



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:22 PM EDT

PDB ID : 4E0S / pdb_00004e0s
Title : Crystal Structure of C5b-6
Authors : Aleshin, A.E.; Stec, B.; DiScipio, R.; Liddington, R.C.
Deposited on : 2012-03-05
Resolution : 4.21 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

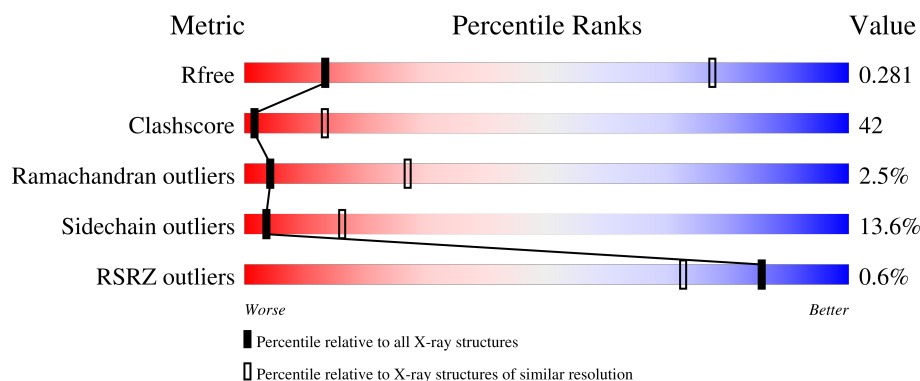
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.21 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	1014 (4.56-3.88)
Clashscore	190562	1033 (4.54-3.90)
Ramachandran outliers	187476	1002 (4.58-3.86)
Sidechain outliers	187428	1030 (4.60-3.84)
RSRZ outliers	180081	1011 (4.56-3.88)

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	1676	
2	B	913	
3	C	2	
3	D	2	
4	E	2	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 19475 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 Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1552	Total	C	N	O	S	0	0	0
			12306	7891	2011	2359	45			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	802	ILE	VAL	SEE REMARK 999	UNP P01031

- Molecule 2 is a protein called Complement component C6.

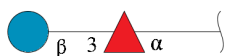
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	898	Total	C	N	O	S	0	0	0
			7046	4353	1239	1383	71			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	E	2	Total	C	O	0	0	0
			21	12	9			

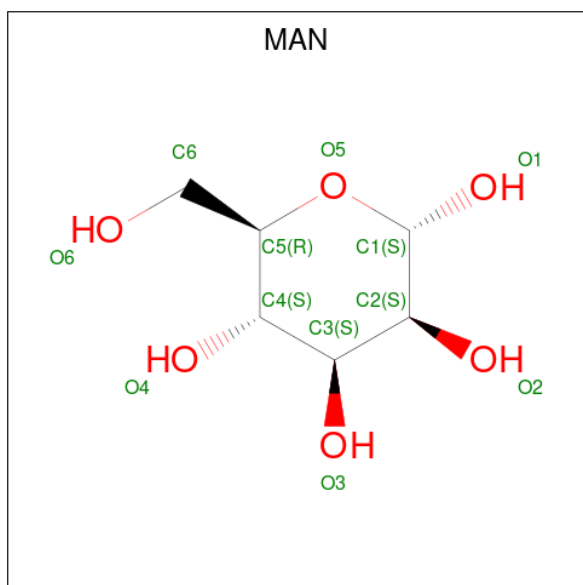
- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		

- Molecule 7 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		

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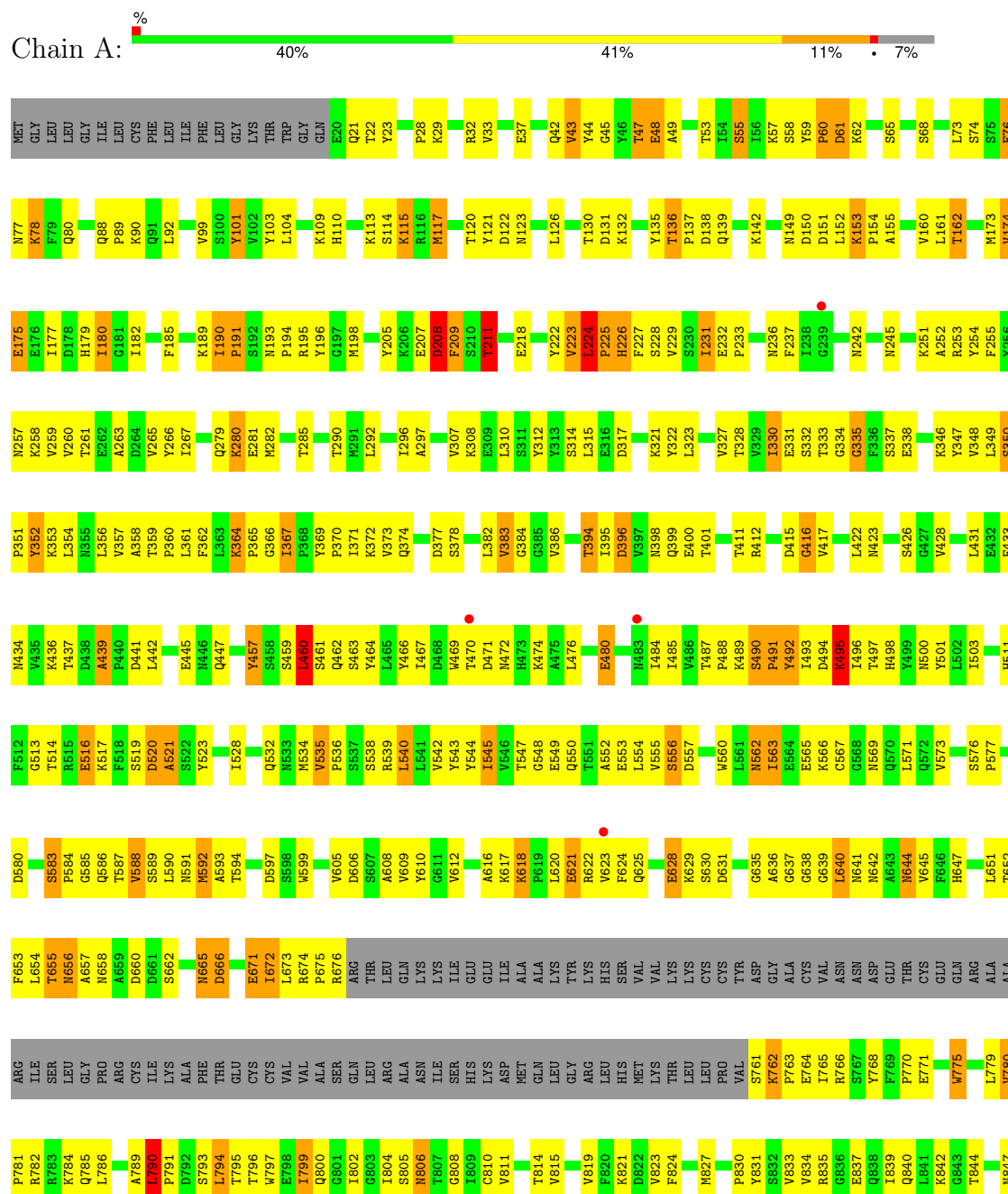
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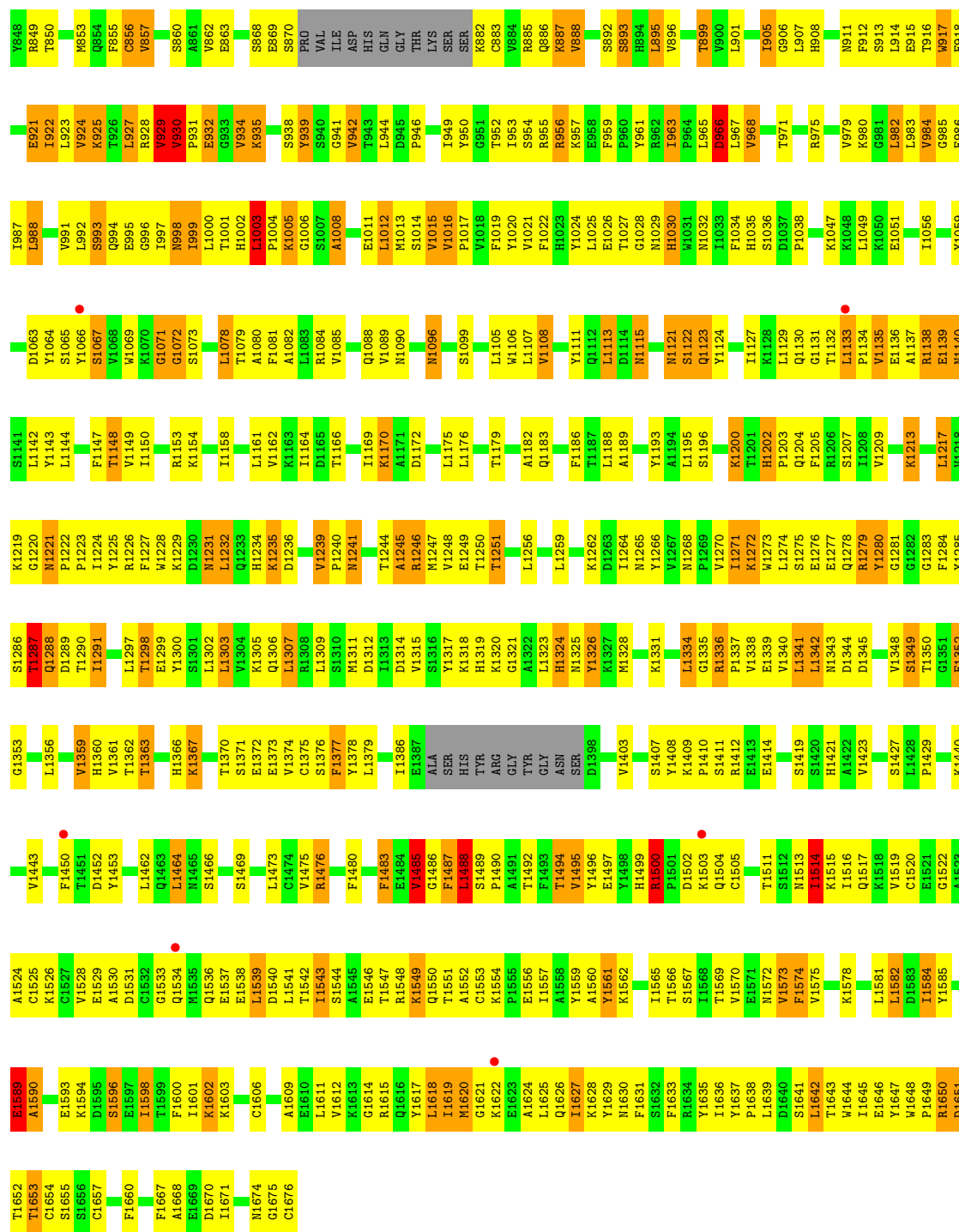
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		

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.

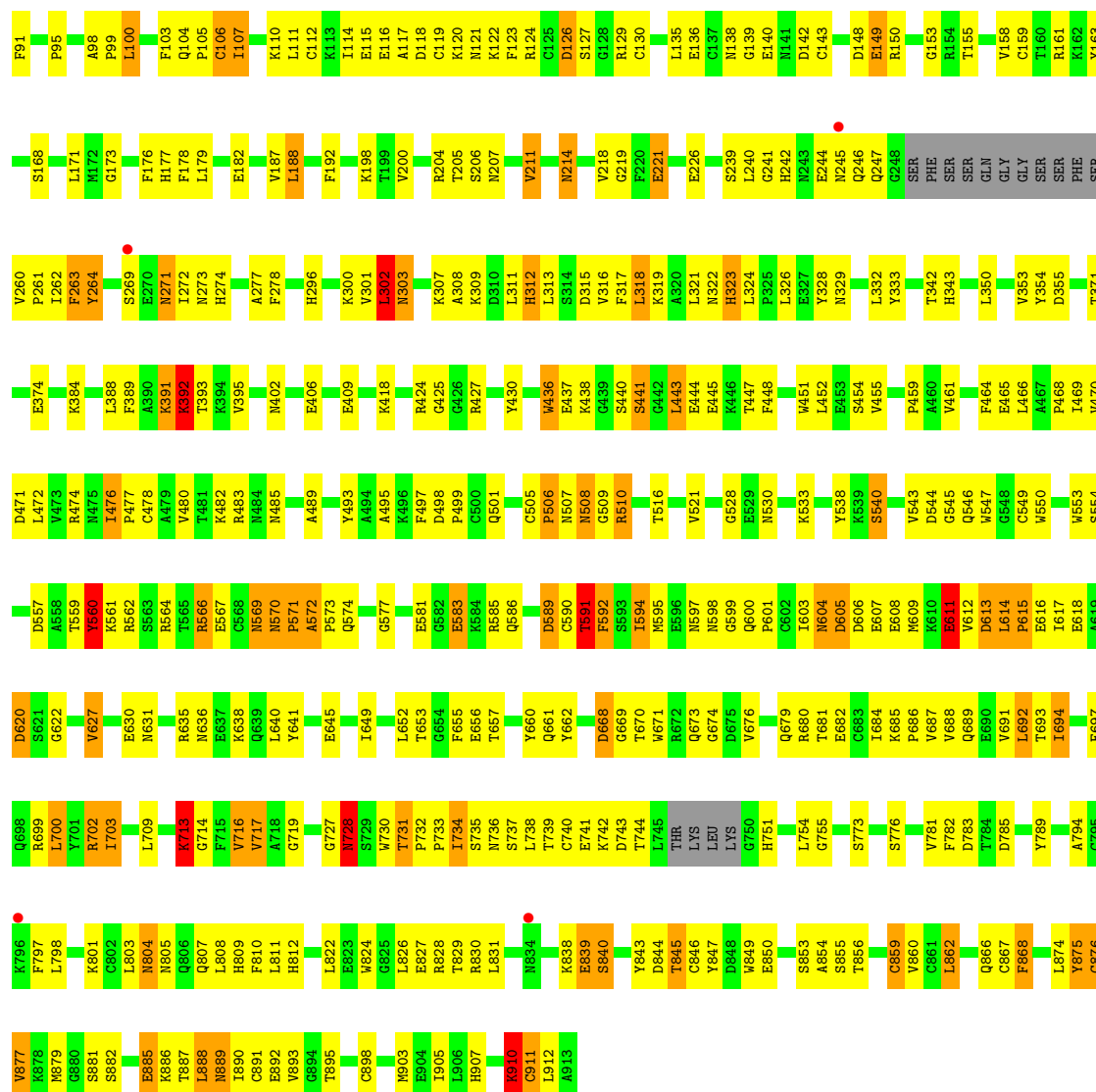
• Molecule 1: Complement C5





• Molecule 2: Complement component C6





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose

Chain E:



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	158.95Å 227.53Å 278.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 4.21 29.93 – 4.21	Depositor EDS
% Data completeness (in resolution range)	81.8 (29.93-4.21) 81.8 (29.93-4.21)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 4.26Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.218 , 0.278 0.219 , 0.281	Depositor DCC
R_{free} test set	1529 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å ²)	113.5	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 130.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19475	wwPDB-VP
Average B, all atoms (Å ²)	192.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: BGC, NAG, NA, FUC, CA, MAN

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	0.80	2/12576 (0.0%)	1.17	92/17068 (0.5%)
2	B	0.79	1/7193 (0.0%)	1.16	55/9708 (0.6%)
All	All	0.80	3/19769 (0.0%)	1.17	147/26776 (0.5%)

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	2
2	B	0	3
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1067	SER	CA-C	6.29	1.60	1.52
1	A	775	TRP	CA-C	-5.53	1.47	1.53
2	B	106	CYS	CA-C	5.31	1.59	1.52

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1584	ILE	N-CA-C	13.29	123.81	111.45
1	A	618	LYS	CA-C-N	-10.30	110.21	120.31
1	A	618	LYS	C-N-CA	-10.30	110.21	120.31
1	A	190	ILE	CA-C-N	9.74	132.02	119.84
1	A	190	ILE	C-N-CA	9.74	132.02	119.84
1	A	930	VAL	CA-C-N	9.49	130.24	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	930	VAL	C-N-CA	9.49	130.24	119.99
1	A	966	ASP	N-CA-C	-9.46	100.27	114.64
2	B	839	GLU	N-CA-C	9.39	121.28	111.14
1	A	1071	GLY	N-CA-C	-9.32	101.55	112.73
1	A	1123	GLN	N-CA-C	-8.94	101.95	112.86
2	B	73	ASP	CA-C-N	-8.80	108.84	119.84
2	B	73	ASP	C-N-CA	-8.80	108.84	119.84
2	B	572	ALA	CA-C-N	8.69	128.73	119.78
2	B	572	ALA	C-N-CA	8.69	128.73	119.78
1	A	1034	PHE	N-CA-C	8.64	121.47	111.11
2	B	627	VAL	CB-CA-C	-8.54	100.96	111.04
1	A	1189	ALA	N-CA-C	8.20	119.91	110.97
2	B	570	ASN	CA-C-N	8.15	130.03	119.84
2	B	570	ASN	C-N-CA	8.15	130.03	119.84
2	B	106	CYS	N-CA-C	8.07	120.38	108.60
2	B	53	ASN	CA-C-N	7.80	131.05	120.44
2	B	53	ASN	C-N-CA	7.80	131.05	120.44
1	A	1287	THR	CA-C-N	-7.38	110.90	120.65
1	A	1287	THR	C-N-CA	-7.38	110.90	120.65
2	B	242	HIS	N-CA-C	7.34	118.93	111.07
1	A	1561	TYR	N-CA-C	7.22	119.54	108.42
1	A	998	ASN	CA-C-N	-7.17	111.74	120.70
1	A	998	ASN	C-N-CA	-7.17	111.74	120.70
1	A	1121	ASN	N-CA-C	7.16	119.09	111.28
2	B	264	TYR	N-CA-C	7.13	119.01	108.60
2	B	731	THR	C-N-CD	-7.08	105.03	120.60
2	B	840	SER	N-CA-C	7.05	119.15	110.91
2	B	853	SER	N-CA-C	7.00	119.48	110.65
2	B	856	THR	N-CA-C	-6.96	103.70	111.28
2	B	50	ARG	N-CA-C	6.75	117.49	108.38
2	B	107	ILE	N-CA-C	6.75	115.64	107.61
2	B	425	GLY	N-CA-C	6.69	118.87	112.04
2	B	98	ALA	CA-C-N	6.69	128.20	119.84
2	B	98	ALA	C-N-CA	6.69	128.20	119.84
1	A	642	ASN	N-CA-C	-6.60	104.25	112.90
1	A	1239	VAL	CA-C-N	6.60	126.04	118.85
1	A	1239	VAL	C-N-CA	6.60	126.04	118.85
1	A	439	ALA	CA-C-N	6.54	126.23	119.56
1	A	439	ALA	C-N-CA	6.54	126.23	119.56
2	B	674	GLY	N-CA-C	6.50	119.47	112.33
1	A	257	ASN	N-CA-C	6.35	120.60	112.86
1	A	226	HIS	N-CA-C	6.33	117.84	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1349	SER	N-CA-C	6.33	118.38	107.93
1	A	834	VAL	CB-CA-C	-6.27	103.37	110.96
1	A	92	LEU	CA-C-N	6.25	125.66	118.85
1	A	92	LEU	C-N-CA	6.25	125.66	118.85
2	B	591	THR	N-CA-C	6.24	117.66	108.86
1	A	211	THR	N-CA-C	6.20	118.98	110.24
1	A	556	SER	N-CA-C	6.19	118.18	108.96
2	B	616	GLU	N-CA-C	6.08	123.76	110.80
2	B	391	LYS	N-CA-C	-6.04	101.10	110.10
1	A	88	GLN	CA-C-N	6.03	127.38	119.84
1	A	88	GLN	C-N-CA	6.03	127.38	119.84
1	A	1224	ILE	N-CA-C	-6.02	106.94	112.96
1	A	666	ASP	N-CA-C	6.01	117.50	111.07
2	B	510	ARG	CB-CA-C	6.01	116.12	110.17
2	B	888	LEU	N-CA-C	6.00	118.29	109.24
1	A	780	VAL	N-CA-C	5.95	113.97	107.60
1	A	621	GLU	N-CA-C	-5.91	104.02	111.11
1	A	350	SER	CA-C-N	5.89	125.59	119.64
1	A	350	SER	C-N-CA	5.89	125.59	119.64
1	A	352	TYR	N-CA-C	5.87	118.33	109.23
1	A	790	LEU	CA-C-N	5.84	125.79	119.78
1	A	790	LEU	C-N-CA	5.84	125.79	119.78
2	B	717	VAL	N-CA-C	5.83	116.58	109.30
1	A	1286	SER	N-CA-C	5.70	118.84	109.72
2	B	570	ASN	C-N-CD	-5.67	101.73	125.00
1	A	245	ASN	N-CA-C	5.67	117.61	108.32
2	B	866	GLN	N-CA-C	5.67	119.71	112.34
1	A	224	LEU	CA-C-N	5.63	126.87	119.84
1	A	224	LEU	C-N-CA	5.63	126.87	119.84
2	B	540	SER	N-CA-C	5.62	117.65	108.55
2	B	24	SER	N-CA-C	5.56	117.64	109.24
2	B	302	LEU	CA-C-N	-5.55	112.64	122.74
2	B	302	LEU	C-N-CA	-5.55	112.64	122.74
1	A	1574	PHE	N-CA-C	5.54	118.29	109.81
1	A	208	ASP	N-CA-C	5.54	119.76	112.89
1	A	930	VAL	N-CA-C	5.53	113.98	107.84
2	B	207	ASN	N-CA-C	5.53	117.71	110.08
1	A	433	PHE	N-CA-C	5.52	117.90	108.90
1	A	1288	GLN	N-CA-CB	5.51	117.96	109.91
1	A	521	ALA	N-CA-C	5.45	119.89	112.04
1	A	520	ASP	N-CA-C	5.44	117.97	111.71
2	B	560	TYR	CA-CB-CG	5.44	123.69	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	90	GLN	N-CA-C	5.41	117.48	108.99
2	B	673	GLN	N-CA-C	5.41	117.33	108.52
1	A	1067	SER	O-C-N	-5.40	115.55	122.94
1	A	1241	ASN	N-CA-C	5.39	117.16	111.28
1	A	117	MET	N-CA-C	5.38	118.83	108.45
1	A	1008	ALA	N-CA-C	-5.35	105.45	111.28
1	A	583	SER	CA-C-N	5.33	126.50	119.84
1	A	583	SER	C-N-CA	5.33	126.50	119.84
1	A	174	VAL	N-CA-C	5.32	114.87	108.06
2	B	910	LYS	N-CA-C	5.31	122.11	110.80
1	A	460	LEU	N-CA-C	-5.31	104.91	111.33
1	A	671	GLU	N-CA-C	-5.31	101.05	108.96
1	A	885	ARG	N-CA-C	5.30	117.38	109.59
1	A	1239	VAL	N-CA-C	5.29	113.53	109.19
2	B	392	LYS	N-CA-C	5.26	118.16	109.85
1	A	1202	HIS	N-CA-C	5.26	117.05	109.48
1	A	279	GLN	N-CA-C	5.25	115.06	108.45
1	A	1272	LYS	N-CA-C	-5.25	105.25	110.97
1	A	153	LYS	CA-C-N	5.24	126.39	119.84
1	A	153	LYS	C-N-CA	5.24	126.39	119.84
2	B	611	GLU	N-CA-C	5.24	116.99	111.28
2	B	308	ALA	N-CA-C	5.23	116.79	111.14
1	A	416	GLY	N-CA-C	-5.23	108.41	115.21
2	B	830	ARG	N-CA-C	-5.20	107.07	113.41
2	B	669	GLY	N-CA-C	-5.18	108.52	114.69
2	B	713	LYS	N-CA-C	5.18	116.62	111.07
1	A	101	TYR	N-CA-C	5.17	117.05	109.24
1	A	868	SER	N-CA-C	5.17	116.60	111.07
1	A	367	ILE	N-CA-C	-5.15	103.19	109.01
2	B	614	LEU	CA-C-N	5.15	126.27	119.84
2	B	614	LEU	C-N-CA	5.15	126.27	119.84
1	A	185	PHE	CA-C-N	5.12	125.05	119.78
1	A	185	PHE	C-N-CA	5.12	125.05	119.78
1	A	1336	ARG	CA-C-N	5.12	126.24	119.84
1	A	1336	ARG	C-N-CA	5.12	126.24	119.84
2	B	505	CYS	CA-C-N	5.12	126.23	119.84
2	B	505	CYS	C-N-CA	5.12	126.23	119.84
1	A	929	VAL	N-CA-C	5.11	116.02	108.45
1	A	616	ALA	N-CA-C	5.11	117.90	109.72
1	A	519	SER	CA-C-N	5.11	127.64	120.28
1	A	519	SER	C-N-CA	5.11	127.64	120.28
1	A	1485	VAL	N-CA-C	-5.09	101.25	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	999	ILE	N-CA-CB	5.09	116.16	110.62
2	B	239	SER	N-CA-C	5.08	116.82	111.28
2	B	808	LEU	N-CA-C	5.08	116.88	108.20
2	B	211	VAL	CA-C-N	5.07	125.08	120.21
2	B	211	VAL	C-N-CA	5.07	125.08	120.21
1	A	856	CYS	N-CA-C	5.07	115.82	107.20
1	A	1359	VAL	N-CA-C	5.06	115.37	107.99
1	A	280	LYS	N-CA-C	5.05	115.82	108.14
1	A	1182	ALA	N-CA-C	5.03	117.84	110.30
2	B	221	GLU	N-CA-C	5.03	116.39	109.15
1	A	1488	LEU	N-CA-C	5.02	115.67	108.74
1	A	1003	LEU	CA-C-N	5.00	126.09	119.84
1	A	1003	LEU	C-N-CA	5.00	126.09	119.84
1	A	1500	ARG	CA-C-N	5.00	126.09	119.84
1	A	1500	ARG	C-N-CA	5.00	126.09	119.84

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	90	LYS	Peptide
1	A	985	GLY	Peptide
2	B	391	LYS	Peptide
2	B	599	GLY	Peptide
2	B	731	THR	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	12306	0	12238	1143	0
2	B	7046	0	6708	496	0
3	C	28	0	25	1	0
3	D	28	0	25	3	0
4	E	21	0	19	0	0
5	A	1	0	0	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	44	0	40	7	0
All	All	19475	0	19055	1604	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 42.

All (1604) 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:A:1598:ILE:HG21	1:A:1637:TYR:CE2	1.45	1.52
1:A:21:GLN:NE2	1:A:45:GLY:HA2	1.32	1.45
1:A:1013:MET:SD	1:A:1129:LEU:HG	1.65	1.35
1:A:1127:ILE:HD12	1:A:1130:GLN:NE2	1.36	1.35
1:A:1539:LEU:HD22	1:A:1540:ASP:N	1.48	1.27
1:A:1598:ILE:CG2	1:A:1637:TYR:HE2	1.46	1.26
1:A:1133:LEU:C	1:A:1133:LEU:HD23	1.61	1.23
1:A:1249:GLU:CG	1:A:1289:ASP:HB3	1.66	1.23
1:A:991:VAL:C	1:A:992:LEU:HD12	1.65	1.22
2:B:655:PHE:HA	2:B:680:ARG:HB3	1.20	1.19
1:A:351:PRO:CG	1:A:442:LEU:HD11	1.71	1.19
1:A:1239:VAL:CG1	1:A:1240:PRO:HD2	1.71	1.18
2:B:734:ILE:HG13	2:B:738:LEU:HB3	1.23	1.17
1:A:21:GLN:HE22	1:A:45:GLY:CA	1.58	1.17
1:A:1538:GLU:CG	1:A:1539:LEU:HD13	1.75	1.16
1:A:59:TYR:CG	1:A:60:PRO:HD2	1.82	1.15
1:A:987:ILE:C	1:A:988:LEU:HD23	1.70	1.15
1:A:672:ILE:HD12	1:A:673:LEU:N	1.60	1.14
1:A:1029:ASN:O	1:A:1030:HIS:CD2	2.00	1.14
2:B:493:TYR:CZ	2:B:497:PHE:CZ	2.36	1.13
1:A:1648:TRP:HB3	1:A:1660:PHE:HE2	1.05	1.12
2:B:543:VAL:CG1	2:B:574:GLN:HB2	1.79	1.11
1:A:991:VAL:CG1	1:A:992:LEU:H	1.63	1.11
2:B:244:GLU:HB3	2:B:269:SER:HA	1.09	1.09
1:A:1005:LYS:HD2	1:A:1005:LYS:C	1.75	1.09
1:A:334:GLY:HA2	1:A:844:THR:HG21	1.27	1.09
1:A:1598:ILE:CG2	1:A:1637:TYR:CE2	2.27	1.09
1:A:351:PRO:HG3	1:A:442:LEU:HD11	1.10	1.09
1:A:131:ASP:HA	1:A:775:TRP:CH2	1.88	1.08
1:A:1016:VAL:HG12	1:A:1017:PRO:HD3	1.17	1.08
1:A:374:GLN:HE22	1:A:675:PRO:HB3	1.12	1.08
1:A:1225:TYR:CE1	1:A:1276:GLU:HG3	1.89	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:991:VAL:O	1:A:992:LEU:HD12	1.52	1.07
2:B:119:CYS:HB3	2:B:124:ARG:HE	0.93	1.07
1:A:1589:GLU:HG2	1:A:1590:ALA:H	1.19	1.06
1:A:1231:ASN:C	1:A:1232:LEU:HD12	1.79	1.06
1:A:461:SER:CB	1:A:463:SER:HB3	1.87	1.05
1:A:1538:GLU:HG2	1:A:1539:LEU:CD1	1.86	1.05
1:A:1013:MET:HB2	1:A:1129:LEU:HD21	1.36	1.05
1:A:1287:THR:HA	1:A:1290:THR:HG22	1.34	1.04
2:B:75:CYS:SG	2:B:319:LYS:HE3	1.97	1.04
1:A:1249:GLU:HG2	1:A:1289:ASP:CB	1.85	1.04
2:B:438:LYS:HA	2:B:441:SER:HB2	1.37	1.04
1:A:374:GLN:NE2	1:A:675:PRO:HB3	1.73	1.04
1:A:1538:GLU:HG2	1:A:1539:LEU:H	1.16	1.04
2:B:178:PHE:HE2	2:B:262:ILE:HD11	1.18	1.03
1:A:1016:VAL:HG12	1:A:1017:PRO:CD	1.89	1.03
2:B:73:ASP:H	2:B:74:PRO:CD	1.66	1.03
2:B:178:PHE:CE2	2:B:262:ILE:HD11	1.92	1.03
1:A:1352:PHE:C	1:A:1352:PHE:HD2	1.66	1.03
2:B:264:TYR:CZ	2:B:466:LEU:HD22	1.93	1.03
1:A:1225:TYR:HE1	1:A:1276:GLU:HG3	1.24	1.02
1:A:991:VAL:HG12	1:A:992:LEU:H	1.17	1.01
2:B:244:GLU:HB3	2:B:269:SER:CA	1.90	1.01
2:B:119:CYS:HB3	2:B:124:ARG:NE	1.73	1.01
1:A:1648:TRP:HB3	1:A:1660:PHE:CE2	1.95	1.01
1:A:1538:GLU:OE2	1:A:1539:LEU:HD11	1.61	1.00
1:A:1538:GLU:HG2	1:A:1539:LEU:HD13	1.01	1.00
1:A:1059:TYR:HB3	1:A:1067:SER:O	1.60	1.00
1:A:209:PHE:HD1	1:A:209:PHE:H	1.08	0.99
1:A:1341:LEU:CB	1:A:1342:LEU:HD13	1.92	0.99
1:A:1239:VAL:HG12	1:A:1240:PRO:HD2	1.42	0.99
1:A:991:VAL:HG12	1:A:992:LEU:N	1.67	0.99
1:A:1245:ALA:O	1:A:1247:MET:N	1.96	0.98
2:B:877:VAL:CG1	2:B:903:MET:HE3	1.93	0.98
1:A:266:TYR:CE2	1:A:1483:PHE:CB	2.46	0.98
1:A:1559:TYR:HH	1:A:1600:PHE:HE1	0.99	0.98
1:A:1013:MET:SD	1:A:1129:LEU:CG	2.52	0.97
1:A:1133:LEU:C	1:A:1133:LEU:CD2	2.35	0.97
1:A:266:TYR:CE2	1:A:1483:PHE:CD2	2.52	0.97
1:A:1241:ASN:O	1:A:1244:THR:HB	1.64	0.97
1:A:1352:PHE:C	1:A:1352:PHE:CD2	2.39	0.96
1:A:266:TYR:CD2	1:A:1483:PHE:CD2	2.53	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:543:VAL:O	2:B:577:GLY:HA3	1.65	0.96
1:A:999:ILE:HG13	1:A:1000:LEU:HD12	1.46	0.96
1:A:42:GLN:HG2	1:A:80:GLN:HG2	1.45	0.96
1:A:1288:GLN:O	1:A:1291:ILE:HG22	1.65	0.96
1:A:1279:ARG:HG3	2:B:601:PRO:CG	1.96	0.95
1:A:334:GLY:CA	1:A:844:THR:HG21	1.94	0.95
1:A:1239:VAL:HG13	1:A:1240:PRO:HD2	1.44	0.95
1:A:665:ASN:HD22	1:A:666:ASP:N	1.64	0.95
1:A:1013:MET:HB2	1:A:1129:LEU:CD2	1.97	0.95
2:B:493:TYR:HH	2:B:497:PHE:HZ	1.13	0.95
1:A:1132:THR:CG2	1:A:1246:ARG:HG2	1.95	0.95
1:A:1279:ARG:HG3	2:B:601:PRO:CD	1.97	0.95
1:A:587:THR:HG22	1:A:789:ALA:HB2	1.47	0.94
2:B:538:TYR:CE2	2:B:540:SER:O	2.21	0.94
2:B:609:MET:SD	2:B:614:LEU:HD11	2.07	0.94
2:B:734:ILE:CG1	2:B:738:LEU:HB3	1.98	0.94
1:A:1127:ILE:CD1	1:A:1130:GLN:NE2	2.30	0.94
2:B:73:ASP:HB3	2:B:323:HIS:CD2	2.02	0.94
1:A:620:LEU:HD13	1:A:811:VAL:HB	1.51	0.93
1:A:1011:GLU:O	1:A:1014:SER:HB2	1.67	0.93
1:A:993:SER:HA	2:B:597:ASN:HD21	1.34	0.93
1:A:362:PHE:CD2	1:A:640:LEU:HB2	2.04	0.92
1:A:362:PHE:HE2	1:A:640:LEU:HD22	1.33	0.92
1:A:395:ILE:HD13	2:B:153:GLY:CA	2.00	0.92
1:A:461:SER:HB3	1:A:463:SER:HB3	1.52	0.92
2:B:493:TYR:CZ	2:B:497:PHE:CE2	2.57	0.92
1:A:855:PHE:HB3	1:A:916:THR:HG22	1.49	0.92
1:A:1132:THR:HG21	1:A:1246:ARG:HG2	1.49	0.92
1:A:1133:LEU:HD23	1:A:1133:LEU:O	1.67	0.92
2:B:114:ILE:HG12	2:B:127:SER:O	1.70	0.92
1:A:576:SER:HB2	1:A:577:PRO:HD3	1.52	0.92
1:A:1280:TYR:CD2	1:A:1281:GLY:N	2.38	0.92
1:A:1627:ILE:HG13	1:A:1627:ILE:O	1.69	0.91
2:B:438:LYS:CA	2:B:441:SER:HB2	2.00	0.91
1:A:1573:VAL:O	1:A:1603:LYS:HB2	1.69	0.91
1:A:395:ILE:HD13	2:B:153:GLY:HA3	1.53	0.91
2:B:392:LYS:H	2:B:392:LYS:HD3	1.34	0.91
1:A:930:VAL:HG13	1:A:931:PRO:HD2	1.53	0.91
1:A:1249:GLU:HG2	1:A:1289:ASP:HB3	0.92	0.90
1:A:855:PHE:CB	1:A:916:THR:HG22	2.00	0.90
2:B:392:LYS:HD3	2:B:392:LYS:N	1.87	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:443:LEU:HD13	2:B:444:GLU:N	1.86	0.90
1:A:991:VAL:CG1	1:A:992:LEU:N	2.28	0.90
1:A:1287:THR:HA	1:A:1290:THR:CG2	2.02	0.90
1:A:1537:GLU:HB3	1:A:1541:LEU:HD11	1.52	0.90
1:A:1024:TYR:HA	1:A:1298:THR:HG23	1.53	0.90
2:B:570:ASN:HB3	2:B:571:PRO:CD	2.03	0.89
1:A:1245:ALA:O	1:A:1246:ARG:C	2.13	0.89
2:B:272:ILE:HG23	2:B:424:ARG:HE	1.37	0.89
1:A:337:SER:OG	1:A:1485:VAL:HG23	1.73	0.89
1:A:266:TYR:CE2	1:A:1483:PHE:CG	2.61	0.89
2:B:178:PHE:HE2	2:B:262:ILE:CD1	1.84	0.89
2:B:119:CYS:CB	2:B:124:ARG:HE	1.84	0.88
2:B:138:ASN:N	2:B:149:GLU:OE2	2.05	0.88
1:A:1028:GLY:HA2	1:A:1302:LEU:HD21	1.55	0.88
1:A:842:LYS:HE2	1:A:1486:GLY:C	1.99	0.88
1:A:1648:TRP:CB	1:A:1660:PHE:HE2	1.85	0.88
1:A:1144:LEU:O	1:A:1148:THR:HG22	1.74	0.88
1:A:266:TYR:HE2	1:A:1483:PHE:CB	1.84	0.88
1:A:1539:LEU:HD22	1:A:1540:ASP:H	1.37	0.88
2:B:831:LEU:HD13	2:B:831:LEU:O	1.74	0.88
1:A:1127:ILE:HD12	1:A:1130:GLN:HE21	1.10	0.88
1:A:1307:LEU:HD13	1:A:1307:LEU:C	1.99	0.88
2:B:543:VAL:HG12	2:B:574:GLN:HB2	1.53	0.88
2:B:22:THR:HA	2:B:50:ARG:O	1.74	0.87
2:B:493:TYR:CZ	2:B:497:PHE:HZ	1.86	0.87
1:A:1029:ASN:O	1:A:1030:HIS:HD2	1.53	0.87
1:A:360:PRO:HG3	1:A:636:ALA:HB3	1.56	0.87
1:A:1352:PHE:CD2	1:A:1353:GLY:N	2.43	0.87
1:A:1629:TYR:CE1	1:A:1630:ASN:ND2	2.43	0.87
1:A:209:PHE:HD1	1:A:209:PHE:N	1.70	0.87
2:B:476:ILE:HB	2:B:477:PRO:HD2	1.53	0.87
2:B:560:TYR:HB2	2:B:589:ASP:HB2	1.56	0.87
1:A:351:PRO:HG3	1:A:442:LEU:CD1	2.01	0.87
1:A:934:VAL:HG12	1:A:1367:LYS:O	1.75	0.87
2:B:474:ARG:HG2	2:B:483:ARG:HH21	1.39	0.86
2:B:804:ASN:N	2:B:804:ASN:HD22	1.72	0.86
1:A:672:ILE:HD12	1:A:673:LEU:H	1.38	0.86
2:B:560:TYR:HB2	2:B:589:ASP:CB	2.05	0.86
1:A:1548:ARG:NH2	1:A:1646:GLU:OE1	2.09	0.86
1:A:109:LYS:HE2	1:A:110:HIS:CE1	2.10	0.86
1:A:1028:GLY:CA	1:A:1302:LEU:HD21	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1552:ALA:HB2	1:A:1620:MET:HE3	1.58	0.86
2:B:493:TYR:CE2	2:B:497:PHE:CE2	2.64	0.86
1:A:618:LYS:HB3	1:A:622:ARG:HD2	1.55	0.86
1:A:1020:TYR:CE2	1:A:1291:ILE:HG13	2.11	0.86
2:B:73:ASP:H	2:B:74:PRO:HD2	1.38	0.86
2:B:274:HIS:N	2:B:277:ALA:HB3	1.91	0.86
1:A:1352:PHE:HD2	1:A:1353:GLY:N	1.74	0.85
1:A:1019:PHE:CD1	1:A:1049:LEU:HD11	2.11	0.85
1:A:1538:GLU:HG2	1:A:1539:LEU:N	1.81	0.85
1:A:1234:HIS:O	1:A:1235:LYS:HB2	1.74	0.85
1:A:1317:TYR:HB3	1:A:1344:ASP:OD2	1.76	0.85
1:A:396:ASP:HB2	1:A:400:GLU:HB3	1.57	0.85
1:A:842:LYS:NZ	1:A:1486:GLY:O	2.10	0.85
2:B:570:ASN:HB3	2:B:571:PRO:HD2	1.56	0.85
1:A:1628:LYS:HB3	1:A:1633:PHE:HD1	1.38	0.85
1:A:1559:TYR:CE2	1:A:1637:TYR:CD1	2.65	0.84
1:A:362:PHE:CE2	1:A:640:LEU:HD22	2.12	0.84
1:A:656:ASN:C	1:A:656:ASN:HD22	1.83	0.84
1:A:461:SER:HB2	1:A:463:SER:HB3	1.58	0.84
1:A:266:TYR:CE2	1:A:1483:PHE:HB2	2.12	0.84
2:B:719:GLY:H	2:B:738:LEU:HD13	1.39	0.84
1:A:459:SER:OG	1:A:461:SER:HB2	1.78	0.84
1:A:988:LEU:HD23	1:A:988:LEU:N	1.90	0.84
2:B:274:HIS:H	2:B:277:ALA:HB3	1.43	0.84
2:B:877:VAL:HG11	2:B:903:MET:HE3	1.59	0.84
1:A:1515:LYS:O	1:A:1516:ILE:HG13	1.78	0.83
2:B:263:PHE:CD1	2:B:263:PHE:C	2.56	0.83
1:A:1538:GLU:OE2	1:A:1539:LEU:CD1	2.26	0.83
2:B:111:LEU:HD12	2:B:112:CYS:H	1.43	0.83
1:A:862:VAL:CG1	1:A:863:GLU:H	1.92	0.83
2:B:681:THR:HB	2:B:703:ILE:HG13	1.61	0.83
1:A:849:ARG:HG2	1:A:918:PHE:CZ	2.14	0.83
1:A:1341:LEU:HB3	1:A:1342:LEU:HD13	1.60	0.83
1:A:1585:TYR:HE1	1:A:1668:ALA:HB1	1.41	0.83
1:A:857:VAL:HG21	1:A:896:VAL:HG11	1.60	0.82
1:A:1620:MET:HB2	1:A:1644:TRP:HB3	1.61	0.82
2:B:333:TYR:HE2	2:B:485:ASN:HB3	1.44	0.82
1:A:882:LYS:HG3	1:A:883:CYS:H	1.43	0.82
1:A:1328:MET:HE2	1:A:1335:GLY:H	1.41	0.82
1:A:672:ILE:HD11	1:A:674:ARG:O	1.80	0.82
1:A:860:SER:HB3	1:A:911:ASN:HB2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1274:LEU:O	1:A:1277:GLU:HB3	1.79	0.82
2:B:70:SER:HB3	2:B:332:LEU:HD11	1.62	0.82
2:B:592:PHE:CD2	2:B:592:PHE:N	2.48	0.82
2:B:681:THR:HB	2:B:703:ILE:CG1	2.10	0.82
1:A:1429:PRO:HG2	1:A:1511:THR:HB	1.62	0.81
1:A:1557:ILE:HD13	1:A:1622:LYS:HG3	1.59	0.81
1:A:1574:PHE:CE2	1:A:1601:ILE:HD12	2.14	0.81
1:A:1203:PRO:HD3	2:B:653:THR:HG22	1.63	0.81
2:B:734:ILE:HG21	2:B:738:LEU:HB2	1.61	0.81
1:A:1239:VAL:HG12	1:A:1240:PRO:CD	2.10	0.81
1:A:1005:LYS:HD2	1:A:1006:GLY:N	1.95	0.81
1:A:1133:LEU:HG	1:A:1143:TYR:CE2	2.15	0.81
1:A:369:TYR:HE2	1:A:371:ILE:HG12	1.44	0.81
1:A:182:ILE:HG13	1:A:804:ILE:HD11	1.62	0.81
1:A:998:ASN:O	1:A:1002:HIS:CD2	2.33	0.81
1:A:1421:HIS:HB2	1:A:1464:LEU:O	1.80	0.81
1:A:1016:VAL:CG1	1:A:1017:PRO:HD3	2.07	0.81
1:A:862:VAL:HG12	1:A:863:GLU:N	1.95	0.81
2:B:418:LYS:HA	2:B:436:TRP:CZ3	2.15	0.81
1:A:149:ASN:HB3	1:A:155:ALA:HB2	1.63	0.80
1:A:999:ILE:CG1	1:A:1000:LEU:HD12	2.12	0.80
1:A:1279:ARG:HG3	2:B:601:PRO:HD2	1.61	0.80
1:A:1307:LEU:HD13	1:A:1307:LEU:O	1.80	0.80
2:B:11:TRP:CE2	2:B:50:ARG:NH2	2.48	0.80
2:B:569:ASN:H	2:B:569:ASN:HD22	1.26	0.80
1:A:1121:ASN:O	1:A:1122:SER:HB3	1.80	0.80
1:A:182:ILE:HG13	1:A:804:ILE:CD1	2.11	0.80
1:A:1538:GLU:CG	1:A:1539:LEU:CD1	2.50	0.80
2:B:655:PHE:HA	2:B:680:ARG:CB	2.10	0.80
1:A:620:LEU:HD13	1:A:811:VAL:CB	2.12	0.80
1:A:1203:PRO:HG3	2:B:652:LEU:HD13	1.64	0.80
1:A:620:LEU:HD13	1:A:811:VAL:CG2	2.12	0.79
1:A:924:VAL:HG12	1:A:924:VAL:O	1.83	0.79
2:B:263:PHE:HD1	2:B:264:TYR:N	1.80	0.79
1:A:1234:HIS:O	1:A:1234:HIS:CG	2.34	0.79
2:B:681:THR:HB	2:B:703:ILE:CD1	2.12	0.79
1:A:1341:LEU:HB2	1:A:1342:LEU:HD13	1.62	0.79
1:A:886:GLN:HG3	1:A:887:LYS:H	1.48	0.79
2:B:178:PHE:CE2	2:B:262:ILE:CD1	2.63	0.79
2:B:569:ASN:HD22	2:B:569:ASN:N	1.81	0.79
1:A:334:GLY:C	1:A:844:THR:HG21	2.08	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ASP:HB3	1:A:417:VAL:H	1.46	0.79
2:B:418:LYS:HA	2:B:436:TRP:HZ3	1.48	0.79
1:A:255:PHE:CE1	1:A:608:ALA:HA	2.17	0.79
1:A:761:SER:O	1:A:762:LYS:HB3	1.80	0.79
1:A:1408:TYR:O	1:A:1410:PRO:HD3	1.81	0.79
1:A:1514:ILE:HG22	1:A:1515:LYS:H	1.46	0.79
2:B:570:ASN:CB	2:B:571:PRO:CD	2.59	0.79
1:A:1225:TYR:HD1	1:A:1273:TRP:HB2	1.48	0.79
1:A:1264:ILE:HD11	1:A:1303:LEU:HD11	1.65	0.79
1:A:1315:VAL:HG12	1:A:1324:HIS:O	1.83	0.79
2:B:73:ASP:C	2:B:74:PRO:O	2.22	0.78
1:A:1539:LEU:CD2	1:A:1540:ASP:N	2.40	0.78
2:B:685:LYS:HD3	2:B:694:ILE:HD11	1.64	0.78
2:B:438:LYS:C	2:B:441:SER:HB2	2.09	0.78
1:A:950:TYR:CE1	2:B:635:ARG:HD3	2.19	0.78
1:A:1001:THR:O	1:A:1003:LEU:HD13	1.83	0.78
2:B:436:TRP:CD1	2:B:436:TRP:C	2.61	0.78
2:B:559:THR:HG22	2:B:560:TYR:H	1.48	0.78
1:A:912:PHE:O	1:A:923:LEU:N	2.14	0.78
1:A:1311:MET:HE3	1:A:1350:THR:HG21	1.65	0.78
1:A:983:LEU:HD13	1:A:984:VAL:N	1.98	0.78
2:B:810:PHE:HB2	2:B:844:ASP:HB2	1.64	0.78
1:A:136:THR:HG23	1:A:139:GLN:HG3	1.65	0.78
2:B:493:TYR:OH	2:B:497:PHE:CZ	2.35	0.78
1:A:1515:LYS:CE	1:A:1603:LYS:HE3	2.13	0.77
1:A:1585:TYR:HE1	1:A:1668:ALA:CB	1.97	0.77
2:B:543:VAL:HG11	2:B:574:GLN:HB2	1.66	0.77
1:A:986:GLU:O	1:A:988:LEU:HD21	1.85	0.77
2:B:464:PHE:CD1	2:B:466:LEU:HD11	2.19	0.77
2:B:438:LYS:HA	2:B:441:SER:CB	2.14	0.77
1:A:577:PRO:HD3	1:A:588:VAL:HG23	1.65	0.77
1:A:1408:TYR:CD2	1:A:1419:SER:HB2	2.19	0.77
1:A:1515:LYS:NZ	1:A:1603:LYS:HE3	2.00	0.77
1:A:609:VAL:O	1:A:612:VAL:HG12	1.84	0.77
1:A:198:MET:HE1	1:A:218:GLU:HG3	1.67	0.77
1:A:1228:TRP:O	1:A:1247:MET:HB2	1.85	0.77
2:B:734:ILE:HD12	2:B:738:LEU:HD23	1.67	0.77
1:A:59:TYR:CD2	1:A:60:PRO:HD2	2.20	0.76
1:A:467:ILE:HD11	1:A:484:ILE:CD1	2.15	0.76
1:A:641:ASN:HB2	1:A:644:ASN:H	1.50	0.76
2:B:804:ASN:HD22	2:B:804:ASN:H	1.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1598:ILE:HG21	1:A:1637:TYR:CD2	2.19	0.76
2:B:73:ASP:O	2:B:74:PRO:C	2.22	0.76
2:B:699:ARG:O	2:B:700:LEU:HD13	1.85	0.76
2:B:74:PRO:HD3	2:B:323:HIS:CE1	2.21	0.76
1:A:1219:LYS:HD3	2:B:606:ASP:HB3	1.67	0.76
2:B:464:PHE:CE1	2:B:466:LEU:HD11	2.20	0.76
1:A:930:VAL:HG13	1:A:931:PRO:CD	2.15	0.76
1:A:1628:LYS:CB	1:A:1633:PHE:HD1	1.99	0.76
2:B:822:LEU:C	2:B:822:LEU:HD13	2.10	0.76
1:A:849:ARG:HG2	1:A:918:PHE:HZ	1.50	0.76
1:A:927:LEU:HD22	1:A:928:ARG:H	1.49	0.76
1:A:1297:LEU:HD21	2:B:595:MET:HE3	1.68	0.76
2:B:244:GLU:CB	2:B:269:SER:HA	2.05	0.76
1:A:1231:ASN:O	1:A:1232:LEU:HD12	1.86	0.76
1:A:362:PHE:CE2	1:A:640:LEU:HB2	2.19	0.76
1:A:1551:THR:O	1:A:1557:ILE:HG13	1.86	0.76
1:A:562:ASN:C	1:A:562:ASN:HD22	1.92	0.76
1:A:351:PRO:HG2	1:A:442:LEU:HD11	1.68	0.75
1:A:367:ILE:HG23	1:A:466:TYR:CD2	2.20	0.75
2:B:11:TRP:CZ2	2:B:50:ARG:CZ	2.69	0.75
1:A:934:VAL:HG22	1:A:935:LYS:N	2.01	0.75
2:B:139:GLY:N	2:B:149:GLU:OE2	2.20	0.75
2:B:388:LEU:O	2:B:389:PHE:CD2	2.39	0.75
2:B:493:TYR:OH	2:B:497:PHE:HZ	1.70	0.75
1:A:131:ASP:HA	1:A:775:TRP:CZ3	2.21	0.75
1:A:330:ILE:HG13	1:A:330:ILE:O	1.86	0.75
1:A:1239:VAL:CG1	1:A:1240:PRO:CD	2.59	0.75
2:B:187:VAL:HG13	2:B:188:LEU:HD13	1.66	0.75
1:A:461:SER:HB3	1:A:463:SER:CB	2.16	0.75
1:A:992:LEU:HD12	1:A:992:LEU:N	2.00	0.75
1:A:266:TYR:HE2	1:A:1483:PHE:HB3	1.51	0.75
2:B:260:VAL:HB	2:B:261:PRO:HD2	1.67	0.75
1:A:988:LEU:HD11	1:A:1268:ASN:OD1	1.87	0.75
1:A:1283:GLY:HA3	2:B:591:THR:OG1	1.86	0.75
1:A:1590:ALA:HB1	1:A:1635:TYR:CE1	2.22	0.74
1:A:335:GLY:CA	1:A:895:LEU:HD21	2.17	0.74
1:A:939:TYR:CD2	1:A:1362:THR:HG22	2.22	0.74
1:A:1549:LYS:HA	1:A:1552:ALA:HB3	1.68	0.74
1:A:842:LYS:CE	1:A:1486:GLY:O	2.36	0.74
1:A:1537:GLU:CB	1:A:1541:LEU:HD11	2.17	0.74
1:A:1234:HIS:O	1:A:1235:LYS:CB	2.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:MET:HB3	1:A:538:SER:OG	1.87	0.74
2:B:11:TRP:CE2	2:B:50:ARG:CZ	2.71	0.74
2:B:333:TYR:CE2	2:B:485:ASN:HB3	2.22	0.74
2:B:681:THR:HB	2:B:703:ILE:HD11	1.69	0.74
1:A:535:VAL:HG23	1:A:536:PRO:HD3	1.70	0.73
1:A:1273:TRP:CE3	1:A:1274:LEU:HA	2.23	0.73
1:A:1131:GLY:O	1:A:1134:PRO:HD2	1.89	0.73
1:A:1280:TYR:CD2	1:A:1280:TYR:C	2.66	0.73
1:A:1647:TYR:O	1:A:1649:PRO:HD3	1.87	0.73
1:A:609:VAL:HG21	1:A:771:GLU:HG3	1.68	0.73
1:A:1008:ALA:O	1:A:1011:GLU:HB2	1.89	0.73
2:B:781:VAL:HG11	2:B:797:PHE:CD1	2.23	0.73
1:A:862:VAL:CG1	1:A:863:GLU:N	2.49	0.73
1:A:120:THR:HG22	1:A:122:ASP:H	1.53	0.73
1:A:1024:TYR:HA	1:A:1298:THR:CG2	2.18	0.73
1:A:266:TYR:OH	1:A:1483:PHE:HB2	1.88	0.73
1:A:1085:VAL:O	1:A:1089:VAL:HG23	1.88	0.73
1:A:1528:VAL:CG2	1:A:1625:LEU:CD2	2.66	0.73
1:A:1559:TYR:CE2	1:A:1637:TYR:HD1	2.04	0.73
2:B:272:ILE:HG23	2:B:424:ARG:NE	2.02	0.73
1:A:109:LYS:HE2	1:A:110:HIS:ND1	2.03	0.73
1:A:672:ILE:HD12	1:A:672:ILE:C	2.13	0.73
1:A:934:VAL:CG2	1:A:935:LYS:N	2.51	0.73
2:B:850:GLU:HA	2:B:862:LEU:HD23	1.71	0.73
1:A:109:LYS:NZ	1:A:110:HIS:HE1	1.86	0.73
2:B:734:ILE:HG13	2:B:738:LEU:CB	2.10	0.73
2:B:480:VAL:HB	2:B:603:ILE:HG23	1.70	0.72
2:B:570:ASN:CB	2:B:571:PRO:HD3	2.19	0.72
1:A:193:ASN:HD21	1:A:935:LYS:NZ	1.87	0.72
1:A:1133:LEU:HD23	1:A:1134:PRO:N	2.04	0.72
1:A:552:ALA:O	1:A:657:ALA:HB1	1.89	0.72
1:A:1539:LEU:O	1:A:1660:PHE:CD1	2.42	0.72
2:B:104:GLN:HB3	2:B:105:PRO:HD2	1.70	0.72
1:A:939:TYR:HB3	1:A:1362:THR:HA	1.70	0.72
1:A:1000:LEU:O	1:A:1003:LEU:HD12	1.90	0.72
1:A:1280:TYR:HD2	1:A:1281:GLY:N	1.88	0.72
1:A:109:LYS:CE	1:A:110:HIS:CE1	2.72	0.72
1:A:1537:GLU:CG	1:A:1541:LEU:HD11	2.20	0.72
1:A:1539:LEU:HD13	1:A:1539:LEU:H	1.53	0.72
1:A:618:LYS:HD2	1:A:622:ARG:HH11	1.55	0.72
2:B:804:ASN:HB3	2:B:807:GLN:CD	2.14	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:ASN:ND2	1:A:666:ASP:OD2	2.22	0.72
1:A:991:VAL:C	1:A:992:LEU:CD1	2.56	0.72
1:A:1229:LYS:HE3	1:A:1247:MET:HE1	1.72	0.72
1:A:131:ASP:HB3	1:A:142:LYS:HB2	1.72	0.71
1:A:576:SER:CB	1:A:577:PRO:HD3	2.19	0.71
1:A:109:LYS:HZ1	1:A:110:HIS:HE1	1.38	0.71
1:A:1121:ASN:O	1:A:1122:SER:CB	2.37	0.71
2:B:538:TYR:HE2	2:B:540:SER:O	1.71	0.71
2:B:660:TYR:O	2:B:676:VAL:HB	1.90	0.71
1:A:109:LYS:NZ	1:A:110:HIS:CE1	2.58	0.71
1:A:395:ILE:CD1	2:B:153:GLY:HA2	2.21	0.71
1:A:1561:TYR:HB3	1:A:1584:ILE:O	1.91	0.71
2:B:476:ILE:CD1	2:B:482:LYS:HD2	2.21	0.71
2:B:681:THR:CB	2:B:703:ILE:CD1	2.69	0.71
1:A:628:GLU:OE2	1:A:674:ARG:NH2	2.24	0.71
1:A:1528:VAL:HG21	1:A:1625:LEU:HD22	1.72	0.71
1:A:209:PHE:N	1:A:209:PHE:CD1	2.45	0.71
1:A:628:GLU:O	1:A:628:GLU:HG3	1.91	0.71
1:A:1279:ARG:HG3	2:B:601:PRO:HG2	1.72	0.71
1:A:254:TYR:HD1	1:A:258:LYS:O	1.74	0.71
1:A:1377:PHE:HB3	1:A:1407:SER:O	1.90	0.71
1:A:1647:TYR:O	1:A:1649:PRO:CD	2.38	0.71
2:B:436:TRP:HD1	2:B:437:GLU:N	1.89	0.71
1:A:182:ILE:HD11	1:A:804:ILE:HG12	1.73	0.70
2:B:73:ASP:O	2:B:74:PRO:O	2.09	0.70
1:A:1528:VAL:HG21	1:A:1625:LEU:CD2	2.21	0.70
2:B:438:LYS:O	2:B:441:SER:HB2	1.91	0.70
1:A:266:TYR:CZ	1:A:1483:PHE:HB2	2.26	0.70
1:A:569:ASN:HD22	1:A:805:SER:CB	2.04	0.70
1:A:987:ILE:O	1:A:988:LEU:HD23	1.91	0.70
1:A:1528:VAL:CG2	1:A:1625:LEU:HD22	2.21	0.70
2:B:263:PHE:CD1	2:B:264:TYR:N	2.60	0.70
1:A:622:ARG:O	1:A:625:GLN:HG2	1.91	0.70
1:A:762:LYS:N	1:A:763:PRO:CD	2.55	0.70
1:A:1011:GLU:O	1:A:1014:SER:CB	2.39	0.70
1:A:770:PRO:O	1:A:797:TRP:HH2	1.74	0.70
1:A:1287:THR:CA	1:A:1290:THR:HG22	2.17	0.70
1:A:467:ILE:HD11	1:A:484:ILE:HD11	1.72	0.70
1:A:1016:VAL:CG1	1:A:1017:PRO:CD	2.68	0.70
1:A:132:LYS:NZ	1:A:139:GLN:HE22	1.90	0.70
2:B:681:THR:CB	2:B:703:ILE:HD11	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:608:GLU:O	2:B:609:MET:HG3	1.92	0.69
1:A:266:TYR:CD2	1:A:1483:PHE:HD2	2.09	0.69
1:A:395:ILE:HD13	2:B:153:GLY:HA2	1.71	0.69
1:A:1372:GLU:HG3	1:A:1409:LYS:HZ2	1.57	0.69
2:B:296:HIS:HA	2:B:354:TYR:O	1.92	0.69
2:B:269:SER:HB2	2:B:271:ASN:ND2	2.07	0.69
2:B:560:TYR:CB	2:B:589:ASP:HB2	2.21	0.69
1:A:1241:ASN:O	1:A:1244:THR:CB	2.39	0.69
1:A:1284:PHE:HB3	1:A:1289:ASP:OD2	1.92	0.69
2:B:322:ASN:C	2:B:324:LEU:H	2.00	0.69
1:A:991:VAL:HG13	1:A:992:LEU:H	1.56	0.69
1:A:1183:GLN:O	1:A:1232:LEU:HD21	1.93	0.69
1:A:1279:ARG:HD3	2:B:600:GLN:HE22	1.56	0.69
1:A:1421:HIS:HE1	1:A:1499:HIS:CE1	2.11	0.69
1:A:1514:ILE:HG22	1:A:1515:LYS:N	2.07	0.69
1:A:1589:GLU:CG	1:A:1590:ALA:H	2.00	0.69
2:B:274:HIS:H	2:B:277:ALA:CB	2.05	0.69
2:B:840:SER:HB3	2:B:844:ASP:O	1.92	0.69
1:A:1538:GLU:CD	1:A:1539:LEU:HD13	2.17	0.69
2:B:824:TRP:CH2	2:B:898:CYS:HA	2.28	0.69
2:B:879:MET:HB2	2:B:882:SER:HB3	1.72	0.69
1:A:43:VAL:HG22	1:A:45:GLY:H	1.57	0.68
1:A:74:SER:OG	1:A:76:GLU:HB3	1.92	0.68
1:A:1012:LEU:C	1:A:1012:LEU:HD13	2.17	0.68
2:B:831:LEU:O	2:B:831:LEU:CD1	2.41	0.68
1:A:395:ILE:CD1	2:B:153:GLY:CA	2.70	0.68
1:A:1539:LEU:HD22	1:A:1539:LEU:C	2.16	0.68
2:B:543:VAL:HG13	2:B:574:GLN:N	2.07	0.68
1:A:21:GLN:NE2	1:A:45:GLY:CA	2.26	0.68
1:A:939:TYR:HD2	1:A:1362:THR:HG22	1.58	0.68
1:A:999:ILE:HG13	1:A:1000:LEU:N	2.08	0.68
2:B:543:VAL:CG1	2:B:574:GLN:CB	2.67	0.68
1:A:29:LYS:HA	1:A:652:THR:HG22	1.74	0.68
1:A:1376:SER:O	1:A:1409:LYS:HB3	1.93	0.68
1:A:1559:TYR:CZ	1:A:1621:GLY:HA3	2.27	0.68
2:B:566:ARG:HD2	2:B:583:GLU:O	1.93	0.68
1:A:1111:TYR:OH	1:A:1121:ASN:ND2	2.26	0.68
1:A:620:LEU:HD11	1:A:624:PHE:CE1	2.28	0.68
1:A:1248:VAL:HG11	1:A:1284:PHE:HD1	1.58	0.68
1:A:356:LEU:HB3	1:A:359:THR:OG1	1.94	0.68
1:A:1027:THR:HG22	1:A:1302:LEU:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:ILE:HB	1:A:1130:GLN:HG3	1.75	0.68
2:B:73:ASP:N	2:B:74:PRO:CD	2.47	0.68
1:A:569:ASN:ND2	1:A:805:SER:CB	2.56	0.68
1:A:1123:GLN:HA	1:A:1123:GLN:HE21	1.58	0.68
1:A:1225:TYR:CD1	1:A:1273:TRP:HB2	2.29	0.68
1:A:1245:ALA:C	1:A:1247:MET:N	2.51	0.68
1:A:995:GLU:O	1:A:998:ASN:HB2	1.94	0.67
1:A:1589:GLU:HG2	1:A:1590:ALA:N	1.98	0.67
2:B:72:CYS:HB2	2:B:78:LYS:O	1.93	0.67
1:A:1497:GLU:HB3	1:A:1500:ARG:HG3	1.76	0.67
1:A:1628:LYS:CB	1:A:1633:PHE:CD1	2.77	0.67
2:B:436:TRP:CD1	2:B:437:GLU:N	2.63	0.67
1:A:842:LYS:HE2	1:A:1486:GLY:O	1.94	0.67
2:B:443:LEU:HD21	2:B:447:THR:OG1	1.94	0.67
2:B:528:GLY:HA3	2:B:533:LYS:HG3	1.76	0.67
1:A:835:ARG:HD3	1:A:905:ILE:HG12	1.76	0.67
1:A:1248:VAL:HG11	1:A:1284:PHE:CD1	2.29	0.67
1:A:1538:GLU:CD	1:A:1539:LEU:CD1	2.67	0.67
1:A:620:LEU:CD1	1:A:624:PHE:CE1	2.78	0.67
1:A:862:VAL:HG12	1:A:863:GLU:H	1.54	0.67
1:A:1225:TYR:HE1	1:A:1276:GLU:CG	2.05	0.67
1:A:1515:LYS:HZ1	1:A:1603:LYS:HE3	1.58	0.67
1:A:1612:VAL:HB	1:A:1615:ARG:HB3	1.77	0.67
1:A:412:ARG:HB3	1:A:415:ASP:HB2	1.75	0.67
1:A:1303:LEU:C	1:A:1303:LEU:HD13	2.20	0.67
1:A:1584:ILE:O	1:A:1585:TYR:HB2	1.94	0.67
2:B:73:ASP:HB3	2:B:323:HIS:NE2	2.09	0.67
2:B:177:HIS:NE2	2:B:493:TYR:OH	2.28	0.67
1:A:369:TYR:HE2	1:A:371:ILE:CG1	2.08	0.67
1:A:516:GLU:CD	1:A:516:GLU:H	2.00	0.67
2:B:111:LEU:HD12	2:B:112:CYS:N	2.09	0.67
1:A:462:GLN:OE1	1:A:462:GLN:HA	1.94	0.66
1:A:1489:SER:OG	1:A:1490:PRO:HD2	1.95	0.66
2:B:822:LEU:HD13	2:B:822:LEU:O	1.94	0.66
1:A:115:LYS:HG2	1:A:654:LEU:HD13	1.75	0.66
1:A:265:VAL:HB	1:A:290:THR:O	1.95	0.66
1:A:1272:LYS:O	1:A:1276:GLU:HG2	1.95	0.66
2:B:507:ASN:C	2:B:509:GLY:H	2.03	0.66
1:A:334:GLY:HA2	1:A:844:THR:CG2	2.16	0.66
1:A:997:ILE:HG23	1:A:1021:VAL:HG11	1.77	0.66
1:A:349:LEU:O	1:A:351:PRO:HD3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:804:ASN:N	2:B:804:ASN:ND2	2.37	0.66
2:B:824:TRP:CZ2	2:B:898:CYS:HA	2.30	0.66
1:A:656:ASN:C	1:A:656:ASN:ND2	2.53	0.66
1:A:770:PRO:O	1:A:797:TRP:CH2	2.48	0.66
1:A:994:GLN:OE1	1:A:1035:HIS:ND1	2.29	0.66
1:A:1536:GLN:HG3	1:A:1537:GLU:H	1.61	0.66
1:A:1675:GLY:O	1:A:1676:CYS:HB2	1.93	0.66
1:A:1228:TRP:HE3	1:A:1251:THR:HB	1.59	0.66
1:A:1542:THR:HG22	1:A:1542:THR:O	1.96	0.66
2:B:11:TRP:CZ2	2:B:50:ARG:NH1	2.63	0.66
1:A:1593:GLU:HB2	1:A:1596:SER:HB2	1.78	0.66
1:A:641:ASN:O	1:A:645:VAL:HG23	1.96	0.65
1:A:236:ASN:HB2	1:A:377:ASP:OD2	1.97	0.65
1:A:1647:TYR:HD1	1:A:1649:PRO:HD3	1.61	0.65
2:B:91:PHE:HD1	2:B:530:ASN:ND2	1.94	0.65
2:B:495:ALA:HB1	7:B:1008:MAN:H61	1.76	0.65
2:B:682:GLU:CD	2:B:702:ARG:HH22	2.04	0.65
1:A:1221:ASN:HA	1:A:1222:PRO:C	2.19	0.65
1:A:930:VAL:CG1	1:A:931:PRO:HD2	2.25	0.65
2:B:264:TYR:CZ	2:B:466:LEU:CD2	2.77	0.65
1:A:946:PRO:HG2	1:A:1353:GLY:O	1.97	0.65
1:A:1066:TYR:CD1	1:A:1079:THR:HA	2.32	0.65
1:A:1273:TRP:O	1:A:1277:GLU:N	2.30	0.65
1:A:149:ASN:HB3	1:A:155:ALA:CB	2.27	0.65
1:A:366:GLY:C	1:A:367:ILE:HD12	2.21	0.65
1:A:1016:VAL:CG1	1:A:1017:PRO:N	2.60	0.65
1:A:1524:ALA:CB	1:A:1629:TYR:HB2	2.25	0.65
2:B:557:ASP:HB2	2:B:561:LYS:O	1.97	0.65
1:A:351:PRO:CG	1:A:442:LEU:CD1	2.64	0.65
1:A:543:TYR:HB3	1:A:556:SER:HB3	1.79	0.65
1:A:1011:GLU:OE2	1:A:1059:TYR:OH	2.14	0.65
1:A:335:GLY:H	1:A:895:LEU:HG	1.62	0.65
1:A:1537:GLU:HB3	1:A:1541:LEU:CD1	2.25	0.65
1:A:1538:GLU:CG	1:A:1539:LEU:H	2.02	0.64
2:B:543:VAL:HG11	2:B:574:GLN:HE21	1.61	0.64
1:A:57:LYS:HE2	1:A:65:SER:HB3	1.80	0.64
2:B:247:GLN:O	2:B:262:ILE:HD12	1.96	0.64
1:A:1421:HIS:CE1	1:A:1499:HIS:CE1	2.86	0.64
1:A:1559:TYR:CZ	1:A:1637:TYR:CD1	2.86	0.64
2:B:803:LEU:CB	2:B:804:ASN:ND2	2.61	0.64
1:A:963:ILE:HG12	1:A:963:ILE:O	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:GLU:OE2	2:B:130:CYS:HB2	1.98	0.64
1:A:369:TYR:CE2	1:A:371:ILE:CG1	2.81	0.64
2:B:498:ASP:OD2	7:B:1008:MAN:O2	2.16	0.64
2:B:507:ASN:C	2:B:509:GLY:N	2.54	0.64
1:A:43:VAL:HG22	1:A:45:GLY:N	2.12	0.64
1:A:260:VAL:HG13	1:A:331:GLU:OE2	1.97	0.64
2:B:443:LEU:HD22	2:B:444:GLU:H	1.62	0.64
2:B:734:ILE:HG21	2:B:738:LEU:CB	2.27	0.64
1:A:784:LYS:HG2	1:A:785:GLN:H	1.61	0.64
1:A:1066:TYR:HD1	1:A:1079:THR:HA	1.62	0.64
1:A:1513:ASN:O	1:A:1514:ILE:HG12	1.98	0.64
2:B:465:GLU:C	2:B:466:LEU:HD12	2.22	0.64
1:A:322:TYR:OH	1:A:346:LYS:HE2	1.98	0.64
1:A:1073:SER:HB3	1:A:1123:GLN:HG2	1.80	0.64
1:A:1138:ARG:O	1:A:1139:GLU:C	2.41	0.64
1:A:1069:TRP:HA	1:A:1069:TRP:CE3	2.32	0.63
2:B:886:LYS:O	2:B:911:CYS:SG	2.56	0.63
1:A:227:PHE:CZ	1:A:338:GLU:HB2	2.33	0.63
1:A:412:ARG:HD2	1:A:415:ASP:HB2	1.80	0.63
1:A:548:GLY:O	1:A:550:GLN:HG3	1.97	0.63
1:A:562:ASN:ND2	1:A:562:ASN:O	2.31	0.63
1:A:1015:VAL:O	1:A:1015:VAL:CG2	2.46	0.63
1:A:58:SER:O	1:A:103:TYR:HD1	1.80	0.63
1:A:138:ASP:HA	1:A:189:LYS:HE3	1.80	0.63
1:A:357:VAL:HG11	1:A:675:PRO:HG3	1.81	0.63
1:A:1019:PHE:CD1	1:A:1049:LEU:CD1	2.80	0.63
1:A:21:GLN:HE22	1:A:45:GLY:HA2	0.83	0.63
1:A:457:TYR:HD2	1:A:457:TYR:C	2.06	0.63
1:A:1629:TYR:CD1	1:A:1630:ASN:ND2	2.67	0.63
2:B:545:GLY:HA2	2:B:571:PRO:O	1.98	0.63
1:A:137:PRO:O	1:A:138:ASP:HB3	1.98	0.63
1:A:1277:GLU:O	1:A:1281:GLY:N	2.27	0.63
1:A:1309:LEU:HD11	1:A:1311:MET:HB2	1.81	0.63
1:A:992:LEU:N	1:A:992:LEU:CD1	2.61	0.63
1:A:1225:TYR:CZ	1:A:1276:GLU:HG3	2.32	0.63
1:A:1231:ASN:C	1:A:1232:LEU:CD1	2.66	0.63
1:A:1341:LEU:HB3	1:A:1342:LEU:CD1	2.27	0.63
1:A:335:GLY:HA3	1:A:895:LEU:HD21	1.80	0.63
1:A:469:TRP:CZ2	1:A:471:ASP:OD1	2.51	0.63
1:A:1193:TYR:CE1	1:A:1256:LEU:HB3	2.34	0.63
1:A:1273:TRP:CE3	1:A:1274:LEU:CA	2.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450:PHE:CZ	1:A:1475:VAL:HB	2.33	0.63
1:A:1539:LEU:O	1:A:1660:PHE:CE1	2.52	0.63
2:B:547:TRP:HE1	7:B:1009:MAN:H5	1.63	0.63
1:A:1307:LEU:C	1:A:1307:LEU:CD1	2.72	0.62
2:B:543:VAL:HG13	2:B:574:GLN:H	1.64	0.62
1:A:949:ILE:HD11	1:A:1306:GLN:HB3	1.81	0.62
2:B:388:LEU:O	2:B:389:PHE:CG	2.52	0.62
1:A:1271:ILE:HD12	1:A:1271:ILE:C	2.25	0.62
1:A:521:ALA:HB1	1:A:523:TYR:O	2.00	0.62
1:A:1244:THR:O	1:A:1246:ARG:N	2.32	0.62
1:A:1562:LYS:HD2	1:A:1648:TRP:HE1	1.63	0.62
1:A:365:PRO:O	1:A:367:ILE:HD12	1.99	0.62
1:A:367:ILE:CG2	1:A:466:TYR:CD2	2.83	0.62
1:A:1123:GLN:HA	1:A:1123:GLN:NE2	2.15	0.62
1:A:1421:HIS:HE1	1:A:1499:HIS:HE1	1.47	0.62
2:B:559:THR:HG22	2:B:560:TYR:N	2.14	0.62
1:A:988:LEU:HD11	1:A:1268:ASN:CG	2.23	0.62
1:A:1528:VAL:CG2	1:A:1625:LEU:HD21	2.30	0.62
1:A:1582:LEU:CD1	1:A:1582:LEU:N	2.62	0.62
2:B:244:GLU:C	2:B:244:GLU:OE1	2.42	0.62
1:A:1273:TRP:HA	1:A:1276:GLU:HB2	1.81	0.62
2:B:11:TRP:CD2	2:B:50:ARG:NH2	2.67	0.62
2:B:567:GLU:O	2:B:569:ASN:ND2	2.33	0.62
1:A:1001:THR:O	1:A:1003:LEU:CD1	2.48	0.62
1:A:1232:LEU:HD12	1:A:1232:LEU:N	2.13	0.62
1:A:1234:HIS:O	1:A:1234:HIS:ND1	2.32	0.62
2:B:591:THR:OG1	2:B:592:PHE:N	2.32	0.62
1:A:576:SER:HB2	1:A:588:VAL:HG23	1.82	0.61
2:B:877:VAL:HG22	2:B:888:LEU:CD2	2.30	0.61
1:A:1213:LYS:HG3	1:A:1266:TYR:CZ	2.35	0.61
2:B:219:GLY:O	2:B:302:LEU:HB2	2.00	0.61
1:A:457:TYR:C	1:A:457:TYR:CD2	2.78	0.61
1:A:1133:LEU:CD2	1:A:1134:PRO:N	2.61	0.61
1:A:1408:TYR:CG	1:A:1419:SER:HB2	2.35	0.61
1:A:1539:LEU:HD13	1:A:1539:LEU:N	2.15	0.61
2:B:608:GLU:C	2:B:609:MET:HG3	2.26	0.61
2:B:681:THR:CG2	2:B:703:ILE:HD11	2.30	0.61
2:B:73:ASP:H	2:B:74:PRO:HD3	1.62	0.61
2:B:493:TYR:CE1	2:B:497:PHE:CZ	2.86	0.61
2:B:622:GLY:CA	2:B:640:LEU:HD11	2.31	0.61
1:A:191:PRO:O	1:A:194:PRO:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:SER:O	1:A:462:GLN:HB2	1.99	0.61
1:A:609:VAL:HG21	1:A:771:GLU:CG	2.31	0.61
1:A:1136:GLU:O	1:A:1137:ALA:HB3	2.01	0.61
1:A:1273:TRP:CE3	1:A:1274:LEU:N	2.68	0.61
1:A:1279:ARG:CG	2:B:601:PRO:CG	2.77	0.61
1:A:1647:TYR:C	1:A:1649:PRO:HD3	2.24	0.61
1:A:1081:PHE:HD1	1:A:1147:PHE:HZ	1.49	0.61
1:A:1169:ILE:HG22	2:B:697:PHE:HE2	1.66	0.61
1:A:1622:LYS:HZ3	1:A:1642:LEU:HD23	1.65	0.61
1:A:113:LYS:HB3	1:A:654:LEU:HD21	1.82	0.61
1:A:467:ILE:HD11	1:A:484:ILE:HD13	1.83	0.61
1:A:1264:ILE:CD1	1:A:1303:LEU:HD11	2.30	0.61
1:A:1409:LYS:HE2	1:A:1411:SER:OG	2.00	0.61
2:B:100:LEU:HD12	2:B:100:LEU:H	1.66	0.61
1:A:493:ILE:HG22	1:A:495:LYS:H	1.65	0.61
1:A:653:PHE:CE1	1:A:660:ASP:HB2	2.36	0.61
1:A:1123:GLN:O	1:A:1124:TYR:C	2.43	0.61
1:A:1279:ARG:CG	2:B:601:PRO:CD	2.78	0.61
2:B:681:THR:CB	2:B:703:ILE:HG13	2.29	0.61
1:A:1084:ARG:HD2	1:A:1154:LYS:HG3	1.83	0.60
1:A:1376:SER:O	1:A:1409:LYS:N	2.25	0.60
1:A:357:VAL:HG23	1:A:374:GLN:HB2	1.81	0.60
1:A:535:VAL:HG11	1:A:566:LYS:O	2.01	0.60
1:A:1514:ILE:CG2	1:A:1515:LYS:H	2.09	0.60
1:A:840:GLN:HG3	1:A:899:THR:CG2	2.31	0.60
1:A:961:TYR:CD1	1:A:1343:ASN:HB2	2.37	0.60
1:A:1544:SER:O	1:A:1548:ARG:HG3	2.02	0.60
2:B:75:CYS:SG	2:B:319:LYS:CE	2.84	0.60
2:B:570:ASN:CG	2:B:571:PRO:HD3	2.26	0.60
1:A:358:ALA:HB3	1:A:372:LYS:HD2	1.83	0.60
1:A:982:LEU:C	1:A:982:LEU:HD13	2.26	0.60
1:A:1020:TYR:CD2	1:A:1291:ILE:HG13	2.36	0.60
2:B:66:PHE:HB3	2:B:81:LYS:HE2	1.82	0.60
2:B:613:ASP:O	2:B:615:PRO:HD3	2.02	0.60
1:A:560:TRP:CD2	1:A:673:LEU:HD23	2.37	0.60
1:A:855:PHE:HB2	1:A:916:THR:HG22	1.83	0.60
1:A:461:SER:C	1:A:463:SER:H	2.10	0.60
1:A:1598:ILE:CG2	1:A:1637:TYR:CD2	2.82	0.60
2:B:493:TYR:CE1	2:B:497:PHE:CE2	2.89	0.60
1:A:42:GLN:HG2	1:A:80:GLN:CG	2.27	0.60
1:A:374:GLN:HE22	1:A:675:PRO:CB	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ASP:O	1:A:474:LYS:HA	2.02	0.60
2:B:389:PHE:HB3	2:B:445:GLU:HB3	1.82	0.60
1:A:459:SER:HG	1:A:461:SER:HB2	1.66	0.60
1:A:562:ASN:C	1:A:562:ASN:ND2	2.59	0.60
1:A:983:LEU:HD13	1:A:983:LEU:C	2.25	0.60
1:A:487:THR:HG22	1:A:523:TYR:HB3	1.84	0.59
1:A:924:VAL:O	1:A:924:VAL:CG1	2.50	0.59
1:A:1421:HIS:CE1	1:A:1499:HIS:HE1	2.20	0.59
2:B:562:ARG:HB2	2:B:590:CYS:SG	2.42	0.59
2:B:877:VAL:CB	2:B:903:MET:HE3	2.32	0.59
1:A:655:THR:CG2	1:A:658:ASN:O	2.49	0.59
1:A:1273:TRP:HE3	1:A:1274:LEU:N	1.99	0.59
1:A:1517:GLN:OE1	1:A:1603:LYS:HE2	2.01	0.59
1:A:1598:ILE:HG21	1:A:1637:TYR:HE2	0.77	0.59
1:A:369:TYR:CE2	1:A:371:ILE:HG12	2.33	0.59
1:A:369:TYR:CD2	1:A:371:ILE:HG13	2.37	0.59
1:A:577:PRO:CD	1:A:588:VAL:HG23	2.31	0.59
1:A:1654:CYS:O	1:A:1657:CYS:SG	2.60	0.59
1:A:535:VAL:HA	1:A:563:ILE:HD11	1.84	0.59
2:B:592:PHE:N	2:B:592:PHE:HD2	2.01	0.59
2:B:877:VAL:HG22	2:B:888:LEU:HD21	1.84	0.59
1:A:372:LYS:HZ1	1:A:470:THR:HG21	1.67	0.59
1:A:1272:LYS:O	1:A:1275:SER:HB3	2.01	0.59
1:A:1551:THR:HA	1:A:1554:LYS:HB2	1.83	0.59
2:B:274:HIS:HB2	2:B:277:ALA:HB2	1.84	0.59
2:B:508:ASN:HD21	2:B:544:ASP:CG	2.10	0.59
1:A:467:ILE:CD1	1:A:484:ILE:HD11	2.32	0.59
1:A:469:TRP:CH2	1:A:471:ASP:OD1	2.55	0.59
1:A:1539:LEU:CD1	1:A:1539:LEU:H	2.15	0.59
2:B:877:VAL:CG1	2:B:903:MET:CE	2.77	0.59
2:B:302:LEU:CD1	2:B:350:LEU:HB3	2.33	0.59
1:A:23:TYR:CE2	1:A:656:ASN:HB2	2.37	0.59
1:A:28:PRO:HG2	1:A:37:GLU:OE2	2.03	0.59
1:A:113:LYS:CD	1:A:654:LEU:HD11	2.33	0.59
1:A:467:ILE:HG22	1:A:557:ASP:HB3	1.85	0.59
1:A:665:ASN:HD22	1:A:665:ASN:C	2.09	0.59
2:B:803:LEU:HB2	2:B:804:ASN:ND2	2.18	0.59
1:A:618:LYS:HD2	1:A:622:ARG:NH1	2.17	0.59
1:A:1005:LYS:C	1:A:1005:LYS:CD	2.59	0.59
1:A:1372:GLU:HG3	1:A:1409:LYS:NZ	2.17	0.59
1:A:1374:VAL:O	1:A:1503:LYS:HA	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1524:ALA:HB2	1:A:1629:TYR:HB2	1.84	0.59
2:B:498:ASP:OD1	2:B:499:PRO:HD2	2.03	0.59
2:B:810:PHE:CB	2:B:844:ASP:HB2	2.31	0.59
1:A:1235:LYS:O	1:A:1235:LYS:HG2	2.03	0.58
1:A:1341:LEU:C	1:A:1342:LEU:HD13	2.28	0.58
1:A:1561:TYR:HE1	1:A:1598:ILE:HD11	1.67	0.58
2:B:655:PHE:HE1	2:B:728:ASN:HD22	1.50	0.58
1:A:365:PRO:O	1:A:367:ILE:CD1	2.51	0.58
1:A:1249:GLU:HG3	1:A:1289:ASP:HB3	1.79	0.58
2:B:538:TYR:CZ	2:B:540:SER:O	2.57	0.58
1:A:1600:PHE:HB3	1:A:1639:LEU:HD11	1.85	0.58
1:A:353:LYS:C	1:A:354:LEU:HD22	2.28	0.58
1:A:356:LEU:HD22	1:A:359:THR:HG21	1.85	0.58
1:A:953:ILE:HD12	1:A:955:ARG:HH12	1.69	0.58
2:B:887:THR:C	2:B:888:LEU:HD22	2.29	0.58
1:A:494:ASP:C	1:A:496:ILE:H	2.10	0.58
1:A:988:LEU:HG	1:A:1300:TYR:OH	2.04	0.58
1:A:1232:LEU:CD1	1:A:1232:LEU:N	2.67	0.58
1:A:280:LYS:HG3	1:A:282:MET:HE3	1.84	0.58
1:A:995:GLU:O	1:A:998:ASN:N	2.36	0.58
2:B:440:SER:O	2:B:443:LEU:HB3	2.03	0.58
2:B:620:ASP:OD1	2:B:620:ASP:N	2.37	0.58
1:A:99:VAL:HG22	1:A:101:TYR:H	1.69	0.58
1:A:198:MET:HE1	1:A:218:GLU:CG	2.33	0.58
1:A:331:GLU:HG2	1:A:334:GLY:HA3	1.86	0.58
2:B:803:LEU:HB3	2:B:804:ASN:ND2	2.19	0.58
1:A:357:VAL:O	1:A:672:ILE:O	2.22	0.58
1:A:995:GLU:O	1:A:996:GLY:C	2.46	0.58
1:A:1132:THR:CG2	1:A:1246:ARG:CG	2.77	0.58
1:A:1314:ASP:HA	1:A:1325:ASN:HB2	1.85	0.58
1:A:1536:GLN:HG3	1:A:1537:GLU:N	2.17	0.58
1:A:1543:ILE:H	1:A:1543:ILE:CD1	2.17	0.58
1:A:1642:LEU:HD13	1:A:1642:LEU:H	1.69	0.58
1:A:23:TYR:CD2	1:A:656:ASN:HB2	2.39	0.57
1:A:59:TYR:CD1	1:A:60:PRO:HD2	2.36	0.57
1:A:357:VAL:CG2	1:A:374:GLN:HB2	2.34	0.57
1:A:437:THR:O	1:A:447:GLN:NE2	2.37	0.57
1:A:503:ILE:HG12	1:A:540:LEU:HB2	1.84	0.57
1:A:592:MET:HB3	1:A:780:VAL:HG11	1.86	0.57
1:A:1067:SER:HB2	1:A:1073:SER:O	2.04	0.57
2:B:822:LEU:C	2:B:822:LEU:CD1	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:ASN:H	2:B:149:GLU:CD	2.10	0.57
1:A:587:THR:HA	1:A:789:ALA:HA	1.86	0.57
1:A:1096:ASN:HD22	1:A:1099:SER:H	1.52	0.57
1:A:1166:THR:O	1:A:1170:LYS:HG2	2.05	0.57
1:A:1628:LYS:HB3	1:A:1633:PHE:CD1	2.28	0.57
2:B:244:GLU:HB3	2:B:269:SER:CB	2.34	0.57
2:B:754:LEU:C	2:B:798:LEU:HD22	2.29	0.57
1:A:967:LEU:HD12	1:A:1366:HIS:O	2.05	0.57
1:A:1008:ALA:O	1:A:1011:GLU:CB	2.53	0.57
1:A:1265:ASN:ND2	2:B:638:LYS:HE2	2.20	0.57
2:B:161:ARG:HD3	2:B:163:TYR:HE2	1.69	0.57
2:B:269:SER:HB2	2:B:271:ASN:HD21	1.68	0.57
2:B:478:CYS:HB2	2:B:482:LYS:HE3	1.87	0.57
2:B:569:ASN:N	2:B:569:ASN:ND2	2.51	0.57
2:B:839:GLU:HB2	2:B:846:CYS:HB2	1.87	0.57
1:A:1262:LYS:HD3	1:A:1303:LEU:HD23	1.86	0.57
1:A:1642:LEU:H	1:A:1642:LEU:CD1	2.17	0.57
2:B:272:ILE:HG22	2:B:272:ILE:O	2.05	0.57
1:A:362:PHE:CE2	1:A:640:LEU:CD2	2.87	0.57
1:A:367:ILE:HG23	1:A:466:TYR:CE2	2.40	0.57
1:A:934:VAL:CG1	1:A:1367:LYS:O	2.49	0.57
2:B:264:TYR:CE1	2:B:466:LEU:HD22	2.40	0.57
2:B:850:GLU:OE2	2:B:859:CYS:HB2	2.05	0.57
1:A:282:MET:HE2	1:A:282:MET:HA	1.86	0.57
1:A:842:LYS:HE2	1:A:1486:GLY:CA	2.35	0.57
1:A:1024:TYR:HB2	1:A:1298:THR:OG1	2.04	0.57
1:A:1403:VAL:HG22	1:A:1476:ARG:HB3	1.86	0.57
1:A:1543:ILE:HD13	1:A:1543:ILE:N	2.20	0.57
2:B:69:TRP:HZ3	2:B:79:GLN:O	1.88	0.57
2:B:264:TYR:OH	2:B:466:LEU:CD2	2.53	0.57
1:A:1088:GLN:OE1	1:A:1154:LYS:HD2	2.05	0.56
1:A:386:VAL:O	1:A:411:THR:HG22	2.04	0.56
1:A:467:ILE:CG1	1:A:484:ILE:HD11	2.35	0.56
1:A:1620:MET:HB2	1:A:1644:TRP:CB	2.32	0.56
1:A:939:TYR:HB2	2:B:660:TYR:HE1	1.69	0.56
1:A:1069:TRP:O	1:A:1072:GLY:CA	2.54	0.56
1:A:1647:TYR:CD1	1:A:1649:PRO:HD3	2.40	0.56
1:A:1654:CYS:O	1:A:1655:SER:OG	2.20	0.56
2:B:176:PHE:CD2	2:B:466:LEU:HD21	2.40	0.56
2:B:668:ASP:HB3	2:B:670:THR:H	1.70	0.56
2:B:714:GLY:O	2:B:742:LYS:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1000:LEU:HD12	1:A:1000:LEU:N	2.20	0.56
1:A:1015:VAL:O	1:A:1015:VAL:HG23	2.05	0.56
2:B:271:ASN:H	2:B:271:ASN:HD22	1.52	0.56
2:B:569:ASN:H	2:B:569:ASN:ND2	1.98	0.56
1:A:672:ILE:HD11	1:A:674:ARG:C	2.31	0.56
1:A:966:ASP:OD1	1:A:966:ASP:N	2.38	0.56
2:B:303:ASN:N	2:B:303:ASN:OD1	2.37	0.56
1:A:1115:ASN:H	1:A:1115:ASN:HD22	1.54	0.56
2:B:115:GLU:O	2:B:116:GLU:HG3	2.05	0.56
1:A:1131:GLY:O	1:A:1134:PRO:CD	2.54	0.56
1:A:1628:LYS:HB2	1:A:1633:PHE:CD1	2.40	0.56
1:A:1524:ALA:CB	1:A:1629:TYR:CB	2.83	0.56
1:A:1567:SER:HB3	1:A:1578:LYS:HB2	1.87	0.56
1:A:939:TYR:HB2	2:B:660:TYR:CE1	2.41	0.56
2:B:543:VAL:HG11	2:B:574:GLN:NE2	2.20	0.56
2:B:681:THR:HG21	2:B:703:ILE:HD11	1.88	0.56
2:B:849:TRP:HB3	2:B:891:CYS:SG	2.46	0.56
1:A:253:ARG:HB2	1:A:259:VAL:HA	1.88	0.56
1:A:844:THR:HG22	1:A:895:LEU:HA	1.88	0.56
1:A:1220:GLY:O	1:A:1223:PRO:HA	2.06	0.56
2:B:471:ASP:HB3	2:B:474:ARG:NH2	2.20	0.56
1:A:394:THR:HG23	1:A:428:VAL:HG23	1.88	0.55
1:A:869:GLU:O	1:A:870:SER:CB	2.54	0.55
2:B:831:LEU:HD12	2:B:849:TRP:HH2	1.70	0.55
1:A:315:LEU:C	1:A:315:LEU:HD23	2.31	0.55
1:A:934:VAL:CG2	1:A:935:LYS:H	2.19	0.55
1:A:1539:LEU:HD22	1:A:1540:ASP:CA	2.31	0.55
1:A:1584:ILE:O	1:A:1585:TYR:CB	2.55	0.55
2:B:604:ASN:O	2:B:606:ASP:N	2.39	0.55
1:A:839:ILE:HG13	1:A:840:GLN:N	2.20	0.55
1:A:956:ARG:HG3	1:A:1349:SER:HB3	1.88	0.55
1:A:1249:GLU:CG	1:A:1289:ASP:CB	2.62	0.55
2:B:438:LYS:O	2:B:441:SER:CB	2.53	0.55
2:B:440:SER:O	2:B:443:LEU:CB	2.55	0.55
1:A:359:THR:HG22	1:A:372:LYS:H	1.71	0.55
1:A:590:LEU:O	1:A:785:GLN:HA	2.07	0.55
1:A:982:LEU:C	1:A:982:LEU:CD1	2.79	0.55
2:B:79:GLN:O	2:B:103:PHE:HB3	2.07	0.55
1:A:605:VAL:HG11	1:A:610:TYR:CE1	2.42	0.55
1:A:794:LEU:HD21	1:A:824:PHE:CD1	2.41	0.55
1:A:1528:VAL:HG22	1:A:1625:LEU:CD2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1539:LEU:HD22	1:A:1540:ASP:CB	2.35	0.55
1:A:993:SER:OG	1:A:995:GLU:OE1	2.24	0.55
1:A:1084:ARG:HD3	1:A:1150:ILE:HG22	1.88	0.55
2:B:126:ASP:OD1	2:B:150:ARG:NH2	2.38	0.55
2:B:350:LEU:HG	2:B:459:PRO:HB2	1.88	0.55
2:B:480:VAL:HG22	2:B:605:ASP:OD2	2.07	0.55
2:B:734:ILE:HB	2:B:737:SER:HB3	1.89	0.55
1:A:554:LEU:CD2	1:A:657:ALA:HB3	2.37	0.55
1:A:979:VAL:HG22	1:A:1359:VAL:HA	1.89	0.55
1:A:1543:ILE:H	1:A:1543:ILE:HD13	1.71	0.55
1:A:132:LYS:HZ1	1:A:139:GLN:HE22	1.52	0.55
1:A:673:LEU:N	1:A:673:LEU:HD12	2.21	0.55
1:A:1487:PHE:CD1	1:A:1488:LEU:N	2.75	0.55
1:A:1654:CYS:C	1:A:1657:CYS:SG	2.90	0.55
2:B:119:CYS:CB	2:B:124:ARG:NE	2.54	0.55
1:A:1127:ILE:HB	1:A:1130:GLN:CG	2.36	0.55
2:B:849:TRP:O	2:B:862:LEU:HD23	2.06	0.55
1:A:198:MET:CE	1:A:218:GLU:HG3	2.36	0.55
1:A:1069:TRP:O	1:A:1072:GLY:N	2.40	0.55
1:A:1531:ASP:HB2	1:A:1641:SER:H	1.72	0.55
1:A:560:TRP:CE2	1:A:673:LEU:HD23	2.42	0.54
1:A:263:ALA:HA	1:A:332:SER:H	1.73	0.54
1:A:543:TYR:CB	1:A:556:SER:HB3	2.37	0.54
1:A:827:MET:HE3	1:A:842:LYS:O	2.06	0.54
1:A:1013:MET:HE1	1:A:1129:LEU:HA	1.89	0.54
1:A:1135:VAL:HG11	1:A:1139:GLU:HG2	1.89	0.54
1:A:1311:MET:CE	1:A:1350:THR:HG21	2.36	0.54
2:B:24:SER:HA	2:B:48:GLU:O	2.07	0.54
1:A:263:ALA:HB3	1:A:292:LEU:HB3	1.89	0.54
1:A:1647:TYR:HD1	1:A:1649:PRO:CD	2.20	0.54
2:B:115:GLU:HB2	2:B:322:ASN:ND2	2.23	0.54
2:B:854:ALA:O	2:B:855:SER:HB2	2.07	0.54
1:A:1574:PHE:CD2	1:A:1601:ILE:HD12	2.43	0.54
1:A:1585:TYR:CE1	1:A:1668:ALA:CB	2.86	0.54
2:B:117:ALA:O	2:B:118:ASP:HB2	2.08	0.54
1:A:1028:GLY:HA2	1:A:1302:LEU:CD2	2.34	0.54
1:A:1539:LEU:CD2	1:A:1539:LEU:C	2.79	0.54
2:B:803:LEU:HB2	2:B:804:ASN:HD22	1.73	0.54
1:A:966:ASP:HB3	1:A:1371:SER:OG	2.08	0.54
1:A:1288:GLN:O	1:A:1291:ILE:CG2	2.49	0.54
1:A:1539:LEU:CD2	1:A:1540:ASP:CB	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:ARG:HH21	2:B:315:ASP:CG	2.16	0.54
1:A:950:TYR:CZ	2:B:635:ARG:HD3	2.42	0.54
1:A:1427:SER:HB3	1:A:1492:THR:H	1.72	0.54
2:B:106:CYS:SG	2:B:107:ILE:N	2.79	0.54
2:B:466:LEU:HD12	2:B:466:LEU:N	2.23	0.54
2:B:613:ASP:OD1	2:B:613:ASP:N	2.40	0.54
1:A:1122:SER:C	1:A:1124:TYR:N	2.63	0.54
1:A:1245:ALA:HB2	1:A:1285:TYR:CE2	2.43	0.54
1:A:996:GLY:O	1:A:997:ILE:C	2.50	0.54
1:A:113:LYS:HG2	1:A:114:SER:H	1.72	0.53
1:A:1205:PHE:O	1:A:1209:VAL:HG23	2.08	0.53
1:A:1515:LYS:HE3	1:A:1603:LYS:CE	2.38	0.53
1:A:1556:GLU:CB	1:A:1622:LYS:HE2	2.38	0.53
1:A:1063:ASP:O	1:A:1064:TYR:HB2	2.08	0.53
2:B:682:GLU:HG2	2:B:702:ARG:NH2	2.23	0.53
1:A:32:ARG:HD3	1:A:150:ASP:OD1	2.08	0.53
1:A:1108:VAL:HG11	1:A:1164:ILE:HG22	1.91	0.53
2:B:73:ASP:N	2:B:74:PRO:HD2	2.16	0.53
2:B:198:LYS:HG3	2:B:211:VAL:HB	1.90	0.53
1:A:493:ILE:HG21	1:A:495:LYS:HG2	1.90	0.53
1:A:1096:ASN:ND2	1:A:1099:SER:H	2.06	0.53
1:A:1515:LYS:CE	1:A:1603:LYS:CE	2.85	0.53
2:B:739:THR:CG2	2:B:740:CYS:N	2.71	0.53
1:A:153:LYS:HB3	1:A:154:PRO:HD2	1.91	0.53
1:A:335:GLY:HA3	1:A:895:LEU:CD2	2.38	0.53
1:A:372:LYS:NZ	1:A:470:THR:HG21	2.23	0.53
1:A:494:ASP:HA	1:A:496:ILE:HD12	1.90	0.53
1:A:1135:VAL:CG1	1:A:1136:GLU:N	2.72	0.53
1:A:1273:TRP:CE3	1:A:1273:TRP:C	2.87	0.53
2:B:322:ASN:C	2:B:324:LEU:N	2.67	0.53
2:B:546:GLN:O	2:B:571:PRO:HD2	2.09	0.53
1:A:1065:SER:HB3	1:A:1106:TRP:CE2	2.43	0.53
2:B:240:LEU:HD13	2:B:273:ASN:HD21	1.74	0.53
1:A:1036:SER:O	1:A:1038:PRO:HD3	2.08	0.53
1:A:1133:LEU:N	1:A:1134:PRO:CD	2.72	0.53
1:A:1338:VAL:CG1	1:A:1339:GLU:N	2.70	0.53
1:A:1644:TRP:O	1:A:1645:ILE:HD13	2.08	0.53
1:A:1360:HIS:CD2	2:B:660:TYR:OH	2.62	0.53
1:A:1386:ILE:O	1:A:1386:ILE:HG23	2.09	0.53
1:A:605:VAL:HG21	1:A:610:TYR:OH	2.09	0.52
1:A:955:ARG:O	1:A:1349:SER:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:998:ASN:O	1:A:1002:HIS:HD2	1.87	0.52
1:A:1005:LYS:HD2	1:A:1005:LYS:O	2.08	0.52
1:A:1273:TRP:CZ3	1:A:1274:LEU:HA	2.44	0.52
2:B:52:CYS:HA	2:B:54:TRP:CE3	2.44	0.52
2:B:824:TRP:NE1	2:B:847:TYR:OH	2.42	0.52
1:A:104:LEU:HB2	1:A:117:MET:HE1	1.89	0.52
1:A:180:ILE:HG21	1:A:599:TRP:NE1	2.24	0.52
1:A:460:LEU:HD12	1:A:460:LEU:O	2.09	0.52
1:A:949:ILE:CD1	1:A:1306:GLN:HB3	2.38	0.52
1:A:1012:LEU:HD13	1:A:1012:LEU:O	2.10	0.52
1:A:1376:SER:O	1:A:1409:LYS:CB	2.58	0.52
1:A:369:TYR:CE2	1:A:371:ILE:HG13	2.44	0.52
1:A:1284:PHE:CD2	2:B:594:ILE:HD11	2.45	0.52
1:A:1648:TRP:CB	1:A:1660:PHE:CE2	2.73	0.52
1:A:1132:THR:OG1	1:A:1249:GLU:OE2	2.26	0.52
1:A:1320:LYS:N	1:A:1344:ASP:OD2	2.42	0.52
1:A:768:TYR:CE2	1:A:770:PRO:HG3	2.45	0.52
1:A:927:LEU:HD22	1:A:928:ARG:N	2.22	0.52
1:A:29:LYS:HD2	1:A:647:HIS:CE1	2.45	0.52
1:A:855:PHE:CE2	1:A:888:VAL:HG13	2.45	0.52
2:B:451:TRP:O	2:B:455:VAL:HG23	2.10	0.52
2:B:476:ILE:HD11	2:B:482:LYS:HD2	1.92	0.52
1:A:986:GLU:O	1:A:988:LEU:CD2	2.55	0.52
2:B:476:ILE:HB	2:B:477:PRO:CD	2.32	0.52
2:B:809:HIS:HB3	2:B:829:THR:HG21	1.92	0.52
1:A:1012:LEU:C	1:A:1012:LEU:CD1	2.83	0.52
1:A:1073:SER:CB	1:A:1123:GLN:HG2	2.39	0.52
1:A:1410:PRO:HG3	1:A:1469:SER:HB3	1.92	0.52
1:A:1671:ILE:HA	1:A:1674:ASN:O	2.10	0.52
2:B:301:VAL:HB	2:B:350:LEU:O	2.09	0.52
2:B:622:GLY:HA3	2:B:640:LEU:HD11	1.91	0.52
1:A:255:PHE:CD1	1:A:608:ALA:HA	2.45	0.52
1:A:766:ARG:O	1:A:924:VAL:HB	2.10	0.52
1:A:1647:TYR:O	1:A:1649:PRO:HD2	2.09	0.52
1:A:908:HIS:HA	1:A:927:LEU:O	2.09	0.52
1:A:1066:TYR:CE1	1:A:1082:ALA:HB3	2.45	0.52
2:B:585:ARG:HG2	2:B:586:GLN:N	2.25	0.52
1:A:398:ASN:O	1:A:399:GLN:HB2	2.11	0.51
1:A:956:ARG:CG	1:A:1349:SER:HB3	2.40	0.51
1:A:1020:TYR:CE2	1:A:1291:ILE:CG1	2.91	0.51
2:B:73:ASP:O	2:B:73:ASP:OD1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:SER:HB3	1:A:68:SER:HB3	1.92	0.51
1:A:461:SER:CB	1:A:463:SER:CB	2.73	0.51
1:A:620:LEU:O	1:A:623:VAL:N	2.43	0.51
1:A:1176:LEU:HB3	1:A:1204:GLN:HG2	1.91	0.51
1:A:1547:THR:O	1:A:1550:GLN:HB2	2.10	0.51
2:B:655:PHE:CA	2:B:680:ARG:HB3	2.14	0.51
1:A:384:GLY:HA2	1:A:411:THR:HG23	1.92	0.51
1:A:618:LYS:HB3	1:A:622:ARG:CD	2.34	0.51
1:A:906:GLY:O	1:A:908:HIS:CE1	2.64	0.51
1:A:1338:VAL:HG12	1:A:1339:GLU:N	2.26	0.51
1:A:965:LEU:C	1:A:966:ASP:OD1	2.54	0.51
1:A:439:ALA:N	1:A:447:GLN:OE1	2.44	0.51
1:A:1550:GLN:O	1:A:1554:LYS:N	2.44	0.51
2:B:8:TRP:HZ3	2:B:26:HIS:HA	1.76	0.51
2:B:498:ASP:OD1	2:B:499:PRO:CD	2.58	0.51
1:A:162:THR:HB	1:A:173:MET:HG3	1.93	0.51
1:A:1450:PHE:HZ	1:A:1475:VAL:HB	1.74	0.51
2:B:828:ARG:HG2	2:B:829:THR:HG23	1.91	0.51
1:A:605:VAL:CG1	1:A:610:TYR:CE1	2.94	0.51
1:A:784:LYS:HG2	1:A:785:GLN:N	2.24	0.51
1:A:1631:PHE:CG	1:A:1631:PHE:O	2.63	0.51
2:B:734:ILE:HG13	2:B:738:LEU:N	2.26	0.51
2:B:877:VAL:HB	2:B:903:MET:HE3	1.93	0.51
2:B:877:VAL:O	2:B:877:VAL:HG23	2.11	0.51
2:B:329:ASN:HD22	2:B:332:LEU:HB2	1.75	0.51
2:B:418:LYS:CA	2:B:436:TRP:HZ3	2.22	0.51
1:A:805:SER:O	1:A:808:GLY:N	2.44	0.51
1:A:1013:MET:CG	1:A:1129:LEU:HG	2.40	0.51
1:A:362:PHE:CE2	1:A:640:LEU:CB	2.92	0.51
1:A:1204:GLN:O	1:A:1207:SER:HB3	2.11	0.51
1:A:1408:TYR:CD2	1:A:1419:SER:N	2.79	0.51
1:A:1622:LYS:NZ	1:A:1642:LEU:HD23	2.26	0.51
2:B:47:GLN:HG2	2:B:48:GLU:N	2.25	0.51
1:A:113:LYS:HD3	1:A:654:LEU:HD11	1.93	0.50
1:A:136:THR:CG2	1:A:139:GLN:HG3	2.39	0.50
1:A:461:SER:C	1:A:463:SER:N	2.68	0.50
1:A:464:TYR:H	1:A:491:PRO:HD3	1.76	0.50
1:A:498:HIS:HB3	1:A:514:THR:HG23	1.93	0.50
1:A:532:GLN:O	1:A:535:VAL:HG22	2.10	0.50
1:A:655:THR:CG2	1:A:656:ASN:N	2.72	0.50
1:A:1069:TRP:O	1:A:1072:GLY:HA3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1262:LYS:HD3	1:A:1303:LEU:CD2	2.41	0.50
1:A:1324:HIS:NE2	1:A:1338:VAL:HG21	2.26	0.50
2:B:79:GLN:HG3	2:B:106:CYS:HB2	1.92	0.50
2:B:877:VAL:HG13	2:B:888:LEU:HD23	1.92	0.50
1:A:1275:SER:HA	2:B:595:MET:CE	2.41	0.50
2:B:178:PHE:HB3	2:B:179:LEU:HD22	1.94	0.50
1:A:547:THR:C	1:A:549:GLU:H	2.19	0.50
1:A:1153:ARG:NH2	1:A:1172:ASP:OD2	2.44	0.50
2:B:79:GLN:O	2:B:103:PHE:CB	2.59	0.50
2:B:507:ASN:O	2:B:509:GLY:N	2.45	0.50
1:A:995:GLU:OE1	1:A:995:GLU:N	2.39	0.50
1:A:292:LEU:HA	1:A:297:ALA:HB2	1.94	0.50
1:A:307:VAL:HG12	1:A:312:TYR:HB2	1.92	0.50
1:A:500:ASN:ND2	1:A:513:GLY:O	2.44	0.50
1:A:610:TYR:CE2	1:A:617:LYS:HB3	2.46	0.50
1:A:934:VAL:HG13	1:A:1367:LYS:H	1.75	0.50
2:B:501:GLN:N	2:B:549:CYS:SG	2.85	0.50
2:B:877:VAL:HG12	2:B:903:MET:HE3	1.90	0.50
1:A:182:ILE:HG13	1:A:804:ILE:HD13	1.93	0.50
1:A:1273:TRP:C	1:A:1273:TRP:CD2	2.90	0.50
1:A:1376:SER:OG	1:A:1503:LYS:HG2	2.10	0.50
2:B:682:GLU:OE2	2:B:702:ARG:NH2	2.42	0.50
2:B:686:PRO:HG3	2:B:730:TRP:NE1	2.26	0.50
2:B:692:LEU:HD22	2:B:709:LEU:HD23	1.93	0.50
2:B:809:HIS:CB	2:B:829:THR:HG21	2.41	0.50
1:A:930:VAL:CB	1:A:931:PRO:HD2	2.41	0.50
1:A:1287:THR:O	1:A:1288:GLN:C	2.50	0.50
1:A:1522:GLY:HA3	1:A:1629:TYR:CZ	2.47	0.50
2:B:273:ASN:HB3	2:B:278:PHE:HB2	1.94	0.50
1:A:123:ASN:HD21	1:A:150:ASP:H	1.60	0.50
1:A:592:MET:HG2	1:A:780:VAL:HG21	1.94	0.50
1:A:1410:PRO:HG3	1:A:1469:SER:CB	2.42	0.50
1:A:1638:PRO:C	1:A:1639:LEU:HD12	2.37	0.50
1:A:862:VAL:HG13	1:A:863:GLU:H	1.71	0.49
1:A:1602:LYS:HB3	1:A:1639:LEU:HD22	1.95	0.49
2:B:309:LYS:HZ3	2:B:474:ARG:HH12	1.60	0.49
2:B:550:TRP:CE3	2:B:564:ARG:HG2	2.47	0.49
1:A:1408:TYR:CD2	1:A:1419:SER:CB	2.95	0.49
1:A:1483:PHE:CD1	1:A:1483:PHE:C	2.90	0.49
2:B:8:TRP:H	7:B:1007:MAN:H2	1.77	0.49
2:B:735:SER:C	2:B:736:ASN:OD1	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:TRP:CZ3	1:A:673:LEU:HB3	2.48	0.49
1:A:1143:TYR:CD1	1:A:1186:PHE:HE2	2.29	0.49
1:A:1186:PHE:CD1	1:A:1250:THR:HG22	2.47	0.49
1:A:1317:TYR:HB3	1:A:1344:ASP:CG	2.37	0.49
2:B:171:LEU:N	2:B:171:LEU:HD12	2.27	0.49
2:B:388:LEU:C	2:B:389:PHE:CD2	2.91	0.49
2:B:427:ARG:N	2:B:454:SER:OG	2.32	0.49
1:A:47:THR:O	1:A:48:GLU:C	2.55	0.49
1:A:1303:LEU:HD13	1:A:1303:LEU:O	2.11	0.49
2:B:585:ARG:HG2	2:B:586:GLN:H	1.77	0.49
2:B:684:ILE:HG22	2:B:700:LEU:HD12	1.94	0.49
2:B:847:TYR:CD2	2:B:850:GLU:CD	2.91	0.49
1:A:193:ASN:HD21	1:A:935:LYS:HZ3	1.61	0.49
1:A:1341:LEU:C	1:A:1342:LEU:CD1	2.85	0.49
2:B:560:TYR:HB2	2:B:589:ASP:HB3	1.91	0.49
1:A:109:LYS:CE	1:A:110:HIS:ND1	2.71	0.49
1:A:472:ASN:HA	1:A:474:LYS:HG3	1.95	0.49
1:A:1066:TYR:HB3	1:A:1078:LEU:CD2	2.43	0.49
1:A:1559:TYR:OH	1:A:1637:TYR:HB3	2.12	0.49
2:B:443:LEU:CD2	2:B:447:THR:OG1	2.59	0.49
2:B:498:ASP:OD1	2:B:499:PRO:N	2.45	0.49
1:A:539:ARG:NH2	1:A:635:GLY:O	2.45	0.49
1:A:554:LEU:HD23	1:A:657:ALA:HB3	1.94	0.49
1:A:640:LEU:H	1:A:644:ASN:HB3	1.77	0.49
1:A:1556:GLU:HB3	1:A:1622:LYS:HE2	1.94	0.49
2:B:618:GLU:CG	2:B:618:GLU:O	2.60	0.49
1:A:366:GLY:O	1:A:489:LYS:HD2	2.12	0.49
1:A:1129:LEU:HD12	1:A:1129:LEU:N	2.28	0.49
2:B:570:ASN:HB3	2:B:571:PRO:HD3	1.80	0.49
1:A:60:PRO:O	1:A:61:ASP:HB3	2.13	0.48
1:A:231:ILE:HD12	1:A:327:VAL:CG2	2.43	0.48
1:A:1225:TYR:CE1	1:A:1272:LYS:HD3	2.48	0.48
1:A:1318:LYS:HG2	1:A:1319:HIS:CE1	2.48	0.48
1:A:1334:LEU:HD12	1:A:1334:LEU:C	2.37	0.48
2:B:828:ARG:CZ	2:B:843:TYR:CE2	2.95	0.48
1:A:335:GLY:HA2	1:A:895:LEU:HD21	1.93	0.48
1:A:1066:TYR:HB3	1:A:1078:LEU:HD23	1.95	0.48
1:A:1071:GLY:O	1:A:1072:GLY:O	2.31	0.48
1:A:1111:TYR:CE1	1:A:1121:ASN:HB2	2.48	0.48
1:A:1317:TYR:CD2	1:A:1344:ASP:HB3	2.47	0.48
1:A:1378:TYR:N	1:A:1407:SER:O	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1540:ASP:O	1:A:1541:LEU:HD23	2.13	0.48
1:A:131:ASP:OD1	1:A:135:TYR:OH	2.24	0.48
1:A:131:ASP:CA	1:A:775:TRP:CH2	2.79	0.48
1:A:226:HIS:O	1:A:255:PHE:HD2	1.96	0.48
1:A:840:GLN:HG3	1:A:899:THR:HG23	1.94	0.48
1:A:1496:TYR:HB3	1:A:1504:GLN:HA	1.96	0.48
1:A:1562:LYS:CD	1:A:1648:TRP:HE1	2.24	0.48
2:B:464:PHE:HD1	2:B:466:LEU:HD11	1.71	0.48
2:B:824:TRP:CZ3	2:B:827:GLU:HG2	2.48	0.48
1:A:461:SER:HB2	1:A:463:SER:H	1.78	0.48
1:A:762:LYS:N	1:A:763:PRO:HD2	2.27	0.48
1:A:1000:LEU:HD12	1:A:1000:LEU:H	1.78	0.48
1:A:1013:MET:SD	1:A:1129:LEU:CB	3.02	0.48
1:A:1013:MET:CE	1:A:1129:LEU:HA	2.42	0.48
1:A:1585:TYR:CE1	1:A:1668:ALA:HB1	2.33	0.48
1:A:266:TYR:CE2	1:A:1483:PHE:HB3	2.35	0.48
1:A:571:LEU:HA	1:A:593:ALA:O	2.13	0.48
1:A:1088:GLN:OE1	1:A:1154:LYS:CD	2.62	0.48
2:B:493:TYR:CE2	2:B:497:PHE:CZ	2.95	0.48
1:A:226:HIS:CD2	1:A:254:TYR:CD2	3.02	0.48
1:A:322:TYR:CZ	1:A:346:LYS:HG3	2.48	0.48
1:A:348:VAL:HG12	1:A:350:SER:N	2.28	0.48
1:A:1122:SER:O	1:A:1123:GLN:HB3	2.12	0.48
1:A:1241:ASN:O	1:A:1244:THR:CG2	2.61	0.48
1:A:1311:MET:HG3	1:A:1312:ASP:H	1.79	0.48
2:B:493:TYR:CE1	2:B:497:PHE:HZ	2.27	0.48
2:B:670:THR:CG2	2:B:671:TRP:N	2.77	0.48
1:A:59:TYR:CB	1:A:60:PRO:HD2	2.42	0.48
1:A:104:LEU:HB2	1:A:117:MET:CE	2.44	0.48
1:A:461:SER:OG	1:A:553:GLU:CD	2.56	0.48
1:A:640:LEU:HB3	1:A:644:ASN:OD1	2.13	0.48
1:A:853:MET:HG2	1:A:888:VAL:HG23	1.96	0.48
1:A:912:PHE:HB2	1:A:923:LEU:HB3	1.94	0.48
1:A:1245:ALA:O	1:A:1248:VAL:N	2.44	0.48
1:A:1421:HIS:CB	1:A:1464:LEU:O	2.56	0.48
2:B:656:GLU:HB3	2:B:680:ARG:HD2	1.94	0.48
1:A:584:PRO:HG2	1:A:821:LYS:HB2	1.95	0.48
1:A:853:MET:HA	1:A:917:TRP:CD1	2.49	0.48
1:A:1245:ALA:C	1:A:1247:MET:H	2.20	0.48
1:A:1572:ASN:C	1:A:1573:VAL:HG23	2.38	0.48
2:B:309:LYS:NZ	2:B:474:ARG:HH12	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:464:PHE:HE1	2:B:466:LEU:HD11	1.74	0.48
1:A:208:ASP:OD1	1:A:208:ASP:N	2.33	0.48
2:B:205:THR:HG22	2:B:205:THR:O	2.14	0.48
2:B:353:VAL:HG12	2:B:355:ASP:HB2	1.95	0.48
2:B:418:LYS:HA	2:B:436:TRP:CE3	2.49	0.48
2:B:569:ASN:HA	2:B:572:ALA:HB2	1.96	0.48
2:B:803:LEU:CB	2:B:804:ASN:HD22	2.25	0.48
1:A:467:ILE:HG12	1:A:484:ILE:HD11	1.95	0.48
1:A:980:LYS:HA	1:A:1334:LEU:HD13	1.96	0.48
1:A:1080:ALA:HB1	1:A:1148:THR:HA	1.96	0.48
2:B:85:VAL:HG11	2:B:516:THR:HG22	1.96	0.48
1:A:23:TYR:CZ	1:A:656:ASN:HB2	2.48	0.47
1:A:1088:GLN:CD	1:A:1154:LYS:HZ2	2.20	0.47
2:B:23:GLN:O	2:B:49:THR:HA	2.14	0.47
2:B:371:THR:HG23	2:B:374:GLU:H	1.79	0.47
1:A:126:LEU:HD11	1:A:205:TYR:CE1	2.49	0.47
1:A:364:LYS:O	1:A:367:ILE:HB	2.14	0.47
1:A:618:LYS:CD	1:A:622:ARG:HH11	2.24	0.47
1:A:849:ARG:CG	1:A:918:PHE:CZ	2.92	0.47
1:A:1113:LEU:HB3	1:A:1115:ASN:ND2	2.29	0.47
1:A:1377:PHE:CD2	1:A:1408:TYR:HA	2.50	0.47
2:B:622:GLY:N	2:B:640:LEU:HD11	2.30	0.47
2:B:739:THR:CG2	2:B:740:CYS:H	2.27	0.47
1:A:226:HIS:CD2	1:A:254:TYR:HD2	2.31	0.47
1:A:267:ILE:HG12	1:A:327:VAL:HG13	1.95	0.47
1:A:1067:SER:CB	1:A:1073:SER:O	2.62	0.47
1:A:1612:VAL:HG23	1:A:1617:TYR:OH	2.14	0.47
1:A:1650:ARG:HG2	1:A:1651:ASP:N	2.29	0.47
2:B:168:SER:HB2	2:B:459:PRO:HG2	1.95	0.47
1:A:493:ILE:HG22	1:A:495:LYS:N	2.29	0.47
1:A:545:ILE:HG22	1:A:554:LEU:HD13	1.97	0.47
1:A:905:ILE:H	1:A:905:ILE:HG13	1.42	0.47
1:A:939:TYR:HD2	1:A:1362:THR:CG2	2.25	0.47
1:A:1247:MET:O	1:A:1248:VAL:C	2.54	0.47
1:A:1642:LEU:CD1	1:A:1642:LEU:N	2.77	0.47
2:B:302:LEU:HD11	2:B:350:LEU:HB3	1.95	0.47
1:A:331:GLU:HB3	1:A:334:GLY:O	2.14	0.47
1:A:599:TRP:CZ3	1:A:779:LEU:HB2	2.49	0.47
1:A:1016:VAL:HG13	1:A:1017:PRO:N	2.29	0.47
1:A:1203:PRO:CD	2:B:653:THR:HG22	2.40	0.47
1:A:1241:ASN:OD1	1:A:1241:ASN:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:LYS:O	2:B:311:LEU:HD21	2.14	0.47
2:B:430:TYR:HB3	2:B:451:TRP:HB2	1.96	0.47
2:B:739:THR:HG22	2:B:740:CYS:N	2.28	0.47
1:A:543:TYR:CD2	1:A:554:LEU:HD12	2.49	0.47
1:A:766:ARG:NH1	1:A:794:LEU:HD13	2.30	0.47
1:A:942:VAL:HG22	1:A:957:LYS:HD2	1.97	0.47
2:B:313:LEU:HD12	2:B:318:LEU:HD13	1.96	0.47
2:B:443:LEU:HD13	2:B:443:LEU:C	2.39	0.47
2:B:493:TYR:CD2	2:B:497:PHE:CE2	3.02	0.47
1:A:49:ALA:CB	1:A:74:SER:HB3	2.45	0.47
1:A:224:LEU:H	1:A:224:LEU:HG	1.25	0.47
1:A:625:GLN:O	1:A:629:LYS:HG2	2.15	0.47
1:A:653:PHE:CD1	1:A:660:ASP:HB2	2.49	0.47
1:A:1028:GLY:N	1:A:1302:LEU:HD21	2.30	0.47
1:A:1217:LEU:HD12	1:A:1227:PHE:CE1	2.50	0.47
1:A:1515:LYS:HE2	1:A:1530:ALA:HB3	1.96	0.47
1:A:1627:ILE:O	1:A:1627:ILE:CG1	2.54	0.47
2:B:342:THR:HG22	2:B:343:HIS:CE1	2.49	0.47
1:A:606:ASP:OD2	1:A:795:THR:HG21	2.15	0.47
1:A:1065:SER:HB3	1:A:1106:TRP:CD2	2.49	0.47
1:A:1244:THR:O	1:A:1245:ALA:C	2.57	0.47
1:A:1326:TYR:N	1:A:1326:TYR:CD2	2.82	0.47
2:B:176:PHE:HD2	2:B:466:LEU:HD21	1.80	0.47
2:B:218:VAL:HA	2:B:303:ASN:O	2.14	0.47
2:B:689:GLN:HB2	2:B:692:LEU:CD1	2.44	0.47
1:A:137:PRO:HG3	1:A:196:TYR:HE1	1.78	0.47
1:A:849:ARG:CG	1:A:918:PHE:HZ	2.21	0.47
1:A:1517:GLN:HB3	1:A:1574:PHE:CE1	2.50	0.47
1:A:576:SER:OG	1:A:589:SER:HB2	2.15	0.47
1:A:1264:ILE:CG1	1:A:1303:LEU:HD11	2.44	0.47
2:B:241:GLY:O	2:B:245:ASN:CG	2.57	0.47
2:B:316:VAL:O	2:B:319:LYS:HB3	2.15	0.47
1:A:222:TYR:OH	1:A:771:GLU:OE1	2.31	0.46
1:A:337:SER:OG	1:A:1485:VAL:CG2	2.57	0.46
1:A:821:LYS:HE2	1:A:921:GLU:OE1	2.15	0.46
1:A:830:PRO:HG3	1:A:1487:PHE:CE1	2.48	0.46
1:A:959:PHE:HE2	1:A:1348:VAL:CG2	2.28	0.46
2:B:10:GLN:HE21	2:B:10:GLN:HB2	1.47	0.46
2:B:54:TRP:CD1	2:B:55:GLN:H	2.32	0.46
2:B:371:THR:HG22	2:B:374:GLU:HG3	1.97	0.46
2:B:443:LEU:HD13	2:B:444:GLU:H	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:567:GLU:C	2:B:569:ASN:HD22	2.22	0.46
1:A:113:LYS:HG2	1:A:114:SER:N	2.28	0.46
1:A:911:ASN:HA	1:A:923:LEU:O	2.15	0.46
1:A:975:ARG:HG3	1:A:1340:VAL:HG21	1.97	0.46
1:A:988:LEU:CD1	1:A:1268:ASN:OD1	2.60	0.46
1:A:49:ALA:HB1	1:A:74:SER:HB3	1.98	0.46
1:A:59:TYR:CG	1:A:60:PRO:CD	2.76	0.46
1:A:123:ASN:H	1:A:211:THR:HG23	1.80	0.46
1:A:180:ILE:HD12	1:A:599:TRP:CD2	2.50	0.46
1:A:357:VAL:CG1	1:A:675:PRO:HG3	2.44	0.46
1:A:1090:ASN:HD22	1:A:1158:ILE:HD13	1.80	0.46
1:A:1245:ALA:HB2	1:A:1285:TYR:HE2	1.80	0.46
1:A:1515:LYS:NZ	1:A:1530:ALA:O	2.47	0.46
2:B:402:ASN:O	2:B:406:GLU:HB2	2.15	0.46
1:A:307:VAL:CG1	1:A:312:TYR:HB2	2.46	0.46
1:A:469:TRP:CH2	1:A:471:ASP:CG	2.93	0.46
1:A:1069:TRP:HA	1:A:1069:TRP:HE3	1.80	0.46
1:A:1121:ASN:O	1:A:1121:ASN:OD1	2.34	0.46
2:B:161:ARG:HD3	2:B:163:TYR:CE2	2.51	0.46
2:B:477:PRO:HG2	2:B:478:CYS:H	1.80	0.46
1:A:487:THR:HG22	1:A:523:TYR:CB	2.44	0.46
1:A:1059:TYR:O	1:A:1067:SER:N	2.32	0.46
2:B:436:TRP:O	2:B:437:GLU:HG3	2.15	0.46
2:B:550:TRP:HB2	7:B:1008:MAN:H5	1.97	0.46
2:B:554:SER:O	2:B:562:ARG:HG3	2.15	0.46
1:A:469:TRP:CZ2	1:A:471:ASP:CG	2.93	0.46
1:A:573:VAL:HA	1:A:591:ASN:O	2.16	0.46
1:A:576:SER:CB	1:A:577:PRO:CD	2.90	0.46
1:A:1540:ASP:OD1	1:A:1541:LEU:N	2.48	0.46
1:A:1546:GLU:O	1:A:1550:GLN:HG3	2.16	0.46
2:B:179:LEU:HD22	2:B:179:LEU:N	2.31	0.46
2:B:854:ALA:O	2:B:855:SER:CB	2.63	0.46
1:A:647:HIS:HA	1:A:651:LEU:O	2.15	0.46
1:A:938:SER:O	1:A:1363:THR:N	2.35	0.46
1:A:1485:VAL:HG22	1:A:1487:PHE:O	2.16	0.46
1:A:1647:TYR:O	1:A:1647:TYR:CD1	2.68	0.46
2:B:11:TRP:CH2	2:B:50:ARG:HD3	2.51	0.46
2:B:119:CYS:C	2:B:124:ARG:HH21	2.24	0.46
1:A:21:GLN:HE22	1:A:45:GLY:N	2.12	0.46
1:A:620:LEU:HD11	1:A:624:PHE:CZ	2.50	0.46
1:A:655:THR:HG21	1:A:658:ASN:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1132:THR:HG22	1:A:1246:ARG:CG	2.46	0.46
2:B:641:TYR:HB3	2:B:645:GLU:OE2	2.16	0.46
1:A:335:GLY:N	1:A:844:THR:HG21	2.31	0.46
1:A:961:TYR:CE1	1:A:1343:ASN:HB2	2.51	0.46
1:A:1121:ASN:OD1	1:A:1121:ASN:C	2.58	0.46
1:A:1138:ARG:O	1:A:1140:ASN:N	2.49	0.46
1:A:1528:VAL:HG22	1:A:1625:LEU:HD22	1.94	0.46
2:B:877:VAL:HG22	2:B:888:LEU:HD23	1.98	0.46
1:A:1515:LYS:HD3	1:A:1530:ALA:O	2.16	0.45
1:A:1537:GLU:HG2	1:A:1541:LEU:HD11	1.96	0.45
2:B:471:ASP:O	2:B:474:ARG:NE	2.49	0.45
2:B:572:ALA:HA	2:B:573:PRO:HD3	1.60	0.45
2:B:755:GLY:N	2:B:798:LEU:HD22	2.32	0.45
1:A:979:VAL:O	1:A:1334:LEU:HD13	2.16	0.45
1:A:1543:ILE:CD1	1:A:1543:ILE:N	2.79	0.45
2:B:52:CYS:HA	2:B:54:TRP:CZ3	2.51	0.45
2:B:123:PHE:CD2	2:B:124:ARG:N	2.84	0.45
2:B:480:VAL:CG2	2:B:605:ASP:OD2	2.64	0.45
2:B:776:SER:CB	2:B:794:ALA:HB3	2.46	0.45
1:A:228:SER:HB3	1:A:255:PHE:CZ	2.51	0.45
1:A:441:ASP:OD2	1:A:441:ASP:N	2.43	0.45
1:A:939:TYR:HB3	1:A:1362:THR:HG22	1.97	0.45
1:A:939:TYR:HA	1:A:1361:VAL:O	2.16	0.45
1:A:1517:GLN:HB3	1:A:1574:PHE:HE1	1.81	0.45
1:A:1600:PHE:CD1	1:A:1637:TYR:HB2	2.51	0.45
2:B:464:PHE:HD1	2:B:466:LEU:CD1	2.28	0.45
1:A:501:TYR:HB3	1:A:542:VAL:HG22	1.98	0.45
1:A:869:GLU:O	1:A:870:SER:HB3	2.16	0.45
1:A:1028:GLY:HA2	1:A:1305:LYS:NZ	2.31	0.45
1:A:1175:LEU:O	1:A:1179:THR:OG1	2.21	0.45
1:A:1241:ASN:O	1:A:1241:ASN:OD1	2.33	0.45
1:A:1560:ALA:O	1:A:1584:ILE:O	2.35	0.45
2:B:468:PRO:HB2	2:B:470:VAL:HG12	1.97	0.45
2:B:694:ILE:H	2:B:694:ILE:HG12	1.38	0.45
1:A:560:TRP:CH2	1:A:562:ASN:HB3	2.51	0.45
1:A:793:SER:O	1:A:819:VAL:HG23	2.17	0.45
1:A:892:SER:HB3	1:A:893:SER:H	1.56	0.45
1:A:939:TYR:O	2:B:660:TYR:HD1	2.00	0.45
1:A:1323:LEU:HD12	1:A:1323:LEU:HA	1.74	0.45
1:A:1376:SER:OG	1:A:1503:LYS:CG	2.64	0.45
1:A:1379:LEU:HD11	1:A:1495:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1453:TYR:CD2	1:A:1453:TYR:C	2.95	0.45
1:A:1488:LEU:HD13	1:A:1489:SER:O	2.17	0.45
2:B:70:SER:O	2:B:71:ASP:O	2.34	0.45
2:B:611:GLU:O	2:B:611:GLU:HG3	2.17	0.45
2:B:735:SER:O	2:B:736:ASN:HB2	2.17	0.45
1:A:762:LYS:H	1:A:763:PRO:HD2	1.82	0.45
1:A:968:VAL:HG23	1:A:971:THR:HG21	1.97	0.45
1:A:1582:LEU:N	1:A:1582:LEU:HD13	2.32	0.45
1:A:33:VAL:HG23	1:A:120:THR:O	2.17	0.45
1:A:914:LEU:HD13	1:A:914:LEU:C	2.41	0.45
1:A:1079:THR:HG22	1:A:1107:LEU:HD11	1.99	0.45
1:A:1221:ASN:OD1	2:B:614:LEU:HD13	2.17	0.45
1:A:1225:TYR:OH	1:A:1276:GLU:HG3	2.17	0.45
2:B:54:TRP:CD1	2:B:55:GLN:OE1	2.70	0.45
2:B:893:VAL:HG22	2:B:903:MET:HE1	1.99	0.45
1:A:496:ILE:HB	1:A:517:LYS:HG3	1.99	0.45
1:A:1279:ARG:CG	2:B:601:PRO:HD2	2.40	0.45
2:B:300:LYS:CD	3:D:1:NAG:H82	2.47	0.45
2:B:476:ILE:CB	2:B:477:PRO:HD2	2.36	0.45
2:B:493:TYR:CE1	2:B:497:PHE:HE2	2.33	0.45
2:B:493:TYR:CD2	2:B:497:PHE:HE2	2.35	0.45
1:A:365:PRO:HB3	1:A:426:SER:O	2.16	0.45
1:A:1000:LEU:H	1:A:1000:LEU:CD1	2.30	0.45
1:A:1013:MET:HB2	1:A:1129:LEU:CG	2.47	0.45
1:A:1408:TYR:HD2	1:A:1419:SER:N	2.14	0.45
1:A:126:LEU:HD11	1:A:205:TYR:CZ	2.52	0.44
1:A:639:GLY:H	1:A:645:VAL:HG22	1.81	0.44
1:A:1221:ASN:HD22	1:A:1221:ASN:C	2.25	0.44
2:B:140:GLU:CD	2:B:158:VAL:HG21	2.42	0.44
2:B:143:CYS:SG	2:B:148:ASP:HB3	2.56	0.44
2:B:689:GLN:HB2	2:B:692:LEU:HD12	1.99	0.44
1:A:567:CYS:HB3	1:A:810:CYS:HB2	1.86	0.44
1:A:882:LYS:HG3	1:A:883:CYS:N	2.21	0.44
1:A:914:LEU:HB3	1:A:921:GLU:HB3	1.98	0.44
1:A:1570:VAL:HG22	1:A:1575:VAL:HG13	1.99	0.44
2:B:8:TRP:CE3	2:B:25:ARG:HG3	2.53	0.44
1:A:460:LEU:HD12	1:A:460:LEU:C	2.42	0.44
1:A:1247:MET:O	1:A:1251:THR:HG23	2.17	0.44
1:A:1375:CYS:SG	1:A:1376:SER:N	2.90	0.44
1:A:1515:LYS:HE3	1:A:1603:LYS:HE2	1.99	0.44
2:B:246:GLN:O	2:B:246:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:630:GLU:O	2:B:631:ASN:HB2	2.17	0.44
1:A:255:PHE:O	1:A:796:THR:OG1	2.23	0.44
1:A:223:VAL:O	1:A:224:LEU:C	2.61	0.44
1:A:855:PHE:HB2	1:A:916:THR:CG2	2.47	0.44
1:A:882:LYS:CG	1:A:883:CYS:H	2.15	0.44
1:A:1277:GLU:OE2	1:A:1284:PHE:CZ	2.70	0.44
2:B:219:GLY:O	2:B:302:LEU:CB	2.64	0.44
2:B:451:TRP:O	2:B:454:SER:HB3	2.18	0.44
1:A:369:TYR:HD2	1:A:371:ILE:HG13	1.82	0.44
1:A:635:GLY:HA2	1:A:671:GLU:HG3	1.99	0.44
1:A:1013:MET:CE	1:A:1129:LEU:HG	2.44	0.44
1:A:1016:VAL:N	1:A:1017:PRO:CD	2.80	0.44
1:A:1200:LYS:H	1:A:1200:LYS:HG2	1.52	0.44
2:B:735:SER:O	2:B:736:ASN:CB	2.65	0.44
1:A:382:LEU:HD22	1:A:416:GLY:HA3	1.98	0.44
1:A:805:SER:O	1:A:806:ASN:C	2.60	0.44
1:A:1311:MET:HE3	1:A:1350:THR:CG2	2.40	0.44
1:A:461:SER:CB	1:A:463:SER:H	2.30	0.44
1:A:500:ASN:OD1	1:A:543:TYR:CZ	2.69	0.44
1:A:1129:LEU:N	1:A:1129:LEU:CD1	2.81	0.44
1:A:1626:GLN:HE21	1:A:1633:PHE:HB3	1.82	0.44
2:B:262:ILE:HG23	2:B:262:ILE:O	2.18	0.44
2:B:877:VAL:O	2:B:877:VAL:CG2	2.66	0.44
1:A:173:MET:HE3	1:A:173:MET:HB2	1.82	0.44
1:A:539:ARG:NH1	1:A:631:ASP:OD1	2.51	0.44
2:B:1:CYS:HB3	2:B:43:ILE:HD11	2.00	0.44
1:A:237:PHE:HE2	1:A:352:TYR:HH	1.62	0.43
1:A:1565:ILE:O	1:A:1614:GLY:HA2	2.18	0.43
1:A:1652:THR:HG22	1:A:1653:THR:N	2.32	0.43
2:B:173:GLY:O	2:B:187:VAL:HG12	2.18	0.43
1:A:605:VAL:HG11	1:A:610:TYR:CZ	2.53	0.43
1:A:790:LEU:HA	1:A:791:PRO:HD3	1.80	0.43
1:A:1170:LYS:HG2	1:A:1170:LYS:H	1.50	0.43
1:A:1202:HIS:HD2	1:A:1204:GLN:N	2.17	0.43
1:A:1372:GLU:CG	1:A:1409:LYS:NZ	2.81	0.43
2:B:119:CYS:CB	2:B:124:ARG:HH21	2.30	0.43
2:B:506:PRO:HG2	2:B:530:ASN:O	2.18	0.43
1:A:835:ARG:CD	1:A:905:ILE:HG12	2.48	0.43
1:A:907:LEU:HG	1:A:908:HIS:N	2.32	0.43
1:A:1225:TYR:CE1	1:A:1276:GLU:CG	2.80	0.43
2:B:905:ILE:HG23	2:B:905:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLU:HG3	1:A:77:ASN:N	2.32	0.43
1:A:983:LEU:C	1:A:983:LEU:CD1	2.89	0.43
1:A:1275:SER:HA	2:B:595:MET:SD	2.59	0.43
1:A:1536:GLN:HB3	1:A:1645:ILE:O	2.17	0.43
2:B:911:CYS:HB3	2:B:912:LEU:H	1.68	0.43
1:A:232:GLU:OE2	1:A:251:LYS:HE2	2.18	0.43
1:A:292:LEU:HD22	1:A:296:ILE:C	2.43	0.43
1:A:786:LEU:N	1:A:786:LEU:HD23	2.32	0.43
1:A:799:ILE:HG23	1:A:815:VAL:HB	1.99	0.43
1:A:934:VAL:HG23	1:A:935:LYS:H	1.83	0.43
1:A:1202:HIS:CD2	1:A:1204:GLN:H	2.37	0.43
1:A:1309:LEU:CD1	1:A:1311:MET:HB2	2.46	0.43
2:B:4:ASP:OD1	7:B:1007:MAN:H3	2.19	0.43
2:B:17:THR:HA	2:B:53:ASN:HD22	1.83	0.43
2:B:176:PHE:HD2	2:B:466:LEU:CD2	2.31	0.43
2:B:240:LEU:CD1	2:B:273:ASN:HD21	2.31	0.43
2:B:828:ARG:NH2	2:B:845:THR:O	2.52	0.43
1:A:113:LYS:CE	1:A:654:LEU:HD11	2.48	0.43
1:A:314:SER:O	1:A:317:ASP:HB2	2.19	0.43
1:A:583:SER:HA	1:A:584:PRO:HD3	1.69	0.43
1:A:766:ARG:NH2	1:A:921:GLU:OE2	2.42	0.43
1:A:1133:LEU:HB2	1:A:1143:TYR:CZ	2.54	0.43
1:A:1209:VAL:O	1:A:1213:LYS:HB2	2.19	0.43
1:A:1231:ASN:C	1:A:1231:ASN:HD22	2.26	0.43
1:A:1526:LYS:HG2	1:A:1627:ILE:HG22	1.99	0.43
2:B:29:ILE:CD1	2:B:46:LYS:HE3	2.48	0.43
2:B:70:SER:O	2:B:71:ASP:C	2.61	0.43
2:B:158:VAL:HG23	2:B:159:CYS:HB2	2.01	0.43
2:B:300:LYS:HD2	3:D:1:NAG:H82	2.01	0.43
1:A:229:VAL:HG22	1:A:252:ALA:HB2	2.00	0.43
1:A:941:GLY:HA2	1:A:1359:VAL:O	2.18	0.43
1:A:1377:PHE:CD1	1:A:1377:PHE:N	2.86	0.43
1:A:1556:GLU:HB3	1:A:1622:LYS:CE	2.49	0.43
1:A:1562:LYS:NZ	1:A:1648:TRP:HZ2	2.16	0.43
1:A:1618:LEU:HD22	1:A:1619:ILE:N	2.33	0.43
2:B:656:GLU:H	2:B:680:ARG:HB2	1.84	0.43
2:B:730:TRP:HB2	2:B:733:PRO:HD3	2.01	0.43
1:A:193:ASN:HD21	1:A:935:LYS:HZ1	1.62	0.43
1:A:913:SER:HA	1:A:922:ILE:HG12	2.01	0.43
1:A:930:VAL:CG1	1:A:931:PRO:CD	2.89	0.43
1:A:1027:THR:HG22	1:A:1302:LEU:CD1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1419:SER:O	1:A:1466:SER:CB	2.67	0.43
1:A:1483:PHE:C	1:A:1483:PHE:HD1	2.27	0.43
1:A:1675:GLY:O	1:A:1676:CYS:CB	2.64	0.43
2:B:443:LEU:CD1	2:B:444:GLU:N	2.71	0.43
2:B:850:GLU:HG2	2:B:860:VAL:O	2.18	0.43
1:A:597:ASP:OD1	1:A:781:PRO:HA	2.19	0.43
1:A:1002:HIS:O	1:A:1003:LEU:HB2	2.19	0.43
1:A:1105:LEU:HA	1:A:1108:VAL:CG1	2.49	0.43
2:B:88:PRO:CB	2:B:516:THR:O	2.67	0.43
2:B:471:ASP:HB3	2:B:474:ARG:HH21	1.83	0.43
2:B:876:CYS:SG	2:B:885:GLU:HB2	2.59	0.43
2:B:877:VAL:HG12	2:B:903:MET:CE	2.47	0.43
2:B:890:ILE:HG13	2:B:891:CYS:N	2.33	0.43
1:A:117:MET:HE3	1:A:117:MET:HB2	1.89	0.43
1:A:224:LEU:HA	1:A:225:PRO:HD3	1.83	0.43
1:A:628:GLU:OE1	1:A:674:ARG:NH1	2.52	0.43
1:A:944:LEU:HB3	1:A:1311:MET:CE	2.48	0.43
1:A:1029:ASN:C	1:A:1030:HIS:CD2	2.88	0.43
1:A:1549:LYS:HZ3	1:A:1670:ASP:CG	2.27	0.43
1:A:1574:PHE:HA	1:A:1603:LYS:HA	2.01	0.43
2:B:679:GLN:O	2:B:680:ARG:HB2	2.19	0.43
2:B:734:ILE:CD1	2:B:738:LEU:HB3	2.48	0.43
1:A:43:VAL:CG2	1:A:44:TYR:N	2.82	0.42
1:A:61:ASP:O	1:A:61:ASP:OD2	2.36	0.42
1:A:569:ASN:ND2	1:A:805:SER:HB3	2.33	0.42
1:A:1344:ASP:O	1:A:1345:ASP:C	2.60	0.42
1:A:1590:ALA:HB3	1:A:1624:ALA:HB1	2.00	0.42
1:A:1629:TYR:O	1:A:1630:ASN:CG	2.61	0.42
1:A:1654:CYS:N	1:A:1657:CYS:SG	2.92	0.42
2:B:466:LEU:N	2:B:466:LEU:CD1	2.82	0.42
2:B:469:ILE:O	2:B:472:LEU:HB2	2.19	0.42
2:B:699:ARG:C	2:B:700:LEU:HD13	2.44	0.42
2:B:889:ASN:OD1	2:B:889:ASN:N	2.52	0.42
1:A:58:SER:O	1:A:103:TYR:CD1	2.67	0.42
1:A:577:PRO:HG2	1:A:586:GLN:NE2	2.34	0.42
1:A:1228:TRP:CE3	1:A:1251:THR:HB	2.46	0.42
1:A:1462:LEU:HD11	1:A:1475:VAL:HG21	2.00	0.42
2:B:2:PHE:O	2:B:5:HIS:HB2	2.19	0.42
2:B:214:ASN:H	2:B:214:ASN:HD22	1.67	0.42
2:B:271:ASN:HD22	2:B:271:ASN:N	2.15	0.42
2:B:474:ARG:O	2:B:605:ASP:OD1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:477:PRO:O	2:B:604:ASN:HB3	2.19	0.42
2:B:493:TYR:CE2	2:B:497:PHE:HE2	2.28	0.42
1:A:149:ASN:CB	1:A:155:ALA:HB2	2.40	0.42
1:A:983:LEU:HD13	1:A:984:VAL:CA	2.48	0.42
1:A:1030:HIS:C	1:A:1032:ASN:H	2.26	0.42
1:A:1143:TYR:HD1	1:A:1186:PHE:HE2	1.65	0.42
2:B:317:PHE:CE1	2:B:321:LEU:HD22	2.54	0.42
2:B:418:LYS:CA	2:B:436:TRP:CZ3	2.97	0.42
2:B:495:ALA:CB	7:B:1008:MAN:H61	2.47	0.42
2:B:608:GLU:H	2:B:608:GLU:HG3	1.59	0.42
2:B:713:LYS:H	2:B:713:LYS:HD3	1.84	0.42
1:A:77:ASN:O	1:A:78:LYS:C	2.61	0.42
1:A:177:ILE:C	1:A:177:ILE:HD12	2.44	0.42
1:A:321:LYS:O	1:A:347:TYR:HB2	2.19	0.42
1:A:655:THR:HG23	1:A:656:ASN:N	2.35	0.42
1:A:882:LYS:CG	1:A:883:CYS:N	2.82	0.42
1:A:1284:PHE:CE2	2:B:594:ILE:HD11	2.54	0.42
2:B:660:TYR:HE2	2:B:662:TYR:HB2	1.83	0.42
2:B:743:ASP:O	2:B:744:THR:HG22	2.19	0.42
2:B:875:TYR:CG	2:B:910:LYS:HA	2.55	0.42
1:A:138:ASP:HA	1:A:189:LYS:CE	2.49	0.42
1:A:1028:GLY:HA2	1:A:1305:LYS:HZ1	1.85	0.42
1:A:1590:ALA:HB1	1:A:1635:TYR:CZ	2.54	0.42
1:A:1631:PHE:O	1:A:1631:PHE:CD2	2.73	0.42
2:B:782:PHE:CE1	2:B:826:LEU:HD12	2.54	0.42
1:A:620:LEU:O	1:A:621:GLU:C	2.61	0.42
1:A:823:VAL:HG22	1:A:847:ASN:HA	2.01	0.42
2:B:716:VAL:HG13	2:B:717:VAL:N	2.35	0.42
1:A:160:VAL:HG22	1:A:175:GLU:HB3	2.02	0.42
1:A:222:TYR:HE1	1:A:224:LEU:HD23	1.84	0.42
1:A:959:PHE:HE2	1:A:1348:VAL:HG23	1.85	0.42
1:A:1127:ILE:CD1	1:A:1130:GLN:HE21	2.03	0.42
2:B:322:ASN:O	2:B:324:LEU:N	2.51	0.42
1:A:485:ILE:HD12	1:A:485:ILE:N	2.35	0.42
1:A:489:LYS:C	1:A:491:PRO:HD2	2.45	0.42
1:A:620:LEU:HG	1:A:624:PHE:HE1	1.84	0.42
1:A:1153:ARG:HH22	2:B:699:ARG:HH22	1.68	0.42
1:A:1176:LEU:HD23	1:A:1195:LEU:HD13	2.01	0.42
2:B:226:GLU:OE2	2:B:384:LYS:NZ	2.52	0.42
2:B:241:GLY:O	2:B:245:ASN:OD1	2.38	0.42
2:B:300:LYS:HD2	3:D:1:NAG:C8	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:437:GLU:O	2:B:441:SER:N	2.53	0.42
1:A:22:THR:HG21	1:A:552:ALA:CB	2.49	0.42
1:A:833:VAL:O	1:A:929:VAL:HA	2.20	0.42
1:A:1066:TYR:CB	1:A:1078:LEU:HD23	2.49	0.42
2:B:508:ASN:OD1	2:B:543:VAL:HA	2.19	0.42
2:B:510:ARG:O	2:B:521:VAL:HB	2.20	0.42
1:A:1259:LEU:HD13	1:A:1299:GLU:HB3	2.01	0.42
1:A:1519:VAL:HG22	1:A:1574:PHE:CE1	2.55	0.42
2:B:389:PHE:HE2	2:B:448:PHE:HD1	1.67	0.42
2:B:483:ARG:NH2	2:B:605:ASP:OD1	2.53	0.42
2:B:493:TYR:O	2:B:497:PHE:CD2	2.73	0.42
2:B:613:ASP:C	2:B:615:PRO:HD3	2.45	0.42
1:A:266:TYR:CZ	1:A:1483:PHE:CG	3.06	0.41
1:A:346:LYS:NZ	1:A:378:SER:HB2	2.34	0.41
1:A:620:LEU:CD1	1:A:811:VAL:HB	2.34	0.41
1:A:1549:LYS:HG3	1:A:1667:PHE:HE1	1.85	0.41
1:A:1589:GLU:CG	1:A:1590:ALA:N	2.70	0.41
2:B:493:TYR:CD1	2:B:497:PHE:HE2	2.38	0.41
2:B:691:VAL:HG11	2:B:739:THR:HG23	2.02	0.41
2:B:874:LEU:O	2:B:875:TYR:C	2.63	0.41
1:A:23:TYR:CG	1:A:656:ASN:HB2	2.55	0.41
1:A:491:PRO:HG3	1:A:544:TYR:OH	2.20	0.41
1:A:762:LYS:HG2	1:A:762:LYS:O	2.19	0.41
1:A:956:ARG:HA	1:A:1348:VAL:O	2.19	0.41
1:A:1135:VAL:HG13	1:A:1136:GLU:N	2.35	0.41
1:A:1226:ARG:NH1	2:B:611:GLU:OE1	2.50	0.41
1:A:1314:ASP:HA	1:A:1325:ASN:CB	2.50	0.41
1:A:1450:PHE:CE1	1:A:1475:VAL:HB	2.55	0.41
1:A:1562:LYS:HD2	1:A:1648:TRP:NE1	2.32	0.41
1:A:57:LYS:HD3	1:A:62:LYS:HB3	2.01	0.41
1:A:396:ASP:CB	1:A:400:GLU:HB3	2.38	0.41
1:A:494:ASP:CA	1:A:496:ILE:HD12	2.50	0.41
1:A:781:PRO:O	1:A:782:ARG:HB2	2.20	0.41
1:A:949:ILE:HG23	1:A:1262:LYS:HD2	2.01	0.41
1:A:961:TYR:CE2	1:A:963:ILE:HG22	2.55	0.41
1:A:1556:GLU:HB2	1:A:1622:LYS:HE2	2.02	0.41
1:A:1654:CYS:C	1:A:1655:SER:HG	2.23	0.41
2:B:444:GLU:O	2:B:447:THR:HB	2.20	0.41
1:A:151:ASP:O	1:A:152:LEU:HB2	2.20	0.41
1:A:335:GLY:CA	1:A:895:LEU:CD2	2.92	0.41
1:A:494:ASP:C	1:A:496:ILE:HD12	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:PHE:HA	1:A:1049:LEU:HD11	2.02	0.41
1:A:1022:PHE:HE2	1:A:1026:GLU:OE2	2.03	0.41
1:A:1066:TYR:HD1	1:A:1079:THR:HG23	1.85	0.41
1:A:1135:VAL:HG11	1:A:1139:GLU:C	2.44	0.41
1:A:1273:TRP:HE3	1:A:1274:LEU:CA	2.30	0.41
1:A:1342:LEU:HD13	1:A:1342:LEU:N	2.36	0.41
2:B:11:TRP:CH2	2:B:50:ARG:CZ	3.03	0.41
2:B:138:ASN:C	2:B:149:GLU:OE2	2.63	0.41
2:B:427:ARG:HB2	2:B:430:TYR:CD2	2.56	0.41
2:B:546:GLN:HB2	2:B:571:PRO:CG	2.50	0.41
1:A:190:ILE:HA	1:A:191:PRO:HD3	1.91	0.41
1:A:1188:LEU:HD12	1:A:1188:LEU:HA	1.86	0.41
1:A:1411:SER:H	1:A:1414:GLU:HB2	1.86	0.41
1:A:1648:TRP:CG	1:A:1648:TRP:O	2.74	0.41
2:B:567:GLU:C	2:B:569:ASN:ND2	2.78	0.41
1:A:103:TYR:HA	1:A:115:LYS:O	2.21	0.41
1:A:494:ASP:HA	1:A:496:ILE:CD1	2.49	0.41
1:A:501:TYR:CB	1:A:542:VAL:HG22	2.51	0.41
1:A:855:PHE:HA	1:A:915:GLU:O	2.21	0.41
1:A:1280:TYR:CD2	1:A:1281:GLY:CA	3.04	0.41
1:A:1487:PHE:CD1	1:A:1487:PHE:C	2.97	0.41
1:A:1572:ASN:O	1:A:1573:VAL:HB	2.21	0.41
2:B:18:CYS:C	2:B:57:CYS:SG	3.04	0.41
2:B:89:SER:HB2	2:B:95:PRO:HA	2.01	0.41
2:B:214:ASN:O	2:B:307:LYS:HB3	2.20	0.41
2:B:734:ILE:N	2:B:734:ILE:HD13	2.36	0.41
1:A:308:LYS:HA	1:A:312:TYR:O	2.20	0.41
1:A:560:TRP:CH2	1:A:673:LEU:HB3	2.56	0.41
1:A:765:ILE:HD13	3:C:2:NAG:H82	2.01	0.41
1:A:856:CYS:N	1:A:915:GLU:O	2.53	0.41
1:A:1226:ARG:O	1:A:1270:VAL:HG22	2.21	0.41
1:A:1247:MET:O	1:A:1251:THR:CG2	2.69	0.41
2:B:328:TYR:OH	2:B:489:ALA:HA	2.21	0.41
2:B:553:TRP:CZ3	2:B:564:ARG:HB2	2.55	0.41
2:B:755:GLY:HA3	2:B:801:LYS:HE3	2.03	0.41
2:B:844:ASP:C	2:B:845:THR:HG22	2.44	0.41
1:A:494:ASP:C	1:A:496:ILE:N	2.78	0.41
1:A:1021:VAL:O	1:A:1025:LEU:HB2	2.20	0.41
1:A:1488:LEU:C	1:A:1488:LEU:HD12	2.46	0.41
2:B:868:PHE:C	2:B:868:PHE:CD2	2.99	0.41
1:A:136:THR:OG1	1:A:831:TYR:OH	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:GLU:OE2	1:A:821:LYS:NZ	2.42	0.41
1:A:793:SER:O	1:A:819:VAL:CG2	2.69	0.41
1:A:925:LYS:HD2	1:A:925:LYS:HA	1.55	0.41
1:A:944:LEU:CB	1:A:1311:MET:HE2	2.51	0.41
1:A:1013:MET:SD	1:A:1287:THR:HB	2.61	0.41
1:A:1204:GLN:OE1	1:A:1204:GLN:HA	2.21	0.41
1:A:1494:THR:HA	1:A:1505:CYS:O	2.21	0.41
2:B:116:GLU:OE2	2:B:130:CYS:CB	2.65	0.41
2:B:546:GLN:N	2:B:571:PRO:HG2	2.35	0.41
1:A:115:LYS:HB3	1:A:117:MET:HE2	2.03	0.41
1:A:123:ASN:HD22	1:A:150:ASP:CG	2.29	0.41
1:A:232:GLU:HA	1:A:233:PRO:HD3	1.88	0.41
1:A:359:THR:CG2	1:A:372:LYS:H	2.34	0.41
1:A:489:LYS:O	1:A:490:SER:HB2	2.21	0.41
1:A:503:ILE:HB	1:A:511:HIS:HB2	2.03	0.41
1:A:543:TYR:HA	1:A:555:VAL:O	2.21	0.41
1:A:586:GLN:HG2	1:A:587:THR:O	2.20	0.41
1:A:589:SER:HB3	1:A:785:GLN:HG2	2.03	0.41
1:A:923:LEU:HD12	1:A:923:LEU:HA	1.54	0.41
1:A:1341:LEU:HD12	1:A:1341:LEU:N	2.36	0.41
1:A:1528:VAL:HG12	1:A:1529:GLU:H	1.85	0.41
1:A:1533:GLY:N	1:A:1606:CYS:SG	2.94	0.41
2:B:838:LYS:HB3	2:B:845:THR:HB	2.02	0.41
1:A:120:THR:HG22	1:A:121:TYR:N	2.37	0.40
1:A:137:PRO:HG3	1:A:196:TYR:CE1	2.56	0.40
1:A:369:TYR:HA	1:A:370:PRO:HD3	1.98	0.40
1:A:488:PRO:O	1:A:491:PRO:HD2	2.21	0.40
2:B:138:ASN:C	2:B:138:ASN:OD1	2.64	0.40
2:B:142:ASP:HB2	2:B:148:ASP:OD1	2.20	0.40
2:B:219:GLY:O	2:B:302:LEU:HA	2.22	0.40
2:B:641:TYR:HD1	2:B:645:GLU:OE1	2.03	0.40
2:B:641:TYR:HD1	2:B:645:GLU:CD	2.29	0.40
1:A:182:ILE:CG1	1:A:804:ILE:CD1	2.92	0.40
1:A:492:TYR:CD2	1:A:493:ILE:N	2.89	0.40
1:A:565:GLU:HB3	1:A:624:PHE:CE2	2.56	0.40
1:A:1030:HIS:C	1:A:1032:ASN:N	2.78	0.40
1:A:1138:ARG:H	1:A:1138:ARG:CD	2.34	0.40
1:A:1647:TYR:HD1	1:A:1649:PRO:CG	2.35	0.40
1:A:1356:LEU:HD23	1:A:1356:LEU:HA	1.83	0.40
1:A:1367:LYS:CD	1:A:1373:GLU:HG2	2.51	0.40
1:A:1549:LYS:NZ	1:A:1670:ASP:CG	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:PHE:CE2	2:B:312:HIS:CD2	3.10	0.40
2:B:508:ASN:OD1	2:B:544:ASP:N	2.39	0.40
2:B:867:CYS:O	2:B:868:PHE:HB2	2.21	0.40
1:A:352:TYR:CE1	1:A:383:VAL:HG11	2.56	0.40
1:A:476:LEU:HD22	1:A:480:GLU:OE2	2.22	0.40
1:A:1601:ILE:O	1:A:1639:LEU:HD13	2.21	0.40
1:A:1622:LYS:CD	1:A:1642:LEU:HD23	2.52	0.40
2:B:783:ASP:OD2	2:B:783:ASP:C	2.64	0.40
1:A:635:GLY:C	1:A:637:GLY:H	2.29	0.40
1:A:1047:LYS:NZ	1:A:1051:GLU:OE2	2.42	0.40
1:A:1342:LEU:CD1	1:A:1342:LEU:N	2.85	0.40
2:B:123:PHE:CD1	2:B:136:GLU:OE1	2.74	0.40
2:B:389:PHE:CE2	2:B:448:PHE:HD1	2.39	0.40
2:B:560:TYR:O	2:B:590:CYS:N	2.46	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	1544/1676 (92%)	1339 (87%)	170 (11%)	35 (2%)	5	29
2	B	892/913 (98%)	770 (86%)	96 (11%)	26 (3%)	3	24
All	All	2436/2589 (94%)	2109 (87%)	266 (11%)	61 (2%)	4	27

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	PRO
1	A	89	PRO
1	A	191	PRO
1	A	335	GLY

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Mol	Chain	Res	Type
1	A	490	SER
1	A	662	SER
1	A	762	LYS
1	A	1072	GLY
1	A	1122	SER
1	A	1235	LYS
1	A	1245	ALA
1	A	1246	ARG
1	A	1573	VAL
2	B	73	ASP
2	B	508	ASN
2	B	571	PRO
2	B	605	ASP
2	B	615	PRO
2	B	727	GLY
2	B	875	TYR
2	B	910	LYS
1	A	48	GLU
1	A	61	ASP
1	A	638	GLY
1	A	1596	SER
2	B	71	ASP
2	B	323	HIS
2	B	773	SER
1	A	480	GLU
1	A	932	GLU
1	A	1004	PRO
1	A	1139	GLU
1	A	1590	ALA
2	B	20	SER
2	B	74	PRO
2	B	99	PRO
2	B	598	ASN
2	B	668	ASP
2	B	728	ASN
2	B	868	PHE
1	A	207	GLU
1	A	585	GLY
1	A	1321	GLY
1	A	1337	PRO
1	A	1589	GLU
2	B	206	SER

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Mol	Chain	Res	Type
2	B	732	PRO
1	A	806	ASN
1	A	1030	HIS
2	B	687	VAL
2	B	812	HIS
1	A	495	LYS
1	A	1003	LEU
1	A	1514	ILE
1	A	1609	ALA
2	B	55	GLN
2	B	506	PRO
2	B	911	CYS
2	B	476	ILE
1	A	491	PRO
1	A	225	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	1379/1484 (93%)	1174 (85%)	205 (15%)	3	14
2	B	797/810 (98%)	707 (89%)	90 (11%)	5	21
All	All	2176/2294 (95%)	1881 (86%)	295 (14%)	3	16

All (295) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	VAL
1	A	47	THR
1	A	53	THR
1	A	55	SER
1	A	73	LEU
1	A	76	GLU
1	A	78	LYS
1	A	115	LYS

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Mol	Chain	Res	Type
1	A	130	THR
1	A	136	THR
1	A	161	LEU
1	A	162	THR
1	A	174	VAL
1	A	175	GLU
1	A	179	HIS
1	A	180	ILE
1	A	195	ARG
1	A	208	ASP
1	A	209	PHE
1	A	211	THR
1	A	223	VAL
1	A	224	LEU
1	A	231	ILE
1	A	242	ASN
1	A	261	THR
1	A	281	GLU
1	A	285	THR
1	A	310	LEU
1	A	323	LEU
1	A	328	THR
1	A	330	ILE
1	A	333	THR
1	A	361	LEU
1	A	364	LYS
1	A	373	VAL
1	A	383	VAL
1	A	394	THR
1	A	396	ASP
1	A	401	THR
1	A	422	LEU
1	A	423	ASN
1	A	431	LEU
1	A	434	ASN
1	A	436	LYS
1	A	445	GLU
1	A	457	TYR
1	A	460	LEU
1	A	492	TYR
1	A	495	LYS
1	A	497	THR

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Mol	Chain	Res	Type
1	A	516	GLU
1	A	520	ASP
1	A	528	ILE
1	A	535	VAL
1	A	540	LEU
1	A	545	ILE
1	A	562	ASN
1	A	563	ILE
1	A	580	ASP
1	A	588	VAL
1	A	592	MET
1	A	594	THR
1	A	628	GLU
1	A	630	SER
1	A	640	LEU
1	A	644	ASN
1	A	655	THR
1	A	656	ASN
1	A	665	ASN
1	A	672	ILE
1	A	676	ARG
1	A	790	LEU
1	A	794	LEU
1	A	799	ILE
1	A	800	GLN
1	A	802	ILE
1	A	814	THR
1	A	837	GLU
1	A	850	THR
1	A	857	VAL
1	A	887	LYS
1	A	888	VAL
1	A	893	SER
1	A	895	LEU
1	A	899	THR
1	A	901	LEU
1	A	905	ILE
1	A	917	TRP
1	A	921	GLU
1	A	922	ILE
1	A	924	VAL
1	A	925	LYS

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Mol	Chain	Res	Type
1	A	927	LEU
1	A	929	VAL
1	A	930	VAL
1	A	932	GLU
1	A	934	VAL
1	A	935	LYS
1	A	939	TYR
1	A	942	VAL
1	A	952	THR
1	A	954	SER
1	A	956	ARG
1	A	963	ILE
1	A	966	ASP
1	A	968	VAL
1	A	982	LEU
1	A	984	VAL
1	A	988	LEU
1	A	993	SER
1	A	1003	LEU
1	A	1005	LYS
1	A	1012	LEU
1	A	1015	VAL
1	A	1016	VAL
1	A	1056	ILE
1	A	1078	LEU
1	A	1096	ASN
1	A	1108	VAL
1	A	1113	LEU
1	A	1115	ASN
1	A	1133	LEU
1	A	1135	VAL
1	A	1138	ARG
1	A	1140	ASN
1	A	1142	LEU
1	A	1148	THR
1	A	1149	VAL
1	A	1161	LEU
1	A	1162	VAL
1	A	1170	LYS
1	A	1196	SER
1	A	1200	LYS
1	A	1213	LYS

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Mol	Chain	Res	Type
1	A	1217	LEU
1	A	1221	ASN
1	A	1231	ASN
1	A	1232	LEU
1	A	1236	ASP
1	A	1251	THR
1	A	1271	ILE
1	A	1278	GLN
1	A	1279	ARG
1	A	1280	TYR
1	A	1287	THR
1	A	1291	ILE
1	A	1298	THR
1	A	1303	LEU
1	A	1307	LEU
1	A	1324	HIS
1	A	1326	TYR
1	A	1331	LYS
1	A	1334	LEU
1	A	1336	ARG
1	A	1341	LEU
1	A	1342	LEU
1	A	1352	PHE
1	A	1363	THR
1	A	1367	LYS
1	A	1370	THR
1	A	1377	PHE
1	A	1412	ARG
1	A	1423	VAL
1	A	1440	LYS
1	A	1443	VAL
1	A	1452	ASP
1	A	1464	LEU
1	A	1473	LEU
1	A	1476	ARG
1	A	1480	PHE
1	A	1483	PHE
1	A	1485	VAL
1	A	1487	PHE
1	A	1488	LEU
1	A	1494	THR
1	A	1495	VAL

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Mol	Chain	Res	Type
1	A	1500	ARG
1	A	1502	ASP
1	A	1514	ILE
1	A	1520	CYS
1	A	1525	CYS
1	A	1534	GLN
1	A	1539	LEU
1	A	1543	ILE
1	A	1549	LYS
1	A	1553	CYS
1	A	1566	THR
1	A	1569	THR
1	A	1581	LEU
1	A	1582	LEU
1	A	1589	GLU
1	A	1594	LYS
1	A	1598	ILE
1	A	1602	LYS
1	A	1611	LEU
1	A	1618	LEU
1	A	1619	ILE
1	A	1620	MET
1	A	1627	ILE
1	A	1636	ILE
1	A	1642	LEU
1	A	1643	THR
1	A	1650	ARG
1	A	1651	ASP
1	A	1653	THR
2	B	5	HIS
2	B	10	GLN
2	B	17	THR
2	B	30	VAL
2	B	51	GLU
2	B	54	TRP
2	B	72	CYS
2	B	80	SER
2	B	85	VAL
2	B	100	LEU
2	B	110	LYS
2	B	120	LYS
2	B	121	ASN

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Mol	Chain	Res	Type
2	B	122	LYS
2	B	126	ASP
2	B	135	LEU
2	B	149	GLU
2	B	155	THR
2	B	182	GLU
2	B	188	LEU
2	B	200	VAL
2	B	204	ARG
2	B	214	ASN
2	B	221	GLU
2	B	263	PHE
2	B	271	ASN
2	B	302	LEU
2	B	303	ASN
2	B	312	HIS
2	B	318	LEU
2	B	326	LEU
2	B	392	LYS
2	B	393	THR
2	B	395	VAL
2	B	409	GLU
2	B	436	TRP
2	B	441	SER
2	B	443	LEU
2	B	452	LEU
2	B	461	VAL
2	B	560	TYR
2	B	566	ARG
2	B	569	ASN
2	B	581	GLU
2	B	583	GLU
2	B	589	ASP
2	B	591	THR
2	B	592	PHE
2	B	594	ILE
2	B	604	ASN
2	B	607	GLU
2	B	611	GLU
2	B	612	VAL
2	B	613	ASP
2	B	617	ILE

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Mol	Chain	Res	Type
2	B	620	ASP
2	B	627	VAL
2	B	636	ASN
2	B	649	ILE
2	B	657	THR
2	B	661	GLN
2	B	688	VAL
2	B	692	LEU
2	B	693	THR
2	B	694	ILE
2	B	700	LEU
2	B	702	ARG
2	B	703	ILE
2	B	713	LYS
2	B	716	VAL
2	B	728	ASN
2	B	734	ILE
2	B	741	GLU
2	B	751	HIS
2	B	785	ASP
2	B	789	TYR
2	B	804	ASN
2	B	805	ASN
2	B	811	LEU
2	B	845	THR
2	B	859	CYS
2	B	862	LEU
2	B	876	CYS
2	B	877	VAL
2	B	881	SER
2	B	885	GLU
2	B	889	ASN
2	B	892	GLU
2	B	895	THR
2	B	907	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	42	GLN
1	A	88	GLN

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Mol	Chain	Res	Type
1	A	91	GLN
1	A	110	HIS
1	A	123	ASN
1	A	139	GLN
1	A	193	ASN
1	A	226	HIS
1	A	289	ASN
1	A	423	ASN
1	A	472	ASN
1	A	483	ASN
1	A	533	ASN
1	A	562	ASN
1	A	574	HIS
1	A	613	GLN
1	A	642	ASN
1	A	647	HIS
1	A	656	ASN
1	A	665	ASN
1	A	787	GLN
1	A	800	GLN
1	A	886	GLN
1	A	909	ASN
1	A	1002	HIS
1	A	1043	GLN
1	A	1096	ASN
1	A	1098	ASN
1	A	1110	ASN
1	A	1115	ASN
1	A	1121	ASN
1	A	1123	GLN
1	A	1140	ASN
1	A	1202	HIS
1	A	1231	ASN
1	A	1265	ASN
1	A	1288	GLN
1	A	1319	HIS
1	A	1332	ASN
1	A	1360	HIS
1	A	1421	HIS
1	A	1448	GLN
1	A	1465	ASN
1	A	1499	HIS

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Mol	Chain	Res	Type
1	A	1513	ASN
1	A	1626	GLN
1	A	1658	GLN
2	B	10	GLN
2	B	23	GLN
2	B	53	ASN
2	B	79	GLN
2	B	90	GLN
2	B	146	ASN
2	B	174	ASN
2	B	190	ASN
2	B	214	ASN
2	B	217	ASN
2	B	223	GLN
2	B	242	HIS
2	B	271	ASN
2	B	273	ASN
2	B	275	ASN
2	B	280	GLN
2	B	286	HIS
2	B	312	HIS
2	B	329	ASN
2	B	491	GLN
2	B	530	ASN
2	B	546	GLN
2	B	569	ASN
2	B	574	GLN
2	B	597	ASN
2	B	600	GLN
2	B	636	ASN
2	B	698	GLN
2	B	726	GLN
2	B	804	ASN
2	B	834	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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
3	NAG	C	1	3,1	14,14,15	0.57	0	17,19,21	1.53	4 (23%)
3	NAG	C	2	3	14,14,15	0.52	0	17,19,21	1.11	2 (11%)
3	NAG	D	1	3,2	14,14,15	0.42	0	17,19,21	1.96	1 (5%)
3	NAG	D	2	3	14,14,15	0.57	0	17,19,21	1.03	2 (11%)
4	FUC	E	1	2,4	10,10,11	0.67	0	14,14,16	1.46	3 (21%)
4	BGC	E	2	4	11,11,12	0.73	0	15,15,17	0.89	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	NAG	D	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
4	FUC	E	1	2,4	-	-	0/1/1/1
4	BGC	E	2	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	C1-O5-C5	6.76	121.25	112.19
4	E	1	FUC	C3-C4-C5	3.46	115.07	109.81
3	C	1	NAG	O5-C1-C2	-3.37	106.07	111.29
3	C	1	NAG	C1-C2-N2	2.84	114.90	110.43
4	E	1	FUC	C1-O5-C5	2.37	118.56	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	O4-C4-C3	-2.34	104.86	110.38
3	D	2	NAG	C1-O5-C5	2.31	115.28	112.19
3	C	2	NAG	C1-C2-N2	2.28	114.03	110.43
3	C	1	NAG	O7-C7-C8	-2.10	118.31	122.05
4	E	1	FUC	O5-C5-C4	2.03	113.21	109.55
3	D	2	NAG	O4-C4-C3	-2.02	105.62	110.38
3	C	2	NAG	O7-C7-N2	2.02	125.54	121.98

There are no chirality outliers.

All (5) torsion outliers are listed below:

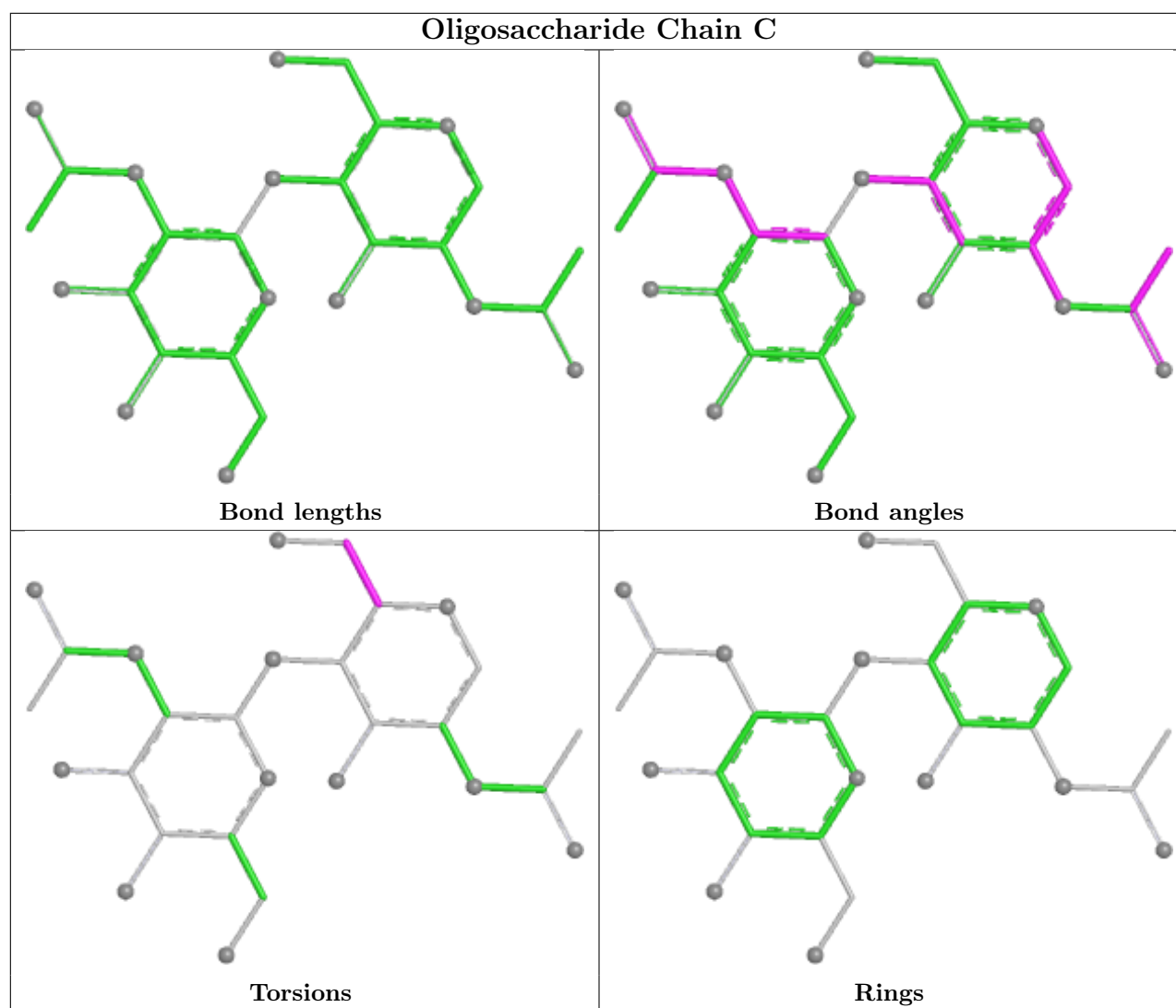
Mol	Chain	Res	Type	Atoms
4	E	2	BGC	O5-C5-C6-O6
4	E	2	BGC	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

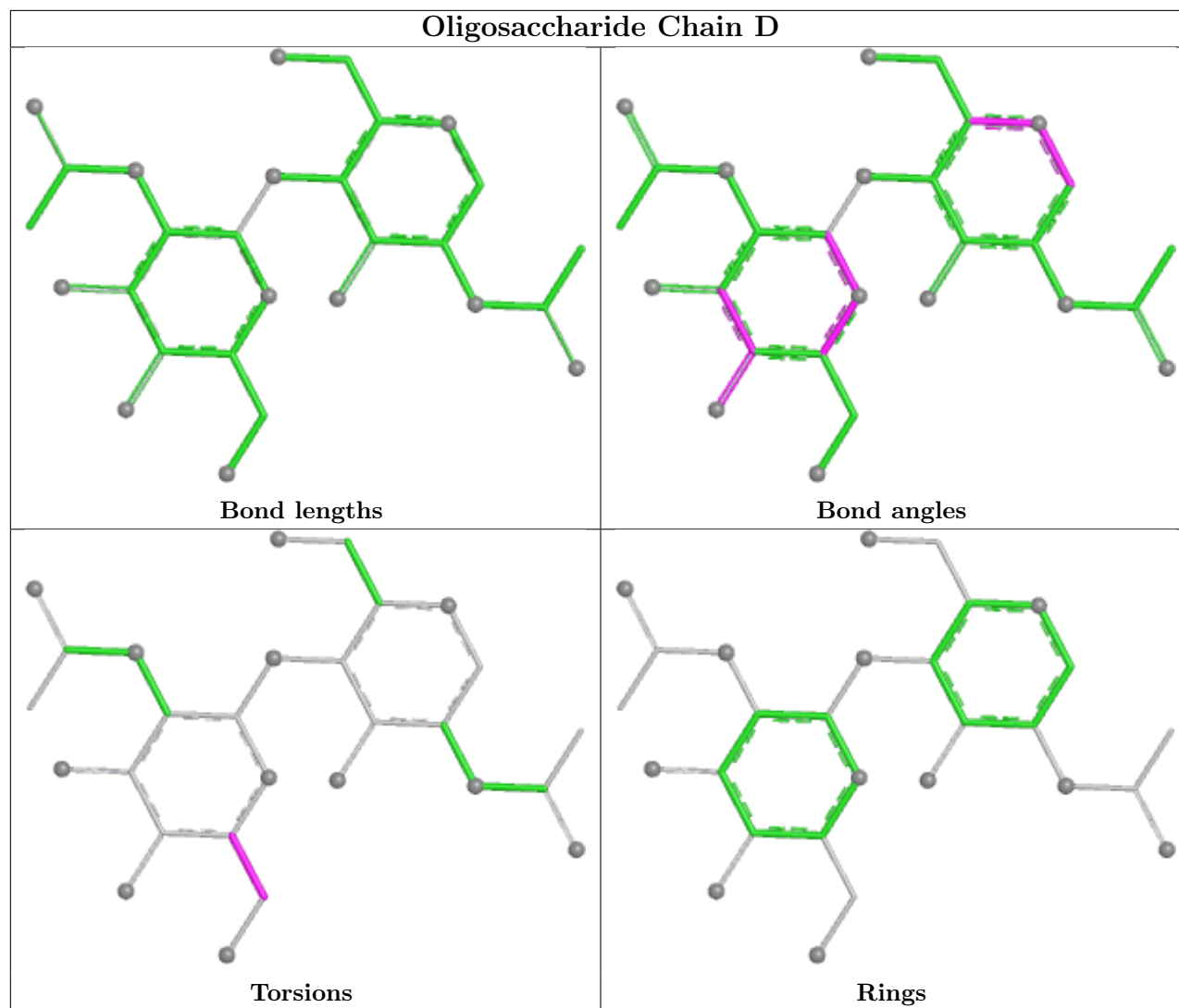
There are no ring outliers.

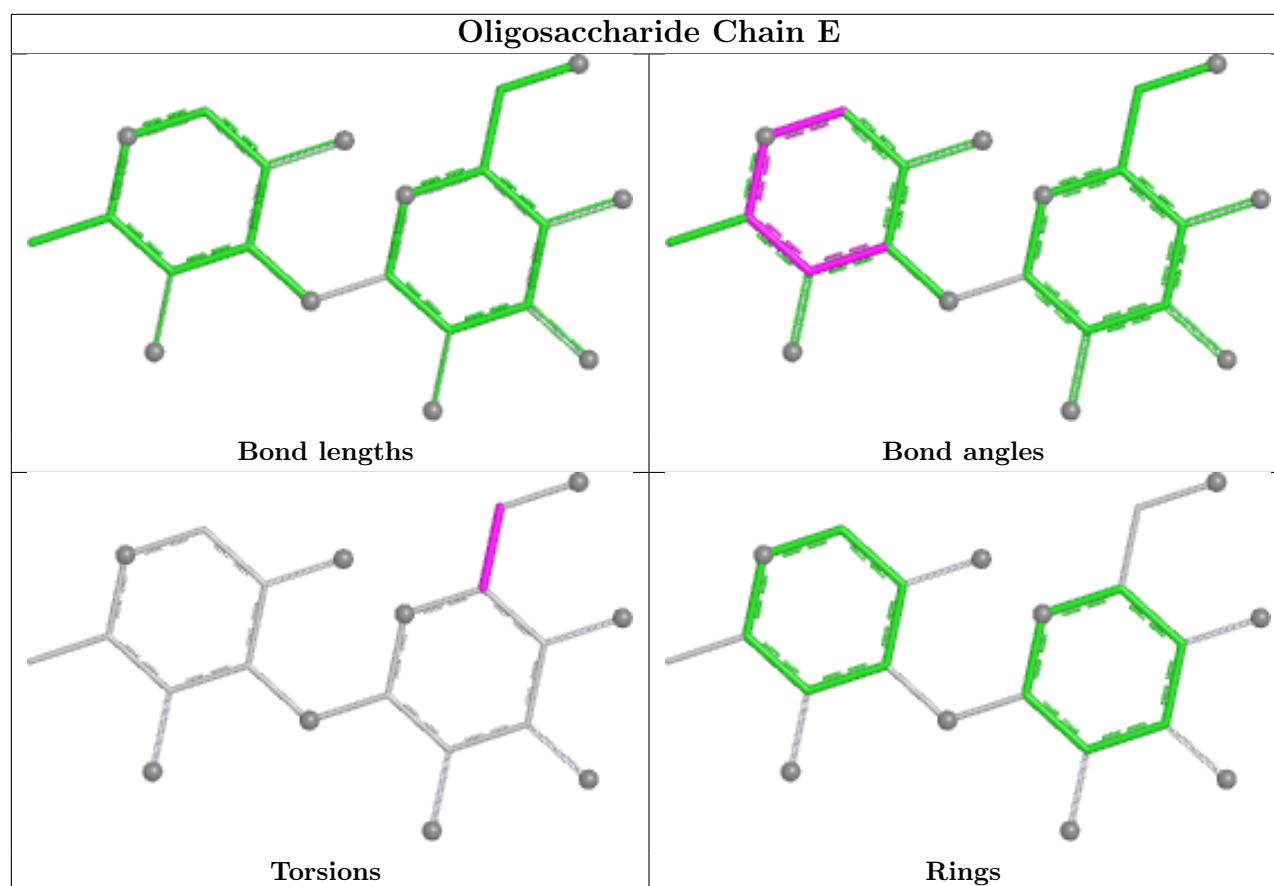
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	NAG	1	0
3	D	1	NAG	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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
7	MAN	B	1009	2	11,11,12	0.61	0	15,15,17	1.10	2 (13%)
7	MAN	B	1008	2	11,11,12	0.66	0	15,15,17	1.47	1 (6%)
7	MAN	B	1007	2	11,11,12	0.69	0	15,15,17	0.84	0
7	MAN	B	1006	2	11,11,12	0.57	0	15,15,17	1.05	1 (6%)

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
7	MAN	B	1009	2	-	0/2/19/22	0/1/1/1
7	MAN	B	1008	2	-	0/2/19/22	0/1/1/1
7	MAN	B	1007	2	-	1/2/19/22	0/1/1/1
7	MAN	B	1006	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1008	MAN	C3-C4-C5	3.70	116.94	110.23
7	B	1009	MAN	C3-C4-C5	2.27	114.34	110.23
7	B	1006	MAN	C1-O5-C5	2.27	115.22	112.19
7	B	1009	MAN	C1-O5-C5	2.24	115.19	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1006	MAN	O5-C5-C6-O6
7	B	1006	MAN	C4-C5-C6-O6
7	B	1007	MAN	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1009	MAN	1	0
7	B	1008	MAN	4	0
7	B	1007	MAN	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1552/1676 (92%)	-0.08	10 (0%) 85 72	110, 177, 258, 386	0
2	B	898/913 (98%)	-0.10	5 (0%) 85 72	121, 201, 282, 389	0
All	All	2450/2589 (94%)	-0.09	15 (0%) 85 72	110, 187, 269, 389	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1133	LEU	4.5
2	B	834	ASN	3.6
2	B	269	SER	3.3
2	B	51	GLU	3.0
1	A	470	THR	2.8
2	B	796	LYS	2.7
1	A	1534	GLN	2.3
1	A	1450	PHE	2.3
1	A	1622	LYS	2.2
1	A	1503	LYS	2.2
1	A	1066	TYR	2.1
1	A	239	GLY	2.1
1	A	483	ASN	2.1
1	A	623	VAL	2.1
2	B	245	ASN	2.0

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

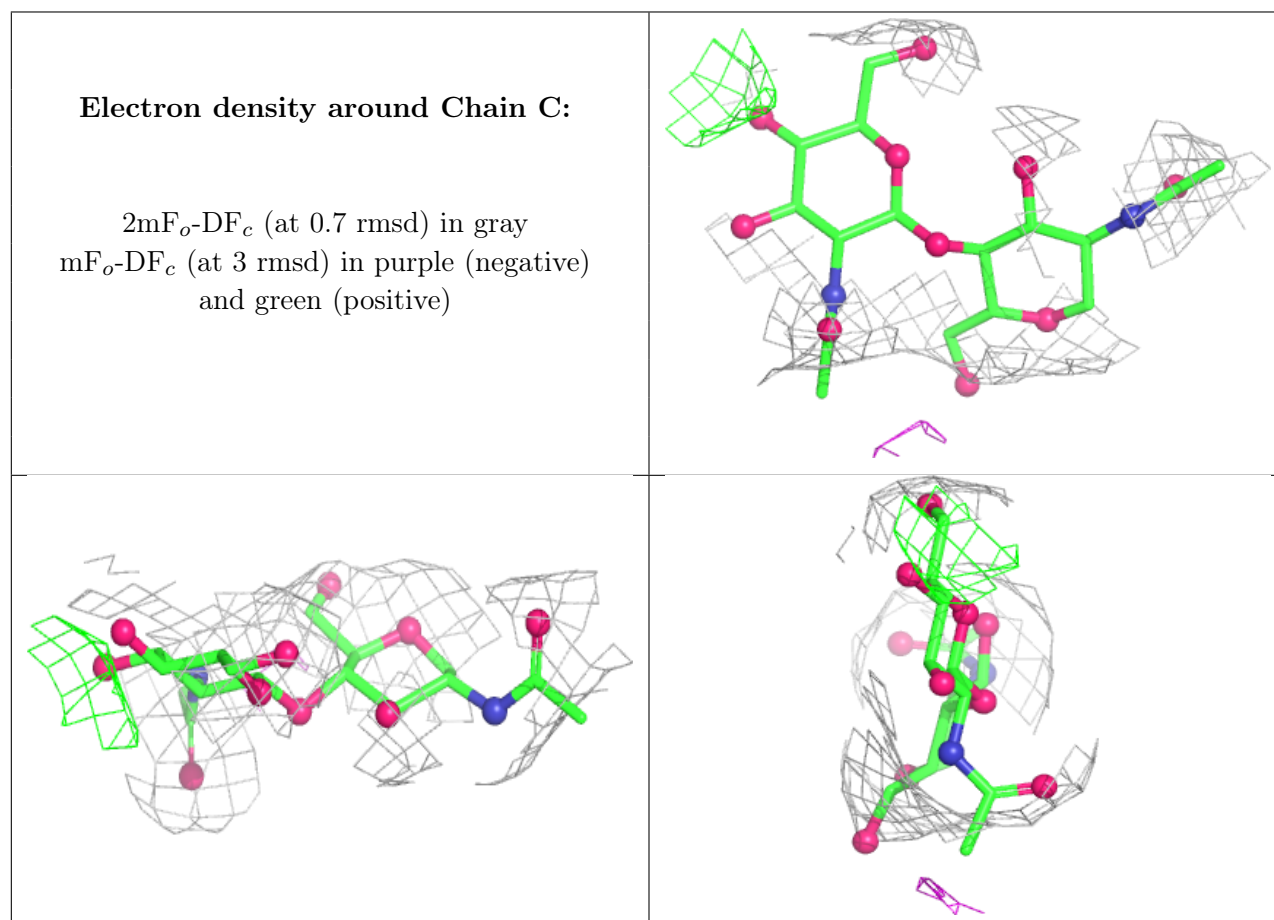
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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.

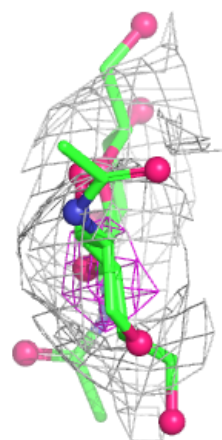
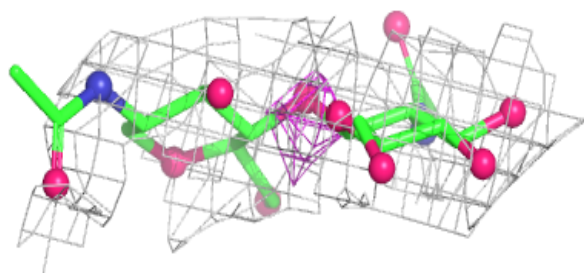
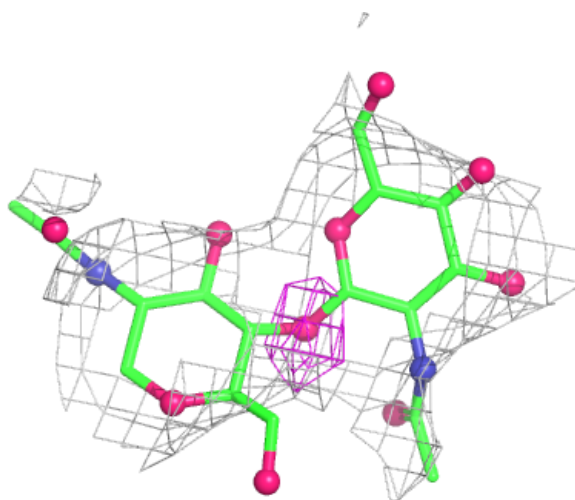
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	D	2	14/15	0.28	0.11	269,286,304,315	0
3	NAG	C	2	14/15	0.79	0.11	207,226,257,262	0
3	NAG	D	1	14/15	0.84	0.12	205,240,279,295	0
4	BGC	E	2	11/12	0.87	0.09	187,198,214,224	0
4	FUC	E	1	10/11	0.95	0.09	174,188,192,196	0
3	NAG	C	1	14/15	0.95	0.07	152,160,185,186	0

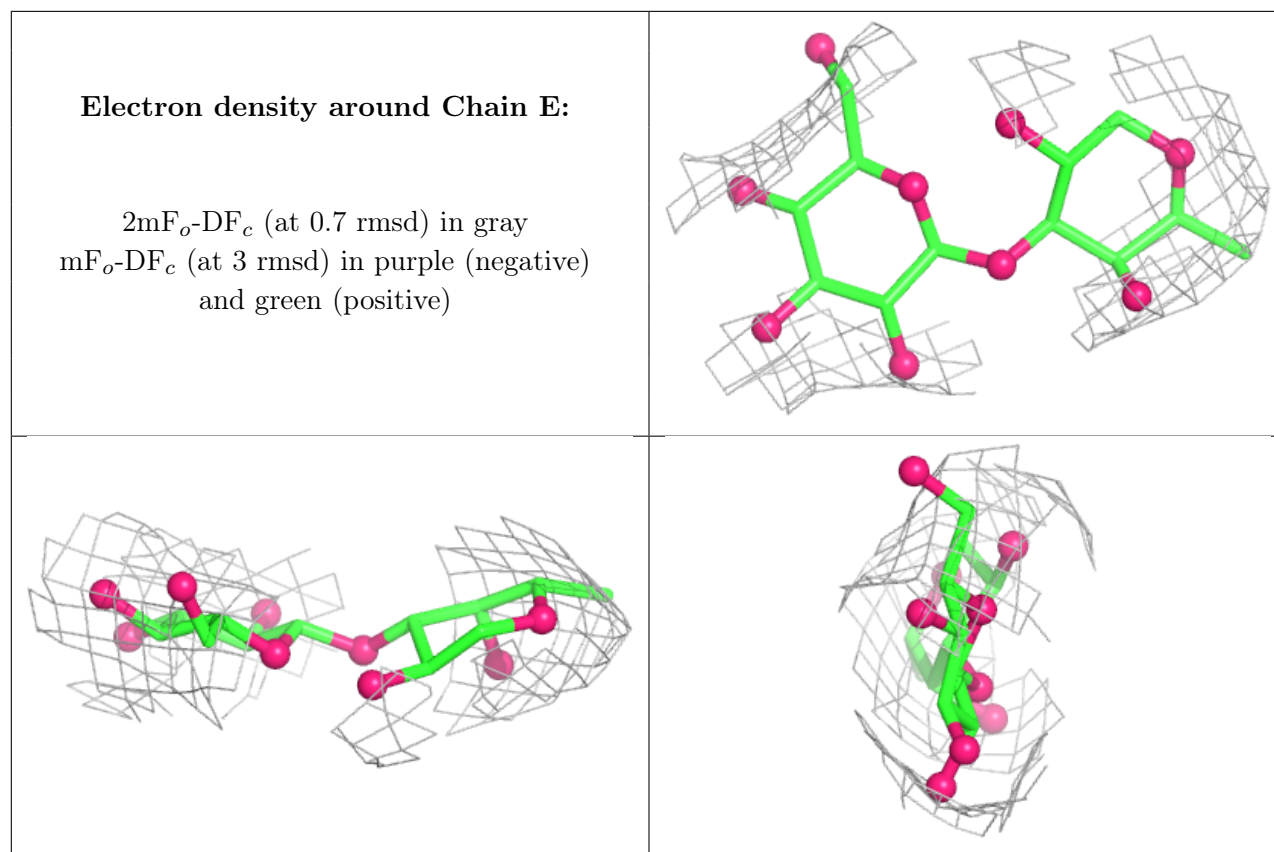
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MAN	B	1007	11/12	0.80	0.13	205,212,234,240	0
5	NA	A	2003	1/1	0.90	0.07	111,111,111,111	0
7	MAN	B	1006	11/12	0.94	0.15	245,260,277,281	0
7	MAN	B	1009	11/12	0.95	0.12	178,190,201,215	0
7	MAN	B	1008	11/12	0.97	0.11	147,167,176,188	0
6	CA	B	1001	1/1	0.99	0.04	167,167,167,167	1

6.5 Other polymers [i](#)

There are no such residues in this entry.