Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 12:33 PM EST

PDB ID	:	4P2R
Title	:	Crystal structure of the 5cc7 TCR in complex with 5c1/I-Ek
Authors	:	Birnbaum, M.E.; Ozkan, E.; Garcia, K.C.
Deposited on	:	2014-03-04
Resolution	:	3.29 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

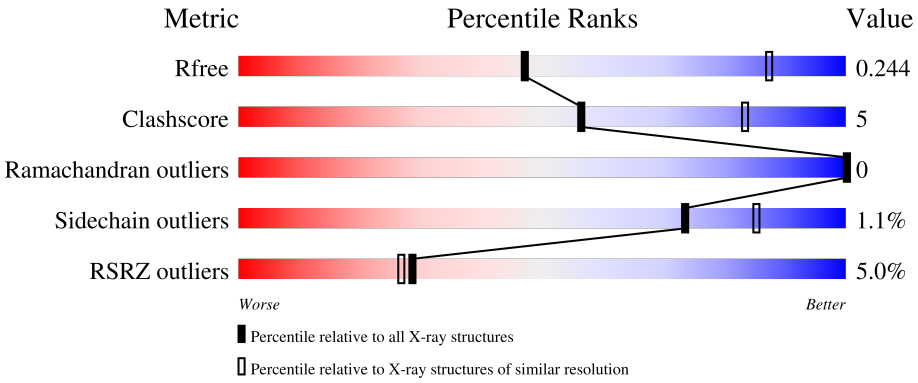
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.29 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 of 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 <=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	72% 16% 12%
1	F	204	% 75% 13% 12%
1	K	204	69% 19% 12%
1	P	204	5% 73% 15% 12%
2	B	212	4% 67% 14% 19%

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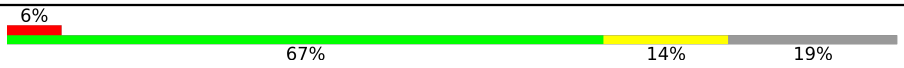
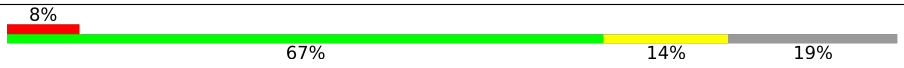
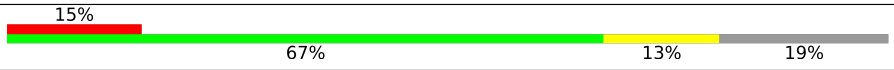
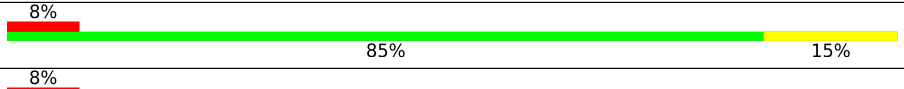
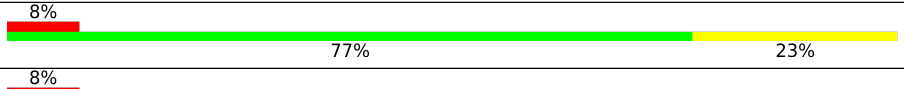
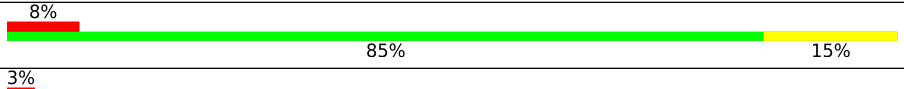
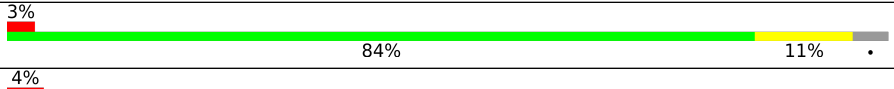
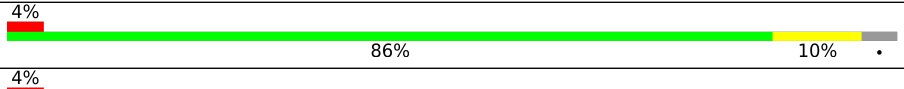
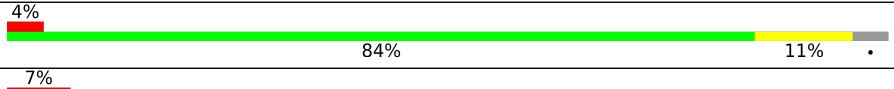
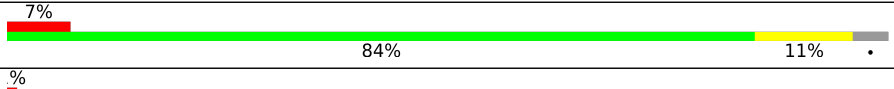
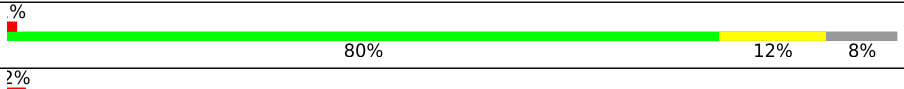
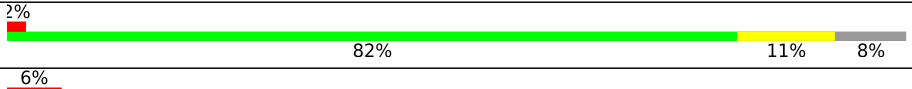
Mol	Chain	Length	Quality of chain
2	G	212	
2	L	212	
2	Q	212	
3	C	13	
3	H	13	
3	M	13	
3	R	13	
4	D	205	
4	I	205	
4	N	205	
4	S	205	
5	E	266	
5	J	266	
5	O	266	
5	T	266	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25651 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 5c1 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			98	68	15	15			
3	H	13	Total	C	N	O	0	0	0
			98	68	15	15			
3	M	13	Total	C	N	O	0	0	0
			98	68	15	15			
3	R	13	Total	C	N	O	0	0	0
			98	68	15	15			

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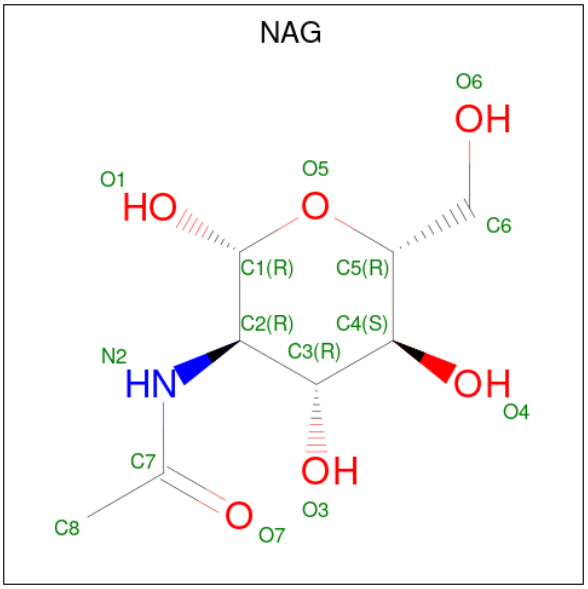
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	196	Total	C	N	O	S	0	0	0
			1523	942	264	309	8			
4	S	196	Total	C	N	O	S	0	0	0
			1523	942	264	309	8			

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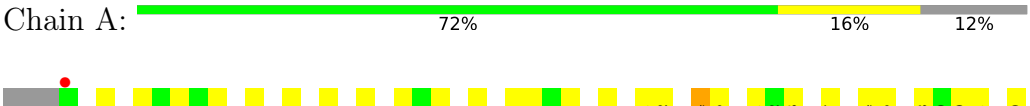
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	K	1	Total	C	N	O	0	0
			14	8	1	5		
6	L	1	Total	C	N	O	0	0
			14	8	1	5		

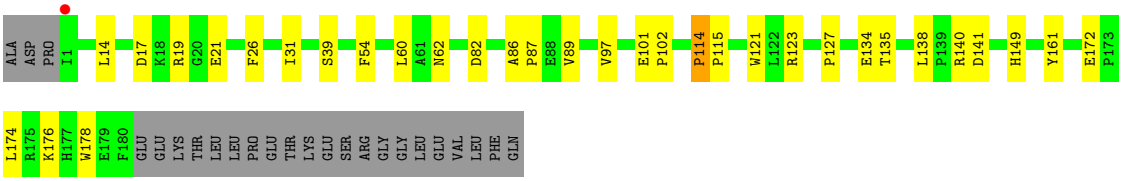
3 Residue-property plots (i)

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

• Molecule 1: H-2 class II histocompatibility antigen, E-K alpha chain

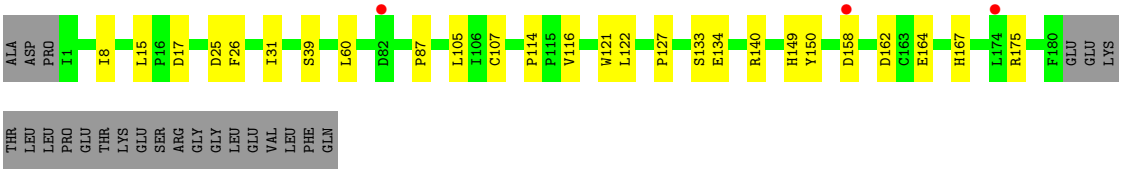
Chain A:





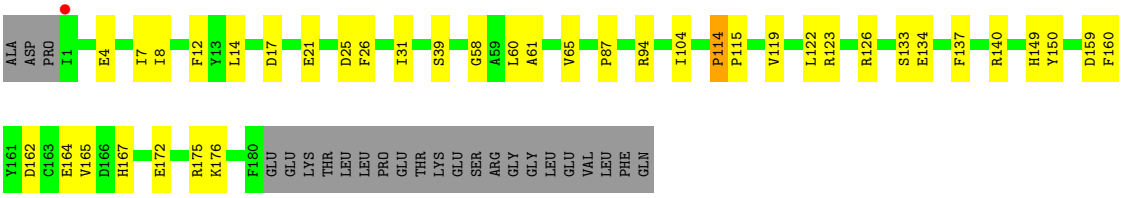
• Molecule 1: H-2 class II histocompatibility antigen, E-K alpha chain

Chain F:



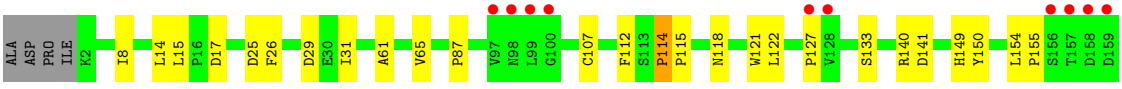
• Molecule 1: H-2 class II histocompatibility antigen, E-K alpha chain

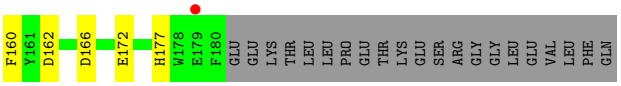
Chain K:



• Molecule 1: H-2 class II histocompatibility antigen, E-K alpha chain

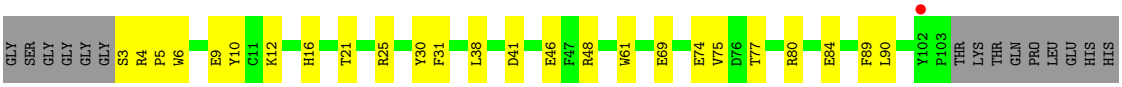
Chain P:





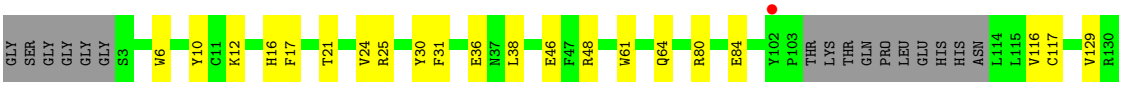
• Molecule 2: MHC class II E-beta-k

Chain B:



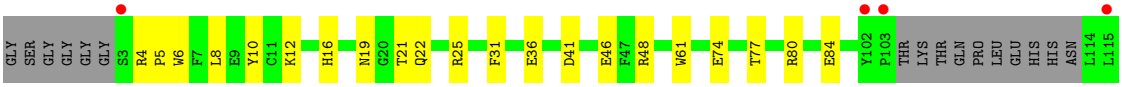
• Molecule 2: MHC class II E-beta-k

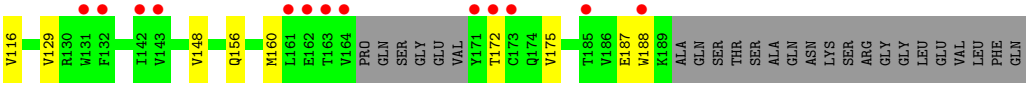
Chain G:



• Molecule 2: MHC class II E-beta-k

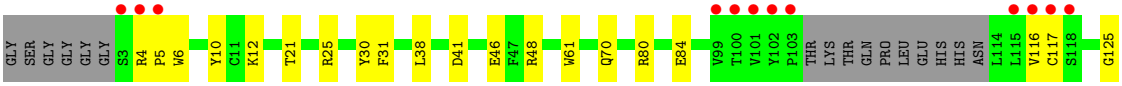
Chain L:

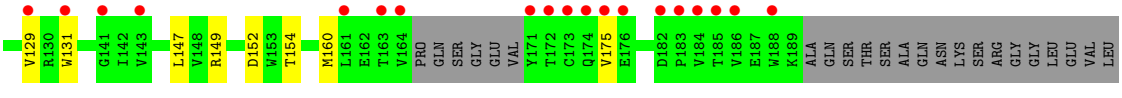




• Molecule 2: MHC class II E-beta-k

Chain Q:



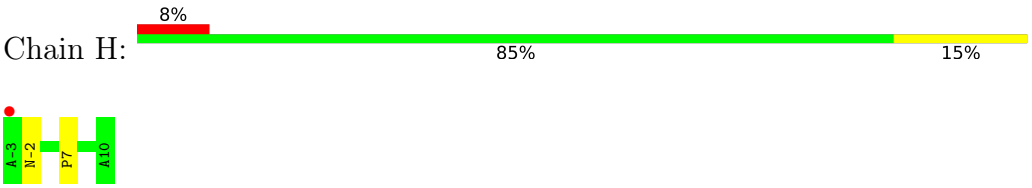


• Molecule 3: 5c1 peptide

Chain C:

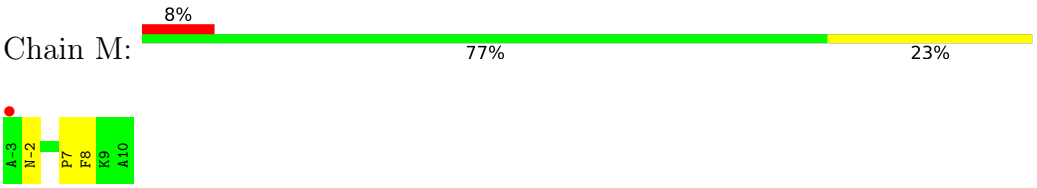
• Molecule 3: 5c1 peptide

Chain H:



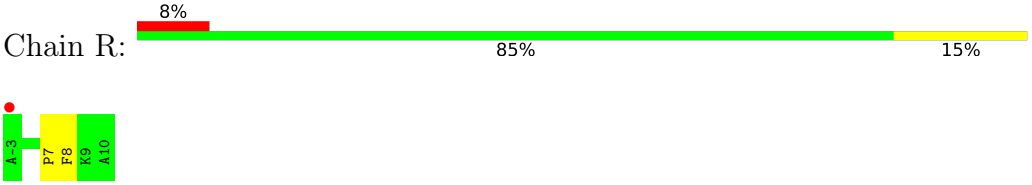
• Molecule 3: 5c1 peptide

Chain M:



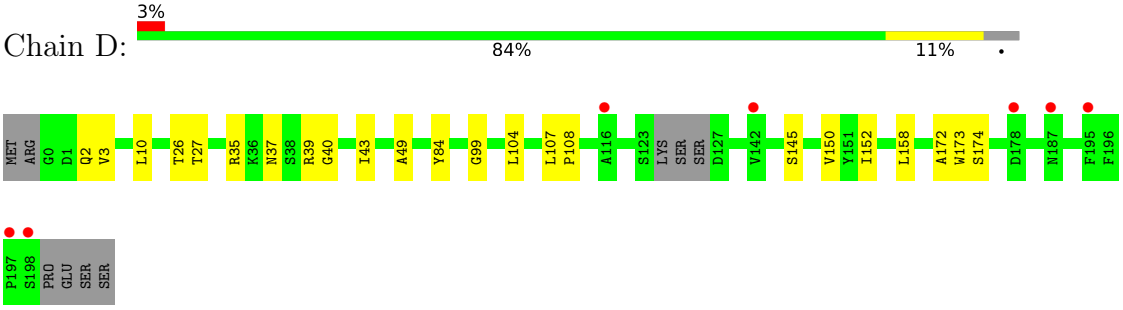
• Molecule 3: 5c1 peptide

Chain R:



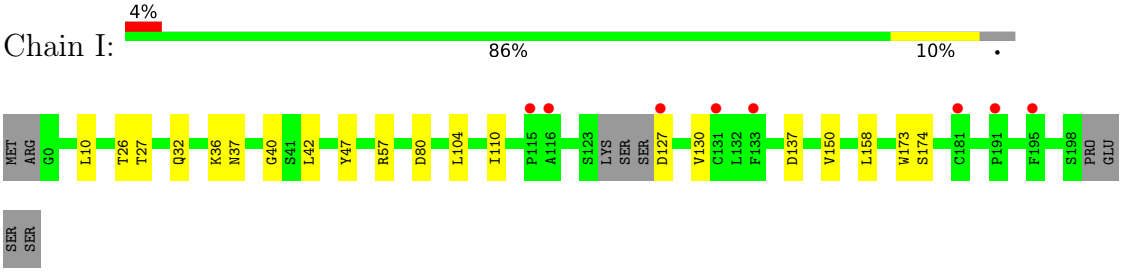
• Molecule 4: 5cc7 T-cell receptor alpha chain

Chain D:



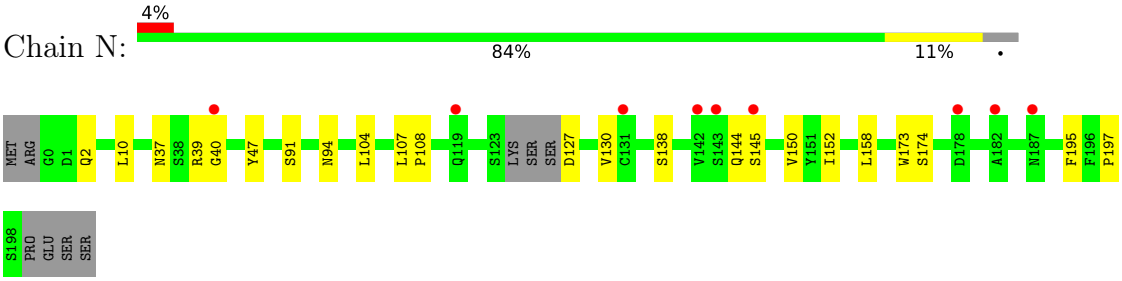
• Molecule 4: 5cc7 T-cell receptor alpha chain

Chain I:



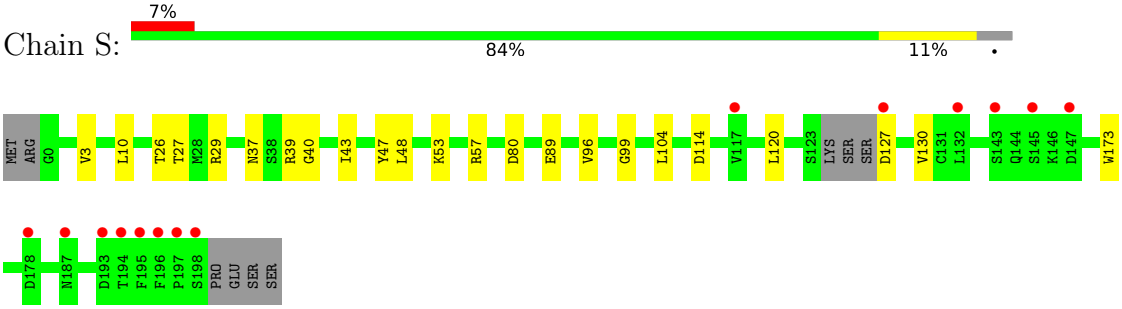
• Molecule 4: 5cc7 T-cell receptor alpha chain

Chain N:



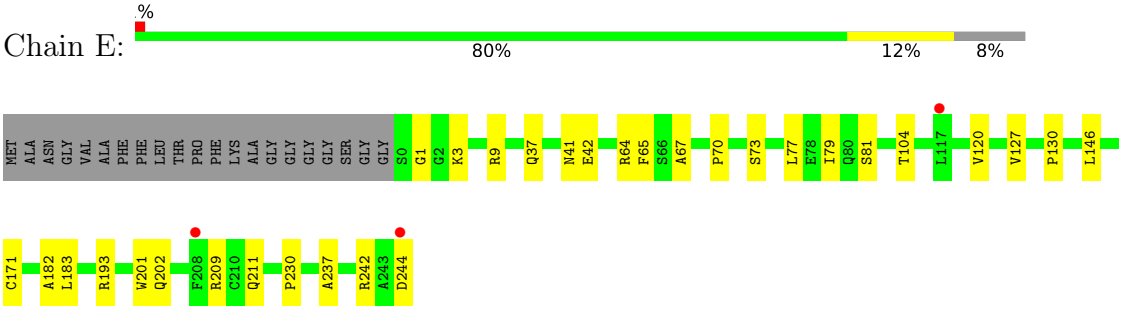
• Molecule 4: 5cc7 T-cell receptor alpha chain

Chain S:



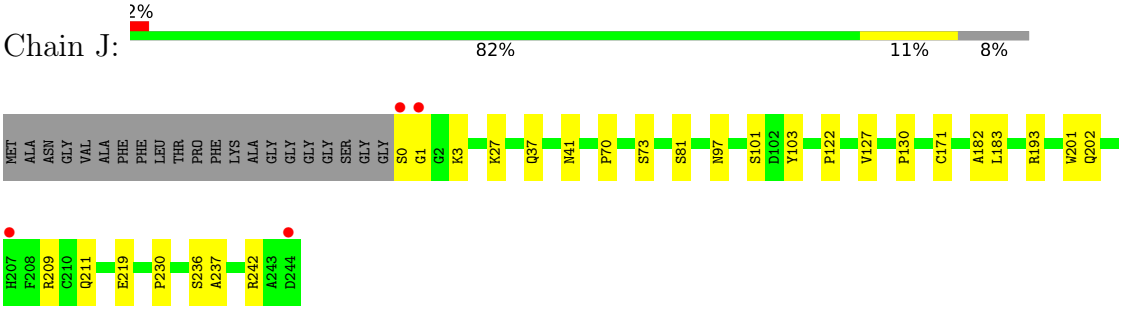
• Molecule 5: 5cc7 T-cell receptor beta chain

Chain E:



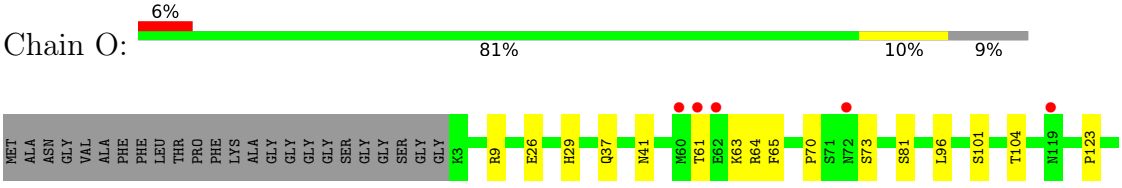
• Molecule 5: 5cc7 T-cell receptor beta chain

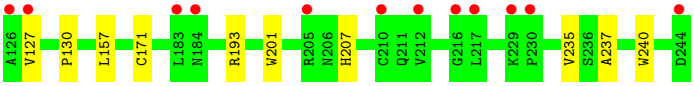
Chain J:



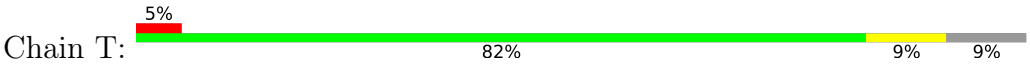
• Molecule 5: 5cc7 T-cell receptor beta chain

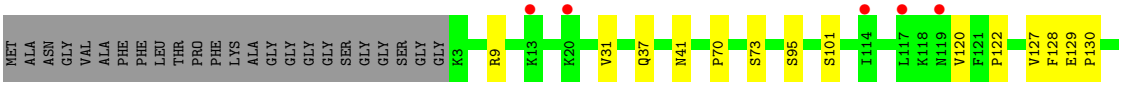
Chain O:

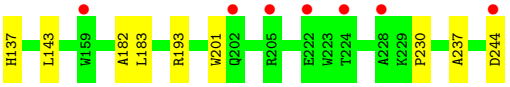




• Molecule 5: 5cc7 T-cell receptor beta chain







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	261.60Å 101.87Å 214.64Å 90.00° 94.89° 90.00°	Depositor
Resolution (Å)	39.45 – 3.29 39.45 – 3.29	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.45-3.29) 98.8 (39.45-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.212 , 0.243 0.214 , 0.244	Depositor DCC
R_{free} test set	4218 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	100.5	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 57.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	25651	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.52	0/1516	0.54	0/2062
1	F	0.38	0/1516	0.45	0/2062
1	K	0.40	0/1512	0.49	0/2058
1	P	0.28	0/1504	0.42	0/2047
2	B	0.53	0/1424	0.48	0/1943
2	G	0.48	0/1419	0.48	0/1937
2	L	0.39	0/1419	0.46	0/1937
2	Q	0.33	0/1419	0.44	0/1937
3	C	0.69	0/101	0.45	0/136
3	H	0.52	0/101	0.43	0/136
3	M	0.50	0/101	0.41	0/136
3	R	0.37	0/101	0.42	0/136
4	D	0.44	0/1551	0.46	0/2098
4	I	0.39	0/1545	0.44	0/2091
4	N	0.39	0/1551	0.47	0/2098
4	S	0.34	0/1551	0.43	0/2098
5	E	0.40	0/1978	0.44	0/2691
5	J	0.34	0/1978	0.42	0/2691
5	O	0.27	0/1969	0.41	0/2678
5	T	0.27	0/1965	0.41	0/2674
All	All	0.39	0/26221	0.45	0/35646

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 (i)

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	20	0
1	F	1473	0	1403	14	0
1	K	1469	0	1391	26	0
1	P	1461	0	1378	20	0
2	B	1387	0	1279	21	0
2	G	1382	0	1272	18	0
2	L	1382	0	1272	21	0
2	Q	1382	0	1273	20	0
3	C	98	0	100	4	0
3	H	98	0	100	1	0
3	M	98	0	100	2	0
3	R	98	0	100	2	0
4	D	1523	0	1441	15	0
4	I	1517	0	1430	12	0
4	N	1523	0	1441	17	0
4	S	1523	0	1441	15	0
5	E	1929	0	1816	19	0
5	J	1929	0	1816	19	0
5	O	1920	0	1816	17	0
5	T	1916	0	1805	14	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	25651	0	24141	250	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 (250) 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)
2:L:48:ARG:NH1	1:P:141:ASP:OD2	2.12	0.81
2:L:21:THR:O	2:L:80:ARG:NH1	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:57:ARG:NH1	4:I:80:ASP:OD2	2.19	0.75
2:B:21:THR:O	2:B:80:ARG:NH1	2.19	0.75
2:G:10:TYR:HB3	2:G:31:PHE:HB2	1.69	0.74
2:Q:10:TYR:HB3	2:Q:31:PHE:HB2	1.70	0.73
2:L:10:TYR:HB3	2:L:31:PHE:HB2	1.70	0.72
1:K:133:SER:HB2	1:K:150:TYR:HB2	1.69	0.72
5:O:70:PRO:HB2	5:O:73:SER:HB2	1.71	0.72
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.70	0.72
5:T:70:PRO:HB2	5:T:73:SER:HB2	1.70	0.72
1:K:26:PHE:HB2	1:K:31:ILE:HD11	1.72	0.71
2:B:10:TYR:HB3	2:B:31:PHE:HB2	1.74	0.70
2:G:21:THR:O	2:G:80:ARG:NH1	2.26	0.69
5:J:70:PRO:HB2	5:J:73:SER:HB2	1.74	0.69
2:B:129:VAL:HG22	2:B:175:VAL:HG22	1.75	0.69
1:P:133:SER:HB2	1:P:150:TYR:HB2	1.75	0.69
1:A:123:ARG:NH1	1:A:161:TYR:OH	2.27	0.68
5:E:70:PRO:HB2	5:E:73:SER:HB2	1.75	0.68
1:K:140:ARG:O	2:L:12:LYS:NZ	2.27	0.68
5:E:209:ARG:NH2	5:E:211:GLN:OE1	2.28	0.67
1:P:118:ASN:HB2	1:P:166:ASP:HB3	1.75	0.67
2:L:46:GLU:OE1	2:L:48:ARG:NH2	2.29	0.66
2:B:46:GLU:OE1	2:B:48:ARG:NH2	2.31	0.63
2:Q:4:ARG:HD2	2:Q:5:PRO:HD2	1.81	0.63
2:L:19:ASN:ND2	2:L:22:GLN:OE1	2.32	0.63
1:P:26:PHE:HB2	1:P:31:ILE:HD11	1.81	0.63
2:Q:129:VAL:HG22	2:Q:175:VAL:HG22	1.80	0.62
1:A:82:ASP:OD2	2:B:3:SER:OG	2.17	0.62
5:E:1:GLY:HA2	5:E:3:LYS:H	1.64	0.62
1:P:122:LEU:HB2	1:P:162:ASP:HB2	1.80	0.61
1:F:133:SER:HB2	1:F:150:TYR:HB2	1.82	0.61
1:A:140:ARG:O	2:B:12:LYS:NZ	2.34	0.61
4:N:158:LEU:HB3	5:O:171:CYS:HB2	1.83	0.61
2:L:4:ARG:HD2	2:L:5:PRO:HD2	1.82	0.61
2:G:129:VAL:HG22	2:G:175:VAL:HG22	1.83	0.60
1:F:114:PRO:HG3	2:G:6:TRP:CD2	2.37	0.60
1:A:141:ASP:OD2	2:G:48:ARG:NH1	2.22	0.59
4:D:145:SER:HB3	4:D:152:ILE:HG13	1.84	0.59
1:F:140:ARG:O	2:G:12:LYS:NZ	2.35	0.59
1:F:164:GLU:OE1	1:F:175:ARG:NH2	2.30	0.59
1:K:94:ARG:HD3	1:K:104:ILE:HD13	1.85	0.58
2:B:4:ARG:HD2	2:B:5:PRO:HD2	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:145:SER:HB2	4:D:150:VAL:HG23	1.85	0.58
5:J:1:GLY:HA2	5:J:3:LYS:H	1.69	0.58
5:J:219:GLU:OE1	5:J:219:GLU:N	2.33	0.58
4:S:57:ARG:NH1	4:S:80:ASP:OD2	2.37	0.58
1:P:107:CYS:HB3	1:P:149:HIS:HB2	1.84	0.57
1:K:114:PRO:HG3	2:L:6:TRP:CE2	2.40	0.57
5:O:37:GLN:HE21	5:O:41:ASN:HA	1.69	0.57
5:E:37:GLN:HE21	5:E:41:ASN:HA	1.70	0.56
1:P:114:PRO:HG3	2:Q:6:TRP:CE2	2.39	0.56
4:S:89:GLU:HB3	4:S:96:VAL:HG22	1.88	0.56
1:K:114:PRO:HG3	2:L:6:TRP:CD2	2.41	0.56
5:J:209:ARG:NH2	5:J:211:GLN:OE1	2.36	0.56
4:N:10:LEU:HD23	4:N:104:LEU:HD13	1.87	0.56
1:F:8:ILE:HB	1:F:25:ASP:HB3	1.87	0.55
2:G:16:HIS:HB2	2:G:25:ARG:HG2	1.88	0.55
2:G:46:GLU:OE1	2:G:48:ARG:NH2	2.39	0.55
1:P:140:ARG:O	2:Q:12:LYS:NZ	2.40	0.55
1:K:164:GLU:OE1	1:K:175:ARG:NH2	2.29	0.54
2:G:80:ARG:O	2:G:84:GLU:HG2	2.07	0.54
2:Q:117:CYS:HB2	2:Q:131:TRP:CZ2	2.43	0.54
1:K:14:LEU:HD22	1:K:115:PRO:HG2	1.89	0.54
5:E:130:PRO:HD2	5:E:201:TRP:CZ2	2.43	0.53
4:D:10:LEU:HD23	4:D:104:LEU:HD13	1.89	0.53
5:E:182:ALA:O	5:E:183:LEU:HB3	2.08	0.53
4:I:32:GLN:HE22	5:J:103:TYR:N	2.07	0.53
4:I:47:TYR:HE1	5:J:101:SER:HB3	1.73	0.53
2:Q:80:ARG:O	2:Q:84:GLU:HG2	2.09	0.53
4:I:158:LEU:HB3	5:J:171:CYS:HB2	1.90	0.53
5:J:182:ALA:O	5:J:183:LEU:HB3	2.09	0.53
1:A:121:TRP:O	1:A:127:PRO:HA	2.09	0.52
1:A:134:GLU:HG3	1:A:149:HIS:NE2	2.25	0.52
5:T:31:VAL:HB	5:T:95:SER:HB3	1.92	0.52
4:S:37:ASN:HD21	4:S:43:ILE:HD13	1.75	0.52
4:N:145:SER:HB3	4:N:152:ILE:HG13	1.91	0.52
5:E:1:GLY:HA2	5:E:3:LYS:N	2.24	0.52
1:A:89:VAL:HG23	1:A:174:LEU:HD23	1.92	0.52
2:Q:21:THR:O	2:Q:80:ARG:NH1	2.43	0.51
1:A:135:THR:HG21	1:A:138:LEU:HD11	1.92	0.51
1:K:134:GLU:HG3	1:K:149:HIS:CE1	2.46	0.51
1:A:39:SER:HB2	1:A:60:LEU:HD11	1.92	0.51
4:N:39:ARG:HH12	5:O:157:LEU:H	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:61:ALA:O	1:P:65:VAL:HG23	2.11	0.51
2:Q:116:VAL:HG22	2:Q:160:MET:HG2	1.92	0.51
1:A:114:PRO:HG3	2:B:6:TRP:CE2	2.46	0.51
5:T:37:GLN:HE21	5:T:41:ASN:HA	1.75	0.51
2:B:80:ARG:O	2:B:84:GLU:HG2	2.11	0.51
2:B:30:TYR:HB2	2:B:38:LEU:HB3	1.92	0.51
4:S:37:ASN:HB2	4:S:40:GLY:HA3	1.92	0.51
1:F:26:PHE:HB2	1:F:31:ILE:HD11	1.92	0.51
1:K:123:ARG:HH22	1:K:160:PHE:N	2.10	0.50
5:J:0:SER:O	5:J:27:LYS:N	2.44	0.50
5:T:182:ALA:O	5:T:183:LEU:HB3	2.10	0.50
1:F:122:LEU:HB2	1:F:162:ASP:HB2	1.94	0.50
4:I:37:ASN:HB2	4:I:40:GLY:HA3	1.92	0.50
5:O:207:HIS:HB2	5:O:240:TRP:CZ3	2.47	0.50
1:F:107:CYS:HB3	1:F:149:HIS:HB2	1.93	0.50
2:Q:25:ARG:NH2	2:Q:41:ASP:OD2	2.41	0.50
2:L:16:HIS:HB2	2:L:25:ARG:HG2	1.94	0.50
4:I:110:ILE:HG13	4:I:137:ASP:HA	1.94	0.50
4:N:39:ARG:HG2	5:O:9:ARG:HH21	1.76	0.49
2:L:129:VAL:HG22	2:L:175:VAL:HG22	1.94	0.49
4:D:37:ASN:HB2	4:D:40:GLY:HA3	1.93	0.49
2:G:132:PHE:HB2	2:G:172:THR:HG23	1.94	0.49
2:G:117:CYS:HB2	2:G:131:TRP:CZ2	2.48	0.49
2:B:69:GLU:HG2	4:D:49:ALA:HB3	1.95	0.49
4:N:195:PHE:CE2	4:N:197:PRO:HG3	2.48	0.49
1:A:114:PRO:HG3	2:B:6:TRP:CD2	2.48	0.48
2:L:148:VAL:HB	2:L:156:GLN:HG3	1.93	0.48
1:K:58:GLY:HA2	4:N:94:ASN:HD21	1.78	0.48
2:G:31:PHE:CE2	2:G:36:GLU:HB2	2.47	0.48
4:N:150:VAL:HG12	4:N:174:SER:HB2	1.95	0.48
1:K:39:SER:HB2	1:K:60:LEU:HD11	1.95	0.48
1:K:87:PRO:HD3	1:K:167:HIS:ND1	2.29	0.48
2:L:80:ARG:O	2:L:84:GLU:HG2	2.13	0.48
4:I:150:VAL:HG12	4:I:174:SER:HB2	1.94	0.48
5:O:26:GLU:HB3	5:O:29:HIS:CG	2.48	0.48
1:P:65:VAL:HG22	3:R:8:PHE:CE1	2.49	0.48
4:I:10:LEU:HD23	4:I:104:LEU:HD13	1.96	0.48
1:A:14:LEU:HD22	1:A:115:PRO:HG2	1.95	0.48
4:N:37:ASN:HB2	4:N:40:GLY:HA3	1.95	0.48
1:K:123:ARG:NH2	1:K:159:ASP:HB3	2.28	0.48
4:D:26:THR:OG1	4:D:27:THR:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:64:GLN:HE22	5:J:97:ASN:HD22	1.62	0.48
1:P:160:PHE:CD2	1:P:177:HIS:HE1	2.32	0.48
4:D:37:ASN:HD21	4:D:43:ILE:HD13	1.78	0.47
1:F:134:GLU:HG3	1:F:149:HIS:CE1	2.49	0.47
4:S:10:LEU:HD23	4:S:104:LEU:HD13	1.96	0.47
2:G:116:VAL:HG22	2:G:160:MET:HG2	1.95	0.47
2:Q:152:ASP:OD1	2:Q:154:THR:OG1	2.25	0.47
5:J:130:PRO:HD2	5:J:201:TRP:CZ2	2.50	0.47
2:B:116:VAL:HG22	2:B:160:MET:HG2	1.97	0.47
4:D:158:LEU:HB3	5:E:171:CYS:HB2	1.97	0.47
5:J:1:GLY:HA2	5:J:3:LYS:N	2.29	0.47
4:I:36:LYS:HB2	4:I:42:LEU:HD23	1.97	0.47
2:B:16:HIS:HB2	2:B:25:ARG:HG2	1.97	0.47
2:G:152:ASP:OD1	2:G:154:THR:OG1	2.31	0.47
4:N:108:PRO:HD2	4:N:138:SER:OG	2.15	0.46
4:S:39:ARG:HG2	5:T:9:ARG:HH21	1.80	0.46
5:J:209:ARG:NH1	5:J:236:SER:OG	2.49	0.46
2:L:61:TRP:CZ2	3:M:7:PRO:HG2	2.51	0.46
1:K:122:LEU:HB2	1:K:162:ASP:HB2	1.98	0.46
1:K:119:VAL:HG22	1:K:165:VAL:HG22	1.97	0.46
5:E:67:ALA:HB2	5:E:77:LEU:HD12	1.98	0.45
5:O:63:LYS:HG3	5:O:64:ARG:HG3	1.98	0.45
5:O:127:VAL:HG23	5:O:237:ALA:HB3	1.97	0.45
2:B:25:ARG:NH2	2:B:41:ASP:OD2	2.49	0.45
1:K:87:PRO:HD3	1:K:167:HIS:HD1	1.81	0.45
2:Q:30:TYR:HB2	2:Q:38:LEU:HB3	1.98	0.45
2:B:25:ARG:HH21	2:B:41:ASP:CG	2.20	0.45
1:F:39:SER:HB2	1:F:60:LEU:HD11	1.98	0.45
1:K:61:ALA:O	1:K:65:VAL:HG23	2.16	0.45
2:L:25:ARG:NH2	2:L:41:ASP:OD2	2.50	0.45
4:S:26:THR:OG1	4:S:27:THR:N	2.50	0.45
5:J:127:VAL:HG23	5:J:237:ALA:HB3	1.98	0.45
5:O:61:THR:HA	5:O:65:PHE:CD1	2.52	0.45
5:E:65:PHE:CE2	5:E:79:ILE:HG12	2.52	0.45
4:N:145:SER:HB2	4:N:150:VAL:HG23	1.97	0.45
5:O:130:PRO:HD2	5:O:201:TRP:CZ2	2.52	0.45
1:A:176:LYS:HA	1:A:176:LYS:HD3	1.75	0.45
5:T:130:PRO:HD3	5:T:143:LEU:HG	1.98	0.45
4:I:130:VAL:HG12	4:I:173:TRP:HB3	1.99	0.44
2:Q:61:TRP:CZ2	3:R:7:PRO:HG2	2.52	0.44
5:E:120:VAL:HG12	5:E:230:PRO:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:116:VAL:HG22	2:L:160:MET:HG2	1.99	0.44
2:B:9:GLU:OE2	3:C:9:LYS:HE3	2.18	0.44
5:J:202:GLN:HA	5:J:242:ARG:O	2.18	0.44
4:N:144:GLN:NE2	4:N:152:ILE:O	2.47	0.44
5:T:130:PRO:HD2	5:T:201:TRP:CZ2	2.52	0.44
1:K:7:ILE:HG12	1:K:26:PHE:HD1	1.83	0.44
1:K:176:LYS:HA	1:K:176:LYS:HD3	1.82	0.44
2:Q:46:GLU:OE1	2:Q:48:ARG:NH2	2.51	0.44
4:S:130:VAL:HG12	4:S:173:TRP:HB3	1.98	0.44
1:K:8:ILE:HB	1:K:25:ASP:HB3	2.00	0.43
1:K:21:GLU:OE2	1:K:137:PHE:N	2.49	0.43
4:N:47:TYR:HE1	5:O:101:SER:HB3	1.82	0.43
1:P:154:LEU:HA	1:P:155:PRO:HD3	1.89	0.43
2:G:30:TYR:HB2	2:G:38:LEU:HB3	2.01	0.43
1:A:19:ARG:NH2	1:A:21:GLU:OE1	2.51	0.43
5:E:81:SER:O	5:E:81:SER:OG	2.29	0.43
5:E:202:GLN:HA	5:E:242:ARG:O	2.18	0.43
5:T:120:VAL:HG12	5:T:230:PRO:HB2	2.00	0.43
1:F:87:PRO:HD3	1:F:167:HIS:ND1	2.34	0.43
1:K:12:PHE:HB2	2:L:8:LEU:HD11	2.01	0.43
4:D:150:VAL:HG12	4:D:174:SER:HB2	2.00	0.43
1:K:65:VAL:HG22	3:M:8:PHE:CE1	2.54	0.43
1:P:114:PRO:HG3	2:Q:6:TRP:CD2	2.53	0.43
2:B:75:VAL:O	2:B:80:ARG:HG3	2.18	0.43
1:K:4:GLU:OE2	2:Q:48:ARG:NH1	2.51	0.43
1:P:14:LEU:HD22	1:P:115:PRO:HG2	2.00	0.43
1:P:121:TRP:O	1:P:127:PRO:HA	2.19	0.43
1:P:160:PHE:HD2	1:P:177:HIS:HE1	1.67	0.43
4:N:107:LEU:HA	4:N:108:PRO:HD3	1.92	0.43
5:T:122:PRO:HD3	5:T:230:PRO:HB3	2.01	0.43
5:J:122:PRO:HD3	5:J:230:PRO:HB3	2.01	0.43
1:P:8:ILE:HB	1:P:25:ASP:HB3	2.01	0.43
5:E:104:THR:O	5:E:104:THR:OG1	2.37	0.42
4:S:47:TYR:HE1	5:T:101:SER:HB3	1.84	0.42
4:S:48:LEU:HD21	4:S:53:LYS:HG3	2.01	0.42
5:T:127:VAL:HG23	5:T:237:ALA:HB3	2.01	0.42
2:G:61:TRP:CZ2	3:H:7:PRO:HG2	2.54	0.42
2:L:77:THR:O	4:N:91:SER:OG	2.27	0.42
1:A:97:VAL:HG21	1:A:178:TRP:HZ2	1.83	0.42
4:D:152:ILE:HG12	4:D:172:ALA:HB2	2.00	0.42
1:F:121:TRP:O	1:F:127:PRO:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:123:ARG:N	1:K:126:ARG:O	2.52	0.42
4:D:35:ARG:HD3	4:D:84:TYR:CZ	2.53	0.42
1:P:87:PRO:HA	1:P:112:PHE:HB3	2.01	0.42
5:E:37:GLN:HA	5:E:42:GLU:O	2.20	0.42
5:O:81:SER:O	5:O:81:SER:OG	2.36	0.42
4:S:3:VAL:HB	4:S:99:GLY:HA2	2.02	0.42
5:J:81:SER:O	5:J:81:SER:OG	2.38	0.42
4:D:107:LEU:HA	4:D:108:PRO:HD3	1.94	0.41
4:N:130:VAL:HG12	4:N:173:TRP:HB3	2.02	0.41
4:S:57:ARG:HH12	4:S:80:ASP:CG	2.21	0.41
4:S:120:LEU:HB3	5:T:128:PHE:HB3	2.02	0.41
2:B:74:GLU:HA	2:B:77:THR:OG1	2.20	0.41
5:E:64:ARG:NH2	5:E:81:SER:O	2.54	0.41
5:J:37:GLN:HE21	5:J:41:ASN:HA	1.85	0.41
5:O:123:PRO:O	5:O:235:VAL:HG11	2.20	0.41
1:A:54:PHE:HD1	3:C:1:VAL:HG22	1.84	0.41
1:A:86:ALA:HA	1:A:87:PRO:HD3	1.90	0.41
4:D:3:VAL:HB	4:D:99:GLY:HA2	2.03	0.41
4:I:26:THR:OG1	4:I:27:THR:N	2.54	0.41
1:P:15:LEU:HD23	1:P:15:LEU:HA	1.91	0.41
4:S:114:ASP:CG	5:T:137:HIS:HE2	2.24	0.41
2:B:61:TRP:CZ2	3:C:7:PRO:HG2	2.56	0.41
4:D:39:ARG:HG2	5:E:9:ARG:HH21	1.86	0.41
1:F:105:LEU:HD23	1:F:105:LEU:HA	1.85	0.41
2:G:17:PHE:CD1	2:G:24:VAL:HG22	2.56	0.41
4:I:47:TYR:CE1	5:J:101:SER:HB3	2.53	0.41
2:L:74:GLU:HA	2:L:77:THR:OG1	2.21	0.41
2:L:172:THR:HB	2:L:187:GLU:CB	2.51	0.41
5:O:104:THR:O	5:O:104:THR:OG1	2.37	0.41
1:P:29:ASP:OD1	2:Q:149:ARG:HD3	2.21	0.41
5:T:129:GLU:HA	5:T:130:PRO:HD3	1.96	0.41
4:D:173:TRP:CD2	5:E:146:LEU:HD11	2.56	0.40
5:O:63:LYS:HB3	5:O:63:LYS:HE2	1.89	0.40
2:L:31:PHE:CE2	2:L:36:GLU:HB2	2.57	0.40
2:Q:25:ARG:HH21	2:Q:41:ASP:CG	2.23	0.40
1:A:101:GLU:HA	1:A:102:PRO:HD3	1.97	0.40
2:B:89:PHE:CE2	2:B:90:LEU:HG	2.57	0.40
2:Q:70:GLN:OE1	4:S:29:ARG:HD3	2.21	0.40
2:Q:125:GLY:HA3	2:Q:147:LEU:HD21	2.03	0.40
1:A:62:ASN:CG	3:C:6:THR:HG22	2.42	0.40
5:E:127:VAL:HG23	5:E:237:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:15:LEU:HD23	1:F:15:LEU:HA	1.95	0.40
4:N:47:TYR:CE1	5:O:101:SER:HB3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	178/204 (87%)	173 (97%)	5 (3%)	0	100	100
1	F	178/204 (87%)	173 (97%)	5 (3%)	0	100	100
1	K	178/204 (87%)	174 (98%)	4 (2%)	0	100	100
1	P	177/204 (87%)	172 (97%)	5 (3%)	0	100	100
2	B	165/212 (78%)	156 (94%)	9 (6%)	0	100	100
2	G	165/212 (78%)	157 (95%)	8 (5%)	0	100	100
2	L	165/212 (78%)	157 (95%)	8 (5%)	0	100	100
2	Q	165/212 (78%)	157 (95%)	8 (5%)	0	100	100
3	C	11/13 (85%)	11 (100%)	0	0	100	100
3	H	11/13 (85%)	11 (100%)	0	0	100	100
3	M	11/13 (85%)	11 (100%)	0	0	100	100
3	R	11/13 (85%)	11 (100%)	0	0	100	100
4	D	192/205 (94%)	186 (97%)	6 (3%)	0	100	100
4	I	192/205 (94%)	186 (97%)	6 (3%)	0	100	100
4	N	192/205 (94%)	186 (97%)	6 (3%)	0	100	100
4	S	192/205 (94%)	186 (97%)	6 (3%)	0	100	100
5	E	243/266 (91%)	232 (96%)	11 (4%)	0	100	100
5	J	243/266 (91%)	232 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	O	240/266 (90%)	230 (96%)	10 (4%)	0	100	100
5	T	240/266 (90%)	230 (96%)	10 (4%)	0	100	100
All	All	3149/3600 (88%)	3031 (96%)	118 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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%)	158 (98%)	3 (2%)	57	77
1	K	160/184 (87%)	157 (98%)	3 (2%)	57	77
1	P	159/184 (86%)	156 (98%)	3 (2%)	57	77
2	B	150/191 (78%)	149 (99%)	1 (1%)	84	90
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%)	148 (100%)	0	100	100
3	C	9/9 (100%)	7 (78%)	2 (22%)	1	3
3	H	9/9 (100%)	8 (89%)	1 (11%)	6	23
3	M	9/9 (100%)	8 (89%)	1 (11%)	6	23
3	R	9/9 (100%)	9 (100%)	0	100	100
4	D	171/181 (94%)	170 (99%)	1 (1%)	86	91
4	I	170/181 (94%)	169 (99%)	1 (1%)	86	91
4	N	171/181 (94%)	169 (99%)	2 (1%)	71	83
4	S	171/181 (94%)	170 (99%)	1 (1%)	86	91
5	E	209/226 (92%)	207 (99%)	2 (1%)	76	86
5	J	209/226 (92%)	208 (100%)	1 (0%)	88	93
5	O	210/226 (93%)	208 (99%)	2 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	T	209/226 (92%)	207 (99%)	2 (1%)	76 86
All	All	2791/3164 (88%)	2760 (99%)	31 (1%)	73 85

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	114	PRO
1	A	172	GLU
2	B	173	CYS
3	C	-2	ASN
3	C	1	VAL
4	D	2	GLN
5	E	193	ARG
5	E	244	ASP
1	F	17	ASP
1	F	116	VAL
1	F	158	ASP
2	G	173	CYS
3	H	-2	ASN
4	I	127	ASP
5	J	193	ARG
1	K	17	ASP
1	K	114	PRO
1	K	172	GLU
2	L	188	TRP
3	M	-2	ASN
4	N	2	GLN
4	N	127	ASP
5	O	96	LEU
5	O	193	ARG
1	P	17	ASP
1	P	114	PRO
1	P	172	GLU
4	S	127	ASP
5	T	193	ARG
5	T	244	ASP

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

Mol	Chain	Res	Type
5	J	97	ASN
5	O	80	GLN
5	T	37	GLN

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	B	901	2	14,14,15	0.39	0	17,19,21	0.56	0
6	NAG	K	901	1	14,14,15	0.44	0	17,19,21	0.54	0
6	NAG	L	901	2	14,14,15	0.52	0	17,19,21	0.50	0
6	NAG	G	901	2	14,14,15	0.35	0	17,19,21	0.80	1 (5%)
6	NAG	A	901	1	14,14,15	0.36	0	17,19,21	0.41	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	B	901	2	-	0/6/23/26	0/1/1/1
6	NAG	K	901	1	-	2/6/23/26	0/1/1/1
6	NAG	L	901	2	-	0/6/23/26	0/1/1/1
6	NAG	G	901	2	-	0/6/23/26	0/1/1/1
6	NAG	A	901	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	901	NAG	C1-O5-C5	2.54	115.63	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

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^{th} 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%)	0.05	1 (0%) 89 90	59, 78, 123, 149	0
1	F	180/204 (88%)	0.18	3 (1%) 70 68	70, 106, 163, 191	0
1	K	180/204 (88%)	0.05	1 (0%) 89 90	77, 97, 146, 184	0
1	P	179/204 (87%)	0.33	11 (6%) 21 20	97, 140, 196, 225	0
2	B	171/212 (80%)	0.24	8 (4%) 31 29	55, 81, 160, 188	0
2	G	171/212 (80%)	0.41	13 (7%) 13 13	60, 88, 169, 199	0
2	L	171/212 (80%)	0.37	17 (9%) 7 7	70, 103, 192, 245	0
2	Q	171/212 (80%)	0.78	31 (18%) 1 1	84, 129, 205, 223	0
3	C	13/13 (100%)	-0.04	0 100 100	58, 64, 83, 105	0
3	H	13/13 (100%)	0.22	1 (7%) 13 12	61, 76, 113, 132	0
3	M	13/13 (100%)	0.19	1 (7%) 13 12	87, 93, 102, 124	0
3	R	13/13 (100%)	0.70	1 (7%) 13 12	91, 111, 126, 162	0
4	D	196/205 (95%)	0.22	7 (3%) 42 40	67, 98, 181, 225	0
4	I	196/205 (95%)	0.34	8 (4%) 37 35	73, 108, 178, 203	0
4	N	196/205 (95%)	0.36	9 (4%) 32 30	81, 107, 189, 239	0
4	S	196/205 (95%)	0.43	14 (7%) 16 16	82, 113, 201, 254	0
5	E	245/266 (92%)	0.04	3 (1%) 79 78	73, 111, 156, 184	0
5	J	245/266 (92%)	0.10	4 (1%) 72 70	85, 114, 162, 196	0
5	O	242/266 (90%)	0.40	17 (7%) 16 16	104, 142, 188, 229	0
5	T	242/266 (90%)	0.44	12 (4%) 28 27	111, 145, 187, 213	0
All	All	3213/3600 (89%)	0.29	162 (5%) 28 27	55, 115, 181, 254	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	-3	ALA	7.3
2	Q	103	PRO	5.5
1	A	1	ILE	5.5
4	S	196	PHE	5.3
4	S	197	PRO	5.2
5	O	127	VAL	4.8
2	Q	131	TRP	4.7
5	J	0	SER	4.7
2	Q	115	LEU	4.6
4	S	198	SER	4.6
2	Q	116	VAL	4.6
5	O	244	ASP	4.4
5	J	244	ASP	4.4
4	S	195	PHE	4.4
4	N	178	ASP	4.4
5	T	117	LEU	4.3
2	Q	102	TYR	4.3
2	Q	163	THR	4.2
2	Q	5	PRO	4.1
2	Q	100	THR	4.1
4	S	127	ASP	4.1
2	L	164	VAL	4.1
5	O	216	GLY	4.1
2	Q	173	CYS	4.0
4	D	197	PRO	4.0
2	L	143	VAL	3.9
1	P	159	ASP	3.9
2	Q	175	VAL	3.8
2	L	163	THR	3.8
4	S	193	ASP	3.8
2	G	143	VAL	3.7
2	Q	101	VAL	3.7
2	Q	117	CYS	3.6
2	B	188	TRP	3.6
2	L	131	TRP	3.5
2	Q	176	GLU	3.5
2	L	171	TYR	3.4
2	G	188	TRP	3.4
5	O	61	THR	3.4
2	G	102	TYR	3.4
2	L	132	PHE	3.4
5	O	126	ALA	3.4
4	N	131	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
4	S	145	SER	3.3
4	S	178	ASP	3.3
2	Q	3	SER	3.3
2	Q	99	VAL	3.3
4	N	187	ASN	3.3
2	Q	186	VAL	3.2
2	Q	185	THR	3.2
5	O	183	LEU	3.1
2	Q	143	VAL	3.1
1	F	82	ASP	3.1
2	G	173	CYS	3.1
4	N	119	GLN	3.1
2	G	160	MET	3.1
2	B	115	LEU	3.1
2	B	161	LEU	3.0
2	L	173	CYS	3.0
5	O	217	LEU	3.0
4	D	198	SER	3.0
1	P	156	SER	2.9
2	Q	183	PRO	2.9
5	E	244	ASP	2.9
1	P	158	ASP	2.9
4	D	187	ASN	2.9
1	P	99	LEU	2.9
2	Q	188	TRP	2.9
4	S	117	VAL	2.9
2	L	188	TRP	2.9
5	T	13	LYS	2.9
2	B	163	THR	2.9
5	T	224	THR	2.9
5	T	114	ILE	2.8
4	D	178	ASP	2.8
5	T	119	ASN	2.8
4	I	191	PRO	2.8
4	I	195	PHE	2.8
1	P	157	THR	2.7
2	Q	129	VAL	2.7
2	L	3	SER	2.7
2	Q	184	VAL	2.7
5	O	210	CYS	2.6
2	G	162	GLU	2.6
4	N	182	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
5	T	244	ASP	2.6
5	T	205	ARG	2.6
2	L	142	ILE	2.6
3	M	-3	ALA	2.6
5	O	212	VAL	2.6
2	G	172	THR	2.6
4	I	133	PHE	2.6
4	I	116	ALA	2.6
5	T	222	GLU	2.6
4	D	195	PHE	2.6
4	N	145	SER	2.6
4	I	127	ASP	2.6
2	B	102	TYR	2.5
5	T	228	ALA	2.5
2	B	162	GLU	2.5
2	G	142	ILE	2.5
1	P	100	GLY	2.4
5	E	208	PHE	2.4
5	O	205	ARG	2.4
4	S	143	SER	2.4
4	S	187	ASN	2.4
4	S	194	THR	2.4
1	P	98	ASN	2.4
2	L	185	THR	2.4
2	Q	172	THR	2.4
5	O	230	PRO	2.4
2	Q	182	ASP	2.4
2	G	164	VAL	2.3
2	L	161	LEU	2.3
1	F	174	LEU	2.3
2	Q	118	SER	2.3
5	E	117	LEU	2.3
5	J	207	HIS	2.3
4	N	143	SER	2.3
2	B	131	TRP	2.3
2	G	163	THR	2.3
4	D	116	ALA	2.3
1	P	128	VAL	2.3
2	L	115	LEU	2.3
2	L	102	TYR	2.3
2	Q	171	TYR	2.3
2	L	162	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	G	136	LYS	2.2
1	K	1	ILE	2.2
5	T	20	LYS	2.2
4	I	115	PRO	2.2
2	B	142	ILE	2.2
4	I	181	CYS	2.2
2	Q	4	ARG	2.2
5	O	72	ASN	2.2
5	J	1	GLY	2.2
1	P	179	GLU	2.2
2	G	131	TRP	2.2
5	O	62	GLU	2.2
5	O	60	MET	2.1
5	O	184	ASN	2.1
1	P	127	PRO	2.1
2	Q	141	GLY	2.1
2	G	174	GLN	2.1
2	Q	174	GLN	2.1
5	O	119	ASN	2.1
4	I	131	CYS	2.1
3	H	-3	ALA	2.1
5	O	229	LYS	2.1
2	L	103	PRO	2.1
2	Q	161	LEU	2.1
4	D	142	VAL	2.1
1	F	158	ASP	2.1
4	S	147	ASP	2.1
4	N	40	GLY	2.0
4	S	132	LEU	2.0
5	T	159	TRP	2.0
1	P	97	VAL	2.0
4	N	142	VAL	2.0
2	Q	164	VAL	2.0
2	L	172	THR	2.0
5	T	202	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^{th} 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^2)	Q<0.9
6	NAG	L	901	14/15	0.69	0.24	79,107,117,119	0
6	NAG	B	901	14/15	0.75	0.23	78,112,126,126	0
6	NAG	G	901	14/15	0.84	0.15	69,84,108,110	0
6	NAG	K	901	14/15	0.91	0.16	95,115,120,132	0
6	NAG	A	901	14/15	0.92	0.21	65,92,106,112	0

6.5 Other polymers (i)

There are no such residues in this entry.