



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 09:33 PM UTC

PDB ID : 3TOP / pdb_00003top
Title : Crystall Structure of the C-terminal Subunit of Human Maltase-Glucoamylase
in Complex with Acarbose
Authors : Shen, Y.; Qin, X.H.; Ren, L.M.
Deposited on : 2011-09-06
Resolution : 2.88 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

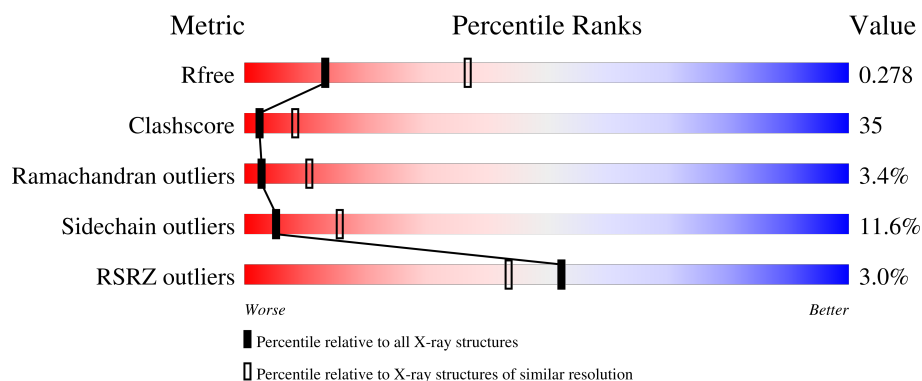
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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

Mol	Chain	Length	Quality of chain
1	A	908	3% 45% 43% 9% ..
1	B	908	3% 44% 44% 10% ..
2	C	3	100%
2	D	3	67% 33%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14388 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 Maltase-glucoamylase, intestinal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	890	Total	C	N	O	S	0	0	0
			7131	4572	1190	1338	31			
1	B	890	Total	C	N	O	S	0	0	0
			7131	4572	1190	1338	31			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	952	TRP	-	expression tag	UNP O43451
A	953	SER	-	expression tag	UNP O43451
A	954	HIS	-	expression tag	UNP O43451
A	955	PRO	-	expression tag	UNP O43451
A	956	GLN	-	expression tag	UNP O43451
A	957	PHE	-	expression tag	UNP O43451
A	958	GLU	-	expression tag	UNP O43451
A	959	LYS	-	expression tag	UNP O43451
A	1854	HIS	-	expression tag	UNP O43451
A	1855	HIS	-	expression tag	UNP O43451
A	1856	HIS	-	expression tag	UNP O43451
A	1857	HIS	-	expression tag	UNP O43451
A	1858	HIS	-	expression tag	UNP O43451
A	1859	HIS	-	expression tag	UNP O43451
B	952	TRP	-	expression tag	UNP O43451
B	953	SER	-	expression tag	UNP O43451
B	954	HIS	-	expression tag	UNP O43451
B	955	PRO	-	expression tag	UNP O43451
B	956	GLN	-	expression tag	UNP O43451
B	957	PHE	-	expression tag	UNP O43451
B	958	GLU	-	expression tag	UNP O43451
B	959	LYS	-	expression tag	UNP O43451
B	1854	HIS	-	expression tag	UNP O43451
B	1855	HIS	-	expression tag	UNP O43451
B	1856	HIS	-	expression tag	UNP O43451

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1857	HIS	-	expression tag	UNP O43451
B	1858	HIS	-	expression tag	UNP O43451
B	1859	HIS	-	expression tag	UNP O43451

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	D	3	Total	C	N	O	0	0	0
			44	25	1	18			

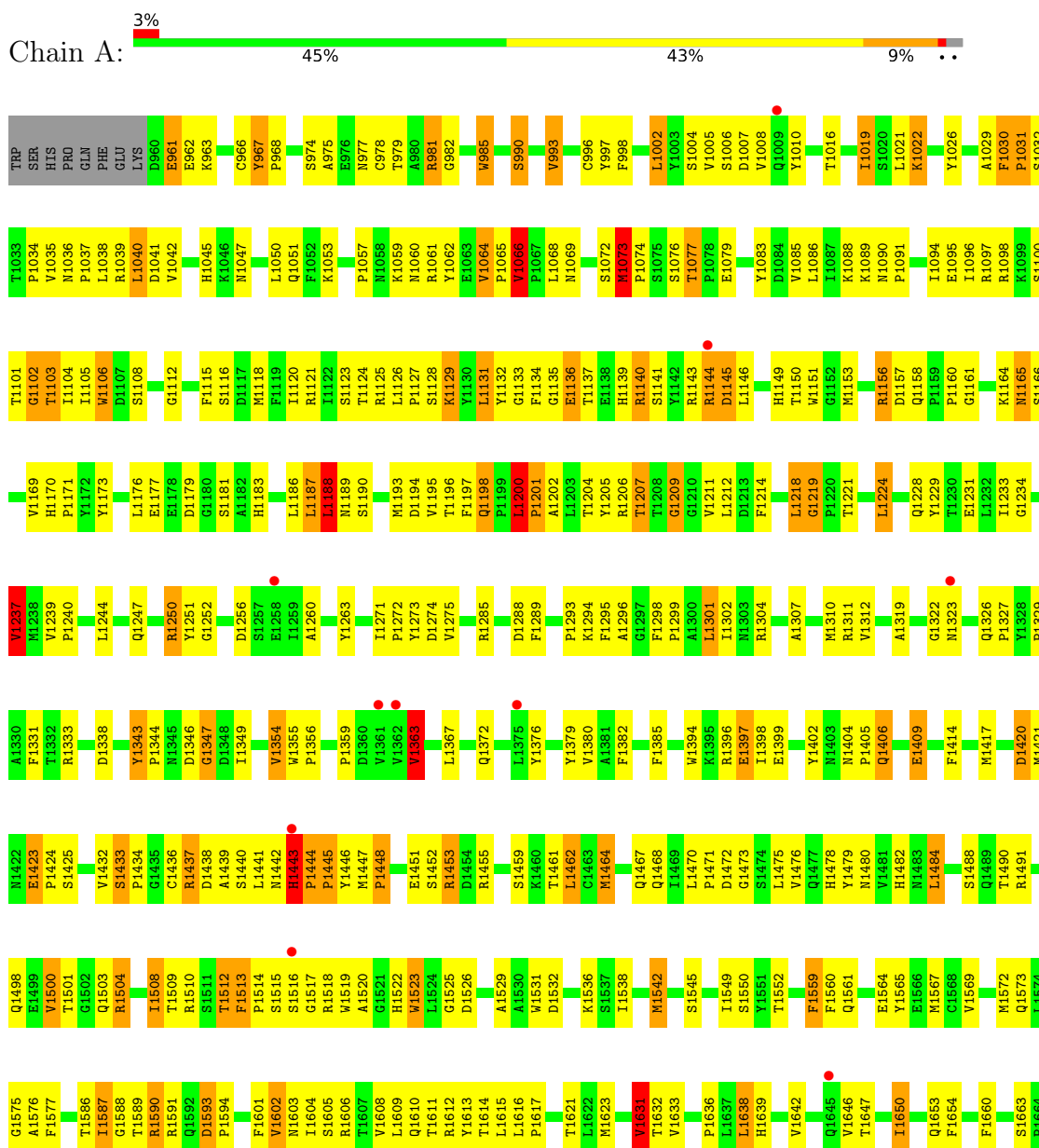
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	8	Total	O	0	0
			8	8		

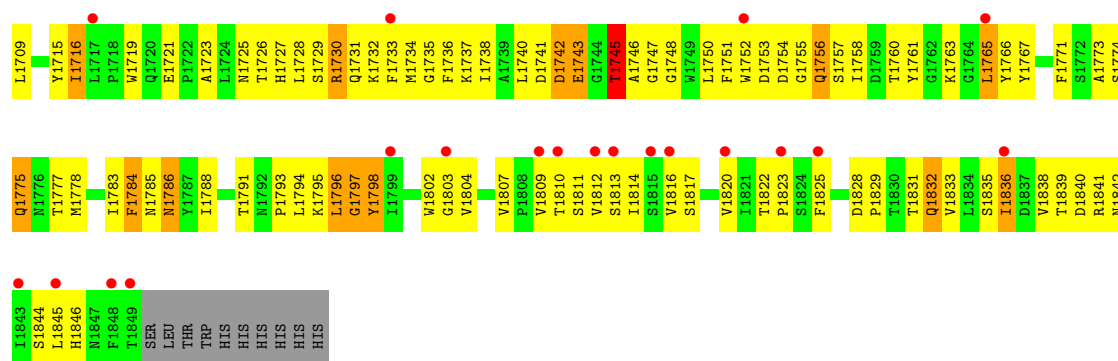
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Maltase-glucoamylase, intestinal





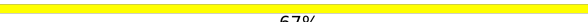


- Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:  100%

GLC1
GLC2
AC13

- Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:  67%  33%

GLC1
GLC2
AC13

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.50Å 105.50Å 516.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.45 – 2.88 36.45 – 2.88	Depositor EDS
% Data completeness (in resolution range)	82.3 (36.45-2.88) 87.8 (36.45-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.218 , 0.284 0.218 , 0.278	Depositor DCC
R_{free} test set	3014 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 79.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14388	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: AC1, GLC

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	0.56	2/7350 (0.0%)	0.96	30/10031 (0.3%)
1	B	0.54	0/7350	0.95	23/10031 (0.2%)
All	All	0.55	2/14700 (0.0%)	0.96	53/20062 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1144	ARG	CB-CG	5.58	1.69	1.52
1	A	1066	VAL	CA-CB	5.43	1.59	1.54

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1742	ASP	N-CA-C	-8.06	102.45	111.71
1	A	1742	ASP	N-CA-C	-7.49	103.25	112.38
1	B	1219	GLY	N-CA-C	-7.05	97.95	112.34
1	A	1663	SER	CA-C-N	7.04	126.96	119.85
1	A	1663	SER	C-N-CA	7.04	126.96	119.85
1	A	1219	GLY	N-CA-C	-6.65	98.77	112.34
1	A	1444	PRO	CA-C-N	6.61	128.10	119.84
1	A	1444	PRO	C-N-CA	6.61	128.10	119.84
1	B	1444	PRO	CA-C-N	6.57	128.05	119.84
1	B	1444	PRO	C-N-CA	6.57	128.05	119.84
1	B	1343	TYR	CA-C-N	6.52	126.10	119.19
1	B	1343	TYR	C-N-CA	6.52	126.10	119.19
1	A	1145	ASP	N-CA-C	6.35	118.00	111.14
1	B	1237	VAL	CB-CA-C	-6.29	102.59	111.28
1	B	1440	SER	N-CA-C	-6.29	105.47	113.02
1	A	1343	TYR	CA-C-N	6.26	125.83	119.19
1	A	1343	TYR	C-N-CA	6.26	125.83	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1237	VAL	CB-CA-C	-6.24	102.67	111.28
1	B	1593	ASP	CA-C-N	6.12	126.02	119.28
1	B	1593	ASP	C-N-CA	6.12	126.02	119.28
1	A	1593	ASP	CA-C-N	6.07	125.96	119.28
1	A	1593	ASP	C-N-CA	6.07	125.96	119.28
1	A	1513	PHE	CA-C-N	-6.05	113.46	119.93
1	A	1513	PHE	C-N-CA	-6.05	113.46	119.93
1	B	1521	GLY	N-CA-C	-5.92	104.64	112.81
1	A	1440	SER	N-CA-C	-5.84	105.92	113.16
1	B	1145	ASP	N-CA-C	5.79	117.40	111.14
1	B	1811	SER	N-CA-C	-5.74	106.32	113.38
1	B	1065	PRO	CA-C-O	-5.72	116.97	121.38
1	A	1030	PHE	CA-C-N	5.68	126.94	119.84
1	A	1030	PHE	C-N-CA	5.68	126.94	119.84
1	B	1663	SER	CA-C-N	5.59	125.50	119.85
1	B	1663	SER	C-N-CA	5.59	125.50	119.85
1	A	1811	SER	N-CA-C	-5.57	106.53	113.38
1	B	1443	HIS	CA-C-N	-5.51	114.71	120.38
1	B	1443	HIS	C-N-CA	-5.51	114.71	120.38
1	A	1198	GLN	CA-C-N	5.45	125.27	119.28
1	A	1198	GLN	C-N-CA	5.45	125.27	119.28
1	A	1363	VAL	N-CA-C	5.35	115.55	107.80
1	A	1065	PRO	CA-C-O	-5.26	117.33	121.38
1	A	1077	THR	CA-C-N	5.18	126.31	119.84
1	A	1077	THR	C-N-CA	5.18	126.31	119.84
1	B	1513	PHE	CA-C-N	-5.17	114.39	119.93
1	B	1513	PHE	C-N-CA	-5.17	114.39	119.93
1	A	1443	HIS	CA-C-N	-5.15	115.08	120.38
1	A	1443	HIS	C-N-CA	-5.15	115.08	120.38
1	B	1030	PHE	N-CA-C	5.08	117.93	109.09
1	A	1073	MET	CA-C-N	5.07	126.17	119.84
1	A	1073	MET	C-N-CA	5.07	126.17	119.84
1	A	1200	LEU	N-CA-C	-5.05	99.45	109.60
1	B	1635	ARG	CA-C-N	5.05	124.96	119.76
1	B	1635	ARG	C-N-CA	5.05	124.96	119.76
1	A	1523	TRP	N-CA-C	-5.00	101.72	109.72

There are no chirality outliers.

There are no planarity outliers.

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	7131	0	6766	486	0
1	B	7131	0	6766	485	0
2	C	44	0	30	8	0
2	D	44	0	30	1	0
3	A	30	0	0	1	0
3	B	8	0	0	2	0
All	All	14388	0	13592	971	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (971) 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:B:967:TYR:CE2	1:B:1030:PHE:HZ	1.72	1.08
1:B:1542:MET:HE1	1:B:1636:PRO:HB3	1.08	1.05
1:B:1734:MET:HE3	1:B:1794:LEU:HD21	1.37	1.05
1:A:1765:LEU:H	1:A:1765:LEU:HD23	1.16	1.05
1:A:1542:MET:HE1	1:A:1636:PRO:CB	1.87	1.05
1:B:981:ARG:NH1	1:B:1030:PHE:HB2	1.71	1.04
1:A:1734:MET:HE3	1:A:1794:LEU:HD21	1.38	1.04
1:B:1441:LEU:HD12	1:B:1464:MET:HB2	1.40	1.04
1:B:1765:LEU:HD23	1:B:1765:LEU:H	1.16	1.03
1:A:967:TYR:CE2	1:A:1030:PHE:HZ	1.78	1.00
1:A:981:ARG:NH1	1:A:1030:PHE:HB2	1.77	1.00
1:A:1542:MET:HE1	1:A:1636:PRO:HB3	1.03	0.99
1:A:1047:ASN:HD21	1:A:1077:THR:H	1.08	0.98
1:A:1681:ARG:HH11	1:A:1742:ASP:H	1.07	0.98
1:B:1542:MET:HE1	1:B:1636:PRO:CB	1.93	0.97
1:B:1047:ASN:HD21	1:B:1077:THR:H	1.12	0.96
1:A:1441:LEU:HD12	1:A:1464:MET:HB2	1.46	0.95
1:B:1681:ARG:HH11	1:B:1742:ASP:H	1.07	0.95
1:A:1538:ILE:O	1:A:1542:MET:HG3	1.68	0.92
1:B:1538:ILE:O	1:B:1542:MET:HG3	1.69	0.92
1:A:1030:PHE:CD2	1:A:1031:PRO:HD2	2.05	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1030:PHE:CD2	1:B:1031:PRO:HD2	2.06	0.91
1:A:1355:TRP:HE1	1:A:1421:MET:HE3	1.37	0.89
1:B:1030:PHE:HD2	1:B:1031:PRO:HD2	1.36	0.89
1:A:1050:LEU:HD21	1:A:1083:TYR:CE1	2.07	0.88
1:B:1441:LEU:CD1	1:B:1464:MET:H	1.87	0.88
1:A:1030:PHE:HD2	1:A:1031:PRO:HD2	1.37	0.88
1:A:1542:MET:CE	1:A:1636:PRO:HB3	1.99	0.87
1:A:1441:LEU:CD1	1:A:1464:MET:H	1.86	0.87
1:A:1784:PHE:HE2	1:A:1786:ASN:HB2	1.41	0.86
1:A:1035:VAL:HG23	1:A:1038:LEU:HD21	1.57	0.86
1:A:1636:PRO:HG2	1:A:1639:HIS:CD2	2.10	0.86
1:A:1156:ARG:HH11	1:A:1158:GLN:HG2	1.40	0.86
1:B:967:TYR:CE2	1:B:1030:PHE:CZ	2.62	0.86
1:B:1035:VAL:HG23	1:B:1038:LEU:HD21	1.57	0.85
1:B:1120:ILE:HG21	1:B:1212:LEU:HD21	1.58	0.85
1:A:1021:LEU:HB2	1:A:1036:ASN:HD21	1.40	0.85
1:B:1816:VAL:HG22	1:B:1820:VAL:HG22	1.58	0.85
1:A:961:GLU:HB3	1:A:1200:LEU:HB3	1.59	0.85
1:B:1256:ASP:HB2	1:B:1295:PHE:HA	1.58	0.85
1:B:1823:PRO:HB3	1:B:1841:ARG:HH21	1.41	0.85
1:B:1021:LEU:HB2	1:B:1036:ASN:HD21	1.39	0.85
1:B:1526:ASP:HB3	1:B:1560:PHE:CE2	2.12	0.85
1:A:1716:ILE:HG12	1:A:1748:GLY:HA3	1.59	0.85
1:A:1716:ILE:HG22	1:A:1738:ILE:HA	1.59	0.85
1:B:1587:ILE:HG23	1:B:1588:GLY:H	1.41	0.84
1:B:1636:PRO:HG2	1:B:1639:HIS:CD2	2.11	0.84
1:B:1716:ILE:HG12	1:B:1748:GLY:HA3	1.55	0.84
1:B:1156:ARG:HH11	1:B:1158:GLN:HG2	1.42	0.84
1:B:1355:TRP:HE1	1:B:1421:MET:HE3	1.41	0.84
1:A:1256:ASP:HB2	1:A:1295:PHE:HA	1.60	0.83
1:B:961:GLU:HB3	1:B:1200:LEU:HB3	1.61	0.83
1:B:1784:PHE:HE2	1:B:1786:ASN:HB2	1.43	0.83
1:B:1716:ILE:HG22	1:B:1738:ILE:HA	1.58	0.82
1:A:1526:ASP:HB3	1:A:1560:PHE:CE2	2.13	0.82
1:A:1681:ARG:HD3	1:A:1741:ASP:HA	1.59	0.82
1:B:1681:ARG:HD3	1:B:1741:ASP:HA	1.60	0.82
1:A:1587:ILE:HG23	1:A:1588:GLY:H	1.44	0.82
1:B:1468:GLN:NE2	1:B:1478:HIS:HD2	1.76	0.82
1:B:1542:MET:CE	1:B:1636:PRO:HB3	2.02	0.81
1:B:1726:THR:O	1:B:1730:ARG:HG2	1.81	0.81
1:A:1517:GLY:HA3	1:A:1549:ILE:HG12	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1816:VAL:HG22	1:A:1820:VAL:HG22	1.63	0.81
1:A:1343:TYR:HB3	1:A:1344:PRO:HD2	1.63	0.80
1:A:967:TYR:CE2	1:A:1030:PHE:CZ	2.67	0.80
1:A:1165:ASN:HD21	1:A:1451:GLU:H	1.29	0.80
1:A:1823:PRO:HB3	1:A:1841:ARG:HH21	1.46	0.80
1:B:1517:GLY:HA3	1:B:1549:ILE:HG12	1.64	0.80
1:B:1050:LEU:HD21	1:B:1083:TYR:CE1	2.18	0.79
1:A:1120:ILE:HG21	1:A:1212:LEU:HD21	1.62	0.79
1:A:1468:GLN:NE2	1:A:1478:HIS:HD2	1.79	0.79
1:B:1421:MET:HE1	2:D:3:AC1:HCB1	1.64	0.79
1:B:1098:ARG:NH1	1:B:1181:SER:HB3	1.97	0.78
1:B:1165:ASN:HD21	1:B:1451:GLU:H	1.31	0.78
1:A:1726:THR:O	1:A:1730:ARG:HG2	1.84	0.78
1:B:1617:PRO:O	1:B:1621:THR:HG23	1.84	0.78
1:A:981:ARG:HG3	1:A:981:ARG:HH11	1.47	0.77
1:A:1088:LYS:HE2	1:A:1095:GLU:HB2	1.64	0.77
1:B:1765:LEU:HD23	1:B:1765:LEU:N	1.99	0.77
1:A:1617:PRO:O	1:A:1621:THR:HG23	1.85	0.77
1:B:1219:GLY:H	1:B:1228:GLN:HE22	1.30	0.77
1:B:1468:GLN:HE21	1:B:1478:HIS:HD2	1.31	0.77
1:B:981:ARG:HH12	1:B:1030:PHE:HB2	1.49	0.76
1:A:1665:VAL:HG22	1:A:1673:VAL:HG11	1.67	0.75
1:A:1219:GLY:H	1:A:1228:GLN:HE22	1.30	0.75
1:A:1039:ARG:HB3	1:A:1057:PRO:HG3	1.66	0.75
1:B:1088:LYS:HE2	1:B:1095:GLU:HB2	1.67	0.75
1:A:1165:ASN:ND2	1:A:1451:GLU:H	1.84	0.75
1:B:1765:LEU:H	1:B:1765:LEU:CD2	1.97	0.75
1:A:1765:LEU:HD23	1:A:1765:LEU:N	1.99	0.75
1:B:1343:TYR:HB3	1:B:1344:PRO:HD2	1.66	0.75
1:A:1559:PHE:CE2	1:A:1586:THR:HB	2.22	0.74
1:A:1421:MET:HE1	2:C:3:AC1:HCB1	1.68	0.74
1:B:1039:ARG:HB3	1:B:1057:PRO:HG3	1.70	0.74
1:A:1653:GLN:HE22	1:A:1676:TYR:H	1.36	0.74
1:B:1723:ALA:HB1	1:B:1728:LEU:HB2	1.69	0.74
1:A:1665:VAL:HG22	1:A:1673:VAL:CG1	2.17	0.74
1:B:981:ARG:HH11	1:B:981:ARG:HG3	1.52	0.74
1:B:1165:ASN:ND2	1:B:1451:GLU:H	1.86	0.73
1:B:1665:VAL:HG22	1:B:1673:VAL:HG11	1.69	0.73
1:A:1468:GLN:HE21	1:A:1478:HIS:HD2	1.36	0.73
1:A:1004:SER:OG	1:A:1022:LYS:HG2	1.87	0.73
1:A:1030:PHE:CB	1:A:1031:PRO:HD2	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1606:ARG:O	1:B:1610:GLN:HG3	1.88	0.73
1:B:1653:GLN:HE22	1:B:1676:TYR:H	1.37	0.72
1:A:1030:PHE:HD2	1:A:1031:PRO:CD	2.01	0.72
1:A:1123:SER:OG	1:A:1204:THR:HG23	1.89	0.72
1:B:1665:VAL:HG22	1:B:1673:VAL:CG1	2.19	0.72
1:A:962:GLU:HG3	1:A:1200:LEU:HD22	1.70	0.72
1:B:1030:PHE:HD2	1:B:1031:PRO:CD	2.02	0.72
1:B:1423:GLU:N	1:B:1424:PRO:HA	2.05	0.72
1:A:1420:ASP:OD1	1:A:1421:MET:HE2	1.90	0.72
1:B:1559:PHE:CE2	1:B:1586:THR:HB	2.25	0.71
1:A:1120:ILE:HB	1:A:1207:THR:HG22	1.72	0.71
1:A:1503:GLN:HE22	1:A:1756:GLN:CD	1.97	0.71
1:B:1146:LEU:HA	1:B:1197:PHE:HB3	1.73	0.71
1:B:1399:GLU:HA	1:B:1500:VAL:HG21	1.71	0.71
1:B:1614:THR:HG23	1:B:1719:TRP:HE3	1.55	0.71
1:A:961:GLU:C	1:A:963:LYS:H	1.98	0.71
1:A:1723:ALA:HB1	1:A:1728:LEU:HB2	1.72	0.71
1:A:1399:GLU:HA	1:A:1500:VAL:HG21	1.73	0.71
1:A:1721:GLU:OE1	1:A:1733:PHE:HB2	1.90	0.71
1:A:1437:ARG:O	1:A:1437:ARG:HG2	1.90	0.71
1:A:1647:THR:HA	1:A:1650:ILE:HG22	1.73	0.71
1:B:1467:GLN:NE2	1:B:1475:LEU:HD13	2.06	0.71
1:B:1681:ARG:HH11	1:B:1742:ASP:N	1.85	0.70
1:B:1004:SER:OG	1:B:1022:LYS:HG2	1.91	0.70
1:B:1251:TYR:CD1	1:B:1587:ILE:HB	2.27	0.70
1:A:1251:TYR:CD1	1:A:1587:ILE:HB	2.27	0.70
1:A:1681:ARG:HH11	1:A:1742:ASP:N	1.85	0.70
1:B:1437:ARG:O	1:B:1437:ARG:HG2	1.92	0.70
1:B:1129:LYS:HD2	1:B:1201:PRO:HG3	1.74	0.70
1:B:1120:ILE:HB	1:B:1207:THR:HG22	1.72	0.70
1:A:1606:ARG:O	1:A:1610:GLN:HG3	1.91	0.70
1:B:1035:VAL:CG2	1:B:1038:LEU:HD21	2.21	0.70
1:B:1444:PRO:O	1:B:1446:TYR:N	2.25	0.70
1:B:1503:GLN:HE22	1:B:1756:GLN:CD	1.99	0.70
1:A:1098:ARG:NH1	1:A:1181:SER:HB3	2.07	0.69
1:B:1420:ASP:OD1	1:B:1421:MET:HE2	1.91	0.69
1:A:1614:THR:HG23	1:A:1719:TRP:HE3	1.57	0.69
1:B:961:GLU:C	1:B:963:LYS:H	2.00	0.69
1:B:1083:TYR:HD2	1:B:1218:LEU:HD11	1.58	0.69
1:A:1047:ASN:HD21	1:A:1077:THR:N	1.87	0.69
1:A:1804:VAL:HG22	1:A:1832:GLN:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1647:THR:HA	1:B:1650:ILE:HG22	1.72	0.69
1:A:1803:GLY:H	1:A:1832:GLN:HB2	1.56	0.69
1:B:1803:GLY:H	1:B:1832:GLN:HB2	1.59	0.68
1:A:981:ARG:HH12	1:A:1030:PHE:HB2	1.54	0.68
1:B:1804:VAL:HG22	1:B:1832:GLN:O	1.93	0.68
1:A:1771:PHE:HB3	1:A:1778:MET:HE2	1.76	0.68
1:A:1030:PHE:HB3	1:A:1031:PRO:HD2	1.75	0.68
1:A:1765:LEU:H	1:A:1765:LEU:CD2	1.97	0.68
1:A:1035:VAL:CG2	1:A:1038:LEU:HD21	2.22	0.68
1:B:962:GLU:HG3	1:B:1200:LEU:HD22	1.76	0.67
1:B:1021:LEU:HB2	1:B:1036:ASN:ND2	2.09	0.67
1:A:1237:VAL:HG22	1:A:1518:ARG:C	2.19	0.67
1:B:1237:VAL:HG22	1:B:1518:ARG:C	2.19	0.67
1:B:1030:PHE:CB	1:B:1031:PRO:HD2	2.24	0.67
1:A:1083:TYR:HD2	1:A:1218:LEU:HD11	1.59	0.67
1:B:1587:ILE:HG23	1:B:1588:GLY:N	2.10	0.67
1:A:1423:GLU:N	1:A:1424:PRO:HA	2.10	0.67
1:A:1587:ILE:HG23	1:A:1588:GLY:N	2.09	0.67
1:A:1129:LYS:HD2	1:A:1201:PRO:HG3	1.76	0.66
1:A:1807:VAL:HG23	1:A:1807:VAL:O	1.94	0.66
1:B:1251:TYR:O	1:B:1587:ILE:HA	1.94	0.66
1:B:1721:GLU:OE1	1:B:1733:PHE:HB2	1.95	0.66
1:A:1674:THR:HG22	1:A:1699:THR:OG1	1.95	0.66
1:B:1120:ILE:CG2	1:B:1212:LEU:HD21	2.25	0.66
1:B:1326:GLN:HB3	1:B:1327:PRO:HD2	1.77	0.66
1:A:1687:THR:OG1	1:A:1689:VAL:HG12	1.95	0.65
1:A:1139:HIS:CD2	1:A:1144:ARG:HD2	2.32	0.65
1:B:1733:PHE:CD1	1:B:1795:LYS:HB3	2.31	0.65
1:A:1131:LEU:HD22	1:A:1173:TYR:CD1	2.32	0.65
1:B:1139:HIS:CG	1:B:1144:ARG:HD2	2.31	0.65
1:A:1437:ARG:O	1:A:1438:ASP:HB2	1.96	0.65
1:B:1302:ILE:HD12	1:B:1312:VAL:HG21	1.77	0.65
1:B:1437:ARG:O	1:B:1438:ASP:HB2	1.95	0.65
1:A:1146:LEU:HA	1:A:1197:PHE:HB3	1.76	0.65
1:A:1421:MET:HE1	2:C:3:AC1:C7B	2.27	0.65
1:A:1139:HIS:CG	1:A:1144:ARG:HD2	2.32	0.65
1:A:1733:PHE:CD1	1:A:1795:LYS:HB3	2.31	0.65
1:B:1200:LEU:O	1:B:1200:LEU:HG	1.97	0.64
1:A:1135:GLY:HA3	1:A:1170:HIS:H	1.61	0.64
1:B:1047:ASN:HD21	1:B:1077:THR:N	1.89	0.64
1:B:1771:PHE:HB3	1:B:1778:MET:HE2	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:LEU:HB2	1:A:1036:ASN:ND2	2.11	0.64
1:B:1687:THR:OG1	1:B:1689:VAL:HG12	1.98	0.64
1:A:1467:GLN:NE2	1:A:1475:LEU:HD13	2.13	0.64
1:B:1719:TRP:NE1	1:B:1735:GLY:HA3	2.12	0.64
1:A:1745:THR:HB	1:A:1773:ALA:O	1.98	0.64
1:B:963:LYS:HE2	1:B:997:TYR:CE2	2.33	0.64
1:B:1734:MET:CE	1:B:1794:LEU:HD21	2.23	0.63
1:A:1120:ILE:CG2	1:A:1212:LEU:HD21	2.28	0.63
1:A:1251:TYR:O	1:A:1587:ILE:HA	1.97	0.63
1:B:1098:ARG:CG	1:B:1100:SER:HB3	2.28	0.63
1:B:1135:GLY:HA3	1:B:1170:HIS:H	1.64	0.63
1:B:1467:GLN:HE22	1:B:1475:LEU:HD13	1.63	0.63
1:A:1289:PHE:CZ	1:A:1397:GLU:HB3	2.34	0.63
1:B:1745:THR:HB	1:B:1773:ALA:O	1.97	0.63
1:A:1433:SER:HB3	1:A:1434:PRO:HD3	1.81	0.62
1:B:1433:SER:HB3	1:B:1434:PRO:HD3	1.80	0.62
1:A:1444:PRO:O	1:A:1446:TYR:N	2.31	0.62
1:A:1513:PHE:CD2	1:A:1514:PRO:HD2	2.34	0.62
1:B:1532:ASP:O	1:B:1536:LYS:HG2	1.99	0.62
1:B:1123:SER:OG	1:B:1204:THR:HG23	1.99	0.62
1:A:1200:LEU:HG	1:A:1200:LEU:O	1.99	0.62
1:A:1784:PHE:C	1:A:1784:PHE:CD2	2.77	0.62
1:B:1550:SER:HB2	1:B:1633:VAL:HG21	1.82	0.62
1:A:1730:ARG:HH12	1:A:1755:GLY:HA3	1.65	0.62
1:B:1030:PHE:HB3	1:B:1031:PRO:HD2	1.82	0.62
1:B:1726:THR:O	1:B:1730:ARG:CG	2.48	0.62
2:C:1:GLC:H62	2:C:2:GLC:O2	2.00	0.62
1:A:981:ARG:NH1	1:A:981:ARG:HG3	2.15	0.61
1:A:1804:VAL:H	1:A:1832:GLN:HB3	1.63	0.61
1:B:1047:ASN:ND2	1:B:1077:THR:H	1.91	0.61
1:B:1531:TRP:CH2	1:B:1567:MET:HA	2.35	0.61
1:A:1513:PHE:H	1:A:1516:SER:HB2	1.65	0.61
1:A:1135:GLY:HA2	1:A:1170:HIS:HB2	1.81	0.61
1:B:1298:PHE:N	1:B:1299:PRO:CD	2.63	0.61
1:A:963:LYS:HE2	1:A:997:TYR:CE2	2.35	0.61
1:B:1118:MET:HE2	3:B:34:HOH:O	1.99	0.61
1:A:961:GLU:HG2	1:A:1200:LEU:N	2.15	0.61
1:A:1421:MET:HE1	2:C:3:AC1:C1B	2.31	0.61
1:A:1326:GLN:HB3	1:A:1327:PRO:HD2	1.81	0.61
1:B:1135:GLY:HA2	1:B:1170:HIS:HB2	1.82	0.61
1:B:1614:THR:HG23	1:B:1719:TRP:CE3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1694:ARG:H	1:B:1696:GLU:HG3	1.66	0.61
1:A:1298:PHE:N	1:A:1299:PRO:CD	2.64	0.61
1:A:1726:THR:O	1:A:1730:ARG:CG	2.49	0.61
1:A:966:CYS:SG	1:A:981:ARG:HD3	2.41	0.60
1:A:1022:LYS:HD2	1:A:1022:LYS:O	2.01	0.60
1:B:966:CYS:SG	1:B:981:ARG:HD3	2.41	0.60
1:B:1139:HIS:CD2	1:B:1144:ARG:HD2	2.37	0.60
1:B:1804:VAL:H	1:B:1832:GLN:HB3	1.65	0.60
1:A:1083:TYR:CD2	1:A:1218:LEU:HD11	2.37	0.60
1:A:1784:PHE:C	1:A:1784:PHE:HD2	2.09	0.60
1:A:1105:ILE:HG23	1:A:1183:HIS:CD2	2.36	0.60
1:A:1631:VAL:HG13	1:A:1632:THR:N	2.16	0.60
1:B:1784:PHE:C	1:B:1784:PHE:HD2	2.10	0.60
1:A:1461:THR:OG1	1:A:1462:LEU:N	2.33	0.60
1:B:1285:ARG:NH2	1:B:1359:PRO:HA	2.17	0.60
1:B:1611:THR:O	1:B:1614:THR:HB	2.02	0.60
1:B:1740:LEU:HA	1:B:1745:THR:O	2.02	0.60
2:C:1:GLC:O3	2:C:2:GLC:H5	2.02	0.60
1:B:1040:LEU:HD12	1:B:1041:ASP:N	2.17	0.60
1:A:1512:THR:HG22	1:A:1516:SER:HB3	1.84	0.60
1:A:1550:SER:HB2	1:A:1633:VAL:HG21	1.84	0.60
1:A:1719:TRP:NE1	1:A:1735:GLY:HA3	2.16	0.60
1:B:1382:PHE:CD2	1:B:1462:LEU:HD21	2.37	0.60
1:A:1694:ARG:H	1:A:1696:GLU:HG3	1.67	0.59
1:B:1674:THR:HG22	1:B:1699:THR:OG1	2.00	0.59
1:B:1838:VAL:HG12	1:B:1838:VAL:O	2.00	0.59
1:B:1135:GLY:CA	1:B:1170:HIS:H	2.15	0.59
1:A:1813:SER:HG	1:A:1825:PHE:HE2	1.50	0.59
1:B:966:CYS:HB3	1:B:996:CYS:SG	2.42	0.59
1:B:1513:PHE:CD2	1:B:1514:PRO:HD2	2.37	0.59
1:B:1064:VAL:HG13	1:B:1066:VAL:HG13	1.84	0.59
1:B:1784:PHE:C	1:B:1784:PHE:CD2	2.78	0.59
1:A:1136:GLU:OE1	1:A:1522:HIS:HE1	1.85	0.59
1:A:1803:GLY:HA2	1:A:1832:GLN:HG3	1.84	0.59
1:B:961:GLU:HG2	1:B:1200:LEU:N	2.18	0.59
1:B:1101:THR:O	1:B:1103:THR:N	2.36	0.59
1:A:1740:LEU:HA	1:A:1745:THR:O	2.02	0.59
1:B:1807:VAL:HG23	1:B:1807:VAL:O	2.01	0.59
1:A:1098:ARG:CG	1:A:1100:SER:HB3	2.32	0.59
1:B:1396:ARG:O	1:B:1399:GLU:HB3	2.03	0.59
1:B:1120:ILE:HG21	1:B:1212:LEU:CD2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1136:GLU:OE1	1:B:1522:HIS:HE1	1.85	0.59
1:B:1512:THR:HG22	1:B:1516:SER:HB3	1.85	0.59
1:B:1289:PHE:CZ	1:B:1397:GLU:HB3	2.38	0.59
1:A:1207:THR:HG23	1:A:1209:GLY:H	1.68	0.58
1:B:1823:PRO:HB3	1:B:1841:ARG:NH2	2.15	0.58
1:A:1302:ILE:HD12	1:A:1312:VAL:HG21	1.84	0.58
1:A:1040:LEU:HD12	1:A:1041:ASP:N	2.17	0.58
1:A:1135:GLY:CA	1:A:1170:HIS:H	2.15	0.58
1:B:1686:TYR:CE2	1:B:1706:HIS:HE1	2.22	0.58
1:A:1614:THR:HG23	1:A:1719:TRP:CE3	2.37	0.58
1:B:1186:LEU:HD12	1:B:1187:LEU:N	2.18	0.58
1:B:1576:ALA:O	1:B:1612:ARG:HD2	2.03	0.58
1:B:1621:THR:HG22	1:B:1751:PHE:H	1.67	0.58
1:B:1745:THR:HG21	1:B:1774:SER:O	2.04	0.58
1:A:1382:PHE:CD2	1:A:1462:LEU:HD21	2.37	0.58
1:B:1083:TYR:CD2	1:B:1218:LEU:HD11	2.36	0.58
2:C:1:GLC:H4	2:C:2:GLC:O2	2.03	0.58
1:A:1621:THR:HG22	1:A:1751:PHE:H	1.67	0.58
1:A:1838:VAL:HG12	1:A:1838:VAL:O	2.03	0.58
1:B:1040:LEU:HD11	1:B:1042:VAL:HG23	1.86	0.58
1:B:1472:ASP:OD1	1:B:1473:GLY:N	2.37	0.58
1:A:1260:ALA:HB2	1:A:1301:LEU:HD11	1.86	0.58
1:B:1104:ILE:O	1:B:1127:PRO:HB3	2.03	0.58
1:B:1615:LEU:HD11	1:B:1660:PHE:CZ	2.39	0.58
1:A:1798:TYR:N	1:A:1798:TYR:CD2	2.71	0.58
1:B:968:PRO:HB3	1:B:1206:ARG:NH1	2.19	0.58
1:A:966:CYS:HB3	1:A:996:CYS:SG	2.44	0.58
1:B:1461:THR:OG1	1:B:1462:LEU:N	2.33	0.58
1:A:1101:THR:O	1:A:1103:THR:N	2.36	0.57
1:B:1470:LEU:HD21	1:B:1476:VAL:HG21	1.86	0.57
1:A:1237:VAL:HG21	1:A:1519:TRP:C	2.29	0.57
1:A:1823:PRO:HB3	1:A:1841:ARG:NH2	2.18	0.57
1:B:1156:ARG:HD3	1:B:1158:GLN:CG	2.34	0.57
1:B:1784:PHE:CE2	1:B:1786:ASN:HB2	2.33	0.57
1:B:1803:GLY:HA2	1:B:1832:GLN:HG3	1.86	0.57
1:B:1813:SER:HG	1:B:1825:PHE:HE2	1.52	0.57
1:B:1367:LEU:HD12	1:B:1376:TYR:OH	2.05	0.57
1:A:1047:ASN:ND2	1:A:1077:THR:H	1.90	0.57
1:B:1098:ARG:HG2	1:B:1100:SER:HB3	1.85	0.57
1:A:1715:TYR:HA	1:A:1747:GLY:O	2.04	0.57
1:B:961:GLU:OE1	1:B:961:GLU:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1022:LYS:HD2	1:B:1022:LYS:O	2.05	0.57
1:B:1716:ILE:CG1	1:B:1748:GLY:HA3	2.30	0.57
1:A:1784:PHE:CE2	1:A:1786:ASN:HB2	2.31	0.57
1:A:1156:ARG:HD3	1:A:1158:GLN:CG	2.35	0.57
1:A:1298:PHE:CZ	1:A:1302:ILE:HD11	2.40	0.57
1:A:1576:ALA:O	1:A:1612:ARG:HD2	2.05	0.57
1:A:1098:ARG:HG2	1:A:1100:SER:HB3	1.86	0.56
1:B:1623:MET:HE2	1:B:1633:VAL:HG11	1.86	0.56
1:A:1532:ASP:O	1:A:1536:LYS:HG2	2.03	0.56
1:B:1131:LEU:HD22	1:B:1173:TYR:CD1	2.40	0.56
1:B:1715:TYR:HA	1:B:1747:GLY:O	2.04	0.56
1:A:1441:LEU:HD13	1:A:1464:MET:H	1.70	0.56
1:A:1531:TRP:CH2	1:A:1567:MET:HA	2.39	0.56
1:B:1237:VAL:HG21	1:B:1519:TRP:C	2.30	0.56
1:A:1086:LEU:HD22	1:B:1097:ARG:CZ	2.36	0.56
1:A:1200:LEU:O	1:A:1201:PRO:C	2.49	0.56
1:A:1745:THR:HG21	1:A:1774:SER:O	2.05	0.56
1:B:1035:VAL:CG2	1:B:1115:PHE:CD2	2.89	0.56
1:B:1750:LEU:HD21	1:B:1752:TRP:HD1	1.71	0.56
1:A:968:PRO:HB3	1:A:1206:ARG:NH1	2.21	0.56
1:B:1432:VAL:HG13	1:B:1433:SER:N	2.19	0.56
1:A:967:TYR:CD2	1:A:1030:PHE:HZ	2.22	0.56
1:A:1040:LEU:HD11	1:A:1042:VAL:HG23	1.88	0.56
1:B:981:ARG:NH1	1:B:981:ARG:HG3	2.20	0.56
1:B:1794:LEU:HD22	1:B:1845:LEU:HD23	1.88	0.56
1:A:1219:GLY:N	1:A:1228:GLN:HE22	2.02	0.56
1:A:1250:ARG:NH2	1:A:1589:THR:HG23	2.21	0.56
1:A:1420:ASP:CG	1:A:1421:MET:N	2.64	0.56
1:A:1022:LYS:O	1:A:1022:LYS:CD	2.54	0.56
1:A:1464:MET:HG3	1:A:1479:TYR:HA	1.88	0.56
1:A:1686:TYR:CE2	1:A:1706:HIS:HE1	2.23	0.56
1:A:961:GLU:HB3	1:A:1200:LEU:CB	2.34	0.55
1:B:1513:PHE:H	1:B:1516:SER:HB2	1.70	0.55
1:B:1399:GLU:HA	1:B:1500:VAL:CG2	2.34	0.55
1:B:1420:ASP:CG	1:B:1421:MET:N	2.63	0.55
1:A:1064:VAL:HG13	1:A:1066:VAL:HG13	1.87	0.55
1:B:1200:LEU:O	1:B:1201:PRO:C	2.49	0.55
1:B:1385:PHE:HB2	1:B:1488:SER:OG	2.05	0.55
1:B:1522:HIS:O	1:B:1552:THR:HA	2.06	0.55
1:B:1741:ASP:C	1:B:1743:GLU:N	2.61	0.55
1:A:1059:LYS:HD3	1:A:1060:ASN:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1601:PHE:O	1:A:1602:VAL:C	2.50	0.55
1:A:1590:ARG:HD3	1:A:1591:ARG:O	2.07	0.55
1:B:1333:ARG:NH2	1:B:1396:ARG:HD3	2.21	0.55
1:A:1399:GLU:HA	1:A:1500:VAL:CG2	2.36	0.55
1:B:1406:GLN:HE21	1:B:1406:GLN:HA	1.72	0.55
1:A:1734:MET:CE	1:A:1794:LEU:HD21	2.25	0.55
1:B:961:GLU:HB3	1:B:1200:LEU:CB	2.34	0.55
1:A:981:ARG:HG2	1:A:982:GLY:H	1.72	0.55
1:A:1165:ASN:H	1:A:1165:ASN:HD22	1.54	0.55
1:A:1467:GLN:HE22	1:A:1475:LEU:HD13	1.71	0.55
1:A:1526:ASP:HB3	1:A:1560:PHE:HE2	1.71	0.55
1:B:1590:ARG:HD3	1:B:1591:ARG:O	2.07	0.55
1:A:1794:LEU:HD22	1:A:1845:LEU:HD23	1.89	0.55
1:B:1237:VAL:HG21	1:B:1520:ALA:N	2.22	0.55
1:A:1237:VAL:HG21	1:A:1520:ALA:N	2.22	0.55
1:A:1716:ILE:CG2	1:A:1738:ILE:HG23	2.37	0.55
1:B:1707:ILE:HD13	1:B:1709:LEU:HD21	1.87	0.55
1:A:1333:ARG:NH2	1:A:1396:ARG:HD3	2.22	0.54
1:A:1406:GLN:HE21	1:A:1406:GLN:HA	1.71	0.54
1:B:1542:MET:CE	1:B:1636:PRO:CB	2.76	0.54
2:C:1:GLC:O3	2:C:2:GLC:C5	2.55	0.54
1:A:1621:THR:HG21	1:A:1750:LEU:HA	1.89	0.54
1:B:1775:GLN:C	1:B:1777:THR:H	2.15	0.54
1:A:961:GLU:O	1:A:963:LYS:N	2.40	0.54
1:A:1707:ILE:HG12	1:A:1708:ASN:N	2.22	0.54
1:B:1153:MET:HE3	1:B:1193:MET:CG	2.37	0.54
1:B:1621:THR:HG21	1:B:1750:LEU:HA	1.89	0.54
1:B:1730:ARG:HH12	1:B:1755:GLY:HA3	1.73	0.54
1:A:1045:HIS:CE1	1:A:1051:GLN:HG2	2.43	0.54
1:A:1145:ASP:O	1:A:1146:LEU:HB2	2.08	0.54
1:A:1611:THR:O	1:A:1614:THR:HB	2.08	0.54
1:B:961:GLU:O	1:B:963:LYS:N	2.40	0.54
1:A:1030:PHE:CG	1:A:1031:PRO:HD2	2.42	0.54
1:B:1681:ARG:NH1	1:B:1742:ASP:HB2	2.23	0.54
1:A:1441:LEU:HD12	1:A:1464:MET:H	1.71	0.54
1:A:1467:GLN:NE2	1:A:1475:LEU:HB3	2.23	0.54
1:A:1623:MET:HE2	1:A:1633:VAL:HG11	1.89	0.54
1:B:1036:ASN:OD1	1:B:1037:PRO:HA	2.07	0.54
1:B:1647:THR:HA	1:B:1650:ILE:CG2	2.38	0.54
1:A:1153:MET:HE3	1:A:1193:MET:CG	2.38	0.54
1:B:1273:TYR:HA	1:B:1613:TYR:OH	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1423:GLU:OE2	1:B:1510:ARG:NH2	2.38	0.54
1:A:981:ARG:HB2	1:A:1030:PHE:CE1	2.44	0.53
1:B:1250:ARG:NH2	1:B:1589:THR:HG23	2.23	0.53
1:B:1529:ALA:C	1:B:1567:MET:HE1	2.33	0.53
1:B:1560:PHE:O	1:B:1561:GLN:HB2	2.08	0.53
1:A:961:GLU:HG2	1:A:1200:LEU:H	1.74	0.53
1:A:1120:ILE:HG21	1:A:1212:LEU:CD2	2.36	0.53
1:A:1319:ALA:HB1	1:A:1380:VAL:CG2	2.38	0.53
1:B:1526:ASP:HB3	1:B:1560:PHE:HE2	1.69	0.53
1:B:1141:SER:HB3	3:B:31:HOH:O	2.09	0.53
1:A:1396:ARG:O	1:A:1399:GLU:HB3	2.08	0.53
1:B:961:GLU:C	1:B:963:LYS:N	2.66	0.53
1:A:1432:VAL:HG13	1:A:1433:SER:N	2.24	0.53
1:A:1750:LEU:HD21	1:A:1752:TRP:HD1	1.73	0.53
1:B:1187:LEU:HD12	1:B:1205:TYR:CD2	2.43	0.53
1:A:1560:PHE:O	1:A:1561:GLN:HB2	2.07	0.53
1:B:1022:LYS:O	1:B:1022:LYS:CD	2.57	0.53
1:B:1260:ALA:HB2	1:B:1301:LEU:HD11	1.90	0.53
1:A:1775:GLN:C	1:A:1777:THR:H	2.17	0.53
1:A:961:GLU:N	1:A:961:GLU:OE1	2.39	0.53
1:B:1263:TYR:CE1	1:B:1310:MET:HG3	2.44	0.53
1:A:1470:LEU:HD21	1:A:1476:VAL:HG21	1.91	0.53
1:B:1646:VAL:HG11	1:B:1676:TYR:CE1	2.43	0.53
1:A:1529:ALA:C	1:A:1567:MET:HE1	2.34	0.53
1:B:1716:ILE:CG2	1:B:1738:ILE:HG23	2.39	0.53
1:B:1814:ILE:CB	1:B:1822:THR:HG22	2.39	0.53
1:A:1035:VAL:CG2	1:A:1115:PHE:CD2	2.92	0.52
1:A:1707:ILE:HD13	1:A:1709:LEU:HD21	1.91	0.52
1:B:1523:TRP:CD1	1:B:1525:GLY:H	2.27	0.52
1:A:1247:GLN:HG2	1:A:1275:VAL:HB	1.90	0.52
1:B:967:TYR:CD2	1:B:1030:PHE:HZ	2.21	0.52
1:A:1083:TYR:CD1	1:A:1083:TYR:C	2.87	0.52
1:A:1442:ASN:C	1:A:1444:PRO:CD	2.82	0.52
1:B:981:ARG:HG2	1:B:982:GLY:H	1.74	0.52
1:B:1423:GLU:N	1:B:1424:PRO:CA	2.72	0.52
1:B:1707:ILE:HG12	1:B:1708:ASN:N	2.23	0.52
1:A:1443:HIS:O	1:A:1444:PRO:C	2.52	0.52
1:B:1512:THR:HG21	1:B:1549:ILE:CD1	2.39	0.52
1:B:981:ARG:HB2	1:B:1030:PHE:CE1	2.44	0.52
1:A:1097:ARG:CZ	1:B:1086:LEU:HD22	2.40	0.52
1:B:1177:GLU:O	1:B:1179:ASP:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1647:THR:HA	1:A:1650:ILE:CG2	2.39	0.52
1:B:1032:SER:HB3	1:B:1116:SER:HB3	1.92	0.52
1:B:1145:ASP:O	1:B:1146:LEU:HB2	2.08	0.52
1:B:1550:SER:HB2	1:B:1633:VAL:CG2	2.38	0.52
1:A:1298:PHE:N	1:A:1299:PRO:HD2	2.25	0.52
1:A:1322:GLY:HA3	1:A:1331:PHE:CE2	2.45	0.52
1:A:1472:ASP:OD1	1:A:1473:GLY:N	2.42	0.52
1:B:975:ALA:HA	1:B:985:TRP:CG	2.45	0.52
1:B:1322:GLY:HA3	1:B:1331:PHE:CE2	2.44	0.52
1:A:1542:MET:CE	1:A:1636:PRO:CB	2.73	0.52
1:A:1615:LEU:HD11	1:A:1660:PHE:CZ	2.46	0.52
1:B:1219:GLY:N	1:B:1228:GLN:HE22	2.03	0.52
1:B:1040:LEU:HD22	1:B:1094:ILE:HD11	1.92	0.51
1:A:1716:ILE:CG2	1:A:1738:ILE:HG12	2.40	0.51
1:A:981:ARG:HD2	1:A:1030:PHE:CD1	2.46	0.51
1:A:1442:ASN:C	1:A:1444:PRO:HD3	2.35	0.51
1:B:1083:TYR:CD1	1:B:1083:TYR:C	2.88	0.51
1:B:1047:ASN:ND2	1:B:1076:SER:HA	2.25	0.51
1:B:1105:ILE:HG23	1:B:1183:HIS:CD2	2.45	0.51
1:B:1153:MET:HE3	1:B:1193:MET:HG3	1.93	0.51
1:B:1247:GLN:HG2	1:B:1275:VAL:HB	1.92	0.51
1:B:1298:PHE:CZ	1:B:1302:ILE:HD11	2.46	0.51
1:B:1441:LEU:HD13	1:B:1464:MET:H	1.69	0.51
1:B:1513:PHE:CG	1:B:1514:PRO:HD2	2.46	0.51
1:A:1186:LEU:HD12	1:A:1187:LEU:N	2.25	0.51
1:A:1423:GLU:OE2	1:A:1510:ARG:NH2	2.36	0.51
1:B:1030:PHE:CG	1:B:1031:PRO:HD2	2.46	0.51
1:B:1045:HIS:CE1	1:B:1051:GLN:HG2	2.46	0.51
1:B:1165:ASN:HD22	1:B:1165:ASN:H	1.57	0.51
1:B:1464:MET:HG3	1:B:1479:TYR:HA	1.92	0.51
1:A:1059:LYS:HD3	1:A:1060:ASN:N	2.26	0.51
1:A:1638:LEU:HD12	1:A:1638:LEU:O	2.10	0.51
1:B:1156:ARG:HD3	1:B:1158:GLN:HG2	1.93	0.51
1:A:1034:PRO:HA	1:A:1116:SER:HA	1.92	0.51
1:A:1187:LEU:HD12	1:A:1205:TYR:CD2	2.46	0.51
1:A:1613:TYR:HA	1:A:1616:LEU:HG	1.93	0.51
1:A:1668:ARG:HD2	3:A:12:HOH:O	2.11	0.51
1:B:1035:VAL:HG21	1:B:1115:PHE:CD2	2.45	0.51
1:B:1433:SER:HB3	1:B:1434:PRO:CD	2.40	0.51
2:C:1:GLC:C4	2:C:2:GLC:O2	2.59	0.51
1:A:1575:GLY:C	1:A:1577:PHE:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1737:LYS:HD3	1:A:1802:TRP:CH2	2.46	0.51
1:A:1050:LEU:HD21	1:A:1083:TYR:CZ	2.45	0.51
1:A:1513:PHE:CG	1:A:1514:PRO:HD2	2.45	0.51
1:B:1765:LEU:N	1:B:1765:LEU:CD2	2.67	0.51
1:A:1032:SER:HB3	1:A:1116:SER:HB3	1.92	0.51
1:A:1522:HIS:O	1:A:1552:THR:HA	2.11	0.51
1:A:1814:ILE:CB	1:A:1822:THR:HG22	2.40	0.51
1:B:1478:HIS:CE1	1:B:1482:HIS:ND1	2.79	0.51
1:A:1150:THR:OG1	1:A:1196:THR:HG23	2.12	0.50
1:A:1177:GLU:O	1:A:1179:ASP:O	2.29	0.50
1:A:1302:ILE:HD12	1:A:1312:VAL:HG11	1.93	0.50
1:A:1731:GLN:O	1:A:1795:LYS:HE3	2.11	0.50
1:B:961:GLU:HG2	1:B:1200:LEU:H	1.76	0.50
1:B:1613:TYR:HA	1:B:1616:LEU:HG	1.92	0.50
1:B:1638:LEU:C	1:B:1638:LEU:HD12	2.36	0.50
1:A:1367:LEU:HD12	1:A:1376:TYR:OH	2.11	0.50
1:A:1741:ASP:C	1:A:1743:GLU:N	2.64	0.50
1:B:1761:TYR:HA	1:B:1766:TYR:CD1	2.47	0.50
1:B:1443:HIS:O	1:B:1444:PRO:C	2.51	0.50
1:B:1491:ARG:HG3	1:B:1519:TRP:CE3	2.47	0.50
1:A:1550:SER:HB2	1:A:1633:VAL:CG2	2.42	0.50
1:B:1402:TYR:CD2	1:B:1500:VAL:HG13	2.46	0.50
1:B:1441:LEU:CD1	1:B:1464:MET:HB2	2.26	0.50
1:B:1683:TYR:CE2	1:B:1740:LEU:O	2.64	0.50
1:A:1681:ARG:NH1	1:A:1742:ASP:HB2	2.25	0.50
1:A:1700:LEU:HD12	1:A:1700:LEU:N	2.27	0.50
1:B:1272:PRO:HB2	1:B:1613:TYR:CE2	2.47	0.50
1:B:1513:PHE:O	1:B:1514:PRO:C	2.54	0.50
1:B:1638:LEU:HD12	1:B:1638:LEU:O	2.11	0.50
1:B:1775:GLN:O	1:B:1777:THR:HG23	2.10	0.50
1:A:1097:ARG:NH1	1:B:1086:LEU:HD22	2.26	0.50
1:A:1153:MET:HE3	1:A:1193:MET:HG3	1.93	0.50
1:A:1273:TYR:HA	1:A:1613:TYR:OH	2.11	0.50
1:A:1285:ARG:NH2	1:A:1359:PRO:HA	2.27	0.50
1:A:1716:ILE:HG22	1:A:1738:ILE:CA	2.38	0.50
1:B:1229:TYR:CZ	1:B:1233:ILE:HD13	2.47	0.50
1:B:1731:GLN:O	1:B:1795:LYS:HE3	2.11	0.50
1:B:1798:TYR:CD2	1:B:1798:TYR:N	2.75	0.50
1:A:975:ALA:HA	1:A:985:TRP:CG	2.47	0.50
1:A:1040:LEU:HD22	1:A:1094:ILE:HD11	1.94	0.50
1:A:1137:THR:HG21	1:A:1151:TRP:CE3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1442:ASN:C	1:B:1444:PRO:CD	2.85	0.50
1:B:1218:LEU:C	1:B:1219:GLY:O	2.49	0.50
1:B:1468:GLN:HE21	1:B:1478:HIS:CD2	2.21	0.50
1:A:1559:PHE:CD2	1:A:1586:THR:HB	2.47	0.50
1:B:1513:PHE:O	1:B:1516:SER:HB2	2.12	0.50
1:B:1783:ILE:HD12	1:B:1783:ILE:H	1.76	0.50
1:A:1189:ASN:HD22	1:A:1190:SER:N	2.10	0.49
1:A:1433:SER:HB3	1:A:1434:PRO:CD	2.42	0.49
1:A:1478:HIS:CE1	1:A:1482:HIS:ND1	2.80	0.49
1:A:1765:LEU:N	1:A:1765:LEU:CD2	2.67	0.49
1:A:990:SER:O	1:A:993:VAL:HG22	2.12	0.49
1:A:1402:TYR:CD2	1:A:1500:VAL:HG13	2.47	0.49
1:B:1467:GLN:NE2	1:B:1475:LEU:HB3	2.27	0.49
1:A:1106:TRP:CZ3	1:A:1108:SER:HB3	2.47	0.49
1:A:1414:PHE:CD1	1:A:1414:PHE:C	2.90	0.49
1:A:1455:ARG:HB2	1:A:1459:SER:HB2	1.94	0.49
1:B:1376:TYR:N	1:B:1376:TYR:CD2	2.79	0.49
1:A:1221:THR:OG1	1:A:1224:LEU:HD23	2.12	0.49
1:A:1447:MET:O	1:A:1453:ARG:HD3	2.13	0.49
1:A:1621:THR:CG2	1:A:1751:PHE:H	2.25	0.49
1:A:1831:THR:O	1:A:1833:VAL:N	2.45	0.49
1:A:1587:ILE:CG2	1:A:1588:GLY:H	2.22	0.49
1:B:1207:THR:HG23	1:B:1209:GLY:H	1.76	0.49
1:B:1455:ARG:HB2	1:B:1459:SER:HB2	1.93	0.49
1:A:1145:ASP:HB3	1:A:1149:HIS:HD2	1.77	0.49
1:B:1189:ASN:HD22	1:B:1190:SER:H	1.60	0.49
1:B:1601:PHE:O	1:B:1602:VAL:C	2.55	0.49
1:B:1621:THR:CG2	1:B:1751:PHE:H	2.26	0.49
1:A:1104:ILE:O	1:A:1127:PRO:HB3	2.11	0.49
1:A:1161:GLY:HA3	1:A:1164:LYS:HD2	1.95	0.49
1:A:1250:ARG:HG3	1:A:1251:TYR:N	2.25	0.49
1:B:990:SER:O	1:B:993:VAL:HG22	2.13	0.49
1:B:1161:GLY:HA3	1:B:1164:LYS:HD2	1.95	0.49
1:A:1086:LEU:HD22	1:B:1097:ARG:NH1	2.27	0.49
1:B:1828:ASP:OD1	1:B:1829:PRO:HD2	2.13	0.49
1:A:1038:LEU:HD11	1:A:1115:PHE:HB3	1.95	0.49
1:A:1761:TYR:HA	1:A:1766:TYR:CD1	2.47	0.49
1:A:1035:VAL:HG21	1:A:1115:PHE:CD2	2.47	0.48
1:A:1036:ASN:OD1	1:A:1037:PRO:HA	2.12	0.48
1:A:1293:PRO:C	1:A:1295:PHE:H	2.20	0.48
1:B:1293:PRO:C	1:B:1295:PHE:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1603:ASN:HA	1:B:1606:ARG:HD3	1.95	0.48
1:B:1716:ILE:CG2	1:B:1738:ILE:HG12	2.44	0.48
1:B:1237:VAL:HG22	1:B:1518:ARG:O	2.12	0.48
1:A:1132:TYR:CE1	1:A:1143:ARG:HB2	2.47	0.48
1:A:1603:ASN:HA	1:A:1606:ARG:HD3	1.95	0.48
1:A:1716:ILE:CG1	1:A:1748:GLY:HA3	2.35	0.48
1:B:1102:GLY:O	1:B:1103:THR:C	2.55	0.48
1:A:1394:TRP:O	1:A:1398:ILE:HG12	2.12	0.48
1:B:1187:LEU:O	1:B:1189:ASN:N	2.42	0.48
1:A:1156:ARG:HD3	1:A:1158:GLN:HG2	1.95	0.48
1:A:1260:ALA:HB2	1:A:1301:LEU:CD1	2.43	0.48
1:A:1513:PHE:O	1:A:1516:SER:HB2	2.14	0.48
1:A:1691:ILE:O	1:A:1698:LYS:NZ	2.46	0.48
1:A:1784:PHE:HD2	1:A:1785:ASN:N	2.11	0.48
1:B:1189:ASN:HD22	1:B:1190:SER:N	2.11	0.48
1:B:1319:ALA:HB1	1:B:1380:VAL:CG2	2.44	0.48
1:B:1716:ILE:HG22	1:B:1738:ILE:CA	2.38	0.48
1:A:1145:ASP:HB3	1:A:1149:HIS:CD2	2.48	0.48
1:A:1189:ASN:HD22	1:A:1190:SER:H	1.59	0.48
1:A:1512:THR:HG21	1:A:1549:ILE:CD1	2.44	0.48
1:B:1038:LEU:HD11	1:B:1115:PHE:HB3	1.95	0.48
1:B:1059:LYS:HD3	1:B:1060:ASN:H	1.79	0.48
1:A:1061:ARG:HD3	1:A:1211:VAL:HG12	1.96	0.48
1:A:1237:VAL:HG22	1:A:1518:ARG:O	2.14	0.48
1:A:1274:ASP:OD1	1:A:1726:THR:HG23	2.14	0.48
1:A:1606:ARG:CB	1:A:1606:ARG:HH11	2.27	0.48
1:A:1784:PHE:CD2	1:A:1785:ASN:N	2.82	0.48
1:B:981:ARG:HD2	1:B:1030:PHE:CD1	2.48	0.48
1:B:1838:VAL:C	1:B:1840:ASP:H	2.21	0.48
1:A:1229:TYR:CZ	1:A:1233:ILE:HD13	2.49	0.48
1:A:1464:MET:HE2	1:A:1479:TYR:HA	1.96	0.48
1:A:1683:TYR:CE2	1:A:1740:LEU:O	2.66	0.48
1:A:1019:ILE:HB	1:A:1038:LEU:HB2	1.96	0.48
1:B:1252:GLY:CA	1:B:1587:ILE:HD12	2.44	0.48
1:B:1509:THR:O	1:B:1522:HIS:HD2	1.96	0.48
1:B:1470:LEU:HB3	1:B:1471:PRO:CD	2.44	0.48
1:B:1831:THR:O	1:B:1833:VAL:N	2.47	0.48
1:A:1446:TYR:O	1:A:1448:PRO:HD3	2.14	0.47
1:B:1145:ASP:HB3	1:B:1149:HIS:HD2	1.79	0.47
1:B:1631:VAL:HG13	1:B:1632:THR:N	2.27	0.47
1:B:1034:PRO:HA	1:B:1116:SER:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1137:THR:HG21	1:B:1151:TRP:CE3	2.49	0.47
1:B:1503:GLN:C	1:B:1758:ILE:HD11	2.40	0.47
1:B:1737:LYS:HD3	1:B:1802:TRP:CH2	2.48	0.47
1:A:1423:GLU:N	1:A:1424:PRO:CA	2.76	0.47
1:A:1565:TYR:O	1:A:1569:VAL:HG23	2.14	0.47
1:A:1838:VAL:C	1:A:1840:ASP:H	2.23	0.47
1:B:1053:LYS:HA	1:B:1212:LEU:O	2.15	0.47
1:B:1478:HIS:HE1	1:B:1482:HIS:ND1	2.13	0.47
1:B:1575:GLY:C	1:B:1577:PHE:H	2.21	0.47
1:A:1047:ASN:ND2	1:A:1076:SER:HA	2.29	0.47
1:A:1118:MET:HE3	1:A:1445:PRO:CG	2.44	0.47
1:A:1134:PHE:CE1	1:A:1195:VAL:HG11	2.48	0.47
1:B:1442:ASN:C	1:B:1444:PRO:HD3	2.39	0.47
1:B:1798:TYR:HE2	1:B:1839:THR:CG2	2.27	0.47
1:A:1218:LEU:C	1:A:1219:GLY:O	2.53	0.47
1:A:1683:TYR:HE2	1:A:1740:LEU:O	1.97	0.47
1:B:1030:PHE:CD2	1:B:1031:PRO:CD	2.86	0.47
1:B:1302:ILE:HD12	1:B:1312:VAL:HG11	1.96	0.47
1:B:1446:TYR:O	1:B:1448:PRO:HD3	2.15	0.47
1:B:1504:ARG:HB3	1:B:1756:GLN:O	2.14	0.47
1:B:1683:TYR:HE2	1:B:1740:LEU:O	1.96	0.47
1:A:961:GLU:O	1:A:962:GLU:HB2	2.14	0.47
1:A:1646:VAL:HG11	1:A:1676:TYR:CE1	2.49	0.47
1:B:1129:LYS:CD	1:B:1201:PRO:HG3	2.44	0.47
1:B:1384:ASP:C	1:B:1384:ASP:OD1	2.56	0.47
1:B:1508:ILE:CD1	1:B:1508:ILE:N	2.78	0.47
1:A:1036:ASN:HA	1:A:1037:PRO:HA	1.59	0.47
1:A:1500:VAL:HG12	1:A:1501:THR:HG23	1.97	0.47
1:A:1704:LEU:O	1:A:1704:LEU:HD12	2.15	0.47
1:B:1118:MET:HE3	1:B:1445:PRO:CG	2.45	0.47
1:B:1498:GLN:OE1	1:B:1504:ARG:HA	2.15	0.47
1:B:1542:MET:HB3	1:B:1542:MET:HE2	1.18	0.47
1:B:1700:LEU:N	1:B:1700:LEU:HD12	2.29	0.47
1:B:1704:LEU:HD12	1:B:1704:LEU:O	2.15	0.47
1:A:1102:GLY:O	1:A:1103:THR:C	2.58	0.47
1:A:1187:LEU:O	1:A:1189:ASN:N	2.44	0.47
1:B:1156:ARG:HG2	1:B:1158:GLN:HB2	1.96	0.47
1:B:1394:TRP:O	1:B:1398:ILE:HG12	2.15	0.47
1:A:1263:TYR:CE1	1:A:1310:MET:HG3	2.49	0.47
1:B:1298:PHE:N	1:B:1299:PRO:HD2	2.29	0.47
1:B:1823:PRO:CB	1:B:1841:ARG:HH21	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:PRO:O	1:A:1333:ARG:HG3	2.15	0.47
1:A:1542:MET:HB3	1:A:1542:MET:HE2	1.19	0.47
1:B:1059:LYS:HD3	1:B:1060:ASN:N	2.29	0.47
1:A:1798:TYR:HE2	1:A:1839:THR:CG2	2.28	0.46
1:B:1134:PHE:CE1	1:B:1195:VAL:HG11	2.50	0.46
1:B:1260:ALA:HB2	1:B:1301:LEU:CD1	2.45	0.46
1:B:1414:PHE:CD1	1:B:1414:PHE:C	2.92	0.46
1:B:1559:PHE:CD2	1:B:1586:THR:HB	2.50	0.46
1:B:1745:THR:O	1:B:1746:ALA:HB2	2.15	0.46
1:B:1788:ILE:HG22	1:B:1846:HIS:CD2	2.50	0.46
1:B:1136:GLU:HG2	1:B:1166:SER:HB3	1.97	0.46
1:B:1470:LEU:HB3	1:B:1471:PRO:HD2	1.97	0.46
1:B:1784:PHE:HD2	1:B:1785:ASN:N	2.14	0.46
1:A:1614:THR:CG2	1:A:1719:TRP:HB2	2.45	0.46
1:A:1716:ILE:HG22	1:A:1738:ILE:HG12	1.96	0.46
1:B:1145:ASP:HB3	1:B:1149:HIS:CD2	2.50	0.46
1:B:1691:ILE:O	1:B:1698:LYS:NZ	2.49	0.46
1:B:1798:TYR:HE2	1:B:1839:THR:HG23	1.81	0.46
1:A:1104:ILE:O	1:A:1104:ILE:HG13	2.15	0.46
1:A:1694:ARG:NH2	1:A:1743:GLU:HB2	2.30	0.46
1:B:1077:THR:HG23	1:B:1080:GLY:H	1.80	0.46
1:B:1681:ARG:NH1	1:B:1742:ASP:H	1.92	0.46
1:B:1784:PHE:CD2	1:B:1785:ASN:N	2.83	0.46
1:B:1189:ASN:HB3	1:B:1193:MET:HE1	1.97	0.46
1:A:1053:LYS:HA	1:A:1212:LEU:O	2.14	0.46
1:A:1064:VAL:CG1	1:A:1066:VAL:HG13	2.45	0.46
1:A:1694:ARG:HH22	1:A:1743:GLU:HB2	1.80	0.46
1:A:1825:PHE:CD1	1:A:1825:PHE:C	2.94	0.46
1:B:1733:PHE:HB3	1:B:1797:GLY:HA3	1.98	0.46
1:A:1165:ASN:ND2	1:A:1165:ASN:H	2.14	0.46
1:A:1513:PHE:O	1:A:1514:PRO:C	2.54	0.46
1:B:1468:GLN:NE2	1:B:1478:HIS:CD2	2.68	0.46
1:B:1573:GLN:HA	1:B:1608:VAL:HG21	1.97	0.46
1:B:1746:ALA:HB3	1:B:1773:ALA:HB3	1.97	0.46
1:A:1733:PHE:HB3	1:A:1797:GLY:HA3	1.98	0.46
1:A:1746:ALA:HB3	1:A:1773:ALA:HB3	1.97	0.46
1:A:1783:ILE:HD12	1:A:1783:ILE:H	1.81	0.46
1:B:1106:TRP:CZ3	1:B:1108:SER:HB3	2.50	0.46
1:B:1136:GLU:OE1	1:B:1522:HIS:CE1	2.68	0.46
1:B:1791:THR:O	1:B:1793:PRO:HD3	2.15	0.46
1:A:1118:MET:HB2	1:A:1445:PRO:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1346:ASP:O	1:A:1347:GLY:O	2.33	0.46
1:A:1090:ASN:HA	1:A:1091:PRO:HA	1.88	0.46
1:A:1156:ARG:HG2	1:A:1158:GLN:HB2	1.97	0.46
1:A:1572:MET:HB3	1:A:1572:MET:HE3	1.78	0.46
1:B:1283:MET:HA	1:B:1290:THR:O	2.16	0.46
1:A:1002:LEU:N	1:A:1002:LEU:HD23	2.31	0.45
1:A:1272:PRO:HB2	1:A:1613:TYR:CE2	2.51	0.45
1:A:1587:ILE:CG2	1:A:1588:GLY:N	2.79	0.45
1:B:1229:TYR:CE1	1:B:1233:ILE:HD13	2.51	0.45
1:B:1609:LEU:HD13	1:B:1609:LEU:HA	1.81	0.45
1:B:1614:THR:CG2	1:B:1719:TRP:HB2	2.46	0.45
1:A:1189:ASN:HB3	1:A:1193:MET:HE1	1.97	0.45
1:A:1240:PRO:HA	1:A:1504:ARG:HH11	1.80	0.45
1:A:1575:GLY:C	1:A:1577:PHE:N	2.74	0.45
1:B:1002:LEU:N	1:B:1002:LEU:HD23	2.31	0.45
1:B:1132:TYR:CE1	1:B:1143:ARG:HB2	2.50	0.45
1:B:1165:ASN:ND2	1:B:1165:ASN:H	2.15	0.45
1:A:1229:TYR:CE1	1:A:1233:ILE:HD13	2.52	0.45
1:B:974:SER:OG	1:B:977:ASN:HB2	2.16	0.45
1:B:1145:ASP:O	1:B:1146:LEU:CB	2.64	0.45
1:B:1221:THR:OG1	1:B:1224:LEU:HD23	2.17	0.45
1:B:1512:THR:HG22	1:B:1516:SER:CB	2.47	0.45
1:A:979:THR:O	1:A:981:ARG:O	2.35	0.45
1:A:1129:LYS:CD	1:A:1201:PRO:HG3	2.45	0.45
1:A:1333:ARG:NH2	1:A:1396:ARG:CD	2.80	0.45
1:A:1508:ILE:CD1	1:A:1508:ILE:N	2.79	0.45
1:A:1513:PHE:CE2	1:A:1514:PRO:HD2	2.51	0.45
1:B:961:GLU:O	1:B:962:GLU:HB2	2.16	0.45
1:B:1606:ARG:HH11	1:B:1606:ARG:CB	2.29	0.45
1:A:1040:LEU:HD12	1:A:1040:LEU:C	2.42	0.45
1:A:1136:GLU:OE1	1:A:1522:HIS:CE1	2.69	0.45
1:B:1333:ARG:NH2	1:B:1396:ARG:CD	2.79	0.45
1:B:1624:HIS:CD2	1:B:1751:PHE:CE2	3.05	0.45
1:A:1157:ASP:HB2	1:A:1425:SER:HB2	1.99	0.45
1:A:1509:THR:O	1:A:1522:HIS:HD2	2.00	0.45
1:A:1513:PHE:CG	1:A:1514:PRO:CD	3.00	0.45
1:B:1329:PRO:O	1:B:1330:ALA:C	2.60	0.45
1:B:1443:HIS:O	1:B:1445:PRO:N	2.50	0.45
1:B:1716:ILE:HG22	1:B:1738:ILE:HG12	1.99	0.45
1:A:1807:VAL:O	1:A:1807:VAL:CG2	2.64	0.45
1:B:1672:ASN:HD22	1:B:1673:VAL:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:GLU:C	1:A:963:LYS:N	2.64	0.45
1:A:1045:HIS:CE1	1:A:1051:GLN:HE21	2.35	0.45
1:A:1145:ASP:O	1:A:1146:LEU:CB	2.65	0.45
1:A:1512:THR:HG22	1:A:1516:SER:CB	2.46	0.45
1:A:1788:ILE:HG22	1:A:1846:HIS:CD2	2.52	0.45
1:B:1264:ASP:OD2	1:B:1304:ARG:NH2	2.49	0.45
1:A:1684:ASP:C	1:A:1684:ASP:OD1	2.59	0.45
1:A:1828:ASP:OD1	1:A:1829:PRO:HD2	2.17	0.45
1:B:1118:MET:HB2	1:B:1445:PRO:HG2	1.99	0.45
1:B:1153:MET:HE2	1:B:1195:VAL:HG13	1.98	0.45
1:A:1638:LEU:HD12	1:A:1638:LEU:C	2.42	0.44
1:B:1131:LEU:HD13	1:B:1132:TYR:N	2.32	0.44
1:B:1306:LYS:HA	1:B:1310:MET:O	2.18	0.44
1:B:1694:ARG:NH2	1:B:1743:GLU:HB2	2.32	0.44
1:A:1289:PHE:CE1	1:A:1397:GLU:HB3	2.53	0.44
1:B:1022:LYS:O	1:B:1022:LYS:CG	2.66	0.44
1:B:1040:LEU:HD11	1:B:1042:VAL:CG2	2.47	0.44
1:B:1188:LEU:HD23	1:B:1188:LEU:HA	1.81	0.44
1:B:1751:PHE:HA	1:B:1767:TYR:O	2.16	0.44
1:A:1593:ASP:HB2	1:A:1594:PRO:HD2	1.99	0.44
1:B:1355:TRP:N	1:B:1356:PRO:CD	2.80	0.44
1:B:1693:ALA:HB1	1:B:1696:GLU:HB2	2.00	0.44
1:B:1730:ARG:HH22	1:B:1754:ASP:C	2.25	0.44
1:A:998:PHE:CZ	1:A:1112:GLY:HA2	2.52	0.44
1:A:1459:SER:O	1:A:1461:THR:HG22	2.16	0.44
1:B:1090:ASN:HA	1:B:1091:PRO:HA	1.91	0.44
1:A:1026:TYR:O	1:A:1029:ALA:HB3	2.18	0.44
1:A:1503:GLN:C	1:A:1758:ILE:HD11	2.42	0.44
1:A:1022:LYS:O	1:A:1022:LYS:CG	2.65	0.44
1:A:1193:MET:HE2	1:A:1207:THR:OG1	2.18	0.44
1:A:1491:ARG:HG3	1:A:1519:TRP:CE3	2.52	0.44
1:A:1751:PHE:HA	1:A:1767:TYR:O	2.17	0.44
1:B:998:PHE:CZ	1:B:1112:GLY:HA2	2.53	0.44
1:B:1040:LEU:HD12	1:B:1040:LEU:C	2.41	0.44
1:B:1240:PRO:HA	1:B:1504:ARG:HH11	1.81	0.44
1:B:1452:SER:HB3	1:B:1455:ARG:HG2	1.99	0.44
1:B:1587:ILE:CG2	1:B:1588:GLY:H	2.21	0.44
1:B:1686:TYR:CE2	1:B:1706:HIS:CE1	3.05	0.44
1:A:1131:LEU:CD1	1:A:1131:LEU:C	2.91	0.44
1:A:1803:GLY:HA2	1:A:1832:GLN:CG	2.47	0.44
1:B:962:GLU:CG	1:B:1200:LEU:HD22	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1050:LEU:HD12	1:B:1096:ILE:HD13	1.99	0.44
1:B:1353:LYS:HE2	1:B:1377:ARG:O	2.17	0.44
1:B:1565:TYR:O	1:B:1569:VAL:HG23	2.17	0.44
1:B:1684:ASP:OD1	1:B:1684:ASP:C	2.61	0.44
1:A:1169:VAL:HG12	1:A:1171:PRO:HD3	2.00	0.44
1:A:1200:LEU:O	1:A:1202:ALA:N	2.51	0.44
1:A:1319:ALA:HB1	1:A:1380:VAL:HG21	2.00	0.44
1:B:1825:PHE:CD1	1:B:1825:PHE:C	2.95	0.44
1:A:1086:LEU:HD13	1:B:1097:ARG:NH2	2.33	0.43
1:A:1355:TRP:HB2	1:A:1356:PRO:HD3	1.99	0.43
1:A:1604:ILE:HG22	1:A:1605:SER:N	2.33	0.43
1:B:1066:VAL:HA	1:B:1067:PRO:HD3	1.84	0.43
1:B:1069:ASN:OD1	1:B:1231:GLU:O	2.35	0.43
1:A:1005:VAL:HG11	1:A:1089:LYS:HA	2.00	0.43
1:A:1503:GLN:NE2	1:A:1756:GLN:CD	2.71	0.43
1:A:1745:THR:O	1:A:1746:ALA:HB2	2.17	0.43
1:A:1798:TYR:HE2	1:A:1839:THR:HG23	1.83	0.43
1:A:1803:GLY:HA2	1:A:1832:GLN:CB	2.48	0.43
1:A:1484:LEU:HD12	1:A:1484:LEU:HA	1.77	0.43
1:B:1272:PRO:O	1:B:1273:TYR:HB3	2.18	0.43
1:B:978:CYS:CB	1:B:985:TRP:HD1	2.32	0.43
1:B:1464:MET:HE2	1:B:1479:TYR:HA	2.01	0.43
1:B:1504:ARG:HH21	1:B:1760:THR:HG23	1.84	0.43
1:B:1725:ASN:OD1	1:B:1727:HIS:HB3	2.19	0.43
1:A:978:CYS:CB	1:A:985:TRP:HD1	2.30	0.43
1:A:1252:GLY:CA	1:A:1587:ILE:HD12	2.48	0.43
1:A:1517:GLY:CA	1:A:1549:ILE:HG12	2.40	0.43
1:A:1681:ARG:HD3	1:A:1741:ASP:CA	2.40	0.43
1:B:1050:LEU:HA	1:B:1050:LEU:HD23	1.70	0.43
1:B:1097:ARG:HG3	1:B:1102:GLY:O	2.18	0.43
1:B:1200:LEU:O	1:B:1202:ALA:N	2.52	0.43
1:B:1217:PHE:HB3	1:B:1228:GLN:HE21	1.84	0.43
1:B:1329:PRO:CB	1:B:1333:ARG:HD2	2.49	0.43
1:B:1508:ILE:N	1:B:1508:ILE:HD12	2.33	0.43
1:B:1650:ILE:CD1	1:B:1653:GLN:HE21	2.31	0.43
1:B:1796:LEU:C	1:B:1796:LEU:CD2	2.92	0.43
1:A:1355:TRP:N	1:A:1356:PRO:CD	2.81	0.43
1:B:1288:ASP:HB3	1:B:1289:PHE:CD2	2.54	0.43
1:B:1061:ARG:NH1	1:B:1061:ARG:HG2	2.33	0.43
1:B:1289:PHE:CE1	1:B:1397:GLU:HB3	2.52	0.43
1:B:1346:ASP:O	1:B:1347:GLY:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1500:VAL:HG12	1:B:1501:THR:HG23	2.00	0.43
1:B:1686:TYR:CD2	1:B:1706:HIS:HE1	2.36	0.43
1:B:1831:THR:C	1:B:1833:VAL:H	2.27	0.43
1:A:1131:LEU:HD13	1:A:1132:TYR:N	2.34	0.43
1:B:1592:GLN:HE21	1:B:1592:GLN:HB3	1.68	0.43
1:B:1775:GLN:C	1:B:1777:THR:N	2.77	0.43
1:A:1069:ASN:OD1	1:A:1231:GLU:O	2.36	0.43
1:A:1693:ALA:HB1	1:A:1696:GLU:HB2	2.01	0.43
1:B:1234:GLY:HA3	1:B:1518:ARG:HD3	2.00	0.43
1:B:1575:GLY:C	1:B:1577:PHE:N	2.75	0.43
1:B:1757:SER:HB2	1:B:1760:THR:HG22	1.99	0.43
1:A:1730:ARG:HE	1:A:1752:TRP:HZ3	1.67	0.43
1:A:1831:THR:C	1:A:1833:VAL:H	2.27	0.43
1:B:1240:PRO:HG2	1:B:1243:SER:HB3	2.01	0.43
1:A:1251:TYR:CE1	1:A:1587:ILE:HB	2.53	0.42
1:A:1311:ARG:NH2	1:A:1756:GLN:OE1	2.52	0.42
1:A:1836:ILE:HG22	1:A:1836:ILE:O	2.18	0.42
1:B:1196:THR:OG1	1:B:1206:ARG:NH2	2.52	0.42
1:B:1407:ASN:HB3	1:B:1409:GLU:OE2	2.19	0.42
1:B:1679:ARG:HD3	1:B:1695:GLY:HA3	2.01	0.42
1:A:974:SER:OG	1:A:977:ASN:HB2	2.19	0.42
1:A:981:ARG:HG2	1:A:982:GLY:N	2.33	0.42
1:A:1304:ARG:O	1:A:1307:ALA:HB3	2.18	0.42
1:A:1529:ALA:O	1:A:1567:MET:HE1	2.19	0.42
1:A:1650:ILE:CD1	1:A:1653:GLN:HE21	2.32	0.42
1:A:1791:THR:O	1:A:1793:PRO:HD3	2.19	0.42
1:B:1045:HIS:CE1	1:B:1051:GLN:HE21	2.36	0.42
1:A:1125:ARG:HA	1:A:1202:ALA:HB2	2.01	0.42
1:A:1329:PRO:CB	1:A:1333:ARG:HD2	2.49	0.42
1:A:1478:HIS:HE1	1:A:1482:HIS:ND1	2.15	0.42
1:A:1573:GLN:HA	1:A:1608:VAL:HG21	2.00	0.42
1:A:1006:SER:OG	1:A:1007:ASP:N	2.52	0.42
1:A:1196:THR:OG1	1:A:1206:ARG:NH2	2.53	0.42
1:A:1221:THR:OG1	1:A:1224:LEU:HB2	2.20	0.42
1:B:1083:TYR:HA	1:B:1097:ARG:O	2.19	0.42
1:B:1304:ARG:O	1:B:1307:ALA:HB3	2.20	0.42
1:A:1404:ASN:OD1	1:A:1405:PRO:HD2	2.19	0.42
1:A:1490:THR:HG22	1:A:1519:TRP:HB2	2.02	0.42
1:A:1775:GLN:O	1:A:1777:THR:HG23	2.19	0.42
1:B:1177:GLU:O	1:B:1178:GLU:C	2.63	0.42
1:B:1531:TRP:CZ2	1:B:1567:MET:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1753:ASP:C	1:B:1755:GLY:N	2.77	0.42
1:B:1835:SER:C	1:B:1836:ILE:HG13	2.44	0.42
1:A:1443:HIS:O	1:A:1445:PRO:N	2.52	0.42
1:B:981:ARG:O	1:B:983:CYS:N	2.51	0.42
1:B:1036:ASN:HA	1:B:1037:PRO:HA	1.58	0.42
1:B:1250:ARG:HG3	1:B:1251:TYR:N	2.30	0.42
1:B:1503:GLN:NE2	1:B:1756:GLN:CD	2.74	0.42
1:B:1803:GLY:HA2	1:B:1832:GLN:CG	2.49	0.42
1:A:1234:GLY:HA3	1:A:1518:ARG:HD3	2.01	0.42
1:A:1730:ARG:HH22	1:A:1754:ASP:C	2.27	0.42
1:B:1050:LEU:HD21	1:B:1083:TYR:CZ	2.54	0.42
1:B:1064:VAL:CG1	1:B:1066:VAL:HG13	2.49	0.42
1:B:1604:ILE:HG22	1:B:1605:SER:N	2.34	0.42
1:A:1272:PRO:O	1:A:1273:TYR:HB3	2.20	0.42
1:A:1409:GLU:H	1:A:1409:GLU:HG3	1.48	0.42
1:A:1672:ASN:HD22	1:A:1673:VAL:N	2.18	0.42
1:A:1730:ARG:HH21	1:A:1752:TRP:HZ3	1.67	0.42
1:B:1019:ILE:HB	1:B:1038:LEU:HB2	2.01	0.42
1:B:1436:CYS:O	1:B:1437:ARG:CD	2.67	0.42
1:B:1694:ARG:HH22	1:B:1743:GLU:HB2	1.83	0.42
1:B:1809:VAL:O	1:B:1809:VAL:HG13	2.20	0.42
1:A:1097:ARG:HG3	1:A:1102:GLY:O	2.19	0.42
1:A:1224:LEU:HD13	1:A:1224:LEU:HA	1.87	0.42
1:B:981:ARG:HG2	1:B:982:GLY:N	2.35	0.42
1:B:1459:SER:O	1:B:1461:THR:HG22	2.20	0.42
1:A:1188:LEU:HD23	1:A:1188:LEU:HA	1.88	0.42
1:A:1730:ARG:NE	1:A:1752:TRP:CZ3	2.87	0.42
1:A:1848:PHE:CD2	1:A:1848:PHE:C	2.97	0.42
1:B:1139:HIS:HD2	1:B:1151:TRP:CH2	2.38	0.42
1:B:1513:PHE:CG	1:B:1514:PRO:CD	3.03	0.42
1:A:981:ARG:HB2	1:A:1030:PHE:HE1	1.84	0.41
1:A:1298:PHE:HB3	1:A:1299:PRO:HD3	2.01	0.41
1:A:1679:ARG:HD3	1:A:1695:GLY:HA3	2.01	0.41
1:A:1686:TYR:CE2	1:A:1706:HIS:CE1	3.07	0.41
1:A:1244:LEU:HA	1:A:1244:LEU:HD23	1.79	0.41
1:B:1251:TYR:CE1	1:B:1587:ILE:HB	2.54	0.41
1:B:1593:ASP:HB2	1:B:1594:PRO:HD2	2.02	0.41
1:B:1730:ARG:HH21	1:B:1752:TRP:HZ3	1.68	0.41
1:B:1750:LEU:HD21	1:B:1752:TRP:CD1	2.53	0.41
1:A:1030:PHE:CD2	1:A:1031:PRO:CD	2.84	0.41
1:A:1296:ALA:C	1:A:1298:PHE:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1438:ASP:OD1	1:A:1439:ALA:N	2.52	0.41
1:A:1508:ILE:N	1:A:1508:ILE:HD12	2.34	0.41
1:B:1131:LEU:CD1	1:B:1131:LEU:C	2.93	0.41
1:B:1355:TRP:HB2	1:B:1356:PRO:HD3	2.01	0.41
1:A:1355:TRP:N	1:A:1356:PRO:HD2	2.36	0.41
1:A:1452:SER:HB3	1:A:1455:ARG:HG2	2.02	0.41
1:A:1523:TRP:CD1	1:A:1525:GLY:H	2.38	0.41
1:B:1061:ARG:HD3	1:B:1211:VAL:HG12	2.02	0.41
1:B:1112:GLY:O	1:B:1113:PHE:C	2.63	0.41
1:B:1298:PHE:HB3	1:B:1299:PRO:HD3	2.02	0.41
1:B:1355:TRP:N	1:B:1356:PRO:HD2	2.35	0.41
1:A:1088:LYS:HD3	1:A:1095:GLU:OE1	2.21	0.41
1:A:1128:SER:O	1:A:1201:PRO:HB3	2.21	0.41
1:A:1498:GLN:OE1	1:A:1504:ARG:HA	2.20	0.41
1:A:1504:ARG:HH21	1:A:1760:THR:HG23	1.86	0.41
1:B:1008:VAL:HG12	1:B:1010:TYR:CE1	2.55	0.41
1:B:1372:GLN:HE22	1:B:1377:ARG:HH22	1.68	0.41
1:B:1730:ARG:NE	1:B:1752:TRP:CZ3	2.88	0.41
1:A:1062:TYR:CE2	1:A:1480:ASN:HB3	2.55	0.41
1:A:1131:LEU:CD2	1:A:1173:TYR:CD1	3.03	0.41
1:A:1239:VAL:HB	1:A:1240:PRO:HD2	2.02	0.41
1:A:1288:ASP:O	1:A:1289:PHE:HB2	2.20	0.41
1:A:1288:ASP:HB3	1:A:1289:PHE:CD2	2.56	0.41
1:A:1385:PHE:HB2	1:A:1488:SER:OG	2.20	0.41
1:A:1682:TRP:HB2	1:A:1691:ILE:HG22	2.03	0.41
1:B:979:THR:O	1:B:981:ARG:O	2.38	0.41
1:B:981:ARG:HB2	1:B:1030:PHE:HE1	1.84	0.41
1:B:1447:MET:O	1:B:1453:ARG:NH1	2.43	0.41
1:B:1736:PHE:CZ	1:B:1771:PHE:CE1	3.09	0.41
1:A:1468:GLN:NE2	1:A:1478:HIS:CD2	2.71	0.41
1:A:1614:THR:HG23	1:A:1719:TRP:HB2	2.03	0.41
1:A:1660:PHE:HZ	1:A:1709:LEU:HD13	1.85	0.41
1:A:1672:ASN:ND2	1:A:1672:ASN:C	2.77	0.41
1:B:1140:ARG:HG3	1:B:1144:ARG:NH2	2.35	0.41
1:B:1375:LEU:C	1:B:1376:TYR:HD2	2.29	0.41
1:A:962:GLU:CG	1:A:1200:LEU:HD22	2.44	0.41
1:A:1398:ILE:HD12	1:A:1417:MET:HE3	2.03	0.41
1:A:1736:PHE:HD2	1:A:1736:PHE:HA	1.80	0.41
1:B:1513:PHE:CE2	1:B:1514:PRO:HD2	2.55	0.41
1:A:1153:MET:HE2	1:A:1195:VAL:HG13	2.02	0.41
1:A:1187:LEU:HG	1:A:1214:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1436:CYS:O	1:A:1437:ARG:CD	2.69	0.41
1:A:1470:LEU:HB3	1:A:1471:PRO:HD2	2.03	0.41
1:A:1726:THR:HA	1:A:1729:SER:HB3	2.03	0.41
1:B:1006:SER:OG	1:B:1007:ASP:N	2.53	0.41
1:B:1098:ARG:HH12	1:B:1181:SER:HB3	1.79	0.41
1:B:1296:ALA:C	1:B:1298:PHE:H	2.28	0.41
1:B:1447:MET:O	1:B:1453:ARG:HD3	2.21	0.41
1:B:1491:ARG:O	1:B:1494:TYR:HB3	2.21	0.41
1:B:1552:THR:O	1:B:1579:PRO:HD2	2.21	0.41
1:A:1753:ASP:C	1:A:1755:GLY:N	2.77	0.41
1:B:1150:THR:OG1	1:B:1196:THR:HG23	2.21	0.41
1:B:1311:ARG:HD2	1:B:1415:ASP:CG	2.46	0.41
1:B:1726:THR:HA	1:B:1729:SER:HB3	2.03	0.41
1:B:1803:GLY:HA2	1:B:1832:GLN:CB	2.51	0.41
1:B:1836:ILE:O	1:B:1836:ILE:HG22	2.20	0.41
1:A:1050:LEU:CD2	1:A:1083:TYR:CZ	3.05	0.40
1:A:1140:ARG:H	1:A:1140:ARG:HG3	1.53	0.40
1:A:1725:ASN:OD1	1:A:1727:HIS:HB3	2.21	0.40
1:B:1193:MET:HE2	1:B:1207:THR:OG1	2.20	0.40
1:B:1655:LEU:HD23	1:B:1661:LEU:HA	2.03	0.40
1:B:1813:SER:OG	1:B:1825:PHE:HE2	2.04	0.40
1:A:998:PHE:CE1	1:A:1112:GLY:HA2	2.55	0.40
1:A:1542:MET:HE3	1:A:1636:PRO:HD3	2.03	0.40
1:A:1789:THR:O	1:A:1790:GLY:C	2.64	0.40
1:A:1835:SER:C	1:A:1836:ILE:HG13	2.46	0.40
1:B:1061:ARG:HG2	1:B:1061:ARG:HH11	1.86	0.40
1:B:1539:ILE:O	1:B:1540:GLY:C	2.64	0.40
1:A:981:ARG:HB2	1:A:1030:PHE:CD1	2.57	0.40
1:A:1073:MET:HB3	1:A:1074:PRO:HD2	2.03	0.40
1:A:1441:LEU:CD1	1:A:1464:MET:HB2	2.33	0.40
1:A:1538:ILE:HG23	1:A:1654:PHE:CD2	2.55	0.40
1:B:994:PRO:HB2	1:B:996:CYS:O	2.22	0.40
1:B:1239:VAL:HB	1:B:1240:PRO:HD2	2.03	0.40
1:B:1443:HIS:N	1:B:1444:PRO:CD	2.85	0.40
1:A:1008:VAL:HG12	1:A:1010:TYR:CE1	2.57	0.40
1:A:1050:LEU:HD12	1:A:1096:ILE:HD13	2.03	0.40
1:A:1363:VAL:HG23	1:A:1376:TYR:CE1	2.56	0.40
1:A:1464:MET:HE1	1:A:1482:HIS:HB2	2.02	0.40
1:B:1432:VAL:CG1	1:B:1433:SER:N	2.83	0.40
1:B:1625:LYS:O	1:B:1629:GLU:HB2	2.22	0.40
1:A:1139:HIS:HD2	1:A:1151:TRP:CH2	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1194:ASP:OD1	1:A:1206:ARG:HB2	2.21	0.40
1:A:1228:GLN:HE21	1:A:1228:GLN:HB2	1.61	0.40
1:A:1271:ILE:HA	1:A:1272:PRO:HD3	1.92	0.40
1:A:1809:VAL:HG13	1:A:1809:VAL:O	2.22	0.40
1:A:1844:SER:OG	1:A:1846:HIS:HD2	2.05	0.40
1:B:1108:SER:C	1:B:1110:LEU:H	2.28	0.40
1:B:1844:SER:OG	1:B:1846:HIS:HD2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	888/908 (98%)	750 (84%)	109 (12%)	29 (3%)	3	11
1	B	888/908 (98%)	745 (84%)	111 (12%)	32 (4%)	2	10
All	All	1776/1816 (98%)	1495 (84%)	220 (12%)	61 (3%)	3	11

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1031	PRO
1	A	1136	GLU
1	A	1347	GLY
1	A	1443	HIS
1	A	1445	PRO
1	A	1631	VAL
1	A	1668	ARG
1	B	1031	PRO
1	B	1136	GLU
1	B	1347	GLY
1	B	1443	HIS

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Mol	Chain	Res	Type
1	B	1445	PRO
1	B	1631	VAL
1	A	1102	GLY
1	A	1559	PHE
1	A	1832	GLN
1	B	1102	GLY
1	B	1188	LEU
1	B	1559	PHE
1	B	1668	ARG
1	B	1832	GLN
1	A	1188	LEU
1	A	1354	VAL
1	B	1338	ASP
1	B	1354	VAL
1	B	1587	ILE
1	B	1732	LYS
1	A	1338	ASP
1	A	1587	ILE
1	A	1745	THR
1	A	1756	GLN
1	B	1515	SER
1	B	1745	THR
1	A	1515	SER
1	A	1678	PRO
1	B	961	GLU
1	B	1209	GLY
1	B	1294	LYS
1	B	1678	PRO
1	B	1786	ASN
1	B	1797	GLY
1	A	961	GLU
1	A	1160	PRO
1	A	1209	GLY
1	A	1797	GLY
1	B	1160	PRO
1	B	1756	GLN
1	A	1448	PRO
1	A	1602	VAL
1	B	1201	PRO
1	A	1201	PRO
1	B	1133	GLY
1	B	1448	PRO

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Mol	Chain	Res	Type
1	A	1433	SER
1	A	1836	ILE
1	A	1133	GLY
1	A	1812	VAL
1	B	1812	VAL
1	B	1836	ILE
1	B	1595	VAL
1	B	1602	VAL

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	773/800 (97%)	685 (89%)	88 (11%)	5	16
1	B	773/800 (97%)	681 (88%)	92 (12%)	5	15
All	All	1546/1600 (97%)	1366 (88%)	180 (12%)	5	16

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	967	TYR
1	A	981	ARG
1	A	985	TRP
1	A	990	SER
1	A	993	VAL
1	A	1002	LEU
1	A	1016	THR
1	A	1019	ILE
1	A	1022	LYS
1	A	1040	LEU
1	A	1064	VAL
1	A	1066	VAL
1	A	1068	LEU
1	A	1072	SER
1	A	1073	MET

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Mol	Chain	Res	Type
1	A	1079	GLU
1	A	1085	VAL
1	A	1103	THR
1	A	1106	TRP
1	A	1121	ARG
1	A	1124	THR
1	A	1126	LEU
1	A	1129	LYS
1	A	1131	LEU
1	A	1140	ARG
1	A	1141	SER
1	A	1156	ARG
1	A	1165	ASN
1	A	1166	SER
1	A	1176	LEU
1	A	1187	LEU
1	A	1188	LEU
1	A	1198	GLN
1	A	1200	LEU
1	A	1207	THR
1	A	1218	LEU
1	A	1224	LEU
1	A	1237	VAL
1	A	1250	ARG
1	A	1294	LYS
1	A	1301	LEU
1	A	1323	ASN
1	A	1349	ILE
1	A	1354	VAL
1	A	1363	VAL
1	A	1372	GLN
1	A	1379	TYR
1	A	1397	GLU
1	A	1406	GLN
1	A	1409	GLU
1	A	1420	ASP
1	A	1423	GLU
1	A	1437	ARG
1	A	1453	ARG
1	A	1462	LEU
1	A	1464	MET
1	A	1484	LEU

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Mol	Chain	Res	Type
1	A	1500	VAL
1	A	1504	ARG
1	A	1508	ILE
1	A	1512	THR
1	A	1542	MET
1	A	1545	SER
1	A	1564	GLU
1	A	1590	ARG
1	A	1609	LEU
1	A	1631	VAL
1	A	1638	LEU
1	A	1642	VAL
1	A	1650	ILE
1	A	1672	ASN
1	A	1673	VAL
1	A	1691	ILE
1	A	1707	ILE
1	A	1716	ILE
1	A	1730	ARG
1	A	1743	GLU
1	A	1745	THR
1	A	1763	LYS
1	A	1765	LEU
1	A	1775	GLN
1	A	1784	PHE
1	A	1794	LEU
1	A	1796	LEU
1	A	1798	TYR
1	A	1810	THR
1	A	1817	SER
1	A	1842	ASN
1	B	967	TYR
1	B	981	ARG
1	B	985	TRP
1	B	990	SER
1	B	993	VAL
1	B	999	VAL
1	B	1002	LEU
1	B	1016	THR
1	B	1019	ILE
1	B	1022	LYS
1	B	1040	LEU

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Mol	Chain	Res	Type
1	B	1064	VAL
1	B	1066	VAL
1	B	1068	LEU
1	B	1072	SER
1	B	1073	MET
1	B	1079	GLU
1	B	1082	LEU
1	B	1085	VAL
1	B	1086	LEU
1	B	1103	THR
1	B	1106	TRP
1	B	1120	ILE
1	B	1121	ARG
1	B	1124	THR
1	B	1126	LEU
1	B	1129	LYS
1	B	1131	LEU
1	B	1140	ARG
1	B	1141	SER
1	B	1156	ARG
1	B	1165	ASN
1	B	1166	SER
1	B	1176	LEU
1	B	1186	LEU
1	B	1187	LEU
1	B	1188	LEU
1	B	1198	GLN
1	B	1200	LEU
1	B	1207	THR
1	B	1218	LEU
1	B	1224	LEU
1	B	1237	VAL
1	B	1250	ARG
1	B	1294	LYS
1	B	1301	LEU
1	B	1323	ASN
1	B	1349	ILE
1	B	1354	VAL
1	B	1363	VAL
1	B	1372	GLN
1	B	1397	GLU
1	B	1406	GLN

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Mol	Chain	Res	Type
1	B	1409	GLU
1	B	1420	ASP
1	B	1423	GLU
1	B	1437	ARG
1	B	1453	ARG
1	B	1462	LEU
1	B	1464	MET
1	B	1484	LEU
1	B	1500	VAL
1	B	1504	ARG
1	B	1508	ILE
1	B	1512	THR
1	B	1528	THR
1	B	1542	MET
1	B	1545	SER
1	B	1564	GLU
1	B	1590	ARG
1	B	1609	LEU
1	B	1631	VAL
1	B	1638	LEU
1	B	1642	VAL
1	B	1650	ILE
1	B	1672	ASN
1	B	1673	VAL
1	B	1691	ILE
1	B	1707	ILE
1	B	1716	ILE
1	B	1730	ARG
1	B	1743	GLU
1	B	1745	THR
1	B	1763	LYS
1	B	1765	LEU
1	B	1775	GLN
1	B	1784	PHE
1	B	1796	LEU
1	B	1798	TYR
1	B	1810	THR
1	B	1817	SER
1	B	1842	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1028	ASN
1	A	1045	HIS
1	A	1047	ASN
1	A	1051	GLN
1	A	1058	ASN
1	A	1165	ASN
1	A	1183	HIS
1	A	1189	ASN
1	A	1191	ASN
1	A	1227	GLN
1	A	1228	GLN
1	A	1255	ASN
1	A	1372	GLN
1	A	1406	GLN
1	A	1467	GLN
1	A	1468	GLN
1	A	1478	HIS
1	A	1503	GLN
1	A	1522	HIS
1	A	1585	ASN
1	A	1592	GLN
1	A	1610	GLN
1	A	1653	GLN
1	A	1672	ASN
1	A	1706	HIS
1	A	1792	ASN
1	A	1846	HIS
1	B	1028	ASN
1	B	1045	HIS
1	B	1047	ASN
1	B	1051	GLN
1	B	1058	ASN
1	B	1149	HIS
1	B	1165	ASN
1	B	1183	HIS
1	B	1227	GLN
1	B	1228	GLN
1	B	1255	ASN
1	B	1323	ASN
1	B	1372	GLN
1	B	1406	GLN
1	B	1467	GLN
1	B	1468	GLN

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Mol	Chain	Res	Type
1	B	1478	HIS
1	B	1503	GLN
1	B	1522	HIS
1	B	1585	ASN
1	B	1592	GLN
1	B	1610	GLN
1	B	1653	GLN
1	B	1672	ASN
1	B	1706	HIS
1	B	1792	ASN
1	B	1846	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 monosaccharides 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	GLC	C	1	2	12,12,12	1.55	3 (25%)	17,17,17	2.74	4 (23%)
2	GLC	C	2	2	11,11,12	1.79	5 (45%)	15,15,17	2.33	4 (26%)
2	AC1	C	3	2	21,22,23	2.00	8 (38%)	22,32,34	1.14	3 (13%)
2	GLC	D	1	2	12,12,12	1.59	2 (16%)	17,17,17	2.42	3 (17%)
2	GLC	D	2	2	11,11,12	1.89	4 (36%)	15,15,17	0.89	1 (6%)
2	AC1	D	3	2	21,22,23	1.89	6 (28%)	22,32,34	1.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2	-	2/2/22/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	AC1	C	3	2	-	3/6/43/46	0/2/2/2
2	GLC	D	1	2	-	1/2/22/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1
2	AC1	D	3	2	-	4/6/43/46	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	AC1	C7B-C5B	3.99	1.38	1.32
2	D	2	GLC	O5-C1	-3.97	1.37	1.43
2	C	3	AC1	C3B-C4A	-3.75	1.47	1.53
2	D	3	AC1	C4A-C5B	-3.69	1.48	1.51
2	D	1	GLC	O2-C2	3.37	1.51	1.43
2	C	3	AC1	C7B-C5B	3.33	1.37	1.32
2	C	3	AC1	C4A-C5B	-3.29	1.48	1.51
2	C	3	AC1	O2-C2	-3.08	1.36	1.43
2	C	2	GLC	O5-C1	-2.93	1.38	1.43
2	C	2	GLC	O5-C5	-2.92	1.37	1.43
2	C	1	GLC	O2-C2	2.84	1.50	1.43
2	C	3	AC1	C3-C4	-2.74	1.48	1.53
2	D	3	AC1	C3-C4	-2.51	1.48	1.53
2	D	2	GLC	O5-C5	-2.47	1.38	1.43
2	D	3	AC1	O2-C2	-2.45	1.38	1.43
2	C	1	GLC	C6-C5	2.36	1.59	1.51
2	C	3	AC1	O4-C4A	-2.35	1.37	1.42
2	C	2	GLC	O3-C3	-2.30	1.37	1.43
2	C	2	GLC	O2-C2	-2.29	1.38	1.43
2	C	1	GLC	C4-C3	-2.25	1.46	1.52
2	D	1	GLC	C6-C5	2.25	1.59	1.51
2	D	2	GLC	O3-C3	-2.23	1.37	1.43
2	D	2	GLC	O2-C2	-2.18	1.38	1.43
2	D	3	AC1	O2B-C2B	-2.16	1.37	1.43
2	C	3	AC1	O3B-C3B	-2.06	1.37	1.43
2	D	3	AC1	C3B-C4A	-2.04	1.50	1.53
2	C	2	GLC	C4-C5	-2.03	1.48	1.53
2	C	3	AC1	O3-C3	2.02	1.48	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GLC	O5-C5-C4	7.73	123.62	109.70
2	D	1	GLC	O5-C5-C4	7.21	122.68	109.70
2	C	1	GLC	C1-C2-C3	6.60	123.83	110.36
2	D	1	GLC	C1-C2-C3	5.64	121.85	110.36
2	C	2	GLC	C1-C2-C3	5.52	117.69	109.64
2	C	2	GLC	C1-O5-C5	4.02	117.57	112.19
2	C	2	GLC	O5-C1-C2	3.38	118.84	110.79
2	C	3	AC1	C6-C5-C4	-2.68	108.66	113.57
2	C	2	GLC	C2-C3-C4	2.55	115.34	110.86
2	C	3	AC1	O3-C3-C4	2.47	114.51	109.58
2	C	1	GLC	C3-C4-C5	-2.42	105.85	110.23
2	C	1	GLC	O5-C1-C2	2.34	114.41	110.30
2	C	3	AC1	O4-C4A-C3B	-2.27	105.81	110.53
2	D	1	GLC	C6-C5-C4	-2.26	107.47	113.02
2	D	2	GLC	O6-C6-C5	-2.05	104.34	111.33

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	AC1	C7B-C5B-C6B-O6B
2	D	3	AC1	C4A-C5B-C6B-O6B
2	D	2	GLC	O5-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6
2	C	3	AC1	C4A-C5B-C6B-O6B
2	C	3	AC1	C7B-C1B-N4A-C4
2	D	3	AC1	C7B-C1B-N4A-C4
2	D	3	AC1	C3-C4-N4A-C1B
2	D	3	AC1	C7B-C5B-C6B-O6B

There are no ring outliers.

4 monomers are involved in 9 short contacts:

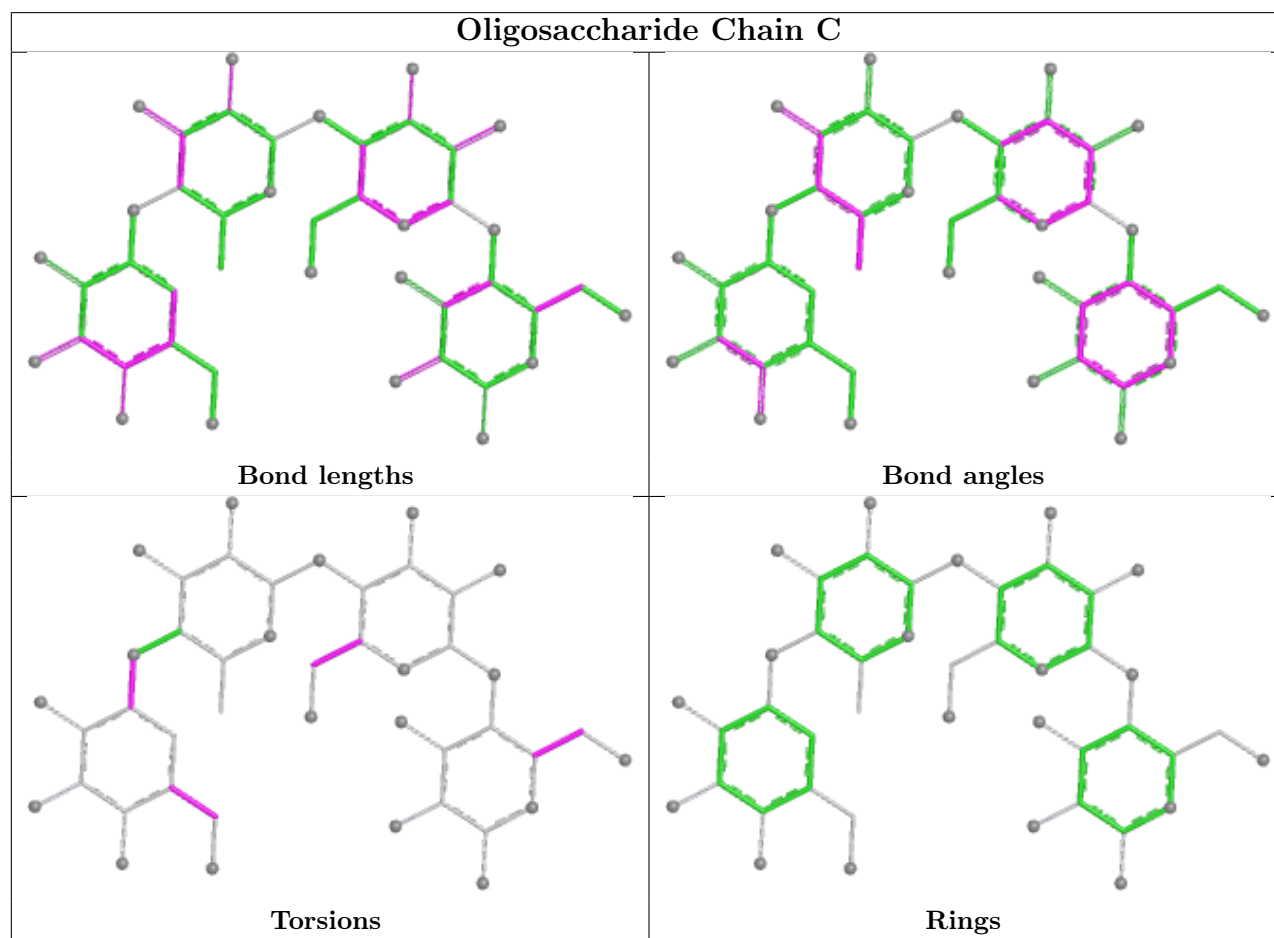
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	GLC	5	0

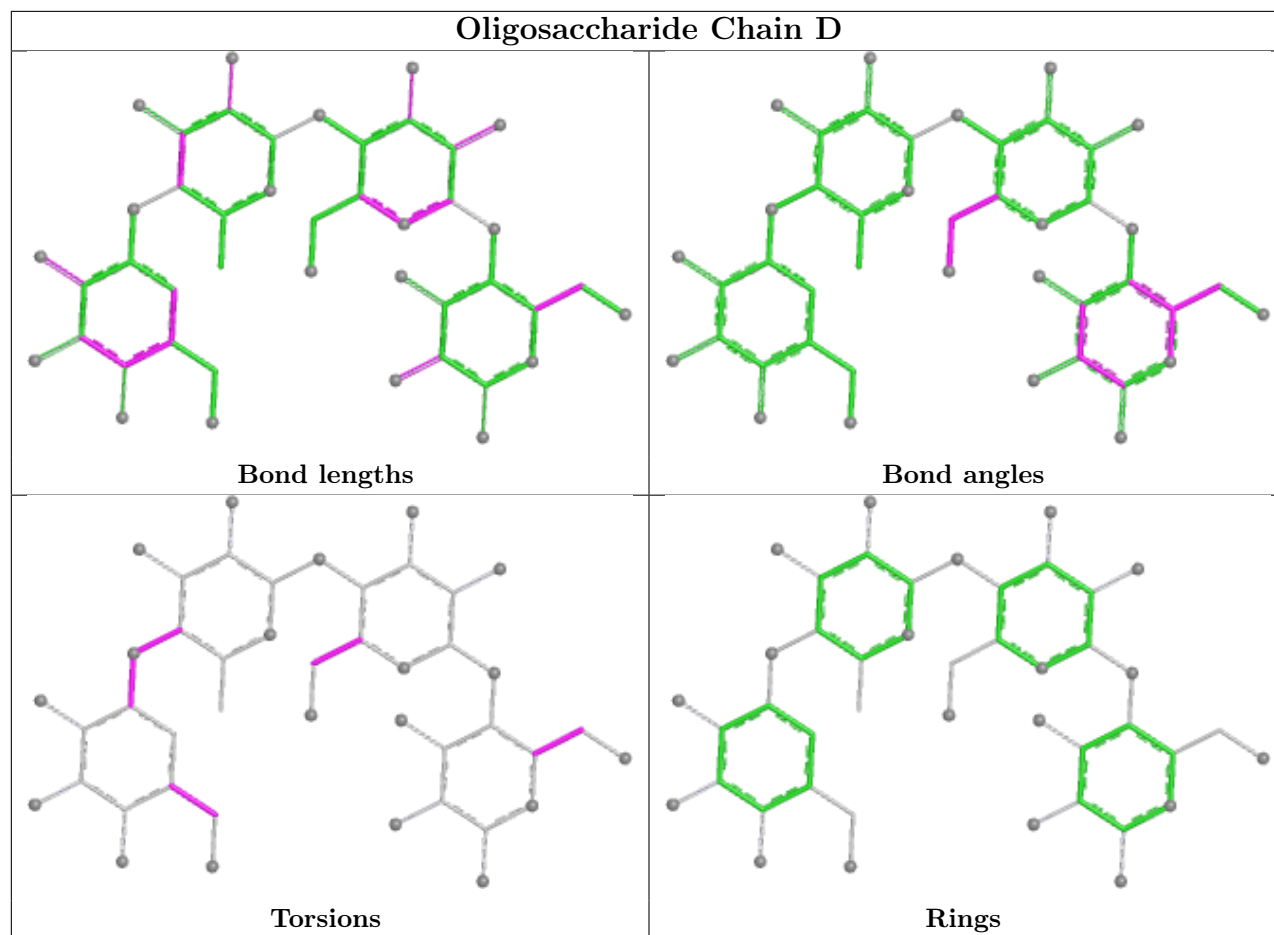
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	AC1	1	0
2	C	1	GLC	5	0
2	C	3	AC1	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	890/908 (98%)	0.24	23 (2%) 57 48	45, 81, 135, 207	0
1	B	890/908 (98%)	0.21	30 (3%) 48 39	50, 85, 141, 211	0
All	All	1780/1816 (98%)	0.22	53 (2%) 52 44	45, 83, 137, 211	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1849	THR	5.1
1	A	1752	TRP	4.8
1	A	1812	VAL	4.7
1	B	1812	VAL	4.2
1	B	1815	SER	4.1
1	A	1849	THR	3.9
1	A	1361	VAL	3.7
1	B	1443	HIS	3.5
1	A	1809	VAL	3.4
1	A	1645	GLN	3.4
1	A	1443	HIS	3.4
1	A	1362	VAL	3.4
1	A	1810	THR	3.2
1	B	1810	THR	3.2
1	B	1809	VAL	3.0
1	B	1733	PHE	3.0
1	B	1752	TRP	3.0
1	A	1323	ASN	2.9
1	B	1599	VAL	2.9
1	B	1820	VAL	2.9
1	B	1765	LEU	2.9
1	B	1816	VAL	2.8
1	A	1821	ILE	2.8
1	A	1842	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1765	LEU	2.8
1	B	1025	VAL	2.7
1	B	1825	PHE	2.6
1	B	1363	VAL	2.6
1	B	1813	SER	2.6
1	A	1516	SER	2.5
1	B	1848	PHE	2.5
1	B	1717	LEU	2.5
1	A	1782	ILE	2.4
1	B	1245	GLY	2.4
1	B	1388	ASN	2.4
1	B	1845	LEU	2.4
1	B	1823	PRO	2.4
1	A	1806	SER	2.4
1	A	1375	LEU	2.3
1	A	1825	PHE	2.3
1	B	1023	SER	2.3
1	A	1009	GLN	2.2
1	B	1836	ILE	2.2
1	A	1813	SER	2.2
1	B	1520	ALA	2.2
1	B	1799	ILE	2.1
1	A	1816	VAL	2.1
1	B	1323	ASN	2.1
1	B	1843	ILE	2.1
1	A	1258	GLU	2.1
1	A	1144	ARG	2.0
1	B	1803	GLY	2.0
1	B	1369	TRP	2.0

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

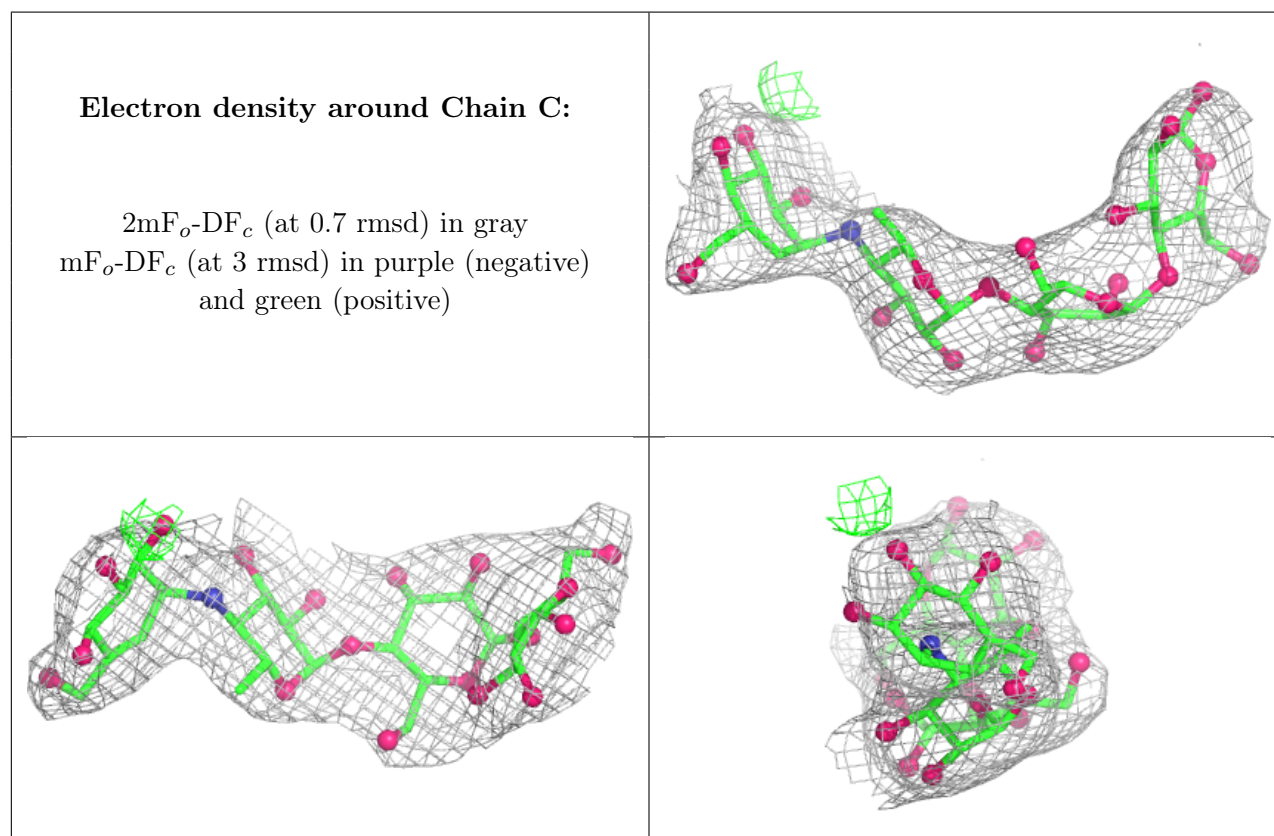
There are no non-standard protein/DNA/RNA residues in this entry.

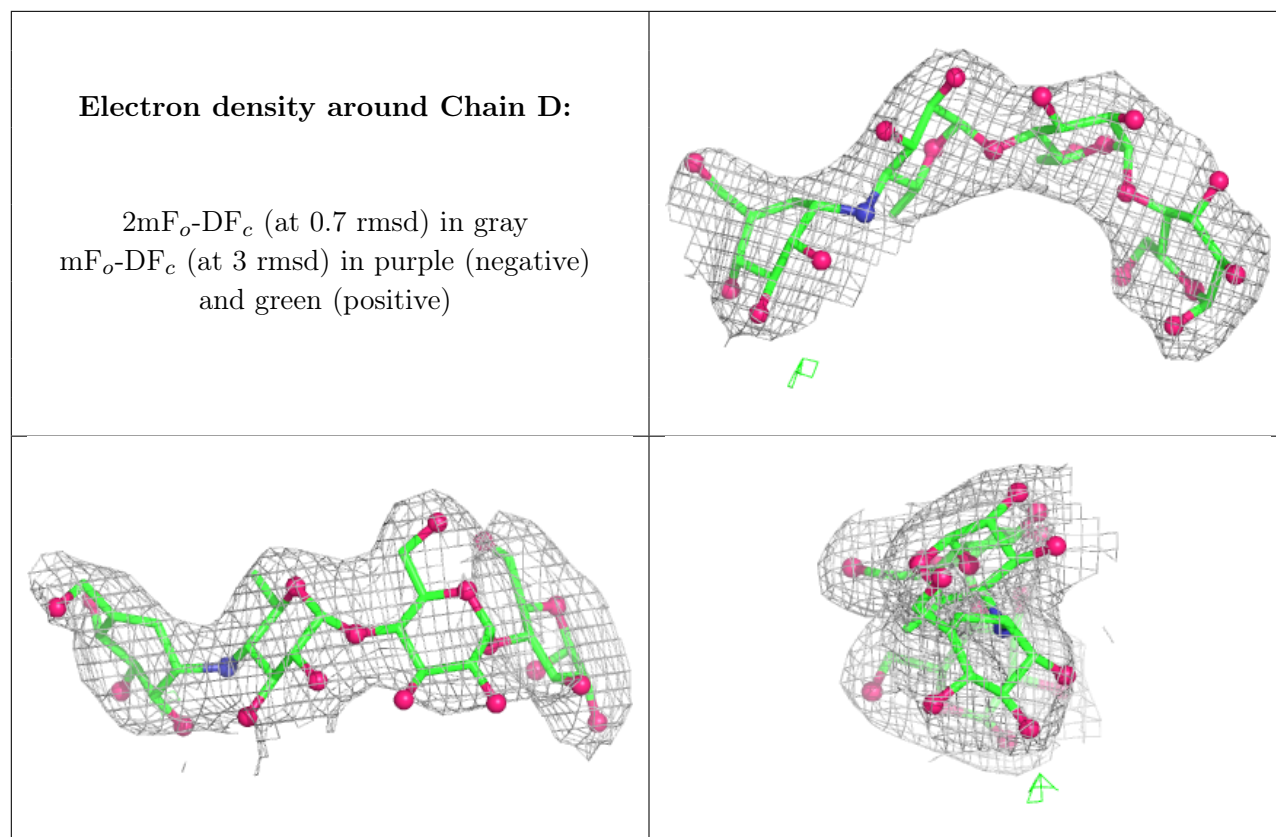
6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	C	1	12/12	0.87	0.11	85,104,117,124	0
2	GLC	D	1	12/12	0.89	0.09	78,88,120,121	0
2	GLC	D	2	11/12	0.93	0.09	54,84,95,102	0
2	GLC	C	2	11/12	0.94	0.10	77,83,115,123	0
2	AC1	C	3	21/22	0.94	0.11	53,73,89,115	0
2	AC1	D	3	21/22	0.96	0.09	56,81,104,109	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.