



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:42 AM UTC

PDB ID : 3ZLE / pdb_00003zle
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

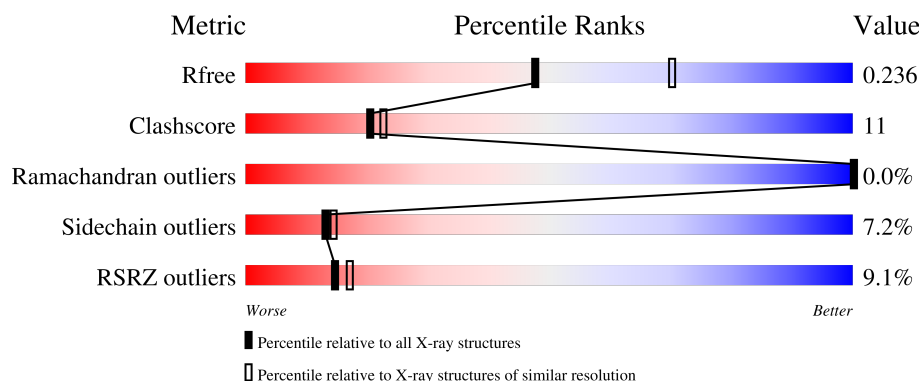
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

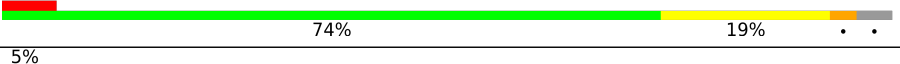
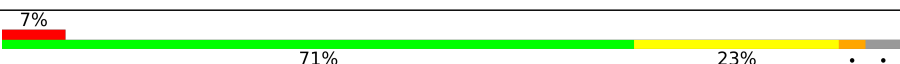
The reported resolution of this entry is 2.35 Å.

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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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 $\leq 5\%$. 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	
1	B	396	
1	C	396	
1	D	396	
1	E	396	

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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	

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
3	GOL	B	1479	-	-	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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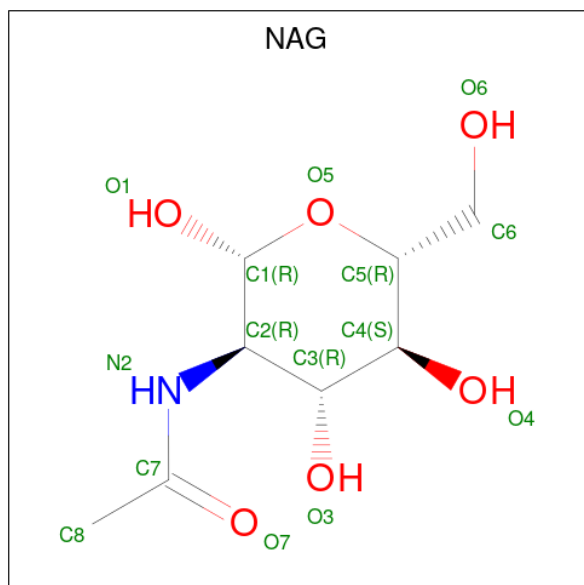
Chain	Residue	Modelled	Actual	Comment	Reference
H	481	ALA	-	expression tag	UNP B6K9M7
H	482	ALA	-	expression tag	UNP B6K9M7
H	483	ALA	-	expression tag	UNP B6K9M7
H	484	LEU	-	expression tag	UNP B6K9M7
H	485	VAL	-	expression tag	UNP B6K9M7
H	486	PRO	-	expression tag	UNP B6K9M7
H	487	ARG	-	expression tag	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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



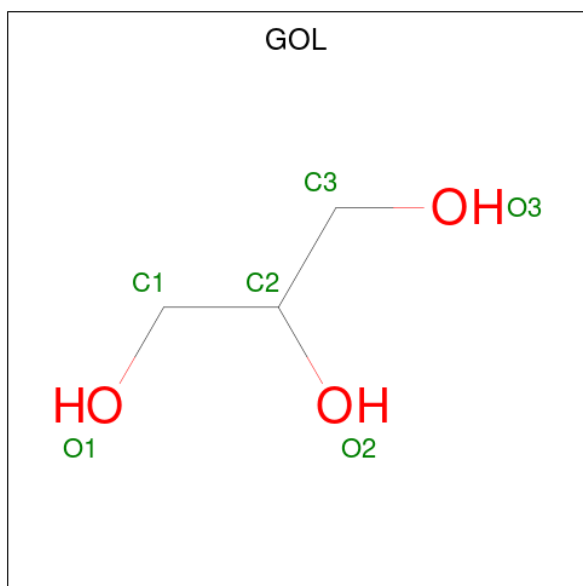
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		

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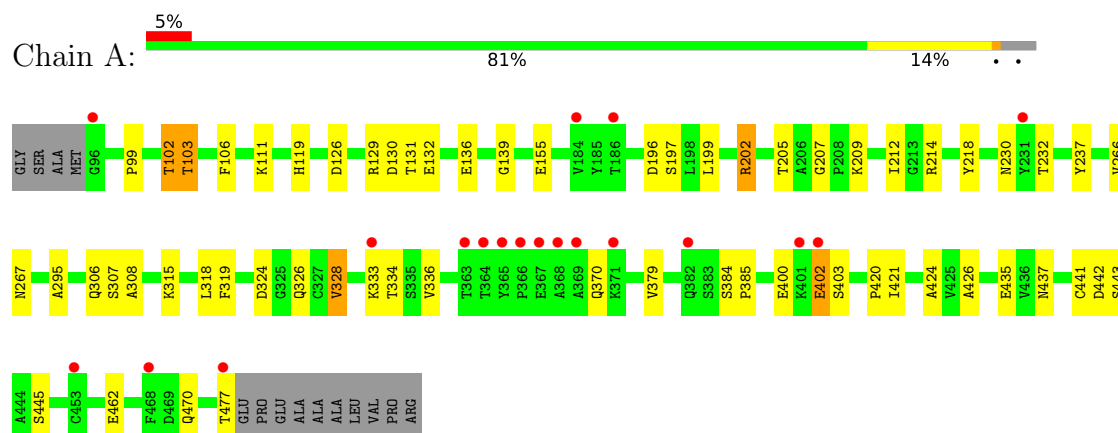
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	164	Total 164	O 164	0	0
4	I	91	Total 91	O 91	0	0
4	J	58	Total 58	O 58	0	0
4	K	88	Total 88	O 88	0	0
4	L	90	Total 90	O 90	0	0

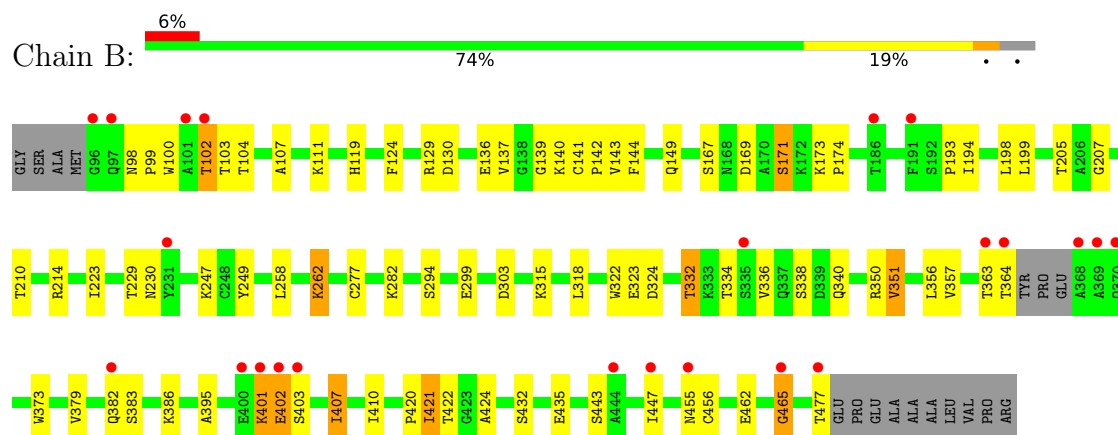
3 Residue-property plots

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.

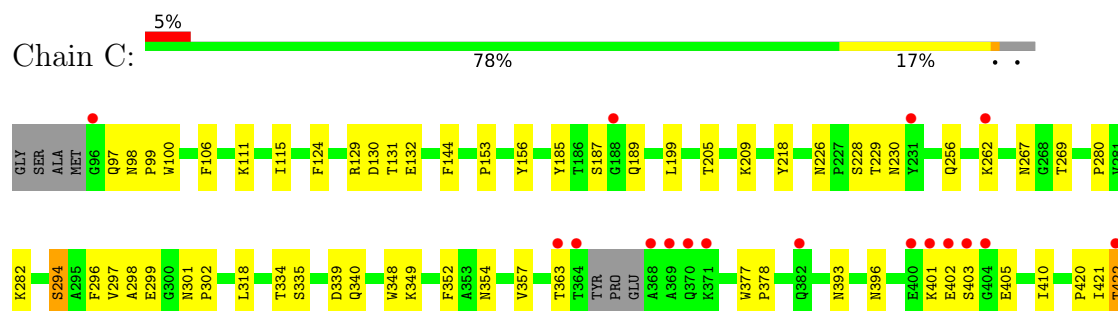
• Molecule 1: APICAL MEMBRANE ANTIGEN 1



• Molecule 1: APICAL MEMBRANE ANTIGEN 1

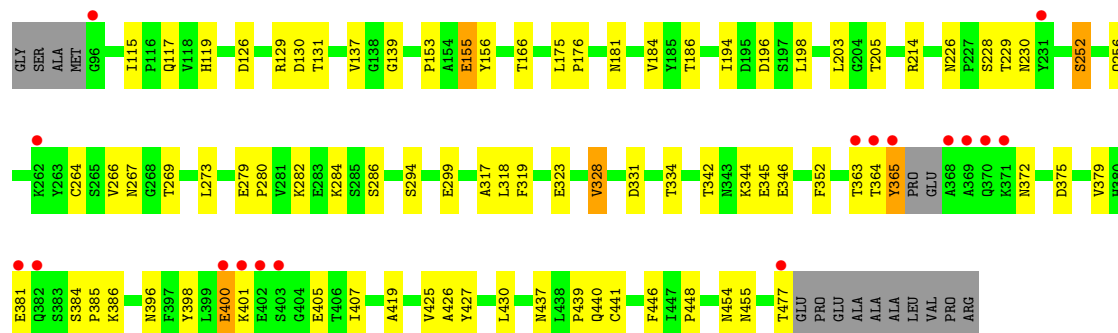
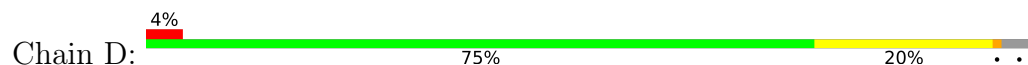


• Molecule 1: APICAL MEMBRANE ANTIGEN 1

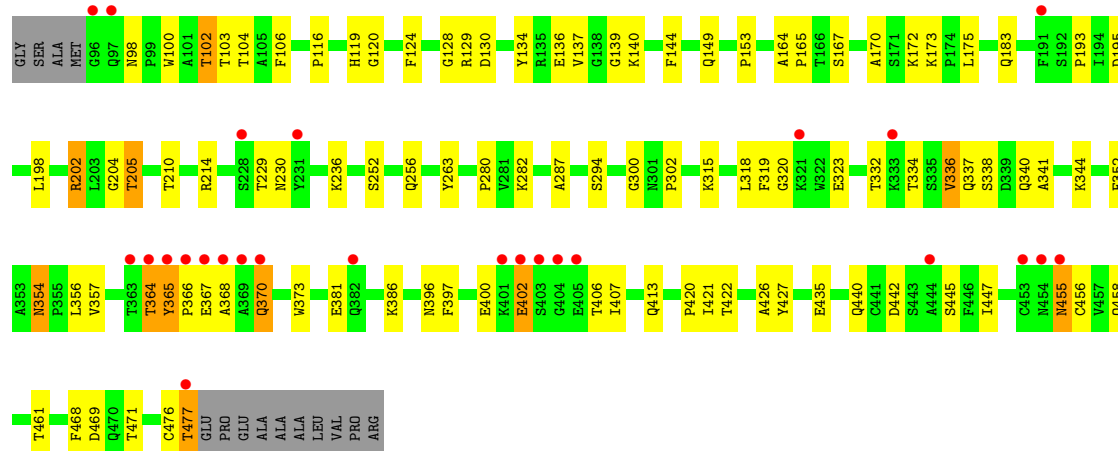




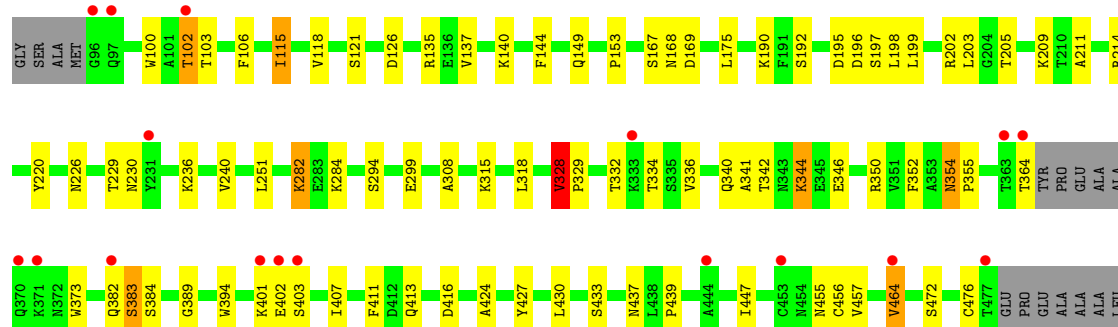
• Molecule 1: APICAL MEMBRANE ANTIGEN 1



• Molecule 1: APICAL MEMBRANE ANTIGEN 1



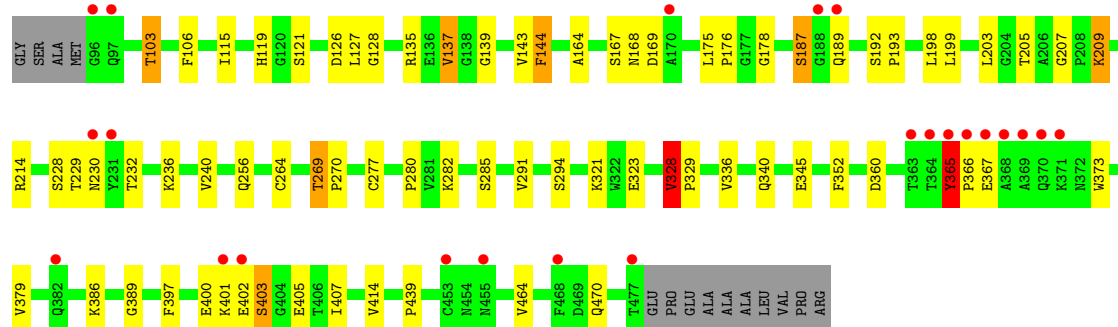
• Molecule 1: APICAL MEMBRANE ANTIGEN 1



VAL
PRO
ARG

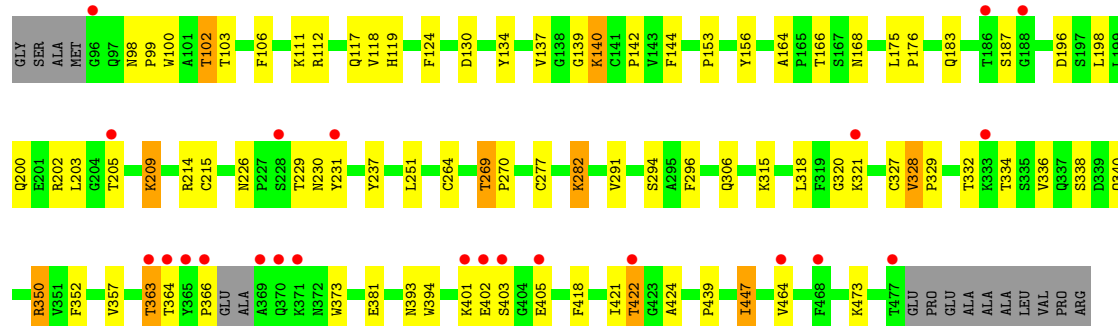
• Molecule 1: APICAL MEMBRANE ANTIGEN 1

Chain G: 



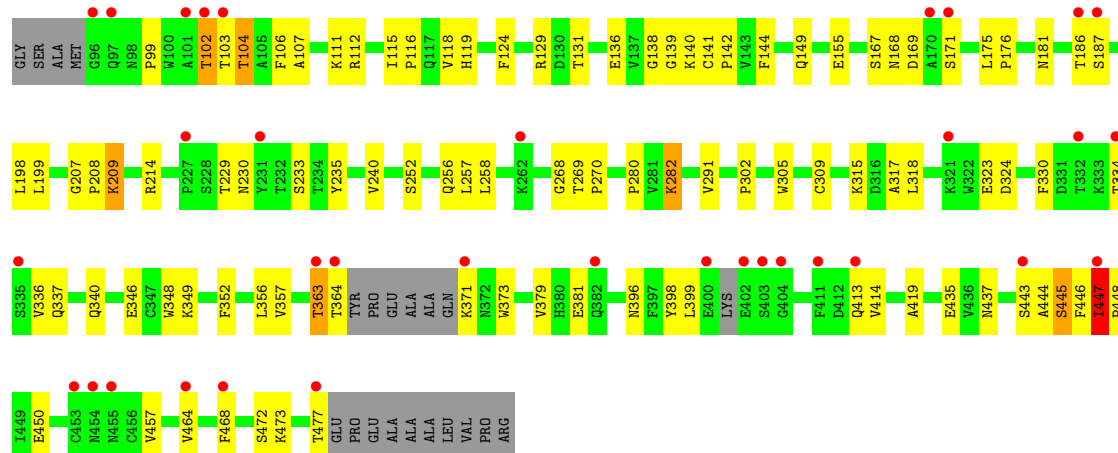
• Molecule 1: APICAL MEMBRANE ANTIGEN 1

Chain H: 



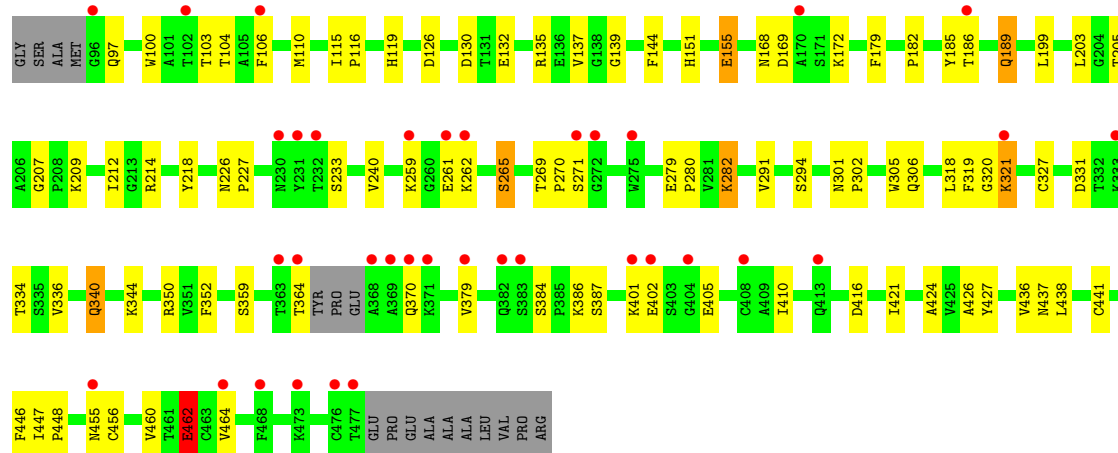
• Molecule 1: APICAL MEMBRANE ANTIGEN 1

Chain I: 



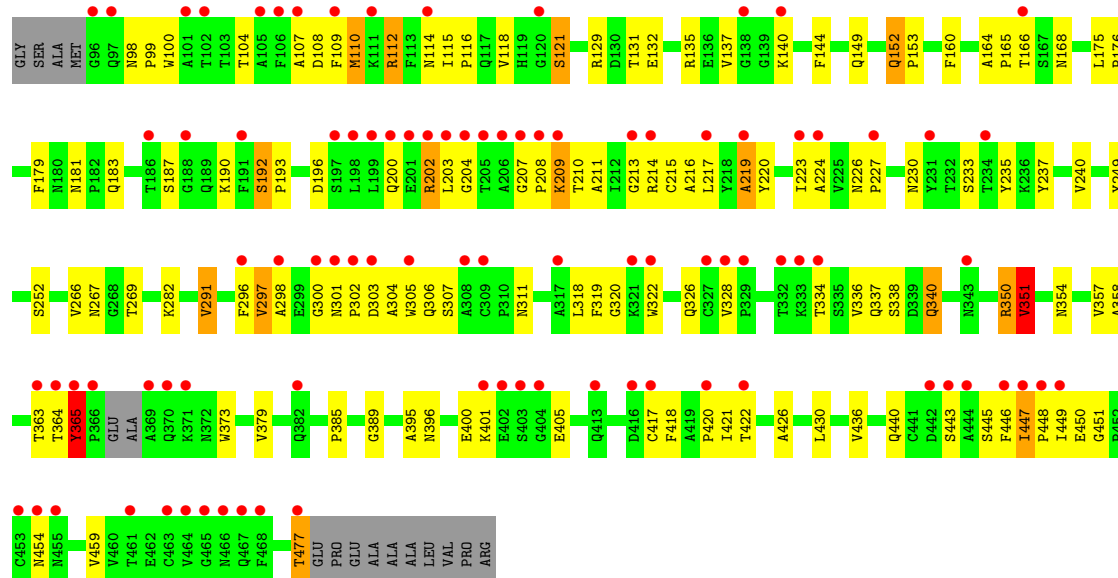
• Molecule 1: APICAL MEMBRANE ANTIGEN 1

Chain J: 



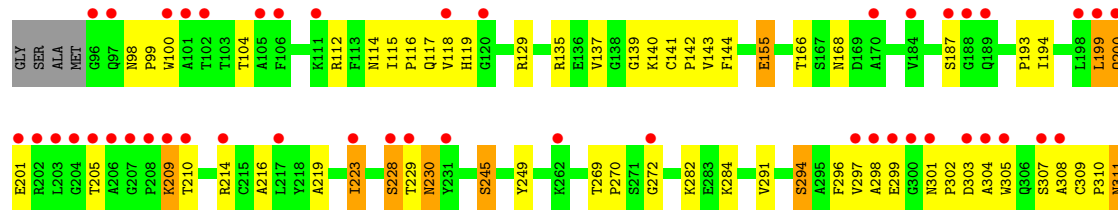
• Molecule 1: APICAL MEMBRANE ANTIGEN 1

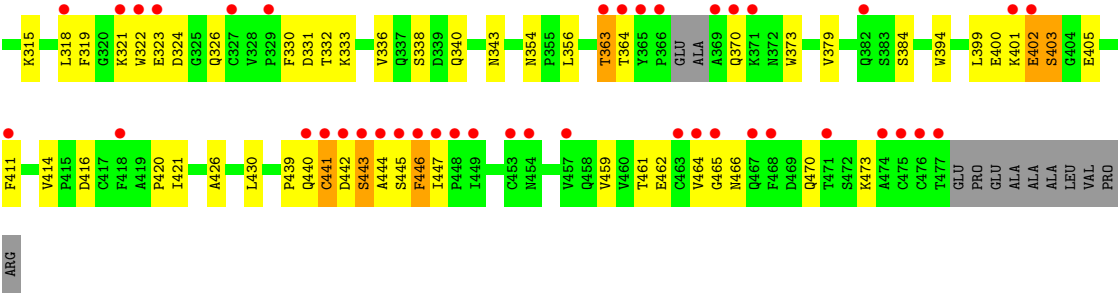
Chain K: 



• Molecule 1: APICAL MEMBRANE ANTIGEN 1

Chain L: 





4 Data and refinement statistics

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) 99.4 (78.04-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	76070 reflections (16.40%)	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)	0.35 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.96	3/2994 (0.1%)	0.91	1/4084 (0.0%)
1	B	0.93	0/2963	0.93	4/4039 (0.1%)
1	C	0.96	0/2963	0.92	2/4039 (0.0%)
1	D	0.95	0/2976	0.91	1/4057 (0.0%)
1	E	0.94	0/2994	0.91	6/4084 (0.1%)
1	F	0.89	0/2953	0.94	4/4025 (0.1%)
1	G	0.92	4/2994 (0.1%)	0.93	4/4084 (0.1%)
1	H	0.91	1/2979 (0.0%)	0.90	3/4062 (0.1%)
1	I	0.74	0/2945	0.86	3/4013 (0.1%)
1	J	0.73	0/2972	0.86	5/4051 (0.1%)
1	K	0.80	0/2990	0.92	9/4076 (0.2%)
1	L	0.82	0/2990	0.89	2/4076 (0.0%)
All	All	0.88	8/35713 (0.0%)	0.91	44/48690 (0.1%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	306	GLN	C-O	-7.66	1.14	1.24
1	A	307	SER	C-O	-6.44	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	308	ALA	C-O	-5.82	1.16	1.23
1	G	144	PHE	C-O	-5.62	1.17	1.24
1	G	143	VAL	C-O	-5.21	1.18	1.24
1	H	118	VAL	C-O	-5.19	1.17	1.24
1	G	137	VAL	N-CA	5.16	1.52	1.46
1	G	115	ILE	CA-CB	5.13	1.57	1.54

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	328	VAL	N-CA-C	9.46	116.91	107.55
1	K	365	TYR	N-CA-C	9.17	118.89	108.25
1	G	365	TYR	CA-C-N	7.23	127.16	119.85
1	G	365	TYR	C-N-CA	7.23	127.16	119.85
1	J	438	LEU	CA-C-N	-6.63	112.95	119.78
1	J	438	LEU	C-N-CA	-6.63	112.95	119.78
1	E	365	TYR	N-CA-C	-6.24	97.18	109.10
1	L	245	SER	N-CA-C	-6.16	105.73	113.18
1	E	287	ALA	N-CA-C	6.09	119.18	111.69
1	K	351	VAL	CB-CA-C	-6.08	104.07	112.04
1	E	175	LEU	CA-C-N	-6.01	113.77	120.14
1	E	175	LEU	C-N-CA	-6.01	113.77	120.14
1	I	447	ILE	N-CA-C	5.89	112.92	107.56
1	D	441	CYS	N-CA-C	-5.83	98.77	108.32
1	H	422	THR	N-CA-C	5.80	119.97	113.01
1	K	451	GLY	CA-C-N	5.74	126.20	120.52
1	K	451	GLY	C-N-CA	5.74	126.20	120.52
1	K	121	SER	N-CA-C	5.62	115.70	108.34
1	F	344	LYS	CB-CA-C	-5.61	101.52	110.84
1	K	152	GLN	CA-C-N	-5.54	113.99	119.92
1	K	152	GLN	C-N-CA	-5.54	113.99	119.92
1	B	350	ARG	N-CA-C	5.45	117.03	111.14
1	I	414	VAL	CA-C-N	5.44	125.34	119.85
1	I	414	VAL	C-N-CA	5.44	125.34	119.85
1	F	328	VAL	N-CA-C	5.43	112.93	107.55
1	C	422	THR	CB-CA-C	5.41	118.55	109.89
1	J	462	GLU	N-CA-C	5.39	116.46	108.86
1	F	115	ILE	CA-C-N	-5.35	113.02	118.85
1	F	115	ILE	C-N-CA	-5.35	113.02	118.85
1	L	343	ASN	N-CA-C	5.31	116.88	108.96
1	C	97	GLN	N-CA-C	5.29	118.21	109.85
1	G	414	VAL	CB-CA-C	-5.28	106.03	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	465	GLY	N-CA-C	-5.19	102.35	111.80
1	E	205	THR	N-CA-C	-5.18	105.70	112.23
1	A	441	CYS	N-CA-C	-5.16	100.29	109.06
1	K	160	PHE	N-CA-C	5.11	119.00	112.87
1	B	207	GLY	CA-C-N	5.06	125.05	119.89
1	B	207	GLY	C-N-CA	5.06	125.05	119.89
1	E	320	GLY	N-CA-C	5.05	119.71	111.27
1	H	164	ALA	CA-C-N	5.04	124.80	119.76
1	H	164	ALA	C-N-CA	5.04	124.80	119.76
1	K	219	ALA	N-CA-C	-5.04	105.86	111.36
1	J	97	GLN	N-CA-C	5.03	117.77	109.72
1	J	271	SER	N-CA-C	5.01	117.85	111.69

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 ⓘ

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	42	0
1	B	2885	0	2707	64	0
1	C	2885	0	2707	40	0
1	D	2897	0	2718	54	0
1	E	2913	0	2731	69	0
1	F	2875	0	2699	55	0
1	G	2913	0	2731	45	0
1	H	2899	0	2718	57	0
1	I	2865	0	2690	58	0
1	J	2891	0	2715	60	0
1	K	2907	0	2733	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2907	0	2731	104	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	4	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	3	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	8	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	2	0
4	K	88	0	0	13	0
4	L	90	0	0	5	0
All	All	36679	0	32872	758	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 (758) 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:K:209:LYS:CA	1:K:209:LYS:HE3	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:B:247:LYS:HZ2	3:B:1479:GOL:H11	1.20	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:K:110:MET:HE1	1:K:418:PHE:CD2	2.01	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:K:110:MET:HE2	1:K:110:MET:HA	1.55	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:K:204:GLY:C	1:K:207:GLY:H	1.83	0.85
1:L:301:ASN:HB3	1:L:304:ALA:HB2	1.56	0.85
1:A:403:SER:OG	4:A:2171:HOH:O	1.95	0.83
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:B:420:PRO:C	1:B:421:ILE:HD13	2.06	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:B:401:LYS:HD2	1.47	0.79
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:A:334:THR:OG1	4:A:2144:HOH:O	2.02	0.77
1:J:130:ASP:O	4:J:2004:HOH:O	2.03	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:O	1:K:220:TYR:CD1	2.39	0.76
1:H:140:LYS:NZ	4:H:2036:HOH:O	2.18	0.76
1:K:203:LEU:HD23	1:K:208:PRO:HD3	1.68	0.75
1:B:247:LYS:HZ2	3:B:1479:GOL:C1	1.99	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:J:269:THR:HA	1:J:270:PRO:C	2.12	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:CE2	2.21	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:K:110:MET:HE1	1:K:418:PHE:HD2	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:209:LYS:H	1:K:303:ASP:CG	1.94	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
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:B:247:LYS:HZ3	3:B:1479:GOL:H11	1.51	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: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:110:MET:HE2	1:K:110:MET:CA	2.18	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:446:PHE:CD1	1:L:446:PHE:C	2.71	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
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:A:209:LYS:NZ	4:A:2075:HOH:O	2.21	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: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:H	1:B:401:LYS:HD3	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:F:102:THR:HG22	1:F:103:THR:N	2.11	0.64
1:J:185:TYR:HD2	1:J:189:GLN:HG2	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:455:ASN:O	1:B:455:ASN:CG	2.41	0.63
1:L:440:GLN:CG	1:L:466:ASN:O	2.47	0.62
1:C:340:GLN:HG3	1:C:405:GLU:CD	2.24	0.62
1:L:115:ILE:HG12	1:L:430:LEU:HD12	1.82	0.62
1:H:447:ILE:O	1:H:447:ILE:CG2	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: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:D:117:GLN:CD	1:H:117:GLN:HE21	2.08	0.61
1:K:209:LYS:C	1:K:214:ARG:HH21	2.09	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:G:464:VAL:HG23	1:G:464:VAL:O	1.99	0.60
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:HG22	1:C:363:THR:O	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:L:210:THR:C	1:L:214:ARG:NH2	2.59	0.60
1:I:363:THR:O	1:I:364:THR:OG1	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:403:SER:HB2	1:G:405:GLU:HB2	1.84	0.59
1:E:364:THR:C	1:E:366:PRO:HD3	2.27	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
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: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
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:I:269:THR:HA	1:I:270:PRO:C	2.29	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:E:420:PRO:C	1:E:421:ILE:HD13	2.28	0.58
1:G:168:ASN:OD1	1:G:169:ASP:N	2.37	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:J:126:ASP:C	1:J:126:ASP:OD1	2.46	0.57
1:D:400:GLU:CG	1:D:407:ILE:HG13	2.28	0.57
1:L:331:ASP:O	1:L:332:THR:C	2.46	0.57
1:D:477:THR:HG22	1:D:477:THR:O	2.04	0.57
1:K:240:VAL:HA	1:K:291:VAL:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:446:PHE:C	1:L:446:PHE:HD1	2.13	0.56
1:A:196:ASP:CG	1:A:214:ARG:NH1	2.63	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: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
1:G:229:THR:O	1:G:230:ASN:HB2	2.04	0.56
1:F:115:ILE:HD13	1:F:430:LEU:HD12	1.88	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: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:D:126:ASP:OD1	1:D:126:ASP:C	2.50	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:L:137:VAL:C	1:L:294:SER:HB2	2.31	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: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:F:190:LYS:NZ	4:F:2046:HOH:O	2.33	0.54
1:J:455:ASN:CG	1:J:455:ASN:O	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG23	1:B:447:ILE:O	2.09	0.53
1:F:202:ARG:O	1:F:202:ARG:HG2	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: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
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: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:J:331:ASP:C	1:J:331:ASP:OD1	2.51	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: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: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: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: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:K:98:ASN:OD1	1:K:100:TRP:N	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:THR:O	1:B:363:THR:HG22	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
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: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: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:L:210:THR:C	1:L:214:ARG:HH21	2.18	0.50
1:I:175:LEU:HD12	1:I:176:PRO:HD2	1.92	0.50
1:B:315:LYS:HB3	1:B:435:GLU:HB3	1.94	0.50
1:F:135:ARG:CZ	1:F:384:SER:HB3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:311:ASN:ND2	1:L:311:ASN:N	2.58	0.50
1:I:464:VAL:HG23	1:I:464:VAL:O	2.11	0.49
1:B:318:LEU:HD21	1:B:424:ALA:HB1	1.94	0.49
1:F:196:ASP:CG	1:F:214:ARG:NH1	2.70	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:L:269:THR:HA	1:L:270:PRO:C	2.36	0.49
1:A:202:ARG:NH1	4:A:2067:HOH:O	2.41	0.49
1:A:442:ASP:OD2	1:A:445:SER:OG	2.28	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
4:E:2121:HOH:O	1:K:300:GLY:CA	2.61	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
1:J:110:MET:HE2	1:J:416:ASP:HA	1.94	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:K:110:MET:CE	1:K:418:PHE:CE2	2.94	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:J:151:HIS:HE2	1:J:279:GLU:CD	2.21	0.48
1:K:132:GLU:CD	1:K:233:SER:HB2	2.37	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
1:J:261[B]:GLU:CD	1:J:261[B]:GLU:H	2.21	0.48
1:K:98:ASN:OD1	1:K:100:TRP:HB2	2.12	0.48
1:E:442:ASP:OD2	1:E:445:SER:OG	2.21	0.48
1:F:226:ASN:C	1:F:226:ASN:OD1	2.56	0.48
1:G:127:LEU:HB3	1:G:135:ARG:HB3	1.95	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:HG23	1:B:194:ILE:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:359:SER:O	1:J:387:SER:HB3	2.14	0.48
1:L:301:ASN:CB	1:L:304:ALA:HB2	2.36	0.48
1:D:264:CYS:C	1:D:273:LEU:HD13	2.39	0.48
1:E:354:ASN:OD1	1:E:354:ASN:C	2.57	0.48
1:H:332:THR:HG22	1:H:338:SER:OG	2.14	0.48
1:B:130:ASP:OD1	1:B:386:LYS:NZ	2.47	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
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:O	1:L:464:VAL:CG2	2.59	0.47
1:E:476:CYS:O	1:E:477:THR:HB	2.13	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
2:K:1:NAG:C7	2:K:1:NAG:HO3	2.26	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:L:420:PRO:C	1:L:421:ILE:HG13	2.39	0.47
1:D:184:VAL:HG23	1:D:184:VAL:O	2.15	0.47
1:D:196:ASP:OD1	1:D:214:ARG:HD2	2.15	0.47
1:E:420:PRO:HG3	1:E:468:PHE:HB3	1.96	0.47
1:G:192:SER:HA	1:G:193:PRO:C	2.40	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:K:266:VAL:O	1:K:267:ASN:C	2.58	0.47
1:L:321:LYS:HA	1:L:416:ASP:OD1	2.14	0.47
1:G:167:SER:HA	1:G:373:TRP:CH2	2.50	0.47
1:K:110:MET:CA	1:K:110:MET:CE	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:114:ASN:O	1:L:118:VAL:HG23	2.15	0.47
1:D:137:VAL:HG12	1:D:294:SER:HB3	1.96	0.47
1:L:98:ASN:OD1	1:L:100:TRP:N	2.47	0.47
1:L:298:ALA:HA	1:L:302:PRO:HA	1.97	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:O7	2:E:1:NAG:O3	2.30	0.46
1:K:179:PHE:N	1:K:179:PHE:CD1	2.83	0.46
1:C:349:LYS:HD2	4:C:2150:HOH:O	2.15	0.46
1:H:269:THR:HA	1:H:270:PRO:C	2.41	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
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: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:181:ASN:HA	1:D:252:SER:HB3	1.98	0.46
1:D:194:ILE:HG23	1:D:194:ILE:O	2.15	0.46
1:F:196:ASP:OD2	1:F:214:ARG:NH1	2.49	0.46
1:G:269:THR:HA	1:G:270:PRO:C	2.39	0.46
1:K:132:GLU:OE2	1:K:233:SER:HB2	2.16	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:416:ASP:OD1	1:F:416:ASP:C	2.58	0.45
1:K:135:ARG:O	1:K:235:TYR:OH	2.17	0.45
1:L:209:LYS:C	1:L:214:ARG:HH21	2.24	0.45
1:F:211:ALA:HA	1:F:214:ARG:NH1	2.32	0.45
3:F:1478:GOL:C1	4:F:2129:HOH:O	2.62	0.45
1:G:128:GLY:O	1:G:386:LYS:HE3	2.16	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:N	1:K:296:PHE:CD1	2.85	0.45
1:A:315:LYS:HB3	1:A:435:GLU:HB3	1.98	0.45
1:C:199:LEU:HD21	1:C:218:TYR:CD1	2.52	0.45
3:C:1478:GOL:H11	4:C:2176:HOH:O	2.17	0.45
1:D:266:VAL:O	1:D:267:ASN:C	2.60	0.45
1:G:464:VAL:O	1:G:464:VAL:CG2	2.64	0.45
1:I:112:ARG:NH1	1:I:309:CYS:O	2.48	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
4:A:2194:HOH:O	1:E:370:GLN:OE1	2.20	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
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
1:K:320:GLY:HA3	1:K:328:VAL:O	2.17	0.44
2:K:1:NAG:O3	2:K:1:NAG:O7	2.30	0.44
1:L:440:GLN:HG2	1:L:466:ASN:O	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:K:447:ILE:CD1	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:B:455:ASN:O	1:B:456:CYS:HB2	2.16	0.44
1:C:318:LEU:HD22	1:C:396:ASN:HB3	1.99	0.44
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: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:A:126:ASP:OD1	1:A:126:ASP:C	2.58	0.44
1:F:126:ASP:OD1	1:F:126:ASP:C	2.60	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:464:VAL:O	1:J:464:VAL:HG13	2.17	0.44
1:L:249:TYR:OH	4:L:2045:HOH:O	2.21	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:K:209:LYS:N	1:K:303:ASP:CG	2.66	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:G:199:LEU:HD23	1:G:199:LEU:HA	1.68	0.43
1:G:203:LEU:HD23	1:G:203:LEU:HA	1.87	0.43
1:K:104:THR:O	1:K:108:ASP:HB2	2.18	0.43
1:K:179:PHE:N	1:K:179:PHE:HD1	2.16	0.43
1:K:364:THR:O	1:K:365:TYR:HD1	2.01	0.43
1:A:196:ASP:CG	1:A:214:ARG:HH11	2.25	0.43
1:B:402:GLU:H	1:B:402:GLU:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:137:VAL:HG12	1:L:294:SER:HB2	2.00	0.43
1:A:199:LEU:HD23	1:A:199:LEU:HA	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:I:477:THR:O	1:I:477:THR:HG22	2.18	0.43
1:C:296:PHE:C	1:C:298:ALA:N	2.75	0.43
1:D:115:ILE:HG12	1:D:430:LEU:HD12	2.01	0.43
1:I:282:LYS:HG3	1:I:348:TRP:CZ2	2.53	0.43
1:I:447:ILE:O	1:I:447:ILE:CG2	2.67	0.43
1:K:168:ASN:HB2	1:K:373:TRP:CD1	2.54	0.43
1:K:208:PRO:CB	1:K:302:PRO:HG2	2.49	0.43
1:A:266:VAL:O	1:A:267:ASN:C	2.61	0.43
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:O	1:H:202:ARG:HG2	2.17	0.43
1:H:464:VAL:HG23	1:H:464:VAL:O	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:318:LEU:HD22	1:D:396:ASN:CG	2.43	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:H	1:J:155:GLU:HG3	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:135:ARG:CZ	1:J:384:SER:HB3	2.49	0.43
1:J:179:PHE:N	1:J:179:PHE:CD1	2.87	0.43
1:J:279:GLU:HA	1:J:280:PRO:HD3	1.85	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:O	1:F:464:VAL:HG22	2.19	0.43
1:G:397:PHE:CD1	1:G:397:PHE:C	2.97	0.43
1:K:210:THR:HB	1:K:305:TRP:HZ2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:98:ASN:HA	1:L:99:PRO:HD2	1.88	0.43
1:A:370:GLN:HE21	1:C:477:THR:HG22	1.83	0.42
3:C:1478:GOL:C1	4:C:2176:HOH:O	2.66	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: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:C:403:SER:HB2	1:C:405:GLU:H	1.84	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:J:455:ASN:O	1:J:456:CYS:HB2	2.18	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:K:220:TYR:CD1	1:K:220:TYR:C	2.98	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE2	1:I:371:LYS:HB3	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:D:331:ASP:OD1	1:D:331:ASP:C	2.63	0.41
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:135:ARG:NH2	1:K:385:PRO:O	2.53	0.41
1:K:350:ARG:HD3	4:K:2078:HOH:O	2.20	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:G:135:ARG:NH1	1:G:360:ASP:O	2.46	0.41
1:H:98:ASN:HA	1:H:99:PRO:HD2	1.85	0.41
1:H:393:ASN:HB2	1:H:394:TRP:CE3	2.55	0.41
1:J:226:ASN:HA	1:J:227:PRO:HD3	1.93	0.41
1:K:152:GLN:O	1:K:153:PRO:C	2.62	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:HD1	1:D:365:TYR:HA	1.67	0.41
1:J:179:PHE:N	1:J:179:PHE:HD1	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:104:THR:HG21	1:L:129:ARG:HA	2.02	0.41
1:B:421:ILE:HD13	1:B:421:ILE:N	2.31	0.41
1:H:315:LYS:O	1:H:315:LYS:HG3	2.20	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:130:ASP:OD2	1:D:386:LYS:NZ	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:366:PRO:O	1:G:367:GLU:C	2.60	0.41
1:I:167:SER:HA	1:I:373:TRP:CH2	2.56	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:B:338:SER:HB2	1:B:407:ILE:HD12	2.03	0.41
1:C:229:THR:O	1:C:230:ASN:HB2	2.21	0.41
1:C:267:ASN:O	1:C:267:ASN:CG	2.64	0.41
1:C:335:SER:HB3	1:C:410:ILE:O	2.20	0.41
1:C:377:TRP:HA	1:C:378:PRO:HD3	1.94	0.41
1:G:198:LEU:HD23	1:G:198:LEU:HA	1.89	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:129:ARG:CZ	1:K:296:PHE:CE2	3.04	0.41
1:K:164:ALA:HB1	1:K:165:PRO:HD2	2.02	0.41
1:K:224:ALA:HB2	1:K:235:TYR:O	2.21	0.41
1:K:226:ASN:HA	1:K:227:PRO:HD3	1.95	0.41
1:K:298:ALA:HA	1:K:302:PRO:HA	2.03	0.41
1:L:140:LYS:HA	1:L:140:LYS:HD2	1.84	0.41
1:L:331:ASP:C	1:L:333:LYS:N	2.77	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:I:169:ASP:OD1	1:I:169:ASP:C	2.62	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:G:126:ASP:OD1	1:G:126:ASP:C	2.63	0.40
1:H:226:ASN:HB3	1:H:229:THR:OG1	2.20	0.40
1:I:446:PHE:CD1	1:I:446:PHE:C	2.99	0.40
1:L:309:CYS:O	1:L:311:ASN:ND2	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:J:350:ARG:HD3	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:K:400:GLU:O	1:K:401:LYS:C	2.63	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:130:ASP:C	1:D:131:THR:HG23	2.47	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:D:454:ASN:O	1:D:455:ASN:C	2.64	0.40
1:E:461:THR:HA	1:E:469:ASP:O	2.22	0.40
1:F:407:ILE:HD13	1:F:407:ILE:HA	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	36	43
1	J	376/396 (95%)	361 (96%)	14 (4%)	1 (0%)	36	43
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 ⓘ

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%)	299 (95%)	16 (5%)	21	26
1	B	312/324 (96%)	289 (93%)	23 (7%)	13	14
1	C	312/324 (96%)	298 (96%)	14 (4%)	24	32
1	D	313/324 (97%)	295 (94%)	18 (6%)	18	22
1	E	315/324 (97%)	292 (93%)	23 (7%)	13	14
1	F	312/324 (96%)	290 (93%)	22 (7%)	13	15
1	G	315/324 (97%)	300 (95%)	15 (5%)	23	29
1	H	314/324 (97%)	290 (92%)	24 (8%)	12	13
1	I	311/324 (96%)	285 (92%)	26 (8%)	10	11
1	J	313/324 (97%)	293 (94%)	20 (6%)	16	18
1	K	315/324 (97%)	280 (89%)	35 (11%)	6	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	315/324 (97%)	280 (89%)	35 (11%)	6	5
All	All	3762/3888 (97%)	3491 (93%)	271 (7%)	13	14

All (271) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	THR
1	A	103	THR
1	A	130	ASP
1	A	155	GLU
1	A	197	SER
1	A	202	ARG
1	A	205	THR
1	A	232	THR
1	A	328	VAL
1	A	336	VAL
1	A	379	VAL
1	A	402	GLU
1	A	421	ILE
1	A	443	SER
1	A	462	GLU
1	A	477	THR
1	B	102	THR
1	B	111	LYS
1	B	143	VAL
1	B	171	SER
1	B	198	LEU
1	B	205	THR
1	B	223	ILE
1	B	262	LYS
1	B	332	THR
1	B	334	THR
1	B	340	GLN
1	B	351	VAL
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	421	ILE

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Mol	Chain	Res	Type
1	B	422	THR
1	B	462	GLU
1	B	477	THR
1	C	111	LYS
1	C	130	ASP
1	C	205	THR
1	C	262	LYS
1	C	269	THR
1	C	294	SER
1	C	299	GLU
1	C	334	THR
1	C	354	ASN
1	C	401	LYS
1	C	402	GLU
1	C	421	ILE
1	C	422	THR
1	C	464	VAL
1	D	155	GLU
1	D	166	THR
1	D	186	THR
1	D	198	LEU
1	D	205	THR
1	D	228	SER
1	D	252	SER
1	D	269	THR
1	D	286	SER
1	D	328	VAL
1	D	334	THR
1	D	363	THR
1	D	365	TYR
1	D	379	VAL
1	D	381	GLU
1	D	400	GLU
1	D	401	LYS
1	D	405	GLU
1	E	102	THR
1	E	104	THR
1	E	140	LYS
1	E	149	GLN
1	E	198	LEU
1	E	202	ARG
1	E	252	SER

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Mol	Chain	Res	Type
1	E	323	GLU
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	413	GLN
1	E	422	THR
1	E	440	GLN
1	E	447	ILE
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	205	THR
1	F	282	LYS
1	F	299	GLU
1	F	328	VAL
1	F	332	THR
1	F	334	THR
1	F	336	VAL
1	F	340	GLN
1	F	342	THR
1	F	354	ASN
1	F	364	THR
1	F	383	SER
1	F	401	LYS
1	F	402	GLU
1	F	403	SER
1	F	413	GLN
1	F	447	ILE
1	F	464	VAL
1	G	103	THR
1	G	187	SER
1	G	205	THR
1	G	209	LYS

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Mol	Chain	Res	Type
1	G	228	SER
1	G	232	THR
1	G	269	THR
1	G	285	SER
1	G	328	VAL
1	G	336	VAL
1	G	365	TYR
1	G	379	VAL
1	G	401	LYS
1	G	402	GLU
1	G	403	SER
1	H	102	THR
1	H	111	LYS
1	H	140	LYS
1	H	166	THR
1	H	187	SER
1	H	198	LEU
1	H	205	THR
1	H	209	LYS
1	H	269	THR
1	H	282	LYS
1	H	321	LYS
1	H	328	VAL
1	H	334	THR
1	H	336	VAL
1	H	340	GLN
1	H	350	ARG
1	H	363	THR
1	H	381	GLU
1	H	401	LYS
1	H	402	GLU
1	H	421	ILE
1	H	422	THR
1	H	447	ILE
1	H	473	LYS
1	I	102	THR
1	I	104	THR
1	I	131	THR
1	I	149	GLN
1	I	171	SER
1	I	186	THR
1	I	187	SER

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Mol	Chain	Res	Type
1	I	198	LEU
1	I	209	LYS
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	349	LYS
1	I	356	LEU
1	I	363	THR
1	I	379	VAL
1	I	381	GLU
1	I	399	LEU
1	I	443	SER
1	I	445	SER
1	I	447	ILE
1	I	450	GLU
1	I	473	LYS
1	J	104	THR
1	J	155	GLU
1	J	186	THR
1	J	189	GLN
1	J	205	THR
1	J	259	LYS
1	J	262	LYS
1	J	265	SER
1	J	282	LYS
1	J	321	LYS
1	J	334	THR
1	J	336	VAL
1	J	340	GLN
1	J	364	THR
1	J	370	GLN
1	J	379	VAL
1	J	401	LYS
1	J	402	GLU
1	J	447	ILE
1	J	462	GLU
1	K	110	MET
1	K	112	ARG
1	K	131	THR

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Mol	Chain	Res	Type
1	K	149	GLN
1	K	166	THR
1	K	187	SER
1	K	192	SER
1	K	196	ASP
1	K	200	GLN
1	K	202[A]	ARG
1	K	202[B]	ARG
1	K	209	LYS
1	K	223	ILE
1	K	269	THR
1	K	282	LYS
1	K	291	VAL
1	K	297	VAL
1	K	307	SER
1	K	334	THR
1	K	336	VAL
1	K	338	SER
1	K	340	GLN
1	K	350	ARG
1	K	351	VAL
1	K	363	THR
1	K	365	TYR
1	K	379	VAL
1	K	422	THR
1	K	436	VAL
1	K	440	GLN
1	K	443	SER
1	K	447	ILE
1	K	450	GLU
1	K	454	ASN
1	K	477	THR
1	L	104	THR
1	L	143	VAL
1	L	155	GLU
1	L	166	THR
1	L	187	SER
1	L	199	LEU
1	L	200	GLN
1	L	201	GLU
1	L	205	THR
1	L	209	LYS

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Mol	Chain	Res	Type
1	L	223	ILE
1	L	228	SER
1	L	230	ASN
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	363	THR
1	L	364	THR
1	L	370	GLN
1	L	379	VAL
1	L	399	LEU
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	462	GLU
1	L	473	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	370	GLN
1	C	200	GLN
1	C	413	GLN
1	D	149	GLN
1	D	189	GLN
1	D	458	GLN
1	E	183	GLN
1	E	370	GLN
1	F	230	ASN
1	F	458	GLN
1	G	149	GLN
1	G	380	HIS
1	G	454	ASN

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Mol	Chain	Res	Type
1	I	183	GLN
1	J	183	GLN
1	J	458	GLN
1	J	470	GLN
1	K	230	ASN
1	K	370	GLN
1	K	413	GLN
1	K	458	GLN
1	L	114	ASN
1	L	152	GLN
1	L	183	GLN
1	L	311	ASN
1	L	326	GLN
1	L	413	GLN
1	L	466	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	L	1479	-	5,5,5	0.41	0	5,5,5	0.48	0
2	NAG	C	1	1	14,14,15	0.76	0	17,19,21	1.16	1 (5%)
3	GOL	B	1479	-	5,5,5	0.47	0	5,5,5	0.76	0
2	NAG	F	1	1	14,14,15	0.30	0	17,19,21	0.57	0
3	GOL	E	1479	-	5,5,5	0.27	0	5,5,5	0.33	0
3	GOL	C	1478	-	5,5,5	0.49	0	5,5,5	0.60	0
3	GOL	D	1478	-	5,5,5	0.15	0	5,5,5	0.70	0
2	NAG	A	1	1	14,14,15	0.30	0	17,19,21	0.56	0
2	NAG	K	1	1	14,14,15	0.36	0	17,19,21	0.96	0
2	NAG	G	1	1	14,14,15	0.29	0	17,19,21	0.56	0
3	GOL	I	1478	-	5,5,5	0.30	0	5,5,5	0.68	0
3	GOL	G	1478	-	5,5,5	0.34	0	5,5,5	0.84	0
3	GOL	A	1478	-	5,5,5	0.18	0	5,5,5	0.63	0
3	GOL	L	1478	-	5,5,5	0.68	0	5,5,5	0.51	0
3	GOL	A	1480	-	5,5,5	0.57	0	5,5,5	0.58	0
3	GOL	E	1478	-	5,5,5	0.51	0	5,5,5	0.92	0
3	GOL	C	1479	-	5,5,5	0.66	0	5,5,5	0.51	0
2	NAG	B	1	1	14,14,15	0.83	0	17,19,21	1.12	1 (5%)
3	GOL	J	1478	-	5,5,5	0.37	0	5,5,5	0.76	0
2	NAG	H	1	1	14,14,15	0.29	0	17,19,21	0.56	0
3	GOL	H	1478	-	5,5,5	0.22	0	5,5,5	0.66	0
2	NAG	L	1	1	14,14,15	0.30	0	17,19,21	0.56	0
3	GOL	F	1478	-	5,5,5	0.23	0	5,5,5	0.68	0
3	GOL	D	1479	-	5,5,5	0.65	0	5,5,5	0.62	0
2	NAG	E	1	1	14,14,15	0.28	0	17,19,21	0.56	0
3	GOL	B	1478	-	5,5,5	0.25	0	5,5,5	0.53	0
3	GOL	A	1479	-	5,5,5	0.73	0	5,5,5	0.46	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	L	1479	-	-	4/4/4/4	-
2	NAG	C	1	1	-	4/6/23/26	0/1/1/1
3	GOL	B	1479	-	-	1/4/4/4	-
2	NAG	F	1	1	-	4/6/23/26	0/1/1/1
3	GOL	E	1479	-	-	2/4/4/4	-
3	GOL	C	1478	-	-	2/4/4/4	-
3	GOL	D	1478	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1	1	-	4/6/23/26	0/1/1/1
2	NAG	K	1	1	-	5/6/23/26	0/1/1/1
2	NAG	G	1	1	-	2/6/23/26	0/1/1/1
3	GOL	I	1478	-	-	2/4/4/4	-
3	GOL	G	1478	-	-	2/4/4/4	-
3	GOL	A	1478	-	-	0/4/4/4	-
3	GOL	L	1478	-	-	4/4/4/4	-
3	GOL	A	1480	-	-	1/4/4/4	-
3	GOL	E	1478	-	-	4/4/4/4	-
3	GOL	C	1479	-	-	1/4/4/4	-
2	NAG	B	1	1	-	2/6/23/26	0/1/1/1
3	GOL	J	1478	-	-	0/4/4/4	-
2	NAG	H	1	1	-	4/6/23/26	0/1/1/1
3	GOL	H	1478	-	-	4/4/4/4	-
2	NAG	L	1	1	-	5/6/23/26	0/1/1/1
3	GOL	F	1478	-	-	1/4/4/4	-
3	GOL	D	1479	-	-	2/4/4/4	-
2	NAG	E	1	1	-	4/6/23/26	0/1/1/1
3	GOL	B	1478	-	-	3/4/4/4	-
3	GOL	A	1479	-	-	1/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	2.13	115.04	112.19
2	C	1	NAG	O5-C1-C2	-2.02	108.16	111.29

There are no chirality outliers.

All (70) 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
2	F	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	L	1	NAG	C1-C2-N2-C7
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
3	B	1478	GOL	C1-C2-C3-O3
3	B	1478	GOL	O2-C2-C3-O3
3	C	1478	GOL	O1-C1-C2-C3
3	D	1478	GOL	O1-C1-C2-O2
3	D	1478	GOL	O1-C1-C2-C3
3	D	1479	GOL	O1-C1-C2-C3
3	E	1478	GOL	C1-C2-C3-O3
3	G	1478	GOL	C1-C2-C3-O3
3	H	1478	GOL	O1-C1-C2-C3
3	H	1478	GOL	C1-C2-C3-O3
3	L	1478	GOL	O1-C1-C2-C3
3	L	1478	GOL	C1-C2-C3-O3
3	L	1479	GOL	O1-C1-C2-C3
3	L	1479	GOL	C1-C2-C3-O3
2	K	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	K	1	NAG	C8-C7-N2-C2
3	L	1478	GOL	O1-C1-C2-O2
2	H	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O7-C7-N2-C2
3	E	1478	GOL	O1-C1-C2-C3
3	E	1479	GOL	O1-C1-C2-C3
3	I	1478	GOL	O1-C1-C2-C3
3	C	1478	GOL	O1-C1-C2-O2
3	E	1478	GOL	O2-C2-C3-O3
3	G	1478	GOL	O2-C2-C3-O3
3	H	1478	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	H	1478	GOL	O2-C2-C3-O3
3	I	1478	GOL	O1-C1-C2-O2
3	L	1478	GOL	O2-C2-C3-O3
3	L	1479	GOL	O1-C1-C2-O2
2	E	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C3-C2-N2-C7
2	K	1	NAG	C3-C2-N2-C7
3	E	1479	GOL	O1-C1-C2-O2
3	L	1479	GOL	O2-C2-C3-O3
2	B	1	NAG	C4-C5-C6-O6
2	A	1	NAG	C4-C5-C6-O6
3	A	1480	GOL	O2-C2-C3-O3
3	D	1479	GOL	O1-C1-C2-O2
3	E	1478	GOL	O1-C1-C2-O2
3	B	1479	GOL	O1-C1-C2-O2
2	A	1	NAG	O5-C5-C6-O6
3	C	1479	GOL	O2-C2-C3-O3
3	F	1478	GOL	O2-C2-C3-O3
3	A	1479	GOL	O2-C2-C3-O3
3	B	1478	GOL	O1-C1-C2-O2
2	C	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2

There are no ring outliers.

15 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1479	GOL	4	0
2	F	1	NAG	2	0
3	C	1478	GOL	3	0
3	D	1478	GOL	2	0
2	A	1	NAG	2	0
2	K	1	NAG	5	0
3	I	1478	GOL	1	0
3	G	1478	GOL	1	0
3	A	1480	GOL	2	0
3	E	1478	GOL	3	0
3	J	1478	GOL	2	0
3	H	1478	GOL	3	0
2	L	1	NAG	2	0
3	F	1478	GOL	3	0
2	E	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	382/396 (96%)	0.14	19 (4%) 34 40	17, 32, 68, 130	0
1	B	379/396 (95%)	0.16	23 (6%) 27 31	14, 32, 66, 91	0
1	C	379/396 (95%)	0.13	18 (4%) 36 42	17, 32, 65, 95	0
1	D	380/396 (95%)	0.12	17 (4%) 38 44	17, 31, 64, 101	0
1	E	382/396 (96%)	0.19	26 (6%) 23 26	16, 32, 63, 105	0
1	F	377/396 (95%)	0.20	17 (4%) 38 44	19, 33, 66, 106	0
1	G	382/396 (96%)	0.26	23 (6%) 27 31	18, 33, 71, 93	0
1	H	380/396 (95%)	0.23	23 (6%) 27 31	20, 34, 66, 99	0
1	I	375/396 (94%)	0.56	34 (9%) 15 17	20, 42, 74, 108	1 (0%)
1	J	379/396 (95%)	0.68	36 (9%) 14 16	24, 44, 78, 104	1 (0%)
1	K	380/396 (95%)	1.25	93 (24%) 2 1	26, 45, 83, 111	1 (0%)
1	L	380/396 (95%)	1.18	87 (22%) 2 1	26, 45, 84, 116	1 (0%)
All	All	4555/4752 (95%)	0.42	416 (9%) 15 17	14, 37, 74, 130	4 (0%)

All (416) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	PRO	9.7
1	H	365	TYR	9.0
1	L	365	TYR	8.9
1	D	365	TYR	8.6
1	E	366	PRO	8.4
1	G	365	TYR	8.1
1	H	369	ALA	7.9
1	L	300	GLY	7.5
1	B	364	THR	7.2
1	B	368	ALA	7.1
1	C	364	THR	7.0

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Mol	Chain	Res	Type	RSRZ
1	E	365	TYR	6.8
1	G	477	THR	6.8
1	I	477	THR	6.7
1	A	477	THR	6.6
1	A	365	TYR	6.6
1	J	364	THR	6.6
1	G	367	GLU	6.4
1	K	205	THR	6.4
1	E	369	ALA	6.3
1	L	369	ALA	6.3
1	E	368	ALA	6.2
1	K	300	GLY	6.2
1	I	364	THR	6.2
1	K	369	ALA	6.1
1	L	208	PRO	6.0
1	K	365	TYR	6.0
1	K	366	PRO	6.0
1	L	477	THR	5.9
1	D	364	THR	5.9
1	J	477	THR	5.9
1	H	366	PRO	5.8
1	G	366	PRO	5.8
1	D	96	GLY	5.6
1	F	364	THR	5.4
1	D	477	THR	5.4
1	K	202[A]	ARG	5.4
1	L	370	GLN	5.4
1	I	363	THR	5.4
1	I	231	TYR	5.4
1	E	367	GLU	5.3
1	L	366	PRO	5.3
1	B	96	GLY	5.3
1	C	368	ALA	5.2
1	D	401	LYS	5.1
1	I	96	GLY	5.1
1	A	401	LYS	5.1
1	K	364	THR	5.1
1	B	369	ALA	5.0
1	J	369	ALA	5.0
1	J	96	GLY	5.0
1	G	368	ALA	5.0
1	E	370	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
1	K	363	THR	4.9
1	H	477	THR	4.9
1	B	401	LYS	4.9
1	D	231	TYR	4.9
1	K	204	GLY	4.8
1	K	231	TYR	4.8
1	B	477	THR	4.7
1	I	102	THR	4.7
1	K	402	GLU	4.7
1	F	464	VAL	4.7
1	E	364	THR	4.7
1	I	371	LYS	4.7
1	J	231	TYR	4.6
1	L	205	THR	4.6
1	G	363	THR	4.5
1	C	401	LYS	4.5
1	F	402	GLU	4.5
1	L	444	ALA	4.5
1	G	96	GLY	4.4
1	F	453	CYS	4.4
1	D	402	GLU	4.4
1	K	468	PHE	4.4
1	C	477	THR	4.4
1	D	363	THR	4.3
1	K	477	THR	4.3
1	H	364	THR	4.3
1	L	371	LYS	4.3
1	H	363	THR	4.3
1	E	96	GLY	4.3
1	K	370	GLN	4.3
1	G	401	LYS	4.3
1	L	401	LYS	4.3
1	J	368	ALA	4.3
1	L	111	LYS	4.2
1	A	364	THR	4.2
1	K	207	GLY	4.2
1	L	442	ASP	4.2
1	K	401	LYS	4.2
1	E	401	LYS	4.1
1	D	368	ALA	4.1
1	L	204	GLY	4.1
1	J	464	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	L	298	ALA	4.1
1	L	231	TYR	4.1
1	E	382	GLN	4.0
1	L	202[A]	ARG	4.0
1	K	197	SER	4.0
1	J	401	LYS	4.0
1	L	441	CYS	4.0
1	F	477	THR	4.0
1	K	97	GLN	3.9
1	L	364	THR	3.9
1	I	468	PHE	3.9
1	L	448	PRO	3.9
1	G	382	GLN	3.9
1	K	96	GLY	3.9
1	K	102	THR	3.9
1	L	102	THR	3.9
1	E	402	GLU	3.8
1	K	321	LYS	3.8
1	A	368	ALA	3.8
1	L	402	GLU	3.8
1	K	217	LEU	3.8
1	L	301	ASN	3.8
1	D	382	GLN	3.8
1	E	477	THR	3.8
1	I	186	THR	3.8
1	K	322	TRP	3.8
1	L	453	CYS	3.8
1	G	231	TYR	3.7
1	K	465	GLY	3.7
1	C	363	THR	3.7
1	I	402	GLU	3.7
1	K	200	GLN	3.7
1	L	322	TRP	3.6
1	G	369	ALA	3.6
1	K	105	ALA	3.6
1	K	223	ILE	3.6
1	A	369	ALA	3.6
1	K	166	THR	3.6
1	H	402	GLU	3.6
1	L	468	PHE	3.6
1	G	364	THR	3.6
1	C	382	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	370	GLN	3.5
1	K	413	GLN	3.5
1	K	444	ALA	3.5
1	J	272	GLY	3.5
1	C	231	TYR	3.5
1	B	400	GLU	3.5
1	I	453	CYS	3.4
1	L	96	GLY	3.4
1	L	203	LEU	3.4
1	A	363	THR	3.4
1	F	363	THR	3.4
1	J	382	GLN	3.4
1	J	271	SER	3.4
1	K	464	VAL	3.4
1	I	101	ALA	3.4
1	A	231	TYR	3.3
1	K	106	PHE	3.3
1	L	474	ALA	3.3
1	F	401	LYS	3.3
1	G	455	ASN	3.3
1	K	309	CYS	3.3
1	I	103	THR	3.3
1	C	371	LYS	3.3
1	J	170	ALA	3.3
1	F	96	GLY	3.3
1	K	209	LYS	3.3
1	L	209	LYS	3.2
1	C	370	GLN	3.2
1	L	207	GLY	3.2
1	L	447	ILE	3.2
1	L	327	CYS	3.2
1	L	446	PHE	3.2
1	L	228	SER	3.2
1	C	369	ALA	3.2
1	A	382	GLN	3.2
1	I	97	GLN	3.2
1	E	404	GLY	3.2
1	K	382	GLN	3.2
1	H	228	SER	3.1
1	G	402	GLU	3.1
1	J	404	GLY	3.1
1	I	464	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	308	ALA	3.1
1	K	453	CYS	3.1
1	H	371	LYS	3.1
1	L	106	PHE	3.1
1	K	198	LEU	3.1
1	K	203	LEU	3.1
1	C	402	GLU	3.0
1	K	111	LYS	3.0
1	K	463	CYS	3.0
1	J	402	GLU	3.0
1	B	363	THR	3.0
1	H	403	SER	3.0
1	H	333	LYS	3.0
1	L	97	GLN	3.0
1	L	454	ASN	3.0
1	K	219	ALA	3.0
1	L	217	LEU	3.0
1	K	199	LEU	2.9
1	L	200	GLN	2.9
1	K	334	THR	2.9
1	E	455	ASN	2.9
1	K	442	ASP	2.9
1	K	302	PRO	2.9
1	A	333	LYS	2.9
1	L	449	ILE	2.9
1	H	422	THR	2.9
1	J	232	THR	2.9
1	L	304	ALA	2.9
1	G	189	GLN	2.9
1	B	447	ILE	2.9
1	A	367	GLU	2.9
1	I	400	GLU	2.9
1	K	201	GLU	2.9
1	L	443	SER	2.9
1	K	448	PRO	2.9
1	L	206	ALA	2.9
1	H	188	GLY	2.8
1	K	333	LYS	2.8
1	G	230	ASN	2.8
1	B	403	SER	2.8
1	K	404	GLY	2.8
1	K	443	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	231	TYR	2.8
1	K	422	THR	2.8
1	K	327	CYS	2.8
1	B	370	GLN	2.8
1	A	402	GLU	2.8
1	C	262	LYS	2.8
1	L	297	VAL	2.8
1	J	275	TRP	2.8
1	K	447	ILE	2.8
1	B	382	GLN	2.8
1	K	467	GLN	2.8
1	K	114	ASN	2.7
1	H	96	GLY	2.7
1	L	198	LEU	2.7
1	K	296	PHE	2.7
1	I	334	THR	2.7
1	J	363	THR	2.7
1	G	188	GLY	2.7
1	C	403	SER	2.7
1	J	473	LYS	2.7
1	K	214	ARG	2.7
1	L	105	ALA	2.7
1	K	109	PHE	2.7
1	F	102	THR	2.7
1	J	455	ASN	2.7
1	E	405	GLU	2.7
1	H	401	LYS	2.7
1	A	453	CYS	2.7
1	F	444	ALA	2.7
1	K	101	ALA	2.7
1	K	107	ALA	2.7
1	C	400	GLU	2.7
1	F	333	LYS	2.7
1	K	371	LYS	2.7
1	I	227	PRO	2.7
1	I	335	SER	2.7
1	E	453	CYS	2.7
1	L	229	THR	2.6
1	K	208	PRO	2.6
1	K	227	PRO	2.6
1	L	199	LEU	2.6
1	B	97	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	370	GLN	2.6
1	F	371	LYS	2.6
1	H	464	VAL	2.6
1	K	328	VAL	2.6
1	L	189	GLN	2.6
1	A	371	LYS	2.6
1	G	371	LYS	2.6
1	J	408	CYS	2.6
1	A	468	PHE	2.6
1	C	422	THR	2.6
1	I	382	GLN	2.5
1	L	323	GLU	2.5
1	L	120	GLY	2.5
1	E	191	PHE	2.5
1	E	321	LYS	2.5
1	E	231	TYR	2.5
1	L	476	CYS	2.5
1	E	363	THR	2.5
1	G	468	PHE	2.5
1	K	305	TRP	2.5
1	D	403	SER	2.5
1	F	97	GLN	2.5
1	L	440	GLN	2.5
1	L	467	GLN	2.5
1	K	206	ALA	2.5
1	L	329	PRO	2.5
1	B	102	THR	2.5
1	B	335	SER	2.5
1	L	307	SER	2.5
1	L	100	TRP	2.5
1	D	371	LYS	2.5
1	I	404	GLY	2.5
1	J	476	CYS	2.4
1	L	214	ARG	2.4
1	I	171	SER	2.4
1	J	383	SER	2.4
1	E	333	LYS	2.4
1	J	370	GLN	2.4
1	L	382	GLN	2.4
1	B	101	ALA	2.4
1	J	102	THR	2.4
1	K	332	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	379	VAL	2.4
1	I	262	LYS	2.4
1	G	370	GLN	2.4
1	D	381	GLU	2.4
1	A	96	GLY	2.4
1	K	298	ALA	2.4
1	L	272	GLY	2.4
1	L	445	SER	2.4
1	L	223	ILE	2.4
1	L	464	VAL	2.4
1	B	455	ASN	2.4
1	L	201	GLU	2.4
1	L	299	GLU	2.4
1	C	404	GLY	2.4
1	L	101	ALA	2.4
1	H	205	THR	2.4
1	J	259	LYS	2.4
1	J	371	LYS	2.4
1	L	363	THR	2.4
1	L	463	CYS	2.4
1	D	400	GLU	2.4
1	L	305	TRP	2.4
1	J	262	LYS	2.3
1	K	188	GLY	2.3
1	K	213	GLY	2.3
1	B	191	PHE	2.3
1	D	370	GLN	2.3
1	D	262	LYS	2.3
1	I	332	THR	2.3
1	E	97	GLN	2.3
1	I	413	GLN	2.3
1	L	411	PHE	2.3
1	K	454	ASN	2.3
1	K	224	ALA	2.3
1	B	402	GLU	2.3
1	I	411	PHE	2.3
1	K	446	PHE	2.3
1	H	231	TYR	2.3
1	I	170	ALA	2.3
1	K	317	ALA	2.3
1	L	210	THR	2.3
1	L	321	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	468	PHE	2.2
1	J	468	PHE	2.2
1	K	191	PHE	2.2
1	L	418	PHE	2.2
1	L	475	CYS	2.2
1	D	369	ALA	2.2
1	E	444	ALA	2.2
1	F	231	TYR	2.2
1	K	186	THR	2.2
1	K	461	THR	2.2
1	E	403	SER	2.2
1	I	443	SER	2.2
1	K	403	SER	2.2
1	J	106	PHE	2.2
1	L	184	VAL	2.2
1	K	455	ASN	2.2
1	H	405	GLU	2.2
1	L	187	SER	2.2
1	K	420	PRO	2.2
1	J	261[A]	GLU	2.2
1	J	321	LYS	2.2
1	K	140	LYS	2.2
1	B	186	THR	2.2
1	L	170	ALA	2.2
1	E	454	ASN	2.2
1	K	343	ASN	2.2
1	J	333	LYS	2.2
1	L	188	GLY	2.2
1	A	186	THR	2.2
1	I	403	SER	2.2
1	J	186	THR	2.2
1	J	230	ASN	2.1
1	I	321	LYS	2.1
1	K	138	GLY	2.1
1	L	465	GLY	2.1
1	K	417	CYS	2.1
1	H	321	LYS	2.1
1	L	118	VAL	2.1
1	C	96	GLY	2.1
1	C	188	GLY	2.1
1	K	120	GLY	2.1
1	B	444	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	447	ILE	2.1
1	K	466	ASN	2.1
1	J	413	GLN	2.1
1	K	329	PRO	2.1
1	L	457	VAL	2.1
1	B	465	GLY	2.1
1	F	403	SER	2.1
1	H	186	THR	2.1
1	G	170	ALA	2.1
1	L	308	ALA	2.1
1	L	318	LEU	2.1
1	I	455	ASN	2.1
1	L	303	ASP	2.1
1	E	228	SER	2.0
1	I	187	SER	2.0
1	K	234	THR	2.0
1	I	454	ASN	2.0
1	K	301	ASN	2.0
1	K	449	ILE	2.0
1	A	184	VAL	2.0
1	L	262	LYS	2.0
1	L	471	THR	2.0
1	F	382	GLN	2.0
1	G	97	GLN	2.0
1	G	453	CYS	2.0
1	K	303	ASP	2.0
1	K	416	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	F	1	14/15	0.35	0.35	83,113,122,127	0
2	NAG	L	1	14/15	0.40	0.30	91,116,127,128	0
2	NAG	A	1	14/15	0.45	0.26	86,125,134,136	0
2	NAG	G	1	14/15	0.48	0.29	109,125,136,141	0
2	NAG	K	1	14/15	0.52	0.25	107,121,129,129	0
2	NAG	H	1	14/15	0.53	0.29	100,133,144,145	0
2	NAG	C	1	14/15	0.60	0.27	87,120,133,134	0
2	NAG	E	1	14/15	0.67	0.22	69,87,96,103	0
3	GOL	L	1478	6/6	0.70	0.27	44,49,55,58	0
2	NAG	B	1	14/15	0.81	0.20	61,95,102,102	0
3	GOL	C	1479	6/6	0.87	0.19	31,45,48,66	0
3	GOL	A	1479	6/6	0.88	0.17	39,49,57,62	0
3	GOL	A	1480	6/6	0.89	0.16	31,40,46,46	0
3	GOL	B	1479	6/6	0.89	0.15	44,47,49,55	0
3	GOL	L	1479	6/6	0.90	0.14	44,53,54,67	0
3	GOL	F	1478	6/6	0.92	0.14	37,41,44,45	0
3	GOL	D	1479	6/6	0.93	0.14	43,47,50,50	0
3	GOL	D	1478	6/6	0.93	0.12	35,38,39,51	0
3	GOL	E	1478	6/6	0.94	0.12	42,48,58,60	0
3	GOL	C	1478	6/6	0.94	0.10	35,40,47,49	0
3	GOL	J	1478	6/6	0.95	0.11	37,39,41,42	0
3	GOL	B	1478	6/6	0.95	0.11	40,43,46,46	0
3	GOL	G	1478	6/6	0.95	0.10	29,31,32,36	0
3	GOL	A	1478	6/6	0.96	0.07	26,28,28,29	0
3	GOL	E	1479	6/6	0.96	0.10	35,43,50,50	0
3	GOL	H	1478	6/6	0.96	0.09	31,35,41,42	0
3	GOL	I	1478	6/6	0.97	0.08	41,43,45,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.