



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2017 – 03:37 AM EDT

PDB ID : 4U33  
Title : Structure of Mtb GlgE bound to maltose  
Authors : Ronning, D.R.; Lindenberger, J.J.  
Deposited on : unknown  
Resolution : 3.29 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : rb-20029824  
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) : rb-20029824

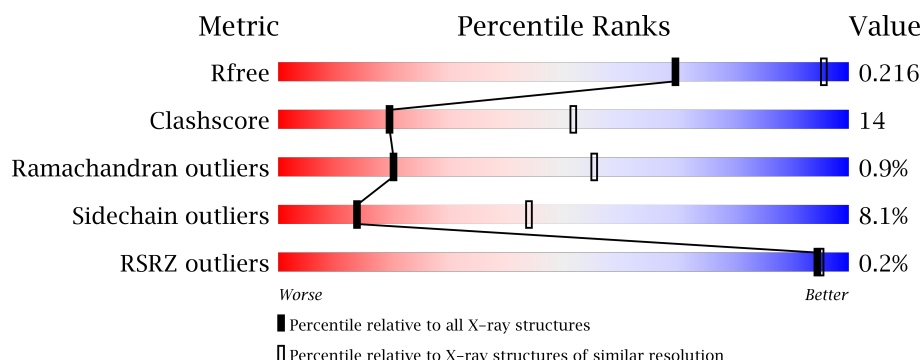
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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	723	
1	B	723	
1	C	723	
1	D	723	
1	E	723	

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Mol	Chain	Length	Quality of chain
1	F	723	<div><div></div><div>65%</div><div>22%</div><div>•</div><div>9%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 31596 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 Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	0	0
			5243	3365	913	951	14			
1	B	661	Total	C	N	O	S	0	0	0
			5243	3365	913	951	14			
1	C	661	Total	C	N	O	S	0	0	0
			5243	3365	913	951	14			
1	D	661	Total	C	N	O	S	0	0	0
			5243	3365	913	951	14			
1	E	661	Total	C	N	O	S	0	0	0
			5243	3365	913	951	14			
1	F	661	Total	C	N	O	S	0	0	0
			5243	3365	913	951	14			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP P9WQ16
A	-20	GLY	-	expression tag	UNP P9WQ16
A	-19	SER	-	expression tag	UNP P9WQ16
A	-18	SER	-	expression tag	UNP P9WQ16
A	-17	HIS	-	expression tag	UNP P9WQ16
A	-16	HIS	-	expression tag	UNP P9WQ16
A	-15	HIS	-	expression tag	UNP P9WQ16
A	-14	HIS	-	expression tag	UNP P9WQ16
A	-13	HIS	-	expression tag	UNP P9WQ16
A	-12	HIS	-	expression tag	UNP P9WQ16
A	-11	SER	-	expression tag	UNP P9WQ16
A	-10	SER	-	expression tag	UNP P9WQ16
A	-9	GLY	-	expression tag	UNP P9WQ16
A	-8	LEU	-	expression tag	UNP P9WQ16
A	-7	GLU	-	expression tag	UNP P9WQ16
A	-6	VAL	-	expression tag	UNP P9WQ16
A	-5	LEU	-	expression tag	UNP P9WQ16

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PHE	-	expression tag	UNP P9WQ16
A	-3	GLN	-	expression tag	UNP P9WQ16
A	-2	GLY	-	expression tag	UNP P9WQ16
A	-1	PRO	-	expression tag	UNP P9WQ16
A	0	HIS	-	expression tag	UNP P9WQ16
B	-21	MET	-	expression tag	UNP P9WQ16
B	-20	GLY	-	expression tag	UNP P9WQ16
B	-19	SER	-	expression tag	UNP P9WQ16
B	-18	SER	-	expression tag	UNP P9WQ16
B	-17	HIS	-	expression tag	UNP P9WQ16
B	-16	HIS	-	expression tag	UNP P9WQ16
B	-15	HIS	-	expression tag	UNP P9WQ16
B	-14	HIS	-	expression tag	UNP P9WQ16
B	-13	HIS	-	expression tag	UNP P9WQ16
B	-12	HIS	-	expression tag	UNP P9WQ16
B	-11	SER	-	expression tag	UNP P9WQ16
B	-10	SER	-	expression tag	UNP P9WQ16
B	-9	GLY	-	expression tag	UNP P9WQ16
B	-8	LEU	-	expression tag	UNP P9WQ16
B	-7	GLU	-	expression tag	UNP P9WQ16
B	-6	VAL	-	expression tag	UNP P9WQ16
B	-5	LEU	-	expression tag	UNP P9WQ16
B	-4	PHE	-	expression tag	UNP P9WQ16
B	-3	GLN	-	expression tag	UNP P9WQ16
B	-2	GLY	-	expression tag	UNP P9WQ16
B	-1	PRO	-	expression tag	UNP P9WQ16
B	0	HIS	-	expression tag	UNP P9WQ16
C	-21	MET	-	expression tag	UNP P9WQ16
C	-20	GLY	-	expression tag	UNP P9WQ16
C	-19	SER	-	expression tag	UNP P9WQ16
C	-18	SER	-	expression tag	UNP P9WQ16
C	-17	HIS	-	expression tag	UNP P9WQ16
C	-16	HIS	-	expression tag	UNP P9WQ16
C	-15	HIS	-	expression tag	UNP P9WQ16
C	-14	HIS	-	expression tag	UNP P9WQ16
C	-13	HIS	-	expression tag	UNP P9WQ16
C	-12	HIS	-	expression tag	UNP P9WQ16
C	-11	SER	-	expression tag	UNP P9WQ16
C	-10	SER	-	expression tag	UNP P9WQ16
C	-9	GLY	-	expression tag	UNP P9WQ16
C	-8	LEU	-	expression tag	UNP P9WQ16
C	-7	GLU	-	expression tag	UNP P9WQ16

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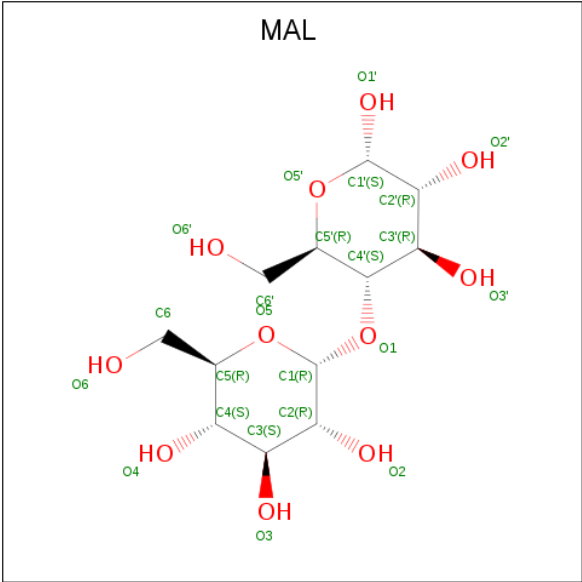
Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	VAL	-	expression tag	UNP P9WQ16
C	-5	LEU	-	expression tag	UNP P9WQ16
C	-4	PHE	-	expression tag	UNP P9WQ16
C	-3	GLN	-	expression tag	UNP P9WQ16
C	-2	GLY	-	expression tag	UNP P9WQ16
C	-1	PRO	-	expression tag	UNP P9WQ16
C	0	HIS	-	expression tag	UNP P9WQ16
D	-21	MET	-	expression tag	UNP P9WQ16
D	-20	GLY	-	expression tag	UNP P9WQ16
D	-19	SER	-	expression tag	UNP P9WQ16
D	-18	SER	-	expression tag	UNP P9WQ16
D	-17	HIS	-	expression tag	UNP P9WQ16
D	-16	HIS	-	expression tag	UNP P9WQ16
D	-15	HIS	-	expression tag	UNP P9WQ16
D	-14	HIS	-	expression tag	UNP P9WQ16
D	-13	HIS	-	expression tag	UNP P9WQ16
D	-12	HIS	-	expression tag	UNP P9WQ16
D	-11	SER	-	expression tag	UNP P9WQ16
D	-10	SER	-	expression tag	UNP P9WQ16
D	-9	GLY	-	expression tag	UNP P9WQ16
D	-8	LEU	-	expression tag	UNP P9WQ16
D	-7	GLU	-	expression tag	UNP P9WQ16
D	-6	VAL	-	expression tag	UNP P9WQ16
D	-5	LEU	-	expression tag	UNP P9WQ16
D	-4	PHE	-	expression tag	UNP P9WQ16
D	-3	GLN	-	expression tag	UNP P9WQ16
D	-2	GLY	-	expression tag	UNP P9WQ16
D	-1	PRO	-	expression tag	UNP P9WQ16
D	0	HIS	-	expression tag	UNP P9WQ16
E	-21	MET	-	expression tag	UNP P9WQ16
E	-20	GLY	-	expression tag	UNP P9WQ16
E	-19	SER	-	expression tag	UNP P9WQ16
E	-18	SER	-	expression tag	UNP P9WQ16
E	-17	HIS	-	expression tag	UNP P9WQ16
E	-16	HIS	-	expression tag	UNP P9WQ16
E	-15	HIS	-	expression tag	UNP P9WQ16
E	-14	HIS	-	expression tag	UNP P9WQ16
E	-13	HIS	-	expression tag	UNP P9WQ16
E	-12	HIS	-	expression tag	UNP P9WQ16
E	-11	SER	-	expression tag	UNP P9WQ16
E	-10	SER	-	expression tag	UNP P9WQ16
E	-9	GLY	-	expression tag	UNP P9WQ16

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	LEU	-	expression tag	UNP P9WQ16
E	-7	GLU	-	expression tag	UNP P9WQ16
E	-6	VAL	-	expression tag	UNP P9WQ16
E	-5	LEU	-	expression tag	UNP P9WQ16
E	-4	PHE	-	expression tag	UNP P9WQ16
E	-3	GLN	-	expression tag	UNP P9WQ16
E	-2	GLY	-	expression tag	UNP P9WQ16
E	-1	PRO	-	expression tag	UNP P9WQ16
E	0	HIS	-	expression tag	UNP P9WQ16
F	-21	MET	-	expression tag	UNP P9WQ16
F	-20	GLY	-	expression tag	UNP P9WQ16
F	-19	SER	-	expression tag	UNP P9WQ16
F	-18	SER	-	expression tag	UNP P9WQ16
F	-17	HIS	-	expression tag	UNP P9WQ16
F	-16	HIS	-	expression tag	UNP P9WQ16
F	-15	HIS	-	expression tag	UNP P9WQ16
F	-14	HIS	-	expression tag	UNP P9WQ16
F	-13	HIS	-	expression tag	UNP P9WQ16
F	-12	HIS	-	expression tag	UNP P9WQ16
F	-11	SER	-	expression tag	UNP P9WQ16
F	-10	SER	-	expression tag	UNP P9WQ16
F	-9	GLY	-	expression tag	UNP P9WQ16
F	-8	LEU	-	expression tag	UNP P9WQ16
F	-7	GLU	-	expression tag	UNP P9WQ16
F	-6	VAL	-	expression tag	UNP P9WQ16
F	-5	LEU	-	expression tag	UNP P9WQ16
F	-4	PHE	-	expression tag	UNP P9WQ16
F	-3	GLN	-	expression tag	UNP P9WQ16
F	-2	GLY	-	expression tag	UNP P9WQ16
F	-1	PRO	-	expression tag	UNP P9WQ16
F	0	HIS	-	expression tag	UNP P9WQ16

- Molecule 2 is MALTOSE (three-letter code: MAL) (formula: C<sub>12</sub>H<sub>22</sub>O<sub>11</sub>).

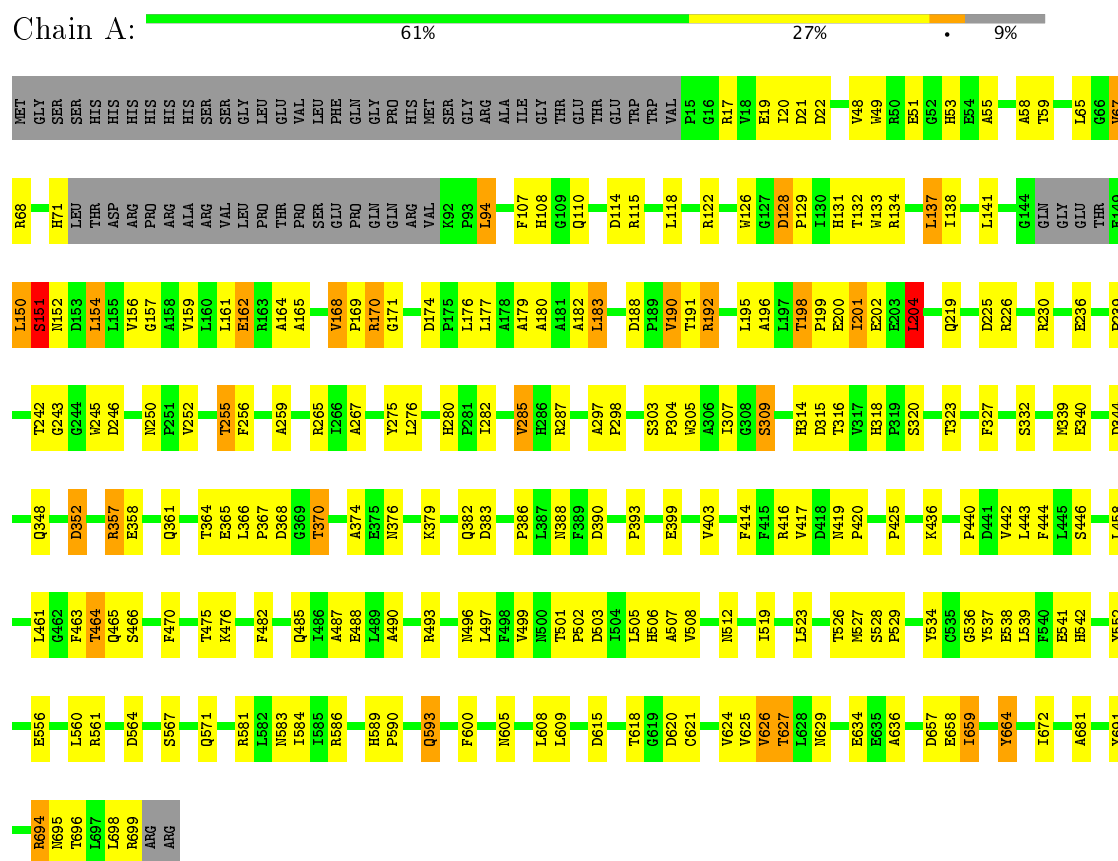


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		
2	C	1	Total	C	O	0	0
			23	12	11		
2	D	1	Total	C	O	0	0
			23	12	11		
2	E	1	Total	C	O	0	0
			23	12	11		
2	F	1	Total	C	O	0	0
			23	12	11		

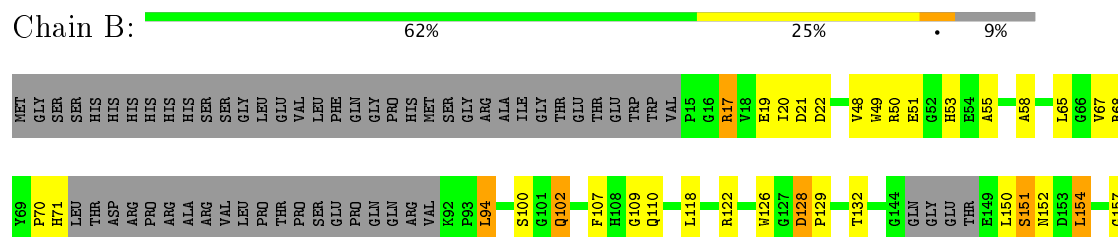
### 3 Residue-property plots

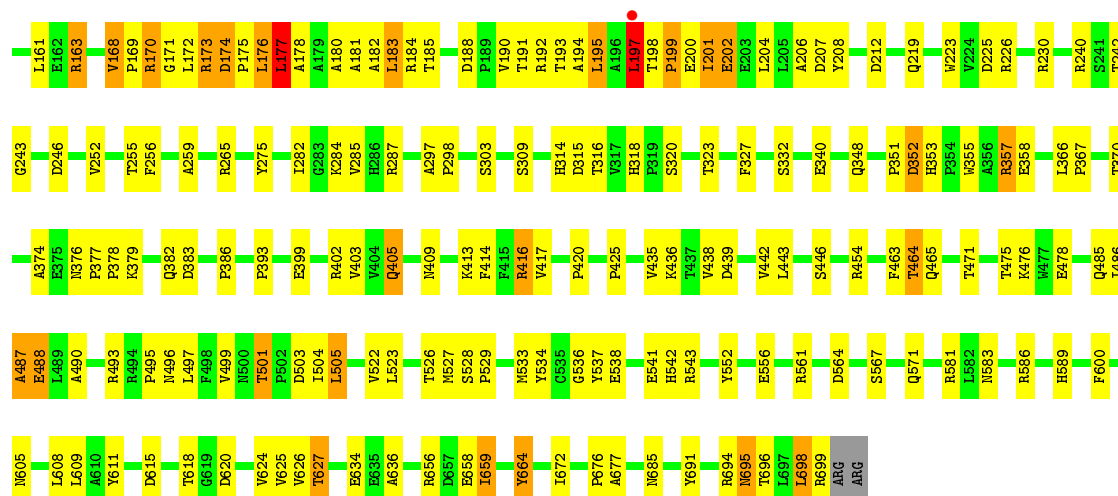
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

- Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase



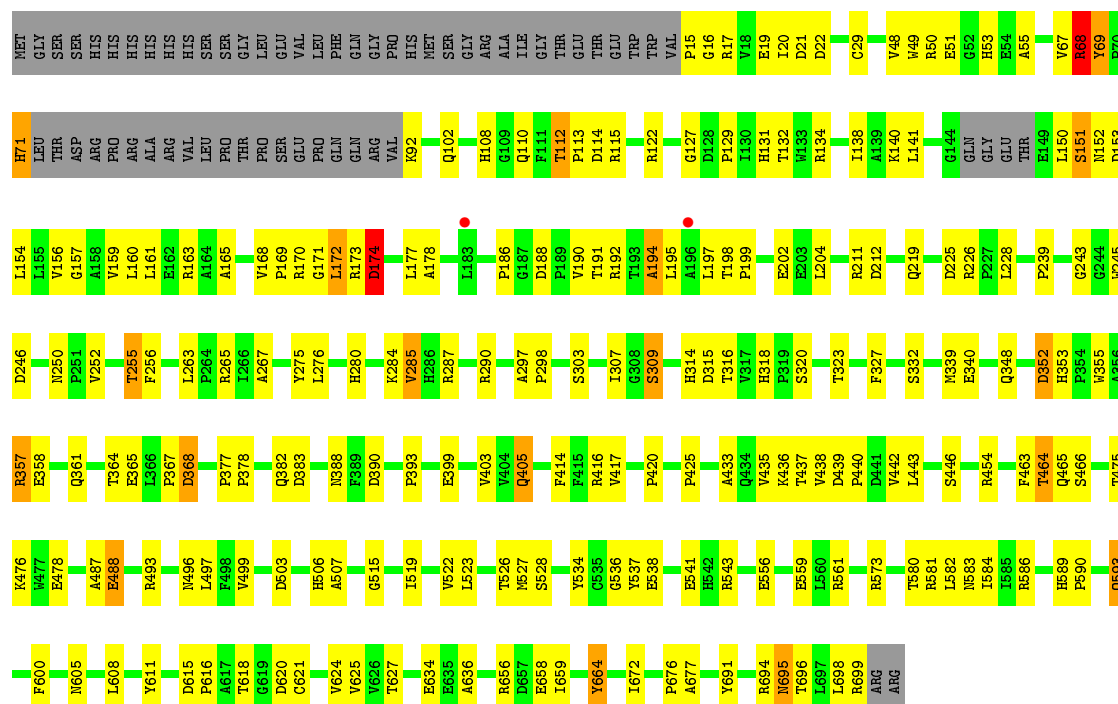
- Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase





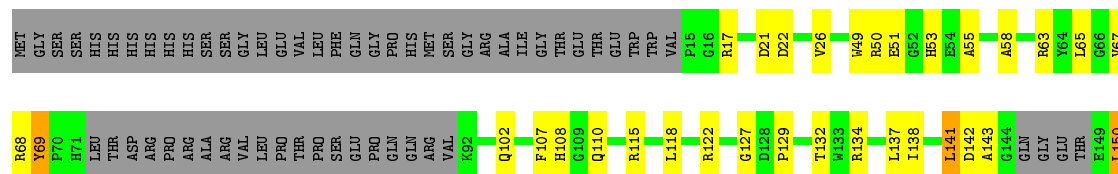
- Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase

Chain C: 62% 27% 9%

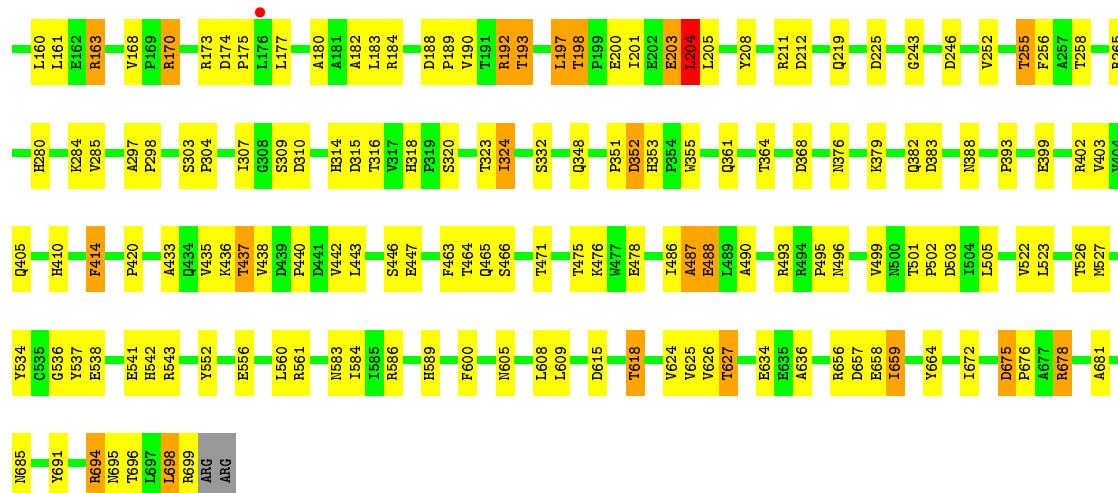


- Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase

Chain D: 63% 25% 9%







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	343.23Å 242.60Å 243.67Å 90.00° 135.15° 90.00°	Depositor
Resolution (Å)	47.64 – 3.29 47.64 – 3.29	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.64-3.29) 90.4 (47.64-3.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.194 , 0.222 0.187 , 0.216	Depositor DCC
$R_{free}$ test set	9696 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	85.1	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 24.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h-2*k,l,h+l 0.000 for -h-k-l,l,k 0.000 for -h+k-l,-l,-k 0.000 for -k+l,-h-l,-l 0.000 for k+l,h+l,-l 0.397 for k-l,h+l,-k 0.389 for h+k+l,-l,-h-l 0.388 for -k-l,-h-l,k 0.389 for h-k+l,l,-h-l 0.000 for h,-k,-h-l 0.450 for h+2*k,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	31596	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.77	1/5407 (0.0%)	0.68	2/7395 (0.0%)
1	B	0.77	0/5407	0.68	5/7395 (0.1%)
1	C	0.76	1/5407 (0.0%)	0.64	1/7395 (0.0%)
1	D	0.76	1/5407 (0.0%)	0.67	3/7395 (0.0%)
1	E	0.76	1/5407 (0.0%)	0.67	3/7395 (0.0%)
1	F	0.77	0/5407	0.65	3/7395 (0.0%)
All	All	0.76	4/32442 (0.0%)	0.66	17/44370 (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	C	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	621	CYS	CB-SG	-5.66	1.72	1.81
1	C	621	CYS	CB-SG	-5.21	1.73	1.81
1	A	621	CYS	CB-SG	-5.13	1.73	1.81
1	E	621	CYS	CB-SG	-5.06	1.73	1.81

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	LEU	CA-CB-CG	8.87	135.71	115.30
1	B	177	LEU	CA-CB-CG	8.50	134.84	115.30
1	D	204	LEU	CA-CB-CG	7.11	131.65	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	204	LEU	CA-CB-CG	7.02	131.45	115.30
1	F	204	LEU	CA-CB-CG	6.22	129.60	115.30
1	C	174	ASP	C-N-CD	-5.84	107.76	120.60
1	A	94	LEU	CA-CB-CG	5.54	128.04	115.30
1	D	487	ALA	C-N-CA	5.48	135.40	121.70
1	F	487	ALA	C-N-CA	5.46	135.36	121.70
1	B	197	LEU	CA-CB-CG	5.32	127.53	115.30
1	F	488	GLU	N-CA-C	5.28	125.25	111.00
1	D	488	GLU	N-CA-C	5.26	125.21	111.00
1	B	488	GLU	N-CA-C	5.22	125.10	111.00
1	E	141	LEU	CA-CB-CG	5.13	127.09	115.30
1	B	94	LEU	CA-CB-CG	5.12	127.07	115.30
1	E	461	LEU	CA-CB-CG	5.03	126.87	115.30
1	B	487	ALA	C-N-CA	5.02	134.25	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	194	ALA	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	5243	0	5051	161	0
1	B	5243	0	5051	157	0
1	C	5243	0	5051	151	0
1	D	5243	0	5051	159	0
1	E	5243	0	5052	147	1
1	F	5243	0	5052	134	1
2	A	23	0	22	1	0
2	B	23	0	22	1	0
2	C	23	0	22	1	0
2	D	23	0	22	1	0
2	E	23	0	22	2	0
2	F	23	0	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31596	0	30440	890	2

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 14.

All (890) 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:D:275:TYR:OH	1:D:416:ARG:NH1	1.98	0.96
1:E:275:TYR:OH	1:E:416:ARG:NH1	2.01	0.94
1:B:275:TYR:OH	1:B:416:ARG:NH1	2.03	0.91
1:C:275:TYR:OH	1:C:416:ARG:NH1	2.02	0.91
1:E:188:ASP:HB2	1:E:191:THR:HG23	1.55	0.89
1:D:589:HIS:NE2	1:D:658:GLU:OE2	2.08	0.87
1:C:589:HIS:NE2	1:C:658:GLU:OE2	2.09	0.86
1:B:589:HIS:NE2	1:B:658:GLU:OE2	2.08	0.85
1:D:184:ARG:H	1:D:192:ARG:HH11	1.22	0.85
1:B:195:LEU:HD22	1:B:201:ILE:HG23	1.59	0.84
1:F:589:HIS:NE2	1:F:658:GLU:OE2	2.08	0.84
1:E:110:GLN:HG2	1:E:694:ARG:HE	1.43	0.84
1:E:493:ARG:HG2	1:E:493:ARG:HH11	1.44	0.83
1:A:352:ASP:OD1	1:A:352:ASP:N	2.12	0.82
1:B:226:ARG:NH1	1:B:340:GLU:OE2	2.13	0.81
1:D:226:ARG:NH1	1:D:340:GLU:OE2	2.13	0.81
1:E:352:ASP:OD1	1:E:352:ASP:N	2.14	0.81
1:A:226:ARG:NH1	1:A:340:GLU:OE2	2.14	0.80
1:B:487:ALA:HB2	1:B:490:ALA:HB2	1.63	0.80
1:A:150:LEU:O	1:A:152:ASN:N	2.14	0.80
1:A:589:HIS:NE2	1:A:658:GLU:OE2	2.12	0.79
1:B:176:LEU:O	1:B:180:ALA:N	2.14	0.79
1:B:177:LEU:HA	1:B:180:ALA:HB3	1.64	0.79
1:F:352:ASP:N	1:F:352:ASP:OD1	2.15	0.79
1:B:656:ARG:NH1	1:B:658:GLU:OE1	2.16	0.78
1:F:656:ARG:NH1	1:F:658:GLU:OE1	2.16	0.78
1:B:55:ALA:H	1:B:132:THR:HG22	1.49	0.78
1:E:656:ARG:NH1	1:E:658:GLU:OE1	2.17	0.78
1:D:174:ASP:HA	1:D:177:LEU:HD13	1.65	0.78
1:F:675:ASP:HB3	1:F:678:ARG:HB2	1.65	0.78
1:E:154:LEU:HD12	1:E:154:LEU:H	1.49	0.78
1:F:695:ASN:HA	1:F:698:LEU:HD13	1.66	0.77
1:D:352:ASP:N	1:D:352:ASP:OD1	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ALA:H	1:A:132:THR:HG22	1.49	0.77
1:E:149:GLU:OE1	1:E:149:GLU:N	2.18	0.77
1:E:150:LEU:HD12	1:E:154:LEU:HD11	1.66	0.77
1:E:465:GLN:OE1	1:E:496:ASN:ND2	2.17	0.77
1:C:656:ARG:NH1	1:C:658:GLU:OE1	2.18	0.76
1:F:487:ALA:HB2	1:F:490:ALA:HB2	1.66	0.76
1:E:154:LEU:HB3	1:E:183:LEU:HD12	1.68	0.76
1:E:589:HIS:NE2	1:E:658:GLU:OE2	2.14	0.76
1:B:695:ASN:HA	1:B:698:LEU:HD13	1.68	0.75
1:C:55:ALA:H	1:C:132:THR:HG22	1.50	0.75
1:F:122:ARG:HB3	1:F:219:GLN:HG2	1.68	0.75
1:A:487:ALA:HB2	1:A:490:ALA:HB2	1.69	0.74
1:F:170:ARG:HA	1:F:173:ARG:HG2	1.69	0.74
1:F:55:ALA:H	1:F:132:THR:HG22	1.53	0.73
1:B:195:LEU:HD21	1:B:200:GLU:HB2	1.68	0.73
1:C:615:ASP:OD2	1:C:618:THR:HG22	1.88	0.73
1:E:183:LEU:HA	1:E:192:ARG:HD3	1.71	0.73
1:D:487:ALA:HB2	1:D:490:ALA:HB2	1.70	0.73
1:E:126:TRP:HZ3	1:E:128:ASP:HB3	1.54	0.73
1:D:55:ALA:H	1:D:132:THR:HG22	1.52	0.73
1:A:615:ASP:OD2	1:A:618:THR:HG22	1.88	0.72
1:B:615:ASP:OD2	1:B:618:THR:HG22	1.87	0.72
1:C:352:ASP:OD1	1:C:352:ASP:N	2.19	0.72
1:B:352:ASP:N	1:B:352:ASP:OD1	2.22	0.72
1:A:122:ARG:HB3	1:A:219:GLN:HG2	1.71	0.72
1:C:150:LEU:HD12	1:C:154:LEU:HD11	1.71	0.71
1:F:676:PRO:O	1:F:678:ARG:NE	2.23	0.71
1:F:126:TRP:HZ3	1:F:128:ASP:HB3	1.55	0.71
1:B:284:LYS:N	1:B:352:ASP:OD2	2.20	0.71
1:B:533:MET:HE2	1:B:537:TYR:HB3	1.72	0.71
1:D:184:ARG:N	1:D:192:ARG:HH11	1.88	0.71
1:C:368:ASP:N	1:C:368:ASP:OD1	2.20	0.71
1:C:188:ASP:O	1:C:192:ARG:HG3	1.90	0.70
1:A:275:TYR:CZ	1:A:416:ARG:HD3	2.26	0.70
1:E:55:ALA:H	1:E:132:THR:HG22	1.56	0.70
1:F:183:LEU:O	1:F:192:ARG:NH1	2.24	0.70
1:D:503:ASP:OD2	2:D:801:MAL:O2'	2.10	0.70
1:C:465:GLN:OE1	1:C:496:ASN:ND2	2.23	0.69
1:D:615:ASP:OD2	1:D:618:THR:HG22	1.92	0.69
1:B:150:LEU:O	1:B:152:ASN:N	2.25	0.69
1:C:605:ASN:HD21	1:C:634:GLU:HG3	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:HIS:ND1	1:F:71:HIS:O	2.25	0.69
1:D:168:VAL:HG22	1:D:170:ARG:NH2	2.08	0.69
1:F:447:GLU:OE2	2:F:801:MAL:O1'	2.11	0.69
1:F:151:SER:HA	1:F:154:LEU:HD23	1.75	0.69
1:C:309:SER:HA	1:C:352:ASP:HB2	1.74	0.69
1:C:365:GLU:OE1	1:C:365:GLU:N	2.19	0.69
1:B:556:GLU:HG3	1:B:561:ARG:HB2	1.74	0.69
1:B:169:PRO:HA	1:B:173:ARG:HE	1.56	0.68
1:B:122:ARG:HB3	1:B:219:GLN:HG2	1.76	0.68
1:B:275:TYR:CZ	1:B:416:ARG:HD2	2.28	0.68
1:C:134:ARG:NH2	1:C:202:GLU:OE1	2.26	0.68
1:B:503:ASP:OD2	2:B:801:MAL:O2'	2.10	0.68
1:F:433:ALA:O	1:F:437:THR:OG1	2.10	0.68
1:A:154:LEU:H	1:A:154:LEU:HD13	1.59	0.68
1:D:420:PRO:HG2	1:D:446:SER:HB2	1.76	0.68
1:B:564:ASP:OD2	1:B:567:SER:OG	2.05	0.68
1:C:275:TYR:CZ	1:C:416:ARG:HD3	2.28	0.68
1:C:420:PRO:HG2	1:C:446:SER:HB2	1.75	0.68
1:C:174:ASP:OD1	1:C:178:ALA:N	2.21	0.68
1:F:50:ARG:NH2	1:F:51:GLU:OE1	2.25	0.67
1:B:174:ASP:OD1	1:B:174:ASP:N	2.28	0.67
1:C:154:LEU:H	1:C:154:LEU:HD12	1.59	0.67
1:D:541:GLU:OE1	1:D:563:ARG:NH1	2.26	0.67
1:D:414:PHE:CE1	1:D:443:LEU:HD12	2.30	0.67
1:D:465:GLN:OE1	1:D:496:ASN:ND2	2.23	0.67
1:C:318:HIS:CD2	1:C:320:SER:HB2	2.30	0.67
1:E:179:ALA:HB1	1:E:195:LEU:HG	1.77	0.67
1:A:67:VAL:HG11	1:A:440:PRO:HG3	1.77	0.67
1:D:154:LEU:HD12	1:D:154:LEU:H	1.60	0.66
1:D:168:VAL:HG22	1:D:170:ARG:CZ	2.23	0.66
1:D:318:HIS:CD2	1:D:320:SER:HB2	2.29	0.66
1:A:618:THR:HG23	1:A:620:ASP:H	1.60	0.66
1:C:170:ARG:HB2	1:C:173:ARG:HB2	1.77	0.66
1:E:50:ARG:NH2	1:E:51:GLU:OE1	2.24	0.66
1:B:501:THR:HG23	1:B:503:ASP:H	1.59	0.66
1:A:365:GLU:OE1	1:A:365:GLU:N	2.19	0.66
1:B:465:GLN:OE1	1:B:496:ASN:ND2	2.20	0.66
1:C:168:VAL:HG21	1:C:204:LEU:HD11	1.76	0.66
1:B:318:HIS:CD2	1:B:320:SER:HB2	2.32	0.65
1:C:503:ASP:OD2	2:C:801:MAL:O2'	2.13	0.65
1:D:436:LYS:HE3	1:D:442:VAL:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:324:ILE:HD11	1:F:410:HIS:CD2	2.32	0.65
1:E:508:VAL:O	1:E:512:ASN:ND2	2.27	0.65
1:F:17:ARG:NH1	1:F:51:GLU:OE2	2.27	0.65
1:D:556:GLU:OE1	1:D:563:ARG:NH2	2.30	0.64
1:D:110:GLN:HB3	1:D:694:ARG:CZ	2.27	0.64
1:A:605:ASN:HD21	1:A:634:GLU:HG3	1.60	0.64
1:C:499:VAL:HG11	1:C:537:TYR:CZ	2.32	0.64
1:C:71:HIS:O	1:C:71:HIS:ND1	2.31	0.64
1:D:151:SER:HA	1:D:154:LEU:HD13	1.80	0.64
1:D:67:VAL:HG11	1:D:440:PRO:HG3	1.80	0.64
1:E:150:LEU:O	1:E:152:ASN:N	2.31	0.64
1:E:162:GLU:HG3	1:E:180:ALA:CB	2.28	0.64
1:A:368:ASP:OD2	1:A:370:THR:OG1	2.16	0.64
1:A:503:ASP:OD2	2:A:801:MAL:O2'	2.15	0.64
1:F:399:GLU:OE1	1:F:402:ARG:NH1	2.31	0.64
1:E:503:ASP:OD2	2:E:801:MAL:O2'	2.12	0.64
1:D:162:GLU:OE1	1:D:184:ARG:NH1	2.32	0.63
1:F:605:ASN:HD21	1:F:634:GLU:HG3	1.63	0.63
1:A:436:LYS:HE3	1:A:442:VAL:O	1.98	0.63
1:E:522:VAL:O	1:E:526:THR:OG1	2.16	0.63
1:D:188:ASP:O	1:D:191:THR:OG1	2.13	0.63
1:D:618:THR:HG23	1:D:620:ASP:H	1.63	0.63
1:B:17:ARG:NH1	1:B:51:GLU:OE2	2.29	0.63
1:F:556:GLU:HG3	1:F:561:ARG:HB2	1.81	0.63
1:B:618:THR:HG23	1:B:620:ASP:H	1.63	0.62
1:E:318:HIS:CD2	1:E:320:SER:HB2	2.34	0.62
1:B:309:SER:HA	1:B:352:ASP:HB2	1.81	0.62
1:B:170:ARG:O	1:B:173:ARG:HD2	2.00	0.62
1:E:265:ARG:NH2	1:E:538:GLU:OE1	2.33	0.62
1:C:436:LYS:HE3	1:C:442:VAL:O	1.99	0.62
1:C:556:GLU:HG3	1:C:561:ARG:HB2	1.81	0.62
1:A:318:HIS:CD2	1:A:320:SER:HB2	2.34	0.62
1:A:275:TYR:OH	1:A:416:ARG:NH1	2.32	0.62
1:B:605:ASN:HD21	1:B:634:GLU:HG3	1.64	0.62
1:C:122:ARG:HB3	1:C:219:GLN:HG2	1.80	0.62
1:C:194:ALA:N	1:C:195:LEU:HA	2.14	0.62
1:C:433:ALA:O	1:C:437:THR:OG1	2.18	0.62
1:F:465:GLN:OE1	1:F:496:ASN:ND2	2.28	0.62
1:D:50:ARG:NH2	1:D:51:GLU:OE1	2.22	0.61
1:F:163:ARG:NH2	1:F:212:ASP:OD1	2.34	0.61
1:D:365:GLU:N	1:D:365:GLU:OE1	2.20	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:605:ASN:HD21	1:D:634:GLU:HG3	1.65	0.61
1:B:151:SER:HA	1:B:154:LEU:HD23	1.83	0.61
1:E:126:TRP:CZ3	1:E:128:ASP:HB3	2.35	0.61
1:D:170:ARG:HH21	1:D:173:ARG:HB2	1.65	0.61
1:D:184:ARG:H	1:D:192:ARG:NH1	1.96	0.61
1:F:284:LYS:N	1:F:352:ASP:OD2	2.25	0.61
1:D:525:ALA:HB1	1:D:586:ARG:HD2	1.83	0.61
1:E:605:ASN:HD21	1:E:634:GLU:HG3	1.66	0.61
1:C:618:THR:HG23	1:C:620:ASP:H	1.63	0.60
1:D:188:ASP:OD1	1:D:191:THR:N	2.33	0.60
1:F:318:HIS:CD2	1:F:320:SER:HB2	2.35	0.60
1:F:382:GLN:N	1:F:382:GLN:OE1	2.31	0.60
1:C:584:ILE:HD13	1:E:664:TYR:HB3	1.83	0.60
1:A:465:GLN:OE1	1:A:496:ASN:ND2	2.25	0.60
1:D:200:GLU:O	1:D:204:LEU:HD13	2.01	0.60
1:E:383:ASP:OD1	1:E:383:ASP:N	2.26	0.60
1:A:605:ASN:ND2	1:A:634:GLU:HG3	2.17	0.60
1:D:383:ASP:N	1:D:383:ASP:OD1	2.30	0.60
1:F:168:VAL:HG12	1:F:208:TYR:HB2	1.82	0.60
1:A:309:SER:HA	1:A:352:ASP:HB2	1.84	0.60
1:D:168:VAL:O	1:D:170:ARG:NH2	2.34	0.60
1:F:503:ASP:OD2	2:F:801:MAL:O2'	2.16	0.60
1:A:368:ASP:OD1	1:B:152:ASN:ND2	2.35	0.60
1:B:154:LEU:HD22	1:B:154:LEU:H	1.65	0.60
1:B:183:LEU:N	1:B:192:ARG:HH11	1.99	0.60
1:A:265:ARG:NH2	1:A:538:GLU:OE1	2.35	0.60
1:A:162:GLU:N	1:A:162:GLU:OE1	2.32	0.59
1:A:487:ALA:CB	1:A:490:ALA:HB2	2.32	0.59
1:D:150:LEU:O	1:D:152:ASN:N	2.35	0.59
1:D:168:VAL:HG23	1:D:208:TYR:CG	2.37	0.59
1:F:67:VAL:HG11	1:F:440:PRO:HG3	1.84	0.59
1:A:169:PRO:O	1:A:171:GLY:N	2.35	0.59
1:B:190:VAL:O	1:B:193:THR:HG22	2.02	0.59
1:F:110:GLN:OE1	1:F:694:ARG:HG3	2.02	0.59
1:A:583:ASN:HA	1:A:586:ARG:HD3	1.84	0.59
1:B:436:LYS:HE3	1:B:442:VAL:O	2.02	0.59
1:C:170:ARG:CB	1:C:173:ARG:HB2	2.32	0.59
1:D:243:GLY:HA3	1:D:252:VAL:O	2.03	0.59
1:E:436:LYS:HE3	1:E:442:VAL:O	2.03	0.59
1:A:499:VAL:HG11	1:A:537:TYR:CZ	2.37	0.59
1:D:195:LEU:HA	1:D:198:THR:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:GLY:HA3	1:C:252:VAL:O	2.02	0.59
1:A:243:GLY:HA3	1:A:252:VAL:O	2.03	0.59
1:C:50:ARG:NH2	1:C:51:GLU:OE1	2.28	0.59
1:B:382:GLN:N	1:B:382:GLN:OE1	2.32	0.58
1:C:150:LEU:O	1:C:152:ASN:N	2.36	0.58
1:D:433:ALA:O	1:D:437:THR:OG1	2.20	0.58
1:E:195:LEU:HA	1:E:201:ILE:HD11	1.85	0.58
1:F:499:VAL:HG11	1:F:537:TYR:CZ	2.37	0.58
1:C:169:PRO:HA	1:C:173:ARG:HD3	1.85	0.58
1:D:122:ARG:HB3	1:D:219:GLN:HG2	1.86	0.58
1:A:133:TRP:HH2	1:A:192:ARG:HH22	1.51	0.58
1:B:163:ARG:NH2	1:B:212:ASP:OD1	2.36	0.58
1:A:176:LEU:O	1:A:180:ALA:N	2.33	0.58
1:C:188:ASP:OD1	1:C:190:VAL:N	2.37	0.58
1:E:695:ASN:HA	1:E:698:LEU:HD13	1.84	0.58
1:F:126:TRP:CZ3	1:F:128:ASP:HB3	2.37	0.58
1:D:157:GLY:O	1:D:161:LEU:HD12	2.03	0.58
1:B:173:ARG:HG2	1:B:174:ASP:OD1	2.04	0.58
1:B:243:GLY:HA3	1:B:252:VAL:O	2.04	0.57
1:D:364:THR:OG1	1:D:388:ASN:ND2	2.27	0.57
1:A:183:LEU:HD12	1:A:192:ARG:HB3	1.85	0.57
1:E:194:ALA:O	1:E:198:THR:OG1	2.20	0.57
1:E:458:LEU:HA	1:E:461:LEU:HD13	1.85	0.57
1:A:382:GLN:N	1:A:382:GLN:OE1	2.32	0.57
1:C:122:ARG:HH11	1:C:219:GLN:HE21	1.53	0.57
1:A:122:ARG:HH11	1:A:219:GLN:HE21	1.51	0.57
1:A:458:LEU:HA	1:A:461:LEU:HD13	1.85	0.57
1:A:196:ALA:O	1:A:201:ILE:HD11	2.05	0.57
1:E:161:LEU:O	1:E:165:ALA:N	2.36	0.57
1:F:243:GLY:HA3	1:F:252:VAL:O	2.04	0.57
1:E:626:VAL:HG12	1:E:681:ALA:HB2	1.87	0.57
1:F:67:VAL:O	1:F:68:ARG:HG2	2.04	0.57
1:F:436:LYS:HE3	1:F:442:VAL:O	2.05	0.57
1:F:157:GLY:O	1:F:161:LEU:HD12	2.05	0.57
1:F:168:VAL:HG23	1:F:173:ARG:HB3	1.86	0.57
1:F:201:ILE:HA	1:F:204:LEU:HG	1.87	0.57
1:F:420:PRO:HG3	1:F:446:SER:HB2	1.86	0.56
1:C:127:GLY:O	1:C:129:PRO:HD3	2.05	0.56
1:C:169:PRO:HA	1:C:173:ARG:HH11	1.71	0.56
1:D:605:ASN:HB2	1:D:636:ALA:HB2	1.88	0.56
1:E:177:LEU:HD12	1:E:177:LEU:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:THR:OG1	1:E:193:THR:O	2.24	0.56
1:E:605:ASN:ND2	1:E:634:GLU:HG3	2.21	0.56
1:D:605:ASN:ND2	1:D:634:GLU:HG3	2.21	0.56
1:A:200:GLU:O	1:A:204:LEU:HD13	2.06	0.56
1:A:526:THR:HG21	1:A:624:VAL:HG21	1.88	0.56
1:D:170:ARG:HG2	1:D:172:LEU:H	1.71	0.56
1:E:110:GLN:HG2	1:E:694:ARG:NE	2.18	0.56
1:B:605:ASN:ND2	1:B:634:GLU:HG3	2.20	0.55
1:C:605:ASN:ND2	1:C:634:GLU:HG3	2.19	0.55
1:D:167:GLY:O	1:D:169:PRO:HD3	2.07	0.55
1:E:243:GLY:HA3	1:E:252:VAL:O	2.05	0.55
1:E:590:PRO:O	1:E:593:GLN:HG3	2.06	0.55
1:E:200:GLU:O	1:E:204:LEU:HD13	2.06	0.55
1:F:180:ALA:O	1:F:184:ARG:HG3	2.07	0.55
1:F:605:ASN:ND2	1:F:634:GLU:HG3	2.20	0.55
1:A:188:ASP:OD2	1:A:190:VAL:N	2.40	0.55
1:C:284:LYS:N	1:C:352:ASP:OD2	2.30	0.55
1:D:58:ALA:HB3	1:D:107:PHE:HD2	1.70	0.55
1:D:275:TYR:HH	1:D:416:ARG:HH11	1.49	0.55
1:E:657:ASP:OD1	1:E:659:ILE:HG13	2.07	0.55
1:D:307:ILE:HG21	1:D:314:HIS:CD2	2.42	0.55
1:C:605:ASN:HB2	1:C:636:ALA:HB2	1.89	0.55
1:D:187:GLY:HA3	1:D:191:THR:HG21	1.89	0.55
1:A:556:GLU:HG3	1:A:561:ARG:HB2	1.88	0.55
1:B:526:THR:HG21	1:B:624:VAL:HG21	1.89	0.55
1:C:157:GLY:O	1:C:161:LEU:HD12	2.07	0.55
1:C:318:HIS:CD2	1:C:320:SER:H	2.25	0.55
1:D:318:HIS:HD2	1:D:320:SER:H	1.55	0.55
1:C:152:ASN:OD1	1:D:367:PRO:HD2	2.07	0.55
1:E:382:GLN:N	1:E:382:GLN:OE1	2.32	0.55
1:A:183:LEU:HB2	1:A:192:ARG:HD3	1.89	0.54
1:B:174:ASP:CG	1:B:177:LEU:HD22	2.28	0.54
1:D:165:ALA:HA	1:D:168:VAL:HG12	1.89	0.54
1:D:182:ALA:HB2	1:D:195:LEU:HD11	1.89	0.54
1:A:420:PRO:HG2	1:A:446:SER:HB2	1.88	0.54
1:C:526:THR:HG21	1:C:624:VAL:HG21	1.90	0.54
1:D:134:ARG:O	1:D:138:ILE:HG13	2.07	0.54
1:A:664:TYR:HB3	1:E:584:ILE:HD13	1.89	0.54
1:B:182:ALA:O	1:B:192:ARG:HD3	2.08	0.54
1:D:522:VAL:O	1:D:526:THR:OG1	2.20	0.54
1:B:199:PRO:HA	1:B:202:GLU:CD	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:ALA:O	1:D:183:LEU:HB2	2.08	0.54
1:A:58:ALA:HB3	1:A:107:PHE:HD2	1.71	0.54
1:A:605:ASN:HB2	1:A:636:ALA:HB2	1.90	0.54
1:E:526:THR:HG21	1:E:624:VAL:HG21	1.90	0.54
1:F:204:LEU:HD12	1:F:205:LEU:N	2.22	0.54
1:F:297:ALA:HB1	1:F:298:PRO:HD2	1.90	0.54
1:F:307:ILE:HG21	1:F:314:HIS:ND1	2.22	0.54
1:A:156:VAL:O	1:A:159:VAL:HG12	2.08	0.54
1:B:420:PRO:HG2	1:B:446:SER:HB2	1.89	0.54
1:D:195:LEU:HA	1:D:198:THR:HG23	1.90	0.54
1:E:556:GLU:HG3	1:E:561:ARG:HB2	1.90	0.54
1:C:140:LYS:NZ	1:C:153:ASP:OD1	2.41	0.53
1:D:309:SER:HA	1:D:352:ASP:HB2	1.89	0.53
1:A:17:ARG:NH1	1:A:51:GLU:OE2	2.36	0.53
1:C:382:GLN:OE1	1:C:382:GLN:N	2.34	0.53
1:E:275:TYR:HH	1:E:416:ARG:HH11	1.48	0.53
1:B:58:ALA:HB3	1:B:107:PHE:HD2	1.73	0.53
1:E:110:GLN:CG	1:E:694:ARG:HE	2.19	0.53
1:F:188:ASP:O	1:F:192:ARG:HG2	2.09	0.53
1:A:297:ALA:HB1	1:A:298:PRO:HD2	1.90	0.53
1:D:176:LEU:O	1:D:180:ALA:N	2.42	0.53
1:A:182:ALA:HB3	1:A:192:ARG:HG3	1.89	0.53
1:B:664:TYR:HB3	1:F:584:ILE:HD13	1.90	0.53
1:C:522:VAL:O	1:C:526:THR:OG1	2.24	0.53
1:D:318:HIS:CD2	1:D:320:SER:H	2.26	0.53
1:D:382:GLN:N	1:D:382:GLN:OE1	2.31	0.53
1:E:149:GLU:HG2	1:E:150:LEU:H	1.73	0.53
1:E:420:PRO:HG3	1:E:446:SER:HB2	1.89	0.53
1:F:615:ASP:OD2	1:F:618:THR:OG1	2.25	0.53
1:A:364:THR:OG1	1:A:388:ASN:ND2	2.27	0.53
1:B:50:ARG:NH2	1:B:51:GLU:OE1	2.24	0.53
1:D:198:THR:OG1	1:D:201:ILE:HD13	2.08	0.53
1:F:315:ASP:OD1	1:F:316:THR:HG23	2.09	0.53
1:F:522:VAL:O	1:F:526:THR:OG1	2.22	0.53
1:A:476:LYS:HE3	1:A:608:LEU:O	2.08	0.53
1:B:157:GLY:O	1:B:161:LEU:HD12	2.09	0.53
1:D:134:ARG:NH2	1:D:202:GLU:OE2	2.41	0.53
1:E:307:ILE:HG21	1:E:314:HIS:ND1	2.24	0.53
1:D:297:ALA:HB1	1:D:298:PRO:HD2	1.91	0.53
1:E:190:VAL:O	1:E:193:THR:HG22	2.09	0.53
1:B:225:ASP:OD1	1:B:436:LYS:NZ	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:GLY:O	1:B:541:GLU:HG3	2.09	0.53
1:C:170:ARG:HG3	1:C:173:ARG:H	1.74	0.53
1:C:534:TYR:OH	1:C:556:GLU:OE1	2.14	0.53
1:F:314:HIS:HB3	1:F:403:VAL:HG11	1.90	0.53
1:A:192:ARG:O	1:A:192:ARG:HG2	2.07	0.53
1:D:529:PRO:O	1:D:586:ARG:NH2	2.42	0.53
1:B:405:GLN:O	1:B:409:ASN:ND2	2.41	0.52
1:C:297:ALA:HB1	1:C:298:PRO:HD2	1.91	0.52
1:B:201:ILE:H	1:B:201:ILE:HD13	1.75	0.52
1:D:170:ARG:HH21	1:D:173:ARG:CB	2.22	0.52
1:E:305:TRP:NE1	1:E:344:ASP:OD2	2.38	0.52
1:E:499:VAL:HG11	1:E:537:TYR:CZ	2.44	0.52
1:E:162:GLU:HG3	1:E:180:ALA:HB2	1.91	0.52
1:B:20:ILE:HG12	1:B:48:VAL:HG12	1.91	0.52
1:C:307:ILE:HG21	1:C:314:HIS:ND1	2.24	0.52
1:F:200:GLU:O	1:F:200:GLU:HG2	2.08	0.52
1:A:150:LEU:C	1:A:152:ASN:H	2.12	0.52
1:C:405:GLN:OE1	1:C:438:VAL:HG21	2.09	0.52
1:D:110:GLN:HB3	1:D:694:ARG:NH1	2.24	0.52
1:F:20:ILE:HG12	1:F:48:VAL:HG12	1.91	0.52
1:B:413:LYS:NZ	1:B:439:ASP:OD1	2.32	0.52
1:D:476:LYS:HE3	1:D:608:LEU:O	2.10	0.52
1:E:173:ARG:HD2	1:E:177:LEU:HD11	1.92	0.52
1:C:487:ALA:O	1:C:488:GLU:HB2	2.10	0.52
1:F:526:THR:HG21	1:F:624:VAL:HG21	1.91	0.52
1:C:20:ILE:HG12	1:C:48:VAL:HG12	1.91	0.52
1:F:309:SER:HA	1:F:352:ASP:HB2	1.92	0.52
1:E:297:ALA:HB1	1:E:298:PRO:HD2	1.92	0.51
1:A:177:LEU:H	1:A:177:LEU:HD12	1.75	0.51
1:B:188:ASP:OD2	1:B:190:VAL:N	2.43	0.51
1:D:285:VAL:HG23	1:D:352:ASP:CG	2.31	0.51
1:F:168:VAL:HG12	1:F:208:TYR:CB	2.40	0.51
1:F:318:HIS:CD2	1:F:320:SER:H	2.28	0.51
1:B:534:TYR:OH	1:B:556:GLU:OE1	2.13	0.51
1:C:695:ASN:O	1:C:698:LEU:HG	2.10	0.51
1:E:315:ASP:OD1	1:E:316:THR:HG23	2.11	0.51
1:A:126:TRP:HZ3	1:A:128:ASP:HB2	1.76	0.51
1:B:184:ARG:N	1:B:192:ARG:NH1	2.58	0.51
1:C:590:PRO:O	1:C:593:GLN:HG3	2.10	0.51
1:E:307:ILE:HG21	1:E:314:HIS:CE1	2.45	0.51
1:B:417:VAL:HG12	1:B:420:PRO:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:MET:CE	1:B:537:TYR:HB3	2.41	0.51
1:C:625:VAL:HG11	1:C:672:ILE:HD13	1.91	0.51
1:D:526:THR:HG21	1:D:624:VAL:HG21	1.92	0.51
1:A:137:LEU:O	1:A:141:LEU:N	2.42	0.51
1:A:307:ILE:HG21	1:A:314:HIS:CE1	2.45	0.51
1:B:318:HIS:CD2	1:B:320:SER:H	2.28	0.51
1:D:102:GLN:HE22	1:D:698:LEU:HD12	1.75	0.51
1:E:155:LEU:HA	1:E:158:ALA:HB3	1.93	0.51
1:A:307:ILE:HG21	1:A:314:HIS:ND1	2.25	0.51
1:B:126:TRP:HZ3	1:B:128:ASP:HB2	1.76	0.51
1:B:476:LYS:HE3	1:B:608:LEU:O	2.11	0.51
1:C:134:ARG:HH21	1:C:197:LEU:HD23	1.76	0.51
1:E:476:LYS:HE3	1:E:608:LEU:O	2.11	0.51
1:A:318:HIS:NE2	1:A:320:SER:HB2	2.26	0.51
1:A:698:LEU:O	1:A:699:ARG:HB2	2.10	0.51
1:B:297:ALA:HB1	1:B:298:PRO:HD2	1.93	0.51
1:B:314:HIS:HB3	1:B:403:VAL:HG11	1.93	0.51
1:C:134:ARG:NH2	1:C:197:LEU:HD23	2.25	0.51
1:E:20:ILE:HG12	1:E:48:VAL:HG12	1.93	0.50
1:E:533:MET:HE1	1:E:579:ILE:HD13	1.93	0.50
1:F:183:LEU:HD23	1:F:192:ARG:HB2	1.93	0.50
1:A:285:VAL:HG23	1:A:352:ASP:OD1	2.11	0.50
1:B:202:GLU:H	1:B:202:GLU:CD	2.14	0.50
1:A:267:ALA:HB2	1:A:339:MET:HE2	1.94	0.50
1:C:367:PRO:HD2	1:D:152:ASN:OD1	2.11	0.50
1:E:157:GLY:O	1:E:161:LEU:HD12	2.12	0.50
1:E:533:MET:HE1	1:E:579:ILE:CD1	2.42	0.50
1:D:142:ASP:OD1	1:D:143:ALA:N	2.45	0.50
1:D:363:PHE:CD1	1:D:363:PHE:N	2.80	0.50
1:C:425:PRO:HG3	1:D:49:TRP:CZ3	2.47	0.50
1:E:487:ALA:O	1:E:488:GLU:HB2	2.09	0.50
1:A:110:GLN:NE2	1:A:694:ARG:HG3	2.27	0.50
1:A:198:THR:O	1:A:201:ILE:HD13	2.11	0.50
1:B:170:ARG:HB2	1:B:172:LEU:HG	1.94	0.50
1:E:275:TYR:CZ	1:E:416:ARG:HD3	2.47	0.50
1:E:284:LYS:N	1:E:352:ASP:OD2	2.29	0.50
1:F:122:ARG:HH11	1:F:219:GLN:HE21	1.58	0.50
1:A:417:VAL:HG12	1:A:420:PRO:HG3	1.94	0.50
1:A:695:ASN:O	1:A:698:LEU:HG	2.11	0.50
1:D:167:GLY:C	1:D:169:PRO:HD3	2.32	0.50
1:A:110:GLN:HB3	1:A:694:ARG:CZ	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:PRO:O	1:B:178:ALA:HB3	2.11	0.50
1:B:443:LEU:HD22	1:B:464:THR:HG21	1.92	0.50
1:D:127:GLY:O	1:D:129:PRO:HD3	2.11	0.49
1:E:605:ASN:HB2	1:E:636:ALA:HB2	1.94	0.49
1:F:134:ARG:O	1:F:138:ILE:HG13	2.12	0.49
1:A:183:LEU:HB2	1:A:192:ARG:CD	2.42	0.49
1:B:315:ASP:OD1	1:B:316:THR:HG23	2.11	0.49
1:C:170:ARG:H	1:C:173:ARG:CZ	2.26	0.49
1:C:307:ILE:HG21	1:C:314:HIS:CE1	2.47	0.49
1:E:185:THR:OG1	1:E:192:ARG:NH2	2.45	0.49
1:E:493:ARG:NH1	1:E:493:ARG:HG2	2.21	0.49
1:A:157:GLY:O	1:A:161:LEU:HD12	2.12	0.49
1:D:185:THR:H	1:D:192:ARG:NH1	2.10	0.49
1:D:305:TRP:NE1	1:D:344:ASP:OD2	2.37	0.49
1:E:182:ALA:HB3	1:E:195:LEU:HD21	1.93	0.49
1:A:285:VAL:HG23	1:A:352:ASP:CG	2.33	0.49
1:C:170:ARG:H	1:C:173:ARG:CD	2.26	0.49
1:E:443:LEU:HD22	1:E:464:THR:HG21	1.94	0.49
1:A:188:ASP:HB3	1:A:191:THR:HG23	1.95	0.49
1:A:20:ILE:HG12	1:A:48:VAL:HG12	1.95	0.49
1:A:305:TRP:NE1	1:A:344:ASP:OD2	2.42	0.49
1:D:169:PRO:O	1:D:170:ARG:HB3	2.13	0.49
1:F:626:VAL:HG12	1:F:681:ALA:HB2	1.95	0.49
1:D:364:THR:HG1	1:D:388:ASN:HD22	1.58	0.49
1:D:698:LEU:O	1:D:699:ARG:HB2	2.13	0.49
1:A:134:ARG:O	1:A:138:ILE:HG13	2.13	0.49
1:A:366:LEU:HB3	1:A:367:PRO:HD2	1.95	0.49
1:C:151:SER:HA	1:C:154:LEU:HD13	1.94	0.49
1:C:170:ARG:H	1:C:173:ARG:NE	2.11	0.49
1:C:170:ARG:HA	1:C:172:LEU:N	2.27	0.49
1:D:183:LEU:HD23	1:D:192:ARG:HB2	1.95	0.49
1:D:272:ASP:N	1:D:272:ASP:OD2	2.46	0.49
1:E:161:LEU:HD12	1:E:161:LEU:H	1.78	0.49
1:F:656:ARG:NH2	1:F:685:ASN:HD22	2.10	0.49
1:A:508:VAL:O	1:A:512:ASN:ND2	2.37	0.48
1:E:318:HIS:CD2	1:E:320:SER:H	2.31	0.48
1:F:583:ASN:HA	1:F:586:ARG:HD3	1.94	0.48
1:C:318:HIS:HD2	1:C:320:SER:H	1.60	0.48
1:E:625:VAL:HG11	1:E:672:ILE:HD13	1.95	0.48
1:F:625:VAL:HG11	1:F:672:ILE:HD13	1.95	0.48
1:A:314:HIS:HB3	1:A:403:VAL:HG11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LEU:HD12	1:B:118:LEU:HD23	1.95	0.48
1:E:698:LEU:O	1:E:699:ARG:HB2	2.13	0.48
1:A:318:HIS:CD2	1:A:320:SER:H	2.32	0.48
1:B:366:LEU:HB3	1:B:367:PRO:HD2	1.94	0.48
1:D:417:VAL:HG12	1:D:420:PRO:HG3	1.96	0.48
1:E:422:THR:OG1	1:E:423:LYS:HE3	2.14	0.48
1:A:67:VAL:HG12	1:A:68:ARG:N	2.28	0.48
1:B:202:GLU:O	1:B:206:ALA:N	2.42	0.48
1:B:242:THR:HG21	1:B:259:ALA:HA	1.96	0.48
1:C:225:ASP:OD1	1:C:436:LYS:NZ	2.36	0.48
1:D:590:PRO:O	1:D:593:GLN:HG3	2.12	0.48
1:E:318:HIS:NE2	1:E:320:SER:HB2	2.29	0.48
1:E:108:HIS:CG	1:E:698:LEU:HG	2.49	0.48
1:F:364:THR:OG1	1:F:388:ASN:ND2	2.33	0.48
1:A:161:LEU:HD12	1:A:161:LEU:H	1.77	0.48
1:A:425:PRO:HG3	1:B:49:TRP:CZ3	2.49	0.48
1:A:536:GLY:O	1:A:541:GLU:HG3	2.14	0.48
1:C:265:ARG:NH2	1:C:538:GLU:OE1	2.45	0.48
1:C:583:ASN:HA	1:C:586:ARG:HD3	1.96	0.48
1:E:198:THR:HB	1:E:201:ILE:HD11	1.95	0.48
1:A:200:GLU:OE1	1:A:200:GLU:N	2.47	0.48
1:D:182:ALA:O	1:D:192:ARG:HB2	2.13	0.48
1:D:275:TYR:CZ	1:D:416:ARG:HD3	2.48	0.48
1:E:170:ARG:O	1:E:173:ARG:HG2	2.14	0.48
1:C:67:VAL:CG1	1:C:440:PRO:HG3	2.44	0.48
1:A:493:ARG:HH11	1:A:493:ARG:HG2	1.78	0.48
1:B:475:THR:OG1	1:B:478:GLU:HG3	2.14	0.48
1:C:536:GLY:O	1:C:541:GLU:HG3	2.14	0.48
1:C:698:LEU:O	1:C:699:ARG:HB2	2.13	0.48
1:D:399:GLU:O	1:D:403:VAL:HG23	2.14	0.48
1:A:49:TRP:CZ3	1:B:425:PRO:HG3	2.49	0.48
1:A:657:ASP:OD1	1:A:659:ILE:HG13	2.13	0.48
1:B:265:ARG:NH2	1:B:538:GLU:OE1	2.47	0.48
1:B:318:HIS:HD2	1:B:320:SER:H	1.61	0.48
1:D:68:ARG:O	1:D:69:TYR:HB2	2.14	0.48
1:F:307:ILE:HG21	1:F:314:HIS:CE1	2.49	0.48
1:B:493:ARG:HG2	1:B:493:ARG:HH11	1.79	0.47
1:C:364:THR:OG1	1:C:388:ASN:ND2	2.31	0.47
1:D:493:ARG:HG2	1:D:493:ARG:HH11	1.79	0.47
1:D:534:TYR:OH	1:D:556:GLU:OE1	2.14	0.47
1:F:285:VAL:HG22	1:F:352:ASP:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LEU:HA	1:A:180:ALA:HB3	1.96	0.47
1:A:230:ARG:O	1:A:529:PRO:HB2	2.14	0.47
1:A:564:ASP:OD2	1:A:567:SER:OG	2.09	0.47
1:C:255:THR:OG1	1:C:256:PHE:N	2.47	0.47
1:D:315:ASP:OD1	1:D:316:THR:HG23	2.14	0.47
1:E:188:ASP:HB2	1:E:191:THR:CG2	2.37	0.47
1:F:285:VAL:HG21	1:F:351:PRO:HB2	1.97	0.47
1:A:315:ASP:OD1	1:A:316:THR:HG23	2.14	0.47
1:B:656:ARG:NH2	1:B:685:ASN:HD22	2.12	0.47
1:C:170:ARG:HA	1:C:171:GLY:C	2.35	0.47
1:C:275:TYR:OH	1:C:416:ARG:HD3	2.14	0.47
1:D:656:ARG:NH1	1:D:658:GLU:OE1	2.44	0.47
1:E:357:ARG:HG2	1:E:358:GLU:N	2.29	0.47
1:A:110:GLN:OE1	1:A:694:ARG:NE	2.46	0.47
1:C:497:LEU:HD22	1:C:528:SER:HB3	1.95	0.47
1:D:694:ARG:HA	1:D:694:ARG:HD2	1.59	0.47
1:E:141:LEU:HD13	1:E:142:ASP:N	2.30	0.47
1:E:280:HIS:C	1:E:318:HIS:HB2	2.35	0.47
1:F:114:ASP:OD1	1:F:115:ARG:NH1	2.48	0.47
1:E:194:ALA:HB3	1:E:195:LEU:HD22	1.97	0.47
1:F:255:THR:OG1	1:F:256:PHE:N	2.48	0.47
1:F:605:ASN:HB2	1:F:636:ALA:HB2	1.96	0.47
1:F:657:ASP:OD1	1:F:659:ILE:HG13	2.15	0.47
1:A:201:ILE:HA	1:A:204:LEU:HD13	1.96	0.47
1:D:168:VAL:HG22	1:D:170:ARG:NH1	2.29	0.47
1:C:170:ARG:H	1:C:173:ARG:HD3	1.79	0.47
1:D:183:LEU:HA	1:D:183:LEU:HD22	1.75	0.47
1:A:534:TYR:OH	1:A:556:GLU:OE1	2.18	0.47
1:C:493:ARG:HG2	1:C:493:ARG:HH11	1.80	0.47
1:F:201:ILE:HG23	1:F:204:LEU:HD11	1.95	0.47
1:C:318:HIS:NE2	1:C:320:SER:HB2	2.29	0.47
1:D:122:ARG:HH11	1:D:219:GLN:HE21	1.62	0.47
1:E:255:THR:OG1	1:E:256:PHE:N	2.47	0.47
1:E:615:ASP:OD2	1:E:618:THR:HG23	2.14	0.47
1:A:225:ASP:OD1	1:A:436:LYS:NZ	2.38	0.47
1:A:383:ASP:OD1	1:A:383:ASP:N	2.26	0.47
1:B:102:GLN:H	1:B:102:GLN:NE2	2.12	0.47
1:E:134:ARG:O	1:E:138:ILE:HG12	2.15	0.46
1:E:656:ARG:NH2	1:E:685:ASN:HD22	2.13	0.46
1:F:154:LEU:HD12	1:F:183:LEU:HD22	1.96	0.46
1:A:590:PRO:O	1:A:593:GLN:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:THR:OG1	1:B:192:ARG:NH2	2.48	0.46
1:A:506:HIS:ND1	1:A:507:ALA:N	2.64	0.46
1:B:110:GLN:OE1	1:B:694:ARG:HD2	2.15	0.46
1:C:150:LEU:CD1	1:C:154:LEU:HD11	2.42	0.46
1:C:245:TRP:HA	1:C:250:ASN:O	2.16	0.46
1:D:363:PHE:HD1	1:D:363:PHE:N	2.14	0.46
1:A:110:GLN:O	1:A:110:GLN:HG2	2.15	0.46
1:D:376:ASN:O	1:D:379:LYS:N	2.48	0.46
1:D:399:GLU:OE2	1:D:402:ARG:NH1	2.48	0.46
1:E:314:HIS:HB3	1:E:403:VAL:HG11	1.96	0.46
1:E:413:LYS:NZ	1:E:439:ASP:OD1	2.38	0.46
1:F:318:HIS:HD2	1:F:320:SER:H	1.61	0.46
1:A:584:ILE:HD13	1:C:664:TYR:HB3	1.96	0.46
1:B:188:ASP:O	1:B:191:THR:OG1	2.33	0.46
1:B:497:LEU:HD22	1:B:528:SER:HB3	1.97	0.46
1:C:357:ARG:HG2	1:C:358:GLU:N	2.29	0.46
1:D:497:LEU:HD22	1:D:528:SER:HB3	1.98	0.46
1:B:499:VAL:HG11	1:B:537:TYR:CZ	2.50	0.46
1:B:583:ASN:HA	1:B:586:ARG:HD3	1.98	0.46
1:F:200:GLU:HA	1:F:203:GLU:OE2	2.16	0.46
1:A:71:HIS:O	1:A:71:HIS:ND1	2.49	0.46
1:B:522:VAL:O	1:B:526:THR:OG1	2.25	0.46
1:C:314:HIS:HB3	1:C:403:VAL:HG11	1.98	0.46
1:C:108:HIS:CG	1:C:698:LEU:HD22	2.51	0.46
1:E:173:ARG:CD	1:E:177:LEU:HD11	2.45	0.46
1:E:288:LYS:HE3	2:E:801:MAL:O4	2.15	0.46
1:C:315:ASP:OD1	1:C:316:THR:HG23	2.15	0.46
1:B:501:THR:HG22	1:B:504:ILE:HG13	1.97	0.46
1:E:161:LEU:O	1:E:164:ALA:HB3	2.16	0.46
1:E:583:ASN:HA	1:E:586:ARG:HD3	1.97	0.46
1:F:152:ASN:O	1:F:156:VAL:HG23	2.15	0.46
1:A:626:VAL:HG12	1:A:681:ALA:HB2	1.98	0.46
1:B:109:GLY:C	1:B:110:GLN:HG3	2.36	0.46
1:C:49:TRP:CZ3	1:D:425:PRO:HG3	2.51	0.46
1:D:65:LEU:HD12	1:D:118:LEU:HD23	1.97	0.46
1:E:475:THR:OG1	1:E:478:GLU:HG3	2.15	0.46
1:F:318:HIS:NE2	1:F:320:SER:HB2	2.30	0.46
1:F:534:TYR:OH	1:F:556:GLU:OE1	2.13	0.46
1:A:255:THR:OG1	1:A:256:PHE:N	2.48	0.45
1:C:188:ASP:O	1:C:192:ARG:CG	2.63	0.45
1:C:68:ARG:O	1:C:69:TYR:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:ASP:OD1	1:F:143:ALA:N	2.49	0.45
1:F:193:THR:O	1:F:197:LEU:HD22	2.16	0.45
1:A:600:PHE:CE1	1:A:609:LEU:HD11	2.51	0.45
1:F:182:ALA:O	1:F:192:ARG:HA	2.15	0.45
1:F:446:SER:HB3	1:F:463:PHE:CD1	2.51	0.45
1:C:15:PRO:HA	1:C:16:GLY:HA2	1.83	0.45
1:C:256:PHE:CE2	1:C:327:PHE:HB2	2.51	0.45
1:D:475:THR:OG1	1:D:478:GLU:HG3	2.16	0.45
1:B:659:ILE:HG13	1:B:659:ILE:H	1.38	0.45
1:C:226:ARG:HH12	1:C:340:GLU:CD	2.19	0.45
1:A:183:LEU:HB2	1:A:192:ARG:CB	2.47	0.45
1:A:501:THR:HB	1:A:502:PRO:HD2	1.99	0.45
1:F:173:ARG:O	1:F:177:LEU:HD12	2.16	0.45
1:F:174:ASP:N	1:F:175:PRO:CD	2.80	0.45
1:B:486:ILE:HD13	1:B:495:PRO:HG3	1.98	0.45
1:C:475:THR:OG1	1:C:478:GLU:HG3	2.16	0.45
1:E:115:ARG:HG3	1:E:115:ARG:HH11	1.82	0.45
1:E:364:THR:OG1	1:E:388:ASN:ND2	2.35	0.45
1:E:536:GLY:O	1:E:541:GLU:HG3	2.17	0.45
1:F:265:ARG:NH2	1:F:538:GLU:OE1	2.49	0.45
1:F:536:GLY:O	1:F:541:GLU:HG3	2.16	0.45
1:B:487:ALA:CB	1:B:490:ALA:HB2	2.40	0.45
1:C:186:PRO:HA	1:C:192:ARG:NH2	2.32	0.45
1:F:177:LEU:H	1:F:177:LEU:HD12	1.82	0.45
1:A:151:SER:C	1:A:154:LEU:HD21	2.37	0.45
1:A:202:GLU:N	1:A:202:GLU:OE1	2.29	0.45
1:C:134:ARG:O	1:C:138:ILE:HG13	2.16	0.45
1:C:156:VAL:O	1:C:160:LEU:HD23	2.17	0.45
1:C:163:ARG:NH2	1:C:212:ASP:OD1	2.50	0.45
1:C:443:LEU:HD22	1:C:464:THR:HG21	1.97	0.45
1:C:476:LYS:HE3	1:C:608:LEU:O	2.16	0.45
1:F:383:ASP:OD1	1:F:383:ASP:N	2.29	0.45
1:A:161:LEU:O	1:A:164:ALA:HB3	2.17	0.45
1:A:443:LEU:HD22	1:A:464:THR:HG21	1.98	0.45
1:C:446:SER:HB3	1:C:463:PHE:CD1	2.52	0.45
1:E:405:GLN:OE1	1:E:438:VAL:HG21	2.16	0.45
1:F:475:THR:OG1	1:F:478:GLU:HG3	2.17	0.45
1:A:304:PRO:O	1:A:307:ILE:HD13	2.17	0.45
1:A:625:VAL:HG11	1:A:672:ILE:HD13	1.99	0.45
1:B:184:ARG:N	1:B:192:ARG:HH11	2.14	0.45
1:D:242:THR:HG21	1:D:259:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:HIS:HD2	1:D:320:SER:N	2.14	0.45
1:A:246:ASP:N	1:A:246:ASP:OD2	2.50	0.44
1:B:698:LEU:O	1:B:699:ARG:HB2	2.18	0.44
1:E:150:LEU:CD1	1:E:154:LEU:HD11	2.43	0.44
1:F:19:GLU:O	1:F:48:VAL:HA	2.17	0.44
1:F:493:ARG:HH11	1:F:493:ARG:HG2	1.83	0.44
1:A:150:LEU:H	1:A:150:LEU:HD23	1.81	0.44
1:C:417:VAL:HG12	1:C:420:PRO:HG3	1.98	0.44
1:E:67:VAL:CG1	1:E:440:PRO:HG3	2.47	0.44
1:F:698:LEU:O	1:F:699:ARG:HB2	2.17	0.44
1:A:275:TYR:CE1	1:A:416:ARG:HD3	2.52	0.44
1:B:170:ARG:O	1:B:172:LEU:N	2.51	0.44
1:B:567:SER:O	1:B:571:GLN:HG3	2.17	0.44
1:E:399:GLU:OE2	1:E:402:ARG:NH1	2.50	0.44
1:F:246:ASP:OD1	1:F:246:ASP:N	2.50	0.44
1:A:256:PHE:CE2	1:A:327:PHE:HB2	2.53	0.44
1:C:197:LEU:O	1:C:199:PRO:HD3	2.17	0.44
1:C:383:ASP:N	1:C:383:ASP:OD1	2.31	0.44
1:E:19:GLU:O	1:E:48:VAL:HA	2.17	0.44
1:A:108:HIS:HB3	1:A:698:LEU:HD22	2.00	0.44
1:B:174:ASP:HB2	1:B:176:LEU:HB2	1.99	0.44
1:B:178:ALA:O	1:B:182:ALA:HB2	2.17	0.44
1:A:245:TRP:HA	1:A:250:ASN:O	2.17	0.44
1:A:357:ARG:HG2	1:A:358:GLU:N	2.32	0.44
1:B:174:ASP:HB2	1:B:176:LEU:H	1.83	0.44
1:D:168:VAL:HG13	1:D:168:VAL:O	2.17	0.44
1:D:416:ARG:HH21	1:D:447:GLU:CG	2.31	0.44
1:D:695:ASN:O	1:D:698:LEU:HG	2.18	0.44
1:F:188:ASP:OD2	1:F:190:VAL:N	2.51	0.44
1:F:675:ASP:OD1	1:F:678:ARG:NH2	2.50	0.44
1:C:263:LEU:HA	1:C:263:LEU:HD23	1.84	0.44
1:E:156:VAL:O	1:E:159:VAL:HG12	2.18	0.44
1:E:366:LEU:HB3	1:E:367:PRO:HD2	2.00	0.44
1:F:201:ILE:N	1:F:201:ILE:HD12	2.32	0.44
1:A:126:TRP:CZ3	1:A:128:ASP:HB2	2.52	0.44
1:A:446:SER:HB3	1:A:463:PHE:CD1	2.53	0.44
1:B:600:PHE:CD1	1:B:611:TYR:HB3	2.53	0.44
1:A:179:ALA:HA	1:A:195:LEU:HB3	2.00	0.44
1:A:600:PHE:HE1	1:A:609:LEU:HD11	1.81	0.44
1:B:282:ILE:O	1:B:287:ARG:NH2	2.51	0.44
1:C:171:GLY:O	1:C:172:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ARG:HB2	1:C:173:ARG:NE	2.33	0.44
1:D:174:ASP:O	1:D:177:LEU:N	2.51	0.44
1:C:454:ARG:HG3	1:D:49:TRP:CE3	2.53	0.44
1:E:156:VAL:HA	1:E:159:VAL:HG12	2.00	0.44
1:F:476:LYS:HE3	1:F:608:LEU:O	2.18	0.44
1:B:21:ASP:OD1	1:B:22:ASP:N	2.48	0.43
1:B:383:ASP:OD1	1:B:383:ASP:N	2.28	0.43
1:C:390:ASP:CG	1:D:17:ARG:HH21	2.21	0.43
1:D:182:ALA:HA	1:D:192:ARG:HB3	2.00	0.43
1:E:114:ASP:OD1	1:E:115:ARG:HG3	2.18	0.43
1:E:242:THR:HG21	1:E:259:ALA:HA	2.00	0.43
1:A:165:ALA:HA	1:A:168:VAL:HG23	2.00	0.43
1:C:68:ARG:HB3	1:C:69:TYR:H	1.47	0.43
1:F:486:ILE:HD13	1:F:495:PRO:HG3	1.99	0.43
1:A:608:LEU:HD23	1:A:627:THR:HA	1.99	0.43
1:C:239:PRO:HD3	1:C:276:LEU:HD22	2.00	0.43
1:C:694:ARG:HD2	1:C:694:ARG:HA	1.84	0.43
1:D:625:VAL:HG11	1:D:672:ILE:HD13	2.01	0.43
1:F:225:ASP:OD1	1:F:436:LYS:NZ	2.42	0.43
1:F:659:ILE:HG13	1:F:659:ILE:H	1.42	0.43
1:A:168:VAL:HA	1:A:169:PRO:HD3	1.81	0.43
1:B:256:PHE:CE2	1:B:327:PHE:HB2	2.53	0.43
1:C:114:ASP:OD1	1:C:115:ARG:HG3	2.17	0.43
1:D:196:ALA:O	1:D:201:ILE:HD11	2.18	0.43
1:D:256:PHE:CE2	1:D:327:PHE:HB2	2.53	0.43
1:E:285:VAL:HG23	1:E:352:ASP:CG	2.39	0.43
1:F:189:PRO:O	1:F:193:THR:HG22	2.18	0.43
1:A:49:TRP:CE3	1:B:454:ARG:HG3	2.53	0.43
1:C:285:VAL:HG13	1:C:352:ASP:OD1	2.19	0.43
1:D:138:ILE:HA	1:D:141:LEU:HD23	2.00	0.43
1:E:182:ALA:O	1:E:192:ARG:HB3	2.17	0.43
1:F:353:HIS:CE1	1:F:355:TRP:CG	3.07	0.43
1:A:150:LEU:HD12	1:A:154:LEU:HD12	2.00	0.43
1:B:181:ALA:O	1:B:192:ARG:NH1	2.51	0.43
1:F:108:HIS:CG	1:F:698:LEU:HG	2.54	0.43
1:F:304:PRO:O	1:F:307:ILE:HD13	2.18	0.43
1:A:282:ILE:O	1:A:287:ARG:NH2	2.50	0.43
1:A:390:ASP:CG	1:B:17:ARG:HH21	2.22	0.43
1:C:156:VAL:O	1:C:159:VAL:HG12	2.19	0.43
1:C:399:GLU:O	1:C:403:VAL:HG23	2.18	0.43
1:D:175:PRO:O	1:D:178:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:ILE:O	1:D:287:ARG:NH2	2.51	0.43
1:D:230:ARG:O	1:D:529:PRO:HB2	2.19	0.43
1:E:162:GLU:CG	1:E:180:ALA:CB	2.96	0.43
1:E:179:ALA:CB	1:E:195:LEU:HG	2.46	0.43
1:F:280:HIS:C	1:F:318:HIS:HB2	2.39	0.43
1:F:505:LEU:HD13	1:F:552:TYR:CZ	2.53	0.43
1:A:567:SER:O	1:A:571:GLN:HG3	2.18	0.43
1:B:173:ARG:HA	1:B:174:ASP:HA	1.48	0.43
1:B:374:ALA:HA	1:B:386:PRO:HG3	2.00	0.43
1:C:17:ARG:HH21	1:D:390:ASP:CG	2.22	0.43
1:C:318:HIS:HD2	1:C:320:SER:N	2.17	0.43
1:C:435:VAL:O	1:C:438:VAL:HG22	2.18	0.43
1:D:506:HIS:ND1	1:D:507:ALA:N	2.66	0.43
1:F:114:ASP:OD1	1:F:115:ARG:HG3	2.19	0.43
1:A:199:PRO:HA	1:A:202:GLU:OE2	2.19	0.43
1:B:102:GLN:H	1:B:102:GLN:CD	2.21	0.43
1:B:126:TRP:CZ3	1:B:128:ASP:HB2	2.53	0.43
1:C:506:HIS:ND1	1:C:507:ALA:N	2.67	0.43
1:D:539:LEU:HA	1:D:539:LEU:HD23	1.74	0.43
1:E:567:SER:O	1:E:571:GLN:HG3	2.19	0.43
1:A:165:ALA:O	1:A:168:VAL:HG23	2.19	0.43
1:B:230:ARG:O	1:B:529:PRO:HB2	2.19	0.43
1:C:177:LEU:HD12	1:C:177:LEU:H	1.84	0.43
1:C:246:ASP:OD1	1:C:246:ASP:N	2.51	0.43
1:E:115:ARG:NH1	1:E:115:ARG:HG3	2.34	0.43
1:B:183:LEU:HA	1:B:192:ARG:HD2	2.01	0.42
1:B:168:VAL:HG12	1:B:208:TYR:CD1	2.54	0.42
1:B:318:HIS:NE2	1:B:320:SER:HB2	2.33	0.42
1:B:19:GLU:O	1:B:48:VAL:HA	2.18	0.42
1:C:19:GLU:O	1:C:48:VAL:HA	2.18	0.42
1:E:305:TRP:O	1:E:348:GLN:NE2	2.51	0.42
1:E:470:PHE:HD1	1:E:482:PHE:CE2	2.36	0.42
1:F:63:ARG:HH22	1:F:92:LYS:HE2	1.84	0.42
1:A:444:PHE:H	1:A:464:THR:HG1	1.67	0.42
1:A:505:LEU:HD13	1:A:552:TYR:CZ	2.54	0.42
1:B:183:LEU:N	1:B:192:ARG:NH1	2.67	0.42
1:B:353:HIS:CE1	1:B:355:TRP:CG	3.06	0.42
1:B:608:LEU:HD23	1:B:627:THR:HA	2.00	0.42
1:A:128:ASP:HA	1:A:129:PRO:HD2	1.93	0.42
1:A:242:THR:HG21	1:A:259:ALA:HA	2.01	0.42
1:D:188:ASP:HB2	1:D:189:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:ARG:NH1	1:E:124:ASP:OD1	2.52	0.42
1:E:309:SER:OG	1:E:310:ASP:N	2.52	0.42
1:F:600:PHE:CE1	1:F:609:LEU:HD11	2.55	0.42
1:B:600:PHE:CE1	1:B:609:LEU:HD11	2.54	0.42
1:D:21:ASP:OD1	1:D:22:ASP:N	2.52	0.42
1:D:318:HIS:NE2	1:D:320:SER:HB2	2.34	0.42
1:E:165:ALA:HA	1:E:168:VAL:HG23	1.99	0.42
1:E:501:THR:HB	1:E:502:PRO:HD2	2.00	0.42
1:A:374:ALA:HA	1:A:386:PRO:HG3	2.00	0.42
1:C:49:TRP:CE3	1:D:454:ARG:HG3	2.54	0.42
1:C:600:PHE:CD1	1:C:611:TYR:HB3	2.55	0.42
1:D:138:ILE:HG23	1:D:141:LEU:HD23	2.02	0.42
1:D:435:VAL:O	1:D:438:VAL:HG22	2.19	0.42
1:D:446:SER:HB3	1:D:463:PHE:CD1	2.53	0.42
1:D:17:ARG:NH1	1:D:51:GLU:OE2	2.38	0.42
1:F:192:ARG:HG2	1:F:192:ARG:H	1.66	0.42
1:A:366:LEU:HA	1:A:366:LEU:HD23	1.81	0.42
1:A:390:ASP:OD2	1:B:17:ARG:NH2	2.53	0.42
1:B:197:LEU:HD13	1:B:198:THR:HG23	2.01	0.42
1:B:405:GLN:OE1	1:B:438:VAL:HG21	2.19	0.42
1:B:676:PRO:O	1:B:677:ALA:HB3	2.20	0.42
1:D:523:LEU:O	1:D:527:MET:HG3	2.20	0.42
1:E:497:LEU:HD22	1:E:528:SER:HB3	2.01	0.42
1:F:160:LEU:HD23	1:F:160:LEU:HA	1.95	0.42
1:F:141:LEU:HD11	1:F:193:THR:HG21	2.01	0.42
1:F:255:THR:HG23	1:F:258:THR:H	1.85	0.42
1:F:676:PRO:C	1:F:678:ARG:H	2.21	0.42
1:B:154:LEU:HD22	1:B:154:LEU:N	2.34	0.42
1:B:376:ASN:O	1:B:379:LYS:N	2.53	0.42
1:C:438:VAL:HG23	1:C:439:ASP:N	2.34	0.42
1:D:629:ASN:ND2	1:D:629:ASN:O	2.52	0.42
1:E:607:ALA:HB3	1:E:634:GLU:HG2	2.01	0.42
1:B:246:ASP:OD1	1:B:246:ASP:N	2.51	0.42
1:B:435:VAL:O	1:B:438:VAL:HG22	2.20	0.42
1:C:280:HIS:C	1:C:318:HIS:HB2	2.40	0.42
1:C:390:ASP:OD2	1:D:17:ARG:NH2	2.50	0.42
1:C:515:GLY:O	1:C:519:ILE:HG13	2.20	0.42
1:E:676:PRO:C	1:E:678:ARG:H	2.22	0.42
1:F:414:PHE:CE1	1:F:443:LEU:HD12	2.55	0.42
1:F:435:VAL:O	1:F:438:VAL:HG22	2.20	0.42
1:F:608:LEU:HD23	1:F:627:THR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:THR:HA	1:B:199:PRO:HD3	1.94	0.42
1:B:285:VAL:HG21	1:B:351:PRO:HB2	2.01	0.42
1:B:605:ASN:HB2	1:B:636:ALA:HB2	2.02	0.42
1:C:161:LEU:O	1:C:165:ALA:N	2.50	0.42
1:C:573:ARG:HG3	1:C:573:ARG:HH11	1.85	0.42
1:D:255:THR:OG1	1:D:256:PHE:N	2.52	0.42
1:E:236:GLU:HB3	1:E:534:TYR:HA	2.02	0.42
1:F:204:LEU:HD12	1:F:205:LEU:HG	2.02	0.42
1:A:497:LEU:HD22	1:A:528:SER:HB3	2.02	0.42
1:A:659:ILE:HG13	1:A:659:ILE:H	1.43	0.42
1:B:128:ASP:HA	1:B:129:PRO:HD2	1.91	0.42
1:B:185:THR:HG23	1:B:192:ARG:NH2	2.34	0.42
1:F:183:LEU:HD23	1:F:192:ARG:CB	2.50	0.42
1:F:318:HIS:HD2	1:F:320:SER:N	2.17	0.42
1:B:168:VAL:HG12	1:B:208:TYR:CG	2.55	0.41
1:B:198:THR:O	1:B:200:GLU:N	2.47	0.41
1:C:21:ASP:OD1	1:C:22:ASP:N	2.50	0.41
1:E:170:ARG:HB2	1:E:171:GLY:H	1.44	0.41
1:F:560:LEU:HA	1:F:560:LEU:HD23	1.75	0.41
1:F:676:PRO:HD2	1:F:678:ARG:HH21	1.85	0.41
1:A:114:ASP:OD1	1:A:115:ARG:HG3	2.21	0.41
1:A:239:PRO:HD3	1:A:276:LEU:HD22	2.02	0.41
1:C:170:ARG:HG2	1:C:171:GLY:HA2	2.01	0.41
1:C:582:LEU:HA	1:C:582:LEU:HD23	1.90	0.41
1:D:536:GLY:O	1:D:541:GLU:HG3	2.19	0.41
1:E:523:LEU:O	1:E:527:MET:HG3	2.20	0.41
1:E:519:ILE:HD13	1:E:627:THR:O	2.20	0.41
1:F:376:ASN:O	1:F:379:LYS:N	2.52	0.41
1:A:65:LEU:HD12	1:A:118:LEU:HD23	2.03	0.41
1:A:280:HIS:C	1:A:318:HIS:HB2	2.41	0.41
1:B:223:TRP:HE1	1:B:436:LYS:HZ3	1.67	0.41
1:E:114:ASP:OD1	1:E:115:ARG:NH1	2.54	0.41
1:E:151:SER:HA	1:E:154:LEU:HD13	2.02	0.41
1:E:255:THR:HG23	1:E:258:THR:H	1.85	0.41
1:E:629:ASN:ND2	1:E:629:ASN:O	2.54	0.41
1:F:523:LEU:O	1:F:527:MET:HG3	2.19	0.41
1:A:19:GLU:O	1:A:48:VAL:HA	2.21	0.41
1:A:236:GLU:HB3	1:A:534:TYR:HA	2.03	0.41
1:A:318:HIS:HD2	1:A:320:SER:H	1.67	0.41
1:A:376:ASN:O	1:A:379:LYS:N	2.53	0.41
1:A:417:VAL:CG1	1:A:420:PRO:HG3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:LEU:HD23	1:A:539:LEU:HA	1.79	0.41
1:C:228:LEU:HD23	1:C:340:GLU:OE1	2.19	0.41
1:D:245:TRP:HA	1:D:250:ASN:O	2.20	0.41
1:B:184:ARG:H	1:B:192:ARG:NH1	2.19	0.41
1:B:199:PRO:HA	1:B:202:GLU:OE2	2.21	0.41
1:B:377:PRO:HA	1:B:378:PRO:HA	1.76	0.41
1:B:505:LEU:HD12	1:B:552:TYR:CD1	2.56	0.41
1:B:67:VAL:HG12	1:B:67:VAL:O	2.21	0.41
1:C:112:THR:HA	1:C:113:PRO:HD3	1.74	0.41
1:C:280:HIS:HB2	1:C:307:ILE:HG23	2.02	0.41
1:D:108:HIS:HB3	1:D:698:LEU:HD22	2.02	0.41
1:F:309:SER:OG	1:F:310:ASP:N	2.54	0.41
1:F:368:ASP:N	1:F:368:ASP:OD1	2.50	0.41
1:A:399:GLU:O	1:A:403:VAL:HG23	2.20	0.41
1:B:183:LEU:HA	1:B:192:ARG:HB3	2.01	0.41
1:D:416:ARG:HH21	1:D:447:GLU:HG3	1.84	0.41
1:B:168:VAL:O	1:B:170:ARG:N	2.48	0.41
1:C:353:HIS:CE1	1:C:355:TRP:CG	3.09	0.41
1:D:160:LEU:O	1:D:164:ALA:N	2.44	0.41
1:D:353:HIS:CE1	1:D:355:TRP:CG	3.09	0.41
1:D:315:ASP:OD2	1:D:402:ARG:NH2	2.54	0.41
1:E:198:THR:HB	1:E:201:ILE:CD1	2.50	0.41
1:F:626:VAL:HG12	1:F:681:ALA:CB	2.51	0.41
1:A:470:PHE:HD1	1:A:482:PHE:CE2	2.39	0.41
1:B:318:HIS:HD2	1:B:320:SER:N	2.18	0.41
1:E:377:PRO:HA	1:E:378:PRO:HA	1.75	0.41
1:E:505:LEU:HD13	1:E:552:TYR:CZ	2.56	0.41
1:F:324:ILE:HD11	1:F:410:HIS:NE2	2.36	0.41
1:A:21:ASP:OD1	1:A:22:ASP:N	2.53	0.41
1:B:185:THR:H	1:B:192:ARG:CZ	2.34	0.41
1:B:625:VAL:HG11	1:B:672:ILE:HD13	2.02	0.41
1:D:626:VAL:HG12	1:D:681:ALA:HB2	2.03	0.41
1:E:185:THR:HA	1:E:186:PRO:HD3	1.95	0.41
1:A:519:ILE:HD13	1:A:627:THR:O	2.21	0.41
1:B:446:SER:HB3	1:B:463:PHE:CD1	2.56	0.41
1:C:377:PRO:HA	1:C:378:PRO:HA	1.81	0.41
1:E:175:PRO:O	1:E:179:ALA:N	2.51	0.41
1:F:102:GLN:CD	1:F:102:GLN:H	2.25	0.41
1:F:115:ARG:HG3	1:F:115:ARG:NH1	2.36	0.41
1:F:501:THR:HB	1:F:502:PRO:HD2	2.03	0.41
1:B:399:GLU:OE2	1:B:402:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ASP:O	1:C:191:THR:HG22	2.21	0.41
1:C:523:LEU:O	1:C:527:MET:HG3	2.21	0.41
1:D:676:PRO:O	1:D:677:ALA:HB3	2.21	0.41
1:E:600:PHE:CE1	1:E:609:LEU:HD11	2.56	0.41
1:F:115:ARG:HH11	1:F:115:ARG:HG3	1.86	0.41
1:B:357:ARG:HB2	1:B:357:ARG:HH11	1.85	0.40
1:D:573:ARG:HH11	1:D:573:ARG:HG3	1.86	0.40
1:E:245:TRP:HA	1:E:250:ASN:O	2.20	0.40
1:E:304:PRO:O	1:E:307:ILE:HD13	2.21	0.40
1:E:433:ALA:O	1:E:437:THR:HG22	2.21	0.40
1:F:197:LEU:HD23	1:F:198:THR:N	2.36	0.40
1:A:419:ASN:N	1:A:420:PRO:HD3	2.36	0.40
1:B:174:ASP:OD2	1:B:177:LEU:HD22	2.22	0.40
1:C:676:PRO:O	1:C:677:ALA:HB3	2.21	0.40
1:D:150:LEU:HG	1:D:154:LEU:HD11	2.02	0.40
1:D:471:THR:O	1:D:506:HIS:CD2	2.74	0.40
1:C:615:ASP:HA	1:C:616:PRO:HD2	1.82	0.40
1:D:246:ASP:OD1	1:D:246:ASP:N	2.54	0.40
1:D:314:HIS:CD2	1:D:353:HIS:HE2	2.40	0.40
1:A:133:TRP:CE2	1:A:157:GLY:HA3	2.57	0.40
1:A:560:LEU:HA	1:A:560:LEU:HD23	1.89	0.40
1:B:357:ARG:HG3	1:B:358:GLU:N	2.37	0.40
1:B:523:LEU:O	1:B:527:MET:HG3	2.21	0.40
1:C:267:ALA:N	1:C:339:MET:HE1	2.36	0.40
1:C:580:THR:O	1:C:584:ILE:HG13	2.21	0.40
1:D:236:GLU:HB3	1:D:534:TYR:HA	2.02	0.40
1:E:539:LEU:HA	1:E:539:LEU:HD23	1.83	0.40
1:E:575:LEU:O	1:E:579:ILE:HG13	2.21	0.40
1:E:676:PRO:O	1:E:677:ALA:HB3	2.21	0.40
1:A:318:HIS:HE2	1:A:320:SER:HB2	1.86	0.40
1:A:523:LEU:O	1:A:527:MET:HG3	2.21	0.40
1:B:177:LEU:O	1:B:181:ALA:N	2.44	0.40
1:C:290:ARG:HH11	1:C:559:GLU:CD	2.25	0.40
1:D:181:ALA:HB1	1:D:192:ARG:HH22	1.86	0.40
1:D:239:PRO:HD3	1:D:276:LEU:HD22	2.02	0.40
1:D:223:TRP:HE1	1:D:436:LYS:HZ2	1.69	0.40
1:D:690:PRO:C	1:D:692:GLU:H	2.24	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:CYS:CB	1:E:29:CYS:SG[2_656]	1.82	0.38
1:F:29:CYS:CB	1:F:29:CYS:SG[2_555]	1.84	0.36

## 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	655/723 (91%)	632 (96%)	18 (3%)	5 (1%)	22	57
1	B	655/723 (91%)	630 (96%)	16 (2%)	9 (1%)	13	46
1	C	655/723 (91%)	632 (96%)	17 (3%)	6 (1%)	20	55
1	D	655/723 (91%)	624 (95%)	25 (4%)	6 (1%)	20	55
1	E	655/723 (91%)	632 (96%)	18 (3%)	5 (1%)	22	57
1	F	655/723 (91%)	631 (96%)	18 (3%)	6 (1%)	20	55
All	All	3930/4338 (91%)	3781 (96%)	112 (3%)	37 (1%)	20	55

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	SER
1	A	170	ARG
1	B	151	SER
1	B	488	GLU
1	C	68	ARG
1	C	69	TYR
1	C	151	SER
1	C	172	LEU
1	C	488	GLU
1	D	69	TYR
1	D	151	SER
1	D	170	ARG
1	D	183	LEU
1	D	488	GLU

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Mol	Chain	Res	Type
1	E	151	SER
1	E	488	GLU
1	F	488	GLU
1	A	67	VAL
1	A	488	GLU
1	B	171	GLY
1	B	194	ALA
1	F	150	LEU
1	B	100	SER
1	E	194	ALA
1	F	68	ARG
1	F	193	THR
1	B	70	PRO
1	B	199	PRO
1	E	171	GLY
1	F	67	VAL
1	A	393	PRO
1	B	168	VAL
1	B	393	PRO
1	E	393	PRO
1	F	393	PRO
1	C	393	PRO
1	D	393	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	543/597 (91%)	497 (92%)	46 (8%)	12	42
1	B	543/597 (91%)	494 (91%)	49 (9%)	11	39
1	C	543/597 (91%)	505 (93%)	38 (7%)	18	52
1	D	543/597 (91%)	500 (92%)	43 (8%)	14	45
1	E	543/597 (91%)	497 (92%)	46 (8%)	12	42
1	F	543/597 (91%)	501 (92%)	42 (8%)	15	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3258/3582 (91%)	2994 (92%)	264 (8%)	14	44

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	59	THR
1	A	94	LEU
1	A	128	ASP
1	A	131	HIS
1	A	137	LEU
1	A	150	LEU
1	A	151	SER
1	A	154	LEU
1	A	162	GLU
1	A	168	VAL
1	A	170	ARG
1	A	174	ASP
1	A	183	LEU
1	A	190	VAL
1	A	192	ARG
1	A	198	THR
1	A	201	ILE
1	A	204	LEU
1	A	255	THR
1	A	285	VAL
1	A	303	SER
1	A	309	SER
1	A	323	THR
1	A	332	SER
1	A	348	GLN
1	A	352	ASP
1	A	357	ARG
1	A	361	GLN
1	A	370	THR
1	A	414	PHE
1	A	464	THR
1	A	466	SER
1	A	475	THR
1	A	485	GLN
1	A	542	HIS
1	A	581	ARG

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Mol	Chain	Res	Type
1	A	593	GLN
1	A	626	VAL
1	A	627	THR
1	A	629	ASN
1	A	659	ILE
1	A	664	TYR
1	A	691	TYR
1	A	694	ARG
1	A	696	THR
1	B	17	ARG
1	B	53	HIS
1	B	68	ARG
1	B	71	HIS
1	B	94	LEU
1	B	102	GLN
1	B	128	ASP
1	B	154	LEU
1	B	163	ARG
1	B	170	ARG
1	B	173	ARG
1	B	174	ASP
1	B	176	LEU
1	B	177	LEU
1	B	183	LEU
1	B	195	LEU
1	B	197	LEU
1	B	201	ILE
1	B	202	GLU
1	B	204	LEU
1	B	207	ASP
1	B	240	ARG
1	B	255	THR
1	B	303	SER
1	B	323	THR
1	B	332	SER
1	B	348	GLN
1	B	352	ASP
1	B	357	ARG
1	B	370	THR
1	B	405	GLN
1	B	414	PHE
1	B	416	ARG

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Mol	Chain	Res	Type
1	B	464	THR
1	B	471	THR
1	B	485	GLN
1	B	501	THR
1	B	505	LEU
1	B	542	HIS
1	B	543	ARG
1	B	581	ARG
1	B	626	VAL
1	B	627	THR
1	B	659	ILE
1	B	664	TYR
1	B	691	TYR
1	B	695	ASN
1	B	696	THR
1	B	698	LEU
1	C	29	CYS
1	C	53	HIS
1	C	68	ARG
1	C	71	HIS
1	C	92	LYS
1	C	102	GLN
1	C	110	GLN
1	C	112	THR
1	C	131	HIS
1	C	141	LEU
1	C	174	ASP
1	C	198	THR
1	C	211	ARG
1	C	255	THR
1	C	285	VAL
1	C	287	ARG
1	C	303	SER
1	C	309	SER
1	C	323	THR
1	C	332	SER
1	C	348	GLN
1	C	352	ASP
1	C	357	ARG
1	C	361	GLN
1	C	368	ASP
1	C	405	GLN

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Mol	Chain	Res	Type
1	C	414	PHE
1	C	464	THR
1	C	466	SER
1	C	543	ARG
1	C	581	ARG
1	C	593	GLN
1	C	627	THR
1	C	659	ILE
1	C	664	TYR
1	C	691	TYR
1	C	695	ASN
1	C	696	THR
1	D	26	VAL
1	D	53	HIS
1	D	63	ARG
1	D	115	ARG
1	D	137	LEU
1	D	141	LEU
1	D	150	LEU
1	D	170	ARG
1	D	172	LEU
1	D	173	ARG
1	D	176	LEU
1	D	183	LEU
1	D	191	THR
1	D	195	LEU
1	D	197	LEU
1	D	198	THR
1	D	201	ILE
1	D	204	LEU
1	D	255	THR
1	D	272	ASP
1	D	303	SER
1	D	309	SER
1	D	323	THR
1	D	348	GLN
1	D	352	ASP
1	D	363	PHE
1	D	370	THR
1	D	405	GLN
1	D	410	HIS
1	D	414	PHE

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Mol	Chain	Res	Type
1	D	437	THR
1	D	464	THR
1	D	471	THR
1	D	563	ARG
1	D	581	ARG
1	D	593	GLN
1	D	626	VAL
1	D	627	THR
1	D	629	ASN
1	D	659	ILE
1	D	664	TYR
1	D	691	TYR
1	D	696	THR
1	E	29	CYS
1	E	53	HIS
1	E	71	HIS
1	E	92	LYS
1	E	112	THR
1	E	115	ARG
1	E	141	LEU
1	E	149	GLU
1	E	168	VAL
1	E	170	ARG
1	E	173	ARG
1	E	183	LEU
1	E	193	THR
1	E	195	LEU
1	E	197	LEU
1	E	198	THR
1	E	201	ILE
1	E	204	LEU
1	E	211	ARG
1	E	219	GLN
1	E	255	THR
1	E	303	SER
1	E	323	THR
1	E	332	SER
1	E	348	GLN
1	E	352	ASP
1	E	357	ARG
1	E	361	GLN
1	E	405	GLN

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Mol	Chain	Res	Type
1	E	410	HIS
1	E	414	PHE
1	E	423	LYS
1	E	464	THR
1	E	471	THR
1	E	493	ARG
1	E	569	LEU
1	E	581	ARG
1	E	593	GLN
1	E	627	THR
1	E	629	ASN
1	E	659	ILE
1	E	663	GLU
1	E	664	TYR
1	E	691	TYR
1	E	694	ARG
1	E	696	THR
1	F	29	CYS
1	F	53	HIS
1	F	68	ARG
1	F	102	GLN
1	F	115	ARG
1	F	151	SER
1	F	153	ASP
1	F	154	LEU
1	F	163	ARG
1	F	170	ARG
1	F	192	ARG
1	F	197	LEU
1	F	198	THR
1	F	203	GLU
1	F	204	LEU
1	F	211	ARG
1	F	255	THR
1	F	303	SER
1	F	323	THR
1	F	324	ILE
1	F	332	SER
1	F	348	GLN
1	F	352	ASP
1	F	361	GLN
1	F	405	GLN

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Mol	Chain	Res	Type
1	F	414	PHE
1	F	437	THR
1	F	464	THR
1	F	466	SER
1	F	471	THR
1	F	542	HIS
1	F	543	ARG
1	F	618	THR
1	F	627	THR
1	F	659	ILE
1	F	664	TYR
1	F	675	ASP
1	F	678	ARG
1	F	691	TYR
1	F	694	ARG
1	F	696	THR
1	F	698	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	318	HIS
1	B	318	HIS
1	C	318	HIS
1	D	314	HIS
1	D	318	HIS
1	E	318	HIS
1	F	318	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

6 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	MAL	A	801	-	24,24,24	0.72	0	35,35,35	0.87	0
2	MAL	B	801	-	24,24,24	0.73	0	35,35,35	0.98	1 (2%)
2	MAL	C	801	-	24,24,24	0.70	0	35,35,35	0.88	0
2	MAL	D	801	-	24,24,24	0.67	0	35,35,35	0.94	2 (5%)
2	MAL	E	801	-	24,24,24	0.71	0	35,35,35	0.99	2 (5%)
2	MAL	F	801	-	24,24,24	0.71	0	35,35,35	0.97	2 (5%)

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	MAL	A	801	-	-	0/8/48/48	0/2/2/2
2	MAL	B	801	-	-	0/8/48/48	0/2/2/2
2	MAL	C	801	-	-	0/8/48/48	0/2/2/2
2	MAL	D	801	-	-	0/8/48/48	0/2/2/2
2	MAL	E	801	-	-	0/8/48/48	0/2/2/2
2	MAL	F	801	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	MAL	O1-C4'-C3'	2.01	112.02	107.19
2	F	801	MAL	C1'-O5'-C5'	2.01	117.01	113.39
2	F	801	MAL	O1-C4'-C3'	2.03	112.09	107.19
2	E	801	MAL	C1'-O5'-C5'	2.10	117.17	113.39
2	E	801	MAL	O1-C4'-C3'	2.11	112.28	107.19
2	B	801	MAL	C1'-O5'-C5'	2.20	117.36	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	MAL	C1'-O5'-C5'	2.38	117.68	113.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	MAL	1	0
2	B	801	MAL	1	0
2	C	801	MAL	1	0
2	D	801	MAL	1	0
2	E	801	MAL	2	0
2	F	801	MAL	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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(Å²)	Q<0.9	
1	A	661/723 (91%)	0.24	0	100	100	47, 65, 120, 146	0
1	B	661/723 (91%)	0.20	1 (0%)	94	95	46, 66, 124, 148	0
1	C	661/723 (91%)	0.25	2 (0%)	93	93	46, 65, 119, 137	0
1	D	661/723 (91%)	0.21	1 (0%)	94	95	45, 65, 123, 144	0
1	E	661/723 (91%)	0.20	3 (0%)	90	90	47, 65, 119, 148	0
1	F	661/723 (91%)	0.22	1 (0%)	94	95	47, 65, 114, 136	0
All	All	3966/4338 (91%)	0.22	8 (0%)	94	95	45, 65, 120, 148	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	197	LEU	3.6
1	D	189	PRO	3.2
1	E	176	LEU	3.0
1	B	197	LEU	2.9
1	C	183	LEU	2.6
1	C	196	ALA	2.3
1	F	176	LEU	2.1
1	E	196	ALA	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
2	MAL	B	801	23/23	0.95	0.24	-0.01	75,80,84,89	0
2	MAL	E	801	23/23	0.95	0.23	-0.15	76,83,90,92	0
2	MAL	D	801	23/23	0.95	0.23	-0.25	76,82,86,87	0
2	MAL	A	801	23/23	0.95	0.23	-0.28	75,83,85,89	0
2	MAL	C	801	23/23	0.96	0.24	-0.44	76,81,86,89	0
2	MAL	F	801	23/23	0.96	0.20	-0.96	74,80,87,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.