



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:39 am 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

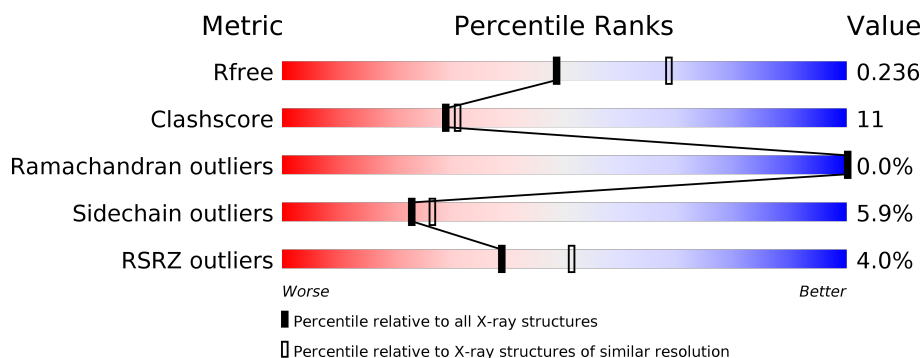
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	396	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• •</div> </div> </div>
1	B	396	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• •</div> </div> </div>
1	C	396	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>• •</div> </div> </div>
1	D	396	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>
1	E	396	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• •</div> </div> </div>
1	F	396	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• 5%</div> </div> </div>

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	F	1	X	-	-	-
3	GOL	C	1479	-	-	-	X
3	GOL	D	1478	-	-	-	X
3	GOL	F	1478	-	-	-	X
3	GOL	G	1478	-	-	-	X
3	GOL	L	1478	-	-	-	X

## 2 Entry composition

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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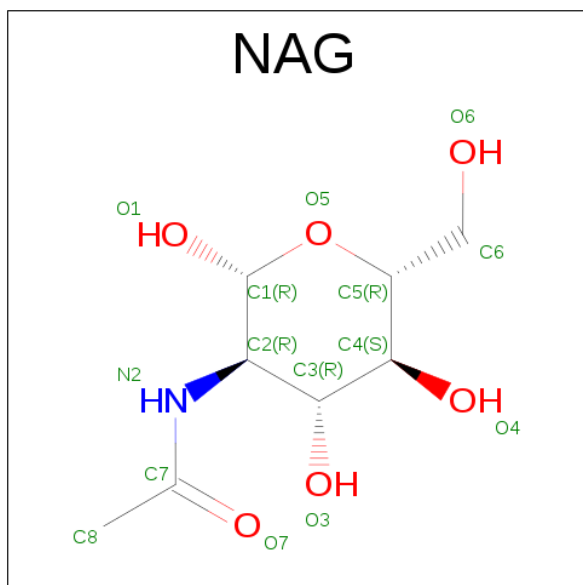
Chain	Residue	Modelled	Actual	Comment	Reference
H	481	ALA	-	EXPRESSION TAG	UNP B6K9M7
H	482	ALA	-	EXPRESSION TAG	UNP B6K9M7
H	483	ALA	-	EXPRESSION TAG	UNP B6K9M7
H	484	LEU	-	EXPRESSION TAG	UNP B6K9M7
H	485	VAL	-	EXPRESSION TAG	UNP B6K9M7
H	486	PRO	-	EXPRESSION TAG	UNP B6K9M7
H	487	ARG	-	EXPRESSION TAG	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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



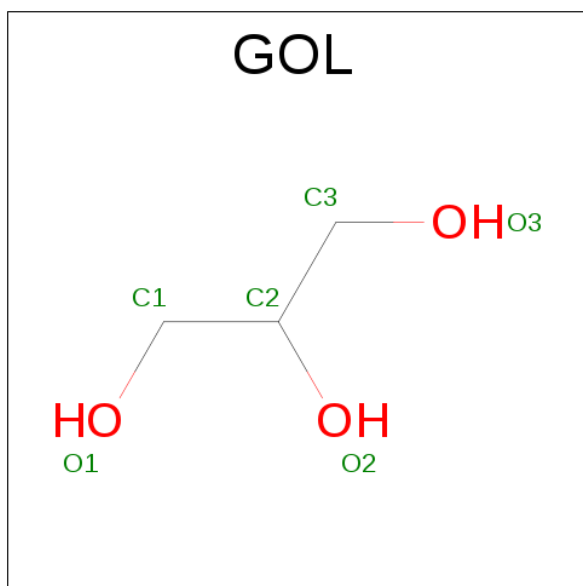
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		

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

- 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	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

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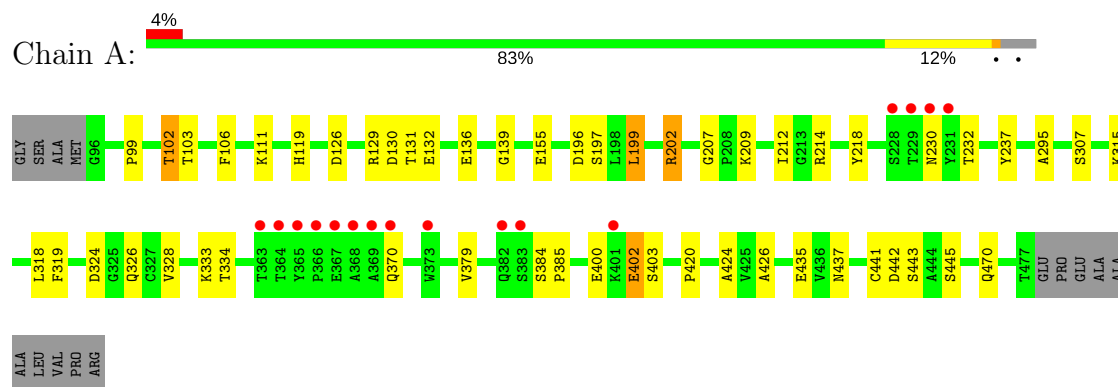
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	164	Total 164	O 164	0	0
4	I	91	Total 91	O 91	0	0
4	J	58	Total 58	O 58	0	0
4	K	88	Total 88	O 88	0	0
4	L	90	Total 90	O 90	0	0

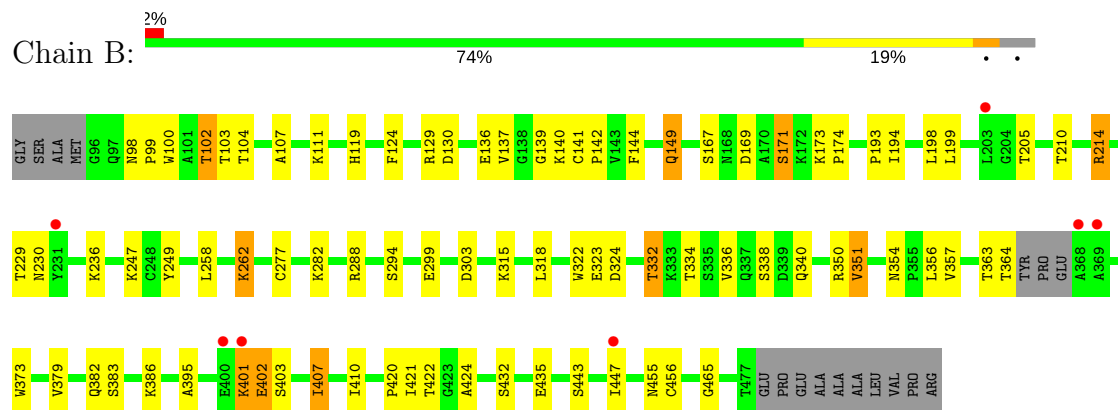
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

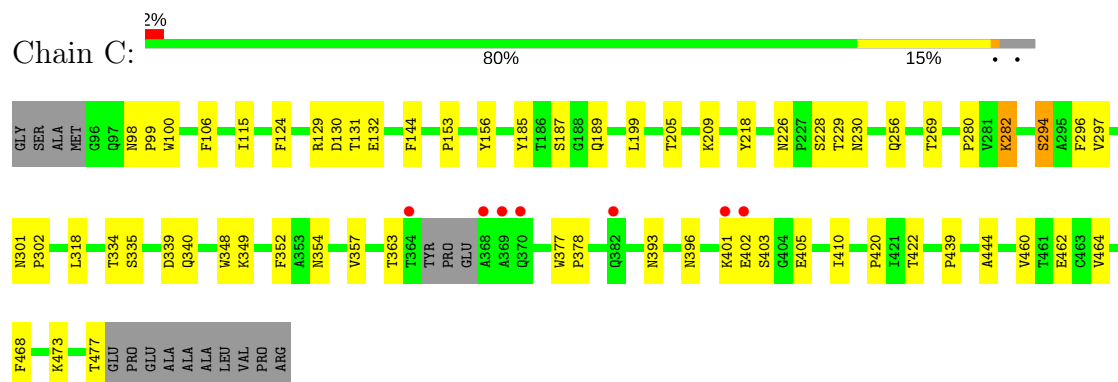
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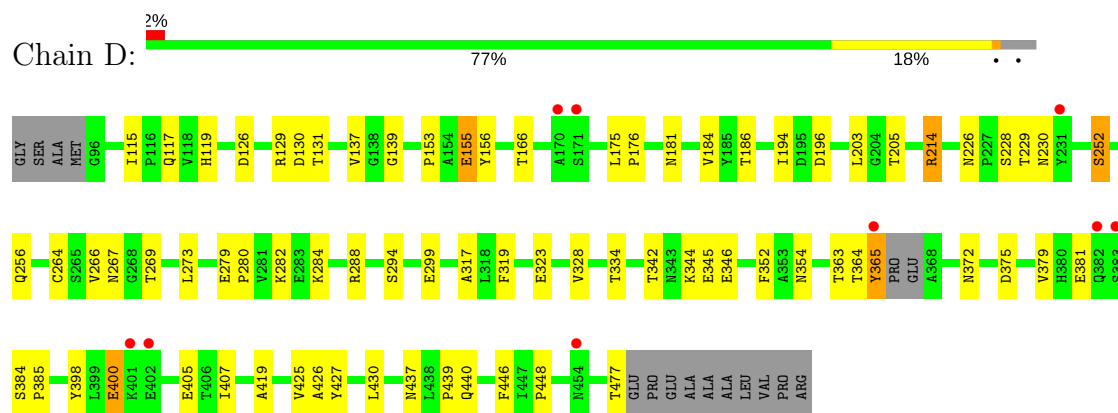
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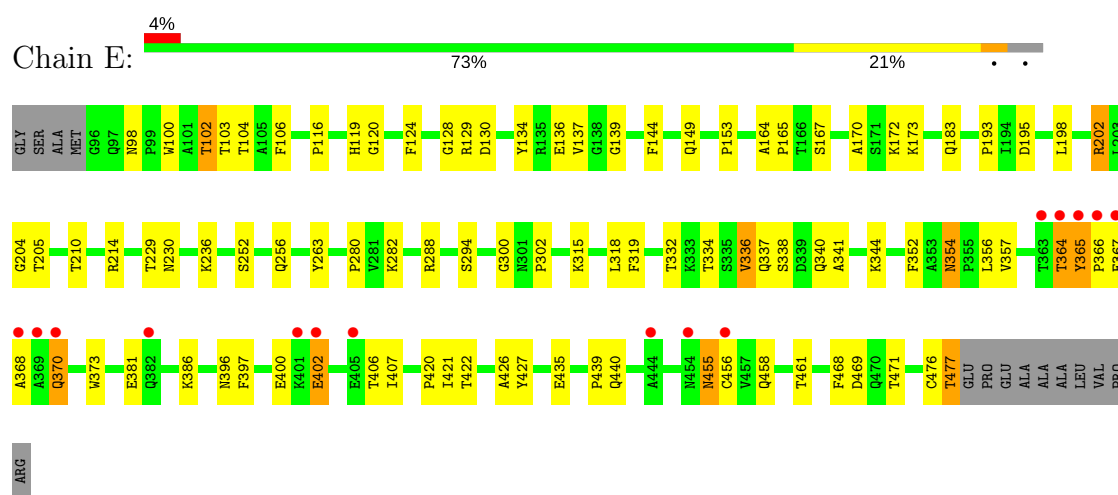
#### • Molecule 1: APICAL MEMBRANE ANTIGEN 1



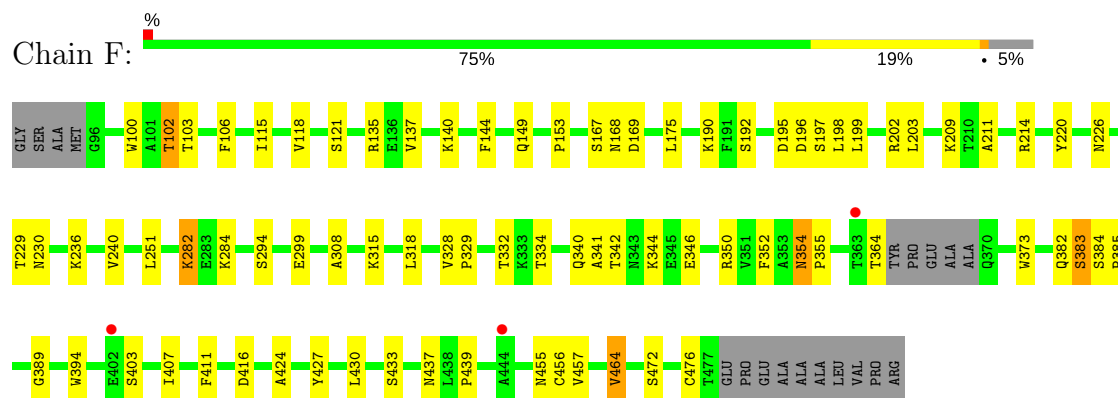
- Molecule 1: APICAL MEMBRANE ANTIGEN 1



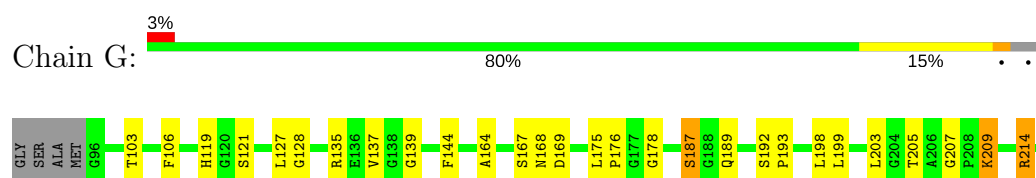
- Molecule 1: APICAL MEMBRANE ANTIGEN 1

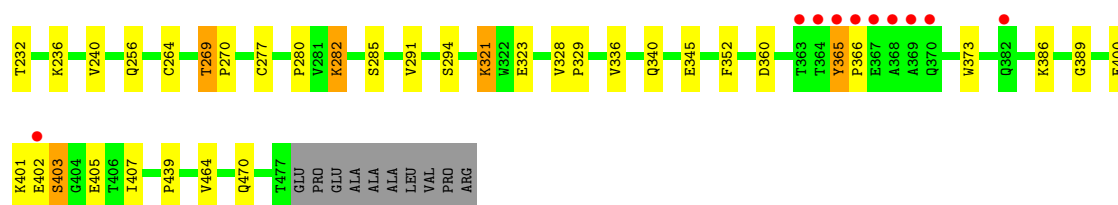


- Molecule 1: APICAL MEMBRANE ANTIGEN 1

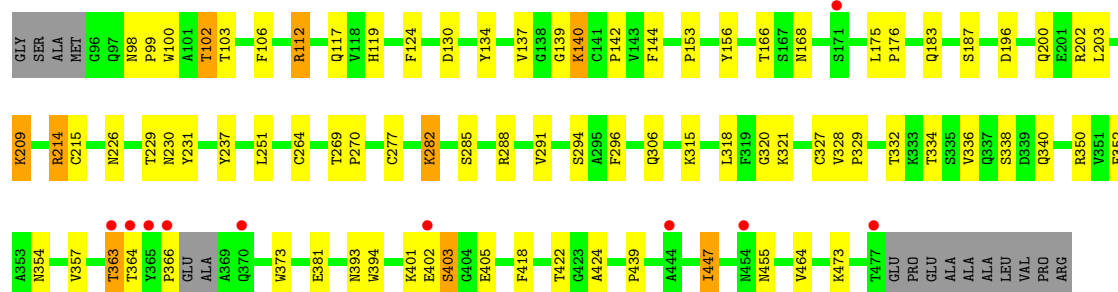
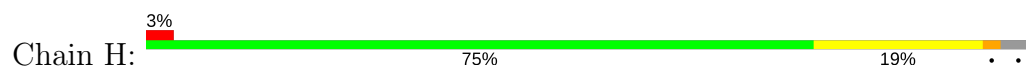


- Molecule 1: APICAL MEMBRANE ANTIGEN 1

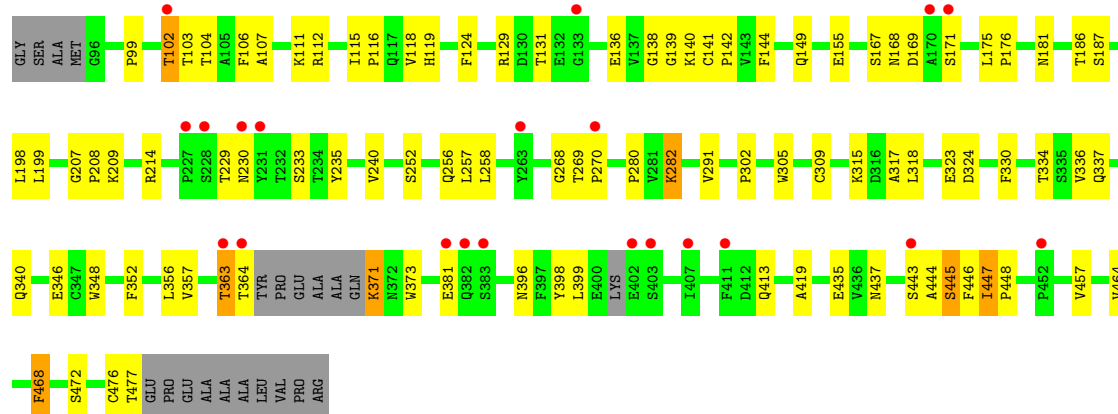




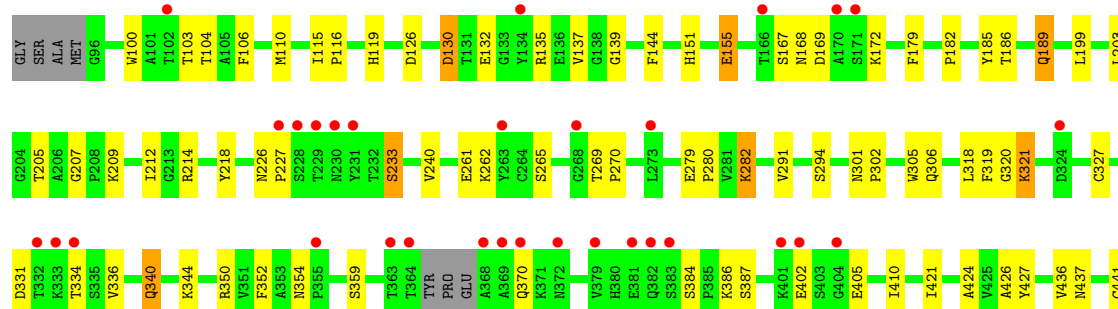
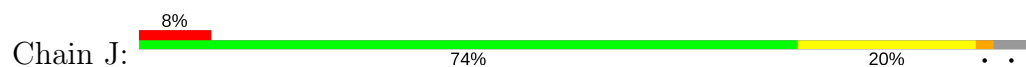
• Molecule 1: APICAL MEMBRANE ANTIGEN 1

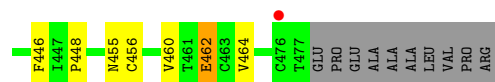


• Molecule 1: APICAL MEMBRANE ANTIGEN 1

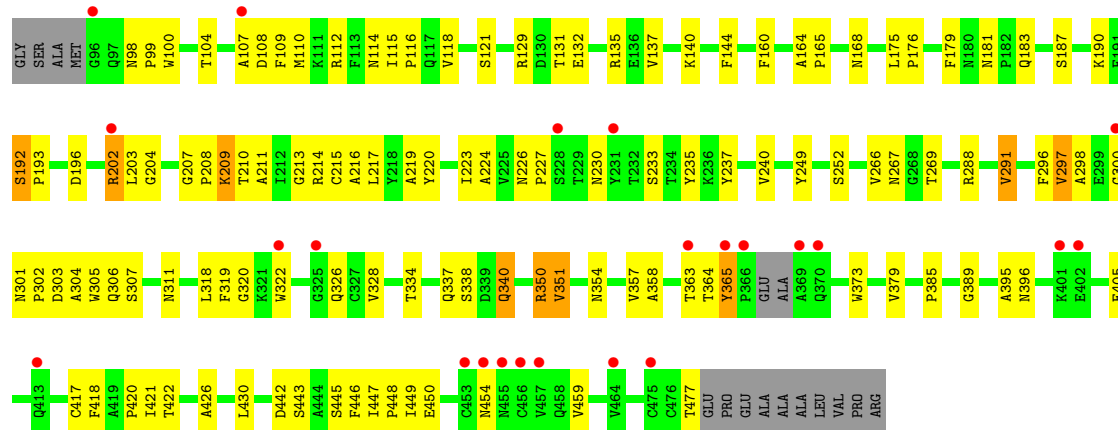


• Molecule 1: APICAL MEMBRANE ANTIGEN 1

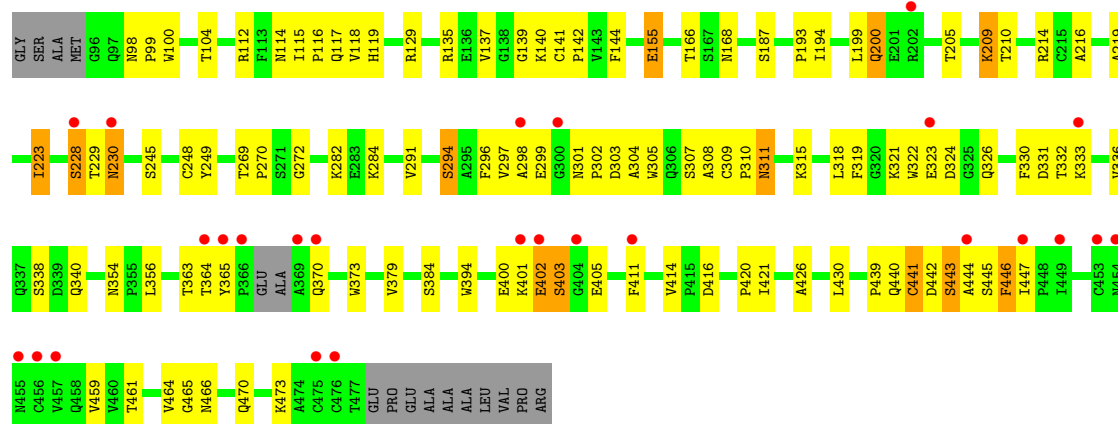




• Molecule 1: APICAL MEMBRANE ANTIGEN 1



• Molecule 1: APICAL MEMBRANE ANTIGEN 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	20500 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.0	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.72	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

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	D	214	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	G	214	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	D	288	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	E	288	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	H	214	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	B	350	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	214	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	214	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	K	288	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	E	365	TYR	N-CA-C	-5.12	97.18	111.00

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:B:247:LYS:NZ	3:B:1479:GOL:H11	1.65	1.10
1:B:144:PHE:O	1:B:282:LYS:HE2	1.49	1.10
1:B:247:LYS:HZ3	3:B:1479:GOL:H11	1.18	1.05
1:K:209:LYS:HE3	1:K:209:LYS:CA	1.80	1.05
1:K:209:LYS:HE3	1:K:209:LYS:HA	1.08	1.04
1:B:351:VAL:CG1	1:B:395:ALA:HB2	1.88	1.02
1:K:209:LYS:N	1:K:303:ASP:OD2	1.91	1.01
1:K:209:LYS:HA	1:K:209:LYS:CE	1.94	0.97
1:B:336:VAL:CG1	1:B:356:LEU:HD12	1.95	0.97
1:B:401:LYS:CD	1:B:401:LYS:H	1.66	0.97
1:A:230:ASN:ND2	2:A:1:NAG:O5	1.98	0.96
1:B:149:GLN:NE2	4:B:2038:HOH:O	1.99	0.95
1:L:229:THR:O	1:L:230:ASN:HB2	1.67	0.95
1:E:365:TYR:HE2	1:E:368:ALA:CB	1.77	0.94
1:L:209:LYS:O	1:L:214:ARG:NH2	1.98	0.94
1:D:400:GLU:HG3	1:D:407:ILE:HG13	1.47	0.93
1:H:403:SER:HB3	1:H:405:GLU:HG2	1.51	0.92
1:I:444:ALA:O	1:I:445:SER:HB3	1.65	0.91
1:E:300:GLY:HA2	1:K:301:ASN:HB2	1.51	0.91
1:L:209:LYS:N	1:L:303:ASP:OD2	2.04	0.90
1:F:230:ASN:HD21	2:F:1:NAG:C1	1.57	0.89
1:L:99:PRO:HD2	1:L:322:TRP:CH2	2.07	0.89
1:F:230:ASN:HD22	2:F:1:NAG:C1	1.60	0.89
1:H:137:VAL:HG12	1:H:294:SER:HB3	1.53	0.88
1:B:351:VAL:HG13	1:B:395:ALA:HB2	1.56	0.88
1:H:229:THR:O	1:H:230:ASN:HB2	1.71	0.87
1:E:183:GLN:OE1	4:E:2051:HOH:O	1.92	0.86
1:L:301:ASN:HB3	1:L:304:ALA:HB2	1.56	0.85
1:K:209:LYS:O	1:K:214:ARG:NH2	2.12	0.83
1:I:129[A]:ARG:NH1	1:I:138:GLY:O	2.12	0.83
1:K:129:ARG:NH1	1:K:296:PHE:CZ	2.48	0.82
1:L:441:CYS:SG	1:L:442:ASP:N	2.52	0.81
1:K:204:GLY:C	1:K:207:GLY:H	1.83	0.81
1:D:175:LEU:HD12	1:D:176:PRO:HD2	1.61	0.81
1:K:129:ARG:NH1	1:K:296:PHE:CE2	2.51	0.79
1:E:318:LEU:HD22	1:E:396:ASN:HB3	1.64	0.79
1:B:401:LYS:HD2	1:B:401:LYS:H	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:PHE:O	1:F:282:LYS:HE2	1.81	0.79
1:L:99:PRO:HD2	1:L:322:TRP:CZ3	2.17	0.79
1:L:301:ASN:OD1	4:L:2067:HOH:O	2.00	0.78
1:F:149:GLN:NE2	4:F:2037:HOH:O	2.05	0.78
1:I:144:PHE:O	1:I:282:LYS:HE2	1.84	0.78
1:B:102:THR:HG22	1:B:103:THR:OG1	1.83	0.78
1:B:443:SER:OG	1:B:465:GLY:O	2.02	0.78
1:E:458:GLN:OE1	4:E:2174:HOH:O	2.02	0.78
1:A:111:LYS:HE3	4:A:2015:HOH:O	1.82	0.78
1:D:344:LYS:HB2	1:D:427:TYR:OH	1.84	0.78
1:B:351:VAL:HG11	1:B:395:ALA:HB2	1.65	0.77
1:L:199:LEU:HD23	1:L:214:ARG:HG2	1.67	0.77
1:H:214:ARG:NH2	1:I:209:LYS:O	2.17	0.77
4:E:2061:HOH:O	1:G:209:LYS:HD3	1.83	0.77
1:J:344:LYS:HB2	1:J:427:TYR:OH	1.85	0.77
1:J:130:ASP:O	4:J:2004:HOH:O	2.03	0.76
1:B:420:PRO:C	1:B:421:ILE:HD13	2.06	0.76
1:E:420:PRO:O	1:E:421:ILE:HD13	1.84	0.76
1:L:363:THR:HG22	1:L:363:THR:O	1.83	0.76
1:F:199:LEU:O	1:F:203:LEU:HB2	1.86	0.76
1:E:336:VAL:HG21	1:E:356:LEU:HD23	1.68	0.76
1:H:364:THR:HG23	1:H:366:PRO:HD3	1.67	0.76
1:K:220:TYR:CD1	1:K:220:TYR:O	2.39	0.76
1:H:140:LYS:NZ	4:H:2036:HOH:O	2.18	0.75
1:K:203:LEU:HD23	1:K:208:PRO:HD3	1.68	0.75
1:E:300:GLY:CA	1:K:301:ASN:HB2	2.16	0.75
1:J:436:VAL:CG1	3:J:1478:GOL:O1	2.33	0.75
1:D:400:GLU:HG3	1:D:407:ILE:CG1	2.14	0.75
1:L:200:GLN:OE1	1:L:214:ARG:NH1	2.19	0.75
1:H:403:SER:HB3	1:H:405:GLU:CG	2.16	0.74
1:K:110:MET:HE1	1:K:418:PHE:CD2	2.22	0.74
1:B:401:LYS:HD2	1:B:401:LYS:N	2.01	0.74
1:E:400:GLU:OE2	4:E:2160:HOH:O	2.05	0.74
1:L:363:THR:O	1:L:363:THR:CG2	2.36	0.73
1:A:209:LYS:NZ	4:A:2075:HOH:O	2.21	0.73
1:E:137:VAL:HG12	1:E:294:SER:HB3	1.70	0.73
1:K:109:PHE:O	1:K:112:ARG:HB2	1.89	0.73
1:G:144:PHE:O	1:G:282:LYS:HE2	1.89	0.73
1:K:211:ALA:O	4:K:2033:HOH:O	2.05	0.73
1:E:144:PHE:O	1:E:282:LYS:HE2	1.89	0.73
1:F:137:VAL:HG12	1:F:294:SER:HB3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:175:LEU:HD12	1:K:176:PRO:HD2	1.71	0.72
1:L:194:ILE:HG23	1:L:199:LEU:HD13	1.71	0.72
1:F:209:LYS:HE2	1:J:209:LYS:HE2	1.70	0.72
1:E:332:THR:HG22	1:E:338:SER:OG	1.90	0.72
1:L:228:SER:O	2:L:1:NAG:O7	2.05	0.72
1:G:470:GLN:OE1	4:G:2114:HOH:O	2.08	0.72
1:L:311:ASN:H	1:L:311:ASN:ND2	1.86	0.72
1:K:204:GLY:O	1:K:207:GLY:N	2.21	0.71
1:L:245:SER:O	4:L:2044:HOH:O	2.06	0.71
2:E:1:NAG:H61	4:E:2005:HOH:O	1.89	0.71
1:B:401:LYS:CD	1:B:401:LYS:N	2.43	0.71
1:I:437:ASN:O	3:I:1478:GOL:H11	1.89	0.71
1:K:140:LYS:O	1:K:297:VAL:HG22	1.90	0.71
1:G:340:GLN:HG3	1:G:405:GLU:OE2	1.91	0.71
1:B:364:THR:HG22	1:B:364:THR:O	1.90	0.70
1:J:269:THR:HA	1:J:270:PRO:C	2.12	0.70
1:C:185:TYR:O	1:C:187:SER:O	2.09	0.70
1:F:209:LYS:CE	1:J:209:LYS:HE2	2.21	0.70
1:H:447:ILE:HG22	1:H:447:ILE:O	1.92	0.70
1:B:447:ILE:HG22	4:B:2168:HOH:O	1.91	0.70
1:B:336:VAL:HG11	1:B:356:LEU:CD1	2.17	0.70
1:G:187:SER:OG	1:G:189:GLN:HG2	1.91	0.70
1:B:332:THR:HG22	1:B:338:SER:OG	1.91	0.70
1:K:477:THR:O	4:K:2088:HOH:O	2.09	0.70
1:H:318:LEU:HD21	1:H:424:ALA:HB1	1.73	0.70
1:L:464:VAL:HG23	1:L:464:VAL:O	1.92	0.70
1:B:247:LYS:HZ2	3:B:1479:GOL:H11	1.54	0.69
1:F:382:GLN:O	1:F:383:SER:CB	2.40	0.69
1:K:203:LEU:HD21	1:K:217:LEU:HD23	1.75	0.69
1:L:403:SER:HB2	1:L:405:GLU:H	1.56	0.69
1:E:455:ASN:O	1:E:456:CYS:HB2	1.92	0.69
1:K:121:SER:O	1:K:389:GLY:HA2	1.92	0.69
1:L:440:GLN:HG3	1:L:466:ASN:O	1.92	0.69
1:H:229:THR:O	1:H:230:ASN:CB	2.41	0.69
1:K:209:LYS:H	1:K:303:ASP:CG	1.94	0.69
1:K:110:MET:HE1	1:K:418:PHE:HD2	1.56	0.69
1:L:336:VAL:HG21	1:L:356:LEU:HD12	1.74	0.68
1:D:226:ASN:HB3	1:D:229:THR:O	1.93	0.68
1:K:115:ILE:HG12	1:K:430:LEU:HD12	1.74	0.68
1:D:203:LEU:HD12	1:D:214:ARG:HG2	1.74	0.68
1:K:175:LEU:HD12	1:K:176:PRO:CD	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:229:THR:O	1:L:230:ASN:CB	2.39	0.68
1:B:420:PRO:O	1:B:421:ILE:HD13	1.93	0.68
1:H:144:PHE:O	1:H:282:LYS:HE2	1.93	0.68
1:C:189:GLN:HB2	4:C:2049:HOH:O	1.93	0.68
1:I:155:GLU:OE2	4:I:2020:HOH:O	2.10	0.68
1:A:400:GLU:OE1	4:A:2171:HOH:O	2.12	0.67
1:E:364:THR:CB	1:E:366:PRO:HD3	2.25	0.67
1:C:256:GLN:O	1:C:280:PRO:HD3	1.94	0.67
1:H:140:LYS:HE2	1:H:296:PHE:O	1.94	0.67
1:D:117:GLN:OE1	1:H:117:GLN:NE2	2.16	0.67
1:L:140:LYS:O	1:L:297:VAL:HG22	1.95	0.67
1:F:196:ASP:OD1	1:F:214:ARG:NH1	2.27	0.67
1:H:403:SER:HB3	1:H:405:GLU:H	1.60	0.67
1:E:365:TYR:HE2	1:E:368:ALA:HB1	1.56	0.66
1:K:100:TRP:CD1	1:K:417:CYS:HB2	2.31	0.66
1:K:318:LEU:HD22	1:K:396:ASN:HB3	1.77	0.66
1:F:153:PRO:HD3	4:F:2039:HOH:O	1.96	0.66
1:H:439:PRO:HA	3:H:1478:GOL:H12	1.78	0.66
1:E:336:VAL:HG21	1:E:356:LEU:CD2	2.26	0.66
1:F:195:ASP:OD1	4:F:2055:HOH:O	2.12	0.66
1:H:203:LEU:HD12	1:H:214:ARG:HG2	1.76	0.66
1:F:102:THR:HG22	1:F:103:THR:N	2.11	0.65
1:J:203:LEU:HD12	1:J:214:ARG:HG2	1.79	0.65
1:A:196:ASP:OD2	1:A:214:ARG:NH1	2.30	0.65
1:L:336:VAL:HG21	1:L:356:LEU:CD1	2.26	0.65
1:B:401:LYS:HD3	1:B:401:LYS:H	1.55	0.65
1:E:229:THR:O	1:E:230:ASN:HB2	1.97	0.64
1:D:328:VAL:HG23	1:D:328:VAL:O	1.97	0.64
1:E:364:THR:HB	1:E:366:PRO:HD3	1.79	0.64
1:J:185:TYR:HD2	1:J:189:GLN:HG2	1.62	0.64
1:L:446:PHE:C	1:L:446:PHE:CD1	2.71	0.64
1:L:194:ILE:CG2	1:L:199:LEU:HD13	2.28	0.64
1:A:131:THR:HG22	1:A:132:GLU:HG3	1.79	0.63
1:C:209:LYS:O	1:D:214:ARG:NH2	2.31	0.63
1:D:439:PRO:HA	3:D:1478:GOL:H12	1.80	0.63
1:K:420:PRO:O	1:K:421:ILE:HD13	1.99	0.63
1:J:137:VAL:HG12	1:J:294:SER:HB3	1.80	0.63
1:G:175:LEU:HD12	1:G:176:PRO:HD2	1.80	0.63
1:G:137:VAL:HG12	1:G:294:SER:HB3	1.81	0.63
1:I:363:THR:O	1:I:364:THR:OG1	2.15	0.63
1:L:440:GLN:CG	1:L:466:ASN:O	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:115:ILE:HG12	1:L:430:LEU:HD12	1.82	0.62
1:H:447:ILE:CG2	1:H:447:ILE:O	2.47	0.62
1:E:195:ASP:H	3:E:1478:GOL:C3	2.11	0.62
1:L:444:ALA:O	1:L:445:SER:CB	2.46	0.62
1:K:337:GLN:NE2	4:K:2073:HOH:O	2.33	0.62
1:L:402:GLU:HG3	1:L:403:SER:N	2.14	0.62
1:F:209:LYS:O	1:J:214:ARG:NH2	2.32	0.62
1:E:365:TYR:CD2	1:E:368:ALA:CB	2.67	0.61
1:F:382:GLN:O	1:F:383:SER:HB3	2.00	0.61
1:L:332:THR:HG22	1:L:338:SER:OG	2.00	0.61
1:A:196:ASP:OD1	1:A:214:ARG:NH1	2.33	0.61
1:E:300:GLY:O	1:E:302:PRO:HD3	2.00	0.61
1:G:464:VAL:HG23	1:G:464:VAL:O	1.99	0.61
1:H:153:PRO:HG2	1:H:156:TYR:CE1	2.35	0.61
1:I:268:GLY:O	4:I:2050:HOH:O	2.16	0.61
1:K:202[A]:ARG:NH1	4:K:2037:HOH:O	2.33	0.61
1:A:103:THR:HB	1:A:106:PHE:CD2	2.35	0.61
1:A:319:PHE:CE2	1:A:426:ALA:HB1	2.35	0.61
1:K:110:MET:HA	1:K:110:MET:HE2	1.82	0.61
1:A:103:THR:HG22	1:A:106:PHE:H	1.66	0.61
1:J:119:HIS:CE1	1:J:139:GLY:HA3	2.35	0.61
1:J:318:LEU:HD21	1:J:424:ALA:HB1	1.83	0.60
1:K:115:ILE:HG12	1:K:430:LEU:CD1	2.31	0.60
1:C:363:THR:O	1:C:363:THR:HG22	2.00	0.60
1:K:447:ILE:HD12	1:K:447:ILE:N	2.16	0.60
1:E:119:HIS:CE1	1:E:139:GLY:HA3	2.36	0.60
1:L:99:PRO:CD	1:L:322:TRP:CH2	2.84	0.60
1:I:330:PHE:HE2	1:I:413:GLN:OE1	1.85	0.60
1:K:144:PHE:CE1	1:K:311:ASN:HB3	2.36	0.60
1:I:140:LYS:HD2	4:I:2062:HOH:O	2.02	0.60
1:J:436:VAL:HG11	3:J:1478:GOL:O1	2.00	0.60
1:G:403:SER:HB2	1:G:405:GLU:HB2	1.84	0.59
1:E:172:LYS:O	1:E:173:LYS:HD3	2.02	0.59
1:E:300:GLY:HA2	1:K:301:ASN:CB	2.29	0.59
1:D:323:GLU:OE2	1:D:328:VAL:HG21	2.03	0.59
1:K:213:GLY:CA	1:K:302:PRO:HB2	2.33	0.59
1:K:132:GLU:OE1	1:K:233:SER:HB2	2.02	0.59
1:K:190:LYS:HE3	1:K:192:SER:O	2.01	0.59
1:D:328:VAL:O	1:D:328:VAL:CG2	2.51	0.59
1:I:99:PRO:HA	1:I:102:THR:HB	1.85	0.59
1:I:107:ALA:O	1:I:111:LYS:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:311:ASN:H	1:L:311:ASN:HD22	1.49	0.59
1:C:144:PHE:O	1:C:282:LYS:HE2	2.03	0.59
1:K:129:ARG:HD2	4:K:2006:HOH:O	2.02	0.58
1:L:303:ASP:HB2	4:L:2067:HOH:O	2.01	0.58
1:H:209:LYS:O	1:I:214:ARG:NH2	2.35	0.58
1:B:169:ASP:OD1	1:B:171:SER:HB3	2.03	0.58
1:I:118:VAL:HG12	1:I:141:CYS:SG	2.44	0.58
1:K:304:ALA:HB2	4:K:2035:HOH:O	2.03	0.58
1:A:119:HIS:CE1	1:A:139:GLY:HA3	2.38	0.58
1:D:119:HIS:CE1	1:D:139:GLY:HA3	2.39	0.58
1:G:175:LEU:HD12	1:G:176:PRO:CD	2.34	0.58
1:L:440:GLN:HG2	1:L:466:ASN:HB3	1.84	0.58
1:A:403:SER:OG	4:A:2171:HOH:O	1.95	0.58
1:B:455:ASN:O	1:B:455:ASN:CG	2.41	0.58
1:J:240:VAL:HA	1:J:291:VAL:O	2.04	0.58
1:K:137:VAL:HG23	4:K:2010:HOH:O	2.03	0.58
1:C:340:GLN:HG3	1:C:405:GLU:CD	2.24	0.58
3:F:1478:GOL:H11	4:F:2129:HOH:O	2.03	0.58
1:H:112:ARG:NH2	1:H:306:GLN:O	2.35	0.58
1:E:98:ASN:O	1:E:102:THR:HB	2.04	0.58
1:H:137:VAL:HG12	1:H:294:SER:CB	2.29	0.58
1:L:336:VAL:CG2	1:L:356:LEU:HD12	2.34	0.58
1:G:168:ASN:OD1	1:G:169:ASP:N	2.37	0.57
1:G:229:THR:O	1:G:230:ASN:HB2	2.04	0.57
1:L:144:PHE:CE1	1:L:311:ASN:HB3	2.39	0.57
1:K:351:VAL:HG13	1:K:395:ALA:HB2	1.85	0.57
1:B:351:VAL:HG11	1:B:395:ALA:CB	2.33	0.57
1:D:400:GLU:CG	1:D:407:ILE:HG13	2.28	0.57
1:D:477:THR:O	1:D:477:THR:HG22	2.04	0.57
1:K:240:VAL:HA	1:K:291:VAL:O	2.04	0.57
1:F:350:ARG:HD3	4:F:2113:HOH:O	2.04	0.57
1:E:193:PRO:HG2	3:E:1478:GOL:H12	1.87	0.57
1:G:282:LYS:HD3	1:G:352:PHE:CG	2.40	0.56
1:H:175:LEU:HD12	1:H:176:PRO:HD2	1.87	0.56
1:L:135:ARG:CZ	1:L:384:SER:HB3	2.35	0.56
1:D:437:ASN:O	3:D:1478:GOL:H32	2.05	0.56
1:E:400:GLU:HG2	1:E:402:GLU:HB2	1.86	0.56
1:H:196:ASP:O	1:H:200:GLN:HG3	2.05	0.56
1:K:209:LYS:C	1:K:214:ARG:HH21	2.09	0.56
1:J:106:PHE:HZ	1:J:441:CYS:HB3	1.70	0.56
1:C:439:PRO:HA	3:C:1478:GOL:H12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:ILE:HD13	1:F:430:LEU:HD12	1.88	0.56
1:L:210:THR:C	1:L:214:ARG:NH2	2.59	0.56
1:L:323:GLU:O	1:L:324:ASP:HB2	2.06	0.56
1:H:403:SER:CB	1:H:405:GLU:HG2	2.28	0.56
1:A:400:GLU:HG2	1:A:402:GLU:HG3	1.88	0.55
1:A:230:ASN:HD21	2:A:1:NAG:C1	2.03	0.55
1:A:334:THR:OG1	4:A:2144:HOH:O	2.02	0.55
1:B:99:PRO:HA	1:B:102:THR:HB	1.87	0.55
1:F:282:LYS:HD3	1:F:352:PHE:CG	2.42	0.55
1:J:168:ASN:OD1	1:J:169:ASP:N	2.39	0.55
1:E:256:GLN:O	1:E:280:PRO:HD3	2.06	0.55
1:G:256:GLN:O	1:G:280:PRO:HD3	2.06	0.55
1:K:99:PRO:HD2	1:K:322:TRP:CH2	2.42	0.55
1:D:319:PHE:CE2	1:D:426:ALA:HB1	2.42	0.55
3:H:1478:GOL:H11	4:H:2155:HOH:O	2.06	0.54
1:E:364:THR:C	1:E:366:PRO:HD3	2.27	0.54
1:K:121:SER:O	1:K:389:GLY:CA	2.54	0.54
1:L:194:ILE:HG21	1:L:199:LEU:CD1	2.37	0.54
1:K:213:GLY:HA3	1:K:302:PRO:HB2	1.88	0.54
1:C:460:VAL:HG12	1:C:462:GLU:HG3	1.89	0.54
1:J:436:VAL:HG12	1:J:437:ASN:O	2.07	0.54
1:G:103:THR:HB	1:G:106:PHE:CD2	2.43	0.54
3:H:1478:GOL:C1	4:H:2155:HOH:O	2.55	0.54
1:D:342:THR:HB	1:D:346:GLU:OE1	2.07	0.54
1:I:175:LEU:HD12	1:I:176:PRO:CD	2.38	0.54
1:K:208:PRO:HB3	1:K:302:PRO:HG2	1.88	0.54
1:K:445:SER:O	1:K:447:ILE:HD12	2.07	0.54
1:D:372:ASN:N	1:D:375:ASP:OD2	2.38	0.54
1:D:282:LYS:HE3	1:D:352:PHE:CD1	2.42	0.54
1:H:209:LYS:HE3	1:I:209:LYS:HE2	1.90	0.54
1:J:132:GLU:OE1	1:J:233:SER:HB2	2.08	0.54
1:F:341:ALA:HA	1:F:346:GLU:OE2	2.08	0.53
1:I:229:THR:O	1:I:230:ASN:HB2	2.08	0.53
1:B:447:ILE:O	1:B:447:ILE:HG23	2.09	0.53
1:F:202:ARG:HG2	1:F:202:ARG:O	2.08	0.53
1:J:318:LEU:HD12	1:J:421:ILE:HD12	1.90	0.53
1:A:102:THR:HG23	1:A:102:THR:O	2.08	0.53
1:C:282:LYS:HD3	1:C:352:PHE:CG	2.43	0.53
1:I:269:THR:HA	1:I:270:PRO:C	2.29	0.53
1:K:449:ILE:HA	4:K:2087:HOH:O	2.08	0.53
1:H:203:LEU:CD1	1:H:214:ARG:HG2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:418:PHE:O	4:H:2003:HOH:O	2.19	0.53
1:D:230:ASN:ND2	4:D:2072:HOH:O	2.36	0.53
1:E:420:PRO:C	1:E:421:ILE:HD13	2.28	0.53
1:G:365:TYR:HD1	1:G:366:PRO:O	1.92	0.53
1:H:209:LYS:CE	1:I:209:LYS:HE2	2.38	0.53
1:L:137:VAL:HG12	1:L:294:SER:CB	2.39	0.53
1:D:130:ASP:O	1:D:131:THR:CG2	2.56	0.53
1:F:229:THR:O	1:F:230:ASN:CB	2.56	0.53
1:D:256:GLN:O	1:D:280:PRO:HD3	2.09	0.53
1:E:344:LYS:HB2	1:E:427:TYR:OH	2.08	0.53
1:I:181:ASN:HA	1:I:252:SER:OG	2.09	0.53
1:G:168:ASN:HB2	1:G:373:TRP:CD1	2.43	0.52
1:K:100:TRP:O	1:K:107:ALA:HA	2.10	0.52
1:A:196:ASP:CG	1:A:214:ARG:NH1	2.63	0.52
1:A:326:GLN:HG2	1:A:328:VAL:HG12	1.91	0.52
1:F:315:LYS:HE2	1:F:437:ASN:OD1	2.09	0.52
1:J:126:ASP:C	1:J:126:ASP:OD1	2.46	0.52
1:C:229:THR:O	1:C:230:ASN:CB	2.58	0.52
1:K:318:LEU:HD22	1:K:396:ASN:CB	2.39	0.52
1:L:118:VAL:HG12	1:L:141:CYS:SG	2.49	0.52
1:L:331:ASP:O	1:L:332:THR:C	2.46	0.52
1:G:321:LYS:HD3	1:G:323:GLU:OE2	2.09	0.52
1:J:350:ARG:HG2	1:J:410:ILE:HD11	1.91	0.52
1:B:137:VAL:HG12	1:B:294:SER:HB3	1.90	0.52
1:I:476:CYS:O	1:I:477:THR:OG1	2.24	0.52
1:K:203:LEU:CD2	1:K:217:LEU:HD23	2.39	0.52
1:E:167:SER:HA	1:E:373:TRP:CH2	2.45	0.52
1:L:115:ILE:N	1:L:116:PRO:CD	2.73	0.52
1:I:119:HIS:CE1	1:I:139:GLY:HA3	2.45	0.52
1:K:215:CYS:HB2	4:K:2033:HOH:O	2.10	0.52
1:K:340:GLN:NE2	1:K:405:GLU:OE2	2.43	0.52
1:L:446:PHE:C	1:L:446:PHE:HD1	2.13	0.52
1:K:98:ASN:OD1	1:K:100:TRP:N	2.39	0.52
1:B:363:THR:HG22	1:B:363:THR:O	2.09	0.52
1:K:301:ASN:HB3	4:K:2035:HOH:O	2.10	0.52
1:L:129:ARG:NH1	1:L:296:PHE:CZ	2.78	0.52
1:G:203:LEU:HD12	1:G:214:ARG:HG2	1.91	0.52
1:L:98:ASN:OD1	1:L:100:TRP:HB2	2.10	0.52
1:H:237:TYR:HB3	1:H:251:LEU:O	2.11	0.51
1:L:119:HIS:CE1	1:L:139:GLY:HA3	2.45	0.51
1:C:405:GLU:OE2	4:C:2165:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:115:ILE:HD12	1:L:394:TRP:CE2	2.45	0.51
1:L:194:ILE:HD13	1:L:199:LEU:HD12	1.93	0.51
1:B:167:SER:HA	1:B:373:TRP:CH2	2.45	0.51
1:G:400:GLU:OE1	1:G:403:SER:OG	2.28	0.51
1:J:103:THR:OG1	1:J:106:PHE:CD2	2.63	0.51
1:I:257:LEU:HD12	1:I:258:LEU:H	1.74	0.51
1:B:144:PHE:O	1:B:282:LYS:CE	2.41	0.51
1:J:460:VAL:HG12	1:J:462:GLU:HG2	1.92	0.51
1:L:194:ILE:CG2	1:L:199:LEU:CD1	2.88	0.51
1:B:229:THR:O	1:B:230:ASN:HB2	2.10	0.51
1:C:131:THR:HG22	1:C:132:GLU:HG3	1.92	0.51
1:D:364:THR:OG1	1:D:365:TYR:N	2.44	0.51
1:E:282:LYS:HD3	1:E:352:PHE:CG	2.46	0.51
1:C:363:THR:O	1:C:363:THR:CG2	2.58	0.51
1:J:207:GLY:O	1:J:209:LYS:HE3	2.11	0.51
1:I:208:PRO:HG3	1:I:302:PRO:HG2	1.93	0.51
1:J:100:TRP:HB3	1:J:110:MET:HG3	1.92	0.51
1:L:210:THR:O	1:L:214:ARG:NH2	2.44	0.51
1:B:351:VAL:CG1	1:B:395:ALA:CB	2.77	0.51
1:E:236:LYS:NZ	4:E:2075:HOH:O	2.45	0.51
1:I:256:GLN:O	1:I:280:PRO:HD3	2.11	0.51
1:B:98:ASN:O	1:B:102:THR:HB	2.11	0.50
1:D:126:ASP:C	1:D:126:ASP:OD1	2.50	0.50
1:E:397:PHE:HA	1:E:407:ILE:O	2.10	0.50
1:I:315:LYS:HB3	1:I:435:GLU:HB3	1.94	0.50
1:I:229:THR:O	1:I:230:ASN:CB	2.60	0.50
1:J:144:PHE:O	1:J:282:LYS:HE2	2.12	0.50
1:K:110:MET:CE	1:K:418:PHE:CE2	2.94	0.50
1:L:137:VAL:C	1:L:294:SER:HB2	2.31	0.50
1:A:99:PRO:O	1:A:102:THR:HB	2.11	0.50
1:A:102:THR:O	1:A:102:THR:CG2	2.59	0.50
1:F:240:VAL:HG23	1:F:251:LEU:HD11	1.92	0.50
1:K:110:MET:CE	1:K:110:MET:HA	2.40	0.50
1:I:175:LEU:HD12	1:I:176:PRO:HD2	1.92	0.50
1:K:110:MET:CE	1:K:110:MET:CA	2.88	0.50
1:B:315:LYS:HB3	1:B:435:GLU:HB3	1.94	0.50
1:J:455:ASN:CG	1:J:455:ASN:O	2.50	0.50
1:F:135:ARG:CZ	1:F:384:SER:HB3	2.42	0.50
1:L:311:ASN:ND2	1:L:311:ASN:N	2.58	0.50
1:I:464:VAL:O	1:I:464:VAL:HG23	2.11	0.49
1:B:318:LEU:HD21	1:B:424:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:442:ASP:OD2	1:K:445:SER:OG	2.24	0.49
1:K:98:ASN:HD22	1:K:322:TRP:HB2	1.78	0.49
1:L:118:VAL:O	1:L:140:LYS:HB2	2.11	0.49
1:A:202:ARG:NH1	4:A:2067:HOH:O	2.41	0.49
1:C:153:PRO:HD2	1:C:156:TYR:CD1	2.48	0.49
1:J:265:SER:HB3	1:J:270:PRO:O	2.12	0.49
2:K:1:NAG:O3	2:K:1:NAG:C7	2.61	0.49
1:F:457:VAL:HG13	1:F:472:SER:HB3	1.95	0.49
1:G:345:GLU:OE2	4:G:2095:HOH:O	2.20	0.49
1:H:142:PRO:HB2	1:H:291:VAL:CG1	2.42	0.49
4:E:2121:HOH:O	1:K:300:GLY:CA	2.61	0.49
1:A:333:LYS:HE2	1:A:333:LYS:HA	1.94	0.49
1:B:351:VAL:CG1	1:B:410:ILE:HG12	2.43	0.49
1:H:363:THR:HG22	1:H:364:THR:N	2.28	0.49
1:K:230:ASN:HD22	2:K:1:NAG:C1	2.12	0.49
1:C:444:ALA:O	4:C:2179:HOH:O	2.17	0.49
1:F:214:ARG:NH2	1:J:209:LYS:O	2.46	0.49
1:E:476:CYS:O	1:E:477:THR:HB	2.13	0.49
1:D:117:GLN:CD	1:H:117:GLN:HE21	2.08	0.49
1:H:229:THR:HB	1:H:231:TYR:CD2	2.48	0.49
1:D:155:GLU:HG2	1:D:156:TYR:HD1	1.77	0.48
1:F:209:LYS:HE3	1:J:209:LYS:HE2	1.96	0.48
1:I:257:LEU:HD12	1:I:258:LEU:N	2.28	0.48
2:K:1:NAG:HO3	2:K:1:NAG:C7	2.25	0.48
1:K:110:MET:HE2	1:K:418:PHE:HE2	1.78	0.48
1:K:98:ASN:OD1	1:K:100:TRP:HB2	2.12	0.48
1:G:127:LEU:HB3	1:G:135:ARG:HB3	1.95	0.48
1:J:331:ASP:C	1:J:331:ASP:OD1	2.51	0.48
1:B:336:VAL:CG1	1:B:356:LEU:CD1	2.81	0.48
1:F:100:TRP:HA	1:F:106:PHE:HB3	1.94	0.48
1:L:446:PHE:CD1	1:L:447:ILE:N	2.82	0.48
1:B:194:ILE:O	1:B:194:ILE:HG23	2.13	0.48
1:D:398:TYR:CD1	1:D:398:TYR:N	2.81	0.48
1:I:444:ALA:O	1:I:445:SER:CB	2.45	0.48
1:J:359:SER:O	1:J:387:SER:HB3	2.14	0.48
1:K:110:MET:CE	1:K:418:PHE:CD2	2.96	0.48
1:L:301:ASN:CB	1:L:304:ALA:HB2	2.36	0.48
1:H:332:THR:HG22	1:H:338:SER:OG	2.14	0.48
1:F:318:LEU:HD21	1:F:424:ALA:HB1	1.96	0.48
1:B:100:TRP:O	1:B:107:ALA:HA	2.14	0.48
1:E:116:PRO:O	1:E:120:GLY:HA2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:140:LYS:O	1:K:297:VAL:CG2	2.62	0.48
1:F:190:LYS:HE3	1:F:192:SER:O	2.13	0.47
1:K:216:ALA:CB	1:K:298:ALA:HB2	2.44	0.47
1:C:403:SER:HB3	1:C:405:GLU:HG3	1.95	0.47
1:D:129:ARG:NH1	4:D:2017:HOH:O	2.07	0.47
1:K:209:LYS:HG2	1:K:303:ASP:OD2	2.14	0.47
1:L:464:VAL:CG2	1:L:464:VAL:O	2.59	0.47
1:E:341:ALA:O	1:E:406:THR:OG1	2.33	0.47
1:G:164:ALA:HA	1:G:178:GLY:O	2.14	0.47
1:L:100:TRP:HH2	1:L:439:PRO:HD2	1.79	0.47
1:L:444:ALA:O	1:L:445:SER:OG	2.30	0.47
1:F:220:TYR:CZ	1:F:236:LYS:HE3	2.49	0.47
1:F:457:VAL:CG1	1:F:472:SER:HB3	2.45	0.47
1:H:124:PHE:HB2	1:H:357:VAL:HG11	1.95	0.47
1:L:229:THR:O	2:L:1:NAG:H81	2.13	0.47
1:A:199:LEU:HD21	1:A:218:TYR:CD1	2.49	0.47
1:A:237:TYR:O	1:A:295:ALA:HB2	2.14	0.47
1:H:320:GLY:HA3	1:H:327:CYS:SG	2.55	0.47
1:L:118:VAL:HG11	1:L:308:ALA:O	2.15	0.47
1:E:420:PRO:HG3	1:E:468:PHE:HB3	1.96	0.47
1:L:321:LYS:HA	1:L:416:ASP:OD1	2.14	0.47
1:D:184:VAL:O	1:D:184:VAL:HG23	2.15	0.47
1:D:196:ASP:OD1	1:D:214:ARG:HD2	2.15	0.47
1:H:168:ASN:HB2	1:H:373:TRP:CD1	2.49	0.47
1:J:169:ASP:HB3	1:J:172:LYS:HB2	1.97	0.47
1:G:167:SER:HA	1:G:373:TRP:CH2	2.50	0.47
1:L:114:ASN:O	1:L:118:VAL:HG23	2.15	0.47
1:B:236:LYS:NZ	4:B:2079:HOH:O	2.44	0.47
1:D:137:VAL:HG12	1:D:294:SER:HB3	1.96	0.47
1:L:298:ALA:HA	1:L:302:PRO:HA	1.97	0.47
1:L:98:ASN:OD1	1:L:100:TRP:N	2.47	0.47
1:F:102:THR:CG2	1:F:103:THR:N	2.77	0.47
1:J:318:LEU:CD2	1:J:424:ALA:HB1	2.44	0.47
1:L:443:SER:OG	1:L:465:GLY:N	2.48	0.47
2:E:1:NAG:O3	2:E:1:NAG:O7	2.30	0.46
1:K:179:PHE:CD1	1:K:179:PHE:N	2.83	0.46
1:C:349:LYS:HD2	4:C:2150:HOH:O	2.15	0.46
1:I:457:VAL:CG1	1:I:472:SER:HB3	2.45	0.46
1:L:193:PRO:HB3	1:L:249:TYR:CE2	2.50	0.46
1:H:183:GLN:NE2	4:H:2053:HOH:O	2.49	0.46
1:H:215:CYS:HB2	4:H:2061:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:340:GLN:NE2	1:J:405:GLU:OE2	2.45	0.46
1:L:330:PHE:CE2	1:L:411:PHE:CE2	3.03	0.46
1:B:323:GLU:O	1:B:324:ASP:HB2	2.15	0.46
1:I:446:PHE:O	1:I:448:PRO:HD3	2.15	0.46
1:C:282:LYS:HG3	1:C:348:TRP:CH2	2.50	0.46
1:K:193:PRO:HB3	1:K:249:TYR:CE2	2.51	0.46
1:L:210:THR:C	1:L:214:ARG:HH21	2.18	0.46
1:C:460:VAL:HG21	1:C:473:LYS:HD3	1.96	0.46
1:H:282:LYS:HD3	1:H:352:PHE:CG	2.51	0.46
1:I:346:GLU:HG3	4:I:2074:HOH:O	2.15	0.46
1:J:106:PHE:CZ	1:J:441:CYS:HB3	2.50	0.46
1:F:455:ASN:O	1:F:456:CYS:HB2	2.16	0.46
1:G:240:VAL:HA	1:G:291:VAL:O	2.16	0.46
1:G:400:GLU:HB2	1:G:407:ILE:HG12	1.98	0.46
1:K:237:TYR:CD1	1:K:252:SER:HA	2.51	0.46
1:K:319:PHE:CE2	1:K:426:ALA:HB1	2.51	0.46
1:L:155:GLU:H	1:L:155:GLU:HG3	1.57	0.46
1:D:194:ILE:HG23	1:D:194:ILE:O	2.15	0.46
1:D:181:ASN:HA	1:D:252:SER:HB3	1.98	0.46
1:F:196:ASP:OD2	1:F:214:ARG:NH1	2.49	0.46
1:K:132:GLU:OE2	1:K:233:SER:HB2	2.16	0.46
1:B:455:ASN:O	1:B:456:CYS:HB2	2.16	0.45
1:E:130:ASP:HA	1:E:134:TYR:O	2.16	0.45
1:L:319:PHE:CE2	1:L:426:ALA:HB1	2.51	0.45
1:A:400:GLU:CG	1:A:402:GLU:HG3	2.45	0.45
1:C:294:SER:O	1:C:297:VAL:HG23	2.15	0.45
1:I:124:PHE:HB2	1:I:357:VAL:HG11	1.98	0.45
1:E:202:ARG:NH1	4:E:2065:HOH:O	2.48	0.45
1:K:135:ARG:O	1:K:235:TYR:OH	2.17	0.45
3:F:1478:GOL:C1	4:F:2129:HOH:O	2.62	0.45
1:F:211:ALA:HA	1:F:214:ARG:NH1	2.32	0.45
1:G:128:GLY:O	1:G:386:LYS:HE3	2.16	0.45
1:K:132:GLU:CD	1:K:233:SER:HB2	2.37	0.45
1:E:102:THR:HG22	1:E:103:THR:N	2.32	0.45
1:E:332:THR:HG22	1:E:338:SER:HG	1.81	0.45
1:I:398:TYR:N	1:I:398:TYR:CD1	2.84	0.45
1:K:220:TYR:O	1:K:220:TYR:HD1	1.92	0.45
1:E:193:PRO:HG2	3:E:1478:GOL:C1	2.47	0.45
1:K:296:PHE:CD1	1:K:296:PHE:N	2.85	0.45
1:A:315:LYS:HB3	1:A:435:GLU:HB3	1.98	0.45
3:C:1478:GOL:H11	4:C:2176:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:LEU:HD21	1:C:218:TYR:CD1	2.52	0.45
1:G:464:VAL:CG2	1:G:464:VAL:O	2.64	0.45
1:I:112:ARG:NH1	1:I:309:CYS:O	2.48	0.45
1:L:269:THR:HA	1:L:270:PRO:C	2.36	0.45
1:F:196:ASP:CG	1:F:214:ARG:NH1	2.70	0.45
1:K:110:MET:HE2	1:K:418:PHE:CE2	2.52	0.45
1:K:357:VAL:HG22	1:K:358:ALA:N	2.31	0.45
1:E:128:GLY:O	1:E:386:LYS:HE2	2.17	0.45
1:E:319:PHE:CE2	1:E:426:ALA:HB1	2.52	0.45
1:L:301:ASN:HB3	1:L:304:ALA:CB	2.38	0.45
1:B:210:THR:N	1:B:303:ASP:OD1	2.49	0.45
1:E:204:GLY:HA2	4:E:2062:HOH:O	2.17	0.45
1:E:210:THR:O	1:E:214:ARG:HG3	2.17	0.45
1:E:263:TYR:CE1	1:E:368:ALA:HB3	2.52	0.45
4:A:2194:HOH:O	1:E:370:GLN:OE1	2.20	0.45
1:H:130:ASP:HA	1:H:134:TYR:O	2.17	0.45
1:L:168:ASN:HB2	1:L:373:TRP:CD1	2.51	0.45
1:B:140:LYS:HE3	1:B:299:GLU:OE2	2.17	0.44
1:F:284:LYS:HE2	1:F:433:SER:OG	2.17	0.44
1:K:112:ARG:NH1	1:K:306:GLN:O	2.48	0.44
1:K:446:PHE:O	1:K:448:PRO:HD3	2.17	0.44
1:C:124:PHE:HB2	1:C:357:VAL:HG11	2.00	0.44
1:F:344:LYS:HB3	1:F:427:TYR:OH	2.17	0.44
1:J:115:ILE:N	1:J:116:PRO:CD	2.80	0.44
2:K:1:NAG:O7	2:K:1:NAG:O3	2.30	0.44
1:K:320:GLY:HA3	1:K:328:VAL:O	2.17	0.44
1:L:440:GLN:HG2	1:L:466:ASN:O	2.17	0.44
1:A:442:ASP:OD2	1:A:445:SER:OG	2.28	0.44
1:E:102:THR:HG22	1:E:103:THR:OG1	2.18	0.44
1:G:121:SER:O	1:G:389:GLY:HA2	2.17	0.44
1:I:282:LYS:HD3	1:I:352:PHE:CG	2.52	0.44
1:J:212:ILE:HG13	4:J:2019:HOH:O	2.17	0.44
1:K:181:ASN:OD1	1:K:183:GLN:HG3	2.17	0.44
1:K:447:ILE:CD1	1:K:447:ILE:N	2.81	0.44
1:C:339:ASP:OD1	4:C:2147:HOH:O	2.21	0.44
1:C:460:VAL:CG1	1:C:462:GLU:HG3	2.47	0.44
1:E:153:PRO:HD3	4:E:2029:HOH:O	2.17	0.44
1:J:199:LEU:HD21	1:J:218:TYR:CD1	2.52	0.44
1:L:112:ARG:O	1:L:310:PRO:HG3	2.16	0.44
1:L:223:ILE:HG22	1:L:223:ILE:O	2.17	0.44
1:C:318:LEU:HD22	1:C:396:ASN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:LYS:HB3	1:E:435:GLU:HB3	1.99	0.44
1:J:130:ASP:OD2	1:J:386:LYS:NZ	2.51	0.44
1:J:151:HIS:HE2	1:J:279:GLU:CD	2.21	0.44
1:L:137:VAL:O	1:L:294:SER:HB2	2.17	0.44
1:L:400:GLU:OE2	1:L:403:SER:OG	2.36	0.44
1:F:439:PRO:HA	3:F:1478:GOL:H12	2.00	0.44
1:J:320:GLY:HA3	1:J:327:CYS:SG	2.58	0.44
1:J:261[B]:GLU:H	1:J:261[B]:GLU:CD	2.21	0.44
1:J:464:VAL:O	1:J:464:VAL:HG13	2.17	0.44
1:A:212:ILE:CD1	3:A:1480:GOL:H2	2.48	0.43
1:A:230:ASN:OD1	1:A:230:ASN:O	2.36	0.43
1:C:129:ARG:HD3	1:C:296:PHE:CE2	2.53	0.43
1:J:455:ASN:O	1:J:456:CYS:HB2	2.18	0.43
1:K:301:ASN:CB	4:K:2035:HOH:O	2.64	0.43
1:L:442:ASP:OD2	1:L:445:SER:OG	2.36	0.43
1:A:384:SER:HA	1:A:385:PRO:HD3	1.90	0.43
1:B:98:ASN:HB2	1:B:322:TRP:CG	2.53	0.43
1:D:384:SER:HA	1:D:385:PRO:HD3	1.86	0.43
1:E:129:ARG:NH1	1:E:136:GLU:OE1	2.48	0.43
1:F:226:ASN:C	1:F:226:ASN:OD1	2.56	0.43
1:G:199:LEU:HA	1:G:199:LEU:HD23	1.68	0.43
1:G:203:LEU:HA	1:G:203:LEU:HD23	1.87	0.43
1:I:477:THR:O	1:I:477:THR:HG22	2.18	0.43
1:K:104:THR:O	1:K:108:ASP:HB2	2.18	0.43
1:K:179:PHE:HD1	1:K:179:PHE:N	2.16	0.43
1:K:364:THR:O	1:K:365:TYR:HD1	2.01	0.43
1:B:402:GLU:HG3	1:B:402:GLU:H	1.28	0.43
1:F:328:VAL:HA	1:F:329:PRO:HD3	1.85	0.43
1:K:354:ASN:O	1:K:357:VAL:HG12	2.18	0.43
1:L:137:VAL:HG12	1:L:294:SER:HB2	2.00	0.43
1:A:199:LEU:HA	1:A:199:LEU:HD23	1.80	0.43
1:B:262:LYS:HB2	4:B:2098:HOH:O	2.19	0.43
1:E:170:ALA:O	1:E:173:LYS:HE2	2.18	0.43
1:I:141:CYS:HA	1:I:142:PRO:HD3	1.87	0.43
1:I:323:GLU:O	1:I:324:ASP:HB2	2.19	0.43
1:D:115:ILE:HG12	1:D:430:LEU:HD12	2.01	0.43
1:E:354:ASN:OD1	1:E:354:ASN:C	2.57	0.43
1:I:282:LYS:HG3	1:I:348:TRP:CZ2	2.53	0.43
1:I:447:ILE:CG2	1:I:447:ILE:O	2.67	0.43
1:K:208:PRO:CB	1:K:302:PRO:HG2	2.49	0.43
1:K:168:ASN:HB2	1:K:373:TRP:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:HB2	1:B:136:GLU:HB3	2.00	0.43
1:F:169:ASP:H	1:F:175:LEU:CD1	2.32	0.43
1:H:202:ARG:HG2	1:H:202:ARG:O	2.17	0.43
1:H:464:VAL:O	1:H:464:VAL:HG23	2.19	0.43
1:I:136:GLU:HG3	1:I:235:TYR:CE1	2.53	0.43
1:L:114:ASN:HA	1:L:414:VAL:HG13	1.99	0.43
1:L:115:ILE:HG12	1:L:430:LEU:CD1	2.48	0.43
1:B:173:LYS:HA	1:B:174:PRO:HA	1.83	0.43
1:D:264:CYS:C	1:D:273:LEU:HD13	2.39	0.43
1:G:236:LYS:HA	4:G:2064:HOH:O	2.19	0.43
1:I:168:ASN:OD1	1:I:169:ASP:N	2.52	0.43
1:L:216:ALA:O	1:L:219:ALA:N	2.47	0.43
1:E:340:GLN:HA	1:E:406:THR:O	2.19	0.43
1:J:155:GLU:HG3	1:J:155:GLU:H	1.43	0.43
1:L:144:PHE:O	1:L:282:LYS:HE2	2.19	0.43
1:D:137:VAL:HG12	1:D:294:SER:CB	2.49	0.43
1:F:121:SER:O	1:F:389:GLY:HA2	2.19	0.43
1:G:119:HIS:CE1	1:G:139:GLY:HA3	2.53	0.43
1:H:99:PRO:HA	1:H:102:THR:HB	2.00	0.43
1:J:179:PHE:CD1	1:J:179:PHE:N	2.87	0.43
1:J:279:GLU:HA	1:J:280:PRO:HD3	1.85	0.43
1:J:135:ARG:CZ	1:J:384:SER:HB3	2.49	0.43
1:K:118:VAL:O	1:K:140:LYS:HB2	2.19	0.43
1:E:124:PHE:HB2	1:E:357:VAL:HG11	2.01	0.43
1:F:464:VAL:HG22	1:F:464:VAL:O	2.19	0.43
1:K:210:THR:HB	1:K:305:TRP:HZ2	1.83	0.43
1:L:98:ASN:HA	1:L:99:PRO:HD2	1.88	0.43
3:C:1478:GOL:C1	4:C:2176:HOH:O	2.66	0.42
1:A:370:GLN:HE21	1:C:477:THR:HG22	1.83	0.42
1:E:318:LEU:HD22	1:E:396:ASN:CB	2.43	0.42
1:E:455:ASN:O	1:E:456:CYS:CB	2.64	0.42
1:F:168:ASN:HB2	1:F:373:TRP:CD1	2.54	0.42
1:F:199:LEU:O	1:F:203:LEU:CB	2.64	0.42
1:K:301:ASN:N	4:K:2066:HOH:O	2.24	0.42
1:K:305:TRP:CD2	1:K:306:GLN:N	2.87	0.42
1:L:402:GLU:CG	1:L:403:SER:N	2.82	0.42
1:A:126:ASP:OD1	1:A:126:ASP:C	2.58	0.42
1:D:153:PRO:O	1:D:156:TYR:HB2	2.20	0.42
1:D:155:GLU:HG2	1:D:156:TYR:N	2.33	0.42
1:H:264:CYS:HB2	1:H:277:CYS:N	2.33	0.42
1:L:420:PRO:C	1:L:421:ILE:HG13	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:SER:HB2	1:C:405:GLU:H	1.84	0.42
1:G:192:SER:HA	1:G:193:PRO:C	2.40	0.42
1:H:100:TRP:CE3	1:H:106:PHE:HB3	2.54	0.42
1:K:217:LEU:N	1:K:298:ALA:HB2	2.35	0.42
1:A:207:GLY:O	1:A:209:LYS:HE3	2.18	0.42
1:A:212:ILE:HD12	3:A:1480:GOL:H2	2.01	0.42
1:B:141:CYS:HA	1:B:142:PRO:HD3	1.87	0.42
1:K:266:VAL:O	1:K:267:ASN:C	2.58	0.42
1:K:326:GLN:OE1	1:K:459:VAL:HG21	2.19	0.42
1:B:124:PHE:HB2	1:B:357:VAL:HG11	2.01	0.42
1:C:301:ASN:HA	1:C:302:PRO:HD3	1.93	0.42
1:E:164:ALA:HB1	1:E:165:PRO:HD2	2.02	0.42
1:F:167:SER:HA	1:F:373:TRP:CH2	2.54	0.42
1:G:264:CYS:HB2	1:G:277:CYS:N	2.34	0.42
1:J:305:TRP:CD2	1:J:306:GLN:N	2.87	0.42
1:L:331:ASP:O	1:L:333:LYS:N	2.52	0.42
1:A:318:LEU:HD21	1:A:424:ALA:HB1	2.02	0.42
1:B:258:LEU:O	1:B:277:CYS:HB3	2.20	0.42
1:G:328:VAL:HA	1:G:329:PRO:HD3	1.95	0.42
1:H:103:THR:HB	1:H:106:PHE:CD2	2.54	0.42
1:K:216:ALA:O	1:K:219:ALA:N	2.53	0.42
1:B:130:ASP:OD1	1:B:386:LYS:NZ	2.47	0.42
1:C:420:PRO:HG3	1:C:468:PHE:HB3	2.01	0.42
1:F:236:LYS:NZ	4:F:2065:HOH:O	2.52	0.42
1:G:207:GLY:O	1:G:209:LYS:HE3	2.20	0.42
1:G:269:THR:HA	1:G:270:PRO:C	2.39	0.42
1:I:318:LEU:HD22	1:I:396:ASN:HB3	2.02	0.42
1:L:459:VAL:HG11	1:L:470:GLN:OE1	2.19	0.42
1:C:100:TRP:CE3	1:C:106:PHE:HB3	2.55	0.42
1:D:425:VAL:HG11	1:D:427:TYR:CZ	2.55	0.42
1:H:102:THR:O	1:H:102:THR:CG2	2.67	0.42
1:I:175:LEU:HA	1:I:176:PRO:HD3	1.85	0.42
1:B:193:PRO:HB3	1:B:249:TYR:CD2	2.54	0.42
1:I:106:PHE:CE1	1:I:468:PHE:HE2	2.38	0.42
1:I:115:ILE:HB	1:I:116:PRO:HD3	2.02	0.42
1:I:207:GLY:O	1:I:209:LYS:HE3	2.20	0.42
1:I:371:LYS:HB3	1:I:371:LYS:HE2	1.78	0.42
1:L:284:LYS:NZ	4:L:2063:HOH:O	2.53	0.42
1:C:98:ASN:HA	1:C:99:PRO:HD2	1.94	0.41
1:D:130:ASP:O	1:D:131:THR:HG23	2.20	0.41
1:H:269:THR:HA	1:H:270:PRO:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:319:PHE:CE2	1:J:426:ALA:HB1	2.55	0.41
1:K:210:THR:O	1:K:210:THR:OG1	2.35	0.41
1:B:119:HIS:CE1	1:B:139:GLY:HA3	2.55	0.41
1:K:98:ASN:ND2	1:K:322:TRP:HB2	2.34	0.41
1:K:350:ARG:HD3	4:K:2078:HOH:O	2.20	0.41
1:K:135:ARG:NH2	1:K:385:PRO:O	2.53	0.41
1:A:315:LYS:HE3	1:A:437:ASN:OD1	2.19	0.41
1:B:144:PHE:HB3	1:B:432:SER:HB2	2.01	0.41
1:E:100:TRP:CE3	1:E:106:PHE:HB3	2.56	0.41
1:F:416:ASP:OD1	1:F:416:ASP:C	2.58	0.41
1:G:135:ARG:NH1	1:G:360:ASP:O	2.46	0.41
1:H:393:ASN:HB2	1:H:394:TRP:CE3	2.55	0.41
1:H:98:ASN:HA	1:H:99:PRO:HD2	1.85	0.41
1:J:226:ASN:HA	1:J:227:PRO:HD3	1.93	0.41
1:A:129:ARG:O	1:A:136:GLU:N	2.40	0.41
1:C:115:ILE:HD12	1:C:393:ASN:HB3	2.03	0.41
1:D:365:TYR:HA	1:D:365:TYR:HD1	1.67	0.41
1:J:179:PHE:HD1	1:J:179:PHE:N	2.19	0.41
1:J:321:LYS:HB2	1:J:321:LYS:HE2	1.75	0.41
1:L:112:ARG:HD3	1:L:309:CYS:O	2.21	0.41
1:L:114:ASN:ND2	1:L:117:GLN:HB2	2.35	0.41
1:B:421:ILE:N	1:B:421:ILE:HD13	2.31	0.41
1:H:315:LYS:O	1:H:315:LYS:HG3	2.20	0.41
1:B:104:THR:HG21	1:L:129:ARG:HA	2.02	0.41
1:A:324:ASP:HA	4:A:2141:HOH:O	2.20	0.41
1:B:364:THR:O	1:B:364:THR:CG2	2.60	0.41
1:D:446:PHE:O	1:D:448:PRO:HD3	2.21	0.41
1:E:336:VAL:CG2	1:E:356:LEU:CD2	2.97	0.41
1:F:394:TRP:HB2	1:F:411:PHE:CZ	2.55	0.41
1:H:350:ARG:HD3	4:H:2134:HOH:O	2.19	0.41
1:I:103:THR:CG2	1:I:104:THR:N	2.84	0.41
1:I:116:PRO:HB2	4:I:2005:HOH:O	2.21	0.41
1:K:445:SER:O	1:K:447:ILE:CD1	2.69	0.41
1:L:318:LEU:HB2	1:L:421:ILE:HD12	2.02	0.41
1:B:351:VAL:HG12	1:B:410:ILE:HG12	2.01	0.41
1:H:119:HIS:CE1	1:H:139:GLY:HA3	2.55	0.41
1:L:305:TRP:HE3	1:L:311:ASN:OD1	2.03	0.41
1:D:299:GLU:O	4:D:2098:HOH:O	2.22	0.41
1:I:167:SER:HA	1:I:373:TRP:CH2	2.56	0.41
1:B:338:SER:HB2	1:B:407:ILE:HD12	2.03	0.41
1:C:335:SER:HB3	1:C:410:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:198:LEU:HD23	1:G:198:LEU:HA	1.89	0.41
1:K:226:ASN:HA	1:K:227:PRO:HD3	1.95	0.41
1:K:224:ALA:HB2	1:K:235:TYR:O	2.21	0.41
1:K:298:ALA:HA	1:K:302:PRO:HA	2.03	0.41
1:A:420:PRO:HD2	1:A:470:GLN:HB2	2.03	0.41
1:B:199:LEU:HD13	1:B:214:ARG:HB3	2.02	0.41
1:C:229:THR:O	1:C:230:ASN:HB2	2.21	0.41
1:C:377:TRP:HA	1:C:378:PRO:HD3	1.94	0.41
1:G:439:PRO:HA	3:G:1478:GOL:H11	2.03	0.41
1:H:203:LEU:HD23	1:H:203:LEU:HA	1.94	0.41
1:J:282:LYS:HD3	1:J:352:PHE:CG	2.55	0.41
1:J:301:ASN:HA	1:J:302:PRO:HD3	1.87	0.41
1:K:164:ALA:HB1	1:K:165:PRO:HD2	2.02	0.41
1:K:129:ARG:CZ	1:K:296:PHE:CE2	3.04	0.41
1:L:140:LYS:HD2	1:L:140:LYS:HA	1.84	0.41
1:F:118:VAL:HG11	1:F:308:ALA:O	2.21	0.41
1:H:328:VAL:HA	1:H:329:PRO:HD3	1.96	0.41
1:E:205:THR:O	1:G:209:LYS:HE2	2.19	0.40
1:F:354:ASN:HA	1:F:355:PRO:HD3	1.93	0.40
1:H:226:ASN:HB3	1:H:229:THR:OG1	2.20	0.40
1:L:309:CYS:O	1:L:311:ASN:ND2	2.54	0.40
1:D:266:VAL:O	1:D:267:ASN:C	2.60	0.40
1:J:282:LYS:NZ	4:J:2032:HOH:O	2.35	0.40
1:K:115:ILE:N	1:K:116:PRO:HD2	2.36	0.40
1:I:240:VAL:HA	1:I:291:VAL:O	2.21	0.40
1:J:446:PHE:O	1:J:448:PRO:HD3	2.21	0.40
1:K:114:ASN:O	1:K:118:VAL:HG23	2.21	0.40
1:L:330:PHE:CD2	1:L:411:PHE:CZ	3.09	0.40
1:D:284:LYS:HE3	1:D:345:GLU:OE1	2.22	0.40
1:J:350:ARG:HD3	1:J:350:ARG:HH11	1.77	0.40
1:J:464:VAL:O	1:J:464:VAL:CG1	2.69	0.40
1:K:320:GLY:CA	1:K:328:VAL:O	2.69	0.40
1:L:142:PRO:HB2	1:L:291:VAL:CG1	2.51	0.40
1:C:226:ASN:OD1	1:C:228:SER:HB2	2.22	0.40
1:D:279:GLU:HA	1:D:280:PRO:HD3	1.85	0.40
1:D:317:ALA:HA	1:D:419:ALA:O	2.22	0.40
1:E:461:THR:HA	1:E:469:ASP:O	2.22	0.40
1:F:407:ILE:HA	1:F:407:ILE:HD13	1.95	0.40
1:I:199:LEU:HD23	1:I:199:LEU:HA	1.82	0.40
1:I:317:ALA:HA	1:I:419:ALA:O	2.21	0.40
1:K:100:TRP:CD1	1:K:417:CYS:CB	3.00	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	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%)	44	53
1	J	376/396 (95%)	361 (96%)	14 (4%)	1 (0%)	44	53
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%)	44	55
1	B	312/324 (96%)	292 (94%)	20 (6%)	20	22
1	C	312/324 (96%)	301 (96%)	11 (4%)	41	52
1	D	313/324 (97%)	298 (95%)	15 (5%)	30	37
1	E	315/324 (97%)	295 (94%)	20 (6%)	21	23
1	F	312/324 (96%)	296 (95%)	16 (5%)	28	33
1	G	315/324 (97%)	301 (96%)	14 (4%)	33	41
1	H	314/324 (97%)	293 (93%)	21 (7%)	19	21
1	I	311/324 (96%)	289 (93%)	22 (7%)	17	18
1	J	313/324 (97%)	295 (94%)	18 (6%)	23	27
1	K	315/324 (97%)	290 (92%)	25 (8%)	14	15
1	L	315/324 (97%)	284 (90%)	31 (10%)	9	8
All	All	3762/3888 (97%)	3539 (94%)	223 (6%)	23	26

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	THR
1	A	130	ASP
1	A	155	GLU
1	A	197	SER
1	A	199	LEU
1	A	202	ARG
1	A	232	THR
1	A	379	VAL
1	A	402	GLU
1	A	443	SER
1	B	102	THR
1	B	111	LYS
1	B	149	GLN
1	B	171	SER
1	B	198	LEU
1	B	205	THR
1	B	262	LYS
1	B	332	THR
1	B	334	THR

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Mol	Chain	Res	Type
1	B	340	GLN
1	B	351	VAL
1	B	354	ASN
1	B	379	VAL
1	B	382	GLN
1	B	383	SER
1	B	401	LYS
1	B	402	GLU
1	B	403	SER
1	B	407	ILE
1	B	422	THR
1	C	130	ASP
1	C	205	THR
1	C	269	THR
1	C	282	LYS
1	C	294	SER
1	C	334	THR
1	C	354	ASN
1	C	401	LYS
1	C	402	GLU
1	C	422	THR
1	C	464	VAL
1	D	155	GLU
1	D	166	THR
1	D	186	THR
1	D	205	THR
1	D	228	SER
1	D	252	SER
1	D	269	THR
1	D	334	THR
1	D	354	ASN
1	D	363	THR
1	D	365	TYR
1	D	379	VAL
1	D	381	GLU
1	D	400	GLU
1	D	405	GLU
1	E	102	THR
1	E	104	THR
1	E	149	GLN
1	E	198	LEU
1	E	202	ARG

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Mol	Chain	Res	Type
1	E	252	SER
1	E	334	THR
1	E	336	VAL
1	E	337	GLN
1	E	354	ASN
1	E	367	GLU
1	E	370	GLN
1	E	381	GLU
1	E	402	GLU
1	E	422	THR
1	E	439	PRO
1	E	440	GLN
1	E	455	ASN
1	E	471	THR
1	E	477	THR
1	F	102	THR
1	F	140	LYS
1	F	197	SER
1	F	198	LEU
1	F	282	LYS
1	F	299	GLU
1	F	332	THR
1	F	334	THR
1	F	340	GLN
1	F	342	THR
1	F	354	ASN
1	F	364	THR
1	F	383	SER
1	F	385	PRO
1	F	403	SER
1	F	464	VAL
1	G	187	SER
1	G	205	THR
1	G	209	LYS
1	G	228	SER
1	G	232	THR
1	G	269	THR
1	G	282	LYS
1	G	285	SER
1	G	321	LYS
1	G	336	VAL
1	G	365	TYR

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Mol	Chain	Res	Type
1	G	401	LYS
1	G	402	GLU
1	G	403	SER
1	H	102	THR
1	H	140	LYS
1	H	166	THR
1	H	187	SER
1	H	209	LYS
1	H	282	LYS
1	H	285	SER
1	H	321	LYS
1	H	334	THR
1	H	336	VAL
1	H	340	GLN
1	H	354	ASN
1	H	363	THR
1	H	381	GLU
1	H	401	LYS
1	H	402	GLU
1	H	403	SER
1	H	422	THR
1	H	447	ILE
1	H	455	ASN
1	H	473	LYS
1	I	102	THR
1	I	131	THR
1	I	149	GLN
1	I	171	SER
1	I	186	THR
1	I	187	SER
1	I	198	LEU
1	I	233	SER
1	I	282	LYS
1	I	334	THR
1	I	336	VAL
1	I	337	GLN
1	I	340	GLN
1	I	356	LEU
1	I	363	THR
1	I	371	LYS
1	I	381	GLU
1	I	399	LEU

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Mol	Chain	Res	Type
1	I	443	SER
1	I	445	SER
1	I	447	ILE
1	I	468	PHE
1	J	104	THR
1	J	130	ASP
1	J	155	GLU
1	J	167	SER
1	J	186	THR
1	J	189	GLN
1	J	205	THR
1	J	233	SER
1	J	262	LYS
1	J	282	LYS
1	J	321	LYS
1	J	334	THR
1	J	336	VAL
1	J	340	GLN
1	J	354	ASN
1	J	370	GLN
1	J	402	GLU
1	J	462	GLU
1	K	131	THR
1	K	160	PHE
1	K	187	SER
1	K	192	SER
1	K	196	ASP
1	K	202[A]	ARG
1	K	202[B]	ARG
1	K	209	LYS
1	K	223	ILE
1	K	269	THR
1	K	291	VAL
1	K	297	VAL
1	K	307	SER
1	K	334	THR
1	K	338	SER
1	K	340	GLN
1	K	350	ARG
1	K	351	VAL
1	K	363	THR
1	K	365	TYR

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Mol	Chain	Res	Type
1	K	379	VAL
1	K	422	THR
1	K	443	SER
1	K	450	GLU
1	K	454	ASN
1	L	104	THR
1	L	155	GLU
1	L	166	THR
1	L	187	SER
1	L	200	GLN
1	L	205	THR
1	L	209	LYS
1	L	223	ILE
1	L	228	SER
1	L	230	ASN
1	L	248	CYS
1	L	294	SER
1	L	299	GLU
1	L	307	SER
1	L	311	ASN
1	L	315	LYS
1	L	326	GLN
1	L	340	GLN
1	L	354	ASN
1	L	364	THR
1	L	365	TYR
1	L	370	GLN
1	L	379	VAL
1	L	401	LYS
1	L	402	GLU
1	L	403	SER
1	L	441	CYS
1	L	443	SER
1	L	446	PHE
1	L	461	THR
1	L	473	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	GLN
1	F	230	ASN

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Mol	Chain	Res	Type
1	H	340	GLN
1	K	230	ASN
1	L	311	ASN
1	L	326	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 carbohydrates 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	$\# Z  > 2$
2	NAG	A	1	1	14,14,15	0.29	0	15,19,21	0.57	0
3	GOL	A	1478	-	5,5,5	0.19	0	5,5,5	0.53	0
3	GOL	A	1479	-	5,5,5	0.70	0	5,5,5	0.43	0
3	GOL	A	1480	-	5,5,5	0.54	0	5,5,5	0.54	0
2	NAG	B	1	1	14,14,15	0.83	0	15,19,21	1.21	1 (6%)
3	GOL	B	1478	-	5,5,5	0.23	0	5,5,5	0.45	0
3	GOL	B	1479	-	5,5,5	0.42	0	5,5,5	0.69	0
2	NAG	C	1	1	14,14,15	0.75	0	15,19,21	1.16	1 (6%)
3	GOL	C	1478	-	5,5,5	0.45	0	5,5,5	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	C	1479	-	5,5,5	0.63	0	5,5,5	0.47	0
3	GOL	D	1478	-	5,5,5	0.17	0	5,5,5	0.57	0
3	GOL	D	1479	-	5,5,5	0.59	0	5,5,5	0.58	0
2	NAG	E	1	1	14,14,15	0.28	0	15,19,21	0.57	0
3	GOL	E	1478	-	5,5,5	0.46	0	5,5,5	0.84	0
3	GOL	E	1479	-	5,5,5	0.25	0	5,5,5	0.29	0
2	NAG	F	1	1	14,14,15	0.29	0	15,19,21	0.58	0
3	GOL	F	1478	-	5,5,5	0.28	0	5,5,5	0.56	0
2	NAG	G	1	1	14,14,15	0.28	0	15,19,21	0.57	0
3	GOL	G	1478	-	5,5,5	0.36	0	5,5,5	0.74	0
2	NAG	H	1	1	14,14,15	0.28	0	15,19,21	0.57	0
3	GOL	H	1478	-	5,5,5	0.18	0	5,5,5	0.57	0
3	GOL	I	1478	-	5,5,5	0.30	0	5,5,5	0.59	0
3	GOL	J	1478	-	5,5,5	0.39	0	5,5,5	0.64	0
2	NAG	K	1	1	14,14,15	0.35	0	15,19,21	1.05	1 (6%)
2	NAG	L	1	1	14,14,15	0.29	0	15,19,21	0.57	0
3	GOL	L	1478	-	5,5,5	0.63	0	5,5,5	0.50	0
3	GOL	L	1479	-	5,5,5	0.37	0	5,5,5	0.37	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
2	NAG	A	1	1	-	0/6/23/26	0/1/1/1
3	GOL	A	1478	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1479	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1480	-	-	0/4/4/4	0/0/0/0
2	NAG	B	1	1	-	0/6/23/26	0/1/1/1
3	GOL	B	1478	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1479	-	-	0/4/4/4	0/0/0/0
2	NAG	C	1	1	-	0/6/23/26	0/1/1/1
3	GOL	C	1478	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1479	-	-	0/4/4/4	0/0/0/0
3	GOL	D	1478	-	-	0/4/4/4	0/0/0/0
3	GOL	D	1479	-	-	0/4/4/4	0/0/0/0
2	NAG	E	1	1	-	0/6/23/26	0/1/1/1
3	GOL	E	1478	-	-	0/4/4/4	0/0/0/0
3	GOL	E	1479	-	-	0/4/4/4	0/0/0/0
2	NAG	F	1	1	1/1/5/7	0/6/23/26	0/1/1/1
3	GOL	F	1478	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	1	-	0/6/23/26	0/1/1/1
3	GOL	G	1478	-	-	0/4/4/4	0/0/0/0
2	NAG	H	1	1	-	0/6/23/26	0/1/1/1
3	GOL	H	1478	-	-	0/4/4/4	0/0/0/0
3	GOL	I	1478	-	-	0/4/4/4	0/0/0/0
3	GOL	J	1478	-	-	0/4/4/4	0/0/0/0
2	NAG	K	1	1	-	0/6/23/26	0/1/1/1
2	NAG	L	1	1	-	2/6/23/26	0/1/1/1
3	GOL	L	1478	-	-	0/4/4/4	0/0/0/0
3	GOL	L	1479	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C1-C2	-2.38	108.16	111.47
2	K	1	NAG	O5-C1-C2	-2.32	108.25	111.47
2	B	1	NAG	C1-O5-C5	2.09	115.04	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	1	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2

There are no ring outliers.

15 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAG	2	0
3	A	1480	GOL	2	0
3	B	1479	GOL	3	0
3	C	1478	GOL	3	0
3	D	1478	GOL	2	0
2	E	1	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1478	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	I	1478	GOL	1	0
3	J	1478	GOL	2	0
2	K	1	NAG	5	0
2	L	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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	382/396 (96%)	0.35	16 (4%)	37 49	17, 32, 68, 130	0
1	B	379/396 (95%)	0.33	7 (1%)	69 78	14, 32, 66, 91	0
1	C	379/396 (95%)	0.35	7 (1%)	69 78	17, 32, 65, 95	0
1	D	380/396 (95%)	0.40	9 (2%)	59 69	17, 31, 64, 101	0
1	E	382/396 (96%)	0.44	15 (3%)	40 52	16, 32, 63, 105	0
1	F	377/396 (95%)	0.21	3 (0%)	86 92	19, 33, 66, 107	0
1	G	382/396 (96%)	0.40	13 (3%)	46 58	18, 33, 71, 93	0
1	H	380/396 (95%)	0.32	10 (2%)	56 66	20, 34, 66, 99	0
1	I	375/396 (94%)	0.46	21 (5%)	25 36	20, 42, 74, 108	0
1	J	379/396 (95%)	0.56	32 (8%)	12 17	24, 44, 78, 104	0
1	K	380/396 (95%)	0.57	23 (6%)	22 31	26, 45, 83, 111	0
1	L	380/396 (95%)	0.59	26 (6%)	18 26	26, 45, 84, 116	0
All	All	4555/4752 (95%)	0.42	182 (3%)	39 51	14, 37, 74, 130	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	365	TYR	9.6
1	L	365	TYR	8.9
1	E	366	PRO	8.7
1	H	365	TYR	8.2
1	G	366	PRO	7.4
1	E	368	ALA	6.9
1	J	369	ALA	6.9
1	D	365	TYR	6.9
1	E	365	TYR	6.6
1	K	366	PRO	6.5
1	G	369	ALA	6.5

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Mol	Chain	Res	Type	RSRZ
1	G	367	GLU	6.3
1	A	365	TYR	6.2
1	A	369	ALA	6.1
1	H	366	PRO	5.9
1	E	369	ALA	5.8
1	K	365	TYR	5.6
1	A	366	PRO	5.5
1	K	369	ALA	5.5
1	L	370	GLN	5.3
1	A	368	ALA	5.2
1	K	370	GLN	5.0
1	G	368	ALA	4.9
1	J	368	ALA	4.9
1	L	476	CYS	4.7
1	E	367	GLU	4.7
1	G	363	THR	4.6
1	I	363	THR	4.5
1	L	366	PRO	4.5
1	L	475	CYS	4.4
1	E	370	GLN	4.2
1	B	368	ALA	4.2
1	E	444	ALA	4.2
1	E	364	THR	4.0
1	I	364	THR	4.0
1	E	363	THR	4.0
1	F	402	GLU	3.9
1	A	370	GLN	3.8
1	L	202[A]	ARG	3.8
1	A	367	GLU	3.8
1	D	382	GLN	3.8
1	K	202[A]	ARG	3.8
1	G	364	THR	3.7
1	L	369	ALA	3.7
1	H	370	GLN	3.6
1	G	228	SER	3.6
1	B	369	ALA	3.6
1	J	379	VAL	3.5
1	J	228	SER	3.5
1	H	402	GLU	3.5
1	J	401	LYS	3.4
1	A	363	THR	3.3
1	L	453	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	J	383	SER	3.3
1	C	370	GLN	3.3
1	K	402	GLU	3.3
1	I	382	GLN	3.2
1	J	230	ASN	3.2
1	A	382	GLN	3.2
1	J	227	PRO	3.2
1	J	363	THR	3.2
1	J	364	THR	3.1
1	I	171	SER	3.1
1	L	333	LYS	3.1
1	I	231	TYR	3.1
1	A	228	SER	3.1
1	J	231	TYR	3.0
1	J	229	THR	3.0
1	L	404	GLY	3.0
1	I	403	SER	3.0
1	J	333	LYS	3.0
1	C	382	GLN	3.0
1	K	453	CYS	3.0
1	A	231	TYR	2.9
1	G	370	GLN	2.9
1	A	401	LYS	2.9
1	D	402	GLU	2.9
1	H	444	ALA	2.9
1	D	454	ASN	2.9
1	L	455	ASN	2.9
1	J	370	GLN	2.9
1	A	364	THR	2.9
1	E	402	GLU	2.9
1	K	300	GLY	2.9
1	C	402	GLU	2.9
1	L	454	ASN	2.9
1	I	228	SER	2.8
1	C	368	ALA	2.8
1	K	401	LYS	2.8
1	K	454	ASN	2.8
1	E	454	ASN	2.8
1	B	401	LYS	2.7
1	K	325	GLY	2.7
1	K	231	TYR	2.7
1	K	455	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	401	LYS	2.6
1	G	382	GLN	2.6
1	B	400	GLU	2.6
1	E	382	GLN	2.6
1	K	96	GLY	2.6
1	J	332	THR	2.6
1	K	322	TRP	2.6
1	J	381	GLU	2.6
1	C	369	ALA	2.6
1	J	382	GLN	2.6
1	J	402	GLU	2.5
1	K	464	VAL	2.5
1	G	230	ASN	2.5
1	I	170	ALA	2.5
1	L	402	GLU	2.5
1	H	364	THR	2.5
1	I	381	GLU	2.5
1	D	171	SER	2.5
1	J	263	TYR	2.5
1	J	334	THR	2.5
1	L	298	ALA	2.5
1	J	324	ASP	2.5
1	H	363	THR	2.4
1	D	383	SER	2.4
1	L	300	GLY	2.4
1	G	402	GLU	2.4
1	I	402	GLU	2.4
1	J	476	CYS	2.4
1	L	323	GLU	2.4
1	I	102	THR	2.4
1	K	475	CYS	2.4
1	I	383	SER	2.4
1	K	413	GLN	2.4
1	B	231	TYR	2.4
1	J	273	LEU	2.4
1	J	170	ALA	2.4
1	K	363	THR	2.4
1	E	456	CYS	2.4
1	I	443	SER	2.4
1	I	227	PRO	2.3
1	G	231	TYR	2.3
1	J	102	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	230	ASN	2.3
1	H	477	THR	2.3
1	D	401	LYS	2.3
1	L	447	ILE	2.3
1	L	411	PHE	2.2
1	I	452	PRO	2.2
1	F	444	ALA	2.2
1	I	230	ASN	2.2
1	J	171	SER	2.2
1	J	134	TYR	2.2
1	L	364	THR	2.2
1	B	447	ILE	2.2
1	A	373	TRP	2.2
1	A	383	SER	2.2
1	J	268	GLY	2.2
1	D	231	TYR	2.1
1	I	411	PHE	2.1
1	H	454	ASN	2.1
1	L	449	ILE	2.1
1	L	456	CYS	2.1
1	D	170	ALA	2.1
1	I	133	GLY	2.1
1	K	456	CYS	2.1
1	J	166	THR	2.1
1	J	372	ASN	2.1
1	K	107	ALA	2.1
1	L	228	SER	2.1
1	B	203	LEU	2.1
1	A	229	THR	2.1
1	C	364	THR	2.1
1	L	401	LYS	2.1
1	J	404	GLY	2.1
1	I	407	ILE	2.0
1	L	444	ALA	2.0
1	K	228	SER	2.0
1	I	270	PRO	2.0
1	J	355	PRO	2.0
1	K	457	VAL	2.0
1	E	405	GLU	2.0
1	F	363	THR	2.0
1	C	401	LYS	2.0
1	L	457	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	230	ASN	2.0
1	I	263	TYR	2.0
1	H	171	SER	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	G	1478	6/6	0.96	0.21	4.97	29,31,32,36	0
3	GOL	F	1478	6/6	0.96	0.21	3.15	37,41,44,45	0
3	GOL	C	1479	6/6	0.85	0.24	2.96	31,45,48,66	0
3	GOL	L	1478	6/6	0.73	0.28	2.94	44,49,55,58	0
3	GOL	D	1478	6/6	0.94	0.20	2.41	35,38,39,51	0
3	GOL	B	1478	6/6	0.94	0.18	1.95	40,43,46,46	0
3	GOL	C	1478	6/6	0.94	0.19	1.75	35,40,47,49	0
3	GOL	A	1479	6/6	0.86	0.19	1.67	39,49,57,62	0
3	GOL	E	1479	6/6	0.97	0.16	1.41	35,43,50,50	0
3	GOL	H	1478	6/6	0.96	0.18	1.28	31,35,41,42	0
3	GOL	A	1480	6/6	0.90	0.18	0.98	31,40,46,46	0
3	GOL	I	1478	6/6	0.95	0.16	0.91	41,43,45,45	0
3	GOL	D	1479	6/6	0.92	0.19	0.51	43,47,50,50	0
3	GOL	A	1478	6/6	0.98	0.16	0.19	26,28,28,29	0
3	GOL	L	1479	6/6	0.94	0.16	-0.70	44,53,54,67	0
3	GOL	J	1478	6/6	0.95	0.13	-0.82	37,39,41,42	0
3	GOL	B	1479	6/6	0.89	0.14	-1.92	44,47,49,55	0
2	NAG	B	1	14/15	0.80	0.15	-	61,95,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
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	L	1	14/15	0.58	0.29	-	91,116,127,128	0
2	NAG	F	1	14/15	0.38	0.33	-	83,113,122,127	0
2	NAG	K	1	14/15	0.74	0.28	-	107,121,129,129	0
2	NAG	H	1	14/15	0.65	0.26	-	100,133,144,145	0
2	NAG	E	1	14/15	0.75	0.25	-	69,87,96,103	0
2	NAG	C	1	14/15	0.65	0.23	-	87,120,133,134	0
3	GOL	E	1478	6/6	0.87	0.23	-	42,48,58,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.