



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2017 – 04:46 AM EDT

PDB ID : 4U3C
Title : Docking Site of Maltohexaose in the Mtb GlgE
Authors : Ronning, D.R.; Lindenberger, J.J.
Deposited on : unknown
Resolution : 3.98 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

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

with specific help available everywhere you see the ⓘ symbol.

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

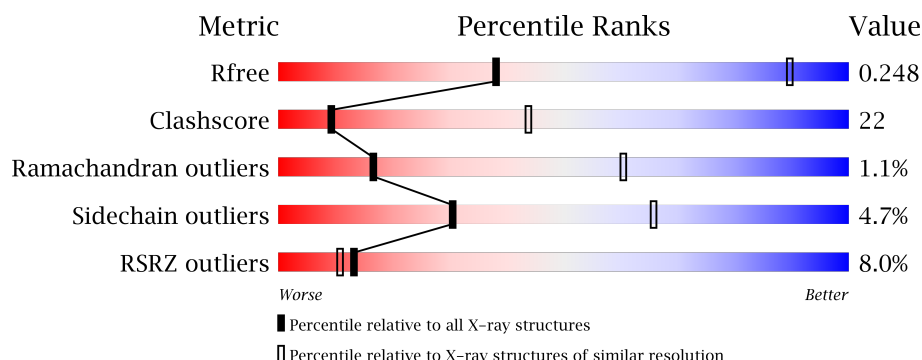
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.98 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	1066 (4.36-3.60)
Clashscore	112137	1163 (4.36-3.60)
Ramachandran outliers	110173	1119 (4.36-3.60)
Sidechain outliers	110143	1108 (4.36-3.60)
RSRZ outliers	101464	1078 (4.36-3.60)

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 ≥ 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	<div> <div>7%</div> <div>55%</div> <div>33%</div> <div>9%</div> </div>
1	B	723	<div> <div>7%</div> <div>58%</div> <div>31%</div> <div>9%</div> </div>
1	C	723	<div> <div>9%</div> <div>55%</div> <div>33%</div> <div>9%</div> </div>
1	D	723	<div> <div>7%</div> <div>50%</div> <div>37%</div> <div>9%</div> </div>
1	E	723	<div> <div>7%</div> <div>53%</div> <div>34%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	723	<div><div></div><div>6%</div><div>56%</div><div>32%</div><div>•</div><div>9%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31938 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	660	Total	C	N	O	S	0	0	0
			5233	3359	910	950	14			
1	B	660	Total	C	N	O	S	0	0	0
			5233	3359	910	950	14			
1	C	660	Total	C	N	O	S	0	0	0
			5233	3359	910	950	14			
1	D	660	Total	C	N	O	S	0	0	0
			5233	3359	910	950	14			
1	E	660	Total	C	N	O	S	0	0	0
			5233	3359	910	950	14			
1	F	660	Total	C	N	O	S	0	0	0
			5233	3359	910	950	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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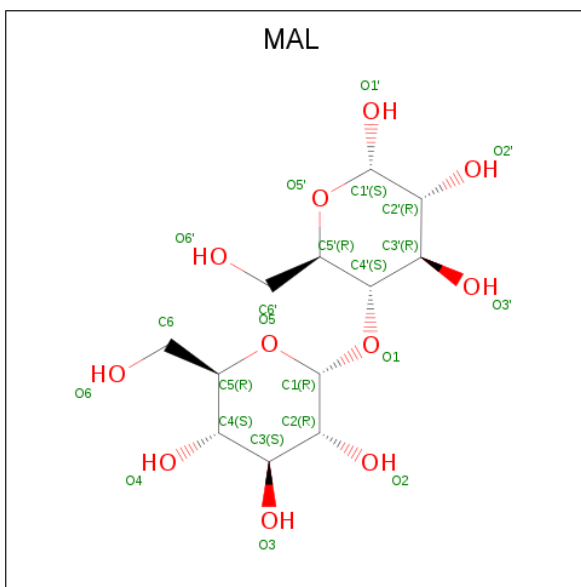
Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	VAL	-	expression tag	UNP P9WQ16
C	-5	LEU	-	expression tag	UNP P9WQ16
C	-4	PHE	-	expression tag	UNP P9WQ16
C	-3	GLN	-	expression tag	UNP P9WQ16
C	-2	GLY	-	expression tag	UNP P9WQ16
C	-1	PRO	-	expression tag	UNP P9WQ16
C	0	HIS	-	expression tag	UNP P9WQ16
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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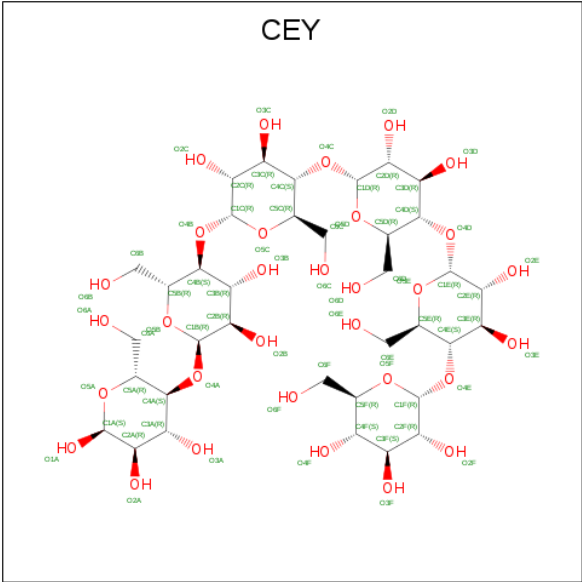
Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	LEU	-	expression tag	UNP P9WQ16
E	-7	GLU	-	expression tag	UNP P9WQ16
E	-6	VAL	-	expression tag	UNP P9WQ16
E	-5	LEU	-	expression tag	UNP P9WQ16
E	-4	PHE	-	expression tag	UNP P9WQ16
E	-3	GLN	-	expression tag	UNP P9WQ16
E	-2	GLY	-	expression tag	UNP P9WQ16
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: C₁₂H₂₂O₁₁).



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		

- Molecule 3 is alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranose (three-letter code: CEY) (formula: C₃₆H₆₂O₃₁).

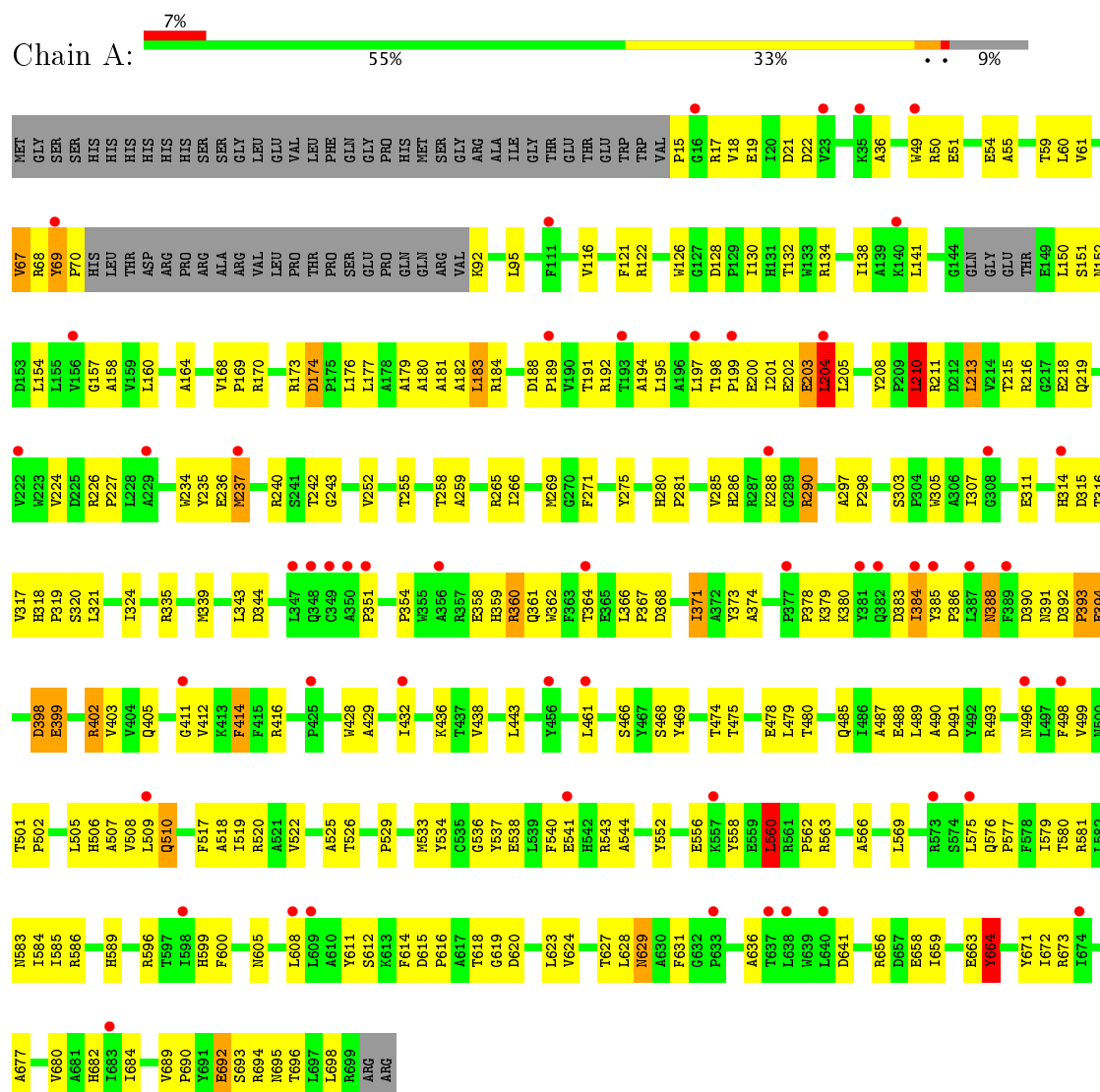


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			67	36	31		
3	B	1	Total	C	O	0	0
			67	36	31		
3	C	1	Total	C	O	0	0
			67	36	31		
3	D	1	Total	C	O	0	0
			67	36	31		
3	E	1	Total	C	O	0	0
			67	36	31		
3	F	1	Total	C	O	0	0
			67	36	31		

3 Residue-property plots

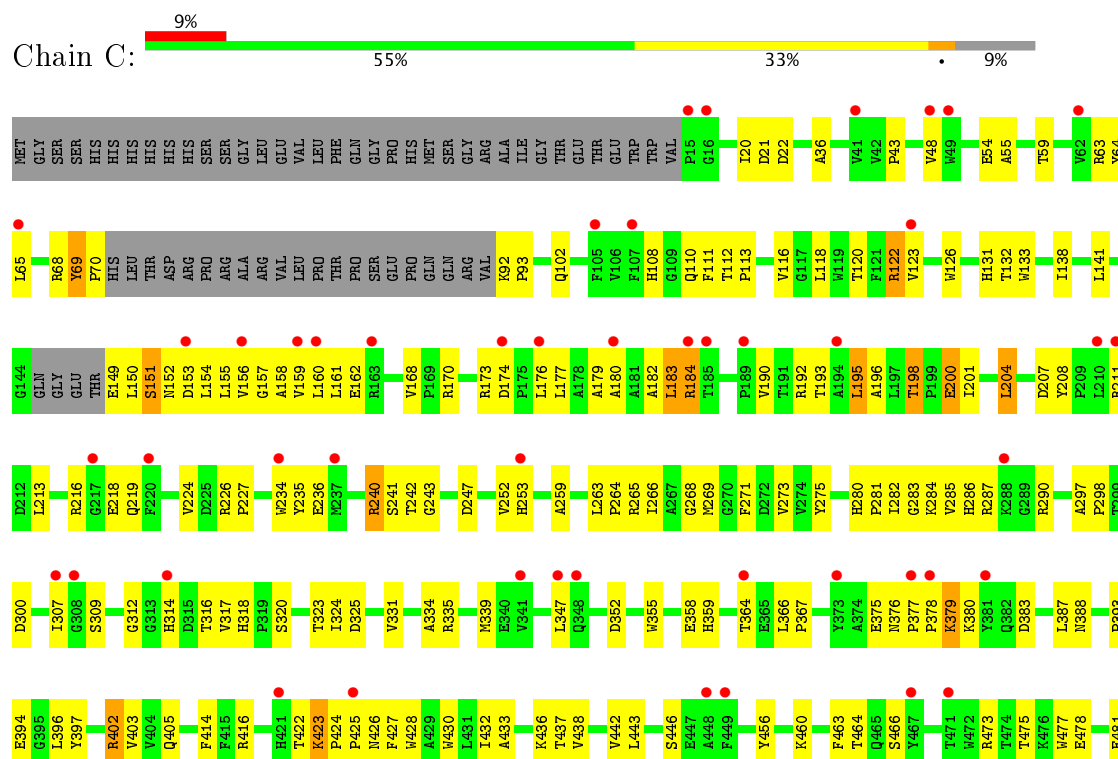
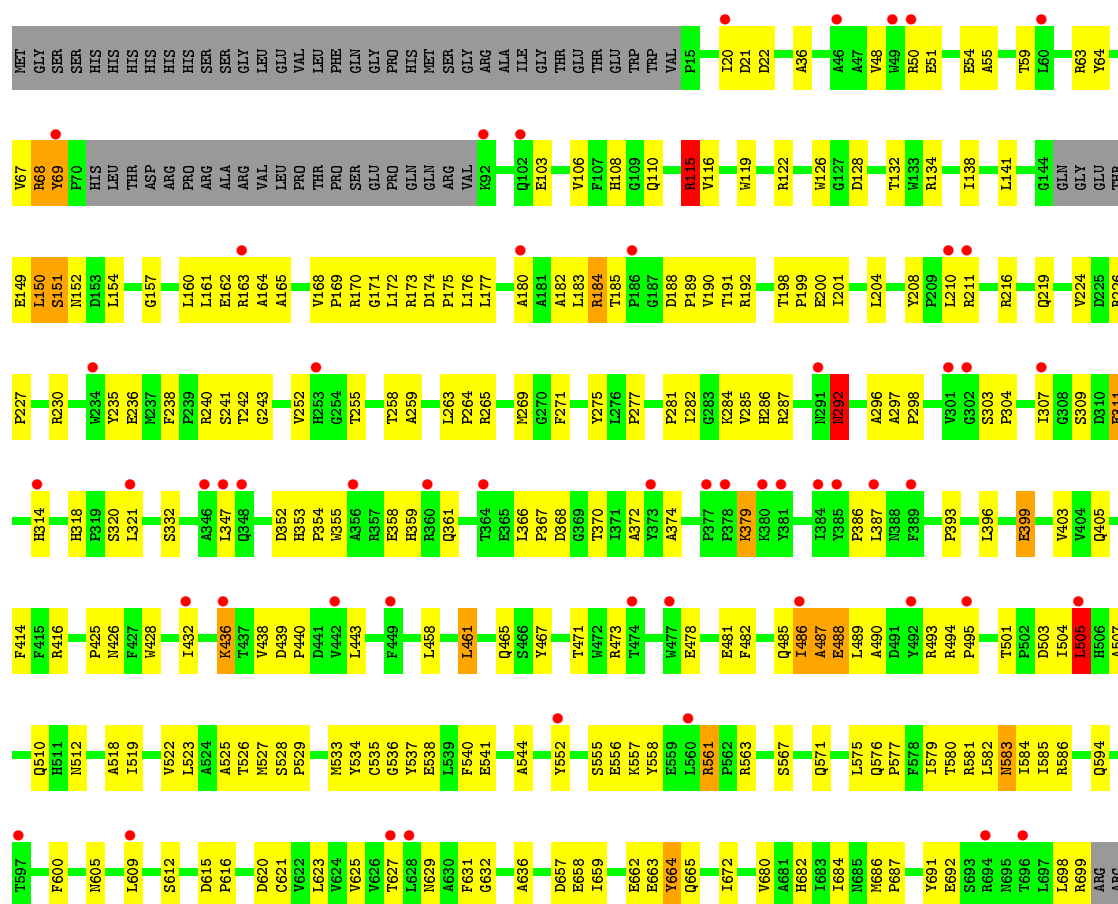
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

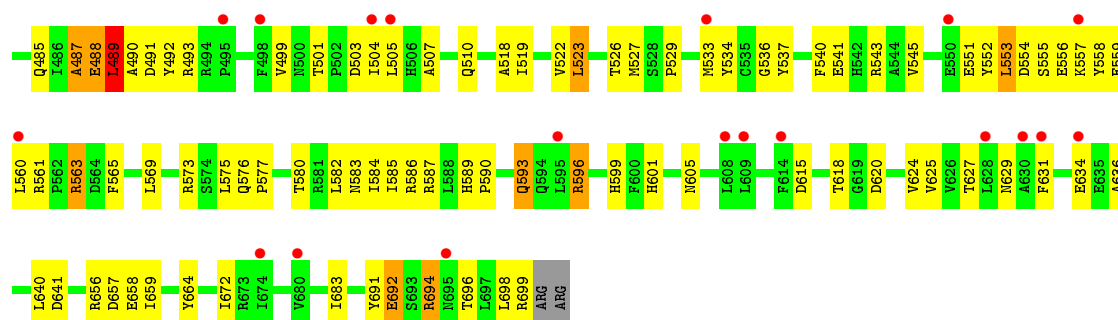
- Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase



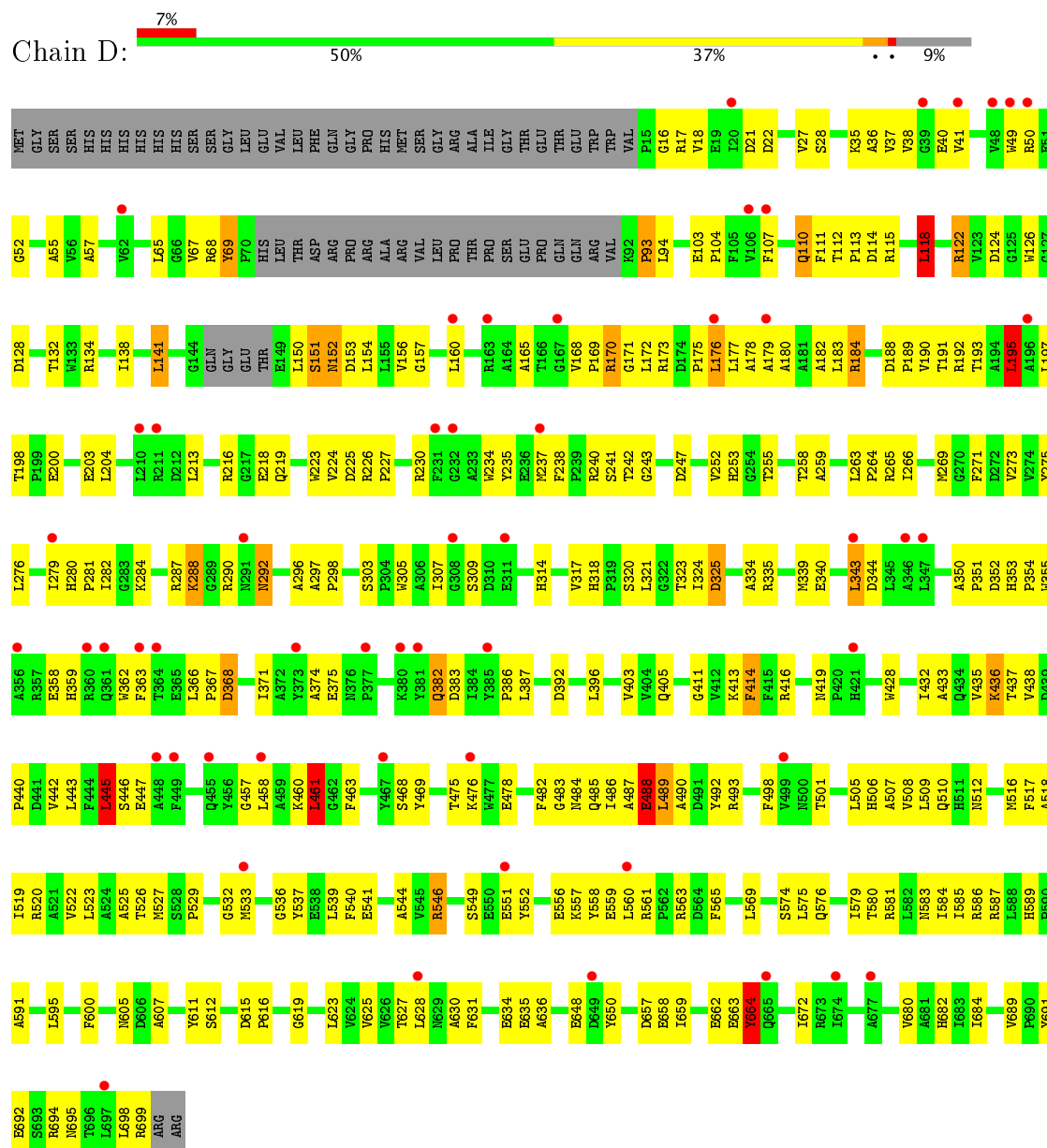
- Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase





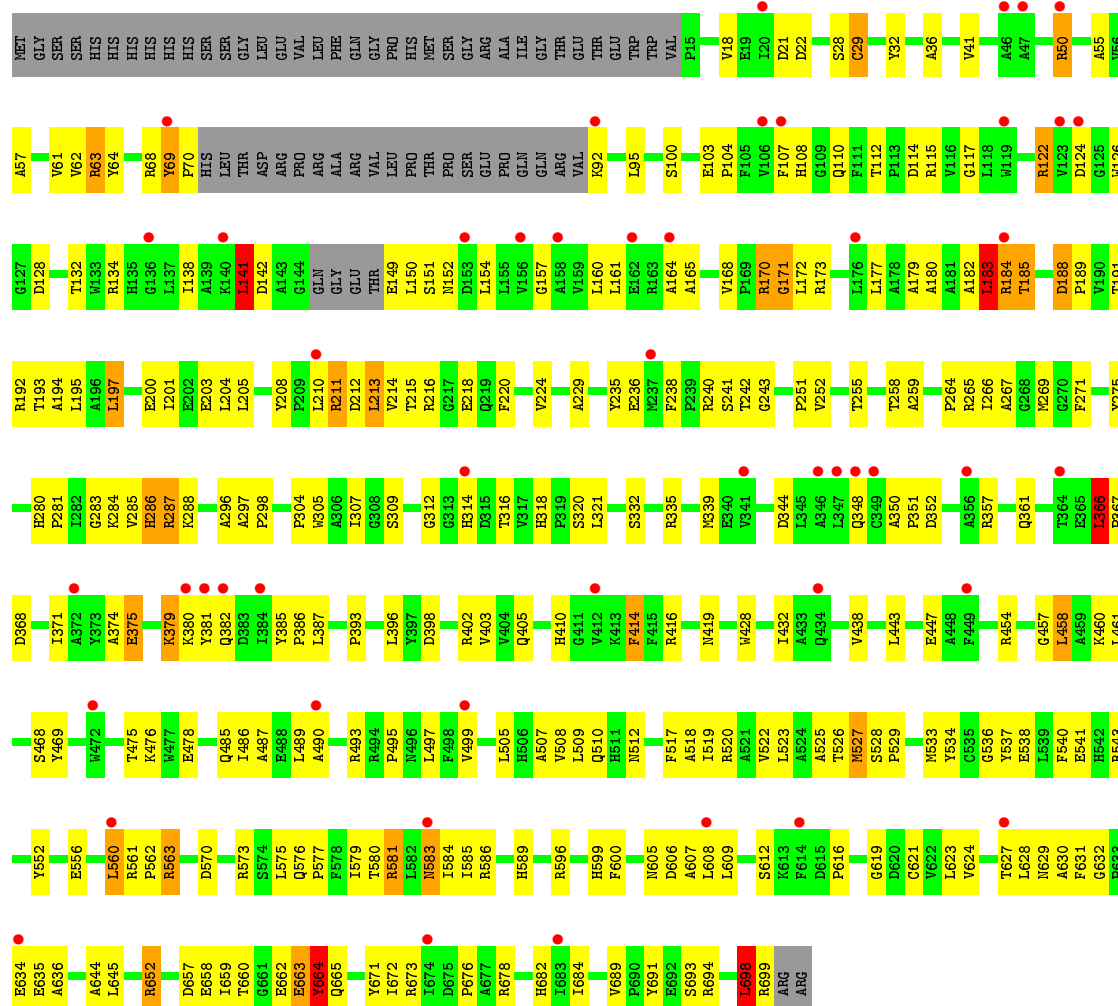


- Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase

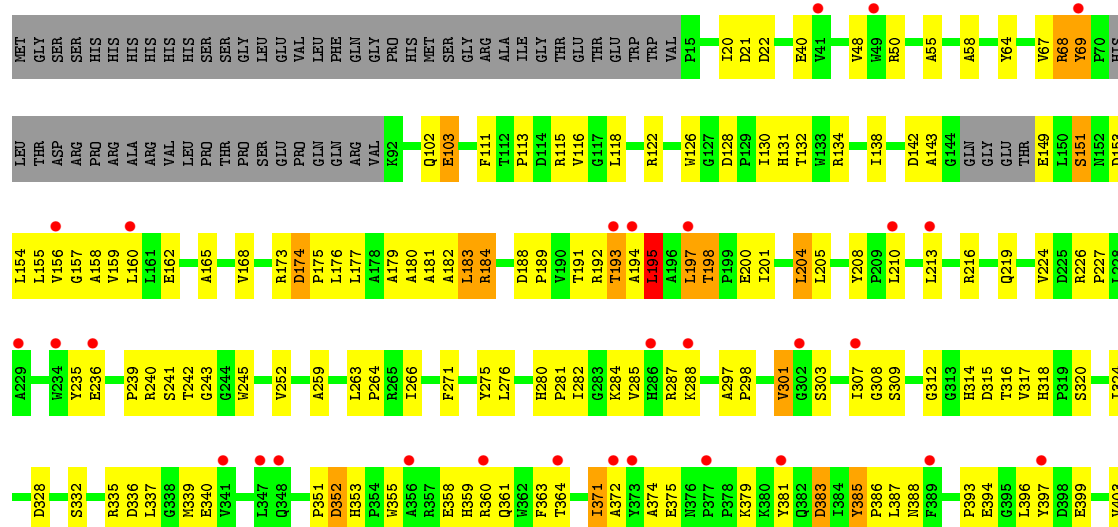


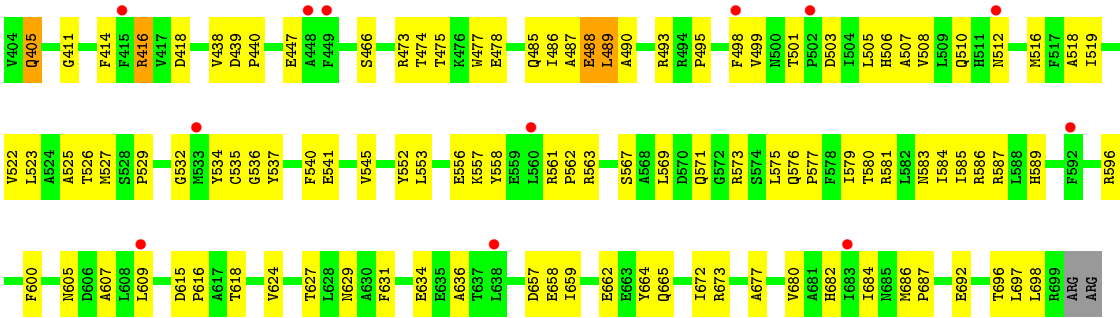
- Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase





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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	338.42Å 239.42Å 239.45Å 90.00° 134.90° 90.00°	Depositor
Resolution (Å)	43.73 – 3.98 43.74 – 3.98	Depositor EDS
% Data completeness (in resolution range)	97.9 (43.73-3.98) 88.0 (43.74-3.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.224 , 0.256 0.221 , 0.248	Depositor DCC
R_{free} test set	5103 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	110.8	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for h+2*k,-h-l 0.000 for k+l,h+l,-l 0.000 for -k+l,-h-l,-l 0.000 for -h+k-l,-l,-k 0.000 for -h-k-l,l,k 0.407 for h-k+l,l,-h-l 0.407 for -k-l,-h-l,k 0.408 for h+k+l,-l,-h-l 0.409 for k-l,h+l,-k 0.000 for h,-k,-h-l 0.409 for -h-2*k,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	31938	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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: MAL, CEY

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	0.38	0/5396	0.74	7/7380 (0.1%)
1	B	0.39	0/5396	0.76	6/7380 (0.1%)
1	C	0.39	0/5396	0.76	5/7380 (0.1%)
1	D	0.41	0/5396	0.81	10/7380 (0.1%)
1	E	0.40	0/5396	0.78	6/7380 (0.1%)
1	F	0.38	0/5396	0.78	8/7380 (0.1%)
All	All	0.39	0/32376	0.77	42/44280 (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	A	0	1
1	B	0	1
1	D	0	3
1	E	0	2
All	All	0	7

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	366	LEU	CA-CB-CG	8.78	135.49	115.30
1	E	698	LEU	CA-CB-CG	8.69	135.29	115.30
1	B	505	LEU	CA-CB-CG	8.41	134.65	115.30
1	A	560	LEU	CA-CB-CG	8.29	134.37	115.30
1	F	195	LEU	CA-CB-CG	7.42	132.37	115.30
1	F	204	LEU	CA-CB-CG	7.16	131.76	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	461	LEU	CA-CB-CG	6.71	130.73	115.30
1	D	461	LEU	CA-CB-CG	6.68	130.66	115.30
1	F	138	ILE	CG1-CB-CG2	-6.67	96.72	111.40
1	E	213	LEU	CA-CB-CG	6.54	130.34	115.30
1	F	184	ARG	N-CA-C	-6.43	93.64	111.00
1	F	360	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	D	176	LEU	CA-CB-CG	6.39	129.99	115.30
1	C	553	LEU	CA-CB-CG	6.38	129.98	115.30
1	D	197	LEU	CA-CB-CG	6.33	129.86	115.30
1	E	183	LEU	N-CA-C	6.30	128.00	111.00
1	A	203	GLU	N-CA-C	6.17	127.65	111.00
1	C	184	ARG	N-CA-C	-6.05	94.65	111.00
1	B	664	TYR	CA-CB-CG	6.05	124.89	113.40
1	D	195	LEU	CA-CB-CG	5.97	129.02	115.30
1	C	489	LEU	CA-CB-CG	5.95	128.98	115.30
1	D	445	LEU	CA-CB-CG	5.93	128.94	115.30
1	A	210	LEU	CA-CB-CG	5.90	128.88	115.30
1	B	115	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	D	195	LEU	CB-CG-CD2	-5.87	101.02	111.00
1	D	292	ASN	CB-CA-C	-5.82	98.76	110.40
1	D	664	TYR	CA-CB-CG	5.76	124.35	113.40
1	C	213	LEU	CA-CB-CG	5.68	128.37	115.30
1	D	288	LYS	CD-CE-NZ	-5.65	98.71	111.70
1	D	118	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	203	GLU	C-N-CA	5.58	135.65	121.70
1	F	197	LEU	CA-CB-CG	5.53	128.01	115.30
1	E	664	TYR	CA-CB-CG	5.48	123.81	113.40
1	A	204	LEU	CA-CB-CG	5.48	127.90	115.30
1	F	213	LEU	CA-CB-CG	5.42	127.77	115.30
1	E	141	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	664	TYR	CA-CB-CG	5.39	123.65	113.40
1	B	487	ALA	C-N-CA	5.32	134.99	121.70
1	A	213	LEU	CA-CB-CG	5.28	127.45	115.30
1	F	183	LEU	N-CA-C	5.26	125.19	111.00
1	B	292	ASN	N-CA-CB	-5.23	101.18	110.60
1	C	487	ALA	N-CA-CB	-5.02	103.08	110.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	B	292	ASN	Sidechain
1	D	292	ASN	Sidechain
1	D	484	ASN	Sidechain
1	D	488	GLU	Peptide
1	E	379	LYS	Mainchain
1	E	62	VAL	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	5233	0	5044	235	0
1	B	5233	0	5044	223	0
1	C	5233	0	5044	229	0
1	D	5233	0	5044	269	0
1	E	5233	0	5045	232	1
1	F	5233	0	5045	209	0
2	A	23	0	22	0	0
2	B	23	0	22	0	0
2	C	23	0	22	2	0
2	D	23	0	22	4	0
2	E	23	0	22	2	0
2	F	23	0	22	1	0
3	A	67	0	62	3	0
3	B	67	0	62	3	0
3	C	67	0	62	3	0
3	D	67	0	62	4	0
3	E	67	0	62	4	0
3	F	67	0	62	5	0
All	All	31938	0	30770	1380	1

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 22.

All (1380) 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:487:ALA:HA	1:D:488:GLU:HB2	1.13	1.11
1:C:487:ALA:HB1	1:C:488:GLU:HB3	1.30	1.08
1:D:154:LEU:HD22	1:D:183:LEU:HD22	1.38	1.03
1:D:487:ALA:HA	1:D:488:GLU:CB	1.90	1.02
1:B:165:ALA:HB1	1:B:173:ARG:HD2	1.43	0.97
1:A:55:ALA:H	1:A:132:THR:HG22	1.32	0.94
1:C:55:ALA:H	1:C:132:THR:HG22	1.33	0.93
1:F:173:ARG:O	1:F:173:ARG:NH1	2.01	0.93
1:E:275:TYR:OH	1:E:416:ARG:NH1	2.00	0.92
1:E:63:ARG:HG3	1:E:64:TYR:N	1.84	0.91
1:D:179:ALA:HA	1:D:195:LEU:HD21	1.55	0.89
1:B:512:ASN:HA	1:B:631:PHE:CZ	2.07	0.89
1:B:512:ASN:HA	1:B:631:PHE:HZ	1.37	0.89
1:C:149:GLU:N	1:C:151:SER:HG	1.72	0.88
1:D:275:TYR:OH	1:D:416:ARG:NH1	2.07	0.86
1:C:275:TYR:OH	1:C:416:ARG:NH1	2.07	0.86
1:A:203:GLU:HG3	1:A:205:LEU:H	1.42	0.85
1:C:347:LEU:O	1:C:423:LYS:NZ	2.09	0.85
1:A:560:LEU:HD23	1:A:562:PRO:HD3	1.58	0.85
1:E:284:LYS:HD3	1:E:352:ASP:HB3	1.59	0.85
1:C:265:ARG:HB2	1:E:673:ARG:HH21	1.41	0.84
1:E:698:LEU:HD12	1:E:699:ARG:HG3	1.58	0.84
1:A:491:ASP:OD1	1:A:596:ARG:NH2	2.11	0.84
1:D:55:ALA:H	1:D:132:THR:HG22	1.42	0.84
1:E:55:ALA:H	1:E:132:THR:HG22	1.39	0.84
1:F:179:ALA:HB1	1:F:195:LEU:HG	1.58	0.84
1:B:55:ALA:H	1:B:132:THR:HG22	1.44	0.83
1:D:18:VAL:HG22	1:D:50:ARG:HD3	1.59	0.83
1:F:173:ARG:HH12	1:F:177:LEU:H	1.23	0.83
1:D:151:SER:OG	1:D:152:ASN:N	2.11	0.82
1:D:37:VAL:N	1:D:40:GLU:OE2	2.12	0.82
1:C:323:THR:HG22	1:C:325:ASP:H	1.44	0.82
1:D:475:THR:HG22	1:D:478:GLU:HG3	1.58	0.82
1:A:629:ASN:C	1:A:629:ASN:HD22	1.84	0.81
1:F:241:SER:OG	1:F:561:ARG:O	1.99	0.81
1:C:170:ARG:HA	1:C:173:ARG:HG2	1.62	0.81
1:A:154:LEU:HD13	1:A:183:LEU:HD13	1.61	0.80
1:F:165:ALA:HB1	1:F:173:ARG:HE	1.44	0.80
1:C:487:ALA:CB	1:C:489:LEU:H	1.94	0.80
1:B:556:GLU:HG3	1:B:561:ARG:HG2	1.63	0.80
1:D:476:LYS:HD3	1:D:628:LEU:HD12	1.63	0.80
1:C:177:LEU:HA	1:C:180:ALA:HB3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:ILE:HA	1:F:204:LEU:HG	1.62	0.80
1:E:63:ARG:HG3	1:E:64:TYR:H	1.44	0.79
1:B:182:ALA:HB1	1:B:192:ARG:HB3	1.62	0.79
1:D:288:LYS:HE3	1:D:382:GLN:HB3	1.62	0.79
1:F:183:LEU:HD11	1:F:191:THR:HG22	1.64	0.79
1:A:164:ALA:HB2	1:A:210:LEU:HD23	1.66	0.78
1:A:405:GLN:HE22	1:A:438:VAL:HG21	1.49	0.78
1:F:558:TYR:HH	2:F:801:MAL:HO3	1.29	0.77
1:A:130:ILE:HD11	1:A:210:LEU:HD21	1.67	0.77
1:E:374:ALA:O	1:E:375:GLU:HB2	1.82	0.77
1:C:487:ALA:HB1	1:C:488:GLU:CB	2.13	0.77
1:D:169:PRO:O	1:D:171:GLY:N	2.15	0.77
1:B:191:THR:HB	1:B:192:ARG:HD2	1.67	0.76
1:C:284:LYS:N	1:C:352:ASP:OD2	2.18	0.76
1:E:28:SER:OG	1:E:460:LYS:HE3	1.86	0.76
1:C:269:MET:HA	1:C:580:THR:HG23	1.68	0.76
1:D:35:LYS:NZ	1:D:463:PHE:O	2.19	0.76
1:B:629:ASN:HD21	1:B:632:GLY:H	1.32	0.76
1:D:288:LYS:HZ3	1:D:383:ASP:HB3	1.51	0.76
1:C:265:ARG:HB2	1:E:673:ARG:NH2	2.00	0.75
1:F:55:ALA:H	1:F:132:THR:HG22	1.51	0.75
1:B:482:PHE:O	1:B:486:ILE:HG22	1.85	0.75
1:D:557:LYS:HE2	2:D:801:MAL:H2	1.68	0.75
1:D:170:ARG:HA	1:D:173:ARG:HG3	1.69	0.75
1:D:241:SER:OG	1:D:561:ARG:O	2.02	0.75
1:E:57:ALA:HA	1:E:107:PHE:HE2	1.51	0.75
1:A:474:THR:HG21	1:A:508:VAL:HG21	1.66	0.75
1:E:149:GLU:N	1:E:149:GLU:OE2	2.20	0.75
1:D:433:ALA:O	1:D:437:THR:OG1	2.04	0.75
1:C:179:ALA:O	1:C:192:ARG:NH1	2.20	0.74
1:F:474:THR:HG21	1:F:508:VAL:HG21	1.69	0.74
1:C:433:ALA:O	1:C:437:THR:OG1	2.05	0.74
1:A:18:VAL:HG21	1:A:213:LEU:HD13	1.70	0.74
1:F:165:ALA:CB	1:F:173:ARG:HE	2.00	0.74
1:E:201:ILE:HA	1:E:204:LEU:HG	1.70	0.74
1:A:265:ARG:NH1	1:A:576:GLN:OE1	2.21	0.74
1:B:318:HIS:CE1	1:B:320:SER:HB3	2.22	0.74
1:C:241:SER:OG	1:C:561:ARG:O	2.05	0.74
1:D:539:LEU:HD12	1:D:563:ARG:HD3	1.69	0.74
1:A:150:LEU:O	1:A:152:ASN:N	2.21	0.74
1:A:275:TYR:OH	1:A:416:ARG:NH1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:TYR:CD2	1:E:460:LYS:HE2	2.23	0.73
1:F:358:GLU:HG3	1:F:359:HIS:ND1	2.04	0.73
1:E:375:GLU:HG3	1:E:380:LYS:HD2	1.70	0.73
1:A:130:ILE:HG12	1:A:210:LEU:HD11	1.70	0.73
1:D:517:PHE:HD2	1:D:540:PHE:HD1	1.35	0.73
1:E:605:ASN:HB2	1:E:636:ALA:HB2	1.69	0.73
1:B:629:ASN:ND2	1:B:632:GLY:H	1.85	0.73
1:F:173:ARG:NH1	1:F:177:LEU:H	1.87	0.73
1:E:266:ILE:HG22	1:E:339:MET:HE1	1.70	0.73
1:B:416:ARG:NH1	1:B:467:TYR:OH	2.22	0.73
1:D:165:ALA:HB2	1:D:176:LEU:HD11	1.71	0.73
1:C:284:LYS:NZ	1:C:309:SER:OG	2.20	0.73
1:E:269:MET:HA	1:E:580:THR:HG23	1.71	0.73
1:E:635:GLU:HB2	1:E:673:ARG:HH11	1.52	0.73
1:F:162:GLU:OE1	1:F:162:GLU:N	2.21	0.73
1:A:179:ALA:O	1:A:192:ARG:HD2	1.90	0.72
1:D:405:GLN:HE22	1:D:438:VAL:HG21	1.54	0.72
1:A:54:GLU:OE1	1:A:54:GLU:N	2.21	0.71
1:C:183:LEU:HB2	1:C:192:ARG:NE	2.05	0.71
1:D:226:ARG:NH1	1:D:340:GLU:OE2	2.22	0.71
1:D:405:GLN:NE2	1:D:438:VAL:HG21	2.05	0.71
1:F:162:GLU:OE2	1:F:184:ARG:NH2	2.22	0.71
1:B:54:GLU:OE1	1:B:54:GLU:N	2.20	0.71
1:A:335:ARG:NH2	1:A:411:GLY:O	2.22	0.71
1:D:539:LEU:HB2	1:D:563:ARG:NH1	2.05	0.71
1:F:335:ARG:NH2	1:F:411:GLY:O	2.24	0.71
1:F:535:CYS:SG	1:F:563:ARG:NH1	2.63	0.71
1:D:318:HIS:CE1	1:D:320:SER:HB3	2.26	0.71
1:D:223:TRP:NE1	1:D:225:ASP:OD1	2.24	0.71
1:F:183:LEU:O	1:F:192:ARG:NH1	2.23	0.70
1:E:281:PRO:HB2	1:E:309:SER:HB3	1.73	0.70
1:E:536:GLY:HA3	1:E:563:ARG:NH1	2.06	0.70
1:B:493:ARG:HD3	1:B:494:ARG:N	2.06	0.70
1:C:378:PRO:O	1:C:380:LYS:NZ	2.24	0.70
1:E:108:HIS:CE1	1:E:698:LEU:HD13	2.27	0.70
1:A:183:LEU:N	1:A:192:ARG:HD3	2.07	0.70
1:B:533:MET:HE3	1:B:537:TYR:HD1	1.56	0.70
1:C:59:THR:HG23	1:C:126:TRP:HE1	1.57	0.70
1:D:488:GLU:OE2	1:D:493:ARG:NH1	2.24	0.70
1:E:183:LEU:HD11	1:E:192:ARG:HB3	1.74	0.70
1:A:618:THR:HG23	1:A:620:ASP:H	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:ALA:HB3	1:C:489:LEU:H	1.56	0.70
1:A:368:ASP:OD2	1:B:152:ASN:ND2	2.24	0.70
1:C:240:ARG:HG3	1:C:240:ARG:HH11	1.57	0.70
1:B:529:PRO:O	1:B:586:ARG:NH2	2.24	0.70
1:B:284:LYS:N	1:B:352:ASP:OD2	2.22	0.69
1:E:486:ILE:HG21	1:E:493:ARG:HH21	1.58	0.69
1:B:493:ARG:NH1	1:B:494:ARG:H	1.89	0.69
1:A:182:ALA:HB3	1:A:192:ARG:HG3	1.73	0.69
1:A:629:ASN:O	1:A:629:ASN:ND2	2.21	0.69
1:D:122:ARG:HH22	1:D:216:ARG:HD3	1.57	0.69
1:C:318:HIS:CE1	1:C:320:SER:HB3	2.26	0.69
1:E:168:VAL:HG13	1:E:173:ARG:HG2	1.73	0.69
1:B:536:GLY:O	1:B:541:GLU:HG3	1.92	0.69
1:F:158:ALA:HB1	1:F:184:ARG:NH1	2.07	0.69
1:D:110:GLN:NE2	1:D:112:THR:OG1	2.25	0.69
1:D:269:MET:HA	1:D:580:THR:HG23	1.72	0.69
1:A:480:THR:HA	1:A:600:PHE:CE1	2.27	0.69
1:C:599:HIS:NE2	1:C:641:ASP:OD2	2.25	0.69
1:F:183:LEU:HB2	1:F:192:ARG:HG3	1.73	0.69
1:D:493:ARG:HG2	1:D:493:ARG:HH11	1.57	0.68
1:A:200:GLU:O	1:A:203:GLU:HB3	1.92	0.68
1:A:517:PHE:HD1	1:A:540:PHE:HD1	1.38	0.68
1:D:487:ALA:CA	1:D:488:GLU:HB2	2.08	0.68
1:F:131:HIS:HA	1:F:134:ARG:HG3	1.74	0.68
1:D:305:TRP:NE1	1:D:344:ASP:OD1	2.26	0.68
1:D:368:ASP:OD1	1:D:368:ASP:N	2.26	0.68
1:E:318:HIS:CE1	1:E:320:SER:HB2	2.28	0.68
1:B:505:LEU:O	1:B:505:LEU:HD12	1.94	0.68
1:D:574:SER:OG	1:D:576:GLN:HG2	1.94	0.68
1:C:268:GLY:HA3	1:E:671:TYR:CD2	2.29	0.67
1:D:151:SER:O	1:D:153:ASP:N	2.27	0.67
1:B:176:LEU:O	1:B:180:ALA:N	2.27	0.67
1:B:241:SER:OG	1:B:561:ARG:O	2.13	0.67
1:E:307:ILE:HG21	1:E:314:HIS:CD2	2.29	0.67
1:F:473:ARG:HD2	1:F:478:GLU:HB3	1.77	0.67
1:B:149:GLU:O	1:B:151:SER:N	2.25	0.67
1:E:195:LEU:O	1:E:201:ILE:HD11	1.94	0.67
1:E:509:LEU:HB3	1:E:517:PHE:HE1	1.59	0.67
1:C:358:GLU:HG3	1:C:359:HIS:CD2	2.29	0.67
1:F:176:LEU:O	1:F:180:ALA:N	2.26	0.67
1:F:309:SER:HA	1:F:352:ASP:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:LEU:HD23	1:B:552:TYR:CD1	2.29	0.67
1:C:394:GLU:N	1:C:394:GLU:OE1	2.25	0.67
1:F:487:ALA:HB2	1:F:490:ALA:HB2	1.76	0.67
1:B:108:HIS:ND1	1:B:698:LEU:HD11	2.10	0.67
1:C:692:GLU:OE1	1:C:692:GLU:HA	1.95	0.67
1:B:150:LEU:O	1:B:152:ASN:N	2.28	0.66
1:D:569:LEU:HD11	1:D:576:GLN:HG3	1.77	0.66
1:C:487:ALA:CB	1:C:488:GLU:HB3	2.15	0.66
1:C:63:ARG:HG3	1:C:93:PRO:HB3	1.76	0.66
1:F:583:ASN:HA	1:F:586:ARG:HD3	1.77	0.66
1:C:618:THR:HG23	1:C:620:ASP:H	1.61	0.66
1:A:629:ASN:C	1:A:629:ASN:ND2	2.48	0.66
1:D:509:LEU:HB3	1:D:517:PHE:HE1	1.60	0.66
1:D:558:TYR:OH	2:D:801:MAL:O3	2.14	0.66
1:A:509:LEU:HD22	1:A:517:PHE:CD2	2.31	0.66
1:C:192:ARG:HB3	1:C:195:LEU:HD22	1.78	0.66
1:B:165:ALA:HB1	1:B:173:ARG:CD	2.23	0.65
1:F:266:ILE:HG22	1:F:339:MET:HE1	1.76	0.65
1:F:318:HIS:CE1	1:F:320:SER:HB2	2.31	0.65
1:A:138:ILE:HA	1:A:141:LEU:HD23	1.78	0.65
1:D:36:ALA:HB1	1:D:40:GLU:OE2	1.97	0.65
1:D:57:ALA:HA	1:D:107:PHE:HE2	1.62	0.65
1:F:149:GLU:OE1	1:F:149:GLU:N	2.29	0.65
1:C:198:THR:OG1	1:C:200:GLU:HG2	1.96	0.65
1:D:476:LYS:HZ2	1:D:628:LEU:HB2	1.61	0.65
1:F:177:LEU:HA	1:F:180:ALA:HB3	1.78	0.65
1:A:510:GLN:NE2	1:A:544:ALA:HB2	2.12	0.65
1:B:493:ARG:HH11	1:B:494:ARG:H	1.45	0.65
1:F:151:SER:HA	1:F:154:LEU:HD13	1.79	0.65
1:F:242:THR:HG21	1:F:259:ALA:HA	1.78	0.65
1:B:533:MET:HE3	1:B:537:TYR:CD1	2.32	0.65
1:B:629:ASN:HD21	1:B:632:GLY:N	1.95	0.65
1:B:347:LEU:HD13	1:B:428:TRP:HH2	1.62	0.65
1:B:541:GLU:OE1	1:B:563:ARG:NH2	2.30	0.65
1:D:605:ASN:HB2	1:D:636:ALA:HB2	1.79	0.64
1:B:432:ILE:HG22	1:B:436:LYS:HZ1	1.62	0.64
1:F:355:TRP:HA	1:F:358:GLU:HG2	1.80	0.64
1:B:465:GLN:HA	1:B:493:ARG:NH1	2.13	0.64
1:A:269:MET:HA	1:A:580:THR:HG23	1.78	0.64
1:B:149:GLU:N	1:B:149:GLU:OE1	2.31	0.64
1:E:50:ARG:HH22	1:E:126:TRP:N	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:ARG:HB3	1:F:219:GLN:HG2	1.79	0.64
1:B:487:ALA:HB1	1:B:489:LEU:N	2.12	0.64
1:C:168:VAL:O	1:C:173:ARG:HD2	1.98	0.64
1:C:54:GLU:N	1:C:54:GLU:OE1	2.20	0.64
1:E:509:LEU:HD21	1:E:520:ARG:HG3	1.80	0.64
1:F:243:GLY:HA3	1:F:252:VAL:O	1.97	0.64
1:F:506:HIS:CE1	1:F:508:VAL:HG23	2.33	0.64
1:A:59:THR:HG23	1:A:126:TRP:HE1	1.63	0.63
1:B:629:ASN:OD1	3:B:802:CEY:O6B	2.15	0.63
1:C:192:ARG:O	1:C:196:ALA:N	2.32	0.63
1:A:203:GLU:HB2	1:A:204:LEU:HD13	1.80	0.63
1:A:237:MET:SD	1:A:266:ILE:HD11	2.39	0.63
1:A:240:ARG:NH2	1:A:556:GLU:O	2.32	0.63
1:B:269:MET:HA	1:B:580:THR:HG23	1.80	0.63
1:E:486:ILE:HD13	1:E:495:PRO:HG3	1.78	0.63
1:C:43:PRO:HD2	1:C:596:ARG:HH11	1.63	0.63
1:E:405:GLN:NE2	1:E:438:VAL:HG21	2.14	0.63
1:F:589:HIS:NE2	1:F:658:GLU:OE2	2.28	0.62
1:A:55:ALA:N	1:A:132:THR:HG22	2.09	0.62
1:B:55:ALA:N	1:B:132:THR:HG22	2.14	0.62
1:B:292:ASN:OD1	1:B:558:TYR:CE2	2.52	0.62
1:D:110:GLN:HG2	1:D:694:ARG:HH22	1.63	0.62
1:E:454:ARG:O	1:E:458:LEU:HD12	1.99	0.62
1:C:522:VAL:O	1:C:526:THR:OG1	2.14	0.62
1:D:419:ASN:HD21	2:D:801:MAL:H6'1	1.63	0.62
1:E:541:GLU:OE1	1:E:563:ARG:NH1	2.32	0.62
1:E:405:GLN:HE22	1:E:438:VAL:HG21	1.64	0.62
1:A:529:PRO:O	1:A:586:ARG:NH2	2.32	0.62
1:C:192:ARG:HA	1:C:195:LEU:HB3	1.80	0.62
1:D:581:ARG:O	1:D:585:ILE:HG12	2.00	0.62
1:A:243:GLY:HA3	1:A:252:VAL:O	1.99	0.62
1:C:487:ALA:HB1	1:C:489:LEU:H	1.63	0.62
1:D:37:VAL:HG11	1:D:227:PRO:HA	1.81	0.62
1:A:318:HIS:CD2	1:A:320:SER:HB3	2.35	0.62
1:C:519:ILE:O	1:C:523:LEU:HD12	2.00	0.62
1:C:563:ARG:HG2	1:C:563:ARG:HH11	1.65	0.62
1:D:325:ASP:N	1:D:325:ASP:OD1	2.28	0.62
1:E:243:GLY:HA3	1:E:252:VAL:O	2.00	0.62
1:E:560:LEU:HD12	1:E:562:PRO:HD3	1.82	0.62
1:F:50:ARG:NH1	1:F:55:ALA:O	2.33	0.62
1:A:475:THR:HG22	1:A:478:GLU:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:ARG:O	1:A:585:ILE:HG13	2.00	0.61
1:D:576:GLN:O	1:D:580:THR:OG1	2.13	0.61
1:F:126:TRP:HZ3	1:F:128:ASP:HB3	1.65	0.61
1:F:508:VAL:O	1:F:512:ASN:ND2	2.33	0.61
1:E:150:LEU:O	1:E:152:ASN:N	2.33	0.61
1:E:487:ALA:HA	1:E:489:LEU:H	1.65	0.61
1:A:682:HIS:HB3	1:A:684:ILE:HD11	1.82	0.61
1:B:63:ARG:HD3	1:B:64:TYR:N	2.16	0.61
1:D:282:ILE:HD12	1:D:318:HIS:HD2	1.64	0.61
1:F:682:HIS:HB3	1:F:684:ILE:HD11	1.82	0.61
1:D:122:ARG:HH21	1:D:124:ASP:CG	2.03	0.61
1:B:486:ILE:HG13	1:B:495:PRO:HG3	1.83	0.61
1:D:28:SER:OG	1:D:460:LYS:NZ	2.25	0.61
1:E:110:GLN:OE1	1:E:110:GLN:N	2.34	0.61
1:A:180:ALA:O	1:A:184:ARG:NE	2.29	0.61
1:C:158:ALA:HB1	1:C:184:ARG:CZ	2.31	0.61
1:C:405:GLN:OE1	1:C:405:GLN:N	2.33	0.61
1:D:37:VAL:O	1:D:40:GLU:HG2	2.01	0.61
1:E:536:GLY:O	1:E:541:GLU:HG3	2.01	0.61
1:B:493:ARG:NH1	1:B:494:ARG:O	2.33	0.60
1:C:475:THR:HG22	1:C:478:GLU:HG3	1.82	0.60
1:E:416:ARG:HH21	1:E:447:GLU:CD	2.03	0.60
1:C:43:PRO:HD2	1:C:596:ARG:NH1	2.15	0.60
1:D:184:ARG:HD2	1:D:184:ARG:N	2.15	0.60
1:E:197:LEU:H	1:E:197:LEU:HD12	1.66	0.60
1:E:583:ASN:HA	1:E:586:ARG:HD3	1.82	0.60
1:D:648:GLU:HG3	1:D:650:TYR:CZ	2.36	0.60
1:B:188:ASP:O	1:B:191:THR:HG23	2.01	0.60
1:C:150:LEU:O	1:C:152:ASN:N	2.34	0.60
1:C:180:ALA:O	1:C:184:ARG:NH2	2.35	0.60
1:C:243:GLY:HA3	1:C:252:VAL:O	2.02	0.60
1:D:416:ARG:HH21	1:D:447:GLU:CD	2.04	0.60
1:E:525:ALA:O	1:E:586:ARG:NH1	2.34	0.60
1:D:525:ALA:HB1	1:D:586:ARG:HD2	1.82	0.60
1:F:155:LEU:O	1:F:159:VAL:HG23	2.01	0.60
1:A:371:ILE:HD11	1:A:385:TYR:CG	2.37	0.60
1:C:198:THR:HG23	1:C:201:ILE:HG13	1.84	0.60
1:C:656:ARG:NH1	1:C:658:GLU:OE1	2.35	0.60
1:F:282:ILE:HD12	1:F:318:HIS:HD2	1.67	0.60
1:A:432:ILE:HG23	1:A:436:LYS:NZ	2.17	0.60
1:E:419:ASN:HD21	2:E:801:MAL:H6'1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:536:GLY:O	1:F:541:GLU:HG3	2.01	0.60
1:A:318:HIS:NE2	1:A:320:SER:HB3	2.16	0.59
1:C:387:LEU:HD13	1:C:396:LEU:HD21	1.84	0.59
1:A:583:ASN:HA	1:A:586:ARG:HD3	1.85	0.59
1:B:138:ILE:HA	1:B:141:LEU:HD23	1.84	0.59
1:B:507:ALA:HA	1:B:510:GLN:OE1	2.02	0.59
1:C:446:SER:HB3	1:C:463:PHE:CD1	2.37	0.59
1:A:19:GLU:OE2	1:A:21:ASP:HB2	2.02	0.59
1:C:536:GLY:O	1:C:541:GLU:HG3	2.03	0.59
1:B:465:GLN:HA	1:B:493:ARG:HH12	1.67	0.59
1:A:181:ALA:HA	1:A:184:ARG:HG2	1.84	0.59
1:E:509:LEU:HD22	1:E:517:PHE:CD1	2.38	0.59
1:B:20:ILE:HG12	1:B:48:VAL:HG12	1.84	0.59
1:C:263:LEU:HD21	1:C:334:ALA:HB2	1.84	0.59
1:C:242:THR:HG21	1:C:259:ALA:HA	1.83	0.59
1:C:529:PRO:O	1:C:586:ARG:NH2	2.33	0.59
1:D:234:TRP:CH2	1:D:445:LEU:HD11	2.38	0.59
1:E:68:ARG:HH11	1:E:68:ARG:HG3	1.68	0.59
1:F:183:LEU:HD13	1:F:192:ARG:HA	1.85	0.59
1:A:509:LEU:HD22	1:A:517:PHE:HD2	1.68	0.59
1:A:525:ALA:O	1:A:586:ARG:NH1	2.36	0.59
1:B:163:ARG:NH1	1:B:210:LEU:HD11	2.18	0.59
1:B:662:GLU:HB3	1:B:664:TYR:HE1	1.67	0.59
1:A:176:LEU:O	1:A:180:ALA:N	2.33	0.58
1:A:126:TRP:CD2	1:A:211:ARG:HG2	2.38	0.58
1:B:149:GLU:C	1:B:151:SER:H	2.06	0.58
1:B:201:ILE:HA	1:B:204:LEU:HB3	1.84	0.58
1:A:152:ASN:ND2	1:B:368:ASP:OD2	2.36	0.58
1:D:416:ARG:HA	1:D:445:LEU:HD13	1.84	0.58
1:D:529:PRO:O	1:D:586:ARG:NH2	2.36	0.58
1:A:480:THR:HA	1:A:600:PHE:HE1	1.67	0.58
1:B:154:LEU:HB3	1:B:183:LEU:HD23	1.86	0.58
1:C:207:ASP:OD1	1:C:208:TYR:N	2.36	0.58
1:D:253:HIS:ND1	1:D:320:SER:OG	2.36	0.58
1:D:539:LEU:HB2	1:D:563:ARG:HH12	1.67	0.58
1:F:485:GLN:NE2	1:F:489:LEU:HD11	2.18	0.58
1:D:509:LEU:HD21	1:D:520:ARG:HG3	1.85	0.58
1:D:533:MET:HG3	1:D:537:TYR:HD2	1.68	0.58
1:A:629:ASN:HB2	3:A:802:CEY:O5B	2.03	0.58
1:B:64:TYR:HD2	1:B:115:ARG:HH11	1.50	0.58
1:C:503:ASP:OD2	2:C:801:MAL:O1'	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:498:PHE:CE1	1:D:532:GLY:HA3	2.39	0.58
1:E:285:VAL:HB	1:E:351:PRO:HG3	1.86	0.58
1:A:615:ASP:OD2	1:A:618:THR:HG22	2.02	0.58
1:C:158:ALA:HB1	1:C:184:ARG:NH2	2.19	0.58
1:E:581:ARG:O	1:E:585:ILE:HG13	2.04	0.58
1:A:203:GLU:HG3	1:A:204:LEU:N	2.18	0.58
1:A:692:GLU:HB3	1:A:695:ASN:HD21	1.67	0.58
1:D:695:ASN:O	1:D:698:LEU:HD13	2.04	0.58
1:F:183:LEU:HD22	1:F:192:ARG:HB2	1.85	0.58
1:B:243:GLY:HA3	1:B:252:VAL:O	2.04	0.58
1:B:486:ILE:HD11	1:B:528:SER:HB2	1.85	0.58
1:C:154:LEU:H	1:C:154:LEU:HD12	1.68	0.58
1:A:183:LEU:HB2	1:A:192:ARG:HB2	1.86	0.57
1:A:285:VAL:HG12	1:A:286:HIS:ND1	2.19	0.57
1:A:205:LEU:HA	1:A:208:TYR:O	2.04	0.57
1:B:116:VAL:HA	1:B:224:VAL:HG23	1.86	0.57
1:B:493:ARG:HH11	1:B:494:ARG:N	2.02	0.57
1:F:475:THR:HG22	1:F:478:GLU:CD	2.25	0.57
1:F:499:VAL:HG11	1:F:537:TYR:CZ	2.39	0.57
1:A:378:PRO:O	1:A:380:LYS:NZ	2.36	0.57
1:E:154:LEU:HD12	1:E:154:LEU:H	1.69	0.57
1:C:153:ASP:O	1:C:156:VAL:HG22	2.04	0.57
1:D:65:LEU:HD12	1:D:118:LEU:HD12	1.86	0.57
1:E:150:LEU:HD12	1:E:154:LEU:HD11	1.86	0.57
1:C:587:ARG:HD3	1:E:665:GLN:OE1	2.03	0.57
1:D:309:SER:HA	1:D:352:ASP:HB2	1.85	0.57
1:F:363:PHE:HB3	1:F:371:ILE:CD1	2.35	0.57
1:A:692:GLU:HA	1:A:692:GLU:OE1	2.04	0.57
1:B:282:ILE:HD12	1:B:318:HIS:HD2	1.70	0.57
1:D:374:ALA:HA	1:D:386:PRO:HD3	1.86	0.57
1:F:275:TYR:CE1	1:F:416:ARG:HG3	2.39	0.57
1:B:230:ARG:NH1	1:B:594:GLN:OE1	2.38	0.57
1:B:50:ARG:NH1	1:B:51:GLU:OE1	2.37	0.57
1:F:631:PHE:CE1	3:F:802:CEY:H3E	2.39	0.57
1:E:487:ALA:HB1	1:E:490:ALA:N	2.20	0.57
1:A:19:GLU:OE1	1:A:49:TRP:NE1	2.38	0.57
1:D:182:ALA:O	1:D:183:LEU:HD12	2.05	0.57
1:F:529:PRO:O	1:F:586:ARG:NH2	2.37	0.57
1:A:255:THR:OG1	1:A:321:LEU:O	2.19	0.57
1:B:168:VAL:HG21	1:B:176:LEU:HD12	1.86	0.57
1:A:318:HIS:HE2	1:A:320:SER:HB3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LEU:HD22	1:B:154:LEU:H	1.69	0.56
1:B:374:ALA:CA	1:B:386:PRO:HD3	2.35	0.56
1:D:247:ASP:N	1:D:247:ASP:OD1	2.38	0.56
1:D:363:PHE:HB3	1:D:371:ILE:HD11	1.87	0.56
1:A:506:HIS:CE1	1:A:508:VAL:HG23	2.40	0.56
1:B:182:ALA:O	1:B:192:ARG:HD3	2.05	0.56
1:B:374:ALA:HA	1:B:386:PRO:HD3	1.86	0.56
1:D:362:TRP:HD1	1:D:392:ASP:HB3	1.69	0.56
1:D:556:GLU:HG3	1:D:561:ARG:HB2	1.87	0.56
1:E:287:ARG:O	1:E:296:ALA:HB2	2.05	0.56
1:A:122:ARG:HB3	1:A:219:GLN:HG2	1.86	0.56
1:C:554:ASP:HB3	1:C:559:GLU:OE2	2.05	0.56
1:F:605:ASN:HB2	1:F:636:ALA:HB2	1.88	0.56
1:A:154:LEU:O	1:A:192:ARG:NH2	2.36	0.56
1:E:157:GLY:O	1:E:161:LEU:HD12	2.05	0.56
1:F:168:VAL:CG2	1:F:173:ARG:HD3	2.34	0.56
1:B:177:LEU:HA	1:B:180:ALA:HB3	1.86	0.56
1:E:182:ALA:O	1:E:183:LEU:HD13	2.05	0.56
1:F:498:PHE:CE1	1:F:532:GLY:HA3	2.41	0.56
1:A:388:ASN:ND2	1:A:391:ASN:H	2.02	0.56
1:B:292:ASN:OD1	1:B:558:TYR:CZ	2.58	0.56
1:C:149:GLU:N	1:C:151:SER:OG	2.37	0.56
1:D:265:ARG:NH1	1:D:269:MET:HE2	2.21	0.56
1:E:387:LEU:HD13	1:E:396:LEU:HD21	1.87	0.56
1:F:317:VAL:HG23	1:F:324:ILE:HG12	1.87	0.56
1:A:536:GLY:O	1:A:541:GLU:HG3	2.05	0.56
1:F:519:ILE:HD13	1:F:627:THR:O	2.05	0.56
1:F:525:ALA:O	1:F:586:ARG:NH1	2.39	0.56
1:C:198:THR:HG23	1:C:201:ILE:CG1	2.36	0.56
1:C:615:ASP:OD2	1:C:618:THR:HG22	2.05	0.56
1:D:282:ILE:HD12	1:D:318:HIS:CD2	2.41	0.56
1:D:366:LEU:HB3	1:D:367:PRO:HD2	1.87	0.56
1:E:476:LYS:HD3	1:E:628:LEU:HD12	1.88	0.56
1:D:122:ARG:HB3	1:D:219:GLN:HG2	1.87	0.56
1:D:154:LEU:H	1:D:154:LEU:HD12	1.70	0.56
1:D:509:LEU:HD22	1:D:517:PHE:CD1	2.41	0.56
1:E:134:ARG:O	1:E:138:ILE:HG12	2.05	0.56
1:E:575:LEU:HD23	1:E:579:ILE:HD11	1.86	0.56
1:A:266:ILE:HG22	1:A:339:MET:HE3	1.87	0.56
1:B:432:ILE:HG22	1:B:436:LYS:NZ	2.20	0.56
1:F:173:ARG:HH12	1:F:177:LEU:N	1.99	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:ASP:OD1	1:C:247:ASP:N	2.39	0.56
1:C:543:ARG:HB3	1:C:553:LEU:HD12	1.88	0.56
1:F:571:GLN:OE1	1:F:573:ARG:NH1	2.38	0.56
1:A:179:ALA:HA	1:A:195:LEU:HD13	1.88	0.55
1:E:486:ILE:HG21	1:E:493:ARG:NH2	2.21	0.55
1:A:92:LYS:HD2	1:A:92:LYS:O	2.06	0.55
1:C:183:LEU:HD22	1:C:192:ARG:HG3	1.87	0.55
1:D:488:GLU:HG3	1:D:489:LEU:C	2.26	0.55
1:B:238:PHE:CE1	1:B:277:PRO:HG2	2.41	0.55
1:C:183:LEU:HB2	1:C:192:ARG:CD	2.37	0.55
1:D:173:ARG:O	1:D:176:LEU:HG	2.05	0.55
1:D:17:ARG:HG2	1:D:213:LEU:HD11	1.88	0.55
1:D:179:ALA:CA	1:D:195:LEU:HD21	2.33	0.55
1:F:287:ARG:NH2	1:F:301:VAL:O	2.34	0.55
1:F:692:GLU:OE1	1:F:692:GLU:HA	2.06	0.55
1:B:581:ARG:O	1:B:585:ILE:HG13	2.06	0.55
1:E:607:ALA:HB3	1:E:634:GLU:HG2	1.88	0.55
1:F:394:GLU:HA	1:F:397:TYR:HB2	1.88	0.55
1:C:120:THR:HG21	1:C:219:GLN:OE1	2.07	0.55
1:D:519:ILE:HD13	1:D:627:THR:O	2.06	0.55
1:E:191:THR:HG23	1:E:192:ARG:HG3	1.87	0.55
1:E:652:ARG:HD3	1:E:665:GLN:NE2	2.22	0.55
1:E:682:HIS:HB3	1:E:684:ILE:HD11	1.88	0.55
1:F:416:ARG:HD2	1:F:416:ARG:C	2.26	0.55
1:C:183:LEU:HB2	1:C:192:ARG:HE	1.70	0.55
1:C:59:THR:OG1	1:C:211:ARG:NH2	2.36	0.55
1:A:195:LEU:O	1:A:201:ILE:HG13	2.06	0.55
1:B:122:ARG:HB3	1:B:219:GLN:HG2	1.88	0.55
1:B:485:GLN:HA	1:B:488:GLU:OE1	2.07	0.55
1:D:536:GLY:O	1:D:541:GLU:HG3	2.06	0.55
1:E:55:ALA:N	1:E:132:THR:HG22	2.15	0.55
1:F:581:ARG:O	1:F:585:ILE:HG13	2.06	0.55
1:D:170:ARG:HA	1:D:173:ARG:CG	2.36	0.55
1:E:519:ILE:HD13	1:E:627:THR:O	2.06	0.55
1:F:198:THR:HG21	1:F:201:ILE:HD13	1.88	0.55
1:B:522:VAL:O	1:B:526:THR:OG1	2.17	0.55
1:C:481:GLU:O	1:C:485:GLN:N	2.40	0.55
1:D:682:HIS:HB3	1:D:684:ILE:HD11	1.89	0.55
1:E:285:VAL:HG12	1:E:286:HIS:CE1	2.41	0.55
1:E:265:ARG:NH1	1:E:576:GLN:OE1	2.40	0.55
1:A:519:ILE:HD13	1:A:627:THR:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ASN:OD1	1:B:558:TYR:OH	2.14	0.54
1:E:671:TYR:HE1	1:E:673:ARG:CZ	2.20	0.54
1:F:180:ALA:O	1:F:184:ARG:CZ	2.55	0.54
1:C:285:VAL:HG12	1:C:286:HIS:ND1	2.22	0.54
1:C:266:ILE:HG22	1:C:339:MET:HE1	1.89	0.54
1:C:505:LEU:HB2	1:C:552:TYR:CE2	2.43	0.54
1:C:505:LEU:HD13	1:C:552:TYR:HE2	1.72	0.54
1:A:188:ASP:HB3	1:A:191:THR:OG1	2.07	0.54
1:A:394:GLU:H	1:A:394:GLU:CD	2.11	0.54
1:B:505:LEU:HB3	1:B:552:TYR:HE1	1.72	0.54
1:B:67:VAL:HG11	1:B:440:PRO:HG3	1.89	0.54
1:E:280:HIS:HB3	1:E:281:PRO:HD2	1.89	0.54
1:E:631:PHE:CE1	3:E:802:CEY:H3E	2.43	0.54
1:F:275:TYR:CZ	1:F:416:ARG:HG3	2.42	0.54
1:B:238:PHE:CD1	1:B:277:PRO:HG2	2.41	0.54
1:E:589:HIS:NE2	1:E:658:GLU:OE2	2.35	0.54
1:D:362:TRP:CD1	1:D:392:ASP:HB3	2.41	0.54
1:A:236:GLU:HB3	1:A:534:TYR:HA	1.89	0.54
1:E:540:PHE:CZ	1:E:575:LEU:HB2	2.43	0.54
1:E:64:TYR:HE2	1:E:117:GLY:HA3	1.71	0.54
1:A:533:MET:HE1	1:A:538:GLU:HB3	1.90	0.54
1:D:153:ASP:O	1:D:156:VAL:HG22	2.08	0.54
1:D:266:ILE:HG22	1:D:339:MET:HE1	1.89	0.54
1:B:575:LEU:HD23	1:B:579:ILE:HD11	1.90	0.54
1:D:242:THR:HG21	1:D:259:ALA:HA	1.88	0.54
1:D:476:LYS:HZ1	3:D:802:CEY:H4A	1.73	0.54
1:E:183:LEU:CD1	1:E:192:ARG:HB3	2.37	0.54
1:C:582:LEU:O	1:C:586:ARG:HG2	2.07	0.54
1:D:335:ARG:NH2	1:D:411:GLY:O	2.41	0.54
1:E:509:LEU:HD22	1:E:517:PHE:HD1	1.72	0.54
1:B:59:THR:HG23	1:B:126:TRP:HE1	1.73	0.54
1:C:176:LEU:O	1:C:180:ALA:N	2.39	0.54
1:C:657:ASP:OD1	1:C:659:ILE:HG12	2.08	0.54
1:E:251:PRO:HB2	1:E:560:LEU:HD11	1.90	0.54
1:C:317:VAL:HG23	1:C:324:ILE:HG12	1.90	0.53
1:C:240:ARG:NH1	1:C:560:LEU:HD23	2.23	0.53
1:D:35:LYS:HD2	1:D:492:TYR:O	2.08	0.53
1:F:111:PHE:CE1	1:F:113:PRO:HG3	2.43	0.53
1:A:158:ALA:HB1	1:A:184:ARG:NE	2.23	0.53
1:B:168:VAL:HG12	1:B:208:TYR:HB2	1.90	0.53
1:C:179:ALA:HA	1:C:195:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:VAL:HG11	1:C:537:TYR:CZ	2.42	0.53
1:C:605:ASN:HB2	1:C:636:ALA:HB2	1.89	0.53
1:D:188:ASP:OD1	1:D:189:PRO:HD2	2.08	0.53
1:B:126:TRP:CZ3	1:B:128:ASP:HB3	2.44	0.53
1:C:92:LYS:HG3	1:C:93:PRO:HD2	1.90	0.53
1:D:134:ARG:O	1:D:138:ILE:HG13	2.08	0.53
1:D:184:ARG:HD2	1:D:184:ARG:H	1.73	0.53
1:A:242:THR:HG21	1:A:259:ALA:HA	1.88	0.53
1:F:485:GLN:O	1:F:489:LEU:HD12	2.08	0.53
1:A:362:TRP:HH2	1:A:399:GLU:HG3	1.74	0.53
1:C:156:VAL:O	1:C:160:LEU:HD23	2.08	0.53
1:E:374:ALA:HB2	1:E:386:PRO:N	2.23	0.53
1:B:387:LEU:HD13	1:B:396:LEU:HD21	1.91	0.53
1:D:190:VAL:HA	1:D:193:THR:OG1	2.08	0.53
1:B:151:SER:HA	1:B:154:LEU:HD23	1.91	0.53
1:D:275:TYR:CZ	1:D:416:ARG:HD3	2.43	0.53
1:F:55:ALA:N	1:F:132:THR:HG22	2.21	0.53
1:F:405:GLN:NE2	1:F:438:VAL:HG21	2.24	0.53
1:E:485:GLN:O	1:E:489:LEU:HG	2.09	0.53
1:A:280:HIS:ND1	1:A:314:HIS:HA	2.24	0.53
1:D:488:GLU:HB3	1:D:490:ALA:HB2	1.91	0.53
1:F:505:LEU:HB2	1:F:552:TYR:CD2	2.43	0.53
1:F:677:ALA:HB2	3:F:802:CEY:H6F	1.91	0.53
1:A:305:TRP:NE1	1:A:344:ASP:OD1	2.39	0.53
1:B:682:HIS:HB3	1:B:684:ILE:HD11	1.90	0.53
1:E:533:MET:HE1	1:E:579:ILE:HG21	1.91	0.53
1:F:569:LEU:HD11	1:F:576:GLN:NE2	2.24	0.53
1:B:103:GLU:OE1	1:B:106:VAL:HG23	2.09	0.52
1:C:207:ASP:OD1	1:C:208:TYR:HD2	1.90	0.52
1:E:398:ASP:OD1	1:E:402:ARG:NH1	2.42	0.52
1:E:663:GLU:C	1:E:664:TYR:HD1	2.13	0.52
1:F:282:ILE:HD12	1:F:318:HIS:CD2	2.43	0.52
1:A:297:ALA:HB1	1:A:298:PRO:HD2	1.90	0.52
1:B:184:ARG:HG3	1:B:185:THR:H	1.73	0.52
1:C:519:ILE:HD13	1:C:627:THR:O	2.09	0.52
1:E:284:LYS:CD	1:E:352:ASP:HB3	2.36	0.52
1:E:621:CYS:HB2	1:E:689:VAL:HG23	1.91	0.52
1:A:134:ARG:O	1:A:138:ILE:HG13	2.09	0.52
1:B:567:SER:O	1:B:571:GLN:HG2	2.08	0.52
1:C:473:ARG:HD2	1:C:478:GLU:HB3	1.91	0.52
1:C:589:HIS:NE2	1:C:658:GLU:OE2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:TRP:CZ3	1:F:128:ASP:HB3	2.45	0.52
1:C:69:TYR:HB3	1:C:70:PRO:HD3	1.92	0.52
1:D:276:LEU:HD11	1:D:343:LEU:HD12	1.92	0.52
1:E:242:THR:HG21	1:E:259:ALA:HA	1.91	0.52
1:F:284:LYS:N	1:F:352:ASP:OD2	2.30	0.52
1:C:265:ARG:HA	1:E:671:TYR:CE1	2.44	0.52
1:D:282:ILE:O	1:D:287:ARG:NH2	2.42	0.52
1:E:580:THR:O	1:E:584:ILE:HG13	2.10	0.52
1:F:130:ILE:HD13	1:F:160:LEU:HD13	1.91	0.52
1:A:15:PRO:N	1:B:426:ASN:HD22	2.07	0.52
1:B:503:ASP:OD1	1:B:557:LYS:HE3	2.10	0.52
1:E:170:ARG:O	1:E:173:ARG:HG3	2.09	0.52
1:E:218:GLU:HG3	1:E:220:PHE:CZ	2.45	0.52
1:A:692:GLU:O	1:A:696:THR:HG23	2.10	0.52
1:F:157:GLY:O	1:F:160:LEU:HB2	2.10	0.52
1:C:176:LEU:HD21	1:C:204:LEU:HD11	1.92	0.52
1:D:457:GLY:O	1:D:460:LYS:HB3	2.09	0.52
1:E:149:GLU:HG2	1:E:150:LEU:H	1.75	0.52
1:E:269:MET:SD	1:E:576:GLN:HG3	2.50	0.52
1:A:374:ALA:HA	1:A:386:PRO:HD3	1.90	0.52
1:A:364:THR:HG22	1:A:388:ASN:HB2	1.91	0.52
1:A:695:ASN:HA	1:A:698:LEU:CD1	2.40	0.52
1:B:662:GLU:HB3	1:B:664:TYR:CE1	2.45	0.52
1:C:133:TRP:CE2	1:C:157:GLY:HA3	2.44	0.52
1:D:27:VAL:HG12	1:D:460:LYS:HE3	1.92	0.52
1:E:21:ASP:OD2	1:E:22:ASP:N	2.43	0.52
1:E:32:TYR:HD2	1:E:460:LYS:HE2	1.74	0.52
1:B:540:PHE:CZ	1:B:575:LEU:HB2	2.44	0.51
1:C:422:THR:HA	1:D:52:GLY:HA2	1.93	0.51
1:D:482:PHE:O	1:D:486:ILE:HG12	2.09	0.51
1:D:698:LEU:O	1:D:699:ARG:HB2	2.10	0.51
1:E:671:TYR:CZ	1:E:673:ARG:HG3	2.44	0.51
1:F:374:ALA:HA	1:F:386:PRO:HD3	1.91	0.51
1:B:665:GLN:OE1	1:F:587:ARG:NH1	2.43	0.51
1:F:657:ASP:OD1	1:F:659:ILE:HG12	2.10	0.51
1:A:656:ARG:NH1	1:A:658:GLU:OE1	2.44	0.51
1:C:156:VAL:O	1:C:159:VAL:HG12	2.09	0.51
1:D:200:GLU:O	1:D:204:LEU:HG	2.10	0.51
1:D:36:ALA:O	1:D:224:VAL:HA	2.10	0.51
1:E:428:TRP:O	1:E:432:ILE:HG13	2.10	0.51
1:E:476:LYS:CD	1:E:628:LEU:HD12	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:TRP:HA	1:C:358:GLU:HG2	1.91	0.51
1:D:103:GLU:HG3	1:D:104:PRO:HD2	1.92	0.51
1:D:200:GLU:O	1:D:203:GLU:HG2	2.10	0.51
1:D:317:VAL:HG23	1:D:324:ILE:HG12	1.91	0.51
1:D:505:LEU:HD12	1:D:552:TYR:CE1	2.46	0.51
1:F:153:ASP:O	1:F:156:VAL:HG22	2.10	0.51
1:F:235:TYR:HB2	1:F:271:PHE:CD1	2.45	0.51
1:F:405:GLN:HE22	1:F:438:VAL:HG21	1.76	0.51
1:A:509:LEU:HB3	1:A:517:PHE:HE2	1.75	0.51
1:D:414:PHE:CE1	1:D:443:LEU:HD12	2.46	0.51
1:F:168:VAL:HG12	1:F:208:TYR:HB2	1.91	0.51
1:F:375:GLU:OE1	1:F:375:GLU:N	2.43	0.51
1:C:583:ASN:HA	1:C:586:ARG:HD3	1.92	0.51
1:F:192:ARG:C	1:F:194:ALA:H	2.14	0.51
1:B:519:ILE:HD13	1:B:627:THR:O	2.10	0.51
1:C:126:TRP:CD2	1:C:211:ARG:HG2	2.46	0.51
1:C:397:TYR:HB3	1:C:430:TRP:CH2	2.45	0.51
1:D:111:PHE:CE1	1:D:113:PRO:HG3	2.46	0.51
1:D:657:ASP:OD2	1:D:659:ILE:HG12	2.11	0.51
1:E:288:LYS:HZ1	1:E:382:GLN:HB2	1.76	0.51
1:E:693:SER:OG	1:E:694:ARG:NH1	2.44	0.51
1:A:399:GLU:O	1:A:403:VAL:HG23	2.11	0.51
1:A:509:LEU:HD21	1:A:520:ARG:HG3	1.93	0.51
1:B:533:MET:HE1	1:B:538:GLU:HG3	1.93	0.51
1:C:149:GLU:N	1:C:149:GLU:OE1	2.43	0.51
1:C:488:GLU:C	1:C:490:ALA:H	2.13	0.51
1:E:505:LEU:HD12	1:E:552:TYR:CE1	2.46	0.51
1:B:698:LEU:O	1:B:699:ARG:HB2	2.11	0.51
1:C:240:ARG:NH2	1:C:556:GLU:O	2.43	0.51
1:D:157:GLY:O	1:D:160:LEU:HB2	2.11	0.51
1:E:657:ASP:OD1	1:E:659:ILE:HG12	2.11	0.51
1:F:416:ARG:NH1	1:F:447:GLU:HB2	2.25	0.51
1:B:173:ARG:O	1:B:173:ARG:HG2	2.10	0.51
1:D:541:GLU:OE2	1:D:563:ARG:NH2	2.44	0.51
1:D:68:ARG:O	1:D:69:TYR:HB2	2.10	0.51
1:A:275:TYR:CZ	1:A:416:ARG:HD3	2.45	0.51
1:D:280:HIS:HB2	1:D:307:ILE:HG23	1.91	0.51
1:B:366:LEU:HG	1:B:372:ALA:HB2	1.93	0.50
1:E:126:TRP:HZ3	1:E:128:ASP:HB2	1.75	0.50
1:A:362:TRP:CD1	1:A:392:ASP:HB3	2.46	0.50
1:A:605:ASN:HB2	1:A:636:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:314:HIS:HB3	1:E:403:VAL:HG11	1.93	0.50
1:A:21:ASP:OD1	1:A:22:ASP:N	2.42	0.50
1:B:236:GLU:HB3	1:B:534:TYR:HA	1.93	0.50
1:B:307:ILE:HG21	1:B:314:HIS:CD2	2.47	0.50
1:C:64:TYR:OH	1:C:116:VAL:O	2.22	0.50
1:C:240:ARG:HG3	1:C:240:ARG:NH1	2.25	0.50
1:D:35:LYS:CG	1:D:492:TYR:HA	2.41	0.50
1:E:275:TYR:CZ	1:E:416:ARG:HD3	2.46	0.50
1:E:371:ILE:HD11	1:E:385:TYR:CE2	2.46	0.50
1:F:173:ARG:HD2	1:F:176:LEU:HD13	1.92	0.50
1:A:428:TRP:O	1:A:432:ILE:HG13	2.11	0.50
1:A:485:GLN:NE2	1:A:489:LEU:HD12	2.25	0.50
1:B:191:THR:CB	1:B:192:ARG:HD2	2.40	0.50
1:C:122:ARG:HG2	1:C:123:VAL:N	2.25	0.50
1:C:375:GLU:OE1	1:C:375:GLU:N	2.45	0.50
1:E:126:TRP:CD2	1:E:211:ARG:HG2	2.47	0.50
1:E:126:TRP:CZ3	1:E:128:ASP:HB2	2.47	0.50
1:E:68:ARG:O	1:E:69:TYR:HB2	2.11	0.50
1:F:179:ALA:O	1:F:195:LEU:HD12	2.11	0.50
1:F:573:ARG:O	1:F:573:ARG:HG2	2.11	0.50
1:A:307:ILE:HG21	1:A:314:HIS:CD2	2.45	0.50
1:B:242:THR:HG21	1:B:259:ALA:HA	1.93	0.50
1:B:512:ASN:CA	1:B:631:PHE:CZ	2.88	0.50
1:C:161:LEU:H	1:C:161:LEU:HD12	1.77	0.50
1:D:630:ALA:O	3:D:802:CEY:O4F	2.28	0.50
1:B:126:TRP:HZ3	1:B:128:ASP:HB3	1.77	0.50
1:D:195:LEU:HA	1:D:198:THR:OG1	2.12	0.50
1:D:288:LYS:NZ	1:D:383:ASP:HB3	2.24	0.50
1:A:499:VAL:HG11	1:A:537:TYR:CZ	2.47	0.50
1:C:366:LEU:HB3	1:C:367:PRO:HD2	1.94	0.50
1:E:507:ALA:O	1:E:510:GLN:HB2	2.11	0.50
1:E:536:GLY:HA3	1:E:563:ARG:HH11	1.75	0.50
1:A:631:PHE:CE1	3:A:802:CEY:H3E	2.47	0.50
1:B:505:LEU:HD11	1:B:544:ALA:HB2	1.94	0.50
1:B:505:LEU:HD23	1:B:552:TYR:CE1	2.47	0.50
1:C:590:PRO:O	1:C:593:GLN:HG3	2.12	0.50
1:C:631:PHE:CE1	3:C:802:CEY:H3E	2.47	0.50
1:E:375:GLU:CD	1:E:379:LYS:O	2.50	0.50
1:E:382:GLN:N	1:E:382:GLN:OE1	2.33	0.50
1:A:414:PHE:CE1	1:A:443:LEU:HB2	2.46	0.50
1:C:314:HIS:HB3	1:C:403:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:LEU:O	1:D:180:ALA:N	2.44	0.50
1:D:583:ASN:O	1:D:587:ARG:HG3	2.11	0.50
1:E:517:PHE:CE2	1:E:540:PHE:HA	2.47	0.50
1:E:366:LEU:HD23	1:E:368:ASP:H	1.77	0.49
1:E:18:VAL:HG11	1:E:50:ARG:CZ	2.42	0.49
1:A:234:TRP:HZ2	1:A:414:PHE:CE2	2.31	0.49
1:A:517:PHE:HD1	1:A:540:PHE:CD1	2.25	0.49
1:A:235:TYR:OH	1:A:538:GLU:OE1	2.18	0.49
1:D:263:LEU:HD21	1:D:334:ALA:HB2	1.94	0.49
1:D:265:ARG:HH21	1:D:565:PHE:HB3	1.77	0.49
1:E:533:MET:HE1	1:E:579:ILE:HD13	1.93	0.49
1:F:151:SER:HA	1:F:154:LEU:CD1	2.41	0.49
1:F:505:LEU:HB2	1:F:552:TYR:CE2	2.46	0.49
1:A:317:VAL:HG23	1:A:324:ILE:HG12	1.94	0.49
1:B:134:ARG:O	1:B:138:ILE:HG23	2.12	0.49
1:D:631:PHE:CE1	3:D:802:CEY:H3E	2.48	0.49
1:E:672:ILE:HD11	1:E:682:HIS:CD2	2.47	0.49
1:A:116:VAL:HA	1:A:224:VAL:HG23	1.93	0.49
1:A:174:ASP:HA	1:A:177:LEU:HD13	1.94	0.49
1:B:157:GLY:O	1:B:161:LEU:HD22	2.13	0.49
1:D:177:LEU:HA	1:D:180:ALA:HB3	1.94	0.49
1:E:200:GLU:O	1:E:203:GLU:HG2	2.12	0.49
1:B:505:LEU:HB3	1:B:552:TYR:CE1	2.46	0.49
1:D:21:ASP:OD1	1:D:22:ASP:N	2.43	0.49
1:D:436:LYS:HG3	1:D:440:PRO:HA	1.93	0.49
1:D:489:LEU:HD23	1:D:492:TYR:OH	2.13	0.49
1:C:183:LEU:N	1:C:192:ARG:HD3	2.27	0.49
1:A:371:ILE:HD11	1:A:385:TYR:CD1	2.48	0.49
1:B:108:HIS:CG	1:B:698:LEU:HD11	2.47	0.49
1:B:534:TYR:OH	1:B:556:GLU:OE1	2.14	0.49
1:C:151:SER:HA	1:C:154:LEU:HD13	1.95	0.49
1:C:182:ALA:C	1:C:192:ARG:HD3	2.33	0.49
1:E:188:ASP:O	1:E:192:ARG:HG3	2.12	0.49
1:F:180:ALA:O	1:F:184:ARG:NH2	2.46	0.49
1:A:479:LEU:HD12	1:A:628:LEU:HD21	1.94	0.49
1:C:491:ASP:OD2	1:C:596:ARG:NH2	2.35	0.49
1:C:631:PHE:CD1	3:C:802:CEY:H3E	2.48	0.49
1:D:169:PRO:C	1:D:171:GLY:H	2.12	0.49
1:D:165:ALA:HA	1:D:176:LEU:HD21	1.95	0.49
1:D:489:LEU:H	1:D:489:LEU:HD12	1.77	0.49
1:F:605:ASN:HD21	1:F:634:GLU:HG3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:MET:HG3	1:A:537:TYR:HD1	1.77	0.49
1:C:583:ASN:O	1:C:587:ARG:HG3	2.12	0.49
1:D:276:LEU:HD13	1:D:279:ILE:HG23	1.94	0.49
1:D:600:PHE:CD1	1:D:611:TYR:HB3	2.47	0.49
1:E:523:LEU:O	1:E:527:MET:HG3	2.13	0.49
1:E:630:ALA:O	3:E:802:CEY:O4F	2.28	0.49
1:F:240:ARG:CZ	1:F:301:VAL:HG11	2.43	0.49
1:F:358:GLU:HG3	1:F:359:HIS:N	2.26	0.49
1:A:468:SER:OG	1:A:469:TYR:N	2.44	0.49
1:A:505:LEU:HB2	1:A:552:TYR:CE2	2.48	0.49
3:D:802:CEY:O2D	3:D:802:CEY:O3C	2.23	0.49
1:F:173:ARG:CZ	1:F:176:LEU:HB2	2.42	0.49
1:B:282:ILE:HD12	1:B:318:HIS:CD2	2.47	0.48
1:B:226:ARG:NE	1:B:443:LEU:HD11	2.28	0.48
1:D:489:LEU:N	1:D:489:LEU:HD12	2.27	0.48
1:D:476:LYS:CD	1:D:628:LEU:HD12	2.40	0.48
1:D:589:HIS:NE2	1:D:658:GLU:OE2	2.36	0.48
1:E:468:SER:OG	1:E:469:TYR:N	2.46	0.48
1:E:508:VAL:O	1:E:512:ASN:ND2	2.32	0.48
1:A:575:LEU:HD23	1:A:579:ILE:HD11	1.95	0.48
1:B:275:TYR:CZ	1:B:416:ARG:HD3	2.48	0.48
1:C:170:ARG:O	1:C:170:ARG:HG3	2.13	0.48
1:D:518:ALA:O	1:D:522:VAL:HG23	2.13	0.48
1:F:122:ARG:HH11	1:F:219:GLN:HE21	1.60	0.48
1:F:153:ASP:OD1	1:F:154:LEU:HD12	2.13	0.48
1:F:155:LEU:HA	1:F:158:ALA:HB3	1.94	0.48
1:A:311:GLU:OE1	1:A:319:PRO:HG3	2.14	0.48
1:A:475:THR:HG22	1:A:478:GLU:CG	2.44	0.48
1:B:405:GLN:NE2	1:B:438:VAL:HG21	2.28	0.48
1:D:265:ARG:NH2	1:D:565:PHE:HB3	2.28	0.48
1:E:180:ALA:O	1:E:184:ARG:HG2	2.13	0.48
1:E:193:THR:O	1:E:195:LEU:N	2.47	0.48
1:E:212:ASP:CG	1:E:213:LEU:HD12	2.34	0.48
1:E:374:ALA:N	1:E:386:PRO:HD3	2.28	0.48
1:C:275:TYR:CZ	1:C:416:ARG:HD3	2.48	0.48
1:D:226:ARG:HH12	1:D:340:GLU:CD	2.17	0.48
1:D:533:MET:HG3	1:D:537:TYR:CD2	2.48	0.48
1:E:179:ALA:HB1	1:E:195:LEU:HD22	1.96	0.48
1:F:21:ASP:OD1	1:F:22:ASP:N	2.46	0.48
1:F:374:ALA:HB3	1:F:381:TYR:HB2	1.96	0.48
1:E:475:THR:OG1	1:E:478:GLU:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:SER:OG	1:E:561:ARG:O	2.21	0.48
1:E:57:ALA:HA	1:E:107:PHE:CE2	2.40	0.48
1:F:336:ASP:OD1	1:F:337:LEU:N	2.47	0.48
1:B:501:THR:OG1	1:B:504:ILE:HG12	2.12	0.48
1:C:157:GLY:O	1:C:160:LEU:HB2	2.13	0.48
1:C:280:HIS:HB3	1:C:281:PRO:HD2	1.94	0.48
1:E:283:GLY:O	1:E:287:ARG:NH2	2.46	0.48
1:A:280:HIS:HB3	1:A:281:PRO:HD2	1.94	0.48
1:A:366:LEU:HB3	1:A:367:PRO:HD2	1.96	0.48
1:A:371:ILE:HD11	1:A:385:TYR:CD2	2.49	0.48
1:C:201:ILE:HA	1:C:204:LEU:HD21	1.95	0.48
1:B:198:THR:OG1	1:B:200:GLU:OE2	2.20	0.48
1:B:240:ARG:NH2	1:B:304:PRO:HG3	2.29	0.48
1:B:269:MET:SD	1:B:576:GLN:HG3	2.53	0.48
1:B:663:GLU:O	1:B:664:TYR:HD1	1.97	0.48
1:C:312:GLY:HA3	1:C:316:THR:OG1	2.14	0.48
1:D:498:PHE:HD2	1:D:501:THR:HG22	1.79	0.48
1:F:503:ASP:OD1	1:F:557:LYS:NZ	2.34	0.48
1:A:432:ILE:HG23	1:A:436:LYS:HZ3	1.78	0.48
1:C:253:HIS:CE1	1:C:320:SER:HG	2.31	0.48
1:D:314:HIS:HB3	1:D:403:VAL:HG11	1.95	0.48
1:D:607:ALA:HB3	1:D:634:GLU:HG2	1.95	0.48
1:E:366:LEU:HD23	1:E:367:PRO:N	2.29	0.48
1:F:314:HIS:HB3	1:F:403:VAL:HG11	1.95	0.48
1:C:20:ILE:HG12	1:C:48:VAL:HG12	1.95	0.48
1:C:569:LEU:HD11	1:C:576:GLN:NE2	2.29	0.48
1:D:662:GLU:HG3	1:D:664:TYR:HE1	1.79	0.48
1:E:141:LEU:HD13	1:E:142:ASP:N	2.29	0.48
1:E:235:TYR:HE1	1:E:538:GLU:OE2	1.95	0.48
1:E:573:ARG:HG2	1:E:573:ARG:O	2.14	0.48
1:F:165:ALA:HB1	1:F:173:ARG:NE	2.20	0.48
1:F:173:ARG:HH12	1:F:177:LEU:HB2	1.79	0.48
1:F:204:LEU:HD12	1:F:205:LEU:HG	1.95	0.48
1:C:436:LYS:NZ	1:C:442:VAL:O	2.30	0.47
1:C:475:THR:HG23	1:C:478:GLU:H	1.79	0.47
1:C:573:ARG:HG3	1:C:573:ARG:O	2.14	0.47
1:D:263:LEU:N	1:D:264:PRO:HD2	2.29	0.47
1:E:235:TYR:HB2	1:E:271:PHE:CD1	2.49	0.47
1:E:283:GLY:HA2	1:E:352:ASP:OD1	2.14	0.47
1:E:267:ALA:HA	1:E:339:MET:HE3	1.95	0.47
1:F:188:ASP:OD1	1:F:189:PRO:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:297:ALA:HB1	1:F:298:PRO:HD2	1.96	0.47
1:F:508:VAL:HG12	1:F:512:ASN:ND2	2.28	0.47
1:A:663:GLU:O	1:A:664:TYR:HD1	1.98	0.47
1:C:265:ARG:CZ	1:C:565:PHE:CD2	2.96	0.47
1:C:92:LYS:HG3	1:C:93:PRO:N	2.29	0.47
1:D:176:LEU:HD12	1:D:177:LEU:N	2.30	0.47
1:E:32:TYR:CE2	1:E:460:LYS:HE2	2.48	0.47
1:E:556:GLU:CD	1:E:563:ARG:HH21	2.16	0.47
1:F:102:GLN:HG2	1:F:103:GLU:H	1.79	0.47
1:A:580:THR:O	1:A:584:ILE:HG13	2.13	0.47
1:B:36:ALA:O	1:B:224:VAL:HA	2.14	0.47
1:B:405:GLN:HE22	1:B:438:VAL:HG21	1.80	0.47
1:B:473:ARG:HD2	1:B:478:GLU:HB3	1.97	0.47
1:B:600:PHE:HE1	1:B:609:LEU:HD11	1.79	0.47
1:E:138:ILE:O	1:E:141:LEU:HD12	2.14	0.47
1:E:297:ALA:HB1	1:E:298:PRO:HD2	1.96	0.47
1:E:476:LYS:NZ	1:E:606:ASP:O	2.27	0.47
1:F:615:ASP:OD2	1:F:618:THR:OG1	2.32	0.47
1:A:269:MET:SD	1:A:576:GLN:HG3	2.55	0.47
1:B:226:ARG:HB2	1:B:227:PRO:HD2	1.97	0.47
1:C:201:ILE:HA	1:C:204:LEU:CD2	2.44	0.47
1:C:563:ARG:HG2	1:C:563:ARG:NH1	2.28	0.47
1:D:271:PHE:HZ	1:D:533:MET:HE2	1.79	0.47
1:D:255:THR:OG1	1:D:321:LEU:O	2.28	0.47
1:D:359:HIS:HD2	1:D:362:TRP:CH2	2.32	0.47
1:D:507:ALA:O	1:D:510:GLN:HB2	2.15	0.47
1:E:161:LEU:O	1:E:165:ALA:N	2.44	0.47
1:E:18:VAL:HG21	1:E:50:ARG:NH1	2.30	0.47
1:A:188:ASP:OD1	1:A:189:PRO:HD2	2.13	0.47
1:A:235:TYR:HB2	1:A:271:PHE:CD1	2.48	0.47
1:C:269:MET:HG3	1:C:271:PHE:CE2	2.50	0.47
1:D:287:ARG:O	1:D:296:ALA:HB2	2.14	0.47
1:C:422:THR:HA	1:D:52:GLY:CA	2.45	0.47
1:B:600:PHE:CE1	1:B:609:LEU:HD11	2.49	0.47
1:C:698:LEU:O	1:C:699:ARG:HB3	2.14	0.47
1:E:375:GLU:HG3	1:E:380:LYS:HA	1.96	0.47
1:A:210:LEU:O	1:A:210:LEU:HD12	2.14	0.47
1:A:499:VAL:HG11	1:A:537:TYR:CE1	2.49	0.47
1:B:235:TYR:HB2	1:B:271:PHE:CD1	2.49	0.47
1:B:582:LEU:O	1:B:586:ARG:HG2	2.15	0.47
1:C:428:TRP:O	1:C:432:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:LYS:HG3	1:C:93:PRO:CD	2.45	0.47
1:D:165:ALA:HB2	1:D:176:LEU:CD1	2.42	0.47
1:F:142:ASP:OD1	1:F:143:ALA:N	2.48	0.47
1:A:361:GLN:CD	1:A:361:GLN:H	2.17	0.47
1:B:21:ASP:OD1	1:B:22:ASP:N	2.46	0.47
1:C:290:ARG:NH2	1:C:300:ASP:OD1	2.48	0.47
1:C:601:HIS:HD1	1:C:640:LEU:HD22	1.80	0.47
1:C:110:GLN:HE22	1:C:694:ARG:NH1	2.12	0.47
1:D:436:LYS:HD2	1:D:442:VAL:O	2.14	0.47
1:E:505:LEU:HD23	1:E:505:LEU:O	2.14	0.47
1:E:663:GLU:O	1:E:664:TYR:HD1	1.98	0.47
1:F:416:ARG:NH1	1:F:418:ASP:HA	2.30	0.47
1:A:589:HIS:NE2	1:A:658:GLU:OE2	2.40	0.47
1:C:263:LEU:N	1:C:264:PRO:HD2	2.30	0.47
1:C:541:GLU:CD	1:C:563:ARG:HH12	2.18	0.47
1:D:485:GLN:NE2	1:D:488:GLU:OE1	2.48	0.47
1:B:161:LEU:HA	1:B:164:ALA:HB3	1.97	0.47
1:B:309:SER:HA	1:B:352:ASP:HB2	1.95	0.47
1:D:253:HIS:HD2	1:D:560:LEU:HD21	1.80	0.47
1:D:662:GLU:HG3	1:D:664:TYR:CE1	2.49	0.47
1:E:173:ARG:O	1:E:177:LEU:HD12	2.14	0.47
1:B:354:PRO:O	1:B:358:GLU:HG2	2.15	0.47
1:B:534:TYR:HE2	1:B:552:TYR:CE2	2.32	0.47
1:C:283:GLY:O	1:C:287:ARG:NE	2.43	0.47
1:C:367:PRO:HG2	1:D:152:ASN:OD1	2.15	0.47
1:F:192:ARG:O	1:F:195:LEU:HB3	2.15	0.47
1:F:615:ASP:HA	1:F:616:PRO:HD2	1.79	0.47
1:A:354:PRO:O	1:A:358:GLU:HG3	2.14	0.46
1:A:695:ASN:O	1:A:698:LEU:HD13	2.15	0.46
1:A:69:TYR:HB3	1:A:70:PRO:HD3	1.97	0.46
1:B:122:ARG:HH11	1:B:219:GLN:HE21	1.63	0.46
1:B:533:MET:CE	1:B:538:GLU:HG3	2.44	0.46
1:B:581:ARG:NH2	1:B:658:GLU:O	2.38	0.46
1:D:512:ASN:ND2	1:D:516:MET:HB2	2.30	0.46
1:D:695:ASN:HA	1:D:698:LEU:CD1	2.46	0.46
1:E:255:THR:OG1	1:E:321:LEU:O	2.28	0.46
1:E:605:ASN:ND2	1:E:635:GLU:O	2.44	0.46
1:B:583:ASN:HA	1:B:586:ARG:HD3	1.96	0.46
1:C:507:ALA:O	1:C:510:GLN:HB2	2.16	0.46
1:D:234:TRP:HH2	1:D:445:LEU:HD11	1.80	0.46
1:D:67:VAL:HG23	1:D:68:ARG:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:ASN:ND2	2:D:801:MAL:H6'1	2.29	0.46
1:A:414:PHE:CD1	1:A:443:LEU:HB2	2.51	0.46
1:B:157:GLY:O	1:B:160:LEU:HB2	2.15	0.46
1:B:297:ALA:HB1	1:B:298:PRO:HD2	1.97	0.46
1:B:556:GLU:HG3	1:B:561:ARG:CG	2.41	0.46
1:C:526:THR:HG21	1:C:624:VAL:HG21	1.97	0.46
1:C:583:ASN:O	1:C:586:ARG:HG3	2.16	0.46
1:D:517:PHE:HD2	1:D:540:PHE:CD1	2.24	0.46
1:E:36:ALA:O	1:E:224:VAL:HA	2.14	0.46
1:E:522:VAL:O	1:E:526:THR:OG1	2.20	0.46
1:E:533:MET:CE	1:E:579:ILE:HD13	2.46	0.46
1:F:475:THR:HG23	1:F:477:TRP:H	1.81	0.46
1:B:255:THR:HG23	1:B:258:THR:H	1.81	0.46
1:B:281:PRO:HB3	1:B:311:GLU:HG2	1.98	0.46
1:B:428:TRP:O	1:B:432:ILE:HG13	2.16	0.46
1:C:216:ARG:HH11	1:C:216:ARG:HG3	1.80	0.46
1:C:309:SER:HA	1:C:352:ASP:HB2	1.97	0.46
1:C:456:TYR:O	1:C:460:LYS:HG3	2.16	0.46
1:D:41:VAL:HG21	1:D:616:PRO:HB2	1.97	0.46
1:D:475:THR:HG22	1:D:478:GLU:CG	2.37	0.46
1:E:280:HIS:ND1	1:E:314:HIS:HA	2.31	0.46
1:B:64:TYR:HD2	1:B:115:ARG:NH1	2.12	0.46
1:C:110:GLN:OE1	1:C:110:GLN:N	2.48	0.46
1:C:235:TYR:HB2	1:C:271:PHE:CD1	2.50	0.46
1:D:297:ALA:HB1	1:D:298:PRO:HD2	1.96	0.46
1:D:575:LEU:HD23	1:D:579:ILE:HD11	1.98	0.46
1:F:522:VAL:O	1:F:526:THR:OG1	2.23	0.46
1:A:183:LEU:HD12	1:A:192:ARG:HB2	1.98	0.46
1:A:677:ALA:HB2	3:A:802:CEY:H6FA	1.98	0.46
1:B:59:THR:OG1	1:B:211:ARG:NH2	2.42	0.46
1:E:698:LEU:CD1	1:E:699:ARG:HG3	2.40	0.46
1:F:130:ILE:HD11	1:F:210:LEU:HD23	1.98	0.46
1:F:371:ILE:HG13	1:F:372:ALA:N	2.30	0.46
1:A:203:GLU:HG3	1:A:204:LEU:H	1.79	0.46
1:B:68:ARG:O	1:B:69:TYR:HB2	2.15	0.46
1:D:175:PRO:O	1:D:178:ALA:HB3	2.15	0.46
1:E:318:HIS:HE1	1:E:320:SER:HB2	1.80	0.46
1:E:499:VAL:HG11	1:E:537:TYR:CZ	2.50	0.46
1:A:358:GLU:C	1:A:359:HIS:HD2	2.19	0.46
1:A:517:PHE:O	1:A:537:TYR:OH	2.23	0.46
1:B:265:ARG:NH2	1:B:538:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:ASP:OD1	1:B:659:ILE:HG13	2.15	0.46
1:C:383:ASP:N	1:C:383:ASP:OD1	2.39	0.46
1:D:37:VAL:HG12	1:D:38:VAL:H	1.81	0.46
1:B:487:ALA:HB1	1:B:490:ALA:N	2.31	0.46
1:C:307:ILE:HG21	1:C:314:HIS:CD2	2.51	0.46
1:C:364:THR:OG1	1:C:388:ASN:HB2	2.16	0.46
1:D:234:TRP:CE2	1:D:273:VAL:HG11	2.51	0.46
1:D:458:LEU:HA	1:D:461:LEU:CD1	2.46	0.46
1:F:263:LEU:N	1:F:264:PRO:HD2	2.31	0.46
1:F:68:ARG:NH2	1:F:118:LEU:HD23	2.30	0.46
1:A:36:ALA:O	1:A:224:VAL:HA	2.15	0.45
1:A:475:THR:CG2	1:A:478:GLU:HG3	2.44	0.45
1:B:150:LEU:HD12	1:B:154:LEU:HD21	1.98	0.45
1:C:331:VAL:O	1:C:335:ARG:HG3	2.16	0.45
1:D:240:ARG:HD3	1:D:560:LEU:HD23	1.98	0.45
1:D:662:GLU:HA	1:D:662:GLU:OE1	2.17	0.45
1:E:631:PHE:CD1	3:E:802:CEY:H3E	2.51	0.45
1:F:387:LEU:HD13	1:F:396:LEU:HD21	1.98	0.45
1:A:290:ARG:HD2	1:A:290:ARG:H	1.80	0.45
1:A:522:VAL:O	1:A:526:THR:OG1	2.20	0.45
1:A:61:VAL:HG22	1:A:95:LEU:HD22	1.98	0.45
1:B:309:SER:O	1:B:354:PRO:HD3	2.16	0.45
1:B:698:LEU:HD12	1:B:699:ARG:H	1.80	0.45
1:F:174:ASP:N	1:F:175:PRO:CD	2.79	0.45
1:A:183:LEU:HB2	1:A:192:ARG:HD3	1.99	0.45
1:C:487:ALA:HB1	1:C:489:LEU:N	2.30	0.45
1:E:371:ILE:HD11	1:E:385:TYR:CZ	2.51	0.45
1:A:195:LEU:HA	1:A:195:LEU:HD23	1.66	0.45
1:C:180:ALA:O	1:C:184:ARG:CZ	2.64	0.45
1:D:122:ARG:NH2	1:D:216:ARG:HD3	2.28	0.45
1:D:475:THR:CG2	1:D:478:GLU:HG3	2.38	0.45
1:D:539:LEU:HD11	1:D:565:PHE:HD1	1.82	0.45
1:E:64:TYR:CE2	1:E:117:GLY:HA3	2.51	0.45
1:E:525:ALA:HB1	1:E:586:ARG:HD2	1.98	0.45
1:F:556:GLU:H	1:F:556:GLU:CD	2.19	0.45
1:A:235:TYR:HE2	1:A:237:MET:HG3	1.82	0.45
1:A:255:THR:HG23	1:A:258:THR:H	1.81	0.45
1:A:280:HIS:N	1:A:280:HIS:CD2	2.82	0.45
1:B:439:ASP:HA	1:B:440:PRO:HD3	1.81	0.45
1:B:692:GLU:OE1	1:B:692:GLU:HA	2.15	0.45
1:C:112:THR:HA	1:C:113:PRO:HD3	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:PRO:HG3	1:D:49:TRP:CZ3	2.51	0.45
1:E:312:GLY:HA3	1:E:316:THR:OG1	2.16	0.45
1:A:673:ARG:NH2	1:E:570:ASP:OD1	2.49	0.45
1:E:693:SER:HG	1:E:694:ARG:NH1	2.15	0.45
1:F:162:GLU:OE2	1:F:180:ALA:HB1	2.15	0.45
1:B:436:LYS:HA	1:B:439:ASP:O	2.17	0.45
1:C:493:ARG:HG2	1:C:493:ARG:NH1	2.30	0.45
1:D:625:VAL:HG11	1:D:672:ILE:HD13	1.97	0.45
1:F:177:LEU:HD12	1:F:180:ALA:HB3	1.99	0.45
1:F:487:ALA:HA	1:F:489:LEU:N	2.31	0.45
1:A:49:TRP:CZ3	1:B:425:PRO:HG3	2.51	0.45
1:B:161:LEU:O	1:B:165:ALA:N	2.49	0.45
1:B:615:ASP:HA	1:B:616:PRO:HD2	1.81	0.45
1:D:237:MET:HG3	1:D:238:PHE:N	2.31	0.45
1:E:188:ASP:O	1:E:191:THR:HG22	2.16	0.45
1:E:41:VAL:HG21	1:E:616:PRO:HB2	1.98	0.45
1:E:529:PRO:O	1:E:586:ARG:NH2	2.45	0.45
1:F:48:VAL:HG21	1:F:58:ALA:HB2	1.97	0.45
1:B:169:PRO:O	1:B:171:GLY:N	2.50	0.45
1:B:629:ASN:HD21	1:B:632:GLY:CA	2.29	0.45
1:C:555:SER:OG	1:C:557:LYS:HG3	2.17	0.45
1:D:165:ALA:CB	1:D:176:LEU:HD11	2.46	0.45
1:D:276:LEU:HD11	1:D:343:LEU:CD1	2.47	0.45
1:E:18:VAL:HB	1:E:215:THR:OG1	2.16	0.45
1:E:211:ARG:HH21	1:E:214:VAL:HG11	1.81	0.45
1:E:458:LEU:HA	1:E:461:LEU:HD13	1.98	0.45
1:F:168:VAL:HG23	1:F:173:ARG:HD3	1.99	0.45
1:F:200:GLU:HG2	1:F:201:ILE:HD12	1.98	0.45
1:F:64:TYR:CD1	1:F:115:ARG:HD2	2.51	0.45
1:A:362:TRP:HD1	1:A:392:ASP:HB3	1.82	0.45
1:A:518:ALA:O	1:A:522:VAL:HG23	2.17	0.45
1:E:122:ARG:NH2	1:E:124:ASP:OD2	2.50	0.45
1:F:280:HIS:HB2	1:F:307:ILE:HG23	1.99	0.45
1:A:130:ILE:CG1	1:A:210:LEU:HD11	2.45	0.45
1:A:318:HIS:CD2	1:A:320:SER:H	2.35	0.45
1:B:162:GLU:CG	1:B:180:ALA:HB1	2.47	0.45
1:B:242:THR:O	1:B:258:THR:HB	2.17	0.45
1:B:698:LEU:HD12	1:B:698:LEU:HA	1.59	0.45
1:C:265:ARG:NE	1:C:576:GLN:OE1	2.50	0.45
1:D:114:ASP:OD1	1:D:115:ARG:HG2	2.17	0.45
1:D:271:PHE:CZ	1:D:533:MET:HE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:ALA:HB2	1:E:443:LEU:HD13	1.99	0.45
1:E:612:SER:HB3	1:E:623:LEU:HD12	1.99	0.45
1:F:583:ASN:O	1:F:587:ARG:HG3	2.16	0.45
1:A:67:VAL:O	1:A:68:ARG:HG2	2.17	0.44
1:C:200:GLU:O	1:C:204:LEU:HD23	2.17	0.44
1:D:37:VAL:HG21	1:D:230:ARG:HB2	1.98	0.44
1:E:255:THR:HG23	1:E:258:THR:H	1.82	0.44
1:E:526:THR:HG21	1:E:624:VAL:HG21	1.98	0.44
1:F:493:ARG:HH11	1:F:493:ARG:HG2	1.82	0.44
1:A:18:VAL:HB	1:A:215:THR:OG1	2.18	0.44
1:B:525:ALA:O	1:B:586:ARG:NH1	2.51	0.44
1:C:424:PRO:O	1:C:427:PHE:HB3	2.18	0.44
1:C:236:GLU:HB3	1:C:534:TYR:HA	1.99	0.44
1:D:323:THR:OG1	1:D:325:ASP:OD1	2.26	0.44
1:D:350:ALA:HB1	1:D:351:PRO:HD2	1.98	0.44
1:B:535:CYS:SG	1:B:563:ARG:NH1	2.91	0.44
1:C:426:ASN:HD21	1:D:17:ARG:NH1	2.15	0.44
1:C:523:LEU:O	1:C:527:MET:HG3	2.17	0.44
1:E:635:GLU:HB2	1:E:673:ARG:HG2	1.98	0.44
1:A:183:LEU:H	1:A:192:ARG:HD3	1.80	0.44
1:A:496:ASN:HD22	1:A:498:PHE:HE1	1.64	0.44
1:C:558:TYR:OH	2:C:801:MAL:O3	2.22	0.44
1:D:122:ARG:NH2	1:D:124:ASP:OD2	2.41	0.44
1:D:243:GLY:HA3	1:D:252:VAL:O	2.17	0.44
1:E:50:ARG:HH12	1:E:126:TRP:HA	1.82	0.44
1:F:307:ILE:HG21	1:F:314:HIS:CE1	2.52	0.44
1:F:498:PHE:HD2	1:F:501:THR:HG22	1.82	0.44
1:A:17:ARG:NH1	1:B:426:ASN:HD21	2.16	0.44
1:A:393:PRO:HG2	1:A:394:GLU:OE1	2.16	0.44
1:A:690:PRO:C	1:A:692:GLU:H	2.20	0.44
1:B:189:PRO:C	1:B:191:THR:H	2.21	0.44
1:B:263:LEU:N	1:B:264:PRO:HD2	2.33	0.44
1:B:493:ARG:HD3	1:B:494:ARG:C	2.38	0.44
1:C:297:ALA:HB1	1:C:298:PRO:HD2	1.99	0.44
1:D:265:ARG:NH2	1:D:576:GLN:OE1	2.51	0.44
1:F:282:ILE:HB	1:F:287:ARG:NH2	2.33	0.44
1:A:128:ASP:O	1:A:132:THR:HG23	2.17	0.44
1:A:509:LEU:HD22	1:A:517:PHE:CE2	2.52	0.44
1:B:138:ILE:O	1:B:141:LEU:HG	2.18	0.44
1:C:195:LEU:C	1:C:198:THR:HG22	2.37	0.44
1:C:271:PHE:CZ	1:C:533:MET:HE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:PRO:HA	1:F:318:HIS:CD2	2.53	0.44
1:F:576:GLN:N	1:F:577:PRO:HD2	2.33	0.44
1:F:607:ALA:HB3	1:F:634:GLU:HG2	1.99	0.44
1:A:614:PHE:HE1	1:A:693:SER:HB2	1.82	0.44
1:C:582:LEU:O	1:C:585:ILE:HG12	2.17	0.44
1:D:280:HIS:HB3	1:D:281:PRO:HD2	2.00	0.44
1:D:549:SER:HG	1:D:551:GLU:CD	2.20	0.44
1:E:533:MET:HE3	1:E:533:MET:HB3	1.75	0.44
1:F:193:THR:O	1:F:197:LEU:HG	2.16	0.44
1:A:360:ARG:O	1:A:360:ARG:HG3	2.18	0.44
1:A:373:TYR:CE1	1:A:385:TYR:HE1	2.36	0.44
1:A:526:THR:OG1	1:A:611:TYR:OH	2.31	0.44
1:A:543:ARG:H	1:A:543:ARG:HG2	1.65	0.44
1:B:165:ALA:CB	1:B:173:ARG:HD2	2.32	0.44
1:B:512:ASN:HA	1:B:631:PHE:CE1	2.52	0.44
1:B:555:SER:OG	1:B:557:LYS:NZ	2.50	0.44
1:B:612:SER:HB3	1:B:623:LEU:HD12	1.99	0.44
1:D:580:THR:O	1:D:584:ILE:HG13	2.16	0.44
1:E:114:ASP:OD2	1:E:115:ARG:HG3	2.17	0.44
1:F:352:ASP:N	1:F:352:ASP:OD1	2.50	0.44
1:B:185:THR:OG1	1:B:192:ARG:NH2	2.47	0.44
1:D:288:LYS:N	1:D:288:LYS:CD	2.81	0.44
1:D:523:LEU:O	1:D:527:MET:HG3	2.17	0.44
1:B:576:GLN:N	1:B:577:PRO:HD2	2.32	0.43
1:B:627:THR:HG22	1:B:680:VAL:O	2.18	0.43
1:C:545:VAL:HA	1:C:553:LEU:CD2	2.48	0.43
1:D:505:LEU:HD23	1:D:505:LEU:O	2.17	0.43
1:F:580:THR:O	1:F:584:ILE:HG13	2.18	0.43
1:A:493:ARG:HH11	1:A:493:ARG:HG2	1.83	0.43
1:A:505:LEU:HB2	1:A:552:TYR:CD2	2.54	0.43
1:C:489:LEU:HD13	1:C:492:TYR:CZ	2.53	0.43
1:D:288:LYS:HZ1	1:D:383:ASP:N	2.16	0.43
1:D:493:ARG:HG2	1:D:493:ARG:NH1	2.26	0.43
1:D:67:VAL:HG23	1:D:68:ARG:N	2.33	0.43
1:F:162:GLU:O	1:F:165:ALA:HB3	2.19	0.43
1:A:50:ARG:HG2	1:A:51:GLU:H	1.83	0.43
1:A:612:SER:HB3	1:A:623:LEU:HD12	2.00	0.43
1:B:110:GLN:N	1:B:110:GLN:OE1	2.51	0.43
1:B:287:ARG:O	1:B:296:ALA:HB2	2.18	0.43
1:B:523:LEU:O	1:B:527:MET:HG3	2.18	0.43
1:C:529:PRO:HB3	1:C:593:GLN:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:THR:HG23	1:D:258:THR:H	1.84	0.43
1:D:488:GLU:HB3	1:D:490:ALA:N	2.33	0.43
1:D:35:LYS:HG3	1:D:492:TYR:HA	2.01	0.43
1:E:61:VAL:HG22	1:E:95:LEU:CD1	2.49	0.43
1:F:508:VAL:CG1	1:F:516:MET:HE3	2.48	0.43
1:F:540:PHE:CZ	1:F:575:LEU:HB2	2.53	0.43
1:F:692:GLU:O	1:F:696:THR:HG23	2.19	0.43
1:F:677:ALA:HB2	3:F:802:CEY:C6F	2.48	0.43
1:A:266:ILE:HG22	1:A:339:MET:CE	2.48	0.43
1:A:429:ALA:HB2	1:A:461:LEU:HD23	2.00	0.43
1:D:354:PRO:O	1:D:358:GLU:HG2	2.18	0.43
1:D:648:GLU:HG3	1:D:650:TYR:CE1	2.53	0.43
1:E:457:GLY:O	1:E:460:LYS:HB3	2.19	0.43
1:A:388:ASN:HD22	1:A:391:ASN:H	1.67	0.43
1:A:501:THR:HB	1:A:502:PRO:HD2	1.99	0.43
1:B:605:ASN:HB2	1:B:636:ALA:HB2	2.00	0.43
1:B:108:HIS:CD2	1:B:698:LEU:HD21	2.54	0.43
1:C:540:PHE:CZ	1:C:575:LEU:HB2	2.54	0.43
1:C:580:THR:O	1:C:584:ILE:HG13	2.19	0.43
1:C:625:VAL:HG11	1:C:672:ILE:HD13	2.01	0.43
1:D:138:ILE:HA	1:D:141:LEU:HD23	2.00	0.43
1:D:445:LEU:HD12	1:D:445:LEU:N	2.34	0.43
1:D:290:ARG:HE	1:D:559:GLU:CD	2.20	0.43
1:E:629:ASN:ND2	1:E:632:GLY:H	2.15	0.43
1:F:523:LEU:O	1:F:527:MET:HG3	2.19	0.43
1:A:398:ASP:O	1:A:402:ARG:NH1	2.51	0.43
1:A:59:THR:HG23	1:A:126:TRP:NE1	2.31	0.43
1:B:255:THR:OG1	1:B:321:LEU:O	2.25	0.43
1:C:234:TRP:CE2	1:C:273:VAL:HG11	2.54	0.43
1:C:493:ARG:HG2	1:C:493:ARG:HH11	1.82	0.43
1:C:543:ARG:HD2	1:C:543:ARG:HA	1.67	0.43
1:D:539:LEU:HA	1:D:539:LEU:HD23	1.76	0.43
1:F:493:ARG:HG2	1:F:493:ARG:NH1	2.33	0.43
1:F:507:ALA:O	1:F:510:GLN:HB2	2.19	0.43
1:F:627:THR:HG22	1:F:680:VAL:O	2.19	0.43
1:F:629:ASN:HB2	3:F:802:CEY:H2B	2.01	0.43
1:A:180:ALA:HB1	1:A:184:ARG:HH21	1.84	0.43
1:C:21:ASP:OD1	1:C:22:ASP:N	2.47	0.43
1:D:184:ARG:CD	1:D:184:ARG:H	2.32	0.43
1:D:387:LEU:HD13	1:D:396:LEU:HD21	2.00	0.43
1:D:226:ARG:NH2	1:D:413:LYS:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:509:LEU:HD22	1:D:517:PHE:HD1	1.80	0.43
1:C:422:THR:HA	1:D:52:GLY:N	2.33	0.43
1:D:487:ALA:HB3	1:D:595:LEU:O	2.19	0.43
1:D:663:GLU:C	1:D:664:TYR:HD1	2.22	0.43
1:F:383:ASP:OD1	1:F:383:ASP:N	2.51	0.43
1:A:126:TRP:CZ3	1:A:128:ASP:HB2	2.54	0.43
1:A:198:THR:C	1:A:200:GLU:H	2.22	0.43
1:A:533:MET:HE3	1:A:537:TYR:CD1	2.54	0.43
1:B:108:HIS:HB3	1:B:698:LEU:HD11	2.01	0.43
1:B:485:GLN:O	1:B:487:ALA:HA	2.19	0.43
1:D:605:ASN:ND2	1:D:635:GLU:O	2.46	0.43
1:F:177:LEU:O	1:F:181:ALA:N	2.51	0.43
1:A:599:HIS:HE1	1:A:641:ASP:OD2	2.02	0.43
1:C:446:SER:HB3	1:C:463:PHE:HD1	1.82	0.43
1:D:40:GLU:O	1:D:112:THR:HG23	2.19	0.43
1:D:517:PHE:CD1	1:D:537:TYR:HE1	2.37	0.43
1:E:398:ASP:O	1:E:402:ARG:HG3	2.19	0.43
1:E:660:THR:HG22	1:E:662:GLU:HG2	2.01	0.43
1:F:631:PHE:CD1	3:F:802:CEY:H3E	2.54	0.43
1:B:399:GLU:O	1:B:403:VAL:HG23	2.19	0.43
1:C:443:LEU:HB3	1:C:464:THR:HG21	2.01	0.43
1:D:168:VAL:HA	1:D:169:PRO:HD3	1.70	0.43
1:D:218:GLU:OE1	1:D:219:GLN:N	2.52	0.43
1:D:461:LEU:H	1:D:461:LEU:HD13	1.84	0.43
1:D:549:SER:OG	1:D:551:GLU:OE1	2.37	0.43
1:E:487:ALA:O	1:E:596:ARG:HA	2.19	0.43
1:E:605:ASN:HD21	1:E:634:GLU:HG3	1.84	0.43
1:F:204:LEU:HD12	1:F:205:LEU:N	2.33	0.43
1:F:351:PRO:HA	1:F:385:TYR:OH	2.19	0.43
1:A:488:GLU:C	1:A:490:ALA:H	2.22	0.42
1:A:493:ARG:NH1	1:A:493:ARG:HG2	2.34	0.42
1:A:608:LEU:HD23	1:A:608:LEU:HA	1.82	0.42
1:B:162:GLU:HG2	1:B:180:ALA:HB1	2.01	0.42
1:B:493:ARG:HH11	1:B:494:ARG:C	2.21	0.42
1:C:111:PHE:CE1	1:C:113:PRO:HG3	2.55	0.42
1:E:170:ARG:HB2	1:E:171:GLY:H	1.50	0.42
1:E:164:ALA:HA	1:E:210:LEU:HD13	2.01	0.42
1:E:619:GLY:O	1:E:689:VAL:N	2.50	0.42
1:A:168:VAL:HG23	1:A:169:PRO:HD2	2.01	0.42
1:A:18:VAL:CG2	1:A:213:LEU:HD13	2.44	0.42
1:C:36:ALA:O	1:C:224:VAL:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:HIS:ND1	1:D:314:HIS:HA	2.34	0.42
1:D:374:ALA:CA	1:D:386:PRO:HD3	2.49	0.42
1:E:168:VAL:O	1:E:173:ARG:HG2	2.18	0.42
1:E:575:LEU:O	1:E:579:ILE:HG13	2.20	0.42
1:E:69:TYR:HB3	1:E:70:PRO:HD3	2.01	0.42
1:F:285:VAL:HG23	1:F:352:ASP:OD1	2.19	0.42
1:F:567:SER:O	1:F:571:GLN:HG3	2.17	0.42
1:A:285:VAL:O	1:A:286:HIS:HB2	2.19	0.42
1:B:379:LYS:H	1:B:379:LYS:HG3	1.35	0.42
1:C:226:ARG:HB2	1:C:227:PRO:HD2	2.02	0.42
1:C:226:ARG:HE	1:C:443:LEU:HD11	1.82	0.42
1:C:605:ASN:HD21	1:C:634:GLU:HG3	1.85	0.42
1:D:40:GLU:O	1:D:40:GLU:HG3	2.19	0.42
1:D:428:TRP:O	1:D:432:ILE:HG13	2.18	0.42
1:C:422:THR:HA	1:D:52:GLY:H	1.84	0.42
1:D:541:GLU:HG2	1:D:563:ARG:HH22	1.84	0.42
1:D:591:ALA:HA	1:D:615:ASP:HB2	2.01	0.42
1:F:439:ASP:HA	1:F:440:PRO:HD3	1.78	0.42
1:A:60:LEU:HD11	1:A:121:PHE:HB2	2.01	0.42
1:A:358:GLU:C	1:A:359:HIS:CD2	2.93	0.42
1:B:518:ALA:O	1:B:522:VAL:HG23	2.19	0.42
1:C:358:GLU:HG3	1:C:359:HIS:CG	2.54	0.42
1:E:205:LEU:HA	1:E:208:TYR:O	2.19	0.42
1:E:497:LEU:HD22	1:E:528:SER:HB3	2.02	0.42
1:E:599:HIS:HD2	1:E:644:ALA:CB	2.31	0.42
1:F:486:ILE:HG23	1:F:495:PRO:HG3	2.01	0.42
1:F:697:LEU:HG	1:F:697:LEU:O	2.20	0.42
1:A:179:ALA:HA	1:A:195:LEU:CD1	2.49	0.42
1:A:475:THR:HG23	1:A:478:GLU:H	1.84	0.42
1:A:556:GLU:CD	1:A:563:ARG:HH12	2.22	0.42
1:B:416:ARG:NH1	1:B:467:TYR:CZ	2.82	0.42
1:C:501:THR:OG1	1:C:504:ILE:HG12	2.19	0.42
1:E:242:THR:O	1:E:258:THR:HB	2.19	0.42
1:A:671:TYR:HD1	1:E:264:PRO:HB2	1.84	0.42
1:E:280:HIS:C	1:E:318:HIS:HB2	2.39	0.42
1:F:364:THR:OG1	1:F:388:ASN:HB2	2.20	0.42
1:A:569:LEU:HD11	1:A:576:GLN:NE2	2.35	0.42
1:A:615:ASP:HA	1:A:616:PRO:HD2	1.79	0.42
1:B:200:GLU:HG2	1:B:201:ILE:HG23	2.01	0.42
1:B:512:ASN:ND2	3:B:802:CEY:O6A	2.51	0.42
1:F:184:ARG:HH11	1:F:192:ARG:NH2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:PRO:HA	1:A:385:TYR:CE2	2.55	0.42
1:A:405:GLN:NE2	1:A:438:VAL:HG21	2.26	0.42
1:B:368:ASP:OD1	1:B:370:THR:HG22	2.19	0.42
3:B:802:CEY:O5E	3:B:802:CEY:H5D	2.18	0.42
1:D:446:SER:HB3	1:D:463:PHE:CD1	2.54	0.42
1:E:414:PHE:CE1	1:E:443:LEU:HB2	2.55	0.42
1:E:238:PHE:CD2	1:E:556:GLU:OE1	2.73	0.42
1:E:608:LEU:HA	1:E:608:LEU:HD23	1.83	0.42
1:F:245:TRP:CZ2	1:F:562:PRO:HB2	2.55	0.42
1:A:18:VAL:HG22	1:A:50:ARG:HD3	2.01	0.42
1:B:172:LEU:O	1:B:175:PRO:HD2	2.20	0.42
1:B:580:THR:O	1:B:584:ILE:HG13	2.19	0.42
1:C:138:ILE:O	1:C:141:LEU:HB3	2.20	0.42
1:C:253:HIS:ND1	1:C:320:SER:OG	2.52	0.42
1:C:475:THR:CG2	1:C:478:GLU:HG3	2.49	0.42
1:C:629:ASN:OD1	3:C:802:CEY:H6B	2.19	0.42
1:D:126:TRP:CZ3	1:D:128:ASP:HB3	2.55	0.42
1:D:509:LEU:HD22	1:D:517:PHE:CE1	2.54	0.42
1:F:353:HIS:CE1	1:F:355:TRP:CG	3.07	0.42
1:F:506:HIS:ND1	1:F:508:VAL:HG23	2.33	0.42
1:A:198:THR:HA	1:A:199:PRO:HD3	1.66	0.42
1:B:126:TRP:CD2	1:B:211:ARG:HG2	2.55	0.42
1:B:172:LEU:C	1:B:174:ASP:H	2.23	0.42
1:C:207:ASP:OD1	1:C:208:TYR:CD2	2.73	0.42
1:C:477:TRP:NE1	1:C:481:GLU:OE2	2.53	0.42
1:D:122:ARG:HH22	1:D:216:ARG:CD	2.29	0.42
1:E:361:GLN:CD	1:E:361:GLN:H	2.23	0.42
1:E:600:PHE:CE1	1:E:609:LEU:HD11	2.54	0.42
1:E:676:PRO:C	1:E:678:ARG:H	2.23	0.42
1:F:312:GLY:HA3	1:F:316:THR:OG1	2.20	0.42
1:A:288:LYS:HZ2	1:A:288:LYS:HG3	1.71	0.42
1:A:526:THR:HG21	1:A:624:VAL:HG21	2.02	0.42
1:A:566:ALA:O	1:A:569:LEU:HB2	2.20	0.42
1:B:366:LEU:HB3	1:B:367:PRO:HD2	2.02	0.42
1:C:108:HIS:ND1	1:C:698:LEU:HD22	2.35	0.42
1:C:487:ALA:HB1	1:C:488:GLU:CA	2.49	0.42
1:C:576:GLN:N	1:C:577:PRO:HD2	2.35	0.42
1:D:188:ASP:O	1:D:191:THR:HG22	2.20	0.42
1:D:353:HIS:CE1	1:D:355:TRP:CG	3.08	0.42
1:D:695:ASN:HA	1:D:698:LEU:HD13	2.02	0.42
1:E:103:GLU:HG3	1:E:104:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:375:GLU:HG3	1:E:381:TYR:H	1.85	0.42
1:F:288:LYS:NZ	1:F:383:ASP:OD1	2.50	0.42
1:B:138:ILE:HA	1:B:141:LEU:CD2	2.50	0.41
1:D:55:ALA:N	1:D:132:THR:HG22	2.23	0.41
1:D:522:VAL:O	1:D:526:THR:OG1	2.18	0.41
1:E:307:ILE:HG21	1:E:314:HIS:HD2	1.78	0.41
1:F:518:ALA:O	1:F:522:VAL:HG23	2.19	0.41
1:A:19:GLU:HG3	1:A:49:TRP:CZ2	2.55	0.41
1:A:558:TYR:N	1:A:558:TYR:CD1	2.87	0.41
1:A:576:GLN:N	1:A:577:PRO:HD2	2.35	0.41
1:B:458:LEU:HA	1:B:461:LEU:HD23	2.02	0.41
1:C:155:LEU:HA	1:C:158:ALA:HB3	2.02	0.41
1:C:190:VAL:O	1:C:193:THR:OG1	2.29	0.41
1:C:226:ARG:NE	1:C:443:LEU:HD11	2.35	0.41
1:C:266:ILE:O	1:C:269:MET:HG2	2.20	0.41
1:E:201:ILE:HG22	1:E:204:LEU:HD21	2.03	0.41
1:E:305:TRP:NE1	1:E:344:ASP:OD2	2.44	0.41
1:E:576:GLN:N	1:E:577:PRO:HD2	2.35	0.41
1:F:508:VAL:HG12	1:F:512:ASN:HD21	1.85	0.41
1:F:526:THR:HG21	1:F:624:VAL:HG21	2.03	0.41
1:A:203:GLU:HG3	1:A:205:LEU:N	2.22	0.41
1:A:255:THR:H	1:A:258:THR:HG1	1.66	0.41
1:A:506:HIS:ND1	1:A:507:ALA:N	2.67	0.41
1:A:517:PHE:CE1	1:A:540:PHE:HA	2.55	0.41
1:A:576:GLN:O	1:A:580:THR:OG1	2.35	0.41
1:B:358:GLU:O	1:B:359:HIS:HD2	2.02	0.41
1:B:471:THR:HG21	1:B:504:ILE:HD12	2.02	0.41
1:B:663:GLU:C	1:B:664:TYR:HD1	2.22	0.41
1:C:541:GLU:OE1	1:C:563:ARG:NH2	2.35	0.41
1:C:505:LEU:HB2	1:C:552:TYR:CD2	2.55	0.41
1:E:350:ALA:HB1	1:E:351:PRO:HD2	2.02	0.41
1:B:318:HIS:HE1	1:B:320:SER:HB3	1.77	0.41
1:B:366:LEU:HD23	1:B:366:LEU:HA	1.89	0.41
1:B:486:ILE:O	1:B:486:ILE:HG12	2.21	0.41
1:C:377:PRO:HA	1:C:378:PRO:HA	1.72	0.41
1:D:110:GLN:HG2	1:D:694:ARG:NH2	2.33	0.41
1:D:37:VAL:HG12	1:D:38:VAL:N	2.35	0.41
1:E:157:GLY:O	1:E:160:LEU:HB2	2.20	0.41
1:E:189:PRO:O	1:E:193:THR:N	2.47	0.41
1:F:308:GLY:HA3	1:F:353:HIS:CD2	2.54	0.41
1:A:343:LEU:HD12	1:A:412:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:HIS:CE1	1:B:355:TRP:CG	3.09	0.41
1:B:625:VAL:HG11	1:B:672:ILE:HD13	2.01	0.41
1:B:64:TYR:HB2	1:B:119:TRP:CE3	2.56	0.41
1:C:402:ARG:HH11	1:C:402:ARG:CG	2.34	0.41
1:C:518:ALA:O	1:C:522:VAL:HG23	2.20	0.41
1:C:683:ILE:N	1:C:683:ILE:HD12	2.36	0.41
1:D:309:SER:HA	1:D:352:ASP:CB	2.48	0.41
1:D:489:LEU:H	1:D:489:LEU:CD1	2.34	0.41
1:E:204:LEU:HD12	1:E:205:LEU:N	2.35	0.41
1:A:194:ALA:HA	1:A:197:LEU:HD12	2.03	0.41
1:A:383:ASP:OD1	1:A:384:ILE:HG13	2.20	0.41
1:C:183:LEU:HB2	1:C:192:ARG:HD3	2.02	0.41
1:D:458:LEU:O	1:D:461:LEU:HD13	2.20	0.41
1:E:267:ALA:HA	1:E:339:MET:CE	2.51	0.41
1:F:173:ARG:NH1	1:F:177:LEU:HB2	2.35	0.41
1:F:416:ARG:O	1:F:416:ARG:HD2	2.20	0.41
1:F:575:LEU:HD23	1:F:579:ILE:HD11	2.03	0.41
1:D:182:ALA:O	1:D:192:ARG:NE	2.52	0.41
1:D:57:ALA:HA	1:D:107:PHE:CE2	2.49	0.41
1:E:185:THR:HG22	1:E:185:THR:H	1.65	0.41
1:F:399:GLU:O	1:F:403:VAL:HG23	2.21	0.41
1:A:157:GLY:O	1:A:160:LEU:HB2	2.21	0.41
1:A:364:THR:CG2	1:A:388:ASN:HB2	2.51	0.41
1:A:388:ASN:ND2	1:A:390:ASP:H	2.19	0.41
1:B:108:HIS:CG	1:B:698:LEU:HD21	2.56	0.41
1:B:507:ALA:O	1:B:510:GLN:HB2	2.21	0.41
1:B:533:MET:CE	1:B:537:TYR:HB3	2.50	0.41
1:F:475:THR:HG23	1:F:477:TRP:N	2.35	0.41
1:F:545:VAL:HA	1:F:553:LEU:HD13	2.02	0.41
1:A:68:ARG:O	1:A:69:TYR:HB2	2.20	0.41
1:D:37:VAL:CG1	1:D:227:PRO:HA	2.49	0.41
1:D:505:LEU:HD22	1:D:544:ALA:HB2	2.02	0.41
1:D:506:HIS:ND1	1:D:508:VAL:HG12	2.36	0.41
1:D:546:ARG:HA	1:D:546:ARG:HD3	1.20	0.41
1:D:619:GLY:O	1:D:689:VAL:N	2.52	0.41
1:E:509:LEU:HB3	1:E:517:PHE:CE1	2.48	0.41
1:E:236:GLU:HB3	1:E:534:TYR:HA	2.02	0.41
2:E:801:MAL:H1	2:E:801:MAL:H62	1.86	0.41
1:F:182:ALA:C	1:F:183:LEU:HD12	2.41	0.41
1:F:20:ILE:HG12	1:F:48:VAL:HG12	2.02	0.41
1:A:226:ARG:HB2	1:A:227:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:THR:HG22	1:A:680:VAL:O	2.21	0.41
1:B:557:LYS:HB2	1:B:558:TYR:CD1	2.56	0.41
1:B:558:TYR:N	1:B:558:TYR:CD1	2.88	0.41
1:C:240:ARG:CG	1:C:240:ARG:HH11	2.31	0.41
1:C:283:GLY:O	1:C:287:ARG:HG3	2.21	0.41
1:A:315:ASP:OD1	1:A:316:THR:HG23	2.20	0.41
1:A:672:ILE:HD12	1:A:673:ARG:H	1.85	0.41
1:B:493:ARG:HD3	1:B:493:ARG:C	2.42	0.41
1:B:686:MET:HB3	1:B:687:PRO:HD2	2.03	0.41
1:D:663:GLU:O	1:D:664:TYR:HD1	2.04	0.41
1:E:629:ASN:OD1	3:E:802:CEY:C6B	2.69	0.41
1:F:195:LEU:HD23	1:F:195:LEU:O	2.21	0.41
1:F:236:GLU:HB3	1:F:534:TYR:HA	2.03	0.41
1:F:600:PHE:CE1	1:F:609:LEU:HD11	2.56	0.41
1:F:686:MET:HB3	1:F:687:PRO:HD2	2.03	0.41
1:A:487:ALA:HA	1:A:488:GLU:HA	1.82	0.40
1:C:155:LEU:O	1:C:158:ALA:HB3	2.20	0.40
1:C:358:GLU:O	1:C:359:HIS:HD2	2.04	0.40
1:D:435:VAL:O	1:D:438:VAL:HG22	2.20	0.40
1:E:100:SER:HB2	1:E:107:PHE:CE1	2.55	0.40
1:E:374:ALA:CA	1:E:386:PRO:HD3	2.50	0.40
1:E:518:ALA:O	1:E:522:VAL:HG23	2.21	0.40
1:F:168:VAL:HG12	1:F:208:TYR:CB	2.49	0.40
1:F:116:VAL:HA	1:F:224:VAL:HG23	2.02	0.40
1:F:226:ARG:HB2	1:F:227:PRO:HD2	2.02	0.40
1:F:266:ILE:HG22	1:F:339:MET:CE	2.48	0.40
1:F:239:PRO:HG3	1:F:276:LEU:HD22	2.03	0.40
1:F:40:GLU:OE1	1:F:596:ARG:NH1	2.53	0.40
1:F:575:LEU:O	1:F:579:ILE:HG13	2.21	0.40
1:B:154:LEU:CD2	1:B:154:LEU:H	2.34	0.40
1:C:65:LEU:HD12	1:C:118:LEU:HD23	2.03	0.40
1:C:271:PHE:N	1:C:271:PHE:CD2	2.90	0.40
1:E:251:PRO:HB2	1:E:560:LEU:CD1	2.50	0.40
1:F:158:ALA:HB1	1:F:184:ARG:HH12	1.81	0.40
1:F:198:THR:OG1	1:F:200:GLU:OE1	2.39	0.40
1:F:68:ARG:HG2	1:F:69:TYR:N	2.37	0.40
1:A:599:HIS:CE1	1:A:641:ASP:OD2	2.74	0.40
1:B:358:GLU:C	1:B:359:HIS:CD2	2.95	0.40
1:B:620:ASP:OD2	1:B:621:CYS:N	2.55	0.40
1:C:218:GLU:HG2	1:C:218:GLU:H	1.66	0.40
1:C:376:ASN:O	1:C:379:LYS:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:LYS:N	1:D:288:LYS:HD3	2.36	0.40
1:D:468:SER:OG	1:D:469:TYR:N	2.54	0.40
1:D:627:THR:HG22	1:D:680:VAL:O	2.21	0.40
1:E:240:ARG:NH2	1:E:304:PRO:HG3	2.36	0.40
1:E:416:ARG:NH2	1:E:447:GLU:OE1	2.54	0.40
1:E:543:ARG:HH11	1:E:543:ARG:HD2	1.76	0.40
1:F:68:ARG:HH22	1:F:118:LEU:HD23	1.85	0.40
1:F:315:ASP:OD1	1:F:316:THR:HG23	2.21	0.40
1:F:317:VAL:HG21	1:F:324:ILE:HA	2.04	0.40
1:A:534:TYR:OH	1:A:556:GLU:OE2	2.37	0.40
1:A:619:GLY:O	1:A:689:VAL:N	2.51	0.40
1:B:285:VAL:HG12	1:B:286:HIS:ND1	2.36	0.40
1:C:545:VAL:HG23	1:C:551:GLU:O	2.21	0.40
1:D:235:TYR:HB2	1:D:271:PHE:CD1	2.56	0.40
1:D:612:SER:HB3	1:D:623:LEU:HD12	2.03	0.40
1:D:93:PRO:HB2	1:D:94:LEU:H	1.71	0.40
1:E:63:ARG:HD2	1:E:92:LYS:O	2.22	0.40
1:F:374:ALA:CA	1:F:386:PRO:HD3	2.51	0.40
1:F:473:ARG:CD	1:F:478:GLU:HB3	2.49	0.40
1:A:150:LEU:CD2	1:A:154:LEU:HG	2.52	0.40
1:A:344:ASP:OD1	1:A:416:ARG:NH1	2.55	0.40
1:A:67:VAL:HG12	1:A:68:ARG:N	2.36	0.40
1:D:442:VAL:C	1:D:443:LEU:HD23	2.41	0.40
1:D:483:GLY:HA3	1:D:600:PHE:CZ	2.57	0.40
1:F:226:ARG:HH12	1:F:340:GLU:CD	2.25	0.40
1:F:672:ILE:HD12	1:F:673:ARG:H	1.85	0.40

All (1) 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_556]	1.75	0.45

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	654/723 (90%)	629 (96%)	20 (3%)	5 (1%)	22	66
1	B	654/723 (90%)	624 (95%)	21 (3%)	9 (1%)	13	55
1	C	654/723 (90%)	628 (96%)	20 (3%)	6 (1%)	20	63
1	D	654/723 (90%)	621 (95%)	24 (4%)	9 (1%)	13	55
1	E	654/723 (90%)	624 (95%)	22 (3%)	8 (1%)	15	59
1	F	654/723 (90%)	629 (96%)	19 (3%)	6 (1%)	20	63
All	All	3924/4338 (90%)	3755 (96%)	126 (3%)	43 (1%)	17	60

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	TYR
1	A	151	SER
1	B	68	ARG
1	B	69	TYR
1	B	150	LEU
1	B	151	SER
1	B	170	ARG
1	C	68	ARG
1	C	69	TYR
1	C	151	SER
1	C	174	ASP
1	C	488	GLU
1	D	16	GLY
1	D	69	TYR
1	D	151	SER
1	D	152	ASN
1	D	170	ARG
1	D	382	GLN
1	D	488	GLU
1	E	69	TYR
1	E	151	SER
1	E	194	ALA
1	F	488	GLU
1	A	67	VAL
1	B	190	VAL
1	D	93	PRO
1	D	172	LEU

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Mol	Chain	Res	Type
1	E	375	GLU
1	A	170	ARG
1	B	488	GLU
1	F	69	TYR
1	F	193	THR
1	F	68	ARG
1	E	171	GLY
1	E	172	LEU
1	E	197	LEU
1	F	67	VAL
1	F	393	PRO
1	B	393	PRO
1	A	393	PRO
1	E	393	PRO
1	B	199	PRO
1	C	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	542/597 (91%)	514 (95%)	28 (5%)	27	63
1	B	542/597 (91%)	525 (97%)	17 (3%)	45	75
1	C	542/597 (91%)	515 (95%)	27 (5%)	28	64
1	D	542/597 (91%)	520 (96%)	22 (4%)	35	69
1	E	542/597 (91%)	508 (94%)	34 (6%)	21	57
1	F	542/597 (91%)	516 (95%)	26 (5%)	30	65
All	All	3252/3582 (91%)	3098 (95%)	154 (5%)	30	66

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	ARG
1	A	174	ASP

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Mol	Chain	Res	Type
1	A	183	LEU
1	A	204	LEU
1	A	210	LEU
1	A	216	ARG
1	A	218	GLU
1	A	237	MET
1	A	290	ARG
1	A	303	SER
1	A	360	ARG
1	A	371	ILE
1	A	379	LYS
1	A	384	ILE
1	A	388	ASN
1	A	394	GLU
1	A	398	ASP
1	A	399	GLU
1	A	402	ARG
1	A	414	PHE
1	A	466	SER
1	A	510	GLN
1	A	560	LEU
1	A	629	ASN
1	A	659	ILE
1	A	664	TYR
1	A	692	GLU
1	A	694	ARG
1	B	115	ARG
1	B	184	ARG
1	B	216	ARG
1	B	303	SER
1	B	311	GLU
1	B	332	SER
1	B	361	GLN
1	B	379	LYS
1	B	399	GLU
1	B	414	PHE
1	B	436	LYS
1	B	481	GLU
1	B	486	ILE
1	B	505	LEU
1	B	561	ARG
1	B	583	ASN

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Mol	Chain	Res	Type
1	B	691	TYR
1	C	102	GLN
1	C	122	ARG
1	C	131	HIS
1	C	162	GLU
1	C	183	LEU
1	C	195	LEU
1	C	198	THR
1	C	200	GLU
1	C	204	LEU
1	C	240	ARG
1	C	282	ILE
1	C	379	LYS
1	C	402	ARG
1	C	414	PHE
1	C	423	LYS
1	C	438	VAL
1	C	466	SER
1	C	489	LEU
1	C	523	LEU
1	C	563	ARG
1	C	593	GLN
1	C	596	ARG
1	C	664	TYR
1	C	691	TYR
1	C	692	GLU
1	C	694	ARG
1	C	696	THR
1	D	110	GLN
1	D	118	LEU
1	D	122	ARG
1	D	141	LEU
1	D	150	LEU
1	D	184	ARG
1	D	195	LEU
1	D	284	LYS
1	D	303	SER
1	D	325	ASP
1	D	343	LEU
1	D	368	ASP
1	D	375	GLU
1	D	414	PHE

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Mol	Chain	Res	Type
1	D	436	LYS
1	D	445	LEU
1	D	461	LEU
1	D	489	LEU
1	D	546	ARG
1	D	664	TYR
1	D	691	TYR
1	D	692	GLU
1	E	29	CYS
1	E	50	ARG
1	E	63	ARG
1	E	112	THR
1	E	122	ARG
1	E	141	LEU
1	E	170	ARG
1	E	183	LEU
1	E	184	ARG
1	E	185	THR
1	E	188	ASP
1	E	211	ARG
1	E	216	ARG
1	E	286	HIS
1	E	287	ARG
1	E	332	SER
1	E	335	ARG
1	E	348	GLN
1	E	357	ARG
1	E	366	LEU
1	E	410	HIS
1	E	414	PHE
1	E	458	LEU
1	E	527	MET
1	E	560	LEU
1	E	563	ARG
1	E	581	ARG
1	E	583	ASN
1	E	645	LEU
1	E	652	ARG
1	E	663	GLU
1	E	664	TYR
1	E	691	TYR
1	E	698	LEU

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Mol	Chain	Res	Type
1	F	103	GLU
1	F	151	SER
1	F	174	ASP
1	F	195	LEU
1	F	198	THR
1	F	216	ARG
1	F	301	VAL
1	F	303	SER
1	F	328	ASP
1	F	332	SER
1	F	352	ASP
1	F	361	GLN
1	F	371	ILE
1	F	379	LYS
1	F	383	ASP
1	F	385	TYR
1	F	405	GLN
1	F	414	PHE
1	F	416	ARG
1	F	466	SER
1	F	488	GLU
1	F	489	LEU
1	F	662	GLU
1	F	664	TYR
1	F	665	GLN
1	F	698	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	HIS
1	A	388	ASN
1	A	405	GLN
1	A	485	GLN
1	A	695	ASN
1	B	314	HIS
1	B	388	ASN
1	B	405	GLN
1	C	314	HIS
1	C	485	GLN
1	D	280	HIS
1	D	314	HIS

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Mol	Chain	Res	Type
1	D	405	GLN
1	D	419	ASN
1	D	484	ASN
1	D	571	GLN
1	E	108	HIS
1	E	286	HIS
1	E	314	HIS
1	E	405	GLN
1	E	419	ASN
1	E	455	GLN
1	F	512	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	0.58	0	35,35,35	1.42	5 (14%)
3	CEY	A	802	-	72,72,72	2.19	31 (43%)	107,107,107	1.32	15 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAL	B	801	-	24,24,24	0.55	0	35,35,35	0.91	2 (5%)
3	CEY	B	802	-	72,72,72	2.20	32 (44%)	107,107,107	1.28	19 (17%)
2	MAL	C	801	-	24,24,24	0.55	0	35,35,35	1.04	2 (5%)
3	CEY	C	802	-	72,72,72	2.17	29 (40%)	107,107,107	1.23	9 (8%)
2	MAL	D	801	-	24,24,24	0.56	0	35,35,35	1.15	2 (5%)
3	CEY	D	802	-	72,72,72	2.21	34 (47%)	107,107,107	1.34	15 (14%)
2	MAL	E	801	-	24,24,24	0.52	0	35,35,35	1.07	3 (8%)
3	CEY	E	802	-	72,72,72	2.17	30 (41%)	107,107,107	1.20	7 (6%)
2	MAL	F	801	-	24,24,24	0.47	0	35,35,35	0.70	1 (2%)
3	CEY	F	802	-	72,72,72	2.20	32 (44%)	107,107,107	1.31	15 (14%)

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
3	CEY	A	802	-	-	0/32/152/152	0/6/6/6
2	MAL	B	801	-	-	0/8/48/48	0/2/2/2
3	CEY	B	802	-	-	0/32/152/152	0/6/6/6
2	MAL	C	801	-	-	0/8/48/48	0/2/2/2
3	CEY	C	802	-	-	0/32/152/152	0/6/6/6
2	MAL	D	801	-	-	0/8/48/48	0/2/2/2
3	CEY	D	802	-	-	0/32/152/152	0/6/6/6
2	MAL	E	801	-	-	0/8/48/48	0/2/2/2
3	CEY	E	802	-	-	0/32/152/152	0/6/6/6
2	MAL	F	801	-	-	0/8/48/48	0/2/2/2
3	CEY	F	802	-	-	0/32/152/152	0/6/6/6

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	CEY	C6C-C5C	-3.65	1.39	1.51
3	A	802	CEY	C6C-C5C	-3.63	1.39	1.51
3	F	802	CEY	C6C-C5C	-3.62	1.39	1.51
3	C	802	CEY	C6C-C5C	-3.57	1.39	1.51
3	E	802	CEY	C6C-C5C	-3.54	1.39	1.51
3	D	802	CEY	C6C-C5C	-3.54	1.39	1.51
3	C	802	CEY	C6F-C5F	-3.39	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	802	CEY	C6E-C5E	-3.37	1.40	1.51
3	D	802	CEY	C6F-C5F	-3.37	1.40	1.51
3	F	802	CEY	C6F-C5F	-3.31	1.40	1.51
3	B	802	CEY	C6F-C5F	-3.30	1.40	1.51
3	A	802	CEY	C6E-C5E	-3.30	1.40	1.51
3	A	802	CEY	C6F-C5F	-3.29	1.40	1.51
3	C	802	CEY	C6E-C5E	-3.29	1.40	1.51
3	E	802	CEY	C6F-C5F	-3.25	1.40	1.51
3	D	802	CEY	C6E-C5E	-3.20	1.41	1.51
3	F	802	CEY	C3E-C2E	-3.16	1.44	1.52
3	F	802	CEY	C2A-C3A	-3.14	1.44	1.52
3	E	802	CEY	C2A-C3A	-3.14	1.44	1.52
3	B	802	CEY	C3D-C2D	-3.14	1.44	1.52
3	C	802	CEY	C2A-C3A	-3.13	1.44	1.52
3	D	802	CEY	C3D-C2D	-3.12	1.44	1.52
3	F	802	CEY	C6E-C5E	-3.10	1.41	1.51
3	A	802	CEY	C3E-C2E	-3.09	1.44	1.52
3	B	802	CEY	C6E-C5E	-3.02	1.41	1.51
3	A	802	CEY	C2A-C3A	-3.01	1.44	1.52
3	C	802	CEY	C3E-C2E	-3.00	1.44	1.52
3	B	802	CEY	C2A-C3A	-2.98	1.44	1.52
3	D	802	CEY	C3E-C2E	-2.98	1.44	1.52
3	C	802	CEY	C3D-C2D	-2.94	1.44	1.52
3	D	802	CEY	C2A-C3A	-2.88	1.45	1.52
3	A	802	CEY	C3D-C2D	-2.88	1.45	1.52
3	F	802	CEY	C3D-C2D	-2.88	1.45	1.52
3	B	802	CEY	C3E-C2E	-2.78	1.45	1.52
3	F	802	CEY	C3C-C2C	-2.74	1.45	1.52
3	E	802	CEY	C3D-C2D	-2.74	1.45	1.52
3	E	802	CEY	C3E-C2E	-2.67	1.45	1.52
3	D	802	CEY	C3C-C2C	-2.65	1.45	1.52
3	C	802	CEY	C3C-C2C	-2.59	1.45	1.52
3	E	802	CEY	C3C-C2C	-2.56	1.45	1.52
3	A	802	CEY	C3C-C2C	-2.54	1.45	1.52
3	F	802	CEY	C6B-C5B	-2.44	1.43	1.51
3	B	802	CEY	C3C-C2C	-2.41	1.46	1.52
3	D	802	CEY	C6B-C5B	-2.36	1.43	1.51
3	A	802	CEY	C6B-C5B	-2.34	1.43	1.51
3	E	802	CEY	C6B-C5B	-2.33	1.43	1.51
3	B	802	CEY	C6B-C5B	-2.33	1.43	1.51
3	C	802	CEY	C6B-C5B	-2.29	1.44	1.51
3	E	802	CEY	C6A-C5A	-2.27	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	CEY	C6A-C5A	-2.26	1.44	1.51
3	F	802	CEY	C6A-C5A	-2.26	1.44	1.51
3	A	802	CEY	C3B-C2B	-2.26	1.46	1.52
3	A	802	CEY	C6A-C5A	-2.22	1.44	1.51
3	E	802	CEY	C3B-C2B	-2.21	1.46	1.52
3	F	802	CEY	C3B-C2B	-2.19	1.46	1.52
3	E	802	CEY	C6D-C5D	-2.19	1.44	1.51
3	C	802	CEY	C6A-C5A	-2.17	1.44	1.51
3	D	802	CEY	C6A-C5A	-2.14	1.44	1.51
3	C	802	CEY	C6D-C5D	-2.13	1.44	1.51
3	C	802	CEY	C3B-C2B	-2.12	1.47	1.52
3	B	802	CEY	C3B-C2B	-2.12	1.47	1.52
3	A	802	CEY	C6D-C5D	-2.11	1.44	1.51
3	F	802	CEY	C3E-C4E	-2.11	1.46	1.52
3	D	802	CEY	C3E-C4E	-2.10	1.46	1.52
3	D	802	CEY	C3B-C2B	-2.09	1.47	1.52
3	F	802	CEY	C6D-C5D	-2.07	1.44	1.51
3	B	802	CEY	C6D-C5D	-2.06	1.44	1.51
3	D	802	CEY	C6D-C5D	-2.03	1.45	1.51
3	A	802	CEY	C3E-C4E	-2.01	1.47	1.52
3	D	802	CEY	C1D-C2D	-2.00	1.46	1.52
3	B	802	CEY	O5D-C1D	2.02	1.46	1.41
3	B	802	CEY	O5F-C1F	2.03	1.46	1.41
3	A	802	CEY	O5E-C1E	2.05	1.46	1.41
3	E	802	CEY	O5C-C1C	2.06	1.46	1.41
3	D	802	CEY	O5E-C1E	2.06	1.46	1.41
3	D	802	CEY	O5D-C1D	2.09	1.47	1.41
3	B	802	CEY	O5A-C1A	2.19	1.47	1.43
3	C	802	CEY	O2A-C2A	2.19	1.48	1.43
3	F	802	CEY	O5C-C1C	2.19	1.47	1.41
3	F	802	CEY	O5E-C1E	2.20	1.47	1.41
3	F	802	CEY	O2A-C2A	2.21	1.48	1.43
3	D	802	CEY	O5C-C1C	2.22	1.47	1.41
3	A	802	CEY	O2F-C2F	2.22	1.48	1.43
3	A	802	CEY	O2A-C2A	2.25	1.48	1.43
3	F	802	CEY	O3B-C3B	2.26	1.48	1.43
3	F	802	CEY	O2F-C2F	2.27	1.48	1.43
3	A	802	CEY	O5A-C1A	2.28	1.47	1.43
3	D	802	CEY	O2A-C2A	2.28	1.48	1.43
3	E	802	CEY	O2A-C2A	2.29	1.48	1.43
3	E	802	CEY	O2F-C2F	2.32	1.48	1.43
3	C	802	CEY	O2F-C2F	2.32	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	CEY	O2A-C2A	2.33	1.48	1.43
3	F	802	CEY	O5A-C1A	2.34	1.47	1.43
3	E	802	CEY	O5A-C1A	2.34	1.47	1.43
3	D	802	CEY	O2F-C2F	2.35	1.48	1.43
3	B	802	CEY	O3B-C3B	2.35	1.48	1.43
3	C	802	CEY	O3B-C3B	2.37	1.48	1.43
3	A	802	CEY	O3B-C3B	2.38	1.48	1.43
3	C	802	CEY	O5A-C1A	2.38	1.47	1.43
3	D	802	CEY	O5A-C1A	2.39	1.47	1.43
3	E	802	CEY	O3B-C3B	2.42	1.48	1.43
3	E	802	CEY	O5B-C1B	2.43	1.47	1.41
3	D	802	CEY	O3B-C3B	2.44	1.48	1.43
3	C	802	CEY	O3C-C3C	2.45	1.48	1.43
3	F	802	CEY	O5B-C1B	2.46	1.47	1.41
3	B	802	CEY	O2F-C2F	2.46	1.48	1.43
3	D	802	CEY	O3C-C3C	2.46	1.48	1.43
3	B	802	CEY	O5E-C1E	2.52	1.48	1.41
3	F	802	CEY	O3C-C3C	2.52	1.48	1.43
3	D	802	CEY	O5B-C1B	2.53	1.48	1.41
3	B	802	CEY	O5B-C1B	2.54	1.48	1.41
3	E	802	CEY	O3D-C3D	2.54	1.48	1.43
3	E	802	CEY	O3C-C3C	2.54	1.48	1.43
3	C	802	CEY	O5B-C1B	2.55	1.48	1.41
3	C	802	CEY	O3D-C3D	2.55	1.48	1.43
3	B	802	CEY	O3D-C3D	2.57	1.48	1.43
3	A	802	CEY	O5B-C1B	2.59	1.48	1.41
3	B	802	CEY	O3C-C3C	2.59	1.48	1.43
3	A	802	CEY	O3D-C3D	2.61	1.49	1.43
3	A	802	CEY	O3C-C3C	2.61	1.49	1.43
3	F	802	CEY	O3D-C3D	2.62	1.49	1.43
3	D	802	CEY	O3D-C3D	2.66	1.49	1.43
3	B	802	CEY	O2D-C2D	2.80	1.49	1.43
3	D	802	CEY	O2D-C2D	2.86	1.49	1.43
3	C	802	CEY	O2E-C2E	2.89	1.49	1.43
3	F	802	CEY	O2E-C2E	2.91	1.49	1.43
3	D	802	CEY	O2E-C2E	2.91	1.49	1.43
3	E	802	CEY	O2E-C2E	2.93	1.49	1.43
3	E	802	CEY	O5E-C5E	2.94	1.51	1.44
3	A	802	CEY	O2E-C2E	2.95	1.49	1.43
3	C	802	CEY	O2D-C2D	3.01	1.49	1.43
3	C	802	CEY	O5E-C5E	3.04	1.51	1.44
3	E	802	CEY	O2D-C2D	3.05	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	802	CEY	O2D-C2D	3.06	1.50	1.43
3	E	802	CEY	O3A-C3A	3.08	1.50	1.43
3	A	802	CEY	O2D-C2D	3.10	1.50	1.43
3	F	802	CEY	O3A-C3A	3.11	1.50	1.43
3	B	802	CEY	O3A-C3A	3.11	1.50	1.43
3	B	802	CEY	O2E-C2E	3.16	1.50	1.43
3	B	802	CEY	O2B-C2B	3.17	1.50	1.43
3	C	802	CEY	O3A-C3A	3.18	1.50	1.43
3	D	802	CEY	O3E-C3E	3.21	1.50	1.43
3	A	802	CEY	O3A-C3A	3.21	1.50	1.43
3	C	802	CEY	O3E-C3E	3.23	1.50	1.43
3	F	802	CEY	O3E-C3E	3.26	1.50	1.43
3	E	802	CEY	O2B-C2B	3.27	1.50	1.43
3	A	802	CEY	O3E-C3E	3.30	1.50	1.43
3	B	802	CEY	O3E-C3E	3.32	1.50	1.43
3	D	802	CEY	O5E-C5E	3.32	1.52	1.44
3	E	802	CEY	O3E-C3E	3.33	1.50	1.43
3	F	802	CEY	O2B-C2B	3.34	1.50	1.43
3	A	802	CEY	O5E-C5E	3.36	1.52	1.44
3	C	802	CEY	O2B-C2B	3.37	1.50	1.43
3	D	802	CEY	O3A-C3A	3.38	1.50	1.43
3	A	802	CEY	O2B-C2B	3.41	1.50	1.43
3	D	802	CEY	O2B-C2B	3.46	1.50	1.43
3	B	802	CEY	O5E-C5E	3.48	1.52	1.44
3	F	802	CEY	O5E-C5E	3.50	1.52	1.44
3	A	802	CEY	O5B-C5B	3.61	1.53	1.44
3	C	802	CEY	O5B-C5B	3.66	1.53	1.44
3	F	802	CEY	O5B-C5B	3.67	1.53	1.44
3	E	802	CEY	O5B-C5B	3.71	1.53	1.44
3	D	802	CEY	O5B-C5B	3.75	1.53	1.44
3	B	802	CEY	O5B-C5B	3.77	1.53	1.44
3	B	802	CEY	O5A-C5A	3.80	1.53	1.44
3	A	802	CEY	O5A-C5A	3.80	1.53	1.44
3	D	802	CEY	O5A-C5A	3.86	1.53	1.44
3	F	802	CEY	O5A-C5A	3.86	1.53	1.44
3	C	802	CEY	O5A-C5A	3.87	1.53	1.44
3	A	802	CEY	O5D-C5D	3.87	1.53	1.44
3	F	802	CEY	O5D-C5D	3.91	1.53	1.44
3	C	802	CEY	O5D-C5D	3.91	1.53	1.44
3	E	802	CEY	O5A-C5A	3.93	1.53	1.44
3	E	802	CEY	O5D-C5D	3.94	1.53	1.44
3	B	802	CEY	O5D-C5D	4.06	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802	CEY	O5D-C5D	4.29	1.54	1.44
3	A	802	CEY	O5C-C5C	4.39	1.55	1.44
3	C	802	CEY	O5C-C5C	4.47	1.55	1.44
3	B	802	CEY	O5C-C5C	4.48	1.55	1.44
3	C	802	CEY	O5F-C5F	4.51	1.55	1.44
3	D	802	CEY	O5F-C5F	4.55	1.55	1.44
3	B	802	CEY	O5F-C5F	4.56	1.55	1.44
3	D	802	CEY	O5C-C5C	4.61	1.55	1.44
3	F	802	CEY	O5F-C5F	4.61	1.55	1.44
3	A	802	CEY	O5F-C5F	4.63	1.55	1.44
3	F	802	CEY	O5C-C5C	4.63	1.55	1.44
3	E	802	CEY	O5C-C5C	4.63	1.55	1.44
3	E	802	CEY	O5F-C5F	4.69	1.55	1.44

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	802	CEY	C1E-O4D-C4D	-3.98	108.29	118.00
3	F	802	CEY	C1D-O4C-C4C	-3.54	109.38	118.00
3	A	802	CEY	C1D-O4C-C4C	-3.38	109.76	118.00
3	B	802	CEY	O6B-C6B-C5B	-3.37	100.00	111.34
3	E	802	CEY	C1E-O4D-C4D	-3.22	110.15	118.00
3	D	802	CEY	C1E-O4D-C4D	-3.19	110.23	118.00
3	D	802	CEY	C1D-O4C-C4C	-3.12	110.40	118.00
3	C	802	CEY	C1D-O4C-C4C	-3.05	110.57	118.00
3	B	802	CEY	C1F-O4E-C4E	-2.75	111.29	118.00
3	E	802	CEY	C1D-O4C-C4C	-2.72	111.37	118.00
3	A	802	CEY	C1E-O4D-C4D	-2.70	111.42	118.00
3	A	802	CEY	C1F-O4E-C4E	-2.67	111.48	118.00
3	E	802	CEY	C1C-O4B-C4B	-2.61	111.64	118.00
3	C	802	CEY	C1F-O4E-C4E	-2.60	111.66	118.00
3	B	802	CEY	C1C-O4B-C4B	-2.58	111.71	118.00
3	F	802	CEY	C1E-O4D-C4D	-2.51	111.88	118.00
3	D	802	CEY	C1F-O4E-C4E	-2.51	111.89	118.00
3	B	802	CEY	O5B-C5B-C4B	-2.48	104.68	109.75
3	D	802	CEY	C1C-O4B-C4B	-2.36	112.24	118.00
3	C	802	CEY	C1C-O4B-C4B	-2.29	112.41	118.00
3	B	802	CEY	C1D-O4C-C4C	-2.28	112.44	118.00
3	B	802	CEY	O5F-C5F-C4F	-2.25	105.51	109.66
3	A	802	CEY	C1B-O4A-C4A	-2.22	112.59	118.00
3	A	802	CEY	C1C-O4B-C4B	-2.20	112.63	118.00
3	B	802	CEY	C1B-O5B-C5B	-2.13	109.70	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	802	CEY	C1B-O4A-C4A	-2.10	112.87	118.00
3	D	802	CEY	O4A-C1B-O5B	-2.10	105.61	110.70
3	A	802	CEY	O4D-C1E-O5E	-2.09	105.63	110.70
3	F	802	CEY	C1F-O4E-C4E	-2.07	112.95	118.00
3	F	802	CEY	C1C-O4B-C4B	-2.03	113.05	118.00
3	B	802	CEY	O4C-C1D-O5D	-2.02	105.78	110.70
2	A	801	MAL	C3'-C4'-C5'	-2.01	106.61	110.88
3	B	802	CEY	C2C-C3C-C4C	2.00	113.76	109.61
3	B	802	CEY	C2E-C3E-C4E	2.01	113.78	109.61
3	B	802	CEY	O5E-C1E-C2E	2.04	114.22	110.30
3	B	802	CEY	O5B-C5B-C6B	2.06	111.33	106.41
3	F	802	CEY	O5E-C5E-C6E	2.06	111.35	106.41
2	E	801	MAL	O5'-C1'-C2'	2.07	113.47	110.04
3	F	802	CEY	O5B-C5B-C6B	2.07	111.37	106.41
3	D	802	CEY	C2E-C3E-C4E	2.07	113.90	109.61
3	C	802	CEY	C2B-C3B-C4B	2.08	113.92	109.61
3	B	802	CEY	C1B-C2B-C3B	2.14	113.96	109.98
3	D	802	CEY	C1E-O5E-C5E	2.17	117.80	113.72
3	B	802	CEY	O5C-C1C-C2C	2.17	114.49	110.30
2	A	801	MAL	C1'-C2'-C3'	2.18	114.58	110.65
3	E	802	CEY	O5C-C1C-C2C	2.20	114.53	110.30
3	A	802	CEY	C1B-C2B-C3B	2.21	114.08	109.98
3	C	802	CEY	C2D-C3D-C4D	2.23	114.23	109.61
3	C	802	CEY	C2A-C3A-C4A	2.27	114.31	109.61
2	F	801	MAL	O5'-C5'-C6'	2.27	111.85	106.41
3	F	802	CEY	C2B-C3B-C4B	2.29	114.35	109.61
3	B	802	CEY	C2A-C3A-C4A	2.29	114.36	109.61
2	B	801	MAL	O1-C4'-C3'	2.29	112.71	107.19
2	E	801	MAL	O5'-C5'-C6'	2.31	111.93	106.41
3	B	802	CEY	O5F-C1F-C2F	2.31	114.75	110.30
3	F	802	CEY	C2E-C3E-C4E	2.35	114.49	109.61
2	B	801	MAL	C2'-C3'-C4'	2.37	114.52	109.61
3	D	802	CEY	O5B-C5B-C6B	2.44	112.26	106.41
3	D	802	CEY	C3E-C4E-C5E	2.46	116.10	110.88
3	E	802	CEY	C2D-C3D-C4D	2.47	114.72	109.61
3	B	802	CEY	O5E-C5E-C6E	2.50	112.40	106.41
3	A	802	CEY	O5E-C5E-C4E	2.53	114.94	109.75
2	A	801	MAL	C1'-O5'-C5'	2.54	117.97	113.39
3	D	802	CEY	O5D-C1D-C2D	2.56	115.23	110.30
2	D	801	MAL	O5'-C5'-C6'	2.57	112.56	106.41
3	F	802	CEY	C3E-C4E-C5E	2.60	116.40	110.88
3	A	802	CEY	C2B-C3B-C4B	2.61	115.02	109.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	MAL	C2'-C3'-C4'	2.63	115.06	109.61
3	D	802	CEY	C3D-C4D-C5D	2.64	116.48	110.88
3	B	802	CEY	C3E-C4E-C5E	2.66	116.51	110.88
2	A	801	MAL	O1-C4'-C3'	2.66	113.59	107.19
3	A	802	CEY	O5C-C1C-C2C	2.69	115.48	110.30
3	F	802	CEY	C1E-O5E-C5E	2.73	118.86	113.72
3	A	802	CEY	O5E-C1E-C2E	2.74	115.58	110.30
3	D	802	CEY	C1D-O5D-C5D	2.78	118.96	113.72
2	C	801	MAL	O1-C4'-C3'	2.81	113.97	107.19
3	F	802	CEY	O5C-C1C-C2C	2.85	115.79	110.30
3	C	802	CEY	C3E-C4E-C5E	2.86	116.95	110.88
3	A	802	CEY	C2A-C3A-C4A	2.91	115.64	109.61
3	A	802	CEY	C3E-C4E-C5E	2.92	117.06	110.88
3	A	802	CEY	C2D-C3D-C4D	3.01	115.84	109.61
3	B	802	CEY	C1E-O5E-C5E	3.02	119.41	113.72
3	F	802	CEY	C2D-C3D-C4D	3.03	115.89	109.61
3	E	802	CEY	C1E-C2E-C3E	3.04	115.63	109.98
3	D	802	CEY	O5E-C1E-C2E	3.16	116.40	110.30
3	A	802	CEY	C1E-O5E-C5E	3.21	119.77	113.72
3	F	802	CEY	C1C-O5C-C5C	3.27	119.88	113.72
3	F	802	CEY	O5E-C1E-C2E	3.27	116.61	110.30
3	C	802	CEY	C2E-C3E-C4E	3.42	116.69	109.61
3	D	802	CEY	O5C-C1C-C2C	3.72	117.47	110.30
3	D	802	CEY	C1C-O5C-C5C	3.72	120.73	113.72
2	E	801	MAL	C1'-O5'-C5'	3.74	120.14	113.39
3	E	802	CEY	C2E-C3E-C4E	3.82	117.53	109.61
2	D	801	MAL	C1'-O5'-C5'	3.89	120.41	113.39
2	A	801	MAL	O5'-C1'-C2'	5.25	118.75	110.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	CEY	3	0
3	B	802	CEY	3	0
2	C	801	MAL	2	0
3	C	802	CEY	3	0
2	D	801	MAL	4	0
3	D	802	CEY	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	801	MAL	2	0
3	E	802	CEY	4	0
2	F	801	MAL	1	0
3	F	802	CEY	5	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	660/723 (91%)	0.94	54 (8%) 12 10	86, 118, 165, 185	0
1	B	660/723 (91%)	0.92	54 (8%) 12 10	86, 117, 162, 185	0
1	C	660/723 (91%)	0.99	66 (10%) 8 7	88, 119, 167, 201	0
1	D	660/723 (91%)	0.90	54 (8%) 12 10	87, 117, 162, 192	0
1	E	660/723 (91%)	0.88	49 (7%) 15 12	85, 119, 165, 191	0
1	F	660/723 (91%)	0.90	41 (6%) 21 16	84, 117, 167, 190	0
All	All	3960/4338 (91%)	0.92	318 (8%) 13 11	84, 118, 165, 201	0

All (318) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	356	ALA	4.8
1	C	377	PRO	4.5
1	D	449	PHE	3.9
1	B	180	ALA	3.8
1	A	347	LEU	3.7
1	E	356	ALA	3.7
1	A	197	LEU	3.7
1	B	373	TYR	3.6
1	D	385	TYR	3.6
1	B	253	HIS	3.6
1	C	107	PHE	3.6
1	E	47	ALA	3.6
1	E	560	LEU	3.6
1	E	449	PHE	3.5
1	C	381	TYR	3.5
1	A	348	GLN	3.4
1	D	179	ALA	3.4
1	D	560	LEU	3.4
1	F	560	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	628	LEU	3.4
1	C	449	PHE	3.4
1	A	364	THR	3.3
1	B	377	PRO	3.3
1	C	16	GLY	3.3
1	F	502	PRO	3.3
1	E	50	ARG	3.3
1	A	385	TYR	3.2
1	F	373	TYR	3.2
1	A	314	HIS	3.2
1	A	573	ARG	3.2
1	B	356	ALA	3.1
1	C	425	PRO	3.1
1	C	156	VAL	3.1
1	C	674	ILE	3.1
1	D	551	GLU	3.1
1	F	288	LYS	3.1
1	F	381	TYR	3.0
1	A	377	PRO	3.0
1	F	194	ALA	3.0
1	A	425	PRO	3.0
1	F	193	THR	3.0
1	D	377	PRO	3.0
1	D	308	GLY	3.0
1	F	341	VAL	3.0
1	C	176	LEU	3.0
1	B	307	ILE	3.0
1	F	347	LEU	3.0
1	C	533	MET	2.9
1	B	381	TYR	2.9
1	B	301	VAL	2.9
1	E	20	ILE	2.9
1	E	372	ALA	2.9
1	A	308	GLY	2.9
1	C	364	THR	2.9
1	C	467	TYR	2.8
1	C	184	ARG	2.8
1	E	176	LEU	2.8
1	A	193	THR	2.8
1	A	69	TYR	2.8
1	F	364	THR	2.8
1	D	364	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	286	HIS	2.8
1	B	347	LEU	2.8
1	E	107	PHE	2.8
1	B	609	LEU	2.8
1	F	229	ALA	2.8
1	D	50	ARG	2.8
1	F	533	MET	2.7
1	E	123	VAL	2.7
1	C	550	GLU	2.7
1	B	385	TYR	2.7
1	D	237	MET	2.7
1	A	608	LEU	2.7
1	B	163	ARG	2.7
1	C	49	TRP	2.7
1	D	20	ILE	2.7
1	D	381	TYR	2.7
1	C	189	PRO	2.7
1	E	674	ILE	2.7
1	B	432	ILE	2.6
1	E	347	LEU	2.6
1	D	41	VAL	2.6
1	A	384	ILE	2.6
1	A	204	LEU	2.6
1	F	160	LEU	2.6
1	F	236	GLU	2.6
1	B	69	TYR	2.6
1	D	361	GLN	2.6
1	A	351	PRO	2.6
1	C	348	GLN	2.6
1	C	504	ILE	2.6
1	D	343	LEU	2.6
1	C	253	HIS	2.6
1	D	210	LEU	2.6
1	C	194	ALA	2.6
1	B	364	THR	2.6
1	C	210	LEU	2.6
1	F	397	TYR	2.6
1	D	48	VAL	2.6
1	A	496	ASN	2.6
1	F	448	ALA	2.6
1	C	628	LEU	2.6
1	C	105	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	363	PHE	2.5
1	A	16	GLY	2.5
1	B	505	LEU	2.5
1	B	210	LEU	2.5
1	C	471	THR	2.5
1	B	291	ASN	2.5
1	D	291	ASN	2.5
1	F	307	ILE	2.5
1	B	486	ILE	2.5
1	C	347	LEU	2.5
1	B	314	HIS	2.5
1	C	307	ILE	2.5
1	E	434	GLN	2.5
1	D	107	PHE	2.5
1	E	472	TRP	2.5
1	E	124	ASP	2.5
1	A	389	PHE	2.5
1	D	649	ASP	2.5
1	C	185	THR	2.5
1	C	308	GLY	2.5
1	E	210	LEU	2.5
1	A	557	LYS	2.5
1	D	106	VAL	2.4
1	B	492	TYR	2.4
1	D	421	HIS	2.4
1	A	461	LEU	2.4
1	D	467	TYR	2.4
1	D	697	LEU	2.4
1	A	199	PRO	2.4
1	E	346	ALA	2.4
1	B	380	LYS	2.4
1	D	176	LEU	2.4
1	D	458	LEU	2.4
1	A	541	GLU	2.4
1	C	421	HIS	2.4
1	C	153	ASP	2.4
1	C	608	LEU	2.4
1	D	499	VAL	2.4
1	A	633	PRO	2.4
1	C	505	LEU	2.4
1	C	288	LYS	2.4
1	E	46	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	302	GLY	2.4
1	A	387	LEU	2.4
1	C	211	ARG	2.4
1	C	237	MET	2.4
1	D	163	ARG	2.4
1	A	637	THR	2.4
1	A	609	LEU	2.3
1	C	48	VAL	2.3
1	F	449	PHE	2.3
1	E	364	THR	2.3
1	A	381	TYR	2.3
1	B	389	PHE	2.3
1	C	614	PHE	2.3
1	D	279	ILE	2.3
1	F	49	TRP	2.3
1	E	381	TYR	2.3
1	C	180	ALA	2.3
1	C	498	PHE	2.3
1	C	609	LEU	2.3
1	E	683	ILE	2.3
1	A	237	MET	2.3
1	D	346	ALA	2.3
1	A	674	ILE	2.3
1	D	628	LEU	2.3
1	B	474	THR	2.3
1	A	509	LEU	2.3
1	A	382	GLN	2.3
1	C	163	ARG	2.3
1	A	156	VAL	2.3
1	E	140	LYS	2.3
1	D	455	GLN	2.3
1	A	140	LYS	2.3
1	B	387	LEU	2.3
1	D	356	ALA	2.3
1	F	197	LEU	2.3
1	C	15	PRO	2.3
1	E	348	GLN	2.3
1	D	49	TRP	2.3
1	D	196	ALA	2.3
1	C	160	LEU	2.3
1	D	160	LEU	2.3
1	E	499	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	449	PHE	2.2
1	B	20	ILE	2.2
1	E	237	MET	2.2
1	D	476	LYS	2.2
1	C	62	VAL	2.2
1	E	162	GLU	2.2
1	C	595	LEU	2.2
1	B	495	PRO	2.2
1	A	456	TYR	2.2
1	B	560	LEU	2.2
1	F	609	LEU	2.2
1	F	592	PHE	2.2
1	A	638	LEU	2.2
1	E	380	LYS	2.2
1	B	378	PRO	2.2
1	D	62	VAL	2.2
1	D	674	ILE	2.2
1	D	373	TYR	2.2
1	F	348	GLN	2.2
1	B	477	TRP	2.2
1	A	23	VAL	2.2
1	B	321	LEU	2.2
1	F	683	ILE	2.2
1	D	448	ALA	2.2
1	B	234	TRP	2.2
1	A	498	PHE	2.2
1	D	39	GLY	2.2
1	F	356	ALA	2.2
1	A	640	LEU	2.2
1	A	111	PHE	2.2
1	A	288	LYS	2.2
1	C	41	VAL	2.2
1	F	69	TYR	2.2
1	B	696	THR	2.1
1	D	347	LEU	2.1
1	E	106	VAL	2.1
1	F	360	ARG	2.1
1	B	346	ALA	2.1
1	B	694	ARG	2.1
1	A	432	ILE	2.1
1	F	512	ASN	2.1
1	E	136	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	495	PRO	2.1
1	E	412	VAL	2.1
1	F	156	VAL	2.1
1	C	631	PHE	2.1
1	F	498	PHE	2.1
1	B	302	GLY	2.1
1	C	174	ASP	2.1
1	B	186	PRO	2.1
1	A	683	ILE	2.1
1	F	415	PHE	2.1
1	C	695	ASN	2.1
1	E	164	ALA	2.1
1	B	92	LYS	2.1
1	C	341	VAL	2.1
1	D	677	ALA	2.1
1	D	231	PHE	2.1
1	A	411	GLY	2.1
1	B	49	TRP	2.1
1	B	597	THR	2.1
1	D	360	ARG	2.1
1	E	341	VAL	2.1
1	B	348	GLN	2.1
1	E	156	VAL	2.1
1	E	382	GLN	2.1
1	F	638	LEU	2.1
1	A	35	LYS	2.1
1	A	49	TRP	2.1
1	C	680	VAL	2.1
1	E	490	ALA	2.1
1	C	557	LYS	2.1
1	B	442	VAL	2.1
1	C	123	VAL	2.1
1	F	389	PHE	2.1
1	E	153	ASP	2.1
1	B	360	ARG	2.1
1	C	378	PRO	2.1
1	A	229	ALA	2.1
1	B	46	ALA	2.1
1	E	614	PHE	2.1
1	F	372	ALA	2.1
1	B	552	TYR	2.1
1	C	634	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	350	ALA	2.1
1	C	630	ALA	2.1
1	E	69	TYR	2.1
1	C	159	VAL	2.1
1	C	314	HIS	2.1
1	A	349	CYS	2.1
1	E	119	TRP	2.1
1	E	583	ASN	2.1
1	A	222	VAL	2.1
1	C	560	LEU	2.1
1	D	232	GLY	2.1
1	E	634	GLU	2.1
1	B	436	LYS	2.0
1	C	65	LEU	2.0
1	D	665	GLN	2.0
1	E	158	ALA	2.0
1	D	211	ARG	2.0
1	E	608	LEU	2.0
1	F	210	LEU	2.0
1	D	380	LYS	2.0
1	B	384	ILE	2.0
1	E	314	HIS	2.0
1	A	575	LEU	2.0
1	E	92	LYS	2.0
1	B	50	ARG	2.0
1	E	384	ILE	2.0
1	B	60	LEU	2.0
1	B	102	GLN	2.0
1	A	189	PRO	2.0
1	D	533	MET	2.0
1	F	234	TRP	2.0
1	C	220	PHE	2.0
1	B	627	THR	2.0
1	C	217	GLY	2.0
1	D	167	GLY	2.0
1	A	598	ILE	2.0
1	B	211	ARG	2.0
1	C	234	TRP	2.0
1	C	373	TYR	2.0
1	F	377	PRO	2.0
1	D	311	GLU	2.0
1	E	184	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	448	ALA	2.0
1	E	349	CYS	2.0
1	E	627	THR	2.0
1	F	41	VAL	2.0
1	F	213	LEU	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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	MAL	E	801	23/23	0.80	0.38	-0.34	121,144,152,156	0
3	CEY	A	802	67/67	0.89	0.35	-0.41	105,125,132,139	0
2	MAL	A	801	23/23	0.75	0.35	-0.55	111,139,149,153	0
2	MAL	B	801	23/23	0.79	0.33	-0.57	117,144,154,155	0
2	MAL	D	801	23/23	0.77	0.34	-0.58	127,147,156,160	0
2	MAL	F	801	23/23	0.77	0.36	-0.62	122,139,148,156	0
3	CEY	D	802	67/67	0.88	0.33	-0.62	109,124,130,134	0
3	CEY	F	802	67/67	0.90	0.33	-0.65	108,121,132,148	0
2	MAL	C	801	23/23	0.76	0.35	-0.83	110,140,153,163	0
3	CEY	B	802	67/67	0.85	0.31	-0.86	106,128,160,171	0
3	CEY	C	802	67/67	0.89	0.32	-0.94	110,125,132,141	0
3	CEY	E	802	67/67	0.87	0.30	-0.96	110,127,134,137	0

6.5 Other polymers [i](#)

There are no such residues in this entry.