wwPDB X-ray Structure Validation Summary Report (i)

Nov 1, 2023 – 10:11 AM JST

PDB ID	:	8W83
Title	:	HLA-DQ2.5-alpha1 gliadin peptide in complex with DQN0344AE02
Authors	:	Irie, M.; Tsushima, T.; Teranishi-Ikawa, Y.; Takahashi, N.; Ishii, S.; Okura, Y.; Fukami, T.A.; Torizawa, T.
Deposited on	:	2023-08-31
Resolution	:	2.82 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
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:

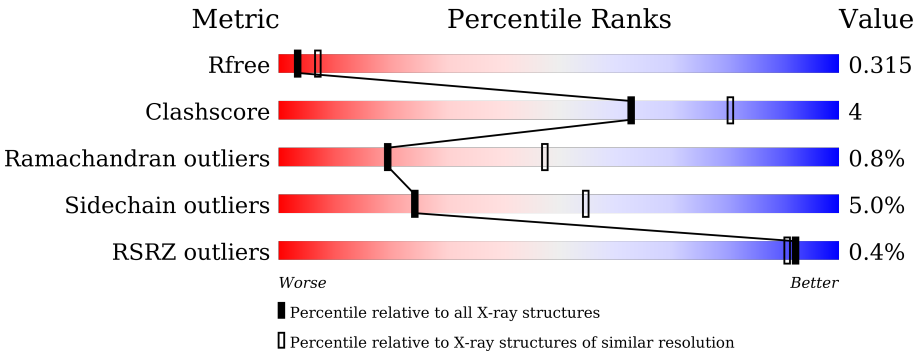
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.82 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	228	86% 10% •
1	E	228	81% 14% • 5%
1	I	228	82% 12% • 5%
1	M	228	3% 78% 12% 10%
2	B	215	87% 10% •
2	F	215	% 81% 14% • •

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Mol	Chain	Length	Quality of chain
2	J	215	
2	N	215	
3	C	189	
3	G	189	
3	K	189	
3	O	189	
4	D	226	
4	H	226	
4	L	226	
4	P	226	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 23643 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 DQN0344AE02 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1620	1025	269	317	9			
1	E	217	Total	C	N	O	S	0	0	0
			1605	1017	262	317	9			
1	I	217	Total	C	N	O	S	0	0	0
			1589	1007	261	312	9			
1	M	206	Total	C	N	O	S	0	0	0
			1506	945	254	298	9			

- Molecule 2 is a protein called DQN0344AE02 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1620	1016	266	333	5			
2	F	212	Total	C	N	O	S	0	0	0
			1522	954	253	310	5			
2	J	209	Total	C	N	O	S	0	0	0
			1548	971	252	321	4			
2	N	212	Total	C	N	O	S	0	0	0
			1529	961	245	318	5			

- Molecule 3 is a protein called HLA class II histocompatibility antigen, DQ alpha 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	179	Total	C	N	O	S	0	0	0
			1407	907	227	271	2			
3	G	179	Total	C	N	O	S	0	0	0
			1357	871	215	269	2			
3	K	179	Total	C	N	O	S	0	0	0
			1354	874	219	259	2			
3	O	178	Total	C	N	O	S	0	0	0
			1370	881	227	260	2			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	47	SER	CYS	engineered mutation	UNP P01909
C	184	LEU	-	expression tag	UNP P01909
C	185	GLU	-	expression tag	UNP P01909
C	186	VAL	-	expression tag	UNP P01909
C	187	LEU	-	expression tag	UNP P01909
C	188	PHE	-	expression tag	UNP P01909
C	189	GLN	-	expression tag	UNP P01909
G	47	SER	CYS	engineered mutation	UNP P01909
G	184	LEU	-	expression tag	UNP P01909
G	185	GLU	-	expression tag	UNP P01909
G	186	VAL	-	expression tag	UNP P01909
G	187	LEU	-	expression tag	UNP P01909
G	188	PHE	-	expression tag	UNP P01909
G	189	GLN	-	expression tag	UNP P01909
K	47	SER	CYS	engineered mutation	UNP P01909
K	184	LEU	-	expression tag	UNP P01909
K	185	GLU	-	expression tag	UNP P01909
K	186	VAL	-	expression tag	UNP P01909
K	187	LEU	-	expression tag	UNP P01909
K	188	PHE	-	expression tag	UNP P01909
K	189	GLN	-	expression tag	UNP P01909
O	47	SER	CYS	engineered mutation	UNP P01909
O	184	LEU	-	expression tag	UNP P01909
O	185	GLU	-	expression tag	UNP P01909
O	186	VAL	-	expression tag	UNP P01909
O	187	LEU	-	expression tag	UNP P01909
O	188	PHE	-	expression tag	UNP P01909
O	189	GLN	-	expression tag	UNP P01909

- Molecule 4 is a protein called MHC class II HLA-DQ-beta-1 - alpha1 gliadin peptide chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	181	Total	C	N	O	S	0	0	0
			1428	917	239	266	6			
4	H	178	Total	C	N	O	S	0	0	0
			1347	861	228	252	6			
4	L	179	Total	C	N	O	S	0	0	0
			1344	851	239	247	7			
4	P	186	Total	C	N	O	S	0	0	0
			1441	916	252	266	7			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	984	GLY	-	linker	PDB ?
D	985	SER	-	linker	PDB ?
D	986	GLY	-	linker	PDB ?
D	987	GLY	-	linker	PDB ?
D	988	GLY	-	linker	PDB ?
D	989	GLY	-	linker	PDB ?
D	990	SER	-	linker	PDB ?
D	991	ILE	-	linker	PDB ?
D	992	GLU	-	linker	PDB ?
D	993	GLY	-	linker	PDB ?
D	994	ARG	-	linker	PDB ?
D	995	GLY	-	linker	PDB ?
D	996	SER	-	linker	PDB ?
D	997	GLY	-	linker	PDB ?
D	998	GLY	-	linker	PDB ?
D	999	GLY	-	linker	PDB ?
D	1000	SER	-	linker	PDB ?
D	1191	LEU	-	expression tag	UNP O19712
D	1192	GLU	-	expression tag	UNP O19712
D	1193	VAL	-	expression tag	UNP O19712
D	1194	LEU	-	expression tag	UNP O19712
D	1195	PHE	-	expression tag	UNP O19712
D	1196	GLN	-	expression tag	UNP O19712
H	984	GLY	-	linker	PDB ?
H	985	SER	-	linker	PDB ?
H	986	GLY	-	linker	PDB ?
H	987	GLY	-	linker	PDB ?
H	988	GLY	-	linker	PDB ?
H	989	GLY	-	linker	PDB ?
H	990	SER	-	linker	PDB ?
H	991	ILE	-	linker	PDB ?
H	992	GLU	-	linker	PDB ?
H	993	GLY	-	linker	PDB ?
H	994	ARG	-	linker	PDB ?
H	995	GLY	-	linker	PDB ?
H	996	SER	-	linker	PDB ?
H	997	GLY	-	linker	PDB ?
H	998	GLY	-	linker	PDB ?
H	999	GLY	-	linker	PDB ?
H	1000	SER	-	linker	PDB ?
H	1191	LEU	-	expression tag	UNP O19712
H	1192	GLU	-	expression tag	UNP O19712

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1193	VAL	-	expression tag	UNP O19712
H	1194	LEU	-	expression tag	UNP O19712
H	1195	PHE	-	expression tag	UNP O19712
H	1196	GLN	-	expression tag	UNP O19712
L	984	GLY	-	linker	PDB ?
L	985	SER	-	linker	PDB ?
L	986	GLY	-	linker	PDB ?
L	987	GLY	-	linker	PDB ?
L	988	GLY	-	linker	PDB ?
L	989	GLY	-	linker	PDB ?
L	990	SER	-	linker	PDB ?
L	991	ILE	-	linker	PDB ?
L	992	GLU	-	linker	PDB ?
L	993	GLY	-	linker	PDB ?
L	994	ARG	-	linker	PDB ?
L	995	GLY	-	linker	PDB ?
L	996	SER	-	linker	PDB ?
L	997	GLY	-	linker	PDB ?
L	998	GLY	-	linker	PDB ?
L	999	GLY	-	linker	PDB ?
L	1000	SER	-	linker	PDB ?
L	1191	LEU	-	expression tag	UNP O19712
L	1192	GLU	-	expression tag	UNP O19712
L	1193	VAL	-	expression tag	UNP O19712
L	1194	LEU	-	expression tag	UNP O19712
L	1195	PHE	-	expression tag	UNP O19712
L	1196	GLN	-	expression tag	UNP O19712
P	984	GLY	-	linker	PDB ?
P	985	SER	-	linker	PDB ?
P	986	GLY	-	linker	PDB ?
P	987	GLY	-	linker	PDB ?
P	988	GLY	-	linker	PDB ?
P	989	GLY	-	linker	PDB ?
P	990	SER	-	linker	PDB ?
P	991	ILE	-	linker	PDB ?
P	992	GLU	-	linker	PDB ?
P	993	GLY	-	linker	PDB ?
P	994	ARG	-	linker	PDB ?
P	995	GLY	-	linker	PDB ?
P	996	SER	-	linker	PDB ?
P	997	GLY	-	linker	PDB ?
P	998	GLY	-	linker	PDB ?

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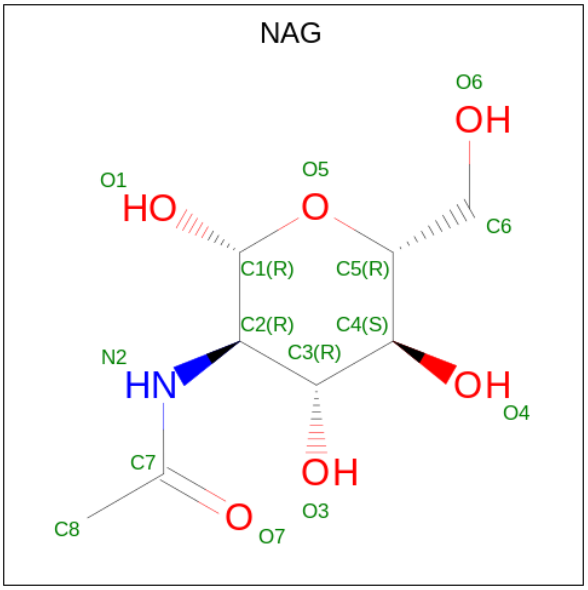
Chain	Residue	Modelled	Actual	Comment	Reference
P	999	GLY	-	linker	PDB ?
P	1000	SER	-	linker	PDB ?
P	1191	LEU	-	expression tag	UNP O19712
P	1192	GLU	-	expression tag	UNP O19712
P	1193	VAL	-	expression tag	UNP O19712
P	1194	LEU	-	expression tag	UNP O19712
P	1195	PHE	-	expression tag	UNP O19712
P	1196	GLN	-	expression tag	UNP O19712

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



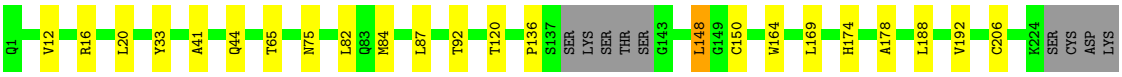
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	K	1	Total C N O 14 8 1 5	0	0
5	O	1	Total C N O 14 8 1 5	0	0

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.

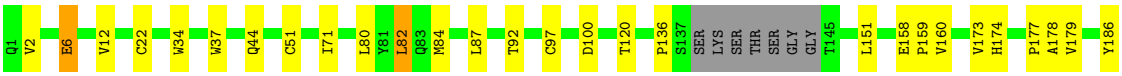
• Molecule 1: DQN0344AE02 Fab heavy chain

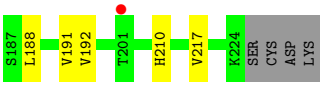
Chain A:



• Molecule 1: DQN0344AE02 Fab heavy chain

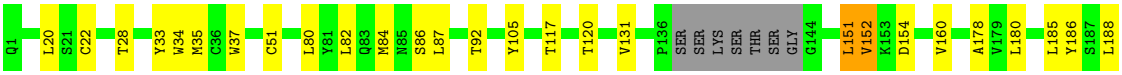
Chain E:





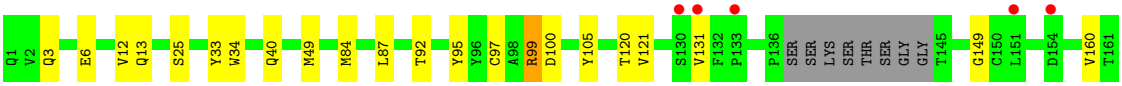
• Molecule 1: DQN0344AE02 Fab heavy chain

Chain I:



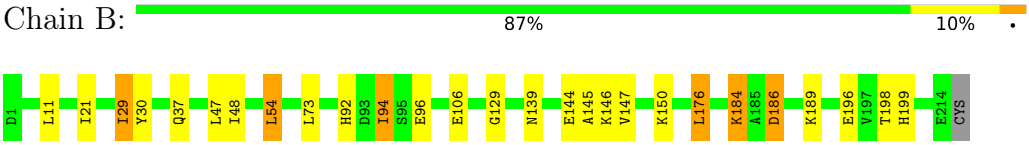
• Molecule 1: DQN0344AE02 Fab heavy chain

Chain M:



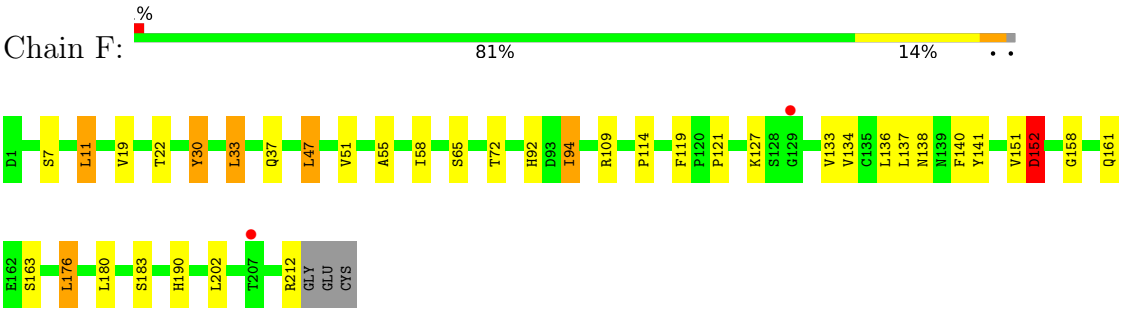
• Molecule 2: DQN0344AE02 Fab light chain

Chain B:



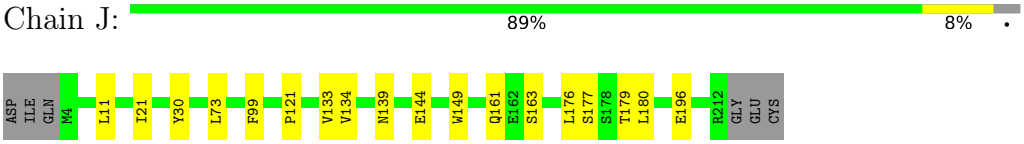
• Molecule 2: DQN0344AE02 Fab light chain

Chain F:



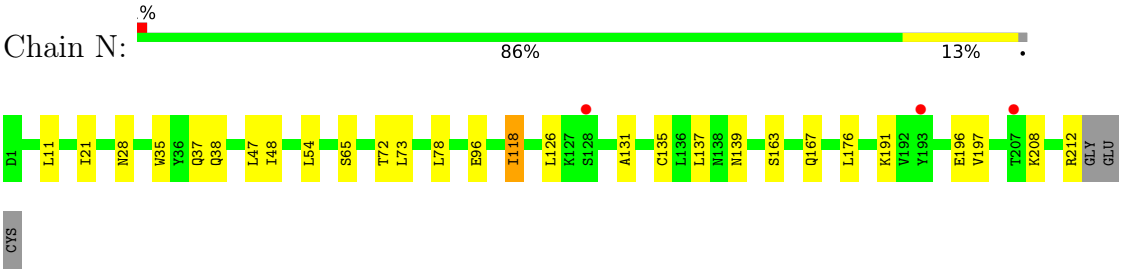
• Molecule 2: DQN0344AE02 Fab light chain

Chain J:



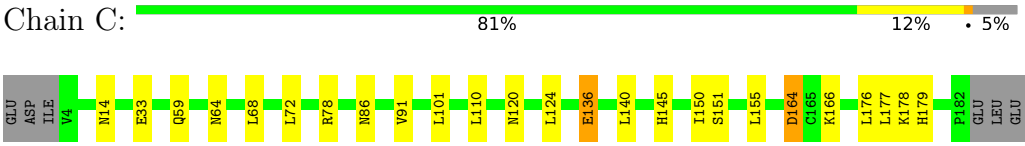
• Molecule 2: DQN0344AE02 Fab light chain

Chain N:



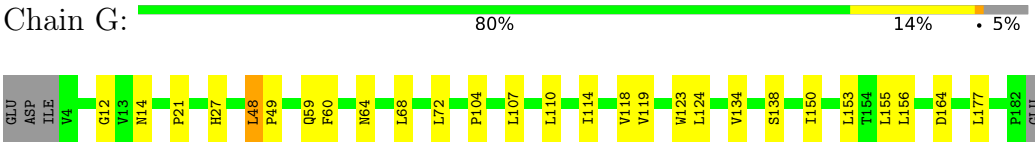
• Molecule 3: HLA class II histocompatibility antigen, DQ alpha 1 chain

Chain C:



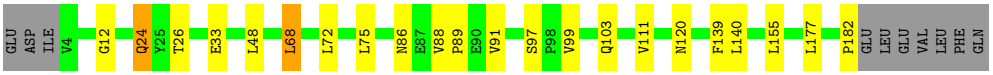
• Molecule 3: HLA class II histocompatibility antigen, DQ alpha 1 chain

Chain G:



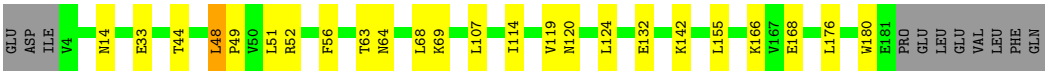
• Molecule 3: HLA class II histocompatibility antigen, DQ alpha 1 chain

Chain K:



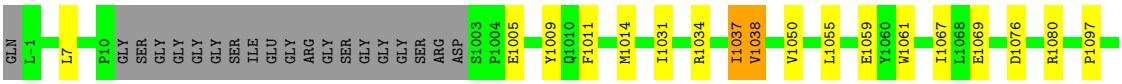
• Molecule 3: HLA class II histocompatibility antigen, DQ alpha 1 chain

Chain O:



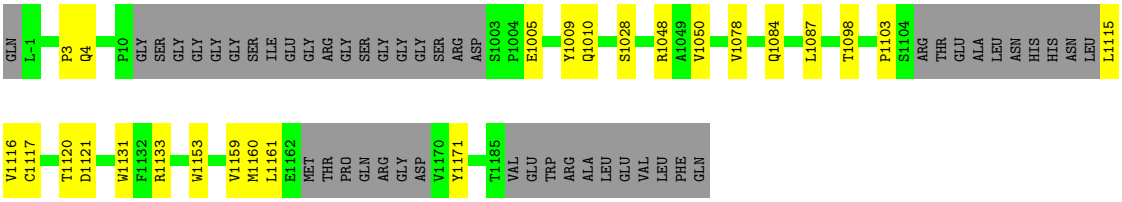
• Molecule 4: MHC class II HLA-DQ-beta-1 - alpha1 gliadin peptide chimeric protein

Chain D:



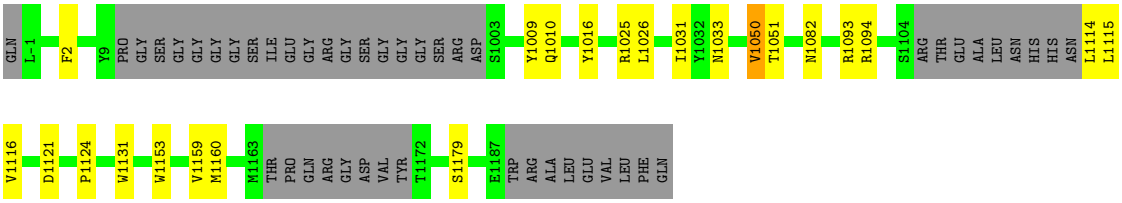
• Molecule 4: MHC class II HLA-DQ-beta-1 - alpha1 gliadin peptide chimeric protein

Chain H:



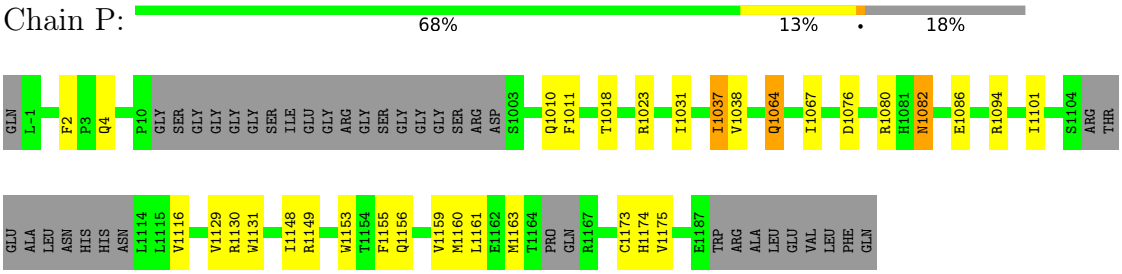
• Molecule 4: MHC class II HLA-DQ-beta-1 - alpha1 gliadin peptide chimeric protein

Chain L:



• Molecule 4: MHC class II HLA-DQ-beta-1 - alpha1 gliadin peptide chimeric protein

Chain P:


68%
13%
18%
GLN L-1 F2 P3 Q4 P10 GLY SER GLY GLY GLY GLY SER ILE GLU GLY ARG GLY SER GLY GLY GLY SER ARG ASP S1003 Q1010 F1011 T1018 R1023 I1031 I1037 V1038 Q1064 I1067 D1076 R1080 H1081 N1082 E1086 R1094 I1101 S1104 ARG THR
GLU ALA LEU ASN HIS HIS ASN L1114 L1115 V1116 V1129 R1130 W1131 I1148 R1149 W1153 T1154 F1155 Q1156 V1159 M1160 L1161 E1162 M1163 T1164 PRO GLN R1167 C1173 H1174 V1175 E1187 TRP ARG ALA LEU GLU VAL LEU PHE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.49Å 174.24Å 129.66Å 90.00° 93.17° 90.00°	Depositor
Resolution (Å)	54.86 – 2.82 54.86 – 2.82	Depositor EDS
% Data completeness (in resolution range)	47.7 (54.86-2.82) 47.7 (54.86-2.82)	Depositor EDS
R_{merge}	0.50	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.11.8 (8-JUN-2022)	Depositor
R, R_{free}	0.278 , 0.321 0.271 , 0.315	Depositor DCC
R_{free} test set	2141 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	35.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , -0.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	23643	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.15% 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	0.17	0/1664	0.35	0/2279
1	E	0.18	0/1649	0.35	0/2260
1	I	0.19	0/1633	0.38	0/2239
1	M	0.18	0/1543	0.35	0/2110
2	B	0.18	0/1655	0.35	0/2253
2	F	0.21	0/1554	0.40	0/2127
2	J	0.17	0/1583	0.35	0/2163
2	N	0.17	0/1563	0.34	0/2139
3	C	0.19	0/1449	0.36	0/1985
3	G	0.19	0/1397	0.36	0/1924
3	K	0.18	0/1395	0.39	0/1920
3	O	0.19	0/1410	0.37	0/1933
4	D	0.19	0/1462	0.38	0/1998
4	H	0.19	0/1381	0.38	0/1893
4	L	0.18	0/1374	0.35	0/1876
4	P	0.18	0/1474	0.36	0/2010
All	All	0.18	0/24186	0.36	0/33109

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	1620	0	1502	11	0
1	E	1605	0	1477	24	0
1	I	1589	0	1446	14	0
1	M	1506	0	1387	14	0
2	B	1620	0	1539	15	0
2	F	1522	0	1392	22	0
2	J	1548	0	1425	7	0
2	N	1529	0	1376	10	0
3	C	1407	0	1330	9	0
3	G	1357	0	1221	16	0
3	K	1354	0	1242	8	0
3	O	1370	0	1278	10	0
4	D	1428	0	1361	15	0
4	H	1347	0	1226	16	0
4	L	1344	0	1234	11	0
4	P	1441	0	1364	17	0
5	C	14	0	13	0	0
5	G	14	0	13	0	0
5	K	14	0	13	0	0
5	O	14	0	13	0	0
All	All	23643	0	21852	197	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 197 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:B:150:LYS:NZ	2:B:196:GLU:HB2	1.88	0.89
3:C:164:ASP:HB3	3:C:179:HIS:HA	1.56	0.87
1:M:160:VAL:HG22	1:M:210:HIS:CD2	2.11	0.84
1:M:40:GLN:HE22	2:N:38:GLN:HE22	1.22	0.83
3:G:14:ASN:HB3	3:G:68:LEU:HD11	1.66	0.75

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	215/228 (94%)	204 (95%)	11 (5%)	0	100	100
1	E	213/228 (93%)	193 (91%)	19 (9%)	1 (0%)	29	59
1	I	213/228 (93%)	192 (90%)	18 (8%)	3 (1%)	11	32
1	M	200/228 (88%)	190 (95%)	10 (5%)	0	100	100
2	B	212/215 (99%)	200 (94%)	9 (4%)	3 (1%)	11	32
2	F	210/215 (98%)	186 (89%)	19 (9%)	5 (2%)	6	19
2	J	207/215 (96%)	188 (91%)	16 (8%)	3 (1%)	11	32
2	N	210/215 (98%)	191 (91%)	18 (9%)	1 (0%)	29	59
3	C	177/189 (94%)	170 (96%)	7 (4%)	0	100	100
3	G	177/189 (94%)	166 (94%)	10 (6%)	1 (1%)	25	54
3	K	177/189 (94%)	171 (97%)	4 (2%)	2 (1%)	14	39
3	O	176/189 (93%)	168 (96%)	8 (4%)	0	100	100
4	D	173/226 (76%)	163 (94%)	9 (5%)	1 (1%)	25	54
4	H	170/226 (75%)	156 (92%)	12 (7%)	2 (1%)	13	37
4	L	171/226 (76%)	157 (92%)	11 (6%)	3 (2%)	8	26
4	P	178/226 (79%)	169 (95%)	9 (5%)	0	100	100
All	All	3079/3432 (90%)	2864 (93%)	190 (6%)	25 (1%)	19	47

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	141	TYR
2	B	139	ASN
2	F	158	GLY
4	H	1121	ASP
2	J	139	ASN

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	173/193 (90%)	167 (96%)	6 (4%)	36	68
1	E	172/193 (89%)	166 (96%)	6 (4%)	36	68
1	I	166/193 (86%)	161 (97%)	5 (3%)	41	73
1	M	160/193 (83%)	154 (96%)	6 (4%)	33	65
2	B	181/188 (96%)	172 (95%)	9 (5%)	24	55
2	F	159/188 (85%)	149 (94%)	10 (6%)	18	44
2	J	168/188 (89%)	164 (98%)	4 (2%)	49	80
2	N	159/188 (85%)	149 (94%)	10 (6%)	18	44
3	C	158/173 (91%)	144 (91%)	14 (9%)	9	27
3	G	146/173 (84%)	138 (94%)	8 (6%)	21	50
3	K	145/173 (84%)	135 (93%)	10 (7%)	15	40
3	O	149/173 (86%)	139 (93%)	10 (7%)	16	41
4	D	155/200 (78%)	144 (93%)	11 (7%)	14	38
4	H	139/200 (70%)	133 (96%)	6 (4%)	29	60
4	L	136/200 (68%)	132 (97%)	4 (3%)	42	74
4	P	153/200 (76%)	145 (95%)	8 (5%)	23	53
All	All	2519/3016 (84%)	2392 (95%)	127 (5%)	24	55

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	27	HIS
3	O	48	LEU
1	I	117	THR
3	O	33	GLU
3	O	176	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	40	GLN
3	O	17	GLN
4	P	1082	ASN
3	O	71	ASN
1	M	210	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	C	1000	-	14,14,15	0.24	0	17,19,21	0.43	0
5	NAG	G	1000	-	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	O	1000	-	14,14,15	0.38	0	17,19,21	0.30	0
5	NAG	K	1000	-	14,14,15	0.24	0	17,19,21	0.38	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
5	NAG	C	1000	-	-	0/6/23/26	0/1/1/1
5	NAG	G	1000	-	-	1/6/23/26	0/1/1/1
5	NAG	O	1000	-	-	0/6/23/26	0/1/1/1
5	NAG	K	1000	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	1000	NAG	O5-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	219/228 (96%)	-0.57	0 100 100	24, 30, 41, 50	0
1	E	217/228 (95%)	-0.46	1 (0%) 91 88	20, 34, 56, 66	0
1	I	217/228 (95%)	-0.42	0 100 100	31, 38, 50, 56	0
1	M	206/228 (90%)	-0.04	7 (3%) 45 35	26, 37, 86, 93	0
2	B	214/215 (99%)	-0.50	0 100 100	23, 36, 48, 55	0
2	F	212/215 (98%)	-0.35	2 (0%) 84 80	26, 42, 60, 69	0
2	J	209/215 (97%)	-0.48	0 100 100	30, 39, 47, 51	0
2	N	212/215 (98%)	-0.16	3 (1%) 75 69	34, 51, 73, 82	0
3	C	179/189 (94%)	-0.59	0 100 100	15, 31, 40, 45	0
3	G	179/189 (94%)	-0.45	0 100 100	23, 36, 50, 52	0
3	K	179/189 (94%)	-0.51	0 100 100	26, 40, 53, 58	0
3	O	178/189 (94%)	-0.43	0 100 100	28, 39, 54, 64	0
4	D	181/226 (80%)	-0.45	0 100 100	27, 32, 43, 50	0
4	H	178/226 (78%)	-0.51	0 100 100	26, 35, 46, 53	0
4	L	179/226 (79%)	-0.46	0 100 100	29, 41, 55, 58	0
4	P	186/226 (82%)	-0.46	0 100 100	28, 38, 50, 56	0
All	All	3145/3432 (91%)	-0.42	13 (0%) 92 91	15, 37, 67, 93	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	151	LEU	4.4
1	M	133	PRO	3.2
1	M	203	THR	2.6
1	M	131	VAL	2.5
1	E	201	THR	2.4

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
5	NAG	O	1000	14/15	0.87	0.25	64,64,64,64	0
5	NAG	G	1000	14/15	0.88	0.22	62,62,62,62	0
5	NAG	C	1000	14/15	0.89	0.20	52,52,52,52	0
5	NAG	K	1000	14/15	0.91	0.17	57,57,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.