	4:S:80:ASP:OD2	2.48	0.45
1:P:114:PRO:HG3	2:Q:6:TRP:CD2	2.51	0.45
1:P:7:ILE:HB	2:Q:15:CYS:HB2	1.99	0.45
1:F:116:VAL:O	1:F:167:HIS:HD2	2.00	0.45
4:I:146:LYS:HG3	5:T:181:PRO:HG2	1.99	0.45
4:D:150:VAL:HG12	4:D:174:SER:HB2	1.99	0.45
4:N:3:VAL:HB	4:N:99:GLY:HA2	1.98	0.45
5:T:130:PRO:HD3	5:T:143:LEU:HG	1.98	0.45
5:T:127:VAL:HG23	5:T:237:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:HB3	1:A:149:HIS:HB2	1.99	0.44
1:F:86:ALA:HA	1:F:87:PRO:HD3	1.85	0.44
5:E:67:ALA:HB2	5:E:77:LEU:HD12	1.99	0.44
5:J:47:ILE:HG13	5:J:57:GLN:HB3	1.99	0.44
1:K:122:LEU:HB2	1:K:162:ASP:HB2	1.99	0.44
1:K:58:GLY:HA2	4:N:94:ASN:HD21	1.83	0.44
4:D:108:PRO:HD2	4:D:138:SER:OG	2.17	0.44
5:E:65:PHE:CE2	5:E:79:ILE:HG12	2.51	0.44
5:E:26:GLU:O	5:E:29:HIS:HB2	2.17	0.44
4:I:3:VAL:HB	4:I:99:GLY:HA2	1.99	0.44
1:K:21:GLU:OE2	1:K:137:PHE:N	2.49	0.44
5:O:52:GLN:HG3	5:O:69:CYS:O	2.18	0.44
5:E:120:VAL:HG12	5:E:230:PRO:HB2	2.00	0.44
4:I:158:LEU:HB3	5:J:171:CYS:HB2	1.99	0.44
2:L:177:HIS:CD2	2:L:178:PRO:HD2	2.52	0.44
2:L:31:PHE:CE2	2:L:36:GLU:HB2	2.52	0.44
4:N:195:PHE:CE2	4:N:197:PRO:HG3	2.52	0.44
1:P:76:ARG:HD3	2:Q:56:PRO:HG2	1.99	0.44
2:B:177:HIS:CD2	2:B:178:PRO:HD2	2.53	0.44
4:S:130:VAL:HG12	4:S:173:TRP:HB3	2.00	0.44
4:S:114:ASP:OD2	5:T:137:HIS:NE2	2.48	0.44
5:O:123:PRO:HB3	5:O:150:PHE:HB3	2.00	0.43
1:P:8:ILE:HB	1:P:25:ASP:HB3	2.00	0.43
2:B:9:GLU:OE2	3:C:9:LYS:HE3	2.18	0.43
2:L:97:PRO:HB3	2:L:122:PHE:HB3	1.99	0.43
5:O:6:GLN:OE1	5:O:92:CYS:N	2.43	0.43
4:D:173:TRP:CD2	5:E:146:LEU:HD11	2.53	0.43
5:E:18:LYS:HD3	5:E:78:GLU:OE2	2.18	0.43
5:E:18:LYS:HE2	5:E:80:GLN:NE2	2.33	0.43
1:K:118:ASN:HB2	1:K:166:ASP:HB3	2.00	0.43
5:O:63:LYS:HG3	5:O:64:ARG:HG3	2.00	0.43
1:A:15:LEU:HD23	1:A:15:LEU:HA	1.76	0.43
1:K:176:LYS:HA	1:K:176:LYS:HD3	1.80	0.43
4:N:130:VAL:HG12	4:N:173:TRP:HB3	2.01	0.43
1:P:87:PRO:HA	1:P:112:PHE:HB3	1.99	0.43
2:Q:31:PHE:CE2	2:Q:36:GLU:HB2	2.54	0.43
5:J:65:PHE:CE2	5:J:79:ILE:HG12	2.54	0.43
4:N:107:LEU:HA	4:N:108:PRO:HD3	1.92	0.43
1:P:26:PHE:HB2	1:P:31:ILE:HD11	2.00	0.43
1:K:87:PRO:HD3	1:K:167:HIS:ND1	2.34	0.43
2:B:152:ASP:OD1	2:B:154:THR:OG1	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:TRP:O	1:F:127:PRO:HA	2.19	0.42
1:P:86:ALA:HA	1:P:87:PRO:HD3	1.81	0.42
4:D:152:ILE:HG12	4:D:172:ALA:HB2	2.00	0.42
5:E:37:GLN:HA	5:E:42:GLU:O	2.18	0.42
1:F:11:GLU:OE1	3:H:6:SER:OG	2.37	0.42
1:K:15:LEU:HA	1:K:15:LEU:HD23	1.87	0.42
1:K:86:ALA:HA	1:K:87:PRO:HD3	1.85	0.42
1:A:89:VAL:HG23	1:A:174:LEU:HD23	2.01	0.42
1:F:17:ASP:OD2	1:F:116:VAL:HG11	2.19	0.42
4:S:120:LEU:HB3	5:T:128:PHE:HB3	2.01	0.42
1:F:176:LYS:HA	1:F:176:LYS:HD3	1.87	0.42
1:K:26:PHE:CD2	2:L:90:LEU:HB3	2.54	0.42
4:N:47:TYR:CE1	5:O:101:SER:HB3	2.52	0.42
1:A:138:LEU:HA	1:A:139:PRO:HD3	1.81	0.42
4:I:10:LEU:HD23	4:I:104:LEU:HD13	2.01	0.42
5:J:0:SER:O	5:J:27:LYS:N	2.52	0.42
4:N:57:ARG:NH1	4:N:80:ASP:OD2	2.39	0.42
1:P:160:PHE:CD2	1:P:177:HIS:HE1	2.38	0.42
5:O:61:THR:HA	5:O:65:PHE:CD1	2.55	0.42
1:A:176:LYS:HD3	1:A:176:LYS:HA	1.81	0.42
4:I:3:VAL:O	4:I:100:THR:HG23	2.20	0.42
2:L:63:SER:O	2:L:65:PRO:HD3	2.19	0.41
1:A:135:THR:HG21	1:A:148:PHE:HB2	2.01	0.41
1:F:92:LEU:HD23	1:F:106:ILE:HB	2.01	0.41
1:F:114:PRO:HG3	2:G:6:TRP:CE2	2.54	0.41
4:S:150:VAL:HG12	4:S:174:SER:HB2	2.02	0.41
5:T:129:GLU:HA	5:T:130:PRO:HD3	1.92	0.41
4:I:78:LEU:HD12	4:I:78:LEU:HA	1.85	0.41
2:L:16:HIS:O	2:L:24:VAL:HA	2.21	0.41
1:K:11:GLU:OE1	3:M:6:SER:OG	2.38	0.41
4:N:39:ARG:NH1	5:O:156:GLU:HA	2.35	0.41
2:L:69:GLU:HG2	4:N:49:ALA:HB3	2.01	0.41
5:T:130:PRO:HD2	5:T:201:TRP:CH2	2.55	0.41
4:D:47:TYR:CE1	5:E:101:SER:HB3	2.54	0.41
5:O:123:PRO:O	5:O:235:VAL:HG11	2.21	0.41
1:P:154:LEU:HA	1:P:155:PRO:HD3	1.89	0.41
5:E:30:PRO:HD2	5:E:96:LEU:HA	2.02	0.41
1:P:176:LYS:HA	1:P:176:LYS:HD3	1.79	0.41
2:G:38:LEU:HD12	2:G:48:ARG:O	2.21	0.41
3:M:5:ARG:NH2	5:O:98:ASN:O	2.53	0.41
2:Q:148:VAL:HB	2:Q:156:GLN:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:207:HIS:HB2	5:E:240:TRP:CZ3	2.56	0.41
1:F:13:TYR:CZ	1:F:67:LYS:HE2	2.56	0.41
5:J:26:GLU:O	5:J:29:HIS:HB2	2.20	0.41
4:S:145:SER:HB2	4:S:150:VAL:HG23	2.02	0.41
2:B:131:TRP:CZ3	2:B:173:CYS:HB3	2.56	0.41
4:I:26:THR:OG1	4:I:27:THR:N	2.54	0.41
1:P:118:ASN:HB2	1:P:166:ASP:HB3	2.02	0.41
1:A:121:TRP:O	1:A:127:PRO:HA	2.21	0.41
1:F:99:LEU:HA	1:F:155:PRO:HB2	2.02	0.41
5:J:127:VAL:HG23	5:J:237:ALA:HB3	2.03	0.41
4:S:26:THR:OG1	4:S:27:THR:N	2.53	0.41
1:F:134:GLU:HG3	1:F:149:HIS:CE1	2.56	0.40
4:D:37:ASN:OD1	4:D:40:GLY:HA3	2.21	0.40
1:F:8:ILE:HB	1:F:25:ASP:HB3	2.02	0.40
2:G:177:HIS:CD2	2:G:178:PRO:HD2	2.57	0.40
1:A:43:TRP:CD1	1:A:49:ALA:HB2	2.57	0.40
5:E:40:ASN:HB3	4:N:139:GLN:HE22	1.86	0.40
5:O:24:ILE:HA	5:O:25:PRO:HD2	1.99	0.40
5:O:49:PHE:CE1	5:O:54:VAL:HG22	2.57	0.40
1:K:154:LEU:HA	1:K:155:PRO:HD3	1.89	0.40
5:O:207:HIS:HB2	5:O:240:TRP:CZ3	2.57	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	178/204 (87%)	173 (97%)	5 (3%)	0	100	100
1	F	178/204 (87%)	174 (98%)	4 (2%)	0	100	100
1	K	178/204 (87%)	174 (98%)	4 (2%)	0	100	100
1	P	177/204 (87%)	171 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	165/212 (78%)	157 (95%)	8 (5%)	0	100	100
2	G	165/212 (78%)	158 (96%)	7 (4%)	0	100	100
2	L	165/212 (78%)	157 (95%)	8 (5%)	0	100	100
2	Q	165/212 (78%)	158 (96%)	7 (4%)	0	100	100
3	C	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
3	H	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
3	M	11/14 (79%)	11 (100%)	0	0	100	100
3	R	11/14 (79%)	11 (100%)	0	0	100	100
4	D	192/205 (94%)	183 (95%)	9 (5%)	0	100	100
4	I	192/205 (94%)	184 (96%)	8 (4%)	0	100	100
4	N	192/205 (94%)	184 (96%)	8 (4%)	0	100	100
4	S	192/205 (94%)	184 (96%)	8 (4%)	0	100	100
5	E	243/266 (91%)	229 (94%)	14 (6%)	0	100	100
5	J	243/266 (91%)	230 (95%)	13 (5%)	0	100	100
5	O	240/266 (90%)	229 (95%)	11 (5%)	0	100	100
5	T	240/266 (90%)	230 (96%)	10 (4%)	0	100	100
All	All	3151/3604 (87%)	3019 (96%)	132 (4%)	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	161/184 (88%)	158 (98%)	3 (2%)	57	77
1	F	161/184 (88%)	160 (99%)	1 (1%)	86	91
1	K	160/184 (87%)	159 (99%)	1 (1%)	86	91
1	P	159/184 (86%)	158 (99%)	1 (1%)	86	91
2	B	150/191 (78%)	148 (99%)	2 (1%)	69	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	148/191 (78%)	147 (99%)	1 (1%)	84	90
2	L	148/191 (78%)	147 (99%)	1 (1%)	84	90
2	Q	148/191 (78%)	147 (99%)	1 (1%)	84	90
3	C	9/9 (100%)	9 (100%)	0	100	100
3	H	9/9 (100%)	9 (100%)	0	100	100
3	M	9/9 (100%)	9 (100%)	0	100	100
3	R	9/9 (100%)	9 (100%)	0	100	100
4	D	171/181 (94%)	169 (99%)	2 (1%)	71	83
4	I	170/181 (94%)	168 (99%)	2 (1%)	71	83
4	N	171/181 (94%)	170 (99%)	1 (1%)	86	91
4	S	171/181 (94%)	168 (98%)	3 (2%)	59	78
5	E	209/226 (92%)	206 (99%)	3 (1%)	67	82
5	J	209/226 (92%)	209 (100%)	0	100	100
5	O	210/226 (93%)	209 (100%)	1 (0%)	88	93
5	T	209/226 (92%)	209 (100%)	0	100	100
All	All	2791/3164 (88%)	2768 (99%)	23 (1%)	81	89

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	152	THR
1	A	172	GLU
2	B	173	CYS
2	B	188	TRP
4	D	2	GLN
4	D	37	ASN
5	E	96	LEU
5	E	104	THR
5	E	193	ARG
1	F	17	ASP
2	G	173	CYS
4	I	37	ASN
4	I	127	ASP
1	K	172	GLU
2	L	173	CYS
4	N	127	ASP

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Mol	Chain	Res	Type
5	O	96	LEU
1	P	172	GLU
2	Q	173	CYS
4	S	37	ASN
4	S	74	ARG
4	S	127	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	2	GLN
5	T	37	GLN
5	T	72	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	NAG	G	901	2	14,14,15	0.38	0	17,19,21	0.74	1 (5%)
6	NAG	B	901	2	14,14,15	0.51	0	17,19,21	0.34	0
6	NAG	A	901	1	14,14,15	0.44	0	17,19,21	0.54	0
6	NAG	L	901	2	14,14,15	0.51	0	17,19,21	0.75	1 (5%)
6	NAG	K	901	1	14,14,15	0.51	0	17,19,21	0.59	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	NAG	G	901	2	-	0/6/23/26	0/1/1/1
6	NAG	B	901	2	-	1/6/23/26	0/1/1/1
6	NAG	A	901	1	-	2/6/23/26	0/1/1/1
6	NAG	L	901	2	-	1/6/23/26	0/1/1/1
6	NAG	K	901	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	901	NAG	C1-O5-C5	2.71	115.87	112.19
6	G	901	NAG	C1-O5-C5	2.64	115.76	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	901	NAG	O5-C5-C6-O6
6	A	901	NAG	C4-C5-C6-O6
6	B	901	NAG	O5-C5-C6-O6
6	L	901	NAG	O5-C5-C6-O6

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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	180/204 (88%)	-0.04	2 (1%) 80 81	57, 83, 146, 185	0
1	F	180/204 (88%)	0.07	3 (1%) 70 68	69, 109, 182, 243	0
1	K	180/204 (88%)	-0.05	0 100 100	77, 101, 163, 207	0
1	P	179/204 (87%)	0.26	9 (5%) 28 27	102, 144, 206, 234	0
2	B	171/212 (80%)	0.20	10 (5%) 23 22	60, 86, 182, 221	0
2	G	171/212 (80%)	0.31	10 (5%) 23 22	60, 94, 167, 207	0
2	L	171/212 (80%)	0.26	12 (7%) 16 16	70, 112, 206, 264	0
2	Q	171/212 (80%)	0.72	28 (16%) 1 2	87, 132, 222, 265	0
3	C	14/14 (100%)	-0.15	0 100 100	56, 69, 120, 125	0
3	H	14/14 (100%)	0.09	0 100 100	69, 88, 118, 141	0
3	M	13/14 (92%)	0.09	0 100 100	87, 101, 132, 146	0
3	R	13/14 (92%)	0.35	1 (7%) 13 12	88, 111, 144, 154	0
4	D	196/205 (95%)	0.13	8 (4%) 37 35	60, 109, 194, 259	0
4	I	196/205 (95%)	0.33	13 (6%) 18 18	72, 121, 194, 246	0
4	N	196/205 (95%)	0.32	16 (8%) 11 11	77, 114, 193, 226	0
4	S	196/205 (95%)	0.35	14 (7%) 16 16	80, 120, 211, 248	0
5	E	245/266 (92%)	0.00	4 (1%) 72 70	65, 113, 166, 201	0
5	J	245/266 (92%)	0.06	5 (2%) 65 64	71, 119, 172, 236	1 (0%)
5	O	242/266 (90%)	0.43	18 (7%) 14 14	93, 155, 212, 258	0
5	T	242/266 (90%)	0.41	15 (6%) 20 20	105, 150, 204, 231	0
All	All	3215/3604 (89%)	0.23	168 (5%) 27 25	56, 119, 197, 265	1 (0%)

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	0	SER	11.5
5	J	1	GLY	6.8
4	S	195	PHE	5.8
1	P	159	ASP	5.6
5	J	244	ASP	5.0
1	A	1	ILE	5.0
2	Q	103	PRO	4.9
5	O	244	ASP	4.8
4	S	196	PHE	4.8
4	S	197	PRO	4.7
2	Q	115	LEU	4.7
5	O	216	GLY	4.6
2	Q	188	TRP	4.5
4	N	178	ASP	4.4
2	Q	173	CYS	4.3
2	L	164	VAL	4.2
4	N	119	GLN	4.2
2	Q	175	VAL	4.2
2	B	115	LEU	4.1
5	T	117	LEU	4.1
2	Q	116	VAL	4.1
2	Q	102	TYR	4.1
4	N	143	SER	4.0
4	S	178	ASP	4.0
5	O	127	VAL	3.9
2	Q	131	TRP	3.9
2	Q	101	VAL	3.8
5	O	183	LEU	3.8
5	O	217	LEU	3.7
4	I	127	ASP	3.7
2	Q	171	TYR	3.7
2	L	188	TRP	3.7
4	N	182	ALA	3.7
2	Q	5	PRO	3.6
2	L	131	TRP	3.5
1	F	82	ASP	3.5
4	S	145	SER	3.5
4	D	116	ALA	3.4
2	Q	163	THR	3.4
2	Q	99	VAL	3.4
5	T	114	ILE	3.4
2	L	132	PHE	3.4
4	S	193	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
4	N	187	ASN	3.3
2	L	185	THR	3.3
5	O	184	ASN	3.3
4	D	187	ASN	3.2
4	N	40	GLY	3.2
2	Q	141	GLY	3.2
4	S	176	LYS	3.2
2	L	163	THR	3.1
4	D	197	PRO	3.1
2	B	161	LEU	3.1
1	P	99	LEU	3.1
2	Q	100	THR	3.1
2	L	142	ILE	3.0
1	P	127	PRO	3.0
2	Q	185	THR	3.0
5	E	208	PHE	3.0
5	E	244	ASP	3.0
5	T	222	GLU	2.9
1	P	156	SER	2.9
2	L	162	GLU	2.9
2	G	102	TYR	2.8
2	B	116	VAL	2.8
2	Q	143	VAL	2.8
2	L	161	LEU	2.8
2	Q	160	MET	2.8
4	S	117	VAL	2.8
2	G	142	ILE	2.8
3	R	-3	ALA	2.8
2	Q	4	ARG	2.8
4	S	194	THR	2.8
4	N	142	VAL	2.8
4	D	198	SER	2.7
5	E	206	ASN	2.7
4	N	183	ASN	2.7
5	O	185	ASP	2.7
5	T	218	SER	2.7
2	L	143	VAL	2.7
2	Q	172	THR	2.7
5	T	159	TRP	2.7
5	O	61	THR	2.7
5	T	244	ASP	2.7
4	N	179	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	102	TYR	2.6
2	B	188	TRP	2.6
2	G	143	VAL	2.6
4	I	133	PHE	2.6
4	I	116	ALA	2.6
4	D	178	ASP	2.5
2	G	160	MET	2.5
5	E	209	ARG	2.5
4	N	150	VAL	2.5
4	I	118	TYR	2.5
4	S	182	ALA	2.5
2	B	142	ILE	2.5
4	I	172	ALA	2.5
4	N	131	CYS	2.5
5	O	115	GLU	2.5
2	Q	3	SER	2.5
5	T	61	THR	2.4
2	L	102	TYR	2.4
4	I	182	ALA	2.4
5	T	13	LYS	2.4
1	P	98	ASN	2.4
2	G	161	LEU	2.4
2	Q	186	VAL	2.4
5	O	62	GLU	2.4
4	S	198	SER	2.4
2	B	143	VAL	2.4
2	Q	159	VAL	2.4
4	I	181	CYS	2.4
5	O	72	ASN	2.4
1	F	84	ASN	2.4
2	Q	162	GLU	2.4
4	I	0	GLY	2.3
4	D	195	PHE	2.3
5	O	210	CYS	2.3
1	P	130	GLU	2.3
4	I	119	GLN	2.3
2	G	173	CYS	2.3
4	I	136	PHE	2.3
5	O	212	VAL	2.3
5	O	211	GLN	2.3
2	B	3	SER	2.3
4	N	145	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	G	115	LEU	2.3
5	T	119	ASN	2.3
5	T	226	ASP	2.3
5	J	208	PHE	2.3
4	S	127	ASP	2.2
5	O	126	ALA	2.2
4	S	181	CYS	2.2
1	P	122	LEU	2.2
5	T	116	ASP	2.2
1	A	157	THR	2.2
2	Q	176	GLU	2.2
4	S	143	SER	2.2
5	J	205	ARG	2.2
2	Q	187	GLU	2.2
5	T	143	LEU	2.2
5	O	181	PRO	2.2
1	F	174	LEU	2.2
2	B	163	THR	2.2
4	I	117	VAL	2.1
4	D	188	SER	2.1
2	G	132	PHE	2.1
4	D	182	ALA	2.1
5	T	79	ILE	2.1
4	I	195	PHE	2.1
2	B	103	PRO	2.1
4	N	41	SER	2.1
2	L	172	THR	2.1
2	G	188	TRP	2.1
4	N	118	TYR	2.1
5	O	144	VAL	2.1
2	Q	180	LEU	2.1
2	Q	129	VAL	2.0
4	I	194	THR	2.0
2	G	184	VAL	2.0
5	T	204	PRO	2.0
5	O	205	ARG	2.0
1	P	158	ASP	2.0
1	P	128	VAL	2.0
5	T	228	ALA	2.0
4	N	173	TRP	2.0
4	N	130	VAL	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, 95th 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(\AA^2)	Q<0.9
6	NAG	B	901	14/15	0.71	0.23	92,139,146,147	0
6	NAG	G	901	14/15	0.78	0.16	90,112,133,144	0
6	NAG	L	901	14/15	0.83	0.18	98,125,137,138	0
6	NAG	K	901	14/15	0.87	0.18	126,144,153,154	0
6	NAG	A	901	14/15	0.89	0.20	98,120,127,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.