



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 08:38 PM BST

PDB ID : 4E0S
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

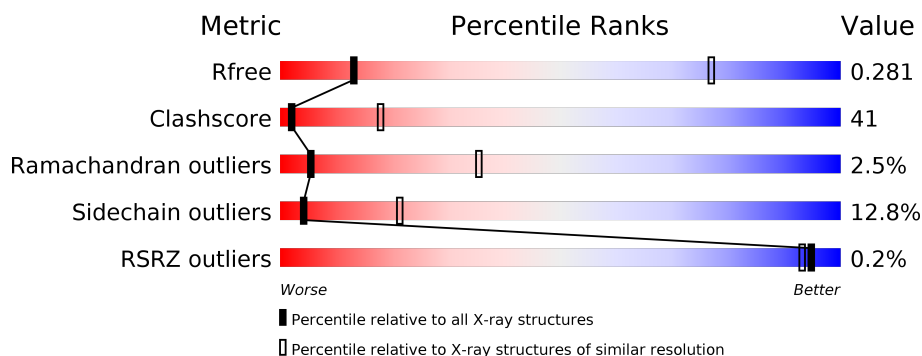
1 Overall quality at a glance ⓘ

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}	130704	1008 (4.66-3.78)
Clashscore	141614	1047 (4.62-3.80)
Ramachandran outliers	138981	1003 (4.62-3.80)
Sidechain outliers	138945	1010 (4.66-3.78)
RSRZ outliers	127900	1064 (4.72-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	<div> <div>42%</div> <div>42%</div> <div>8%</div> <div>7%</div> </div>
2	B	913	<div> <div>54%</div> <div>37%</div> <div>7%</div> <div>••</div> </div>
3	C	2	<div> <div>50%</div> <div>50%</div> </div>
3	D	2	<div> <div>50%</div> <div>50%</div> </div>
4	E	2	<div> <div>50%</div> <div>50%</div> </div>

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.

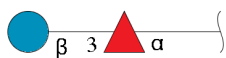
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	898	Total	C	N	O	S	0	0	0
			7046	4353	1239	1383	71			

- 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			

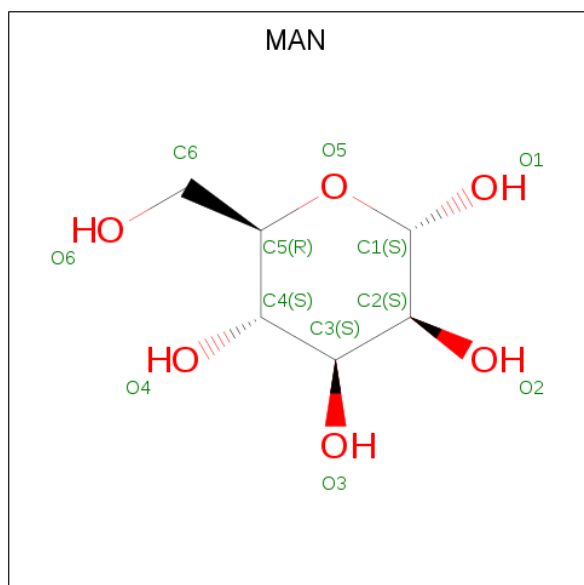
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).

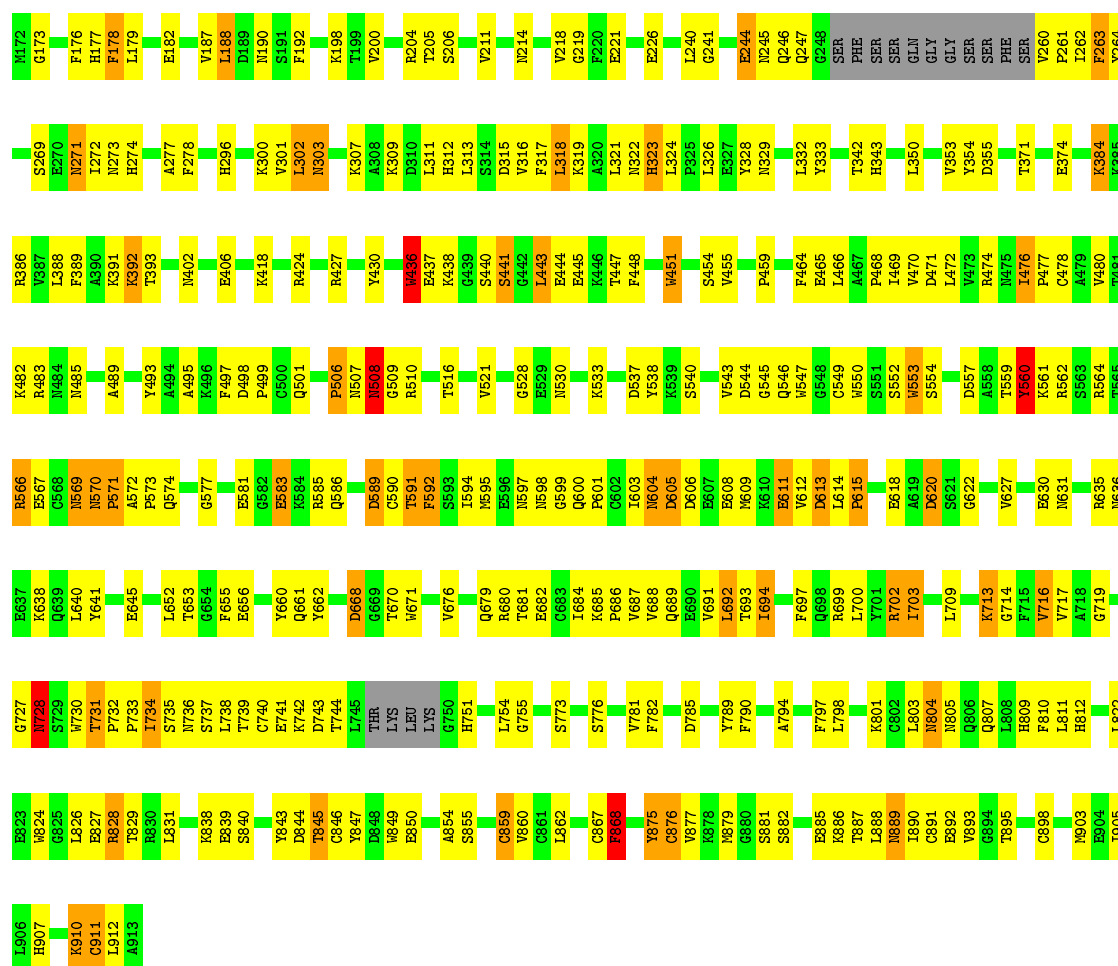


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		

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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		



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

Chain C: 50% 50%



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

Chain D: 50% 50%



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

Chain E: 50% 50%



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) 82.1 (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 (5.07%)	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)	0.20 , 124.8	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, CA, FUC, 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	0.58	6/12576 (0.0%)	0.80	4/17068 (0.0%)
2	B	0.58	5/7193 (0.1%)	0.78	5/9708 (0.1%)
All	All	0.58	11/19769 (0.1%)	0.79	9/26776 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	3
All	All	0	5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	917	TRP	CD2-CE2	5.98	1.48	1.41
1	A	1273	TRP	CD2-CE2	5.97	1.48	1.41
1	A	797	TRP	CD2-CE2	5.75	1.48	1.41
1	A	1077	TRP	CD2-CE2	5.30	1.47	1.41
2	B	436	TRP	CD2-CE2	5.27	1.47	1.41
2	B	8	TRP	CD2-CE2	5.24	1.47	1.41
1	A	773	TRP	CD2-CE2	5.23	1.47	1.41
2	B	54	TRP	CD2-CE2	5.19	1.47	1.41
2	B	451	TRP	CD2-CE2	5.17	1.47	1.41
1	A	1644	TRP	CD2-CE2	5.12	1.47	1.41
2	B	553	TRP	CD2-CE2	5.02	1.47	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	570	ASN	C-N-CD	-8.57	101.73	120.60
2	B	731	THR	C-N-CD	-7.08	105.03	120.60
1	A	794	LEU	CB-CG-CD2	-5.78	101.18	111.00
2	B	627	VAL	CB-CA-C	-5.50	100.96	111.40
2	B	560	TYR	CA-CB-CG	5.41	123.69	113.40
1	A	1113	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	323	LEU	CA-CB-CG	5.10	127.04	115.30
2	B	443	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	640	LEU	CA-CB-CG	5.02	126.85	115.30

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	1116	0
2	B	7046	0	6708	482	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
7	B	44	0	40	7	0
All	All	19475	0	19055	1562	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 41.

All (1562) 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:1249:GLU:CG	1:A:1289:ASP:HB3	1.66	1.23
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:1133:LEU:HD23	1:A:1133:LEU:C	1.61	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:991:VAL:C	1:A:992:LEU:HD12	1.65	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:1029:ASN:O	1:A:1030:HIS:CD2	2.00	1.14
1:A:672:ILE:HD12	1:A:673:LEU:N	1.60	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
1:A:987:ILE:C	1:A:988:LEU:HD23	1.70	1.10
2:B:244:GLU:HB3	2:B:269:SER:HA	1.09	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:1016:VAL:HG12	1:A:1017:PRO:HD3	1.17	1.08
1:A:131:ASP:HA	1:A:775:TRP:CH2	1.88	1.08
1:A:991:VAL:HG12	1:A:992:LEU:N	1.67	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
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: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:1005:LYS:HD2	1:A:1005:LYS:C	1.75	1.04
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:178:PHE:CE2	2:B:262:ILE:HD11	1.92	1.03
2:B:73:ASP:H	2:B:74:PRO:CD	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
2:B:244:GLU:HB3	2:B:269:SER:CA	1.90	1.01
1:A:1231:ASN:C	1:A:1232:LEU:HD12	1.79	1.01
1:A:991:VAL:HG12	1:A:992:LEU:H	1.17	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:1341:LEU:CB	1:A:1342:LEU:HD13	1.92	0.99
1:A:209:PHE:H	1:A:209:PHE:HD1	1.08	0.99
1:A:1239:VAL:HG12	1:A:1240:PRO:HD2	1.42	0.99
1:A:1245:ALA:O	1:A:1247:MET:N	1.96	0.98
1:A:1352:PHE:HD2	1:A:1352:PHE:C	1.66	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: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:266:TYR:CD2	1:A:1483:PHE:CD2	2.53	0.96
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:1288:GLN:O	1:A:1291:ILE:HG22	1.65	0.96
1:A:42:GLN:HG2	1:A:80:GLN:HG2	1.45	0.96
1:A:1538:GLU:HG2	1:A:1539:LEU:N	1.81	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:1013:MET:HB2	1:A:1129:LEU:CD2	1.97	0.95
1:A:665:ASN:HD22	1:A:666:ASP:N	1.64	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
2:B:538:TYR:CE2	2:B:540:SER:O	2.21	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:THR:HG22	1:A:789:ALA:HB2	1.47	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
2:B:493:TYR:HH	2:B:497:PHE:HZ	1.15	0.93
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:1133:LEU:C	1:A:1133:LEU:CD2	2.35	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:1352:PHE:CD2	1:A:1352:PHE:C	2.39	0.92
1:A:461:SER:HB3	1:A:463:SER:HB3	1.52	0.92
1:A:395:ILE:HD13	2:B:153:GLY:CA	2.00	0.92
2:B:493:TYR:CZ	2:B:497:PHE:CE2	2.57	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
1:A:855:PHE:HB3	1:A:916:THR:HG22	1.49	0.92
2:B:114:ILE:HG12	2:B:127:SER:O	1.70	0.92
1:A:1280:TYR:CD2	1:A:1281:GLY:N	2.38	0.92
1:A:576:SER:HB2	1:A:577:PRO:HD3	1.52	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:HD3	2:B:392:LYS:H	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:N	2:B:392:LYS:HD3	1.87	0.90
2:B:443:LEU:HD13	2:B:444:GLU:N	1.86	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:991:VAL:CG1	1:A:992:LEU:N	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1539:LEU:HD22	1:A:1540:ASP:H	1.37	0.88
1:A:266:TYR:HE2	1:A:1483:PHE:CB	1.84	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
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: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:360:PRO:HG3	1:A:636:ALA:HB3	1.56	0.87
1:A:209:PHE:N	1:A:209:PHE:HD1	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
2:B:493:TYR:CE2	2:B:497:PHE:CE2	2.64	0.86
1:A:1020:TYR:CE2	1:A:1291:ILE:HG13	2.11	0.86
1:A:618:LYS:HB3	1:A:622:ARG:HD2	1.55	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: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:842:LYS:NZ	1:A:1486:GLY:O	2.10	0.85
1:A:396:ASP:HB2	1:A:400:GLU:HB3	1.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1245:ALA:O	1:A:1246:ARG:C	2.13	0.84
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: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
2:B:877:VAL:HG11	2:B:903:MET:HE3	1.59	0.84
1:A:459:SER:OG	1:A:461:SER:HB2	1.78	0.84
1:A:988:LEU:N	1:A:988:LEU:HD23	1.90	0.84
2:B:274:HIS:H	2:B:277:ALA:HB3	1.43	0.84
1:A:1515:LYS:O	1:A:1516:ILE:HG13	1.78	0.83
1:A:842:LYS:HE2	1:A:1486:GLY:C	1.99	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:1307:LEU:HD13	1:A:1307:LEU:C	1.99	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:672:ILE:HD11	1:A:674:ARG:O	1.80	0.82
1:A:1274:LEU:O	1:A:1277:GLU:HB3	1.79	0.82
1:A:860:SER:HB3	1:A:911:ASN:HB2	1.61	0.82
2:B:70:SER:HB3	2:B:332:LEU:HD11	1.62	0.82
2:B:592:PHE:N	2:B:592:PHE:CD2	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:1574:PHE:CE2	1:A:1601:ILE:HD12	2.14	0.81
1:A:1557:ILE:HD13	1:A:1622:LYS:HG3	1.59	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:1421:HIS:HB2	1:A:1464:LEU:O	1.80	0.81
1:A:182:ILE:HG13	1:A:804:ILE:HD11	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:998:ASN:O	1:A:1002:HIS:CD2	2.33	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:1203:PRO:HG3	2:B:652:LEU:HD13	1.64	0.80
1:A:656:ASN:C	1:A:656:ASN:HD22	1.83	0.80
1:A:620:LEU:HD13	1:A:811:VAL:CB	2.12	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:CG	1:A:1234:HIS:O	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:415:ASP:HB3	1:A:417:VAL:H	1.46	0.79
2:B:263:PHE:CD1	2:B:263:PHE:C	2.56	0.79
2:B:418:LYS:HA	2:B:436:TRP:HZ3	1.48	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
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
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
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
1:A:1001:THR:O	1:A:1003:LEU:HD13	1.83	0.78
1:A:950:TYR:CE1	2:B:635:ARG:HD3	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:983:LEU:HD13	1:A:984:VAL:N	1.98	0.78
1:A:1297:LEU:HD21	2:B:595:MET:HE3	1.65	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:1585:TYR:HE1	1:A:1668:ALA:CB	1.97	0.77
1:A:1515:LYS:CE	1:A:1603:LYS:HE3	2.13	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: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:467:ILE:HD11	1:A:484:ILE:CD1	2.15	0.76
1:A:59:TYR:CD2	1:A:60:PRO:HD2	2.20	0.76
1:A:641:ASN:HB2	1:A:644:ASN:H	1.50	0.76
2:B:804:ASN:H	2:B:804:ASN:HD22	1.31	0.76
1:A:1598:ILE:HG21	1:A:1637:TYR:CD2	2.19	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:1628:LYS:CB	1:A:1633:PHE:HD1	1.99	0.76
1:A:930:VAL:HG13	1:A:931:PRO:CD	2.15	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
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:1551:THR:O	1:A:1557:ILE:HG13	1.86	0.76
1:A:362:PHE:CE2	1:A:640:LEU:HB2	2.19	0.76
2:B:877:VAL:CG1	2:B:903:MET:HE3	2.14	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:1589:GLU:HG2	1:A:1590:ALA:N	1.98	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1239:VAL:CG1	1:A:1240:PRO:CD	2.59	0.75
1:A:330:ILE:HG13	1:A:330:ILE:O	1.86	0.75
1:A:131:ASP:HA	1:A:775:TRP:CZ3	2.21	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:N	1:A:992:LEU:HD12	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:1549:LYS:HA	1:A:1552:ALA:HB3	1.68	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: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
2:B:73:ASP:C	2:B:74:PRO:O	2.22	0.74
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:1273:TRP:CE3	1:A:1274:LEU:HA	2.23	0.73
1:A:535:VAL:HG23	1:A:536:PRO:HD3	1.70	0.73
1:A:1131:GLY:O	1:A:1134:PRO:HD2	1.89	0.73
1:A:1647:TYR:O	1:A:1649:PRO:HD3	1.87	0.73
2:B:438:LYS:C	2:B:441:SER:HB2	2.09	0.73
1:A:1008:ALA:O	1:A:1011:GLU:HB2	1.89	0.73
1:A:609:VAL:HG21	1:A:771:GLU:HG3	1.68	0.73
2:B:436:TRP:CD1	2:B:436:TRP:C	2.61	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:1024:TYR:HA	1:A:1298:THR:CG2	2.18	0.73
1:A:120:THR:HG22	1:A:122:ASP:H	1.53	0.73
1:A:1085:VAL:O	1:A:1089:VAL:HG23	1.88	0.73
1:A:266:TYR:OH	1:A:1483:PHE:HB2	1.88	0.73
1:A:1559:TYR:CE2	1:A:1637:TYR:HD1	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1528:VAL:CG2	1:A:1625:LEU:CD2	2.66	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: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:1133:LEU:HD23	1:A:1134:PRO:N	2.04	0.72
1:A:334:GLY:C	1:A:844:THR:HG21	2.08	0.72
1:A:193:ASN:HD21	1:A:935:LYS:NZ	1.87	0.72
1:A:1539:LEU:O	1:A:1660:PHE:CD1	2.42	0.72
1:A:552:ALA:O	1:A:657:ALA:HB1	1.89	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
2:B:804:ASN:N	2:B:804:ASN:ND2	2.37	0.72
1:A:109:LYS:CE	1:A:110:HIS:CE1	2.72	0.72
1:A:1539:LEU:H	1:A:1539:LEU:HD13	1.53	0.72
1:A:1537:GLU:CG	1:A:1541:LEU:HD11	2.20	0.72
1:A:618:LYS:HD2	1:A:622:ARG:HH11	1.55	0.72
1:A:665:ASN:ND2	1:A:666:ASP:OD2	2.22	0.72
2:B:73:ASP:O	2:B:74:PRO:C	2.22	0.71
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
2:B:822:LEU:HD13	2:B:822:LEU:C	2.10	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:1528:VAL:HG21	1:A:1625:LEU:HD22	1.72	0.71
1:A:562:ASN:HD22	1:A:562:ASN:C	1.92	0.71
1:A:628:GLU:OE2	1:A:674:ARG:NH2	2.24	0.71
1:A:209:PHE:CD1	1:A:209:PHE:N	2.45	0.71
1:A:628:GLU:HG3	1:A:628:GLU:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1279:ARG:HG3	2:B:601:PRO:HG2	1.72	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
1:A:254:TYR:HD1	1:A:258:LYS:O	1.74	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:1528:VAL:CG2	1:A:1625:LEU:HD22	2.21	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
2:B:263:PHE:CD1	2:B:264:TYR:N	2.60	0.70
1:A:1011:GLU:O	1:A:1014:SER:CB	2.39	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:1287:THR:CA	1:A:1290:THR:HG22	2.17	0.70
1:A:770:PRO:O	1:A:797:TRP:HH2	1.74	0.70
1:A:1016:VAL:CG1	1:A:1017:PRO:CD	2.68	0.70
1:A:467:ILE:HD11	1:A:484:ILE:HD11	1.72	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
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
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
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:1279:ARG:HD3	2:B:600:GLN:HE22	1.56	0.69
2:B:840:SER:HB3	2:B:844:ASP:O	1.92	0.69
1:A:1183:GLN:O	1:A:1232:LEU:HD21	1.93	0.69
1:A:1280:TYR:CD2	1:A:1280:TYR:C	2.66	0.69
1:A:1589:GLU:CG	1:A:1590:ALA:H	2.00	0.69
1:A:991:VAL:HG13	1:A:992:LEU:H	1.56	0.69
2:B:274:HIS:H	2:B:277:ALA:CB	2.05	0.69
2:B:879:MET:HB2	2:B:882:SER:HB3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:824:TRP:CH2	2:B:898:CYS:HA	2.28	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
2:B:831:LEU:CD1	2:B:831:LEU:O	2.41	0.68
1:A:395:ILE:CD1	2:B:153:GLY:CA	2.70	0.68
2:B:543:VAL:HG13	2:B:574:GLN:N	2.07	0.68
1:A:999:ILE:HG13	1:A:1000:LEU:N	2.08	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
2:B:543:VAL:CG1	2:B:574:GLN:CB	2.67	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
1:A:29:LYS:HA	1:A:652:THR:HG22	1.74	0.68
1:A:672:ILE:C	1:A:672:ILE:HD12	2.13	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:1248:VAL:HG11	1:A:1284:PHE:HD1	1.58	0.68
1:A:620:LEU:HD11	1:A:624:PHE:CE1	2.28	0.68
1:A:1127:ILE:HB	1:A:1130:GLN:HG3	1.75	0.68
1:A:1027:THR:HG22	1:A:1302:LEU:HD13	1.75	0.68
1:A:356:LEU:HB3	1:A:359:THR:OG1	1.94	0.68
2:B:73:ASP:N	2:B:74:PRO:CD	2.47	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:569:ASN:ND2	1:A:805:SER:CB	2.56	0.68
2:B:427:ARG:H	2:B:454:SER:HG	1.38	0.68
1:A:991:VAL:C	1:A:992:LEU:CD1	2.56	0.67
1:A:995:GLU:O	1:A:998:ASN:HB2	1.94	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:1248:VAL:HG11	1:A:1284:PHE:CD1	2.29	0.67
1:A:835:ARG:HD3	1:A:905:ILE:HG12	1.76	0.67
2:B:804:ASN:HB3	2:B:807:GLN:CD	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:822:LEU:HD13	2:B:822:LEU:O	1.94	0.67
1:A:412:ARG:HB3	1:A:415:ASP:HB2	1.75	0.67
1:A:1584:ILE:O	1:A:1585:TYR:HB2	1.94	0.67
2:B:177:HIS:NE2	2:B:493:TYR:OH	2.28	0.67
2:B:73:ASP:HB3	2:B:323:HIS:NE2	2.09	0.67
1:A:369:TYR:HE2	1:A:371:ILE:CG1	2.08	0.67
1:A:462:GLN:OE1	1:A:462:GLN:HA	1.94	0.67
2:B:111:LEU:HD12	2:B:112:CYS:N	2.09	0.67
1:A:1489:SER:OG	1:A:1490:PRO:HD2	1.95	0.66
1:A:115:LYS:HG2	1:A:654:LEU:HD13	1.75	0.66
1:A:1272:LYS:O	1:A:1276:GLU:HG2	1.95	0.66
1:A:265:VAL:HB	1:A:290:THR:O	1.95	0.66
1:A:997:ILE:HG23	1:A:1021:VAL:HG11	1.77	0.66
1:A:334:GLY:HA2	1:A:844:THR:CG2	2.16	0.66
1:A:349:LEU:O	1:A:351:PRO:HD3	1.96	0.66
2:B:824:TRP:CZ2	2:B:898:CYS:HA	2.30	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:770:PRO:O	1:A:797:TRP:CH2	2.48	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
1:A:270:GLY:HA3	1:A:282:MET:HE1	1.78	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:1647:TYR:HD1	1:A:1649:PRO:HD3	1.61	0.65
1:A:236:ASN:HB2	1:A:377:ASP:OD2	1.97	0.65
2:B:495:ALA:HB1	7:B:1008:MAN:H61	1.76	0.65
2:B:91:PHE:HD1	2:B:530:ASN:ND2	1.94	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: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:946:PRO:HG2	1:A:1353:GLY:O	1.97	0.65
1:A:1016:VAL:CG1	1:A:1017:PRO:N	2.60	0.65
1:A:149:ASN:HB3	1:A:155:ALA:CB	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:GLU:OE2	1:A:1059:TYR:OH	2.14	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:1537:GLU:HB3	1:A:1541:LEU:CD1	2.25	0.65
1:A:335:GLY:H	1:A:895:LEU:HG	1.62	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
2:B:116:GLU:OE2	2:B:130:CYS:HB2	1.98	0.64
2:B:322:ASN:C	2:B:324:LEU:H	2.00	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
1:A:1012:LEU:C	1:A:1012:LEU:HD13	2.17	0.64
1:A:1538:GLU:CD	1:A:1539:LEU:HD13	2.17	0.64
1:A:260:VAL:HG13	1:A:331:GLU:OE2	1.97	0.64
1:A:43:VAL:HG22	1:A:45:GLY:N	2.12	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: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
1:A:784:LYS:HG2	1:A:785:GLN:H	1.61	0.64
1:A:1073:SER:HB3	1:A:1123:GLN:HG2	1.80	0.64
1:A:322:TYR:OH	1:A:346:LYS:HE2	1.98	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:1015:VAL:CG2	1:A:1015:VAL:O	2.46	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:O	1:A:562:ASN:ND2	2.31	0.63
1:A:1019:PHE:CD1	1:A:1049:LEU:CD1	2.80	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:58:SER:O	1:A:103:TYR:HD1	1.80	0.63
1:A:1629:TYR:CD1	1:A:1630:ASN:ND2	2.67	0.63
1:A:21:GLN:HE22	1:A:45:GLY:HA2	0.83	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:545:GLY:HA2	2:B:571:PRO:O	1.98	0.63
1:A:1277:GLU:O	1:A:1281:GLY:N	2.27	0.63
1:A:137:PRO:O	1:A:138:ASP:HB3	1.98	0.63
1:A:1245:ALA:C	1:A:1247:MET:N	2.51	0.63
1:A:1309:LEU:HD11	1:A:1311:MET:HB2	1.81	0.63
1:A:1225:TYR:CZ	1:A:1276:GLU:HG3	2.32	0.63
1:A:1341:LEU:HB3	1:A:1342:LEU:CD1	2.27	0.63
1:A:992:LEU:N	1:A:992:LEU:CD1	2.61	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
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
1:A:469:TRP:CZ2	1:A:471:ASP:OD1	2.51	0.63
1:A:335:GLY:HA3	1:A:895:LEU:HD21	1.80	0.63
2:B:547:TRP:HE1	7:B:1009:MAN:H5	1.63	0.63
2:B:543:VAL:HG13	2:B:574:GLN:H	1.64	0.62
2:B:877:VAL:CG1	2:B:903:MET:CE	2.77	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:1539:LEU:HD22	1:A:1539:LEU:C	2.16	0.62
1:A:1538:GLU:CD	1:A:1539:LEU:CD1	2.67	0.62
1:A:1244:THR:O	1:A:1246:ARG:N	2.32	0.62
1:A:1303:LEU:C	1:A:1303:LEU:HD13	2.20	0.62
1:A:1562:LYS:HD2	1:A:1648:TRP:HE1	1.63	0.62
1:A:521:ALA:HB1	1:A:523:TYR:O	2.00	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
1:A:367:ILE:CG2	1:A:466:TYR:CD2	2.83	0.62
1:A:365:PRO:O	1:A:367:ILE:HD12	1.99	0.62
2:B:559:THR:HG22	2:B:560:TYR:N	2.14	0.62
1:A:1528:VAL:CG2	1:A:1625:LEU:HD21	2.30	0.62
1:A:1582:LEU:N	1:A:1582:LEU:CD1	2.62	0.62
1:A:516:GLU:H	1:A:516:GLU:CD	2.00	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:N	1:A:1232:LEU:HD12	2.13	0.62
1:A:1234:HIS:ND1	1:A:1234:HIS:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:507:ASN:C	2:B:509:GLY:H	2.03	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
1:A:656:ASN:C	1:A:656:ASN:ND2	2.53	0.61
2:B:219:GLY:O	2:B:302:LEU:HB2	2.00	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:N	1:A:1539:LEU:HD13	2.15	0.61
2:B:681:THR:CG2	2:B:703:ILE:HD11	2.30	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
2:B:73:ASP:H	2:B:74:PRO:HD3	1.62	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:191:PRO:O	1:A:194:PRO:HG3	2.00	0.61
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:1279:ARG:CG	2:B:601:PRO:CG	2.77	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:1221:ASN:HA	1:A:1222:PRO:C	2.19	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
1:A:467:ILE:HD11	1:A:484:ILE:HD13	1.83	0.61
2:B:100:LEU:H	2:B:100:LEU:HD12	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: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:1372:GLU:HG3	1:A:1409:LYS:HZ2	1.66	0.60
1:A:1376:SER:O	1:A:1409:LYS:N	2.25	0.60
2:B:682:GLU:CD	2:B:702:ARG:HH22	2.04	0.60
1:A:357:VAL:HG23	1:A:374:GLN:HB2	1.81	0.60
1:A:1514:ILE:CG2	1:A:1515:LYS:H	2.09	0.60
1:A:535:VAL:HG11	1:A:566:LYS:O	2.01	0.60
1:A:1544:SER:O	1:A:1548:ARG:HG3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:CYS:SG	2:B:319:LYS:CE	2.84	0.60
1:A:1020:TYR:CD2	1:A:1291:ILE:HG13	2.36	0.60
1:A:358:ALA:HB3	1:A:372:LYS:HD2	1.83	0.60
2:B:613:ASP:O	2:B:615:PRO:HD3	2.02	0.60
2:B:66:PHE:HB3	2:B:81:LYS:HE2	1.82	0.60
1:A:366:GLY:C	1:A:367:ILE:HD12	2.21	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: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:374:GLN:HE22	1:A:675:PRO:CB	2.00	0.60
1:A:42:GLN:HG2	1:A:80:GLN:CG	2.27	0.60
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:1421:HIS:CE1	1:A:1499:HIS:HE1	2.20	0.59
1:A:487:THR:HG22	1:A:523:TYR:HB3	1.84	0.59
1:A:924:VAL:CG1	1:A:924:VAL:O	2.50	0.59
2:B:562:ARG:HB2	2:B:590:CYS:SG	2.42	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:655:THR:CG2	1:A:658:ASN:O	2.49	0.59
1:A:369:TYR:CE2	1:A:371:ILE:HG12	2.33	0.59
2:B:507:ASN:C	2:B:509:GLY:N	2.54	0.59
1:A:1654:CYS:O	1:A:1657:CYS:SG	2.60	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:535:VAL:HA	1:A:563:ILE:HD11	1.84	0.59
2:B:465:GLU:C	2:B:466:LEU:HD12	2.22	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: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
1:A:1539:LEU:H	1:A:1539:LEU:CD1	2.15	0.59
1:A:469:TRP:CH2	1:A:471:ASP:OD1	2.55	0.59
1:A:467:ILE:CD1	1:A:484:ILE:HD11	2.32	0.59
1:A:1138:ARG:O	1:A:1139:GLU:C	2.41	0.59
2:B:302:LEU:CD1	2:B:350:LEU:HB3	2.33	0.59
1:A:1235:LYS:HG2	1:A:1235:LYS:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:467:ILE:HG22	1:A:557:ASP:HB3	1.85	0.59
1:A:113:LYS:CD	1:A:654:LEU:HD11	2.33	0.59
2:B:803:LEU:HB2	2:B:804:ASN:ND2	2.18	0.59
1:A:1374:VAL:O	1:A:1503:LYS:HA	2.03	0.59
1:A:1372:GLU:HG3	1:A:1409:LYS:NZ	2.17	0.59
1:A:1524:ALA:HB2	1:A:1629:TYR:HB2	1.84	0.59
1:A:618:LYS:HD2	1:A:622:ARG:NH1	2.17	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:1536:GLN:HG3	1:A:1537:GLU:N	2.17	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:1249:GLU:HG3	1:A:1289:ASP:HB3	1.79	0.58
1:A:365:PRO:O	1:A:367:ILE:CD1	2.51	0.58
1:A:457:TYR:C	1:A:457:TYR:HD2	2.06	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:1307:LEU:C	1:A:1307:LEU:CD1	2.72	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
1:A:1232:LEU:CD1	1:A:1232:LEU:N	2.67	0.58
1:A:988:LEU:HG	1:A:1300:TYR:OH	2.04	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:N	2:B:620:ASP:OD1	2.37	0.58
1:A:99:VAL:HG22	1:A:101:TYR:H	1.69	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: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:1543:ILE:CD1	1:A:1543:ILE:H	2.17	0.58
1:A:1642:LEU:HD13	1:A:1642:LEU:H	1.69	0.58
1:A:357:VAL:O	1:A:672:ILE:O	2.22	0.58
1:A:23:TYR:CD2	1:A:656:ASN:HB2	2.39	0.57
1:A:1067:SER:HB2	1:A:1073:SER:O	2.04	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:59:TYR:CD1	1:A:60:PRO:HD2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:MET:HB3	1:A:780:VAL:HG11	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
1:A:587:THR:HA	1:A:789:ALA:HA	1.86	0.57
2:B:244:GLU:OE1	2:B:244:GLU:C	2.42	0.57
2:B:244:GLU:HB3	2:B:269:SER:CB	2.34	0.57
1:A:1008:ALA:O	1:A:1011:GLU:CB	2.53	0.57
1:A:967:LEU:HD12	1:A:1366:HIS:O	2.05	0.57
1:A:988:LEU:HD11	1:A:1268:ASN:CG	2.23	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:ND2	2:B:569:ASN:N	2.51	0.57
1:A:1265:ASN:ND2	2:B:638:LYS:HE2	2.20	0.57
2:B:839:GLU:HB2	2:B:846:CYS:HB2	1.87	0.57
1:A:109:LYS:HZ1	1:A:110:HIS:HE1	1.53	0.57
1:A:1262:LYS:HD3	1:A:1303:LEU:HD23	1.86	0.57
1:A:1642:LEU:CD1	1:A:1642:LEU:H	2.17	0.57
2:B:272:ILE:O	2:B:272:ILE:HG22	2.05	0.57
1:A:1271:ILE:C	1:A:1271:ILE:HD12	2.25	0.57
1:A:367:ILE:HG23	1:A:466:TYR:CE2	2.40	0.57
1:A:362:PHE:CE2	1:A:640:LEU:CD2	2.87	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: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:842:LYS:HE2	1:A:1486:GLY:CA	2.35	0.57
1:A:1543:ILE:HD13	1:A:1543:ILE:N	2.20	0.57
2:B:264:TYR:OH	2:B:466:LEU:CD2	2.53	0.57
2:B:69:TRP:HZ3	2:B:79:GLN:O	1.88	0.57
1:A:1088:GLN:OE1	1:A:1154:LYS:HD2	2.05	0.56
1:A:944:LEU:CB	1:A:1311:MET:HE2	2.35	0.56
1:A:457:TYR:CD2	1:A:457:TYR:C	2.78	0.56
1:A:1620:MET:HB2	1:A:1644:TRP:CB	2.32	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
2:B:608:GLU:C	2:B:609:MET:HG3	2.26	0.56
1:A:1069:TRP:O	1:A:1072:GLY:CA	2.54	0.56
1:A:1647:TYR:C	1:A:1649:PRO:HD3	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1647:TYR:CD1	1:A:1649:PRO:HD3	2.40	0.56
1:A:939:TYR:HB2	2:B:660:TYR:HE1	1.69	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
1:A:1000:LEU:N	1:A:1000:LEU:HD12	2.20	0.56
1:A:1015:VAL:HG23	1:A:1015:VAL:O	2.05	0.56
1:A:982:LEU:HD13	1:A:982:LEU:C	2.26	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:966:ASP:OD1	1:A:966:ASP:N	2.38	0.56
2:B:303:ASN:OD1	2:B:303:ASN:N	2.37	0.56
1:A:1115:ASN:HD22	1:A:1115:ASN:H	1.54	0.56
2:B:115:GLU:O	2:B:116:GLU:HG3	2.05	0.56
1:A:1123:GLN:O	1:A:1124:TYR:C	2.43	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:104:LEU:HB2	1:A:117:MET:HE3	1.86	0.56
2:B:543:VAL:HG11	2:B:574:GLN:NE2	2.20	0.56
1:A:939:TYR:HB2	2:B:660:TYR:CE1	2.41	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:1220:GLY:O	1:A:1223:PRO:HA	2.06	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
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: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
1:A:934:VAL:CG2	1:A:935:LYS:H	2.19	0.55
2:B:604:ASN:O	2:B:606:ASP:N	2.39	0.55
1:A:1249:GLU:CG	1:A:1289:ASP:CB	2.62	0.55
1:A:956:ARG:HG3	1:A:1349:SER:HB3	1.88	0.55
1:A:839:ILE:HG13	1:A:840:GLN:N	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:79:GLN:O	2:B:103:PHE:HB3	2.07	0.55
1:A:1528:VAL:HG22	1:A:1625:LEU:CD2	2.35	0.55
1:A:1539:LEU:HD22	1:A:1540:ASP:CB	2.35	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:1084:ARG:HD3	1:A:1150:ILE:HG22	1.88	0.55
1:A:983:LEU:C	1:A:983:LEU:HD13	2.25	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:1543:ILE:H	1:A:1543:ILE:HD13	1.71	0.55
1:A:198:MET:CE	1:A:218:GLU:HG3	2.36	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:132:LYS:HZ1	1:A:139:GLN:HE22	1.52	0.55
1:A:1487:PHE:CD1	1:A:1488:LEU:N	2.75	0.55
1:A:673:LEU:N	1:A:673:LEU:HD12	2.21	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: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
2:B:570:ASN:CG	2:B:571:PRO:HD3	2.26	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
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
2:B:508:ASN:HD21	2:B:544:ASP:CG	2.10	0.54
2:B:24:SER:HA	2:B:48:GLU:O	2.07	0.54
1:A:1311:MET:HE3	1:A:1350:THR:HG21	1.89	0.54
1:A:1647:TYR:HD1	1:A:1649:PRO:CD	2.20	0.54
1:A:263:ALA:HB3	1:A:292:LEU:HB3	1.89	0.54
2:B:106:CYS:SG	2:B:107:ILE:N	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:993:SER:OG	1:A:995:GLU:OE1	2.24	0.54
2:B:803:LEU:HB2	2:B:804:ASN:HD22	1.73	0.54
1:A:1288:GLN:O	1:A:1291:ILE:CG2	2.49	0.54
1:A:1341:LEU:C	1:A:1342:LEU:HD13	2.28	0.54
1:A:966:ASP:HB3	1:A:1371:SER:OG	2.08	0.54
1:A:1539:LEU:CD2	1:A:1540:ASP:CB	2.86	0.54
1:A:494:ASP:C	1:A:496:ILE:H	2.10	0.54
1:A:1427:SER:HB3	1:A:1492:THR:H	1.72	0.54
2:B:466:LEU:N	2:B:466:LEU:HD12	2.23	0.54
2:B:613:ASP:OD1	2:B:613:ASP:N	2.40	0.54
1:A:950:TYR:CZ	2:B:635:ARG:HD3	2.42	0.54
1:A:1245:ALA:HB2	1:A:1285:TYR:CE2	2.43	0.54
1:A:461:SER:C	1:A:463:SER:H	2.10	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:353:LYS:C	1:A:354:LEU:HD22	2.28	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
2:B:887:THR:C	2:B:888:LEU:HD22	2.29	0.53
1:A:1108:VAL:HG11	1:A:1164:ILE:HG22	1.91	0.53
1:A:32:ARG:HD3	1:A:150:ASP:OD1	2.08	0.53
2:B:198:LYS:HG3	2:B:211:VAL:HB	1.90	0.53
2:B:73:ASP:N	2:B:74:PRO:HD2	2.16	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
1:A:493:ILE:HG21	1:A:495:LYS:HG2	1.90	0.53
2:B:739:THR:CG2	2:B:740:CYS:N	2.71	0.53
1:A:1135:VAL:CG1	1:A:1136:GLU:N	2.72	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1338:VAL:CG1	1:A:1339:GLU:N	2.70	0.53
1:A:995:GLU:O	1:A:996:GLY:C	2.46	0.53
1:A:1005:LYS:C	1:A:1005:LYS:CD	2.59	0.53
1:A:1644:TRP:O	1:A:1645:ILE:HD13	2.08	0.53
2:B:822:LEU:C	2:B:822:LEU:CD1	2.77	0.53
1:A:1386:ILE:O	1:A:1386:ILE:HG23	2.09	0.53
2:B:138:ASN:H	2:B:149:GLU:CD	2.10	0.53
1:A:1360:HIS:CD2	2:B:660:TYR:OH	2.62	0.53
2:B:754:LEU:C	2:B:798:LEU:HD22	2.29	0.53
1:A:1005:LYS:O	1:A:1005:LYS:HD2	2.08	0.52
1:A:1273:TRP:CZ3	1:A:1274:LEU:HA	2.44	0.52
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
1:A:998:ASN:O	1:A:1002:HIS:HD2	1.87	0.52
2:B:52:CYS:HA	2:B:54:TRP:CE3	2.44	0.52
1:A:1012:LEU:O	1:A:1012:LEU:HD13	2.10	0.52
1:A:1376:SER:O	1:A:1409:LYS:CB	2.58	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: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:369:TYR:CE2	1:A:371:ILE:HG13	2.44	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:655:THR:CG2	1:A:656:ASN:N	2.72	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:1328:MET:CE	1:A:1335:GLY:H	2.22	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1647:TYR:O	1:A:1649:PRO:HD2	2.09	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
2:B:824:TRP:NE1	2:B:847:TYR:OH	2.42	0.52
1:A:1066:TYR:CE1	1:A:1082:ALA:HB3	2.45	0.52
1:A:908:HIS:HA	1:A:927:LEU:O	2.09	0.52
2:B:585:ARG:HG2	2:B:586:GLN:N	2.25	0.52
1:A:1020:TYR:CE2	1:A:1291:ILE:CG1	2.91	0.51
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
2:B:73:ASP:O	2:B:73:ASP:OD1	2.28	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
1:A:461:SER:CB	1:A:463:SER:CB	2.73	0.51
1:A:55:SER:HB3	1:A:68:SER:HB3	1.92	0.51
1:A:620:LEU:O	1:A:623:VAL:N	2.43	0.51
1:A:672:ILE:HD11	1:A:674:ARG:C	2.31	0.51
2:B:655:PHE:CA	2:B:680:ARG:HB3	2.14	0.51
1:A:1338:VAL:HG12	1:A:1339:GLU:N	2.26	0.51
1:A:384:GLY:HA2	1:A:411:THR:HG23	1.92	0.51
1:A:562:ASN:C	1:A:562:ASN:ND2	2.59	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:1550:GLN:O	1:A:1554:LYS:N	2.44	0.51
1:A:439:ALA:N	1:A:447:GLN:OE1	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:1450:PHE:HZ	1:A:1475:VAL:HB	1.74	0.51
1:A:162:THR:HB	1:A:173:MET:HG3	1.93	0.51
2:B:828:ARG:HG2	2:B:829:THR:HG23	1.91	0.51
1:A:1631:PHE:O	1:A:1631:PHE:CG	2.63	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
2:B:734:ILE:HG13	2:B:738:LEU:N	2.26	0.51
2:B:877:VAL:O	2:B:877:VAL:HG23	2.11	0.51
1:A:944:LEU:HB2	1:A:1311:MET:HE2	1.93	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:1013:MET:CG	1:A:1129:LEU:HG	2.40	0.51
1:A:315:LEU:HD23	1:A:315:LEU:C	2.31	0.51
1:A:805:SER:O	1:A:808:GLY:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:362:PHE:CE2	1:A:640:LEU:CB	2.92	0.51
2:B:47:GLN:HG2	2:B:48:GLU:N	2.25	0.51
1:A:1069:TRP:O	1:A:1072:GLY:HA3	2.11	0.50
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
1:A:136:THR:CG2	1:A:139:GLN:HG3	2.39	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:113:LYS:HD3	1:A:654:LEU:HD11	1.93	0.50
1:A:982:LEU:C	1:A:982:LEU:CD1	2.79	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: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:1654:CYS:C	1:A:1657:CYS:SG	2.90	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
1:A:1376:SER:OG	1:A:1503:LYS:HG2	2.10	0.50
1:A:182:ILE:HG13	1:A:804:ILE:HD13	1.93	0.50
2:B:692:LEU:HD22	2:B:709:LEU:HD23	1.93	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:809:HIS:CB	2:B:829:THR:HG21	2.41	0.50
1:A:1522:GLY:HA3	1:A:1629:TYR:CZ	2.47	0.50
1:A:665:ASN:C	1:A:665:ASN:HD22	2.09	0.50
1:A:930:VAL:CB	1:A:931:PRO:HD2	2.41	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:1410:PRO:HG3	1:A:1469:SER:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:MET:HG2	1:A:780:VAL:HG21	1.94	0.50
1:A:1602:LYS:HB3	1:A:1639:LEU:HD22	1.95	0.49
1:A:862:VAL:HG13	1:A:863:GLU:H	1.71	0.49
1:A:996:GLY:O	1:A:997:ILE:C	2.50	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
2:B:8:TRP:H	7:B:1007:MAN:H2	1.77	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:560:TRP:CZ3	1:A:673:LEU:HB3	2.48	0.49
2:B:171:LEU:HD12	2:B:171:LEU:N	2.27	0.49
2:B:427:ARG:N	2:B:454:SER:OG	2.32	0.49
1:A:1303:LEU:HD13	1:A:1303:LEU:O	2.11	0.49
1:A:131:ASP:OD1	1:A:135:TYR:OH	2.24	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
1:A:1539:LEU:CD2	1:A:1539:LEU:C	2.79	0.49
1:A:193:ASN:HD21	1:A:935:LYS:HZ3	1.61	0.49
2:B:129:ARG:HH21	2:B:315:ASP:CG	2.16	0.49
2:B:560:TYR:HB2	2:B:589:ASP:HB3	1.91	0.49
1:A:1066:TYR:HB3	1:A:1078:LEU:CD2	2.43	0.49
1:A:109:LYS:CE	1:A:110:HIS:ND1	2.71	0.49
1:A:1559:TYR:OH	1:A:1637:TYR:HB3	2.12	0.49
1:A:472:ASN:HA	1:A:474:LYS:HG3	1.95	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:1013:MET:CE	1:A:1129:LEU:HA	2.42	0.49
1:A:1556:GLU:HB3	1:A:1622:LYS:HE2	1.94	0.49
1:A:539:ARG:NH2	1:A:635:GLY:O	2.45	0.49
1:A:640:LEU:H	1:A:644:ASN:HB3	1.77	0.49
1:A:554:LEU:HD23	1:A:657:ALA:HB3	1.94	0.49
2:B:618:GLU:O	2:B:618:GLU:CG	2.60	0.49
1:A:1122:SER:O	1:A:1123:GLN:HB3	2.12	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: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:231:ILE:HD12	1:A:327:VAL:CG2	2.43	0.48
1:A:60:PRO:O	1:A:61:ASP:HB3	2.13	0.48
2:B:828:ARG:CZ	2:B:843:TYR:CE2	2.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1122:SER:C	1:A:1124:TYR:N	2.63	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
1:A:1540:ASP:O	1:A:1541:LEU:HD23	2.13	0.48
1:A:335:GLY:HA2	1:A:895:LEU:HD21	1.93	0.48
1:A:1273:TRP:C	1:A:1273:TRP:CE3	2.87	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
1:A:226:HIS:O	1:A:255:PHE:HD2	1.96	0.48
1:A:131:ASP:CA	1:A:775:TRP:CH2	2.79	0.48
1:A:840:GLN:HG3	1:A:899:THR:HG23	1.94	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:1000:LEU:H	1:A:1000:LEU:HD12	1.78	0.48
1:A:1013:MET:SD	1:A:1129:LEU:CB	3.02	0.48
1:A:1585:TYR:CE1	1:A:1668:ALA:HB1	2.33	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
2:B:309:LYS:HZ3	2:B:474:ARG:HH12	1.62	0.48
2:B:322:ASN:C	2:B:324:LEU:N	2.67	0.48
1:A:1088:GLN:OE1	1:A:1154:LYS:CD	2.62	0.48
1:A:1287:THR:O	1:A:1288:GLN:C	2.50	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
2:B:493:TYR:CE2	2:B:497:PHE:CZ	2.95	0.48
2:B:739:THR:HG22	2:B:740:CYS:N	2.28	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
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
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:104:LEU:HB2	1:A:117:MET:CE	2.44	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
1:A:59:TYR:CB	1:A:60:PRO:HD2	2.42	0.48
1:A:640:LEU:HB3	1:A:644:ASN:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:464:PHE:HE1	2:B:466:LEU:HD11	1.74	0.48
2:B:309:LYS:NZ	2:B:474:ARG:HH12	2.11	0.48
1:A:208:ASP:OD1	1:A:208:ASP:N	2.33	0.48
2:B:205:THR:O	2:B:205:THR:HG22	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:1080:ALA:HB1	1:A:1148:THR:HA	1.96	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
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
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:1113:LEU:HB3	1:A:1115:ASN:ND2	2.29	0.47
1:A:126:LEU:HD11	1:A:205:TYR:CE1	2.49	0.47
1:A:1377:PHE:CD2	1:A:1408:TYR:HA	2.50	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
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: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
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
2:B:168:SER:HB2	2:B:459:PRO:HG2	1.95	0.47
1:A:1642:LEU:CD1	1:A:1642:LEU:N	2.77	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
2:B:302:LEU:HD11	2:B:350:LEU:HB3	1.95	0.47
1:A:1016:VAL:HG13	1:A:1017:PRO:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:1203:PRO:CD	2:B:653:THR:HG22	2.40	0.47
1:A:109:LYS:HZ3	1:A:110:HIS:CE1	2.32	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:493:TYR:CD2	2:B:497:PHE:CE2	3.02	0.47
1:A:1217:LEU:HD12	1:A:1227:PHE:CE1	2.50	0.47
1:A:1627:ILE:O	1:A:1627:ILE:CG1	2.54	0.47
1:A:653:PHE:CD1	1:A:660:ASP:HB2	2.49	0.47
2:B:342:THR:HG22	2:B:343:HIS:CE1	2.49	0.47
1:A:1012:LEU:CD1	1:A:1012:LEU:C	2.83	0.47
1:A:1028:GLY:N	1:A:1302:LEU:HD21	2.30	0.47
1:A:1515:LYS:HE2	1:A:1530:ALA:HB3	1.96	0.47
1:A:224:LEU:H	1:A:224:LEU:HG	1.25	0.47
1:A:49:ALA:CB	1:A:74:SER:HB3	2.45	0.47
1:A:625:GLN:O	1:A:629:LYS:HG2	2.15	0.47
1:A:1065:SER:HB3	1:A:1106:TRP:CD2	2.49	0.47
1:A:1326:TYR:CD2	1:A:1326:TYR:N	2.82	0.47
1:A:606:ASP:OD2	1:A:795:THR:HG21	2.15	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:1517:GLN:HB3	1:A:1574:PHE:CE1	2.50	0.47
1:A:849:ARG:CG	1:A:918:PHE:HZ	2.21	0.47
1:A:1264:ILE:CG1	1:A:1303:LEU:HD11	2.44	0.47
1:A:198:MET:HE1	1:A:218:GLU:HG3	1.97	0.47
1:A:576:SER:OG	1:A:589:SER:HB2	2.15	0.47
1:A:965:LEU:C	1:A:966:ASP:OD1	2.54	0.47
2:B:316:VAL:O	2:B:319:LYS:HB3	2.15	0.47
1:A:959:PHE:HE2	1:A:1348:VAL:CG2	2.28	0.46
1:A:830:PRO:HG3	1:A:1487:PHE:CE1	2.48	0.46
1:A:337:SER:OG	1:A:1485:VAL:CG2	2.57	0.46
1:A:222:TYR:OH	1:A:771:GLU:OE1	2.31	0.46
1:A:821:LYS:HE2	1:A:921:GLU:OE1	2.15	0.46
2:B:10:GLN:HB2	2:B:10:GLN:HE21	1.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:113:LYS:HG2	1:A:114:SER:N	2.28	0.46
1:A:988:LEU:CD1	1:A:1268:ASN:OD1	2.60	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:1090:ASN:HD22	1:A:1158:ILE:HD13	1.80	0.46
1:A:123:ASN:H	1:A:211:THR:HG23	1.80	0.46
1:A:1245:ALA:HB2	1:A:1285:TYR:HE2	1.80	0.46
1:A:180:ILE:HD12	1:A:599:TRP:CD2	2.50	0.46
1:A:59:TYR:CG	1:A:60:PRO:CD	2.76	0.46
1:A:357:VAL:CG1	1:A:675:PRO:HG3	2.44	0.46
1:A:49:ALA:HB1	1:A:74:SER:HB3	1.98	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: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
1:A:307:VAL:CG1	1:A:312:TYR:HB2	2.46	0.46
1:A:944:LEU:HB3	1:A:1311:MET:HE2	1.97	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:1059:TYR:O	1:A:1067:SER:N	2.32	0.46
1:A:487:THR:HG22	1:A:523:TYR:CB	2.44	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: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
1:A:461:SER:C	1:A:463:SER:N	2.68	0.46
1:A:576:SER:CB	1:A:577:PRO:CD	2.90	0.46
1:A:573:VAL:HA	1:A:591:ASN:O	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:1275:SER:HA	2:B:595:MET:HE2	1.98	0.46
1:A:1485:VAL:HG22	1:A:1487:PHE:O	2.16	0.46
1:A:1647:TYR:CD1	1:A:1647:TYR:O	2.68	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
2:B:11:TRP:CH2	2:B:50:ARG:HD3	2.51	0.46
1:A:1132:THR:HG22	1:A:1246:ARG:CG	2.46	0.46
1:A:21:GLN:HE22	1:A:45:GLY:N	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:641:TYR:HB3	2:B:645:GLU:OE2	2.16	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
1:A:547:THR:C	1:A:549:GLU:H	2.19	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
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: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:52:CYS:HA	2:B:54:TRP:CZ3	2.51	0.45
2:B:776:SER:CB	2:B:794:ALA:HB3	2.46	0.45
1:A:1273:TRP:CD2	1:A:1273:TRP:C	2.90	0.45
1:A:939:TYR:HB3	1:A:1362:THR:HG22	1.97	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
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:HA	1:A:1361:VAL:O	2.16	0.45
2:B:464:PHE:HD1	2:B:466:LEU:CD1	2.28	0.45
1:A:1028:GLY:HA2	1:A:1305:LYS:NZ	2.31	0.45
1:A:1241:ASN:OD1	1:A:1241:ASN:O	2.33	0.45
1:A:1560:ALA:O	1:A:1584:ILE:O	2.35	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
2:B:468:PRO:HB2	2:B:470:VAL:HG12	1.97	0.45
2:B:694:ILE:HG12	2:B:694:ILE:H	1.38	0.45
1:A:1323:LEU:HD12	1:A:1323:LEU:HA	1.74	0.45
1:A:1379:LEU:HD11	1:A:1495:VAL:HG13	1.99	0.45
1:A:1488:LEU:HD13	1:A:1489:SER:O	2.17	0.45
1:A:1376:SER:OG	1:A:1503:LYS:CG	2.64	0.45
1:A:1638:PRO:C	1:A:1639:LEU:HD12	2.37	0.45
1:A:560:TRP:CH2	1:A:562:ASN:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:611:GLU:HG3	2:B:611:GLU:O	2.17	0.45
1:A:939:TYR:O	2:B:660:TYR:HD1	2.00	0.45
2:B:70:SER:O	2:B:71:ASP:O	2.34	0.45
2:B:735:SER:O	2:B:736:ASN:HB2	2.17	0.45
1:A:1582:LEU:N	1:A:1582:LEU:HD13	2.32	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:1079:THR:HG22	1:A:1107:LEU:HD11	1.99	0.45
1:A:33:VAL:HG23	1:A:120:THR:O	2.17	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
1:A:1375:CYS:SG	1:A:1376:SER:N	2.90	0.45
1:A:1483:PHE:CD1	1:A:1483:PHE:C	2.90	0.45
2:B:54:TRP:CD1	2:B:55:GLN:OE1	2.70	0.45
2:B:735:SER:C	2:B:736:ASN:OD1	2.55	0.45
1:A:496:ILE:HB	1:A:517:LYS:HG3	1.99	0.45
2:B:300:LYS:CD	3:D:1:NAG:H82	2.47	0.45
2:B:388:LEU:C	2:B:389:PHE:CD2	2.91	0.45
2:B:476:ILE:CB	2:B:477:PRO:HD2	2.36	0.45
2:B:493:TYR:CD2	2:B:497:PHE:HE2	2.35	0.45
2:B:493:TYR:CE1	2:B:497:PHE:HE2	2.33	0.45
1:A:1279:ARG:CG	2:B:601:PRO:HD2	2.40	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:1341:LEU:C	1:A:1342:LEU:CD1	2.85	0.45
1:A:1408:TYR:HD2	1:A:1419:SER:N	2.14	0.45
1:A:365:PRO:HB3	1:A:426:SER:O	2.16	0.45
1:A:47:THR:O	1:A:48:GLU:C	2.55	0.45
2:B:847:TYR:CD2	2:B:850:GLU:CD	2.91	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
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:1231:ASN:C	1:A:1232:LEU:CD1	2.66	0.44
1:A:1570:VAL:HG22	1:A:1575:VAL:HG13	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
2:B:8:TRP:CE3	2:B:25:ARG:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1247:MET:O	1:A:1251:THR:HG23	2.17	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
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:804:ILE:HG13	1:A:804:ILE:O	2.18	0.44
2:B:877:VAL:HG12	2:B:903:MET:CE	2.47	0.44
1:A:1277:GLU:OE2	1:A:1284:PHE:CZ	2.70	0.44
1:A:1334:LEU:C	1:A:1334:LEU:HD12	2.37	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
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
2:B:735:SER:O	2:B:736:ASN:CB	2.65	0.44
1:A:1016:VAL:N	1:A:1017:PRO:CD	2.80	0.44
1:A:1013:MET:CE	1:A:1129:LEU:HG	2.44	0.44
1:A:1200:LYS:HG2	1:A:1200:LYS:H	1.52	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:382:LEU:HD22	1:A:416:GLY:HA3	1.98	0.44
1:A:1129:LEU:CD1	1:A:1129:LEU:N	2.81	0.44
1:A:1626:GLN:HE21	1:A:1633:PHE:HB3	1.82	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
2:B:262:ILE:O	2:B:262:ILE:HG23	2.18	0.44
2:B:877:VAL:O	2:B:877:VAL:CG2	2.66	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: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
1:A:237:PHE:HE2	1:A:352:TYR:HH	1.62	0.43
2:B:173:GLY:O	2:B:187:VAL:HG12	2.18	0.43
1:A:1170:LYS:H	1:A:1170:LYS:HG2	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
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
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:1225:TYR:CE1	1:A:1276:GLU:CG	2.80	0.43
1:A:364:LYS:HZ1	1:A:557:ASP:CG	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:905:ILE:HG23	2:B:905:ILE:O	2.18	0.43
1:A:1536:GLN:HB3	1:A:1645:ILE:O	2.17	0.43
1:A:461:SER:OG	1:A:553:GLU:CD	2.56	0.43
1:A:76:GLU:HG3	1:A:77:ASN:N	2.32	0.43
1:A:1275:SER:HA	2:B:595:MET:SD	2.59	0.43
2:B:911:CYS:HB3	2:B:912:LEU:H	1.68	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
1:A:232:GLU:OE2	1:A:251:LYS:HE2	2.18	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
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:240:LEU:CD1	2:B:273:ASN:HD21	2.31	0.43
2:B:176:PHE:HD2	2:B:466:LEU:CD2	2.31	0.43
2:B:828:ARG:NH2	2:B:845:THR:O	2.52	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:1526:LYS:HG2	1:A:1627:ILE:HG22	1.99	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:113:LYS:CE	1:A:654:LEU:HD11	2.48	0.43
1:A:766:ARG:NH2	1:A:921:GLU:OE2	2.42	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
2:B:29:ILE:CD1	2:B:46:LYS:HE3	2.48	0.43
1:A:941:GLY:HA2	1:A:1359:VAL:O	2.18	0.43
1:A:1377:PHE:N	1:A:1377:PHE:CD1	2.86	0.43
1:A:1562:LYS:NZ	1:A:1648:TRP:HZ2	2.16	0.43
1:A:1572:ASN:C	1:A:1573:VAL:HG23	2.38	0.43
1:A:1618:LEU:HD22	1:A:1619:ILE:N	2.33	0.43
1:A:1556:GLU:HB3	1:A:1622:LYS:CE	2.49	0.43
1:A:229:VAL:HG22	1:A:252:ALA:HB2	2.00	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:1027:THR:HG22	1:A:1302:LEU:CD1	2.45	0.43
1:A:1419:SER:O	1:A:1466:SER:CB	2.67	0.43
1:A:1675:GLY:O	1:A:1676:CYS:CB	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:A:1088:GLN:CD	1:A:1154:LYS:HZ2	2.20	0.43
1:A:1317:TYR:HB3	1:A:1344:ASP:CG	2.37	0.43
1:A:597:ASP:OD1	1:A:781:PRO:HA	2.19	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:88:PRO:CB	2:B:516:THR:O	2.67	0.43
2:B:890:ILE:HG13	2:B:891:CYS:N	2.33	0.43
1:A:944:LEU:HB3	1:A:1311:MET:CE	2.48	0.43
1:A:1574:PHE:HA	1:A:1603:LYS:HA	2.01	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
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:1241:ASN:OD1	1:A:1241:ASN:C	2.57	0.42
1:A:1247:MET:O	1:A:1248:VAL:C	2.54	0.42
1:A:1590:ALA:HB3	1:A:1624:ALA:HB1	2.00	0.42
1:A:1654:CYS:N	1:A:1657:CYS:SG	2.92	0.42
1:A:43:VAL:CG2	1:A:44:TYR:N	2.82	0.42
1:A:569:ASN:ND2	1:A:805:SER:HB3	2.33	0.42
1:A:61:ASP:O	1:A:61:ASP:OD2	2.36	0.42
2:B:241:GLY:O	2:B:245:ASN:CG	2.57	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:889:ASN:N	2:B:889:ASN:OD1	2.52	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
1:A:577:PRO:HG2	1:A:586:GLN:NE2	2.34	0.42
1:A:58:SER:O	1:A:103:TYR:CD1	2.67	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
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
2:B:2:PHE:O	2:B:5:HIS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:TYR:HD1	1:A:1186:PHE:HE2	1.65	0.42
1:A:1328:MET:HE2	1:A:1335:GLY:H	1.84	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
2:B:495:ALA:CB	7:B:1008:MAN:H61	2.47	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:443:LEU:C	2:B:443:LEU:HD13	2.39	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:1284:PHE:CE2	2:B:594:ILE:HD11	2.54	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
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:1590:ALA:HB1	1:A:1635:TYR:CZ	2.54	0.42
1:A:1552:ALA:HB2	1:A:1620:MET:CE	2.49	0.42
1:A:1631:PHE:CD2	1:A:1631:PHE:O	2.73	0.42
2:B:782:PHE:CE1	2:B:826:LEU:HD12	2.54	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:1127:ILE:CD1	1:A:1130:GLN:HE21	2.03	0.42
1:A:1244:THR:O	1:A:1245:ALA:C	2.57	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:372:LYS:HZ2	1:A:470:THR:HG21	1.84	0.42
1:A:959:PHE:HE2	1:A:1348:VAL:HG23	1.85	0.42
2:B:322:ASN:O	2:B:324:LEU:N	2.51	0.42
1:A:1176:LEU:HD23	1:A:1195:LEU:HD13	2.01	0.42
1:A:485:ILE:N	1:A:485:ILE:HD12	2.35	0.42
1:A:620:LEU:HG	1:A:624:PHE:HE1	1.84	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:437:GLU:O	2:B:441:SER:N	2.53	0.42
1:A:1153:ARG:HH22	2:B:699:ARG:HH22	1.68	0.42
2:B:300:LYS:HD2	3:D:1:NAG:C8	2.50	0.42
1:A:1066:TYR:CB	1:A:1078:LEU:HD23	2.49	0.42
1:A:1245:ALA:C	1:A:1247:MET:H	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:510:ARG:O	2:B:521:VAL:HB	2.20	0.42
2:B:508:ASN:OD1	2:B:543:VAL:HA	2.19	0.42
2:B:567:GLU:C	2:B:569:ASN:HD22	2.22	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:493:TYR:O	2:B:497:PHE:CD2	2.73	0.42
2:B:483:ARG:NH2	2:B:605:ASP:OD1	2.53	0.42
1:A:266:TYR:CZ	1:A:1483:PHE:CG	3.06	0.41
1:A:1589:GLU:CG	1:A:1590:ALA:N	2.70	0.41
1:A:1549:LYS:HG3	1:A:1667:PHE:HE1	1.85	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
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
1:A:1135:VAL:HG13	1:A:1136:GLU:N	2.35	0.41
1:A:1314:ASP:HA	1:A:1325:ASN:CB	2.50	0.41
1:A:1372:GLU:CG	1:A:1409:LYS:HZ1	2.33	0.41
1:A:1450:PHE:CE1	1:A:1475:VAL:HB	2.55	0.41
1:A:337:SER:HG	1:A:1485:VAL:HG23	1.78	0.41
1:A:1562:LYS:HD2	1:A:1648:TRP:NE1	2.32	0.41
1:A:491:PRO:HG3	1:A:544:TYR:OH	2.20	0.41
1:A:23:TYR:CG	1:A:656:ASN:HB2	2.55	0.41
1:A:762:LYS:O	1:A:762:LYS:HG2	2.19	0.41
1:A:956:ARG:HA	1:A:1348:VAL:O	2.19	0.41
1:A:1226:ARG:NH1	2:B:611:GLU:OE1	2.50	0.41
1:A:949:ILE:HG23	1:A:1262:LYS:HD2	2.01	0.41
1:A:1556:GLU:HB2	1:A:1622:LYS:HE2	2.02	0.41
1:A:396:ASP:CB	1:A:400:GLU:HB3	2.38	0.41
1:A:469:TRP:CH2	1:A:471:ASP:CG	2.93	0.41
1:A:494:ASP:CA	1:A:496:ILE:HD12	2.50	0.41
1:A:57:LYS:HD3	1:A:62:LYS:HB3	2.01	0.41
1:A:781:PRO:O	1:A:782:ARG:HB2	2.20	0.41
1:A:961:TYR:CE2	1:A:963:ILE:HG22	2.55	0.41
2:B:444:GLU:O	2:B:447:THR:HB	2.20	0.41
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:1273:TRP:HE3	1:A:1274:LEU:CA	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1342:LEU:N	1:A:1342:LEU:HD13	2.36	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
2:B:427:ARG:HB2	2:B:430:TYR:CD2	2.56	0.41
2:B:11:TRP:CH2	2:B:50:ARG:CZ	3.03	0.41
2:B:546:GLN:HB2	2:B:571:PRO:CG	2.50	0.41
1:A:1188:LEU:HA	1:A:1188:LEU:HD12	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
1:A:190:ILE:HA	1:A:191:PRO:HD3	1.91	0.41
1:A:469:TRP:CZ2	1:A:471:ASP:CG	2.93	0.41
1:A:103:TYR:HA	1:A:115:LYS:O	2.21	0.41
1:A:1280:TYR:CD2	1:A:1281:GLY:CA	3.04	0.41
1:A:1572:ASN:O	1:A:1573:VAL:HB	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
2:B:214:ASN:O	2:B:307:LYS:HB3	2.20	0.41
2:B:734:ILE:HD13	2:B:734:ILE:N	2.36	0.41
2:B:89:SER:HB2	2:B:95:PRO:HA	2.01	0.41
1:A:1247:MET:O	1:A:1251:THR:CG2	2.69	0.41
1:A:1226:ARG:O	1:A:1270:VAL:HG22	2.21	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
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
1:A:1021:VAL:O	1:A:1025:LEU:HB2	2.20	0.41
1:A:1028:GLY:HA2	1:A:1305:LYS:HZ1	1.86	0.41
1:A:1121:ASN:C	1:A:1121:ASN:OD1	2.58	0.41
2:B:119:CYS:C	2:B:124:ARG:HH21	2.24	0.41
1:A:793:SER:O	1:A:819:VAL:CG2	2.69	0.41
1:A:136:THR:OG1	1:A:831:TYR:OH	2.25	0.41
2:B:116:GLU:OE2	2:B:130:CYS:CB	2.65	0.41
1:A:1204:GLN:OE1	1:A:1204:GLN:HA	2.21	0.41
1:A:1013:MET:SD	1:A:1287:THR:HB	2.61	0.41
1:A:1494:THR:HA	1:A:1505:CYS:O	2.21	0.41
1:A:925:LYS:HA	1:A:925:LYS:HD2	1.55	0.41
2:B:546:GLN:N	2:B:571:PRO:HG2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:140:GLU:CD	2:B:158:VAL:HG21	2.42	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: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
1:A:1138:ARG:H	1:A:1138:ARG:CD	2.34	0.40
1:A:1328:MET:HE3	1:A:1335:GLY:H	1.85	0.40
1:A:1647:TYR:HD1	1:A:1649:PRO:CG	2.35	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:182:ILE:CG1	1:A:804:ILE:CD1	2.92	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:1453:TYR:CD2	1:A:1453:TYR:C	2.95	0.40
1:A:461:SER:HG	1:A:553:GLU:CD	2.24	0.40
1:A:914:LEU:HD13	1:A:914:LEU:C	2.41	0.40
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
2:B:893:VAL:HG22	2:B:903:MET:HE3	2.02	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	6	37
2	B	892/913 (98%)	770 (86%)	96 (11%)	26 (3%)	4	33
All	All	2436/2589 (94%)	2109 (87%)	266 (11%)	61 (2%)	5	35

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	1183 (86%)	196 (14%)	3	19
2	B	797/810 (98%)	715 (90%)	82 (10%)	7	28
All	All	2176/2294 (95%)	1898 (87%)	278 (13%)	4	21

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	SER
1	A	59	TYR
1	A	73	LEU
1	A	76	GLU
1	A	78	LYS
1	A	115	LYS
1	A	116	ARG
1	A	130	THR
1	A	136	THR
1	A	144	ARG
1	A	161	LEU
1	A	162	THR
1	A	179	HIS
1	A	194	PRO
1	A	195	ARG
1	A	208	ASP
1	A	209	PHE
1	A	211	THR
1	A	223	VAL

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Mol	Chain	Res	Type
1	A	224	LEU
1	A	242	ASN
1	A	253	ARG
1	A	261	THR
1	A	280	LYS
1	A	281	GLU
1	A	285	THR
1	A	310	LEU
1	A	317	ASP
1	A	323	LEU
1	A	330	ILE
1	A	333	THR
1	A	361	LEU
1	A	364	LYS
1	A	383	VAL
1	A	394	THR
1	A	396	ASP
1	A	401	THR
1	A	419	SER
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
1	A	500	ASN
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	580	ASP
1	A	588	VAL
1	A	592	MET
1	A	594	THR
1	A	628	GLU

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Mol	Chain	Res	Type
1	A	630	SER
1	A	644	ASN
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	857	VAL
1	A	887	LYS
1	A	888	VAL
1	A	893	SER
1	A	899	THR
1	A	901	LEU
1	A	905	ILE
1	A	909	ASN
1	A	917	TRP
1	A	921	GLU
1	A	922	ILE
1	A	924	VAL
1	A	925	LYS
1	A	927	LEU
1	A	929	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	975	ARG
1	A	982	LEU
1	A	984	VAL

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Mol	Chain	Res	Type
1	A	988	LEU
1	A	993	SER
1	A	1003	LEU
1	A	1005	LYS
1	A	1013	MET
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	1138	ARG
1	A	1140	ASN
1	A	1142	LEU
1	A	1148	THR
1	A	1161	LEU
1	A	1162	VAL
1	A	1196	SER
1	A	1200	LYS
1	A	1206	ARG
1	A	1213	LYS
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	1291	ILE
1	A	1312	ASP
1	A	1324	HIS
1	A	1326	TYR
1	A	1330	ASP
1	A	1331	LYS
1	A	1334	LEU
1	A	1336	ARG
1	A	1341	LEU

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Mol	Chain	Res	Type
1	A	1342	LEU
1	A	1352	PHE
1	A	1360	HIS
1	A	1367	LYS
1	A	1370	THR
1	A	1377	PHE
1	A	1398	ASP
1	A	1412	ARG
1	A	1423	VAL
1	A	1452	ASP
1	A	1453	TYR
1	A	1456	LYS
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	1494	THR
1	A	1495	VAL
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	1583	ASP
1	A	1589	GLU
1	A	1594	LYS
1	A	1598	ILE
1	A	1602	LYS
1	A	1608	ASN
1	A	1611	LEU

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Mol	Chain	Res	Type
1	A	1618	LEU
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	47	GLN
2	B	54	TRP
2	B	56	ARG
2	B	72	CYS
2	B	80	SER
2	B	100	LEU
2	B	121	ASN
2	B	126	ASP
2	B	135	LEU
2	B	149	GLU
2	B	155	THR
2	B	159	CYS
2	B	178	PHE
2	B	182	GLU
2	B	188	LEU
2	B	190	ASN
2	B	200	VAL
2	B	204	ARG
2	B	221	GLU
2	B	244	GLU
2	B	263	PHE
2	B	271	ASN
2	B	302	LEU
2	B	303	ASN
2	B	318	LEU
2	B	326	LEU
2	B	384	LYS
2	B	386	ARG
2	B	392	LYS

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Mol	Chain	Res	Type
2	B	393	THR
2	B	436	TRP
2	B	441	SER
2	B	508	ASN
2	B	537	ASP
2	B	552	SER
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	604	ASN
2	B	611	GLU
2	B	612	VAL
2	B	613	ASP
2	B	620	ASP
2	B	636	ASN
2	B	661	GLN
2	B	688	VAL
2	B	692	LEU
2	B	693	THR
2	B	694	ILE
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	790	PHE
2	B	804	ASN
2	B	805	ASN
2	B	811	LEU
2	B	828	ARG
2	B	845	THR
2	B	859	CYS

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Mol	Chain	Res	Type
2	B	868	PHE
2	B	876	CYS
2	B	881	SER
2	B	889	ASN
2	B	892	GLU
2	B	895	THR
2	B	907	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	42	GLN
1	A	110	HIS
1	A	123	ASN
1	A	139	GLN
1	A	193	ASN
1	A	226	HIS
1	A	399	GLN
1	A	423	ASN
1	A	472	ASN
1	A	483	ASN
1	A	562	ASN
1	A	613	GLN
1	A	642	ASN
1	A	647	HIS
1	A	656	ASN
1	A	665	ASN
1	A	800	GLN
1	A	886	GLN
1	A	909	ASN
1	A	1002	HIS
1	A	1030	HIS
1	A	1043	GLN
1	A	1090	ASN
1	A	1096	ASN
1	A	1098	ASN
1	A	1115	ASN
1	A	1121	ASN
1	A	1123	GLN
1	A	1125	GLN
1	A	1140	ASN

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Mol	Chain	Res	Type
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	1499	HIS
1	A	1513	ASN
1	A	1626	GLN
1	A	1658	GLN
2	B	10	GLN
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	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	569	ASN
2	B	574	GLN
2	B	597	ASN
2	B	600	GLN
2	B	636	ASN
2	B	756	GLN
2	B	804	ASN
2	B	805	ASN
2	B	834	ASN
2	B	872	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	1,3	14,14,15	0.58	0	17,19,21	1.52	5 (29%)
3	NAG	C	2	3	14,14,15	0.54	0	17,19,21	1.08	1 (5%)
3	NAG	D	1	3,2	14,14,15	0.43	0	17,19,21	1.95	2 (11%)
3	NAG	D	2	3	14,14,15	0.58	0	17,19,21	1.01	2 (11%)
4	FUC	E	1	2,4	10,10,11	0.67	0	14,14,16	1.50	3 (21%)
4	BGC	E	2	4	11,11,12	0.75	0	15,15,17	1.02	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	1,3	-	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 (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	C1-O5-C5	6.69	121.25	112.19
4	E	1	FUC	C3-C4-C5	3.40	115.07	109.77
3	C	1	NAG	O5-C1-C2	-3.30	106.07	111.29
3	C	1	NAG	C1-C2-N2	2.58	114.90	110.49
4	E	1	FUC	C1-O5-C5	2.55	118.56	112.78
3	C	1	NAG	O4-C4-C3	-2.37	104.86	110.35
3	D	2	NAG	C1-O5-C5	2.28	115.28	112.19
3	C	2	NAG	C1-C2-N2	2.07	114.03	110.49
4	E	1	FUC	O5-C5-C4	2.06	113.21	109.52
3	D	2	NAG	O4-C4-C3	-2.05	105.62	110.35
3	D	1	NAG	C6-C5-C4	-2.03	108.25	113.00
3	C	1	NAG	O7-C7-C8	-2.02	118.31	122.06
3	C	1	NAG	O5-C5-C6	2.01	110.35	107.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

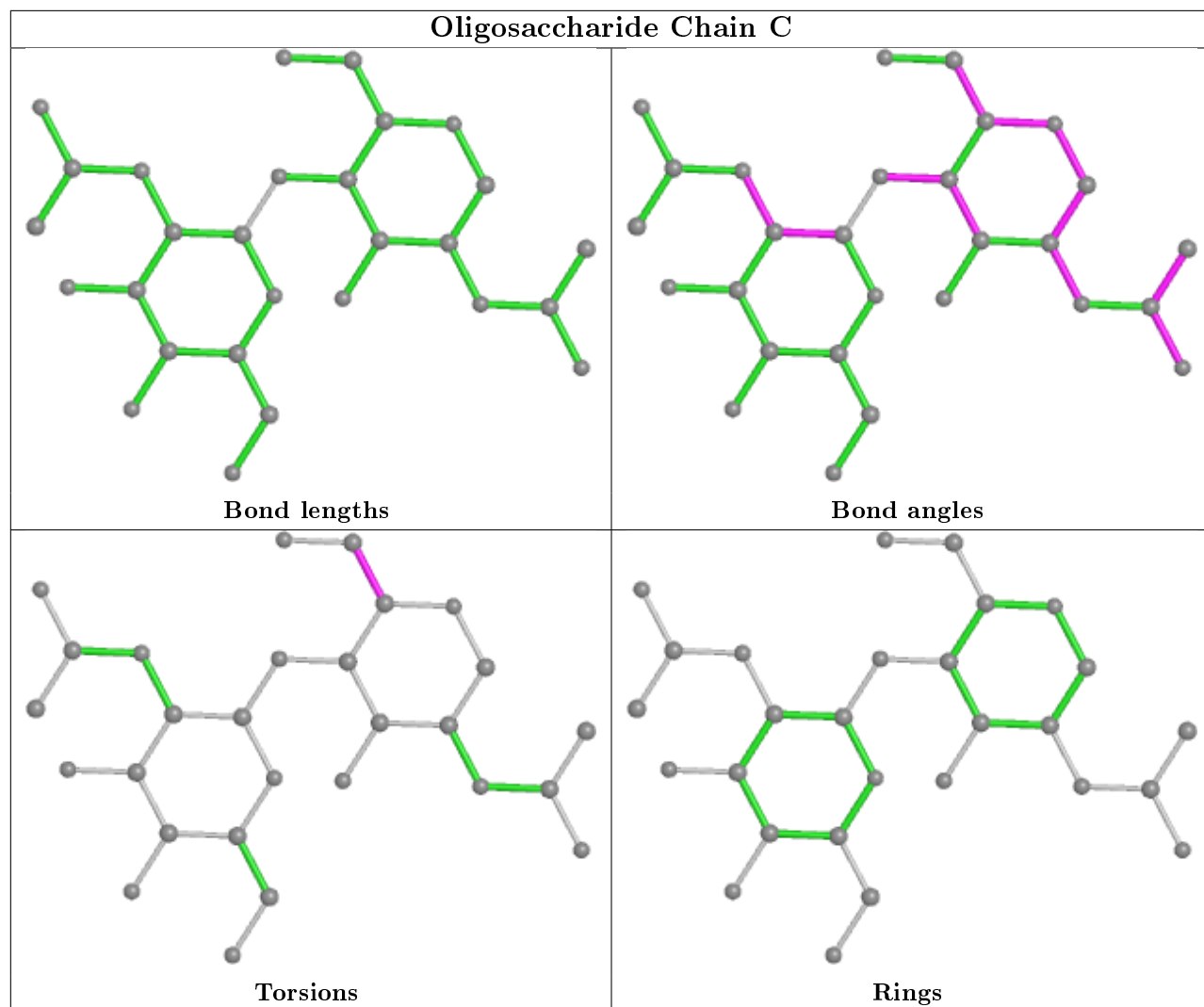
Mol	Chain	Res	Type	Atoms
4	E	2	BGC	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
4	E	2	BGC	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

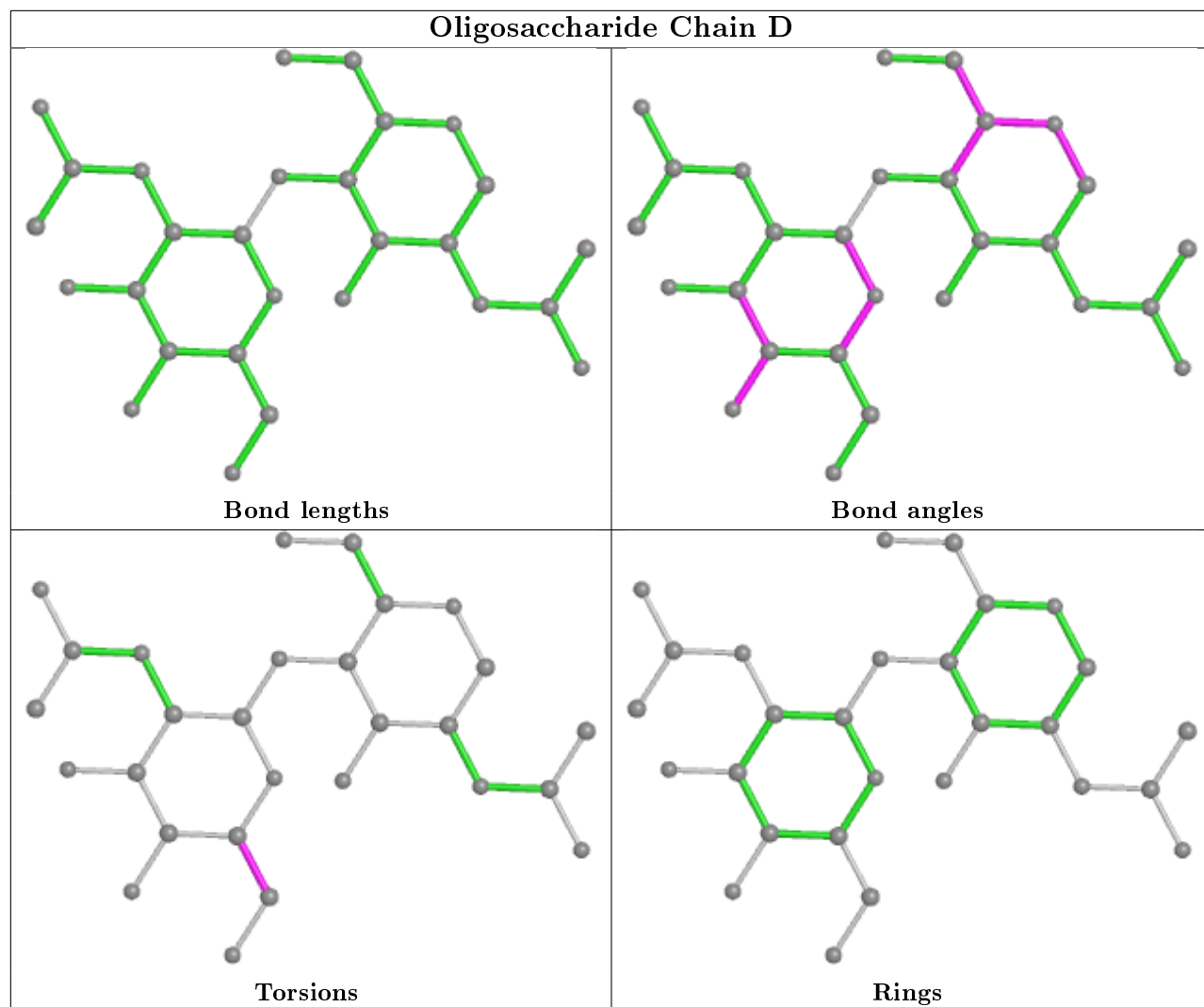
There are no ring outliers.

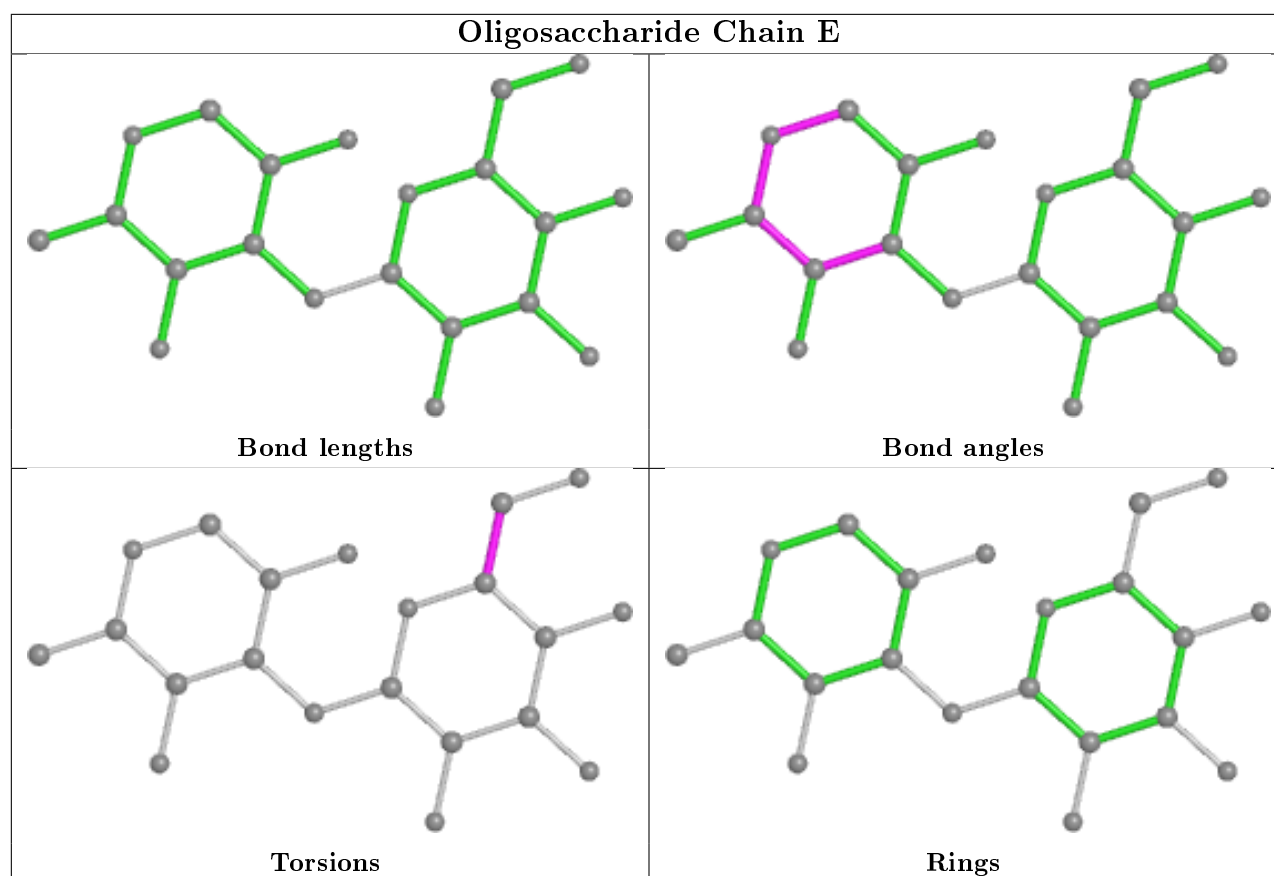
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	3	0
3	C	2	NAG	1	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	1007	2	11,11,12	0.70	0	15,15,17	0.89	0
7	MAN	B	1008	2	11,11,12	0.68	0	15,15,17	1.58	2 (13%)
7	MAN	B	1009	2	11,11,12	0.62	0	15,15,17	1.24	3 (20%)
7	MAN	B	1006	2	11,11,12	0.58	0	15,15,17	1.08	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	1007	2	-	1/2/19/22	0/1/1/1
7	MAN	B	1008	2	-	0/2/19/22	0/1/1/1
7	MAN	B	1009	2	-	0/2/19/22	0/1/1/1
7	MAN	B	1006	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1008	MAN	C3-C4-C5	3.76	116.94	110.24
7	B	1009	MAN	O5-C1-C2	-2.83	106.41	110.77
7	B	1008	MAN	O5-C1-C2	-2.44	107.00	110.77
7	B	1009	MAN	C3-C4-C5	2.30	114.34	110.24
7	B	1006	MAN	C1-O5-C5	2.24	115.22	112.19
7	B	1009	MAN	C1-O5-C5	2.21	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	1007	MAN	2	0
7	B	1008	MAN	4	0
7	B	1009	MAN	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.63	4 (0%) 94 90	110, 177, 258, 386	0
2	B	898/913 (98%)	-0.54	0 100 100	121, 201, 282, 389	0
All	All	2450/2589 (94%)	-0.60	4 (0%) 95 93	110, 187, 269, 389	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1238	SER	5.1
1	A	1006	GLY	2.7
1	A	1237	SER	2.4
1	A	1005	LYS	2.0

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

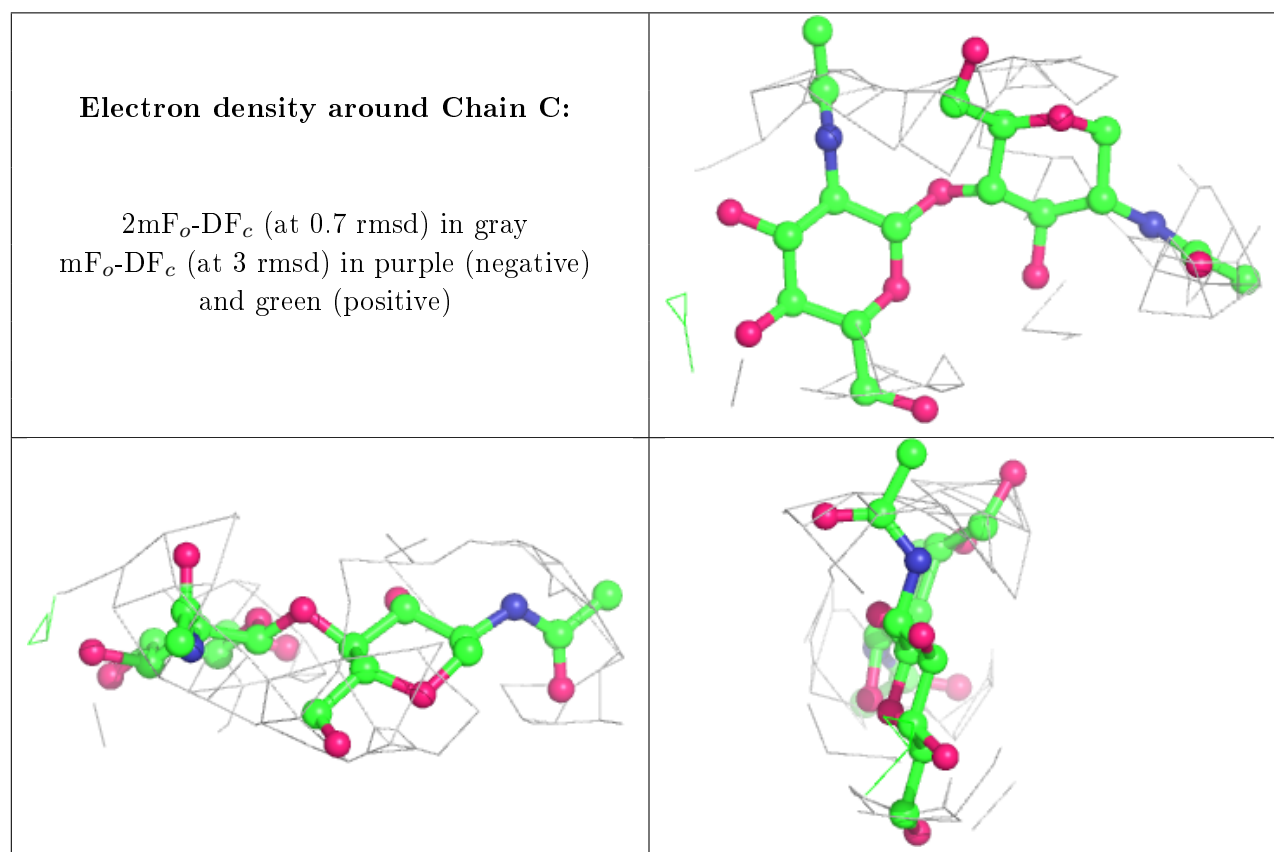
There are no non-standard protein/DNA/RNA residues in this entry.

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.

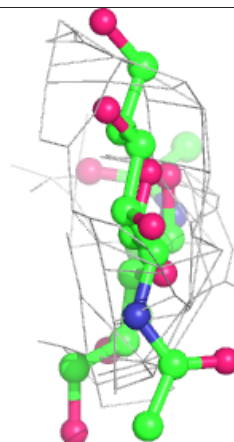
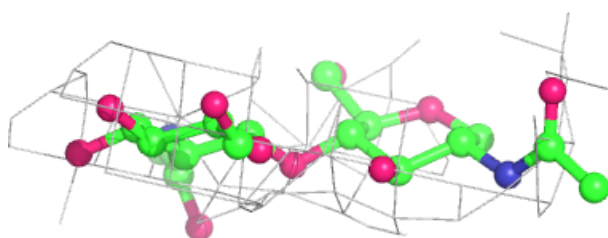
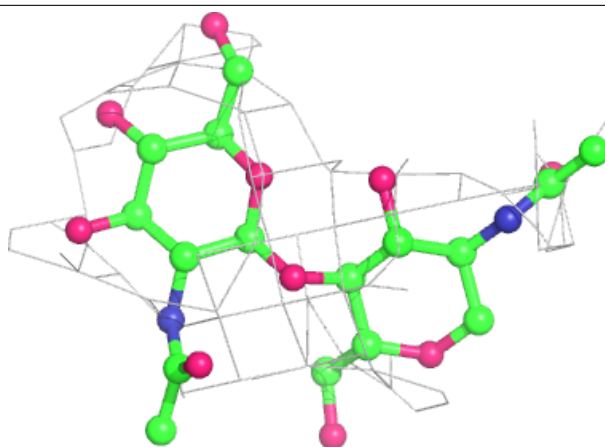
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	D	2	14/15	0.80	0.52	269,286,304,315	0
3	NAG	D	1	14/15	0.81	0.38	205,240,279,295	0
3	NAG	C	2	14/15	0.83	0.28	207,226,257,262	0
4	BGC	E	2	11/12	0.90	0.29	187,198,214,224	0
3	NAG	C	1	14/15	0.93	0.21	152,160,185,186	0
4	FUC	E	1	10/11	0.97	0.20	174,188,192,196	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.

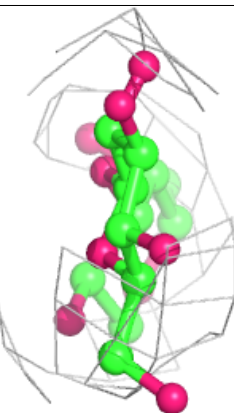
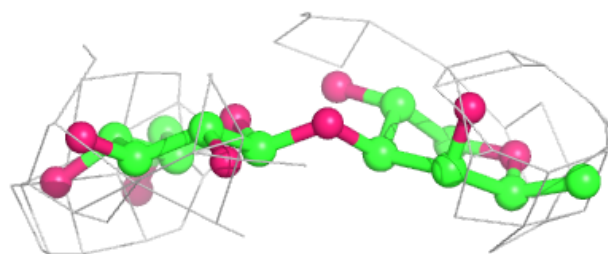
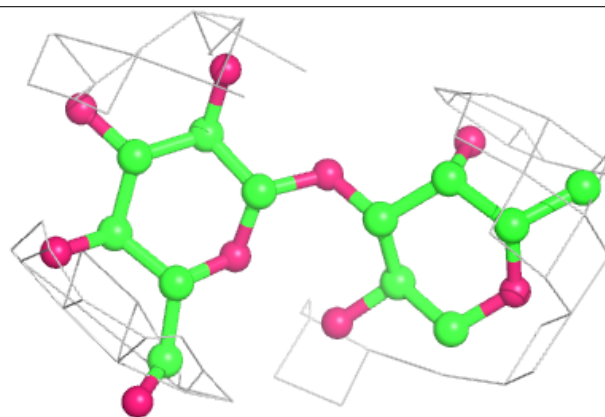


Electron density around Chain D:

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

**Electron density around Chain E:**

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
5	NA	A	2003	1/1	0.81	0.33	111,111,111,111	0
7	MAN	B	1006	11/12	0.88	0.25	245,260,277,281	0
7	MAN	B	1007	11/12	0.89	0.22	205,212,234,240	0
6	CA	B	1001	1/1	0.90	0.06	167,167,167,167	1
7	MAN	B	1009	11/12	0.94	0.25	178,190,201,215	0
7	MAN	B	1008	11/12	0.96	0.23	147,167,176,188	0

6.5 Other polymers [i](#)

There are no such residues in this entry.