wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 06:07 pm GMT

PDB ID	:	3ZLE
Title	:	Crystal structure of Toxoplasma gondii sporozoite AMA1
Authors	:	Tonkin, M.L.; Boulanger, M.J.
Deposited on	:	2013-01-30
Resolution	:	2.35 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:

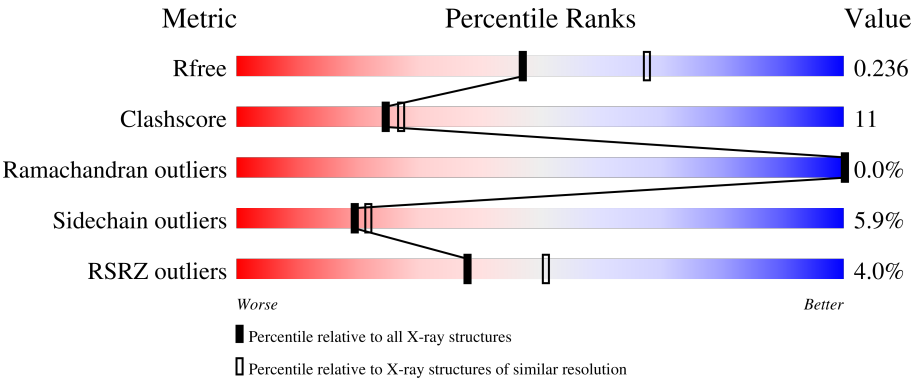
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	396	4% 83% 12%
1	B	396	2% 74% 19%
1	C	396	2% 80% 15%
1	D	396	2% 77% 18%
1	E	396	4% 73% 21%

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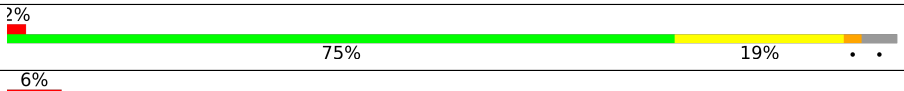
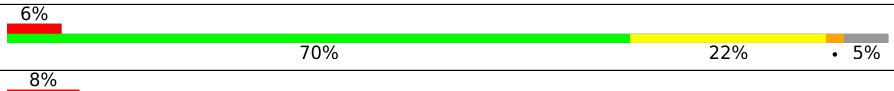
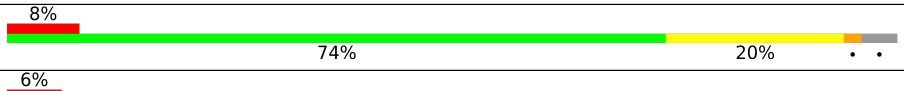
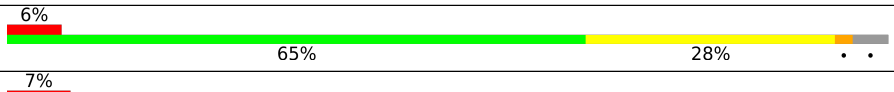
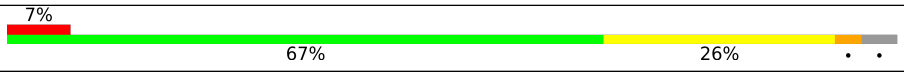
Mol	Chain	Length	Quality of chain
1	F	396	
1	G	396	
1	H	396	
1	I	396	
1	J	396	
1	K	396	
1	L	396	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 36679 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 APICAL MEMBRANE ANTIGEN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2913	1837	483	575	18			
1	B	379	Total	C	N	O	S	0	0	0
			2885	1818	480	569	18			
1	C	379	Total	C	N	O	S	0	0	0
			2885	1818	480	569	18			
1	D	380	Total	C	N	O	S	0	0	0
			2897	1827	481	571	18			
1	E	382	Total	C	N	O	S	0	0	0
			2913	1837	483	575	18			
1	F	377	Total	C	N	O	S	0	0	0
			2875	1812	478	567	18			
1	G	382	Total	C	N	O	S	0	0	0
			2913	1837	483	575	18			
1	H	380	Total	C	N	O	S	0	0	0
			2899	1829	481	571	18			
1	I	375	Total	C	N	O	S	0	1	0
			2865	1806	477	564	18			
1	J	379	Total	C	N	O	S	0	1	0
			2891	1822	480	571	18			
1	K	380	Total	C	N	O	S	0	1	0
			2907	1834	484	571	18			
1	L	380	Total	C	N	O	S	0	1	0
			2907	1834	484	571	18			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	GLY	-	expression tag	UNP B6K9M7
A	93	SER	-	expression tag	UNP B6K9M7
A	94	ALA	-	expression tag	UNP B6K9M7
A	95	MET	-	expression tag	UNP B6K9M7
A	96	GLY	-	expression tag	UNP B6K9M7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	481	ALA	-	expression tag	UNP B6K9M7
A	482	ALA	-	expression tag	UNP B6K9M7
A	483	ALA	-	expression tag	UNP B6K9M7
A	484	LEU	-	expression tag	UNP B6K9M7
A	485	VAL	-	expression tag	UNP B6K9M7
A	486	PRO	-	expression tag	UNP B6K9M7
A	487	ARG	-	expression tag	UNP B6K9M7
B	92	GLY	-	expression tag	UNP B6K9M7
B	93	SER	-	expression tag	UNP B6K9M7
B	94	ALA	-	expression tag	UNP B6K9M7
B	95	MET	-	expression tag	UNP B6K9M7
B	96	GLY	-	expression tag	UNP B6K9M7
B	481	ALA	-	expression tag	UNP B6K9M7
B	482	ALA	-	expression tag	UNP B6K9M7
B	483	ALA	-	expression tag	UNP B6K9M7
B	484	LEU	-	expression tag	UNP B6K9M7
B	485	VAL	-	expression tag	UNP B6K9M7
B	486	PRO	-	expression tag	UNP B6K9M7
B	487	ARG	-	expression tag	UNP B6K9M7
C	92	GLY	-	expression tag	UNP B6K9M7
C	93	SER	-	expression tag	UNP B6K9M7
C	94	ALA	-	expression tag	UNP B6K9M7
C	95	MET	-	expression tag	UNP B6K9M7
C	96	GLY	-	expression tag	UNP B6K9M7
C	481	ALA	-	expression tag	UNP B6K9M7
C	482	ALA	-	expression tag	UNP B6K9M7
C	483	ALA	-	expression tag	UNP B6K9M7
C	484	LEU	-	expression tag	UNP B6K9M7
C	485	VAL	-	expression tag	UNP B6K9M7
C	486	PRO	-	expression tag	UNP B6K9M7
C	487	ARG	-	expression tag	UNP B6K9M7
D	92	GLY	-	expression tag	UNP B6K9M7
D	93	SER	-	expression tag	UNP B6K9M7
D	94	ALA	-	expression tag	UNP B6K9M7
D	95	MET	-	expression tag	UNP B6K9M7
D	96	GLY	-	expression tag	UNP B6K9M7
D	481	ALA	-	expression tag	UNP B6K9M7
D	482	ALA	-	expression tag	UNP B6K9M7
D	483	ALA	-	expression tag	UNP B6K9M7
D	484	LEU	-	expression tag	UNP B6K9M7
D	485	VAL	-	expression tag	UNP B6K9M7
D	486	PRO	-	expression tag	UNP B6K9M7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	487	ARG	-	expression tag	UNP B6K9M7
E	92	GLY	-	expression tag	UNP B6K9M7
E	93	SER	-	expression tag	UNP B6K9M7
E	94	ALA	-	expression tag	UNP B6K9M7
E	95	MET	-	expression tag	UNP B6K9M7
E	96	GLY	-	expression tag	UNP B6K9M7
E	481	ALA	-	expression tag	UNP B6K9M7
E	482	ALA	-	expression tag	UNP B6K9M7
E	483	ALA	-	expression tag	UNP B6K9M7
E	484	LEU	-	expression tag	UNP B6K9M7
E	485	VAL	-	expression tag	UNP B6K9M7
E	486	PRO	-	expression tag	UNP B6K9M7
E	487	ARG	-	expression tag	UNP B6K9M7
F	92	GLY	-	expression tag	UNP B6K9M7
F	93	SER	-	expression tag	UNP B6K9M7
F	94	ALA	-	expression tag	UNP B6K9M7
F	95	MET	-	expression tag	UNP B6K9M7
F	96	GLY	-	expression tag	UNP B6K9M7
F	481	ALA	-	expression tag	UNP B6K9M7
F	482	ALA	-	expression tag	UNP B6K9M7
F	483	ALA	-	expression tag	UNP B6K9M7
F	484	LEU	-	expression tag	UNP B6K9M7
F	485	VAL	-	expression tag	UNP B6K9M7
F	486	PRO	-	expression tag	UNP B6K9M7
F	487	ARG	-	expression tag	UNP B6K9M7
G	92	GLY	-	expression tag	UNP B6K9M7
G	93	SER	-	expression tag	UNP B6K9M7
G	94	ALA	-	expression tag	UNP B6K9M7
G	95	MET	-	expression tag	UNP B6K9M7
G	96	GLY	-	expression tag	UNP B6K9M7
G	481	ALA	-	expression tag	UNP B6K9M7
G	482	ALA	-	expression tag	UNP B6K9M7
G	483	ALA	-	expression tag	UNP B6K9M7
G	484	LEU	-	expression tag	UNP B6K9M7
G	485	VAL	-	expression tag	UNP B6K9M7
G	486	PRO	-	expression tag	UNP B6K9M7
G	487	ARG	-	expression tag	UNP B6K9M7
H	92	GLY	-	expression tag	UNP B6K9M7
H	93	SER	-	expression tag	UNP B6K9M7
H	94	ALA	-	expression tag	UNP B6K9M7
H	95	MET	-	expression tag	UNP B6K9M7
H	96	GLY	-	expression tag	UNP B6K9M7

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Chain	Residue	Modelled	Actual	Comment	Reference
H	481	ALA	-	expression tag	UNP B6K9M7
H	482	ALA	-	expression tag	UNP B6K9M7
H	483	ALA	-	expression tag	UNP B6K9M7
H	484	LEU	-	expression tag	UNP B6K9M7
H	485	VAL	-	expression tag	UNP B6K9M7
H	486	PRO	-	expression tag	UNP B6K9M7
H	487	ARG	-	expression tag	UNP B6K9M7
I	92	GLY	-	expression tag	UNP B6K9M7
I	93	SER	-	expression tag	UNP B6K9M7
I	94	ALA	-	expression tag	UNP B6K9M7
I	95	MET	-	expression tag	UNP B6K9M7
I	96	GLY	-	expression tag	UNP B6K9M7
I	481	ALA	-	expression tag	UNP B6K9M7
I	482	ALA	-	expression tag	UNP B6K9M7
I	483	ALA	-	expression tag	UNP B6K9M7
I	484	LEU	-	expression tag	UNP B6K9M7
I	485	VAL	-	expression tag	UNP B6K9M7
I	486	PRO	-	expression tag	UNP B6K9M7
I	487	ARG	-	expression tag	UNP B6K9M7
J	92	GLY	-	expression tag	UNP B6K9M7
J	93	SER	-	expression tag	UNP B6K9M7
J	94	ALA	-	expression tag	UNP B6K9M7
J	95	MET	-	expression tag	UNP B6K9M7
J	96	GLY	-	expression tag	UNP B6K9M7
J	481	ALA	-	expression tag	UNP B6K9M7
J	482	ALA	-	expression tag	UNP B6K9M7
J	483	ALA	-	expression tag	UNP B6K9M7
J	484	LEU	-	expression tag	UNP B6K9M7
J	485	VAL	-	expression tag	UNP B6K9M7
J	486	PRO	-	expression tag	UNP B6K9M7
J	487	ARG	-	expression tag	UNP B6K9M7
K	92	GLY	-	expression tag	UNP B6K9M7
K	93	SER	-	expression tag	UNP B6K9M7
K	94	ALA	-	expression tag	UNP B6K9M7
K	95	MET	-	expression tag	UNP B6K9M7
K	96	GLY	-	expression tag	UNP B6K9M7
K	481	ALA	-	expression tag	UNP B6K9M7
K	482	ALA	-	expression tag	UNP B6K9M7
K	483	ALA	-	expression tag	UNP B6K9M7
K	484	LEU	-	expression tag	UNP B6K9M7
K	485	VAL	-	expression tag	UNP B6K9M7
K	486	PRO	-	expression tag	UNP B6K9M7

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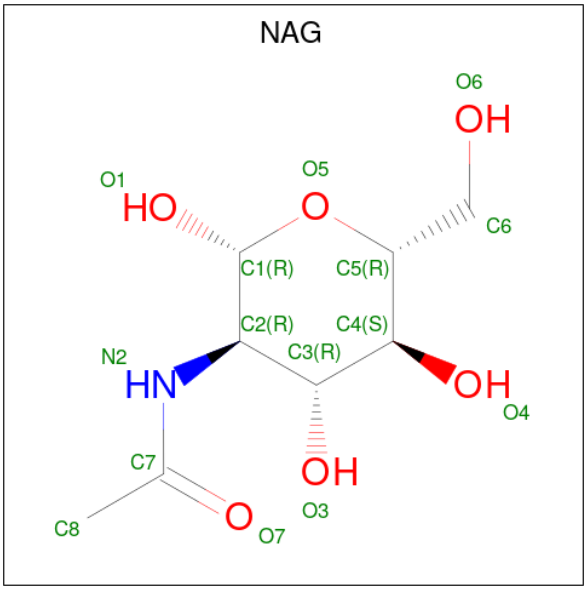
Chain	Residue	Modelled	Actual	Comment	Reference
K	487	ARG	-	expression tag	UNP B6K9M7
L	92	GLY	-	expression tag	UNP B6K9M7
L	93	SER	-	expression tag	UNP B6K9M7
L	94	ALA	-	expression tag	UNP B6K9M7
L	95	MET	-	expression tag	UNP B6K9M7
L	96	GLY	-	expression tag	UNP B6K9M7
L	481	ALA	-	expression tag	UNP B6K9M7
L	482	ALA	-	expression tag	UNP B6K9M7
L	483	ALA	-	expression tag	UNP B6K9M7
L	484	LEU	-	expression tag	UNP B6K9M7
L	485	VAL	-	expression tag	UNP B6K9M7
L	486	PRO	-	expression tag	UNP B6K9M7
L	487	ARG	-	expression tag	UNP B6K9M7

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



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

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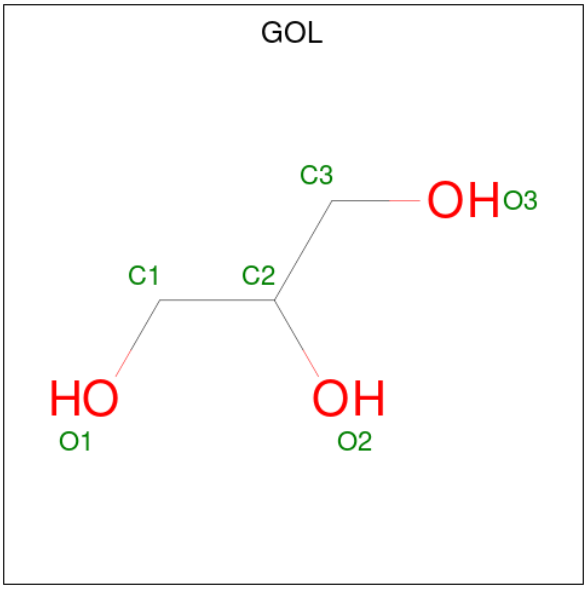
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C N O 14 8 1 5	0	0
2	G	1	Total C N O 14 8 1 5	0	0
2	H	1	Total C N O 14 8 1 5	0	0
2	K	1	Total C N O 14 8 1 5	0	0
2	L	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	I	1	Total C O 6 3 3	0	0
3	J	1	Total C O 6 3 3	0	0
3	L	1	Total C O 6 3 3	0	0
3	L	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	207	Total O 207 207	0	0
4	B	172	Total O 172 172	0	0
4	C	188	Total O 188 188	0	0
4	D	165	Total O 165 165	0	0
4	E	180	Total O 180 180	0	0
4	F	139	Total O 139 139	0	0
4	G	153	Total O 153 153	0	0

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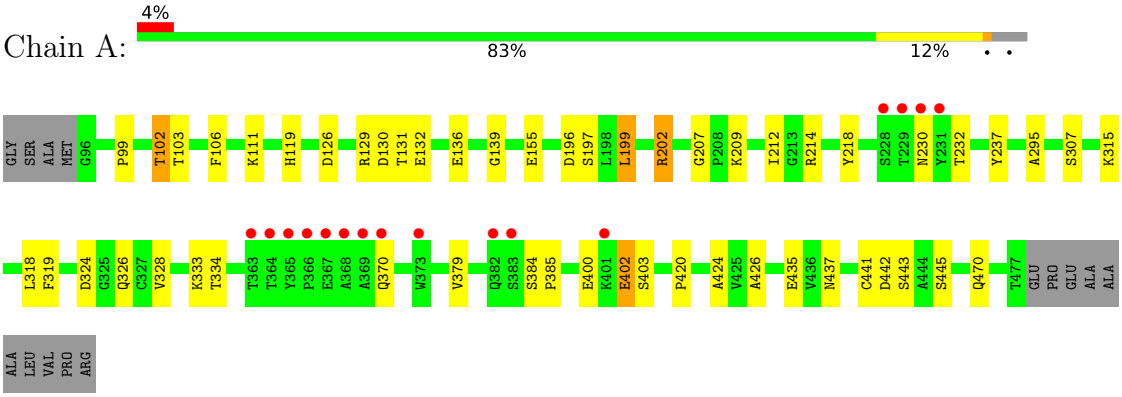
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	164	Total O 164 164	0	0
4	I	91	Total O 91 91	0	0
4	J	58	Total O 58 58	0	0
4	K	88	Total O 88 88	0	0
4	L	90	Total O 90 90	0	0

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.

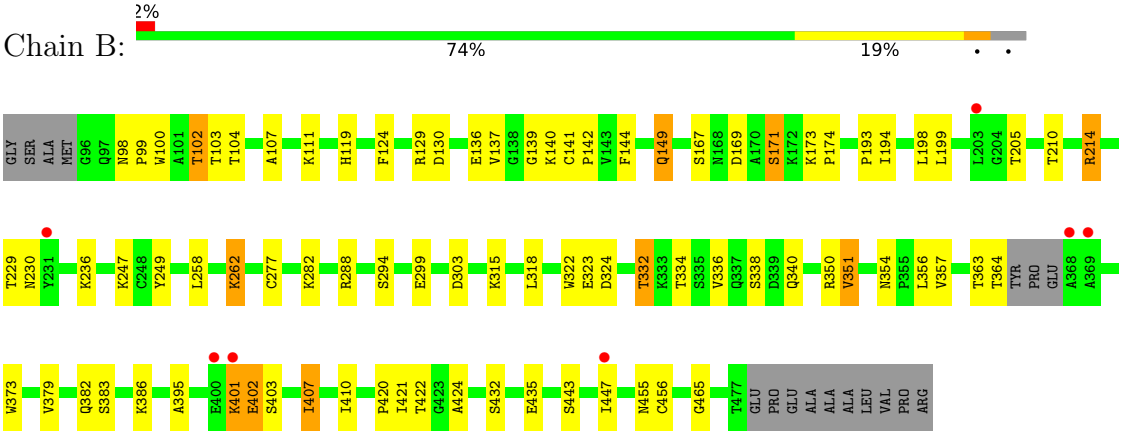
• Molecule 1: APICAL MEMBRANE ANTIGEN 1

Chain A:



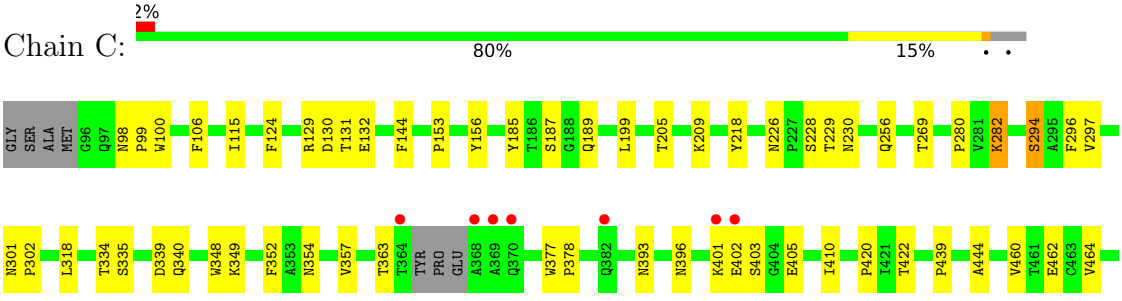
• Molecule 1: APICAL MEMBRANE ANTIGEN 1

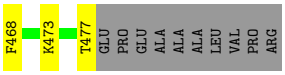
Chain B:



• Molecule 1: APICAL MEMBRANE ANTIGEN 1

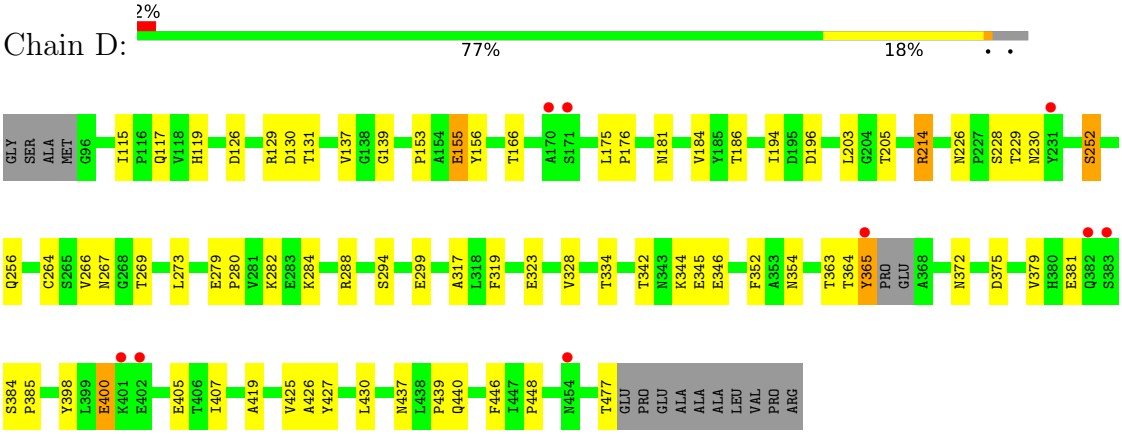
Chain C:





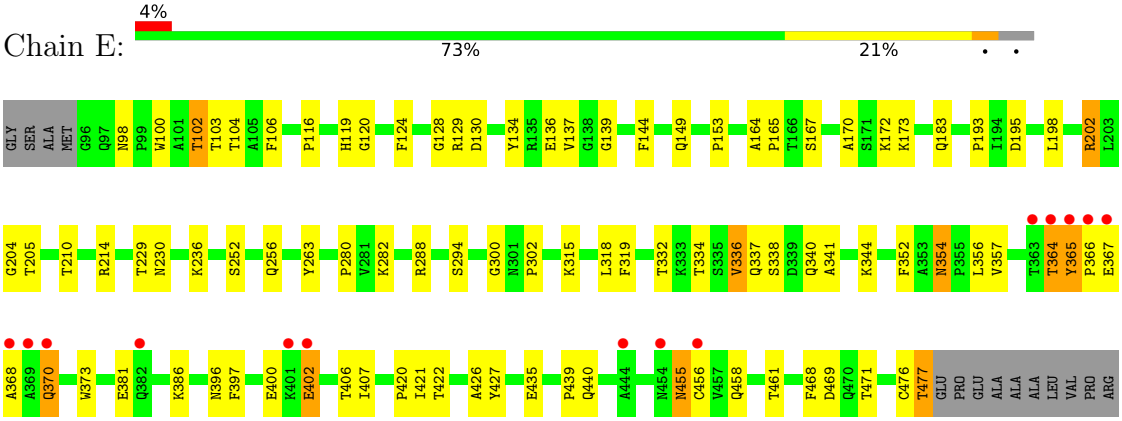
• Molecule 1: APICAL MEMBRANE ANTIGEN 1

Chain D:



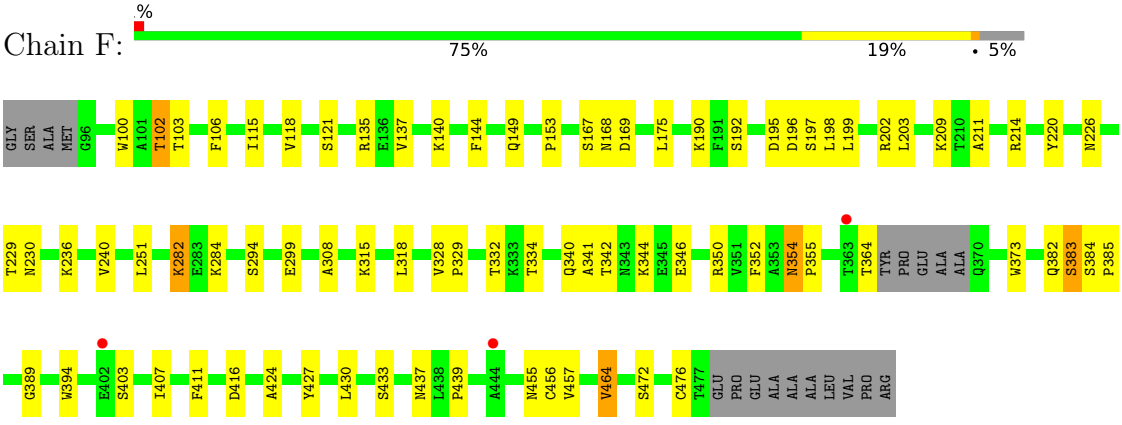
• Molecule 1: APICAL MEMBRANE ANTIGEN 1

Chain E:



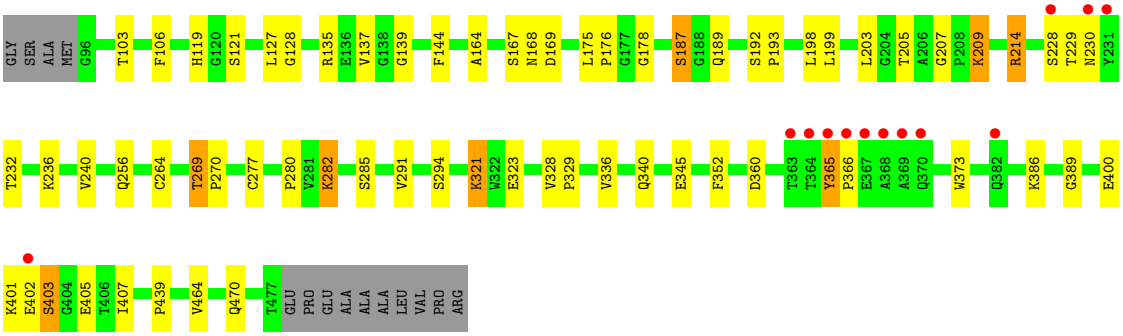
• Molecule 1: APICAL MEMBRANE ANTIGEN 1

Chain F:



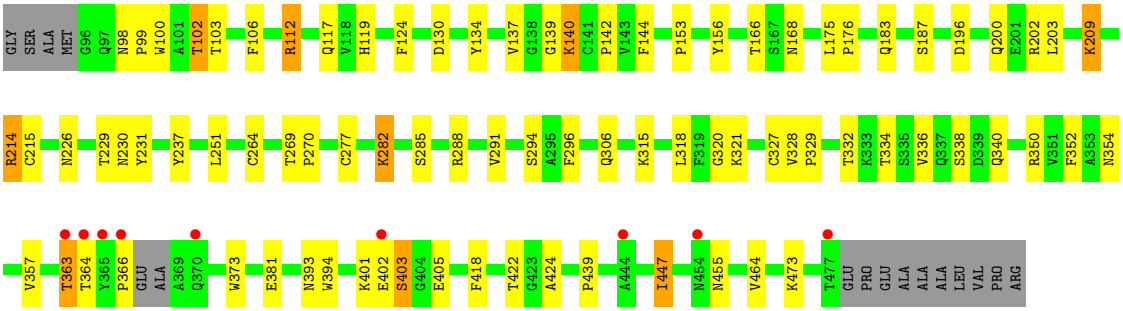
• Molecule 1: APICAL MEMBRANE ANTIGEN 1

Chain G:



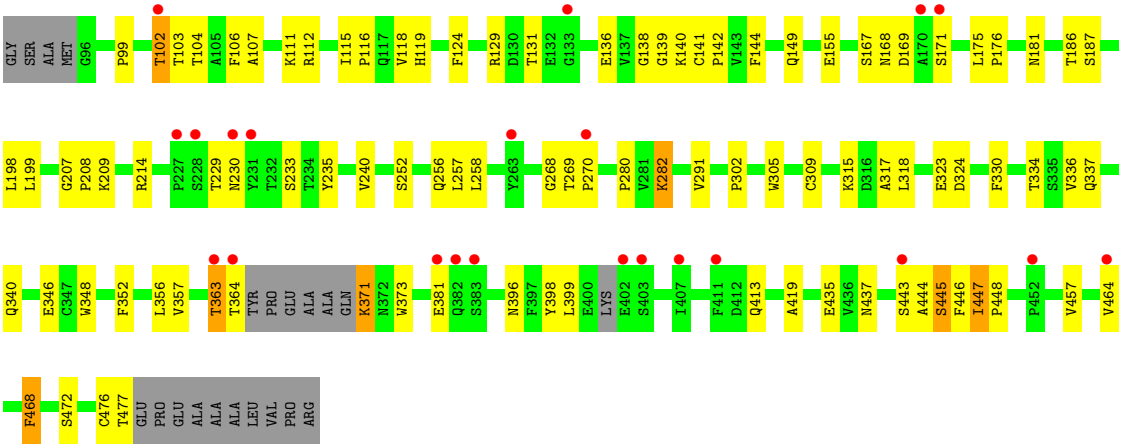
• Molecule 1: APICAL MEMBRANE ANTIGEN 1

Chain H:



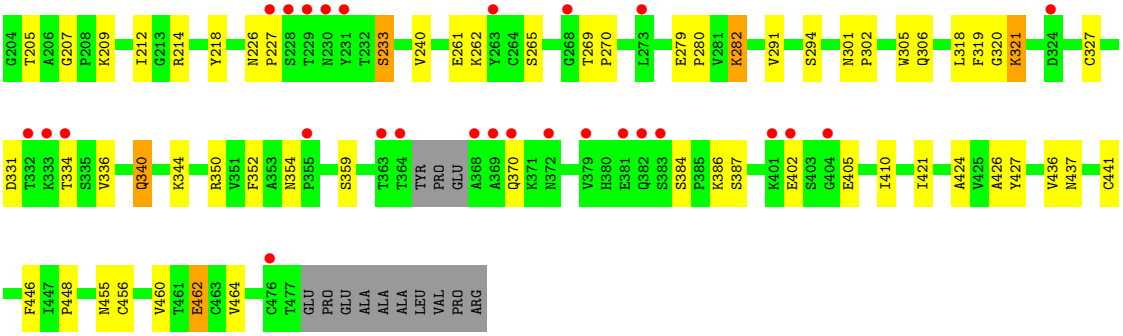
• Molecule 1: APICAL MEMBRANE ANTIGEN 1

Chain I:



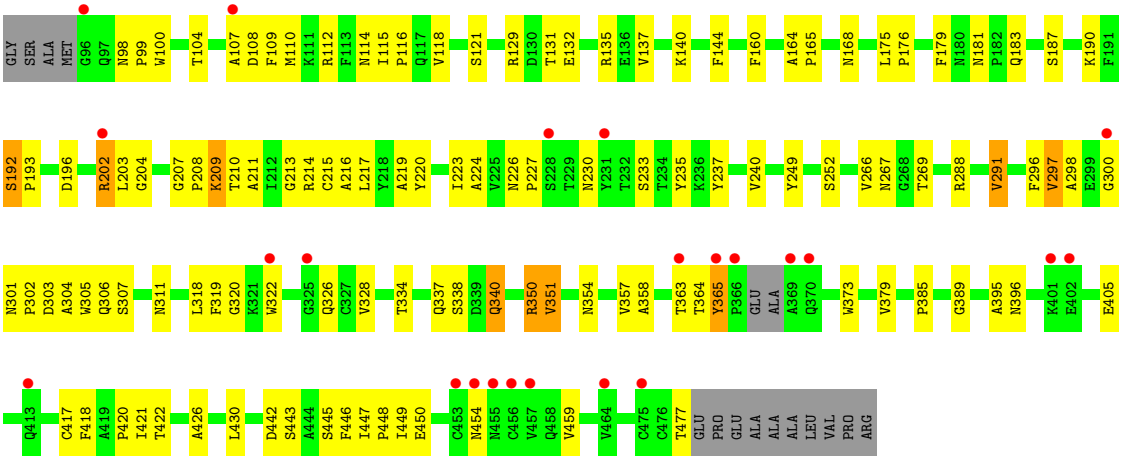
• Molecule 1: APICAL MEMBRANE ANTIGEN 1

Chain J:



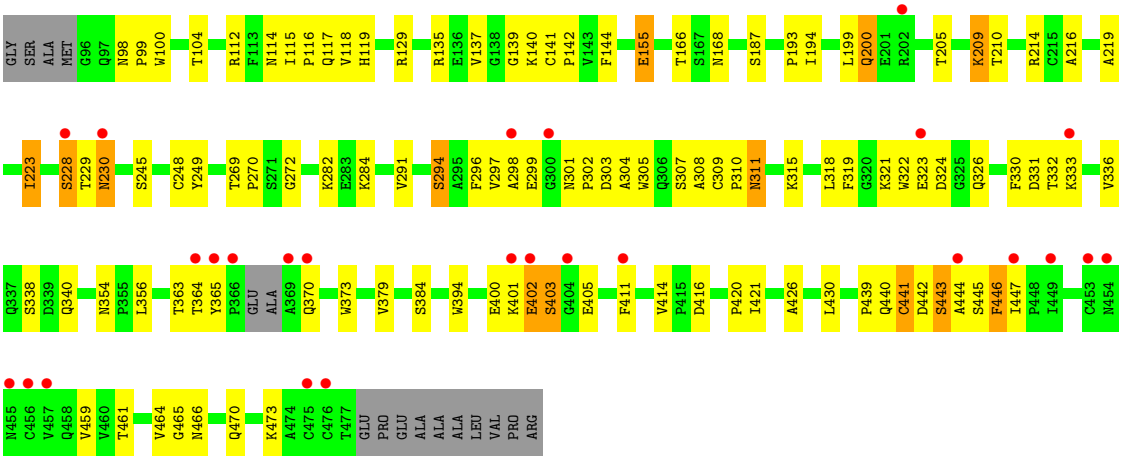
• Molecule 1: APICAL MEMBRANE ANTIGEN 1

Chain K:



• Molecule 1: APICAL MEMBRANE ANTIGEN 1

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	179.19Å 155.52Å 180.59Å 90.00° 92.31° 90.00°	Depositor
Resolution (Å)	78.04 – 2.35 78.04 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (78.04-2.35) 99.5 (78.04-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	13.32 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.209 , 0.244 0.203 , 0.236	Depositor DCC
R_{free} test set	20508 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	43.0	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.006 for h,-k,-l 0.089 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	36679	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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, GOL

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	0.72	2/2994 (0.1%)	0.65	0/4084
1	B	0.70	0/2963	0.70	4/4039 (0.1%)
1	C	0.73	0/2963	0.67	0/4039
1	D	0.72	0/2976	0.67	2/4057 (0.0%)
1	E	0.71	0/2994	0.67	2/4084 (0.0%)
1	F	0.68	0/2953	0.64	0/4025
1	G	0.68	0/2994	0.64	1/4084 (0.0%)
1	H	0.69	0/2979	0.70	5/4062 (0.1%)
1	I	0.56	0/2945	0.58	0/4013
1	J	0.55	0/2972	0.58	0/4051
1	K	0.58	0/2990	0.60	1/4076 (0.0%)
1	L	0.62	0/2990	0.61	0/4076
All	All	0.67	2/35713 (0.0%)	0.64	15/48690 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
1	F	0	1
1	L	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	SER	CB-OG	-5.74	1.34	1.42
1	A	441	CYS	CB-SG	-5.01	1.73	1.81

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	112	ARG	NE-CZ-NH2	-10.90	114.85	120.30
1	B	288	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	H	288	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	H	112	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	H	288	ARG	NE-CZ-NH2	-6.78	116.91	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	440	GLN	Peptide
1	E	364	THR	Peptide
1	F	476	CYS	Peptide
1	L	272	GLY	Peptide

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	2913	0	2731	40	0
1	B	2885	0	2707	64	0
1	C	2885	0	2707	38	0
1	D	2897	0	2718	49	0
1	E	2913	0	2731	68	0
1	F	2875	0	2699	54	0
1	G	2913	0	2731	42	0
1	H	2899	0	2718	57	0
1	I	2865	0	2690	57	0
1	J	2891	0	2715	60	0
1	K	2907	0	2733	116	0
1	L	2907	0	2731	101	0
2	A	14	0	13	2	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	E	14	0	13	2	0
2	F	14	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	14	0	13	0	0
2	H	14	0	13	0	0
2	K	14	0	13	5	0
2	L	14	0	13	2	0
3	A	18	0	24	2	0
3	B	12	0	16	3	0
3	C	12	0	16	3	0
3	D	12	0	16	2	0
3	E	12	0	16	3	0
3	F	6	0	8	3	0
3	G	6	0	8	1	0
3	H	6	0	8	3	0
3	I	6	0	8	1	0
3	J	6	0	8	2	0
3	L	12	0	16	0	0
4	A	207	0	0	8	0
4	B	172	0	0	4	0
4	C	188	0	0	7	0
4	D	165	0	0	3	0
4	E	180	0	0	10	0
4	F	139	0	0	7	0
4	G	153	0	0	3	0
4	H	164	0	0	7	0
4	I	91	0	0	5	0
4	J	58	0	0	3	0
4	K	88	0	0	13	0
4	L	90	0	0	4	0
All	All	36679	0	32872	739	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 11.

The worst 5 of 739 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:230:ASN:HD21	2:K:1:NAG:C1	1.24	1.49
1:E:365:TYR:CE2	1:E:368:ALA:HB2	1.56	1.39
1:E:365:TYR:CD2	1:E:368:ALA:HB2	1.76	1.19
1:E:365:TYR:CE2	1:E:368:ALA:CB	2.30	1.15
1:B:336:VAL:HG11	1:B:356:LEU:HD12	1.30	1.11

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	380/396 (96%)	370 (97%)	10 (3%)	0	100	100
1	B	375/396 (95%)	358 (96%)	17 (4%)	0	100	100
1	C	375/396 (95%)	359 (96%)	16 (4%)	0	100	100
1	D	376/396 (95%)	361 (96%)	15 (4%)	0	100	100
1	E	380/396 (96%)	362 (95%)	18 (5%)	0	100	100
1	F	373/396 (94%)	358 (96%)	15 (4%)	0	100	100
1	G	380/396 (96%)	367 (97%)	13 (3%)	0	100	100
1	H	376/396 (95%)	364 (97%)	12 (3%)	0	100	100
1	I	370/396 (93%)	352 (95%)	17 (5%)	1 (0%)	41	47
1	J	376/396 (95%)	361 (96%)	14 (4%)	1 (0%)	41	47
1	K	377/396 (95%)	351 (93%)	26 (7%)	0	100	100
1	L	377/396 (95%)	350 (93%)	27 (7%)	0	100	100
All	All	4515/4752 (95%)	4313 (96%)	200 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	305	TRP
1	J	182	PRO

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	315/324 (97%)	305 (97%)	10 (3%)	39	47
1	B	312/324 (96%)	292 (94%)	20 (6%)	17	18
1	C	312/324 (96%)	301 (96%)	11 (4%)	36	44
1	D	313/324 (97%)	298 (95%)	15 (5%)	25	30
1	E	315/324 (97%)	295 (94%)	20 (6%)	18	19
1	F	312/324 (96%)	296 (95%)	16 (5%)	24	27
1	G	315/324 (97%)	301 (96%)	14 (4%)	28	34
1	H	314/324 (97%)	293 (93%)	21 (7%)	16	17
1	I	311/324 (96%)	289 (93%)	22 (7%)	14	15
1	J	313/324 (97%)	295 (94%)	18 (6%)	20	22
1	K	315/324 (97%)	290 (92%)	25 (8%)	12	12
1	L	315/324 (97%)	284 (90%)	31 (10%)	8	7
All	All	3762/3888 (97%)	3539 (94%)	223 (6%)	19	22

5 of 223 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	336	VAL
1	L	461	THR
1	I	381	GLU
1	L	443	SER
1	L	223	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	230	ASN
1	L	311	ASN
1	L	326	GLN
1	F	230	ASN
1	A	183	GLN

5.3.3 RNA

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)

27 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	$\#\|Z\| > 2$
3	GOL	I	1478	-	5,5,5	0.29	0	5,5,5	0.63	0
3	GOL	A	1478	-	5,5,5	0.17	0	5,5,5	0.57	0
3	GOL	J	1478	-	5,5,5	0.36	0	5,5,5	0.69	0
3	GOL	C	1478	-	5,5,5	0.48	0	5,5,5	0.55	0
2	NAG	L	1	1	14,14,15	0.30	0	17,19,21	0.61	0
2	NAG	E	1	1	14,14,15	0.28	0	17,19,21	0.62	0
2	NAG	H	1	1	14,14,15	0.29	0	17,19,21	0.62	0
2	NAG	K	1	1	14,14,15	0.36	0	17,19,21	0.93	0
3	GOL	E	1479	-	5,5,5	0.27	0	5,5,5	0.30	0
3	GOL	B	1479	-	5,5,5	0.45	0	5,5,5	0.72	0
2	NAG	F	1	1	14,14,15	0.30	0	17,19,21	0.62	0
3	GOL	F	1478	-	5,5,5	0.22	0	5,5,5	0.61	0
3	GOL	G	1478	-	5,5,5	0.33	0	5,5,5	0.77	0
3	GOL	A	1479	-	5,5,5	0.72	0	5,5,5	0.45	0
2	NAG	G	1	1	14,14,15	0.29	0	17,19,21	0.62	0
3	GOL	B	1478	-	5,5,5	0.25	0	5,5,5	0.48	0
3	GOL	C	1479	-	5,5,5	0.64	0	5,5,5	0.48	0
3	GOL	L	1479	-	5,5,5	0.40	0	5,5,5	0.43	0
3	GOL	D	1479	-	5,5,5	0.62	0	5,5,5	0.59	0
3	GOL	L	1478	-	5,5,5	0.65	0	5,5,5	0.50	0
3	GOL	H	1478	-	5,5,5	0.21	0	5,5,5	0.60	0
3	GOL	E	1478	-	5,5,5	0.49	0	5,5,5	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	D	1478	-	5,5,5	0.14	0	5,5,5	0.63	0
3	GOL	A	1480	-	5,5,5	0.55	0	5,5,5	0.55	0
2	NAG	A	1	1	14,14,15	0.30	0	17,19,21	0.61	0
2	NAG	B	1	1	14,14,15	0.84	0	17,19,21	1.13	1 (5%)
2	NAG	C	1	1	14,14,15	0.75	0	17,19,21	1.20	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
3	GOL	I	1478	-	-	2/4/4/4	-
3	GOL	A	1478	-	-	0/4/4/4	-
3	GOL	J	1478	-	-	0/4/4/4	-
3	GOL	C	1478	-	-	2/4/4/4	-
2	NAG	L	1	1	-	5/6/23/26	0/1/1/1
2	NAG	E	1	1	-	5/6/23/26	0/1/1/1
2	NAG	H	1	1	-	4/6/23/26	0/1/1/1
2	NAG	K	1	1	-	6/6/23/26	0/1/1/1
3	GOL	E	1479	-	-	2/4/4/4	-
3	GOL	B	1479	-	-	2/4/4/4	-
2	NAG	F	1	1	-	4/6/23/26	0/1/1/1
3	GOL	F	1478	-	-	2/4/4/4	-
3	GOL	G	1478	-	-	2/4/4/4	-
3	GOL	A	1479	-	-	1/4/4/4	-
2	NAG	G	1	1	-	2/6/23/26	0/1/1/1
3	GOL	B	1478	-	-	3/4/4/4	-
3	GOL	C	1479	-	-	1/4/4/4	-
3	GOL	L	1479	-	-	4/4/4/4	-
3	GOL	D	1479	-	-	2/4/4/4	-
3	GOL	L	1478	-	-	4/4/4/4	-
3	GOL	H	1478	-	-	4/4/4/4	-
3	GOL	E	1478	-	-	4/4/4/4	-
3	GOL	D	1478	-	-	2/4/4/4	-
3	GOL	A	1480	-	-	1/4/4/4	-
2	NAG	A	1	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	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})
2	B	1	NAG	C1-O5-C5	2.10	115.04	112.19

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NAG	C8-C7-N2-C2
2	A	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2

There are no ring outliers.

15 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1478	GOL	1	0
3	J	1478	GOL	2	0
3	C	1478	GOL	3	0
2	L	1	NAG	2	0
2	E	1	NAG	2	0
2	K	1	NAG	5	0
3	B	1479	GOL	3	0
2	F	1	NAG	2	0
3	F	1478	GOL	3	0
3	G	1478	GOL	1	0
3	H	1478	GOL	3	0
3	E	1478	GOL	3	0
3	D	1478	GOL	2	0
3	A	1480	GOL	2	0
2	A	1	NAG	2	0

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	382/396 (96%)	0.35	16 (4%)	36	48	17, 32, 68, 130	0
1	B	379/396 (95%)	0.33	7 (1%)	68	77	14, 32, 66, 91	0
1	C	379/396 (95%)	0.36	7 (1%)	68	77	17, 32, 65, 95	0
1	D	380/396 (95%)	0.40	9 (2%)	59	68	17, 31, 64, 101	0
1	E	382/396 (96%)	0.44	14 (3%)	41	54	16, 32, 63, 105	0
1	F	377/396 (95%)	0.21	3 (0%)	86	91	19, 33, 66, 106	0
1	G	382/396 (96%)	0.40	13 (3%)	45	57	18, 33, 71, 93	0
1	H	380/396 (95%)	0.32	9 (2%)	59	68	20, 34, 66, 99	0
1	I	375/396 (94%)	0.46	22 (5%)	22	33	20, 42, 74, 108	0
1	J	379/396 (95%)	0.56	32 (8%)	11	16	24, 44, 78, 104	0
1	K	380/396 (95%)	0.58	23 (6%)	21	31	26, 45, 83, 111	0
1	L	380/396 (95%)	0.59	26 (6%)	17	25	26, 45, 84, 116	0
All	All	4555/4752 (95%)	0.42	181 (3%)	38	51	14, 37, 74, 130	0

The worst 5 of 181 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	365	TYR	9.7
1	L	365	TYR	8.9
1	E	366	PRO	8.8
1	H	365	TYR	8.2
1	G	366	PRO	7.5

6.2 Non-standard residues in protein, DNA, RNA chains

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
2	NAG	F	1	14/15	0.39	0.33	83,113,122,127	0
2	NAG	L	1	14/15	0.58	0.29	91,116,127,128	0
2	NAG	H	1	14/15	0.65	0.26	100,133,144,145	0
2	NAG	C	1	14/15	0.65	0.23	87,120,133,134	0
3	GOL	L	1478	6/6	0.73	0.28	44,49,55,58	0
2	NAG	K	1	14/15	0.74	0.28	107,121,129,129	0
2	NAG	E	1	14/15	0.75	0.26	69,87,96,103	0
2	NAG	G	1	14/15	0.76	0.34	109,125,136,141	0
2	NAG	A	1	14/15	0.79	0.38	86,125,134,136	0
2	NAG	B	1	14/15	0.79	0.15	61,95,102,102	0
3	GOL	C	1479	6/6	0.84	0.24	31,45,48,66	0
3	GOL	A	1479	6/6	0.86	0.19	39,49,57,62	0
3	GOL	E	1478	6/6	0.87	0.23	42,48,58,60	0
3	GOL	B	1479	6/6	0.89	0.14	44,47,49,55	0
3	GOL	A	1480	6/6	0.90	0.18	31,40,46,46	0
3	GOL	D	1479	6/6	0.92	0.19	43,47,50,50	0
3	GOL	C	1478	6/6	0.94	0.19	35,40,47,49	0
3	GOL	B	1478	6/6	0.94	0.18	40,43,46,46	0
3	GOL	D	1478	6/6	0.94	0.20	35,38,39,51	0
3	GOL	L	1479	6/6	0.94	0.16	44,53,54,67	0
3	GOL	J	1478	6/6	0.95	0.13	37,39,41,42	0
3	GOL	G	1478	6/6	0.95	0.21	29,31,32,36	0
3	GOL	I	1478	6/6	0.95	0.16	41,43,45,45	0
3	GOL	F	1478	6/6	0.96	0.21	37,41,44,45	0
3	GOL	H	1478	6/6	0.96	0.18	31,35,41,42	0
3	GOL	E	1479	6/6	0.97	0.16	35,43,50,50	0
3	GOL	A	1478	6/6	0.98	0.16	26,28,28,29	0

6.5 Other polymers (i)

There are no such residues in this entry.