Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 03:10 PM EDT

PDB ID	:	4HG6
Title	:	Structure of a cellulose synthase - cellulose translocation intermediate
Authors	:	Zimmer, J.
Deposited on	:	2012-10-07
Resolution	:	3.25 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

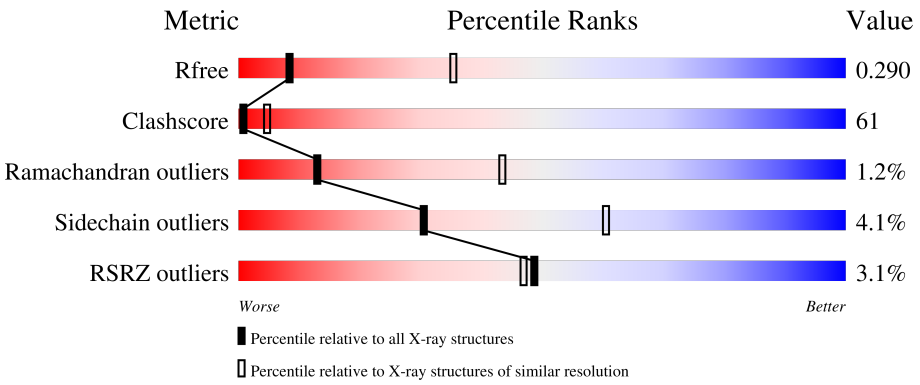
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	802	3%; 40%; 51%; • ; 7%
2	B	707	3%; 42%; 45%; 5%; 7%
3	C	18	11%; 28%; 61%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BGC	C	5	-	-	X	-
4	UDP	A	919	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11029 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 Cellulose Synthase Subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	747	5893	3822	1029	1011	31	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	789	HIS	-	expression tag	UNP Q3J125
A	790	HIS	-	expression tag	UNP Q3J125
A	791	HIS	-	expression tag	UNP Q3J125
A	792	HIS	-	expression tag	UNP Q3J125
A	793	HIS	-	expression tag	UNP Q3J125
A	794	HIS	-	expression tag	UNP Q3J125
A	795	LYS	-	expression tag	UNP Q3J125
A	796	LEU	-	expression tag	UNP Q3J125
A	797	HIS	-	expression tag	UNP Q3J125
A	798	HIS	-	expression tag	UNP Q3J125
A	799	HIS	-	expression tag	UNP Q3J125
A	800	HIS	-	expression tag	UNP Q3J125
A	801	HIS	-	expression tag	UNP Q3J125
A	802	HIS	-	expression tag	UNP Q3J125

- Molecule 2 is a protein called Cellulose Synthase Subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	655	4887	3100	864	907	16	0	0	0

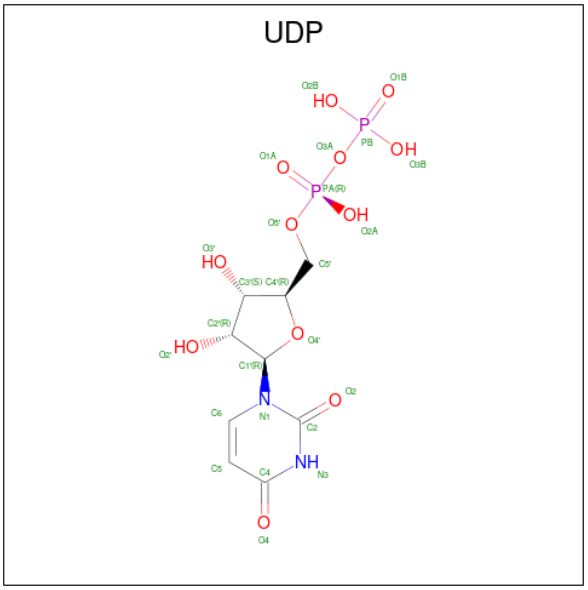
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	19	MET	-	expression tag	UNP Q3J126
B	20	GLY	-	expression tag	UNP Q3J126

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

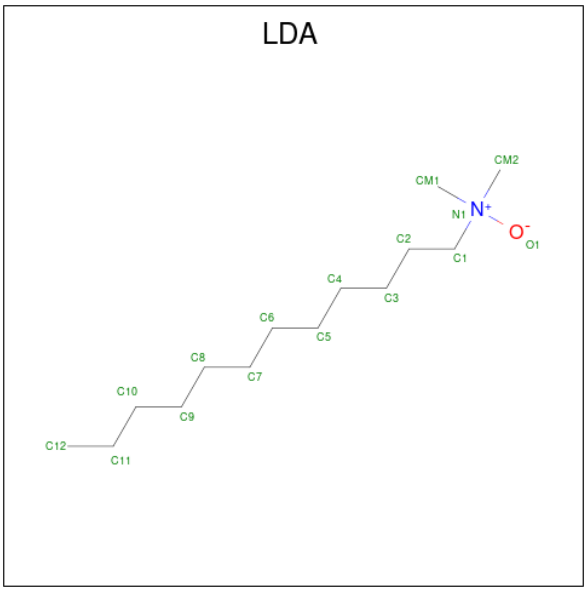
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	C	18	199	108	91	0	0	0

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	25	9	2	12	2	0	0

- Molecule 5 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



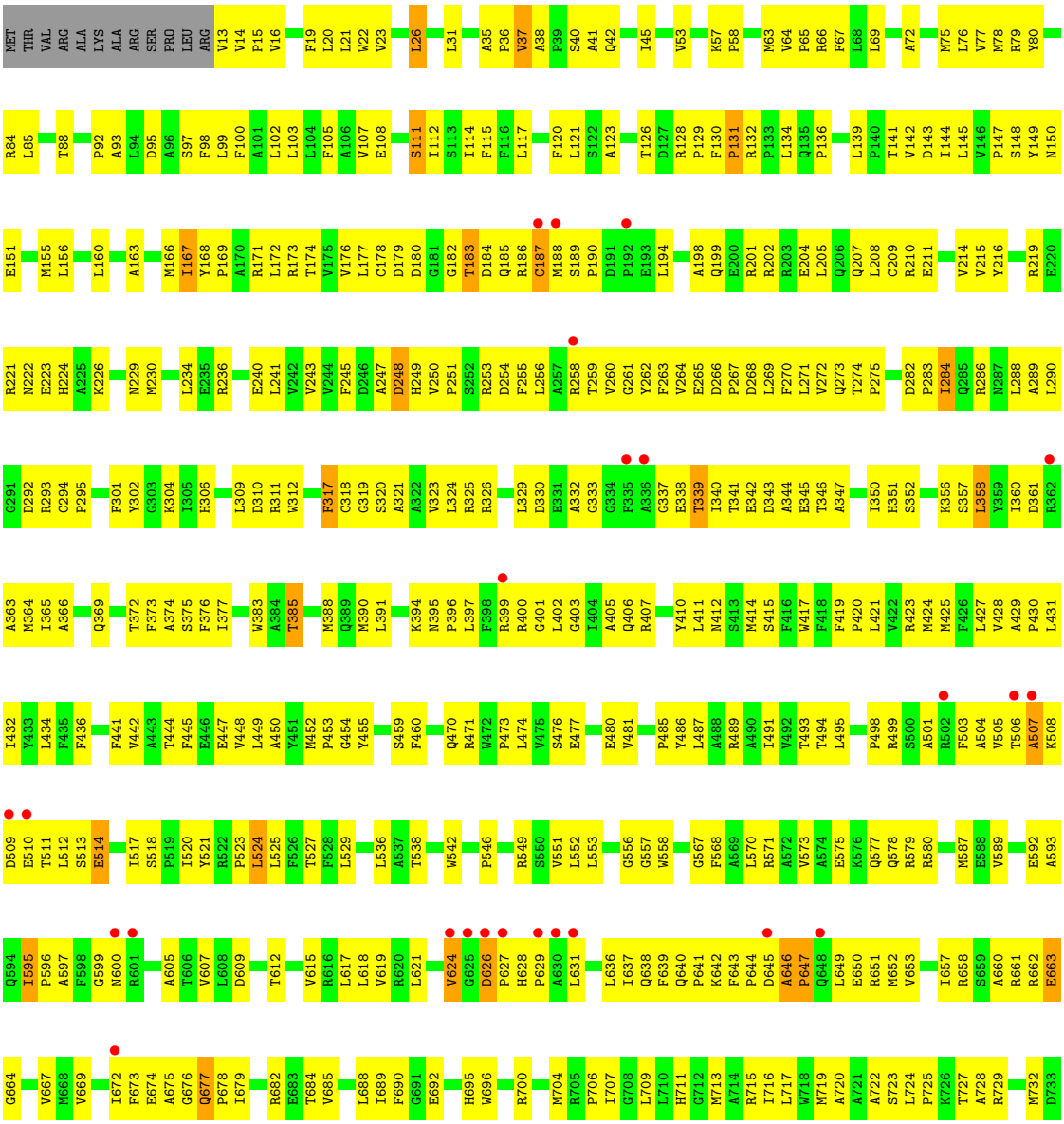
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	9	7	1	1	0	0
			Total	C	N	O		
5	A	1	16	14	1	1	0	0

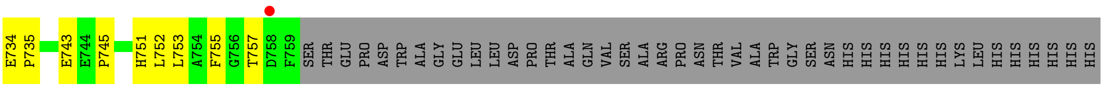
3 Residue-property plots (i)

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

- Molecule 1: Cellulose Synthase Subunit A

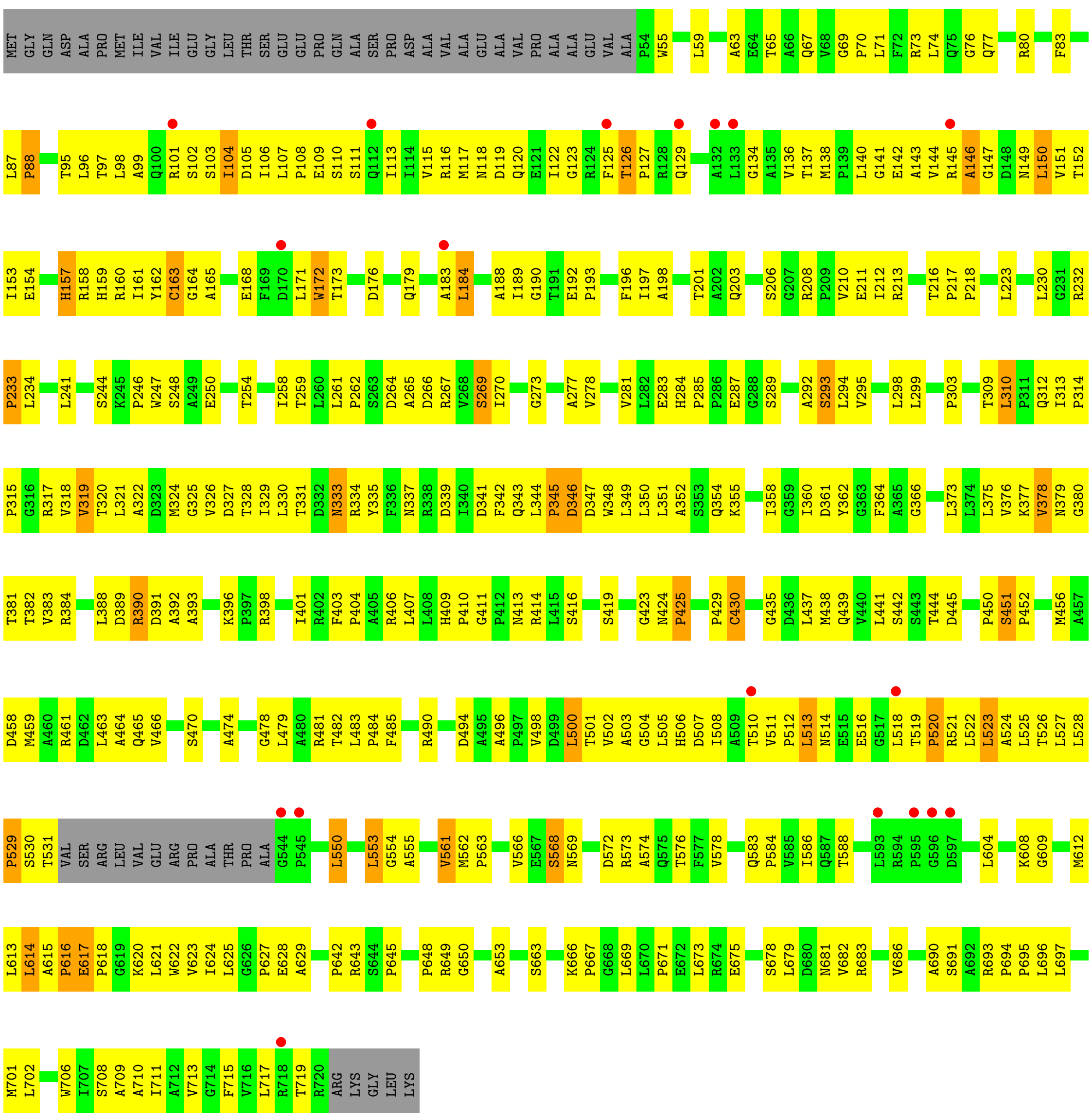
Chain A:





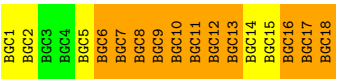
• Molecule 2: Cellulose Synthase Subunit B

Chain B:



• Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4) -beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-gluc opyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1 -4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-gl ucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain C:


BGC1
BGC2
BGC3
BGC4
BGC5
BGC6
BGC7
BGC8
BGC9
BGC10
BGC11
BGC12
BGC13
BGC14
BGC15
BGC16
BGC17
BGC18

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	103.12Å 103.12Å 468.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.81 – 3.25 34.81 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.81-3.25) 99.9 (34.81-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.91 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.213 , 0.282 0.229 , 0.290	Depositor DCC
R_{free} test set	2055 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	117.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 95.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11029	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, BGC, UDP

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	0.41	0/6044	0.63	2/8217 (0.0%)
2	B	0.39	1/5006 (0.0%)	0.63	2/6865 (0.0%)
All	All	0.40	1/11050 (0.0%)	0.63	4/15082 (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
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	345	PRO	N-CD	-10.24	1.33	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	346	ASP	CB-CA-C	-7.15	96.10	110.40
2	B	345	PRO	CA-N-CD	6.14	120.30	111.70
1	A	646	ALA	C-N-CD	-6.03	107.33	120.60
1	A	663	GLU	N-CA-C	-5.53	96.06	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	390	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5893	0	5996	742	0
2	B	4887	0	4966	603	0
3	C	199	0	165	29	0
4	A	25	0	11	2	0
5	A	25	0	45	7	0
All	All	11029	0	11183	1350	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 61.

All (1350) 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)
2:B:330:LEU:CD2	2:B:439:GLN:HG3	1.33	1.58
2:B:377:LYS:CG	2:B:382:THR:HG22	1.32	1.56
1:A:643:PHE:HB3	1:A:646:ALA:CB	1.42	1.49
2:B:107:LEU:CD1	2:B:160:ARG:HA	1.47	1.41
1:A:317:PHE:CE2	1:A:347:ALA:HB2	1.58	1.38
2:B:118:ASN:CG	2:B:144:VAL:HG11	1.42	1.37
2:B:377:LYS:HG2	2:B:382:THR:CG2	1.55	1.36
2:B:107:LEU:HD11	2:B:160:ARG:CA	1.61	1.30
2:B:321:LEU:HA	2:B:324:MET:CG	1.59	1.30
1:A:269:LEU:HD13	1:A:269:LEU:O	1.25	1.29
1:A:262:TYR:CE1	1:A:360:ILE:CD1	2.17	1.28
1:A:571:ARG:CD	1:A:723:SER:HB2	1.62	1.27
1:A:262:TYR:CE1	1:A:360:ILE:HD11	1.70	1.26
1:A:103:LEU:HD13	1:A:425:MET:CE	1.65	1.26
2:B:122:ILE:CG2	2:B:140:LEU:HB3	1.66	1.25
1:A:178:CYS:SG	1:A:180:ASP:HB3	1.77	1.24
1:A:269:LEU:O	1:A:269:LEU:CD1	1.87	1.23
1:A:637:ILE:HD13	1:A:657:ILE:CG2	1.69	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:PHE:CE2	1:A:347:ALA:CB	2.21	1.22
2:B:96:LEU:CD2	2:B:137:THR:HG22	1.68	1.21
2:B:117:MET:SD	2:B:151:VAL:HG22	1.79	1.20
2:B:122:ILE:HG21	2:B:140:LEU:CB	1.71	1.20
2:B:321:LEU:HA	2:B:324:MET:CB	1.70	1.20
2:B:106:ILE:HB	2:B:160:ARG:HD3	1.20	1.19
2:B:73:ARG:CD	2:B:172:TRP:HE3	1.55	1.18
1:A:643:PHE:CB	1:A:646:ALA:HB3	1.72	1.17
1:A:271:LEU:HD11	1:A:317:PHE:CB	1.76	1.16
1:A:646:ALA:CB	1:A:647:PRO:HD3	1.74	1.15
2:B:266:ASP:HB2	2:B:285:PRO:CD	1.76	1.15
1:A:434:LEU:HD13	1:A:538:THR:HG23	1.26	1.15
1:A:317:PHE:HE2	1:A:347:ALA:CB	1.57	1.14
2:B:330:LEU:HD21	2:B:439:GLN:CG	1.76	1.14
1:A:271:LEU:CD1	1:A:317:PHE:HB3	1.78	1.13
1:A:571:ARG:HD2	1:A:723:SER:CB	1.79	1.13
2:B:615:ALA:CB	2:B:621:LEU:HG	1.77	1.13
2:B:424:ASN:HB3	2:B:425:PRO:HD3	1.21	1.12
1:A:364:MET:O	1:A:365:ILE:HG23	1.49	1.12
2:B:321:LEU:HD23	2:B:324:MET:HG3	1.23	1.12
2:B:122:ILE:HG22	2:B:140:LEU:HD13	1.24	1.12
2:B:459:MET:SD	2:B:613:LEU:HD22	1.89	1.12
1:A:514:GLU:CA	1:A:578:GLN:HB2	1.80	1.11
2:B:330:LEU:CD2	2:B:439:GLN:CG	2.28	1.11
1:A:272:VAL:CG2	1:A:358:LEU:HD11	1.79	1.11
1:A:399:ARG:HH22	1:A:410:TYR:HB2	1.00	1.11
2:B:419:SER:HB3	2:B:438:MET:CE	1.79	1.11
1:A:84:ARG:HA	1:A:88:THR:OG1	1.50	1.11
2:B:107:LEU:CD1	2:B:160:ARG:CA	2.24	1.11
2:B:615:ALA:HB2	2:B:621:LEU:HG	1.29	1.11
2:B:678:SER:O	2:B:682:VAL:HG23	1.50	1.11
2:B:350:LEU:CD1	2:B:451:SER:HB2	1.79	1.10
1:A:103:LEU:CD1	1:A:425:MET:HE1	1.80	1.10
1:A:259:THR:HG21	1:A:323:VAL:CG2	1.82	1.10
2:B:118:ASN:HB2	2:B:144:VAL:CG2	1.81	1.10
1:A:258:ARG:NH2	1:A:364:MET:HE2	1.64	1.10
2:B:344:LEU:HB3	2:B:345:PRO:HD2	1.14	1.10
1:A:271:LEU:HD11	1:A:317:PHE:HB3	1.13	1.10
1:A:452:MET:CE	1:A:558:TRP:HE1	1.65	1.10
2:B:520:PRO:HD2	2:B:522:LEU:HG	1.30	1.09
1:A:14:VAL:HG13	1:A:15:PRO:HD3	1.30	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ARG:HH22	1:A:410:TYR:CB	1.64	1.09
2:B:96:LEU:HD23	2:B:137:THR:HG22	1.24	1.09
2:B:328:THR:HG22	2:B:442:SER:H	1.18	1.08
2:B:528:LEU:HB3	2:B:529:PRO:HD3	1.27	1.08
1:A:259:THR:CG2	1:A:323:VAL:HG21	1.84	1.08
1:A:595:ILE:HG22	1:A:596:PRO:CD	1.83	1.08
1:A:643:PHE:HB3	1:A:646:ALA:HB3	1.20	1.08
1:A:643:PHE:CB	1:A:646:ALA:CB	2.30	1.08
2:B:566:VAL:HG11	3:C:5:BGC:H6C2	1.35	1.08
1:A:546:PRO:HA	1:A:549:ARG:HE	1.15	1.07
2:B:266:ASP:HB2	2:B:285:PRO:HD3	1.34	1.07
1:A:595:ILE:HG22	1:A:596:PRO:HD2	1.09	1.07
2:B:73:ARG:HD3	2:B:172:TRP:CE3	1.89	1.07
2:B:350:LEU:HD11	2:B:451:SER:CB	1.84	1.07
1:A:399:ARG:NH2	1:A:410:TYR:HB2	1.69	1.07
1:A:186:ARG:HG3	1:A:199:GLN:HG2	1.34	1.06
1:A:258:ARG:HH21	1:A:364:MET:HE2	0.96	1.06
1:A:452:MET:HE1	1:A:558:TRP:HE1	1.18	1.06
2:B:456:MET:SD	2:B:671:PRO:HB3	1.96	1.06
1:A:399:ARG:NH1	1:A:407:ARG:HA	1.71	1.05
2:B:693:ARG:HD3	2:B:696:LEU:HD23	1.35	1.05
2:B:419:SER:HB3	2:B:438:MET:HE1	1.39	1.04
1:A:64:VAL:HB	1:A:65:PRO:HD3	1.39	1.04
2:B:118:ASN:CB	2:B:144:VAL:HG21	1.88	1.04
1:A:434:LEU:HD13	1:A:538:THR:CG2	1.88	1.04
1:A:637:ILE:HD13	1:A:657:ILE:HG21	1.10	1.04
2:B:321:LEU:HA	2:B:324:MET:HB2	1.35	1.04
1:A:262:TYR:CZ	1:A:360:ILE:HD11	1.92	1.03
1:A:272:VAL:HG22	1:A:358:LEU:HD11	1.04	1.03
1:A:339:THR:CG2	1:A:345:GLU:HG3	1.87	1.03
2:B:73:ARG:HD3	2:B:172:TRP:HE3	1.17	1.03
2:B:107:LEU:HB3	2:B:110:SER:CB	1.88	1.03
2:B:682:VAL:O	2:B:686:VAL:HG23	1.58	1.03
2:B:163:CYS:O	2:B:423:GLY:HA3	1.58	1.02
1:A:434:LEU:CD2	1:A:538:THR:HG22	1.89	1.02
1:A:144:ILE:HG22	1:A:243:VAL:HB	1.36	1.02
1:A:646:ALA:HB3	1:A:647:PRO:CD	1.90	1.02
1:A:142:VAL:HG22	1:A:241:LEU:HB2	1.41	1.01
1:A:288:LEU:N	1:A:288:LEU:HD12	1.74	1.01
1:A:364:MET:O	1:A:365:ILE:CG2	2.08	1.00
2:B:118:ASN:HB2	2:B:144:VAL:HG21	1.03	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:PHE:HZ	2:B:138:MET:HG3	1.23	1.00
2:B:147:GLY:HA3	2:B:303:PRO:HG2	1.39	0.99
2:B:673:LEU:HD13	2:B:675:GLU:O	1.60	0.99
1:A:514:GLU:HA	1:A:578:GLN:CB	1.93	0.99
1:A:658:ARG:CG	1:A:672:ILE:HD11	1.92	0.99
2:B:73:ARG:CD	2:B:172:TRP:CE3	2.45	0.99
2:B:107:LEU:HB3	2:B:110:SER:HB2	1.44	0.99
1:A:272:VAL:HG22	1:A:358:LEU:CD1	1.91	0.99
1:A:434:LEU:CD1	1:A:538:THR:CG2	2.41	0.99
1:A:751:HIS:HD1	1:A:752:LEU:N	1.59	0.99
1:A:571:ARG:HD2	1:A:723:SER:HB2	1.00	0.98
1:A:272:VAL:HG13	1:A:358:LEU:HD21	1.44	0.98
1:A:317:PHE:CD2	1:A:347:ALA:CB	2.46	0.98
2:B:270:ILE:HB	2:B:281:VAL:HG22	1.44	0.97
1:A:273:GLN:OE1	1:A:317:PHE:HA	1.61	0.97
2:B:379:ASN:HD21	2:B:413:ASN:HD22	1.11	0.97
2:B:616:PRO:O	2:B:617:GLU:HG3	1.63	0.97
2:B:616:PRO:C	2:B:617:GLU:HG3	1.83	0.96
2:B:377:LYS:CD	2:B:382:THR:HG22	1.95	0.96
1:A:434:LEU:HD22	1:A:538:THR:HG22	1.48	0.96
1:A:752:LEU:O	1:A:753:LEU:HB2	1.63	0.95
2:B:377:LYS:HD3	2:B:382:THR:CG2	1.97	0.95
1:A:259:THR:HG21	1:A:323:VAL:HG21	0.98	0.95
1:A:514:GLU:HA	1:A:578:GLN:HB2	0.97	0.95
2:B:63:ALA:HB3	2:B:67:GLN:HE22	1.27	0.95
2:B:122:ILE:HG22	2:B:140:LEU:CD1	1.96	0.95
2:B:115:VAL:HG12	2:B:123:GLY:O	1.64	0.95
2:B:377:LYS:CG	2:B:382:THR:CG2	2.27	0.95
1:A:84:ARG:CD	1:A:88:THR:HG21	1.97	0.94
2:B:330:LEU:HD23	2:B:439:GLN:HG3	1.48	0.94
2:B:398:ARG:HH12	2:B:444:THR:HA	1.32	0.94
2:B:118:ASN:OD1	2:B:144:VAL:HG11	1.65	0.94
1:A:37:VAL:HG13	1:A:41:ALA:HB3	1.50	0.93
1:A:637:ILE:CD1	1:A:657:ILE:HG21	1.98	0.93
2:B:101:ARG:HG2	2:B:173:THR:HG23	1.51	0.93
2:B:526:THR:HG21	2:B:604:LEU:HG	1.49	0.93
2:B:321:LEU:CA	2:B:324:MET:HB2	2.00	0.92
1:A:473:PRO:O	1:A:716:ILE:HD13	1.70	0.92
2:B:344:LEU:CB	2:B:345:PRO:HD2	1.92	0.91
2:B:321:LEU:HD12	2:B:442:SER:HA	1.52	0.91
1:A:121:LEU:CD2	1:A:412:ASN:HD21	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:TYR:HE1	1:A:360:ILE:CD1	1.68	0.91
1:A:568:PHE:CD1	1:A:720:ALA:HA	2.06	0.91
2:B:350:LEU:HD11	2:B:451:SER:HB2	0.93	0.91
2:B:125:PHE:HZ	2:B:138:MET:CG	1.84	0.91
1:A:646:ALA:HB3	1:A:647:PRO:HD3	0.94	0.91
2:B:528:LEU:CB	2:B:529:PRO:HD3	1.95	0.91
1:A:340:ILE:HD11	1:A:501:ALA:HB2	1.50	0.90
2:B:377:LYS:CD	2:B:382:THR:CG2	2.48	0.90
1:A:186:ARG:HG3	1:A:199:GLN:CG	2.00	0.90
1:A:429:ALA:O	1:A:432:ILE:HG22	1.72	0.90
2:B:566:VAL:CG1	3:C:5:BGC:H6C2	2.01	0.90
1:A:595:ILE:CG2	1:A:596:PRO:HD2	1.99	0.90
1:A:568:PHE:HD1	1:A:720:ALA:HA	1.36	0.90
2:B:266:ASP:HA	2:B:284:HIS:HA	1.51	0.90
2:B:321:LEU:CA	2:B:324:MET:CG	2.48	0.90
2:B:73:ARG:HD2	2:B:172:TRP:HE3	1.36	0.90
1:A:504:ALA:O	1:A:506:THR:HG23	1.71	0.90
1:A:501:ALA:HB1	1:A:503:PHE:HE2	1.35	0.89
2:B:409:HIS:H	2:B:413:ASN:HD21	0.93	0.89
2:B:321:LEU:HA	2:B:324:MET:HG2	1.54	0.89
1:A:141:THR:O	1:A:240:GLU:HB2	1.72	0.89
1:A:145:LEU:O	1:A:145:LEU:HD12	1.73	0.89
2:B:321:LEU:CD2	2:B:324:MET:HG3	2.02	0.89
1:A:358:LEU:HD13	1:A:358:LEU:H	1.38	0.89
1:A:571:ARG:HG2	1:A:727:THR:HB	1.52	0.89
2:B:349:LEU:C	2:B:350:LEU:HD12	1.93	0.89
2:B:505:LEU:CD2	2:B:523:LEU:CD2	2.51	0.89
2:B:615:ALA:HB2	2:B:621:LEU:CG	2.03	0.88
1:A:643:PHE:HB3	1:A:646:ALA:HB2	1.52	0.88
2:B:184:LEU:HD23	2:B:188:ALA:HB3	1.54	0.88
1:A:571:ARG:CD	1:A:723:SER:CB	2.45	0.88
1:A:72:ALA:O	1:A:75:MET:HG2	1.73	0.88
2:B:424:ASN:CB	2:B:425:PRO:HD3	2.04	0.88
1:A:178:CYS:SG	1:A:180:ASP:CB	2.61	0.88
1:A:317:PHE:HE2	1:A:347:ALA:HB2	0.95	0.87
2:B:266:ASP:HB2	2:B:285:PRO:HD2	1.54	0.87
1:A:340:ILE:HD11	1:A:501:ALA:CB	2.04	0.87
2:B:99:ALA:HB3	2:B:129:GLN:OE1	1.72	0.87
1:A:14:VAL:CG1	1:A:15:PRO:HD3	2.04	0.87
1:A:612:THR:OG1	1:A:753:LEU:HA	1.75	0.87
3:C:7:BGC:O3	3:C:8:BGC:O5	1.93	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:920:LDA:HM23	2:B:708:SER:OG	1.75	0.87
2:B:118:ASN:CG	2:B:144:VAL:CG1	2.37	0.86
2:B:566:VAL:CG1	3:C:5:BGC:C6	2.53	0.86
2:B:409:HIS:H	2:B:413:ASN:ND2	1.72	0.86
1:A:643:PHE:HB3	1:A:646:ALA:HB1	1.58	0.86
2:B:107:LEU:CD1	2:B:160:ARG:CB	2.52	0.86
1:A:37:VAL:CG1	1:A:41:ALA:HB3	2.06	0.86
2:B:107:LEU:CB	2:B:110:SER:HB2	2.05	0.86
1:A:262:TYR:CE1	1:A:360:ILE:HD12	2.09	0.86
1:A:132:ARG:HB2	1:A:265:GLU:OE2	1.75	0.85
1:A:234:LEU:HB3	1:A:326:ARG:HH21	1.40	0.85
2:B:330:LEU:HD21	2:B:439:GLN:HG3	0.85	0.85
2:B:106:ILE:CB	2:B:160:ARG:HD3	2.04	0.85
1:A:501:ALA:HB1	1:A:503:PHE:CE2	2.10	0.85
1:A:599:GLY:O	1:A:600:ASN:HB2	1.75	0.85
2:B:201:THR:HG22	2:B:234:LEU:HD21	1.59	0.85
2:B:398:ARG:NH2	2:B:445:ASP:CG	2.30	0.85
1:A:117:LEU:O	1:A:121:LEU:HD13	1.77	0.85
2:B:107:LEU:HD13	2:B:160:ARG:HA	1.55	0.84
2:B:107:LEU:HB3	2:B:110:SER:OG	1.77	0.84
2:B:266:ASP:CB	2:B:285:PRO:HD3	2.07	0.84
1:A:185:GLN:HG3	1:A:222:ASN:HD21	1.43	0.84
1:A:95:ASP:O	1:A:99:LEU:CD1	2.24	0.84
1:A:103:LEU:HD13	1:A:425:MET:HE1	0.86	0.84
1:A:302:TYR:OH	3:C:17:BGC:H6C1	1.77	0.84
2:B:107:LEU:HD11	2:B:160:ARG:HA	0.86	0.84
1:A:144:ILE:HG13	1:A:144:ILE:O	1.78	0.84
2:B:360:ILE:HD12	2:B:401:ILE:HD11	1.59	0.84
2:B:98:LEU:CD1	2:B:179:GLN:HB2	2.08	0.84
1:A:399:ARG:NH2	1:A:410:TYR:CB	2.33	0.84
2:B:158:ARG:O	2:B:171:LEU:CD2	2.26	0.83
2:B:118:ASN:ND2	2:B:144:VAL:HG11	1.93	0.83
1:A:53:VAL:HG13	1:A:69:LEU:HD11	1.59	0.83
1:A:271:LEU:HD11	1:A:317:PHE:CG	2.13	0.83
1:A:136:PRO:HA	1:A:139:LEU:HD12	1.58	0.83
2:B:474:ALA:HB2	2:B:503:ALA:HB2	1.58	0.83
1:A:269:LEU:HD13	1:A:269:LEU:C	1.98	0.83
1:A:207:GLN:O	1:A:211:GLU:HG3	1.77	0.82
1:A:374:ALA:HA	1:A:377:ILE:HD12	1.62	0.82
1:A:524:LEU:HA	1:A:527:THR:HG22	1.61	0.82
1:A:649:LEU:HG	1:A:684:THR:HG22	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:SER:CB	2:B:438:MET:CE	2.57	0.82
1:A:641:PRO:HB2	1:A:643:PHE:CE1	2.14	0.82
4:A:919:UDP:O3B	3:C:18:BGC:H6C1	1.80	0.81
2:B:321:LEU:HA	2:B:324:MET:HG3	1.61	0.81
2:B:163:CYS:O	2:B:163:CYS:SG	2.37	0.81
1:A:643:PHE:HB2	1:A:647:PRO:HD3	1.60	0.81
1:A:84:ARG:HD2	1:A:88:THR:HG21	1.61	0.81
1:A:507:ALA:HB1	1:A:509:ASP:OD1	1.81	0.81
1:A:358:LEU:CD1	1:A:358:LEU:H	1.94	0.81
2:B:102:SER:HB3	2:B:172:TRP:CD1	2.16	0.81
2:B:566:VAL:HG13	3:C:5:BGC:C6	2.11	0.81
1:A:185:GLN:HG3	1:A:222:ASN:ND2	1.96	0.81
2:B:144:VAL:C	2:B:145:ARG:HG3	2.01	0.81
1:A:53:VAL:HG13	1:A:69:LEU:CD1	2.10	0.81
1:A:284:ILE:O	1:A:288:LEU:HD13	1.81	0.81
2:B:98:LEU:HD11	2:B:179:GLN:HB2	1.62	0.81
1:A:643:PHE:HB2	1:A:646:ALA:HB3	1.63	0.80
2:B:572:ASP:O	2:B:576:THR:HG23	1.80	0.80
1:A:144:ILE:HD11	1:A:163:ALA:HB1	1.63	0.80
2:B:102:SER:HB3	2:B:172:TRP:NE1	1.96	0.80
1:A:95:ASP:O	1:A:99:LEU:HD12	1.81	0.80
1:A:546:PRO:HA	1:A:549:ARG:NE	1.96	0.80
1:A:507:ALA:CB	1:A:509:ASP:OD1	2.30	0.80
2:B:520:PRO:CD	2:B:522:LEU:HG	2.12	0.80
1:A:503:PHE:O	1:A:503:PHE:CD1	2.35	0.79
1:A:290:LEU:N	1:A:290:LEU:HD23	1.97	0.79
2:B:513:LEU:HD13	2:B:513:LEU:O	1.83	0.79
2:B:95:THR:HG22	2:B:96:LEU:N	1.97	0.79
2:B:145:ARG:O	2:B:146:ALA:HB2	1.83	0.79
1:A:339:THR:HG22	1:A:345:GLU:HG3	1.64	0.79
1:A:441:PHE:HB3	3:C:9:BGC:H4	1.64	0.79
1:A:713:MET:O	1:A:717:LEU:HD12	1.82	0.79
2:B:346:ASP:OD1	2:B:346:ASP:O	1.99	0.79
2:B:345:PRO:O	2:B:346:ASP:CB	2.30	0.79
1:A:288:LEU:HD12	1:A:288:LEU:H	1.44	0.78
1:A:658:ARG:HG2	1:A:672:ILE:HD11	1.63	0.78
2:B:615:ALA:CB	2:B:621:LEU:CG	2.58	0.78
2:B:366:GLY:HA2	2:B:392:ALA:HB2	1.64	0.78
2:B:328:THR:HG22	2:B:442:SER:N	1.97	0.78
1:A:676:GLY:C	1:A:678:PRO:HD3	2.03	0.78
2:B:360:ILE:CD1	2:B:401:ILE:HD11	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:ILE:CG2	2:B:140:LEU:HD13	2.11	0.78
1:A:364:MET:C	1:A:365:ILE:HG23	2.04	0.78
1:A:182:GLY:O	1:A:183:THR:C	2.20	0.77
1:A:506:THR:O	1:A:507:ALA:HB3	1.85	0.77
1:A:510:GLU:HG2	1:A:512:LEU:HD11	1.67	0.77
2:B:161:ILE:HG23	2:B:162:TYR:HD2	1.49	0.77
2:B:223:LEU:HD12	2:B:479:LEU:HD21	1.67	0.77
1:A:36:PRO:HD3	2:B:683:ARG:NH1	1.99	0.77
1:A:589:VAL:HB	1:A:607:VAL:CG2	2.14	0.77
1:A:647:PRO:CG	1:A:649:LEU:HB3	2.14	0.77
2:B:375:LEU:HD12	2:B:375:LEU:N	1.99	0.77
2:B:409:HIS:N	2:B:413:ASN:HD21	1.79	0.77
2:B:122:ILE:HD13	2:B:140:LEU:O	1.84	0.77
1:A:141:THR:HB	1:A:240:GLU:HG2	1.66	0.77
1:A:144:ILE:HG22	1:A:243:VAL:CB	2.13	0.77
2:B:118:ASN:O	2:B:119:ASP:HB2	1.83	0.77
1:A:751:HIS:HD1	1:A:752:LEU:H	0.78	0.77
2:B:63:ALA:CB	2:B:67:GLN:HE22	1.98	0.77
2:B:107:LEU:HD11	2:B:160:ARG:CB	2.12	0.77
2:B:125:PHE:CE1	2:B:136:VAL:HG21	2.20	0.77
2:B:145:ARG:O	2:B:146:ALA:CB	2.32	0.77
1:A:288:LEU:HB2	1:A:290:LEU:HD21	1.66	0.76
2:B:321:LEU:HB3	2:B:326:VAL:CG1	2.16	0.76
2:B:516:GLU:HG3	2:B:666:LYS:HE2	1.67	0.76
1:A:223:GLU:O	1:A:224:HIS:HB2	1.85	0.76
1:A:84:ARG:CA	1:A:88:THR:OG1	2.30	0.76
1:A:272:VAL:HG13	1:A:358:LEU:CD2	2.14	0.76
1:A:342:GLU:O	1:A:346:THR:HG23	1.85	0.76
2:B:117:MET:SD	2:B:151:VAL:CG2	2.69	0.76
2:B:125:PHE:CZ	2:B:138:MET:HG3	2.15	0.76
1:A:258:ARG:NH2	1:A:364:MET:CE	2.48	0.76
1:A:288:LEU:HD23	1:A:568:PHE:CD2	2.20	0.76
1:A:752:LEU:O	1:A:753:LEU:CB	2.31	0.76
2:B:147:GLY:CA	2:B:303:PRO:HG2	2.16	0.76
1:A:546:PRO:CA	1:A:549:ARG:HE	1.98	0.75
2:B:419:SER:HB2	2:B:438:MET:SD	2.26	0.75
1:A:284:ILE:O	1:A:288:LEU:CD1	2.34	0.75
2:B:259:THR:O	2:B:281:VAL:HA	1.87	0.75
2:B:348:TRP:CE2	2:B:350:LEU:HD13	2.20	0.75
1:A:339:THR:HG21	1:A:345:GLU:HG3	1.68	0.75
1:A:121:LEU:HD21	1:A:412:ASN:HD21	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLY:O	1:A:185:GLN:N	2.20	0.75
1:A:643:PHE:CB	1:A:647:PRO:HD3	2.15	0.75
1:A:148:SER:OG	1:A:151:GLU:HB2	1.87	0.75
2:B:508:ILE:HG21	2:B:511:VAL:HB	1.67	0.74
4:A:919:UDP:O1A	4:A:919:UDP:O1B	2.05	0.74
2:B:122:ILE:CG2	2:B:140:LEU:HD22	2.17	0.74
2:B:161:ILE:HG23	2:B:162:TYR:CD2	2.22	0.74
2:B:514:ASN:CB	2:B:518:LEU:HA	2.18	0.74
1:A:658:ARG:CD	1:A:672:ILE:HD11	2.17	0.74
1:A:647:PRO:HB2	1:A:649:LEU:H	1.52	0.74
2:B:118:ASN:OD1	2:B:144:VAL:CG1	2.36	0.74
2:B:292:ALA:HA	2:B:295:VAL:HG12	1.69	0.74
1:A:317:PHE:CE2	1:A:347:ALA:HB3	2.23	0.74
1:A:658:ARG:CG	1:A:672:ILE:CD1	2.65	0.74
2:B:511:VAL:N	2:B:512:PRO:CD	2.51	0.73
2:B:122:ILE:CG2	2:B:140:LEU:CB	2.47	0.73
2:B:273:GLY:HA2	2:B:278:VAL:HA	1.69	0.73
1:A:92:PRO:HA	1:A:98:PHE:CD1	2.23	0.73
1:A:258:ARG:HE	1:A:364:MET:CE	2.01	0.73
2:B:345:PRO:HG2	2:B:348:TRP:HB3	1.70	0.73
2:B:505:LEU:HD23	2:B:523:LEU:CD2	2.16	0.73
2:B:518:LEU:HD12	2:B:519:THR:H	1.54	0.73
2:B:76:GLY:O	2:B:77:GLN:HB2	1.88	0.73
2:B:419:SER:HB3	2:B:438:MET:HE2	1.70	0.73
2:B:666:LYS:HG2	2:B:667:PRO:HD2	1.69	0.73
1:A:100:PHE:CD2	1:A:432:ILE:HD11	2.24	0.73
1:A:304:LYS:CG	1:A:470:GLN:OE1	2.37	0.73
2:B:158:ARG:O	2:B:171:LEU:HD21	1.88	0.73
2:B:344:LEU:HB3	2:B:345:PRO:CD	2.06	0.73
1:A:637:ILE:HD13	1:A:657:ILE:HG23	1.71	0.72
1:A:269:LEU:HD21	1:A:358:LEU:HD12	1.71	0.72
1:A:317:PHE:CD2	1:A:347:ALA:HB1	2.23	0.72
2:B:107:LEU:N	2:B:107:LEU:HD12	2.03	0.72
2:B:111:SER:OG	2:B:157:HIS:HA	1.89	0.72
5:A:921:LDA:H123	5:A:921:LDA:H81	1.70	0.72
2:B:373:LEU:HA	2:B:388:LEU:HG	1.70	0.72
1:A:145:LEU:HD12	1:A:145:LEU:C	2.10	0.72
2:B:223:LEU:CD1	2:B:479:LEU:HD21	2.19	0.72
1:A:13:VAL:HG12	1:A:14:VAL:H	1.55	0.72
2:B:107:LEU:CD1	2:B:107:LEU:H	2.03	0.71
2:B:383:VAL:CG2	2:B:403:PHE:HB3	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LEU:HD22	1:A:407:ARG:HH11	1.55	0.71
1:A:486:TYR:OH	1:A:524:LEU:HD12	1.89	0.71
1:A:658:ARG:HD3	1:A:672:ILE:HD11	1.71	0.71
2:B:96:LEU:CD2	2:B:137:THR:CG2	2.62	0.71
1:A:169:PRO:HB2	1:A:171:ARG:HG2	1.72	0.71
2:B:107:LEU:HD12	2:B:107:LEU:H	1.56	0.71
2:B:424:ASN:HB3	2:B:425:PRO:CD	2.12	0.71
1:A:452:MET:HE1	1:A:558:TRP:NE1	2.02	0.71
1:A:571:ARG:HD3	1:A:723:SER:HB2	1.70	0.71
1:A:675:ALA:CB	1:A:757:THR:O	2.38	0.71
2:B:514:ASN:HB2	2:B:518:LEU:HA	1.71	0.71
1:A:269:LEU:O	1:A:269:LEU:HD12	1.87	0.71
1:A:646:ALA:CB	1:A:647:PRO:CD	2.60	0.71
1:A:258:ARG:NE	1:A:364:MET:HE1	2.06	0.71
2:B:107:LEU:HD13	2:B:160:ARG:CA	2.15	0.71
1:A:84:ARG:NE	1:A:88:THR:HG21	2.06	0.70
2:B:189:ILE:HG13	2:B:190:GLY:N	2.06	0.70
2:B:122:ILE:HG22	2:B:140:LEU:CG	2.21	0.70
2:B:384:ARG:HD3	2:B:401:ILE:HG23	1.72	0.70
2:B:464:ALA:HB2	2:B:642:PRO:HB3	1.70	0.70
1:A:66:ARG:NH1	1:A:123:ALA:O	2.25	0.70
1:A:288:LEU:N	1:A:288:LEU:CD1	2.51	0.70
1:A:42:GLN:HG3	1:A:450:ALA:HB1	1.74	0.70
1:A:219:ARG:HD3	1:A:229:ASN:ND2	2.07	0.70
1:A:317:PHE:HD2	1:A:347:ALA:HB1	1.55	0.70
1:A:507:ALA:O	1:A:508:LYS:C	2.30	0.70
2:B:390:ARG:C	2:B:391:ASP:OD1	2.30	0.70
2:B:73:ARG:HD2	2:B:172:TRP:CE3	2.20	0.70
2:B:348:TRP:CZ2	2:B:350:LEU:HD13	2.27	0.70
1:A:167:ILE:HD13	1:A:253:ARG:HB2	1.73	0.70
1:A:149:TYR:HB2	1:A:179:ASP:HB3	1.74	0.70
1:A:510:GLU:HG2	1:A:512:LEU:CD1	2.21	0.70
1:A:78:MET:HE3	1:A:78:MET:HA	1.74	0.69
2:B:102:SER:HB3	2:B:172:TRP:HE1	1.56	0.69
1:A:751:HIS:ND1	1:A:752:LEU:N	2.30	0.69
2:B:613:LEU:C	2:B:614:LEU:HD12	2.13	0.69
1:A:647:PRO:CB	1:A:649:LEU:HB3	2.22	0.69
1:A:571:ARG:HH11	1:A:723:SER:CB	2.05	0.69
1:A:676:GLY:C	1:A:678:PRO:CD	2.61	0.69
2:B:508:ILE:CG2	2:B:511:VAL:HB	2.22	0.69
1:A:64:VAL:HB	1:A:65:PRO:CD	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:MET:CE	1:A:558:TRP:NE1	2.48	0.69
1:A:592:GLU:HG3	1:A:642:LYS:HE3	1.74	0.69
1:A:649:LEU:O	1:A:684:THR:CG2	2.40	0.69
2:B:616:PRO:O	2:B:617:GLU:CG	2.38	0.69
1:A:612:THR:O	1:A:673:PHE:HD1	1.75	0.69
1:A:643:PHE:HB2	1:A:647:PRO:CD	2.22	0.69
1:A:644:PRO:O	1:A:645:ASP:HB2	1.93	0.69
1:A:675:ALA:HB3	1:A:757:THR:O	1.93	0.69
1:A:676:GLY:O	1:A:678:PRO:HD2	1.92	0.69
2:B:107:LEU:CB	2:B:110:SER:CB	2.64	0.69
1:A:444:THR:OG1	1:A:447:GLU:HG2	1.92	0.69
1:A:132:ARG:N	1:A:265:GLU:OE2	2.26	0.69
1:A:172:LEU:O	1:A:172:LEU:HD12	1.93	0.69
1:A:452:MET:HE2	1:A:558:TRP:HE1	1.52	0.69
1:A:262:TYR:HE1	1:A:360:ILE:HD12	1.49	0.68
1:A:341:THR:HG22	1:A:341:THR:O	1.93	0.68
1:A:402:LEU:HG	1:A:403:GLY:H	1.57	0.68
1:A:275:PRO:HG2	1:A:363:ALA:CA	2.23	0.68
1:A:182:GLY:O	1:A:184:ASP:N	2.26	0.68
1:A:179:ASP:HB2	1:A:229:ASN:OD1	1.92	0.68
1:A:510:GLU:CG	1:A:512:LEU:HD11	2.23	0.68
1:A:631:LEU:CD1	1:A:667:VAL:HG11	2.23	0.68
2:B:511:VAL:N	2:B:512:PRO:HD2	2.08	0.68
2:B:125:PHE:CZ	2:B:138:MET:CG	2.73	0.68
2:B:116:ARG:HB2	2:B:152:THR:OG1	1.94	0.68
2:B:248:SER:HB2	2:B:250:GLU:OE2	1.94	0.68
2:B:321:LEU:HB3	2:B:326:VAL:HG12	1.75	0.68
1:A:95:ASP:O	1:A:99:LEU:HD13	1.94	0.68
1:A:186:ARG:CG	1:A:199:GLN:HG2	2.20	0.68
1:A:434:LEU:CD1	1:A:538:THR:HG23	2.08	0.68
1:A:388:MET:HG3	1:A:491:ILE:HD13	1.76	0.68
1:A:642:LYS:O	1:A:644:PRO:HD3	1.94	0.68
1:A:689:ILE:HB	1:A:690:PHE:CD2	2.29	0.68
1:A:144:ILE:CD1	1:A:163:ALA:HB1	2.23	0.67
1:A:341:THR:HG22	1:A:344:ALA:HB3	1.76	0.67
1:A:649:LEU:O	1:A:684:THR:HG22	1.95	0.67
2:B:122:ILE:HD11	2:B:143:ALA:CB	2.25	0.67
1:A:145:LEU:HD22	1:A:177:LEU:HD11	1.74	0.67
1:A:258:ARG:NE	1:A:364:MET:CE	2.58	0.67
1:A:455:TYR:OH	3:C:12:BGC:C6	2.43	0.67
2:B:351:LEU:CD1	2:B:691:SER:HB2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:PHE:CZ	1:A:306:HIS:HD2	2.12	0.67
1:A:647:PRO:CB	1:A:649:LEU:H	2.06	0.67
2:B:710:ALA:HA	2:B:713:VAL:HG12	1.76	0.67
1:A:219:ARG:NH1	1:A:223:GLU:H	1.93	0.67
1:A:596:PRO:HD3	1:A:636:LEU:O	1.95	0.67
2:B:163:CYS:O	2:B:423:GLY:CA	2.38	0.66
2:B:383:VAL:HG12	2:B:401:ILE:HG21	1.76	0.66
1:A:84:ARG:HD2	1:A:88:THR:CG2	2.24	0.66
2:B:523:LEU:CD1	2:B:523:LEU:H	2.08	0.66
2:B:108:PRO:O	2:B:109:GLU:HB2	1.95	0.66
2:B:715:PHE:O	2:B:719:THR:HG23	1.95	0.66
1:A:434:LEU:HD21	1:A:538:THR:HG22	1.78	0.66
1:A:107:VAL:HG21	1:A:425:MET:HG2	1.77	0.66
1:A:19:PHE:O	1:A:23:VAL:HG23	1.94	0.66
1:A:267:PRO:HA	1:A:325:ARG:HH22	1.61	0.66
1:A:345:GLU:HA	1:A:390:MET:HE3	1.76	0.66
2:B:122:ILE:CG2	2:B:140:LEU:CG	2.74	0.66
2:B:339:ASP:HB3	2:B:414:ARG:HE	1.61	0.66
2:B:345:PRO:HG2	2:B:346:ASP:H	1.60	0.66
2:B:398:ARG:HH21	2:B:445:ASP:CG	2.00	0.66
1:A:317:PHE:CD2	1:A:347:ALA:HB2	2.18	0.66
1:A:452:MET:HB3	1:A:453:PRO:HD3	1.78	0.66
1:A:624:VAL:O	1:A:627:PRO:HD2	1.95	0.66
2:B:168:GLU:OE2	2:B:334:ARG:HG3	1.96	0.66
2:B:352:ALA:HB3	2:B:354:GLN:OE1	1.96	0.66
1:A:434:LEU:HD11	1:A:538:THR:CG2	2.23	0.65
2:B:377:LYS:HG2	2:B:382:THR:HG22	0.66	0.65
1:A:35:ALA:O	1:A:79:ARG:NH2	2.29	0.65
1:A:460:PHE:HB3	1:A:709:LEU:HD21	1.78	0.65
1:A:511:THR:HB	1:A:580:ARG:HH12	1.59	0.65
1:A:592:GLU:OE2	1:A:642:LYS:CE	2.44	0.65
1:A:628:HIS:HB2	1:A:629:PRO:HD3	1.77	0.65
1:A:169:PRO:C	1:A:171:ARG:H	2.00	0.65
1:A:751:HIS:ND1	1:A:752:LEU:O	2.29	0.65
1:A:301:PHE:CZ	1:A:306:HIS:CD2	2.85	0.65
1:A:513:SER:O	1:A:514:GLU:HB2	1.96	0.65
2:B:65:THR:OG1	2:B:67:GLN:HG3	1.97	0.65
1:A:506:THR:O	1:A:507:ALA:CB	2.45	0.65
1:A:580:ARG:HE	1:A:752:LEU:HD21	1.62	0.65
2:B:379:ASN:ND2	2:B:413:ASN:HD22	1.88	0.65
2:B:126:THR:H	2:B:127:PRO:HD3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:PRO:O	2:B:346:ASP:HB3	1.95	0.65
1:A:662:ARG:HH12	1:A:664:GLY:HA2	1.60	0.64
2:B:342:PHE:HE2	2:B:344:LEU:HD21	1.61	0.64
1:A:31:LEU:HD11	2:B:682:VAL:HG11	1.79	0.64
1:A:304:LYS:HG2	1:A:470:GLN:OE1	1.97	0.64
1:A:429:ALA:HB3	1:A:430:PRO:HD3	1.79	0.64
2:B:213:ARG:HG2	2:B:244:SER:HB2	1.80	0.64
2:B:373:LEU:HD12	2:B:375:LEU:CD1	2.27	0.64
2:B:709:ALA:O	2:B:713:VAL:HG12	1.97	0.64
1:A:442:VAL:CG2	1:A:442:VAL:O	2.44	0.64
1:A:674:GLU:O	1:A:675:ALA:HB3	1.97	0.64
1:A:549:ARG:O	1:A:553:LEU:HD13	1.97	0.64
2:B:122:ILE:HG21	2:B:140:LEU:HB3	0.77	0.64
1:A:201:ARG:O	1:A:205:LEU:HD23	1.97	0.64
1:A:428:VAL:HA	1:A:431:LEU:HD12	1.80	0.64
2:B:161:ILE:HA	2:B:429:PRO:HG3	1.79	0.64
2:B:381:THR:HG22	2:B:561:VAL:HG13	1.78	0.64
2:B:389:ASP:OD1	2:B:390:ARG:HG3	1.98	0.64
2:B:452:PRO:HB3	2:B:681:ASN:OD1	1.97	0.64
2:B:531:THR:HG23	2:B:608:LYS:HE2	1.80	0.64
1:A:498:PRO:O	1:A:499:ARG:HB2	1.97	0.64
1:A:269:LEU:CD2	1:A:358:LEU:HD12	2.28	0.64
2:B:122:ILE:HD11	2:B:143:ALA:HB2	1.80	0.63
1:A:352:SER:O	1:A:401:GLY:HA3	1.98	0.63
1:A:542:TRP:HZ3	1:A:553:LEU:HD12	1.61	0.63
1:A:682:ARG:HG2	1:A:755:PHE:CE2	2.34	0.63
2:B:419:SER:CB	2:B:438:MET:HE1	2.21	0.63
1:A:658:ARG:HG3	1:A:672:ILE:HG13	1.79	0.63
2:B:98:LEU:HD11	2:B:179:GLN:CB	2.28	0.63
2:B:379:ASN:HD21	2:B:413:ASN:ND2	1.91	0.63
2:B:627:PRO:O	2:B:628:GLU:HB2	1.98	0.63
3:C:10:BGC:O3	3:C:11:BGC:O5	2.15	0.63
2:B:95:THR:CG2	2:B:96:LEU:N	2.61	0.63
3:C:11:BGC:O3	3:C:12:BGC:O5	2.12	0.63
1:A:31:LEU:HD12	5:A:921:LDA:H91	1.80	0.63
1:A:272:VAL:CG1	1:A:358:LEU:HD21	2.25	0.63
2:B:346:ASP:HA	2:B:410:PRO:HB2	1.81	0.63
2:B:649:ARG:O	2:B:663:SER:HB3	1.99	0.63
1:A:751:HIS:CG	1:A:752:LEU:H	2.15	0.63
2:B:106:ILE:HG13	2:B:160:ARG:HE	1.64	0.63
2:B:523:LEU:HD22	2:B:524:ALA:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:PRO:C	1:A:399:ARG:HG3	2.20	0.63
1:A:640:GLN:HB3	1:A:652:MET:HA	1.80	0.63
2:B:321:LEU:CA	2:B:324:MET:HG3	2.25	0.63
1:A:169:PRO:O	1:A:171:ARG:N	2.26	0.62
1:A:658:ARG:HG3	1:A:672:ILE:CD1	2.29	0.62
2:B:101:ARG:HG2	2:B:173:THR:CG2	2.26	0.62
1:A:644:PRO:C	1:A:646:ALA:H	2.01	0.62
2:B:710:ALA:HA	2:B:713:VAL:CG1	2.29	0.62
1:A:184:ASP:OD1	1:A:188:MET:HG2	2.00	0.62
2:B:614:LEU:HD12	2:B:614:LEU:N	2.14	0.62
1:A:121:LEU:CD2	1:A:412:ASN:ND2	2.58	0.62
1:A:373:PHE:CE1	1:A:377:ILE:HD11	2.34	0.62
2:B:107:LEU:CD1	2:B:160:ARG:HB2	2.29	0.62
2:B:63:ALA:HB3	2:B:67:GLN:NE2	2.08	0.62
2:B:163:CYS:HB2	2:B:430:CYS:H	1.64	0.62
2:B:126:THR:H	2:B:127:PRO:CD	2.12	0.62
2:B:666:LYS:HB3	2:B:669:LEU:HG	1.80	0.62
2:B:96:LEU:HD11	2:B:98:LEU:HD21	1.81	0.62
2:B:98:LEU:HD12	2:B:176:ASP:HB3	1.81	0.62
1:A:270:PHE:HD2	1:A:356:LYS:O	1.82	0.62
1:A:546:PRO:HB3	1:A:549:ARG:HH21	1.64	0.62
1:A:649:LEU:HG	1:A:649:LEU:O	1.99	0.62
1:A:255:PHE:HA	1:A:364:MET:HE3	1.81	0.62
1:A:358:LEU:CD1	1:A:358:LEU:N	2.59	0.62
2:B:334:ARG:NH1	2:B:430:CYS:HB3	2.14	0.62
1:A:549:ARG:O	1:A:553:LEU:CD1	2.48	0.61
2:B:126:THR:N	2:B:127:PRO:CD	2.63	0.61
1:A:542:TRP:HA	1:A:552:LEU:CD1	2.30	0.61
1:A:571:ARG:HH11	1:A:723:SER:HB2	1.65	0.61
2:B:505:LEU:HD23	2:B:523:LEU:HD23	1.82	0.61
2:B:616:PRO:C	2:B:617:GLU:CG	2.59	0.61
1:A:644:PRO:C	1:A:646:ALA:N	2.52	0.61
2:B:615:ALA:HB2	2:B:621:LEU:CD2	2.29	0.61
1:A:312:TRP:HB3	1:A:405:ALA:HB1	1.82	0.61
2:B:566:VAL:HG13	3:C:5:BGC:O6	1.99	0.61
2:B:98:LEU:HD11	2:B:179:GLN:C	2.21	0.61
2:B:398:ARG:HH22	2:B:445:ASP:CG	2.04	0.61
2:B:211:GLU:OE1	2:B:250:GLU:HG3	2.00	0.61
2:B:266:ASP:CA	2:B:285:PRO:HD3	2.31	0.61
2:B:566:VAL:HG12	2:B:568:SER:H	1.66	0.61
1:A:288:LEU:CB	1:A:290:LEU:HD21	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:THR:CG2	1:A:344:ALA:HB3	2.31	0.61
2:B:360:ILE:CD1	2:B:401:ILE:CD1	2.78	0.61
2:B:97:THR:HB	2:B:136:VAL:CG1	2.30	0.61
2:B:398:ARG:HH22	2:B:445:ASP:H	1.47	0.61
1:A:270:PHE:CD2	1:A:271:LEU:N	2.69	0.60
2:B:59:LEU:HD13	2:B:83:PHE:CG	2.36	0.60
2:B:115:VAL:HG23	2:B:153:ILE:HG12	1.83	0.60
2:B:344:LEU:CB	2:B:345:PRO:CD	2.70	0.60
1:A:144:ILE:CG2	1:A:243:VAL:HB	2.20	0.60
1:A:183:THR:HA	1:A:202:ARG:HH12	1.65	0.60
2:B:96:LEU:HD22	2:B:137:THR:HG22	1.79	0.60
2:B:358:ILE:HG13	2:B:403:PHE:HE2	1.64	0.60
1:A:361:ASP:OD1	1:A:700:ARG:NH1	2.35	0.60
1:A:709:LEU:HD13	1:A:709:LEU:C	2.21	0.60
2:B:481:ARG:NH1	2:B:504:GLY:CA	2.64	0.60
2:B:321:LEU:HD23	2:B:324:MET:CG	2.16	0.60
2:B:441:LEU:O	2:B:444:THR:HG23	2.01	0.60
2:B:349:LEU:HD22	2:B:456:MET:HG2	1.82	0.60
2:B:505:LEU:CD1	2:B:528:LEU:HD13	2.31	0.60
1:A:272:VAL:HA	1:A:358:LEU:CD1	2.32	0.60
1:A:275:PRO:CD	1:A:363:ALA:H	2.15	0.60
1:A:396:PRO:O	1:A:399:ARG:HG3	2.02	0.60
2:B:351:LEU:HD12	2:B:691:SER:HB2	1.83	0.60
2:B:612:MET:HG2	2:B:614:LEU:HD11	1.82	0.60
1:A:272:VAL:HA	1:A:358:LEU:HD13	1.83	0.60
1:A:275:PRO:CG	1:A:363:ALA:H	2.15	0.60
1:A:329:LEU:O	1:A:332:ALA:HB3	2.01	0.60
1:A:399:ARG:CZ	1:A:410:TYR:HB2	2.30	0.60
1:A:445:PHE:CE2	1:A:449:LEU:HD11	2.36	0.60
1:A:507:ALA:HB3	1:A:509:ASP:OD1	2.02	0.60
2:B:73:ARG:HD3	2:B:172:TRP:CZ3	2.36	0.60
2:B:117:MET:N	2:B:120:GLN:O	2.30	0.60
1:A:487:LEU:HD12	1:A:487:LEU:N	2.16	0.60
2:B:144:VAL:C	2:B:145:ARG:CG	2.70	0.60
1:A:329:LEU:HD12	1:A:330:ASP:N	2.17	0.59
1:A:599:GLY:O	1:A:600:ASN:CB	2.45	0.59
2:B:96:LEU:C	2:B:96:LEU:HD13	2.22	0.59
2:B:344:LEU:HB2	2:B:410:PRO:HA	1.84	0.59
1:A:183:THR:O	1:A:187:CYS:N	2.19	0.59
1:A:647:PRO:HB2	1:A:649:LEU:CB	2.31	0.59
2:B:383:VAL:HG22	2:B:403:PHE:HB3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:694:PRO:N	2:B:695:PRO:HD2	2.17	0.59
1:A:595:ILE:CG2	1:A:596:PRO:CD	2.71	0.59
1:A:262:TYR:CZ	1:A:360:ILE:CD1	2.69	0.59
1:A:321:ALA:HB2	1:A:365:ILE:HD13	1.83	0.59
2:B:510:THR:C	2:B:512:PRO:HD2	2.23	0.59
2:B:523:LEU:HD13	2:B:523:LEU:N	2.17	0.59
1:A:63:MET:HE3	1:A:67:PHE:CZ	2.38	0.59
2:B:122:ILE:HG22	2:B:140:LEU:HD22	1.85	0.59
2:B:315:PRO:HB3	2:B:450:PRO:HA	1.84	0.59
2:B:419:SER:CB	2:B:438:MET:SD	2.90	0.59
1:A:442:VAL:O	1:A:442:VAL:HG23	2.00	0.59
2:B:107:LEU:CD1	2:B:107:LEU:N	2.65	0.59
2:B:583:GLN:HB3	2:B:584:PRO:HD3	1.84	0.59
1:A:589:VAL:HB	1:A:607:VAL:HG22	1.85	0.59
2:B:350:LEU:HD12	2:B:350:LEU:N	2.14	0.59
2:B:459:MET:HE3	2:B:653:ALA:HB2	1.85	0.59
2:B:500:LEU:HA	2:B:621:LEU:O	2.03	0.59
1:A:270:PHE:CG	1:A:271:LEU:N	2.71	0.59
1:A:513:SER:O	1:A:514:GLU:CB	2.51	0.59
2:B:458:ASP:OD1	2:B:461:ARG:NH1	2.36	0.59
2:B:483:LEU:HB2	2:B:484:PRO:HD3	1.84	0.59
1:A:132:ARG:CB	1:A:265:GLU:OE2	2.51	0.58
1:A:662:ARG:NH1	1:A:664:GLY:HA2	2.18	0.58
2:B:165:ALA:HB1	2:B:335:TYR:HB2	1.84	0.58
2:B:393:ALA:HB3	2:B:396:LYS:HG2	1.85	0.58
2:B:569:ASN:OD1	2:B:572:ASP:HB2	2.03	0.58
1:A:21:LEU:HB3	2:B:711:ILE:HD13	1.85	0.58
1:A:75:MET:O	1:A:79:ARG:HG3	2.02	0.58
1:A:121:LEU:HD21	1:A:412:ASN:ND2	2.18	0.58
1:A:177:LEU:N	1:A:177:LEU:HD23	2.18	0.58
1:A:486:TYR:OH	1:A:524:LEU:CD1	2.51	0.58
1:A:647:PRO:HD2	1:A:647:PRO:O	2.03	0.58
2:B:341:ASP:OD2	2:B:645:PRO:CG	2.50	0.58
2:B:501:THR:HG22	2:B:622:TRP:CD1	2.39	0.58
2:B:528:LEU:CB	2:B:529:PRO:CD	2.78	0.58
2:B:615:ALA:CA	2:B:621:LEU:HG	2.33	0.58
1:A:486:TYR:CE1	1:A:523:PRO:HG2	2.39	0.58
2:B:95:THR:HG22	2:B:96:LEU:H	1.68	0.58
2:B:373:LEU:CD1	2:B:375:LEU:HD11	2.34	0.58
2:B:505:LEU:CD2	2:B:523:LEU:HD23	2.31	0.58
1:A:682:ARG:HG2	1:A:755:PHE:HE2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:HD2	1:A:199:GLN:HE21	1.69	0.58
1:A:317:PHE:CE1	1:A:319:GLY:HA2	2.38	0.58
1:A:345:GLU:HA	1:A:390:MET:CE	2.33	0.58
1:A:577:GLN:O	1:A:577:GLN:HG2	2.04	0.58
2:B:246:PRO:O	2:B:247:TRP:HB2	2.03	0.58
2:B:459:MET:HE3	2:B:653:ALA:CB	2.33	0.58
1:A:251:PRO:HA	1:A:365:ILE:HG22	1.84	0.58
2:B:211:GLU:CD	2:B:250:GLU:HG3	2.24	0.58
1:A:23:VAL:O	1:A:26:LEU:HB2	2.03	0.58
2:B:409:HIS:HB3	2:B:410:PRO:HD2	1.85	0.58
1:A:92:PRO:HA	1:A:98:PHE:CE1	2.37	0.58
1:A:722:ALA:O	1:A:725:PRO:HD2	2.03	0.58
1:A:172:LEU:HD12	1:A:172:LEU:C	2.24	0.57
1:A:663:GLU:O	1:A:664:GLY:C	2.40	0.57
1:A:503:PHE:O	1:A:503:PHE:CG	2.57	0.57
2:B:310:LEU:HD12	2:B:310:LEU:N	2.19	0.57
2:B:321:LEU:HD12	2:B:442:SER:CA	2.31	0.57
2:B:383:VAL:CG1	2:B:383:VAL:O	2.51	0.57
1:A:271:LEU:CD2	1:A:317:PHE:HB3	2.35	0.57
1:A:317:PHE:HE1	1:A:319:GLY:HA2	1.69	0.57
2:B:373:LEU:CD1	2:B:375:LEU:CD1	2.82	0.57
2:B:673:LEU:CD1	2:B:675:GLU:O	2.46	0.57
2:B:88:PRO:HD3	2:B:198:ALA:CB	2.35	0.57
2:B:383:VAL:CG2	2:B:403:PHE:CB	2.82	0.57
1:A:434:LEU:CD1	1:A:538:THR:HG22	2.31	0.57
2:B:562:MET:HB2	2:B:563:PRO:HD2	1.86	0.57
1:A:78:MET:HA	1:A:78:MET:CE	2.35	0.57
1:A:198:ALA:O	1:A:202:ARG:HG3	2.04	0.57
1:A:487:LEU:N	1:A:487:LEU:CD1	2.68	0.57
2:B:98:LEU:HD11	2:B:179:GLN:O	2.04	0.57
2:B:101:ARG:NH2	2:B:157:HIS:HB3	2.19	0.57
2:B:326:VAL:HG22	2:B:327:ASP:O	2.04	0.57
2:B:360:ILE:HD11	2:B:376:VAL:HG21	1.87	0.57
2:B:361:ASP:OD2	2:B:398:ARG:NH1	2.30	0.57
2:B:87:LEU:HD12	2:B:88:PRO:O	2.05	0.57
1:A:399:ARG:HH11	1:A:407:ARG:HA	1.63	0.57
2:B:320:THR:O	2:B:442:SER:O	2.23	0.57
2:B:693:ARG:CD	2:B:696:LEU:HD23	2.24	0.57
1:A:445:PHE:O	1:A:449:LEU:HD13	2.05	0.57
1:A:452:MET:HE2	1:A:558:TRP:NE1	2.16	0.57
1:A:542:TRP:HA	1:A:552:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:GLU:CG	1:A:642:LYS:HE3	2.35	0.57
2:B:456:MET:SD	2:B:671:PRO:CB	2.84	0.57
1:A:339:THR:CG2	1:A:345:GLU:CG	2.74	0.56
1:A:399:ARG:NH2	1:A:410:TYR:HB3	2.17	0.56
2:B:521:ARG:O	2:B:524:ALA:HB3	2.06	0.56
2:B:522:LEU:HA	2:B:525:LEU:HD13	1.86	0.56
1:A:121:LEU:HD22	1:A:412:ASN:HD21	1.69	0.56
1:A:249:HIS:HD2	1:A:320:SER:OG	1.87	0.56
1:A:271:LEU:O	1:A:358:LEU:CD1	2.53	0.56
2:B:104:ILE:HG22	2:B:159:HIS:CE1	2.39	0.56
2:B:141:GLY:O	2:B:142:GLU:HB2	2.06	0.56
2:B:320:THR:O	2:B:321:LEU:HB2	2.06	0.56
2:B:351:LEU:CD1	2:B:691:SER:CB	2.83	0.56
2:B:383:VAL:CG1	2:B:401:ILE:HG21	2.35	0.56
2:B:501:THR:CG2	2:B:622:TRP:CD2	2.88	0.56
1:A:143:ASP:OD1	1:A:173:ARG:HD2	2.05	0.56
1:A:151:GLU:HG2	1:A:247:ALA:HB3	1.87	0.56
2:B:95:THR:CG2	2:B:96:LEU:H	2.18	0.56
2:B:118:ASN:CB	2:B:144:VAL:HG11	2.32	0.56
1:A:402:LEU:CG	1:A:403:GLY:N	2.68	0.56
1:A:651:ARG:HG2	1:A:684:THR:HG21	1.86	0.56
2:B:360:ILE:HD11	2:B:401:ILE:CD1	2.35	0.56
1:A:219:ARG:HD2	1:A:229:ASN:HA	1.87	0.56
2:B:105:ASP:O	2:B:105:ASP:OD2	2.24	0.56
2:B:459:MET:HG3	2:B:621:LEU:CD2	2.35	0.56
2:B:466:VAL:HG23	2:B:470:SER:OG	2.04	0.56
1:A:144:ILE:O	1:A:144:ILE:CG1	2.52	0.56
1:A:271:LEU:HD11	1:A:317:PHE:CD2	2.40	0.56
1:A:676:GLY:O	1:A:678:PRO:CD	2.53	0.56
1:A:304:LYS:HG3	1:A:470:GLN:OE1	2.05	0.56
2:B:59:LEU:HD13	2:B:83:PHE:HB3	1.87	0.56
2:B:122:ILE:CG2	2:B:140:LEU:CD2	2.84	0.56
1:A:510:GLU:HG2	1:A:510:GLU:O	2.05	0.56
2:B:381:THR:OG1	2:B:407:LEU:HD13	2.05	0.56
1:A:84:ARG:HD3	1:A:441:PHE:CE1	2.40	0.56
1:A:258:ARG:CZ	1:A:364:MET:CE	2.84	0.56
1:A:84:ARG:HD3	1:A:441:PHE:CZ	2.40	0.55
1:A:605:ALA:HB1	1:A:617:LEU:HD21	1.88	0.55
2:B:383:VAL:HG21	2:B:403:PHE:CB	2.36	0.55
2:B:409:HIS:O	2:B:413:ASN:OD1	2.25	0.55
1:A:424:MET:O	1:A:428:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:ARG:HA	2:B:244:SER:O	2.06	0.55
2:B:320:THR:O	2:B:321:LEU:CB	2.55	0.55
2:B:349:LEU:O	2:B:350:LEU:HD12	2.06	0.55
2:B:481:ARG:HH12	2:B:504:GLY:CA	2.19	0.55
1:A:402:LEU:HG	1:A:403:GLY:N	2.21	0.55
1:A:628:HIS:CB	1:A:629:PRO:HD3	2.35	0.55
2:B:526:THR:O	2:B:608:LYS:HA	2.06	0.55
1:A:360:ILE:HG22	1:A:361:ASP:N	2.21	0.55
1:A:117:LEU:HG	1:A:412:ASN:HD22	1.71	0.55
1:A:498:PRO:O	1:A:499:ARG:CB	2.54	0.55
1:A:658:ARG:HG3	1:A:672:ILE:CG1	2.36	0.55
1:A:339:THR:O	1:A:342:GLU:HG2	2.05	0.55
1:A:677:GLN:N	1:A:678:PRO:HD3	2.21	0.55
2:B:264:ASP:OD1	2:B:264:ASP:N	2.40	0.55
1:A:184:ASP:HB2	1:A:221:ARG:HA	1.87	0.55
1:A:364:MET:O	1:A:365:ILE:HG22	2.03	0.55
1:A:473:PRO:O	1:A:716:ILE:CD1	2.50	0.55
1:A:571:ARG:HH11	1:A:723:SER:HB3	1.70	0.55
1:A:612:THR:CB	1:A:753:LEU:HA	2.37	0.55
2:B:104:ILE:HG22	2:B:159:HIS:NE2	2.21	0.55
2:B:115:VAL:O	2:B:115:VAL:HG13	2.07	0.55
2:B:105:ASP:O	2:B:105:ASP:CG	2.45	0.55
2:B:505:LEU:HD13	2:B:528:LEU:HD13	1.87	0.55
2:B:693:ARG:HD3	2:B:696:LEU:CD2	2.25	0.55
1:A:14:VAL:HG13	1:A:15:PRO:CD	2.20	0.55
1:A:93:ALA:C	1:A:95:ASP:H	2.08	0.55
1:A:100:PHE:CG	1:A:432:ILE:CD1	2.89	0.55
2:B:391:ASP:O	2:B:396:LYS:HE2	2.07	0.55
2:B:505:LEU:CD2	2:B:523:LEU:HD21	2.34	0.55
1:A:444:THR:HG23	1:A:447:GLU:OE1	2.07	0.54
2:B:501:THR:HG22	2:B:622:TRP:CG	2.42	0.54
1:A:258:ARG:HE	1:A:364:MET:HE1	1.67	0.54
1:A:715:ARG:HG2	1:A:719:MET:HE3	1.88	0.54
1:A:166:MET:HE2	1:A:251:PRO:HB2	1.89	0.54
1:A:139:LEU:HD22	1:A:168:TYR:HE1	1.72	0.54
1:A:255:PHE:HA	1:A:364:MET:SD	2.47	0.54
1:A:394:LYS:O	1:A:395:ASN:C	2.44	0.54
2:B:364:PHE:HE1	2:B:391:ASP:C	2.10	0.54
2:B:122:ILE:HG22	2:B:140:LEU:CD2	2.37	0.54
2:B:350:LEU:CD1	2:B:350:LEU:N	2.71	0.54
2:B:377:LYS:HD3	2:B:382:THR:HG21	1.84	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:TRP:HB2	2:B:711:ILE:HG21	1.89	0.54
2:B:514:ASN:HB3	2:B:518:LEU:HA	1.90	0.54
1:A:339:THR:HG21	1:A:345:GLU:CG	2.38	0.54
1:A:346:THR:O	1:A:350:ILE:HG13	2.08	0.54
1:A:402:LEU:CG	1:A:403:GLY:H	2.17	0.54
1:A:485:PRO:HG2	1:A:524:LEU:HB3	1.89	0.54
2:B:518:LEU:HD12	2:B:519:THR:N	2.20	0.54
2:B:521:ARG:O	2:B:525:LEU:HD12	2.08	0.54
1:A:421:LEU:HD13	1:A:491:ILE:HG21	1.90	0.54
1:A:423:ARG:NH1	1:A:480:GLU:OE1	2.41	0.54
2:B:292:ALA:O	2:B:294:LEU:N	2.41	0.54
2:B:345:PRO:HG2	2:B:346:ASP:N	2.23	0.54
1:A:658:ARG:HD3	1:A:672:ILE:CD1	2.37	0.54
2:B:523:LEU:CD1	2:B:523:LEU:N	2.69	0.54
2:B:586:ILE:HG22	2:B:586:ILE:O	2.07	0.54
2:B:107:LEU:HD11	2:B:160:ARG:HG3	1.90	0.54
1:A:258:ARG:CZ	1:A:364:MET:HE2	2.33	0.53
1:A:273:GLN:OE1	1:A:318:CYS:N	2.38	0.53
1:A:524:LEU:CA	1:A:527:THR:HG22	2.36	0.53
2:B:347:ASP:C	2:B:347:ASP:OD1	2.47	0.53
1:A:37:VAL:CG1	1:A:38:ALA:N	2.70	0.53
1:A:318:CYS:HB3	3:C:17:BGC:H5	1.89	0.53
1:A:434:LEU:HD11	1:A:538:THR:HG21	1.90	0.53
1:A:609:ASP:O	1:A:615:VAL:HG22	2.08	0.53
2:B:103:SER:O	2:B:104:ILE:HB	2.08	0.53
2:B:262:PRO:HA	2:B:284:HIS:O	2.08	0.53
1:A:292:ASP:OD1	1:A:293:ARG:N	2.42	0.53
2:B:145:ARG:HA	2:B:149:ASN:HD21	1.74	0.53
2:B:345:PRO:O	2:B:346:ASP:HB2	2.09	0.53
1:A:419:PHE:CD2	1:A:420:PRO:HD3	2.43	0.53
2:B:373:LEU:HD12	2:B:375:LEU:HD11	1.90	0.53
2:B:481:ARG:HH12	2:B:504:GLY:HA2	1.73	0.53
1:A:188:MET:O	1:A:189:SER:C	2.44	0.53
1:A:269:LEU:HD21	1:A:358:LEU:CD1	2.39	0.53
1:A:474:LEU:HA	1:A:477:GLU:OE1	2.09	0.53
2:B:321:LEU:CA	2:B:324:MET:HG2	2.28	0.53
2:B:391:ASP:HB2	2:B:396:LYS:NZ	2.23	0.53
1:A:139:LEU:HD22	1:A:168:TYR:CE1	2.44	0.53
1:A:649:LEU:O	1:A:684:THR:HG21	2.08	0.53
2:B:345:PRO:HG2	2:B:348:TRP:CB	2.38	0.53
2:B:383:VAL:CG1	2:B:401:ILE:CG2	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:615:ALA:HB1	2:B:621:LEU:HG	1.84	0.53
1:A:271:LEU:HD21	1:A:317:PHE:HB3	1.90	0.53
1:A:330:ASP:O	1:A:333:GLY:N	2.41	0.53
2:B:318:VAL:HG23	2:B:445:ASP:HB3	1.91	0.53
2:B:523:LEU:O	2:B:527:LEU:HG	2.09	0.53
1:A:108:GLU:O	1:A:112:ILE:HG13	2.08	0.53
1:A:647:PRO:HB2	1:A:649:LEU:N	2.20	0.53
1:A:103:LEU:HD22	1:A:425:MET:HE3	1.91	0.53
1:A:271:LEU:HD21	1:A:317:PHE:CB	2.39	0.53
5:A:920:LDA:HM23	2:B:708:SER:CB	2.38	0.53
2:B:189:ILE:HG13	2:B:190:GLY:H	1.73	0.53
2:B:346:ASP:O	2:B:346:ASP:CG	2.45	0.53
2:B:615:ALA:HB1	2:B:621:LEU:CD1	2.39	0.53
1:A:149:TYR:HD1	1:A:179:ASP:O	1.92	0.52
1:A:288:LEU:HD23	1:A:568:PHE:CE2	2.43	0.52
1:A:417:TRP:O	1:A:491:ILE:HD12	2.09	0.52
2:B:107:LEU:HD11	2:B:160:ARG:CG	2.39	0.52
2:B:380:GLY:HA3	2:B:561:VAL:HG21	1.91	0.52
2:B:505:LEU:HD21	2:B:523:LEU:CD2	2.35	0.52
2:B:710:ALA:CA	2:B:713:VAL:HG12	2.39	0.52
3:C:9:BGC:O3	3:C:10:BGC:O5	2.26	0.52
2:B:59:LEU:O	2:B:59:LEU:HD12	2.10	0.52
2:B:103:SER:C	2:B:104:ILE:HG13	2.29	0.52
2:B:478:GLY:O	2:B:481:ARG:HG2	2.09	0.52
1:A:120:PHE:O	1:A:123:ALA:HB3	2.10	0.52
2:B:197:ILE:HD11	2:B:299:LEU:HD22	1.92	0.52
1:A:689:ILE:HB	1:A:690:PHE:CE2	2.45	0.52
2:B:516:GLU:HG3	2:B:666:LYS:CE	2.37	0.52
1:A:131:PRO:HB2	1:A:265:GLU:OE2	2.10	0.52
1:A:358:LEU:O	1:A:358:LEU:HD22	2.09	0.52
1:A:612:THR:OG1	1:A:753:LEU:CA	2.53	0.52
2:B:206:SER:HB2	2:B:208:ARG:HH11	1.73	0.52
1:A:77:VAL:HG22	1:A:78:MET:N	2.25	0.52
1:A:84:ARG:HA	1:A:88:THR:HG1	1.71	0.52
2:B:96:LEU:CD1	2:B:98:LEU:HD21	2.40	0.52
2:B:254:THR:O	2:B:277:ALA:HB3	2.09	0.52
1:A:130:PHE:O	1:A:131:PRO:C	2.46	0.52
1:A:340:ILE:HD11	1:A:501:ALA:HB1	1.87	0.52
1:A:360:ILE:CG2	1:A:361:ASP:N	2.72	0.52
2:B:97:THR:HG22	2:B:98:LEU:N	2.24	0.52
2:B:713:VAL:O	2:B:717:LEU:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:PHE:CD2	1:A:432:ILE:CD1	2.92	0.52
1:A:626:ASP:H	1:A:627:PRO:HD2	1.75	0.52
2:B:625:LEU:HD12	2:B:625:LEU:N	2.24	0.52
1:A:542:TRP:CZ3	1:A:549:ARG:HB3	2.45	0.52
1:A:661:ARG:C	1:A:667:VAL:HG23	2.30	0.52
2:B:292:ALA:O	2:B:293:SER:C	2.48	0.52
2:B:351:LEU:HD12	2:B:691:SER:CB	2.39	0.52
2:B:553:LEU:O	2:B:555:ALA:N	2.42	0.52
1:A:77:VAL:CG2	1:A:78:MET:N	2.72	0.51
1:A:517:ILE:HB	1:A:734:GLU:HG3	1.92	0.51
2:B:163:CYS:HB2	2:B:430:CYS:N	2.24	0.51
2:B:505:LEU:HD23	2:B:523:LEU:HD21	1.90	0.51
1:A:42:GLN:OE1	1:A:79:ARG:NH1	2.43	0.51
1:A:373:PHE:O	1:A:377:ILE:HG13	2.10	0.51
1:A:525:LEU:O	1:A:529:LEU:HG	2.10	0.51
2:B:383:VAL:HG21	2:B:403:PHE:HB3	1.93	0.51
1:A:141:THR:HB	1:A:240:GLU:CG	2.37	0.51
1:A:685:VAL:O	1:A:689:ILE:HG13	2.10	0.51
2:B:138:MET:SD	2:B:140:LEU:HD12	2.51	0.51
2:B:506:HIS:O	2:B:507:ASP:C	2.47	0.51
2:B:614:LEU:N	2:B:614:LEU:CD1	2.72	0.51
1:A:63:MET:HE3	1:A:67:PHE:CE2	2.45	0.51
2:B:362:TYR:HA	2:B:439:GLN:O	2.10	0.51
1:A:121:LEU:HD22	1:A:412:ASN:ND2	2.25	0.51
1:A:524:LEU:CD1	1:A:524:LEU:H	2.23	0.51
2:B:313:ILE:HG12	2:B:319:VAL:HG11	1.92	0.51
1:A:167:ILE:O	1:A:167:ILE:HG22	2.10	0.51
1:A:275:PRO:HG2	1:A:363:ALA:N	2.25	0.51
1:A:358:LEU:HD22	1:A:358:LEU:C	2.30	0.51
1:A:512:LEU:HD12	1:A:512:LEU:N	2.26	0.51
1:A:542:TRP:NE1	1:A:549:ARG:NH1	2.58	0.51
2:B:59:LEU:HD13	2:B:83:PHE:CB	2.41	0.51
1:A:121:LEU:HD12	1:A:121:LEU:N	2.26	0.51
1:A:546:PRO:O	1:A:549:ARG:HG3	2.11	0.51
2:B:391:ASP:O	2:B:392:ALA:C	2.46	0.51
1:A:45:ILE:HG23	1:A:75:MET:HE3	1.92	0.51
1:A:174:THR:HG23	1:A:214:VAL:HB	1.92	0.51
1:A:184:ASP:OD1	1:A:188:MET:CG	2.59	0.51
1:A:219:ARG:HD3	1:A:229:ASN:HD22	1.76	0.51
1:A:271:LEU:CD1	1:A:317:PHE:CD2	2.94	0.51
2:B:261:LEU:O	2:B:283:GLU:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:375:LEU:N	2:B:375:LEU:CD1	2.71	0.51
2:B:459:MET:CE	2:B:653:ALA:HB2	2.40	0.51
1:A:445:PHE:O	1:A:448:VAL:HG22	2.10	0.51
1:A:647:PRO:CD	1:A:647:PRO:O	2.59	0.51
1:A:166:MET:CE	1:A:251:PRO:CB	2.89	0.51
2:B:330:LEU:HD23	2:B:439:GLN:HA	1.92	0.51
2:B:345:PRO:CG	2:B:348:TRP:CB	2.89	0.51
2:B:464:ALA:CB	2:B:642:PRO:HB3	2.40	0.51
1:A:338:GLU:OE2	1:A:499:ARG:NH2	2.42	0.50
1:A:419:PHE:CG	1:A:420:PRO:HD3	2.46	0.50
1:A:134:LEU:HD11	1:A:261:GLY:HA2	1.94	0.50
1:A:147:PRO:HD2	1:A:245:PHE:O	2.11	0.50
1:A:156:LEU:O	1:A:160:LEU:HG	2.11	0.50
1:A:255:PHE:HA	1:A:364:MET:CE	2.40	0.50
1:A:271:LEU:HG	1:A:324:LEU:CD2	2.42	0.50
1:A:340:ILE:HG22	1:A:341:THR:H	1.77	0.50
2:B:101:ARG:NE	2:B:173:THR:OG1	2.43	0.50
2:B:292:ALA:C	2:B:294:LEU:N	2.63	0.50
2:B:310:LEU:HD12	2:B:310:LEU:H	1.75	0.50
1:A:63:MET:CE	1:A:67:PHE:CE2	2.94	0.50
1:A:275:PRO:HG2	1:A:363:ALA:HA	1.91	0.50
1:A:412:ASN:HA	1:A:415:SER:OG	2.10	0.50
1:A:612:THR:CG2	1:A:753:LEU:HA	2.41	0.50
1:A:647:PRO:CB	1:A:649:LEU:CB	2.88	0.50
1:A:651:ARG:CG	1:A:684:THR:HG21	2.42	0.50
1:A:677:GLN:N	1:A:678:PRO:CD	2.74	0.50
1:A:692:GLU:HB3	1:A:695:HIS:CD2	2.47	0.50
2:B:109:GLU:HA	2:B:126:THR:OG1	2.11	0.50
1:A:570:LEU:HD13	1:A:570:LEU:O	2.11	0.50
1:A:617:LEU:C	1:A:617:LEU:HD23	2.32	0.50
2:B:321:LEU:CD1	2:B:442:SER:HA	2.33	0.50
2:B:390:ARG:O	2:B:391:ASP:OD1	2.30	0.50
2:B:463:LEU:HD22	2:B:648:PRO:HG2	1.93	0.50
2:B:107:LEU:CD1	2:B:160:ARG:HG3	2.41	0.50
2:B:459:MET:HG3	2:B:621:LEU:HD23	1.93	0.50
2:B:678:SER:H	2:B:681:ASN:HB3	1.76	0.50
1:A:517:ILE:HD12	1:A:734:GLU:HG3	1.94	0.50
1:A:571:ARG:NH1	1:A:723:SER:HB2	2.27	0.50
1:A:612:THR:HG21	1:A:753:LEU:HA	1.92	0.50
2:B:115:VAL:HG11	2:B:138:MET:SD	2.52	0.50
2:B:342:PHE:CE2	2:B:344:LEU:HD21	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:VAL:CB	1:A:65:PRO:HD3	2.27	0.50
1:A:169:PRO:C	1:A:171:ARG:N	2.62	0.50
1:A:477:GLU:HG3	3:C:13:BGC:O6	2.12	0.50
1:A:571:ARG:HD3	1:A:723:SER:CB	2.31	0.50
2:B:524:ALA:O	2:B:528:LEU:CB	2.60	0.50
2:B:625:LEU:HB3	2:B:629:ALA:HB2	1.92	0.50
1:A:112:ILE:O	1:A:115:PHE:HB3	2.12	0.50
1:A:486:TYR:HE1	1:A:520:ILE:HG12	1.76	0.50
2:B:330:LEU:HD23	2:B:439:GLN:CG	2.23	0.50
2:B:514:ASN:ND2	2:B:519:THR:HG23	2.27	0.50
2:B:615:ALA:HB1	2:B:621:LEU:CG	2.42	0.50
1:A:84:ARG:O	1:A:88:THR:OG1	2.30	0.49
1:A:88:THR:HG23	1:A:441:PHE:CE2	2.47	0.49
1:A:396:PRO:CA	1:A:399:ARG:HE	2.25	0.49
2:B:103:SER:O	2:B:104:ILE:CB	2.57	0.49
2:B:550:LEU:CD2	2:B:550:LEU:H	2.25	0.49
1:A:85:LEU:HD13	1:A:105:PHE:CZ	2.46	0.49
1:A:121:LEU:HD23	1:A:309:LEU:CD1	2.42	0.49
1:A:45:ILE:HG23	1:A:75:MET:CE	2.42	0.49
1:A:182:GLY:HA3	1:A:222:ASN:OD1	2.12	0.49
1:A:345:GLU:HB2	1:A:390:MET:HE1	1.93	0.49
1:A:510:GLU:OE1	1:A:510:GLU:N	2.36	0.49
2:B:223:LEU:CD1	2:B:479:LEU:CD2	2.90	0.49
2:B:321:LEU:CB	2:B:324:MET:HB2	2.41	0.49
1:A:128:ARG:NH1	1:A:310:ASP:OD1	2.38	0.49
2:B:345:PRO:CG	2:B:348:TRP:HB3	2.38	0.49
1:A:340:ILE:HG22	1:A:341:THR:N	2.27	0.49
1:A:377:ILE:CD1	1:A:520:ILE:HG21	2.43	0.49
1:A:505:VAL:O	1:A:505:VAL:CG1	2.61	0.49
2:B:627:PRO:O	2:B:628:GLU:CB	2.60	0.49
1:A:273:GLN:OE1	1:A:317:PHE:CA	2.49	0.49
1:A:284:ILE:O	1:A:288:LEU:HD12	2.11	0.49
2:B:378:VAL:CG2	2:B:378:VAL:O	2.61	0.49
2:B:524:ALA:O	2:B:528:LEU:HB3	2.13	0.49
1:A:21:LEU:HB3	2:B:711:ILE:CD1	2.42	0.49
1:A:617:LEU:CD2	1:A:619:VAL:HG22	2.43	0.49
1:A:626:ASP:N	1:A:627:PRO:HD2	2.28	0.49
2:B:318:VAL:HG21	2:B:445:ASP:CG	2.34	0.49
2:B:324:MET:HB2	2:B:326:VAL:HG12	1.94	0.49
2:B:364:PHE:CE1	2:B:391:ASP:C	2.86	0.49
1:A:250:VAL:HB	1:A:690:PHE:CD1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:VAL:HG23	1:A:449:LEU:HD12	1.94	0.49
1:A:183:THR:O	1:A:187:CYS:HB2	2.13	0.48
1:A:351:HIS:CE1	1:A:357:SER:OG	2.66	0.48
1:A:390:MET:SD	1:A:394:LYS:HG3	2.53	0.48
1:A:275:PRO:CG	1:A:363:ALA:N	2.76	0.48
1:A:330:ASP:O	1:A:333:GLY:CA	2.62	0.48
1:A:455:TYR:OH	3:C:12:BGC:H6C2	2.12	0.48
1:A:596:PRO:HG3	1:A:636:LEU:HB3	1.96	0.48
2:B:203:GLN:HG2	2:B:210:VAL:HG22	1.96	0.48
2:B:318:VAL:O	2:B:318:VAL:HG13	2.12	0.48
2:B:360:ILE:CG2	2:B:361:ASP:N	2.77	0.48
1:A:330:ASP:C	1:A:333:GLY:H	2.16	0.48
2:B:463:LEU:C	2:B:465:GLN:H	2.15	0.48
1:A:396:PRO:O	1:A:399:ARG:NE	2.46	0.48
1:A:636:LEU:C	1:A:637:ILE:HD12	2.34	0.48
2:B:96:LEU:HD11	2:B:98:LEU:CD2	2.43	0.48
2:B:160:ARG:O	2:B:429:PRO:HB3	2.13	0.48
2:B:553:LEU:C	2:B:555:ALA:H	2.16	0.48
1:A:84:ARG:O	1:A:88:THR:CB	2.62	0.48
1:A:388:MET:CG	1:A:491:ILE:HD13	2.43	0.48
1:A:595:ILE:O	1:A:599:GLY:CA	2.62	0.48
2:B:69:GLY:O	2:B:71:LEU:N	2.47	0.48
2:B:666:LYS:CG	2:B:667:PRO:HD2	2.38	0.48
1:A:288:LEU:O	1:A:289:ALA:C	2.51	0.48
1:A:397:LEU:HA	1:A:407:ARG:HD2	1.95	0.48
1:A:578:GLN:HG2	1:A:579:ARG:H	1.78	0.48
2:B:144:VAL:O	2:B:145:ARG:CG	2.61	0.48
2:B:144:VAL:HG12	2:B:145:ARG:N	2.28	0.48
2:B:377:LYS:HG2	2:B:382:THR:CB	2.37	0.48
1:A:84:ARG:O	1:A:88:THR:HB	2.14	0.48
1:A:128:ARG:NH1	1:A:310:ASP:OD2	2.46	0.48
1:A:166:MET:CE	1:A:251:PRO:HB2	2.44	0.48
1:A:385:THR:HG22	1:A:494:THR:OG1	2.13	0.48
1:A:631:LEU:HD11	1:A:667:VAL:HG11	1.95	0.48
2:B:107:LEU:HB2	2:B:110:SER:HB2	1.90	0.48
2:B:192:GLU:HG2	2:B:193:PRO:HD2	1.96	0.48
2:B:373:LEU:HD12	2:B:375:LEU:HD12	1.95	0.48
1:A:121:LEU:N	1:A:121:LEU:CD1	2.77	0.48
1:A:674:GLU:O	1:A:675:ALA:CB	2.62	0.48
2:B:107:LEU:CD1	2:B:160:ARG:CG	2.92	0.48
2:B:345:PRO:CG	2:B:346:ASP:H	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:TYR:HB2	1:A:573:VAL:HG11	1.95	0.47
1:A:743:GLU:O	1:A:745:PRO:HD3	2.14	0.47
2:B:273:GLY:CA	2:B:278:VAL:HA	2.41	0.47
2:B:501:THR:CG2	2:B:622:TRP:CG	2.97	0.47
1:A:204:GLU:HG3	1:A:205:LEU:HD22	1.96	0.47
5:A:920:LDA:CM2	2:B:708:SER:OG	2.55	0.47
2:B:264:ASP:CG	2:B:265:ALA:H	2.17	0.47
2:B:404:PRO:HB3	2:B:406:ARG:NH1	2.30	0.47
1:A:121:LEU:HD23	1:A:309:LEU:HD12	1.96	0.47
1:A:155:MET:SD	1:A:248:ASP:HA	2.54	0.47
1:A:288:LEU:HB2	1:A:290:LEU:CD2	2.42	0.47
1:A:514:GLU:HG2	1:A:578:GLN:CD	2.35	0.47
5:A:920:LDA:H21	5:A:920:LDA:HM11	1.52	0.47
1:A:345:GLU:HG2	1:A:394:LYS:HE3	1.95	0.47
1:A:396:PRO:HA	1:A:399:ARG:HE	1.79	0.47
2:B:398:ARG:HH22	2:B:445:ASP:N	2.11	0.47
1:A:130:PHE:HB3	1:A:131:PRO:HD2	1.96	0.47
1:A:215:VAL:HG12	1:A:216:TYR:N	2.29	0.47
1:A:597:ALA:C	1:A:599:GLY:H	2.17	0.47
2:B:523:LEU:H	2:B:523:LEU:HD13	1.74	0.47
2:B:527:LEU:CB	2:B:609:GLY:O	2.63	0.47
1:A:441:PHE:CB	3:C:9:BGC:H4	2.40	0.47
1:A:578:GLN:O	1:A:579:ARG:HB2	2.15	0.47
2:B:69:GLY:C	2:B:71:LEU:N	2.67	0.47
2:B:211:GLU:OE2	2:B:250:GLU:HG3	2.14	0.47
2:B:364:PHE:CZ	2:B:396:LYS:HE3	2.50	0.47
2:B:383:VAL:HG22	2:B:403:PHE:CB	2.43	0.47
2:B:612:MET:HG2	2:B:614:LEU:CD1	2.43	0.47
1:A:103:LEU:CD1	1:A:425:MET:CE	2.60	0.47
1:A:142:VAL:CG2	1:A:241:LEU:HB2	2.30	0.47
1:A:216:TYR:C	1:A:216:TYR:CD2	2.88	0.47
1:A:288:LEU:H	1:A:288:LEU:CD1	2.19	0.47
1:A:487:LEU:CD1	1:A:487:LEU:H	2.28	0.47
1:A:593:ALA:HA	1:A:639:PHE:HA	1.96	0.47
1:A:597:ALA:C	1:A:599:GLY:N	2.68	0.47
2:B:122:ILE:HD11	2:B:143:ALA:HB3	1.95	0.47
2:B:150:LEU:HD23	2:B:150:LEU:O	2.13	0.47
2:B:343:GLN:HA	2:B:411:GLY:O	2.15	0.47
2:B:398:ARG:NH2	2:B:445:ASP:H	2.12	0.47
2:B:501:THR:HG21	2:B:622:TRP:CE2	2.49	0.47
2:B:615:ALA:HB1	2:B:621:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:TYR:CZ	1:A:524:LEU:HD12	2.50	0.47
2:B:266:ASP:CB	2:B:285:PRO:CD	2.66	0.47
2:B:321:LEU:O	2:B:325:GLY:N	2.48	0.47
1:A:22:TRP:HZ2	5:A:920:LDA:HM11	1.79	0.47
1:A:57:LYS:N	1:A:58:PRO:CD	2.77	0.47
1:A:144:ILE:HG22	1:A:243:VAL:CG2	2.45	0.47
1:A:184:ASP:OD1	1:A:184:ASP:C	2.53	0.47
2:B:518:LEU:O	2:B:522:LEU:HD12	2.15	0.47
1:A:53:VAL:HG22	1:A:69:LEU:HD12	1.97	0.47
2:B:73:ARG:HH11	2:B:172:TRP:HZ3	1.63	0.47
2:B:97:THR:HB	2:B:136:VAL:HG12	1.96	0.47
2:B:217:PRO:HA	2:B:218:PRO:HD3	1.81	0.47
2:B:464:ALA:HB2	2:B:642:PRO:CB	2.42	0.47
1:A:650:GLU:H	1:A:650:GLU:HG2	1.55	0.46
2:B:527:LEU:C	2:B:527:LEU:HD12	2.35	0.46
1:A:660:ALA:HA	1:A:669:VAL:HA	1.96	0.46
2:B:269:SER:HB2	2:B:298:LEU:CD1	2.45	0.46
2:B:80:ARG:HG2	2:B:154:GLU:HB3	1.98	0.46
1:A:267:PRO:HA	1:A:325:ARG:NH2	2.29	0.46
1:A:275:PRO:HG2	1:A:363:ALA:HB2	1.97	0.46
1:A:524:LEU:CD2	1:A:570:LEU:HA	2.44	0.46
2:B:106:ILE:HB	2:B:160:ARG:CD	2.14	0.46
2:B:216:THR:HA	2:B:217:PRO:HD2	1.70	0.46
2:B:507:ASP:O	2:B:508:ILE:HG13	2.16	0.46
1:A:366:ALA:HB2	1:A:696:TRP:CZ2	2.51	0.46
1:A:514:GLU:HG2	1:A:578:GLN:OE1	2.16	0.46
1:A:647:PRO:CG	1:A:649:LEU:H	2.28	0.46
2:B:266:ASP:CA	2:B:284:HIS:HA	2.34	0.46
2:B:569:ASN:HB3	2:B:573:ARG:HD2	1.95	0.46
1:A:76:LEU:HD21	1:A:454:GLY:C	2.35	0.46
1:A:605:ALA:HA	1:A:618:LEU:O	2.16	0.46
1:A:84:ARG:HD2	1:A:88:THR:OG1	2.15	0.46
1:A:128:ARG:HH12	1:A:310:ASP:CG	2.19	0.46
1:A:345:GLU:CG	1:A:394:LYS:HE3	2.46	0.46
2:B:113:ILE:N	2:B:125:PHE:O	2.49	0.46
2:B:531:THR:HG23	2:B:608:LYS:CE	2.45	0.46
1:A:267:PRO:HA	1:A:325:ARG:HH12	1.80	0.46
1:A:301:PHE:HB2	3:C:16:BGC:O2	2.15	0.46
1:A:397:LEU:HD22	1:A:407:ARG:NH1	2.26	0.46
2:B:550:LEU:O	2:B:550:LEU:HG	2.16	0.46
1:A:128:ARG:HA	1:A:129:PRO:HD3	1.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:VAL:HA	1:A:251:PRO:HD3	1.63	0.46
1:A:270:PHE:CE1	1:A:271:LEU:HB2	2.50	0.46
1:A:494:THR:O	1:A:498:PRO:HG3	2.16	0.46
2:B:501:THR:HG21	2:B:622:TRP:CD2	2.51	0.46
1:A:182:GLY:C	1:A:184:ASP:N	2.69	0.46
1:A:194:LEU:O	1:A:198:ALA:CB	2.64	0.46
1:A:288:LEU:CD2	1:A:568:PHE:CD2	2.96	0.46
1:A:182:GLY:HA2	1:A:219:ARG:O	2.16	0.45
1:A:186:ARG:HB2	1:A:202:ARG:HH11	1.80	0.45
1:A:312:TRP:HB3	1:A:405:ALA:CB	2.45	0.45
2:B:232:ARG:N	2:B:233:PRO:HD2	2.31	0.45
2:B:344:LEU:CB	2:B:410:PRO:HA	2.46	0.45
1:A:400:ARG:HD3	1:A:400:ARG:HA	1.74	0.45
1:A:417:TRP:O	1:A:420:PRO:HD2	2.16	0.45
1:A:423:ARG:HD2	1:A:480:GLU:CB	2.46	0.45
2:B:320:THR:C	2:B:322:ALA:H	2.20	0.45
1:A:130:PHE:O	1:A:131:PRO:O	2.35	0.45
1:A:145:LEU:C	1:A:145:LEU:CD1	2.82	0.45
1:A:189:SER:O	1:A:190:PRO:C	2.54	0.45
1:A:267:PRO:O	1:A:268:ASP:HB2	2.16	0.45
1:A:471:ARG:NH1	1:A:476:SER:OG	2.40	0.45
1:A:689:ILE:HB	1:A:690:PHE:HD2	1.81	0.45
1:A:692:GLU:OE1	1:A:692:GLU:HA	2.16	0.45
3:C:11:BGC:C3	3:C:12:BGC:O5	2.63	0.45
2:B:456:MET:O	2:B:461:ARG:NH2	2.50	0.45
2:B:193:PRO:O	2:B:196:PHE:HB3	2.17	0.45
1:A:481:VAL:O	1:A:485:PRO:HD3	2.17	0.45
2:B:125:PHE:CZ	2:B:138:MET:SD	3.10	0.45
2:B:398:ARG:NH1	2:B:444:THR:HA	2.15	0.45
1:A:286:ARG:NH2	1:A:575:GLU:OE1	2.50	0.45
2:B:313:ILE:HA	2:B:314:PRO:HD3	1.70	0.45
2:B:350:LEU:CD1	2:B:451:SER:CB	2.66	0.45
2:B:673:LEU:HD12	2:B:673:LEU:O	2.17	0.45
2:B:702:LEU:C	2:B:702:LEU:HD23	2.37	0.45
1:A:129:PRO:O	1:A:130:PHE:C	2.54	0.45
1:A:518:SER:O	1:A:521:TYR:HB3	2.17	0.45
1:A:657:ILE:HG13	1:A:657:ILE:O	2.17	0.45
1:A:254:ASP:OD1	1:A:364:MET:SD	2.75	0.45
1:A:372:THR:HB	1:A:375:SER:H	1.80	0.45
1:A:704:MET:O	1:A:706:PRO:HD3	2.16	0.45
2:B:317:ARG:HG3	2:B:318:VAL:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:348:TRP:CE3	2:B:348:TRP:C	2.90	0.45
2:B:384:ARG:HH21	3:C:6:BGC:H3	1.81	0.45
2:B:211:GLU:HG2	2:B:244:SER:OG	2.17	0.45
1:A:79:ARG:HD2	2:B:701:MET:CE	2.47	0.44
1:A:128:ARG:NH1	1:A:310:ASP:CG	2.71	0.44
1:A:477:GLU:OE2	3:C:13:BGC:O6	2.32	0.44
2:B:574:ALA:O	2:B:578:VAL:HG23	2.17	0.44
2:B:612:MET:CG	2:B:614:LEU:HD11	2.46	0.44
1:A:78:MET:HE3	1:A:78:MET:CA	2.45	0.44
1:A:358:LEU:HD13	1:A:358:LEU:N	2.12	0.44
1:A:751:HIS:CG	1:A:752:LEU:N	2.84	0.44
2:B:65:THR:OG1	2:B:67:GLN:NE2	2.49	0.44
1:A:80:TYR:CD2	1:A:80:TYR:C	2.91	0.44
1:A:207:GLN:HA	1:A:210:ARG:NH1	2.32	0.44
1:A:219:ARG:NH1	1:A:223:GLU:O	2.49	0.44
1:A:263:PHE:O	1:A:325:ARG:NH1	2.51	0.44
1:A:272:VAL:HG22	1:A:358:LEU:CG	2.46	0.44
1:A:275:PRO:HD2	1:A:363:ALA:H	1.81	0.44
1:A:411:LEU:HD23	1:A:411:LEU:O	2.17	0.44
1:A:447:GLU:OE1	2:B:355:LYS:HE2	2.16	0.44
1:A:542:TRP:CE2	1:A:549:ARG:HD3	2.53	0.44
1:A:546:PRO:HB3	1:A:549:ARG:NH2	2.31	0.44
1:A:658:ARG:CD	1:A:672:ILE:CD1	2.93	0.44
2:B:118:ASN:OD1	2:B:144:VAL:CB	2.65	0.44
2:B:351:LEU:HD11	2:B:691:SER:HB2	1.97	0.44
2:B:523:LEU:HD22	2:B:523:LEU:C	2.37	0.44
1:A:208:LEU:HD12	1:A:208:LEU:O	2.18	0.44
1:A:270:PHE:CD2	1:A:356:LYS:O	2.66	0.44
1:A:271:LEU:CG	1:A:317:PHE:HB3	2.45	0.44
1:A:412:ASN:HA	1:A:415:SER:HG	1.82	0.44
2:B:164:GLY:HA2	2:B:423:GLY:H	1.82	0.44
1:A:111:SER:O	1:A:114:ILE:HG13	2.18	0.44
1:A:679:ILE:N	1:A:679:ILE:HD12	2.33	0.44
1:A:674:GLU:C	1:A:676:GLY:H	2.20	0.44
1:A:707:ILE:CD1	1:A:711:HIS:HD2	2.30	0.44
2:B:329:ILE:N	2:B:329:ILE:HD12	2.33	0.44
2:B:456:MET:O	2:B:461:ARG:NH1	2.51	0.44
2:B:482:THR:HG22	2:B:502:VAL:HB	2.00	0.44
2:B:525:LEU:HD12	2:B:525:LEU:H	1.83	0.44
1:A:263:PHE:CE1	1:A:270:PHE:O	2.71	0.44
1:A:271:LEU:O	1:A:358:LEU:HD13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:TRP:CZ2	3:C:17:BGC:H4	2.53	0.44
1:A:403:GLY:HA3	1:A:406:GLN:OE1	2.18	0.44
1:A:551:VAL:HG22	3:C:8:BGC:H6C1	2.00	0.44
2:B:254:THR:O	2:B:277:ALA:CB	2.65	0.44
2:B:623:VAL:C	2:B:624:ILE:HD12	2.39	0.44
1:A:145:LEU:HB2	1:A:177:LEU:HD21	1.99	0.44
1:A:270:PHE:CD1	1:A:350:ILE:HG21	2.53	0.44
1:A:274:THR:OG1	1:A:321:ALA:HB1	2.18	0.44
1:A:419:PHE:O	1:A:420:PRO:C	2.54	0.44
1:A:542:TRP:HZ3	1:A:553:LEU:CD1	2.29	0.44
2:B:99:ALA:O	2:B:134:GLY:CA	2.66	0.44
2:B:345:PRO:HG3	2:B:348:TRP:HB2	1.99	0.44
1:A:145:LEU:HD13	1:A:177:LEU:CD1	2.48	0.43
1:A:148:SER:CB	1:A:156:LEU:HD21	2.48	0.43
1:A:578:GLN:HG2	1:A:579:ARG:N	2.33	0.43
1:A:647:PRO:HG2	1:A:649:LEU:H	1.82	0.43
1:A:675:ALA:HB2	1:A:757:THR:O	2.18	0.43
2:B:523:LEU:HD13	2:B:524:ALA:H	1.82	0.43
1:A:37:VAL:HG13	1:A:38:ALA:N	2.32	0.43
2:B:459:MET:H	2:B:650:GLY:H	1.65	0.43
1:A:53:VAL:HG13	1:A:69:LEU:HD12	1.97	0.43
1:A:209:CYS:HA	1:A:214:VAL:HG22	2.01	0.43
1:A:219:ARG:NH1	1:A:223:GLU:N	2.62	0.43
1:A:310:ASP:O	1:A:311:ARG:C	2.56	0.43
2:B:113:ILE:HB	2:B:125:PHE:HB2	1.99	0.43
2:B:267:ARG:HA	2:B:294:LEU:HD13	1.99	0.43
1:A:343:ASP:N	1:A:343:ASP:OD1	2.51	0.43
2:B:550:LEU:H	2:B:550:LEU:HD23	1.83	0.43
2:B:566:VAL:CG1	3:C:5:BGC:O6	2.64	0.43
1:A:16:VAL:O	1:A:20:LEU:HG	2.19	0.43
2:B:341:ASP:HA	2:B:413:ASN:O	2.19	0.43
1:A:580:ARG:NH2	1:A:751:HIS:O	2.46	0.43
2:B:77:GLN:OE1	2:B:337:ASN:ND2	2.52	0.43
2:B:377:LYS:HB2	2:B:416:SER:HB2	1.99	0.43
2:B:625:LEU:HB3	2:B:629:ALA:CB	2.48	0.43
2:B:625:LEU:HD23	2:B:629:ALA:HB1	2.00	0.43
1:A:317:PHE:HD1	1:A:319:GLY:H	1.64	0.43
2:B:333:ASN:OD1	2:B:333:ASN:N	2.51	0.43
1:A:226:LYS:O	1:A:230:MET:HG2	2.19	0.43
1:A:595:ILE:O	1:A:599:GLY:HA2	2.19	0.43
2:B:310:LEU:HD11	2:B:643:ARG:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:VAL:HG23	2:B:445:ASP:CB	2.48	0.43
2:B:320:THR:HA	2:B:444:THR:O	2.19	0.43
2:B:330:LEU:CD2	2:B:439:GLN:CB	2.94	0.43
2:B:481:ARG:O	2:B:484:PRO:HD2	2.19	0.43
2:B:583:GLN:HB3	2:B:584:PRO:CD	2.47	0.43
1:A:177:LEU:HB3	1:A:229:ASN:HB3	2.01	0.43
1:A:275:PRO:HG2	1:A:363:ALA:CB	2.48	0.43
1:A:282:ASP:HB3	1:A:369:GLN:NE2	2.34	0.43
1:A:288:LEU:HB3	1:A:568:PHE:CZ	2.54	0.43
1:A:732:MET:O	1:A:735:PRO:HD2	2.19	0.43
2:B:563:PRO:HG3	2:B:576:THR:OG1	2.19	0.43
2:B:616:PRO:O	2:B:617:GLU:CB	2.63	0.43
1:A:549:ARG:C	1:A:553:LEU:HD13	2.39	0.43
2:B:106:ILE:CG1	2:B:160:ARG:HE	2.28	0.43
2:B:230:LEU:HD11	2:B:258:ILE:HD13	2.01	0.43
2:B:373:LEU:HD11	2:B:375:LEU:HD11	2.00	0.43
2:B:383:VAL:O	2:B:383:VAL:HG13	2.19	0.43
1:A:78:MET:CE	1:A:78:MET:CA	2.96	0.42
1:A:149:TYR:O	1:A:150:ASN:HB3	2.19	0.42
1:A:151:GLU:HG2	1:A:247:ALA:CB	2.48	0.42
1:A:264:VAL:HG22	1:A:264:VAL:O	2.18	0.42
1:A:337:GLY:HA3	1:A:342:GLU:OE1	2.18	0.42
1:A:373:PHE:O	1:A:376:PHE:HB3	2.19	0.42
1:A:432:ILE:O	1:A:436:PHE:HB2	2.19	0.42
1:A:567:GLY:HA3	1:A:724:LEU:HD21	2.01	0.42
1:A:649:LEU:O	1:A:649:LEU:CG	2.66	0.42
2:B:87:LEU:CD1	2:B:88:PRO:O	2.66	0.42
2:B:360:ILE:HG22	2:B:362:TYR:HD2	1.84	0.42
2:B:389:ASP:OD1	2:B:390:ARG:CG	2.65	0.42
2:B:527:LEU:HB2	2:B:609:GLY:O	2.19	0.42
1:A:166:MET:HE2	1:A:251:PRO:CB	2.48	0.42
2:B:74:LEU:O	2:B:172:TRP:HA	2.18	0.42
2:B:364:PHE:HE1	2:B:392:ALA:N	2.16	0.42
1:A:13:VAL:HB	1:A:15:PRO:HD2	2.00	0.42
1:A:126:THR:HG22	1:A:311:ARG:CZ	2.49	0.42
1:A:321:ALA:CB	1:A:365:ILE:HD13	2.49	0.42
2:B:617:GLU:CB	2:B:618:PRO:HD2	2.49	0.42
2:B:620:LYS:C	2:B:621:LEU:HD12	2.38	0.42
1:A:258:ARG:HB3	1:A:364:MET:HE1	2.01	0.42
1:A:417:TRP:O	1:A:491:ILE:CD1	2.67	0.42
1:A:504:ALA:O	1:A:505:VAL:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:GLU:OE2	1:A:642:LYS:HE3	2.18	0.42
2:B:345:PRO:CG	2:B:346:ASP:N	2.78	0.42
2:B:530:SER:O	2:B:531:THR:O	2.38	0.42
2:B:55:TRP:O	2:B:183:ALA:HA	2.20	0.42
2:B:98:LEU:HD13	2:B:179:GLN:HB2	1.97	0.42
2:B:321:LEU:HB3	2:B:326:VAL:HG13	1.96	0.42
3:C:17:BGC:O3	3:C:18:BGC:O5	2.28	0.42
1:A:283:PRO:HG2	1:A:373:PHE:HA	2.02	0.42
1:A:351:HIS:CE1	1:A:357:SER:HG	2.32	0.42
1:A:399:ARG:NH1	1:A:410:TYR:HB2	2.34	0.42
1:A:647:PRO:HG2	1:A:649:LEU:N	2.34	0.42
2:B:321:LEU:HB3	2:B:324:MET:HB2	2.02	0.42
3:C:10:BGC:HC	3:C:11:BGC:C1	2.31	0.42
1:A:88:THR:CG2	1:A:441:PHE:CZ	3.02	0.42
1:A:131:PRO:C	1:A:265:GLU:OE2	2.58	0.42
1:A:176:VAL:C	1:A:177:LEU:HD23	2.40	0.42
1:A:266:ASP:C	1:A:267:PRO:O	2.57	0.42
1:A:330:ASP:O	1:A:333:GLY:HA2	2.19	0.42
1:A:431:LEU:H	1:A:431:LEU:HG	1.68	0.42
2:B:59:LEU:HD13	2:B:83:PHE:CD1	2.55	0.42
2:B:529:PRO:HD2	2:B:529:PRO:O	2.19	0.42
1:A:489:ARG:O	1:A:493:THR:HG23	2.20	0.42
1:A:587:MET:HE1	1:A:688:LEU:HD12	2.02	0.42
1:A:637:ILE:CG2	1:A:638:GLN:N	2.83	0.42
2:B:96:LEU:HD23	2:B:137:THR:CG2	2.18	0.42
2:B:521:ARG:O	2:B:524:ALA:N	2.53	0.42
1:A:219:ARG:HH12	1:A:223:GLU:N	2.16	0.42
2:B:496:ALA:O	2:B:498:VAL:HG23	2.19	0.42
1:A:318:CYS:O	3:C:18:BGC:H2	2.20	0.42
1:A:329:LEU:HD12	1:A:329:LEU:C	2.40	0.42
1:A:352:SER:HB2	1:A:401:GLY:HA3	2.02	0.42
1:A:725:PRO:O	1:A:728:ALA:HB3	2.20	0.42
2:B:435:GLY:O	2:B:437:LEU:HD12	2.20	0.42
1:A:117:LEU:CD2	1:A:412:ASN:HB3	2.49	0.41
1:A:262:TYR:CE1	1:A:360:ILE:HD13	2.41	0.41
1:A:524:LEU:H	1:A:524:LEU:HD13	1.83	0.41
1:A:536:LEU:HD12	1:A:536:LEU:O	2.20	0.41
1:A:549:ARG:O	1:A:553:LEU:HD12	2.19	0.41
2:B:96:LEU:C	2:B:96:LEU:CD1	2.87	0.41
2:B:230:LEU:CD1	2:B:258:ILE:HD13	2.50	0.41
2:B:624:ILE:HD12	2:B:624:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:679:LEU:HD12	2:B:679:LEU:N	2.35	0.41
1:A:234:LEU:C	1:A:236:ARG:N	2.72	0.41
1:A:255:PHE:CD1	1:A:255:PHE:C	2.93	0.41
1:A:139:LEU:O	1:A:171:ARG:NH1	2.53	0.41
1:A:186:ARG:CB	1:A:202:ARG:HH11	2.32	0.41
1:A:423:ARG:NH2	3:C:13:BGC:O6	2.52	0.41
1:A:421:LEU:N	1:A:421:LEU:HD12	2.35	0.41
1:A:167:ILE:CD1	1:A:167:ILE:N	2.83	0.41
1:A:542:TRP:CA	1:A:552:LEU:HD13	2.50	0.41
1:A:709:LEU:C	1:A:709:LEU:CD1	2.89	0.41
2:B:706:TRP:C	2:B:708:SER:H	2.23	0.41
1:A:35:ALA:HA	1:A:36:PRO:HD2	1.95	0.41
1:A:258:ARG:CZ	1:A:364:MET:HE1	2.51	0.41
1:A:391:LEU:HD13	1:A:414:MET:HB2	2.03	0.41
1:A:638:GLN:HA	1:A:653:VAL:O	2.21	0.41
2:B:69:GLY:C	2:B:71:LEU:H	2.22	0.41
2:B:162:TYR:CD2	2:B:162:TYR:N	2.89	0.41
2:B:285:PRO:C	2:B:287:GLU:N	2.74	0.41
2:B:505:LEU:CD2	2:B:523:LEU:HD22	2.45	0.41
1:A:84:ARG:C	1:A:88:THR:OG1	2.59	0.41
1:A:256:LEU:O	1:A:260:VAL:HB	2.20	0.41
1:A:274:THR:HB	1:A:275:PRO:HD2	2.03	0.41
1:A:294:CYS:HA	1:A:295:PRO:HD3	1.95	0.41
1:A:612:THR:HG21	1:A:753:LEU:CA	2.50	0.41
1:A:642:LYS:C	1:A:644:PRO:HD3	2.40	0.41
1:A:725:PRO:O	1:A:729:ARG:HG3	2.21	0.41
2:B:458:ASP:HB2	2:B:649:ARG:HG2	2.03	0.41
1:A:351:HIS:NE2	1:A:357:SER:OG	2.46	0.41
1:A:352:SER:O	1:A:401:GLY:CA	2.67	0.41
1:A:423:ARG:O	1:A:427:LEU:HG	2.19	0.41
2:B:69:GLY:HA2	2:B:70:PRO:HD2	1.94	0.41
2:B:212:ILE:HA	2:B:258:ILE:O	2.20	0.41
2:B:485:PHE:CE2	2:B:502:VAL:HG11	2.56	0.41
2:B:490:ARG:HD2	2:B:490:ARG:HA	1.96	0.41
2:B:550:LEU:O	2:B:550:LEU:CG	2.68	0.41
2:B:617:GLU:CB	2:B:618:PRO:CD	2.98	0.41
2:B:690:ALA:HB1	2:B:697:LEU:HD22	2.03	0.41
1:A:103:LEU:HB3	1:A:425:MET:HE3	2.03	0.41
1:A:288:LEU:HB3	1:A:568:PHE:CE2	2.55	0.41
2:B:360:ILE:HG22	2:B:361:ASP:N	2.35	0.41
3:C:10:BGC:C3	3:C:11:BGC:O5	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LEU:O	1:A:198:ALA:HB2	2.21	0.40
1:A:267:PRO:CA	1:A:325:ARG:HH22	2.32	0.40
1:A:640:GLN:HA	1:A:641:PRO:HD2	1.87	0.40
2:B:122:ILE:CD1	2:B:143:ALA:HB2	2.50	0.40
2:B:326:VAL:HG13	2:B:326:VAL:O	2.21	0.40
1:A:394:LYS:HA	1:A:394:LYS:HD3	1.72	0.40
1:A:592:GLU:OE2	1:A:642:LYS:NZ	2.54	0.40
1:A:626:ASP:N	1:A:627:PRO:CD	2.83	0.40
2:B:63:ALA:CB	2:B:67:GLN:NE2	2.77	0.40
1:A:361:ASP:OD1	1:A:361:ASP:C	2.58	0.40
1:A:395:ASN:N	1:A:396:PRO:CD	2.84	0.40
1:A:491:ILE:O	1:A:495:LEU:HB2	2.22	0.40
2:B:625:LEU:N	2:B:625:LEU:CD1	2.84	0.40
2:B:694:PRO:N	2:B:695:PRO:CD	2.83	0.40
1:A:263:PHE:CZ	1:A:270:PHE:O	2.73	0.40
1:A:556:GLY:O	1:A:557:GLY:C	2.60	0.40
1:A:696:TRP:HA	1:A:696:TRP:HE3	1.86	0.40
2:B:241:LEU:HD12	2:B:241:LEU:N	2.37	0.40
2:B:391:ASP:OD1	2:B:391:ASP:N	2.49	0.40
2:B:459:MET:HE3	2:B:648:PRO:HB2	2.03	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	745/802 (93%)	674 (90%)	64 (9%)	7 (1%)	17	50
2	B	651/707 (92%)	574 (88%)	67 (10%)	10 (2%)	10	39
All	All	1396/1509 (92%)	1248 (89%)	131 (9%)	17 (1%)	13	43

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	PRO
1	A	514	GLU
1	A	647	PRO
2	B	146	ALA
2	B	529	PRO
2	B	104	ILE
2	B	425	PRO
1	A	677	GLN
2	B	293	SER
2	B	554	GLY
1	A	183	THR
2	B	520	PRO
1	A	507	ALA
2	B	88	PRO
1	A	624	VAL
2	B	126	THR
2	B	616	PRO

5.3.2 Protein sidechains (i)

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	614/661 (93%)	595 (97%)	19 (3%)	40	67
2	B	520/559 (93%)	492 (95%)	28 (5%)	22	53
All	All	1134/1220 (93%)	1087 (96%)	47 (4%)	30	60

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	37	VAL
1	A	40	SER
1	A	97	SER
1	A	102	LEU
1	A	111	SER
1	A	167	ILE

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Mol	Chain	Res	Type
1	A	187	CYS
1	A	248	ASP
1	A	284	ILE
1	A	317	PHE
1	A	339	THR
1	A	358	LEU
1	A	385	THR
1	A	459	SER
1	A	524	LEU
1	A	595	ILE
1	A	621	LEU
1	A	626	ASP
2	B	150	LEU
2	B	157	HIS
2	B	163	CYS
2	B	172	TRP
2	B	184	LEU
2	B	233	PRO
2	B	269	SER
2	B	289	SER
2	B	309	THR
2	B	310	LEU
2	B	312	GLN
2	B	319	VAL
2	B	331	THR
2	B	333	ASN
2	B	378	VAL
2	B	430	CYS
2	B	451	SER
2	B	494	ASP
2	B	500	LEU
2	B	513	LEU
2	B	523	LEU
2	B	550	LEU
2	B	553	LEU
2	B	561	VAL
2	B	568	SER
2	B	588	THR
2	B	614	LEU
2	B	617	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	GLN
1	A	199	GLN
1	A	249	HIS
1	A	306	HIS
1	A	412	ASN
1	A	515	ASN
1	A	711	HIS
2	B	67	GLN
2	B	337	ASN
2	B	343	GLN
2	B	413	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

18 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	BGC	C	1	3	12,12,12	0.49	0	17,17,17	1.86	3 (17%)
3	BGC	C	10	3	11,11,12	0.64	0	15,15,17	1.06	1 (6%)
3	BGC	C	11	3	11,11,12	0.85	0	15,15,17	1.34	2 (13%)
3	BGC	C	12	3	11,11,12	0.99	1 (9%)	15,15,17	1.85	3 (20%)
3	BGC	C	13	3	11,11,12	0.75	0	15,15,17	1.65	4 (26%)
3	BGC	C	14	3	11,11,12	0.62	0	15,15,17	2.77	6 (40%)
3	BGC	C	15	3	11,11,12	0.58	0	15,15,17	1.37	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	BGC	C	16	3	11,11,12	0.62	0	15,15,17	1.38	3 (20%)
3	BGC	C	17	3	11,11,12	0.71	0	15,15,17	2.62	5 (33%)
3	BGC	C	18	3	11,11,12	0.70	0	15,15,17	1.94	3 (20%)
3	BGC	C	2	3	11,11,12	0.66	0	15,15,17	2.16	3 (20%)
3	BGC	C	3	3	11,11,12	0.59	0	15,15,17	1.07	0
3	BGC	C	4	3	11,11,12	0.62	0	15,15,17	0.80	0
3	BGC	C	5	3	11,11,12	0.64	0	15,15,17	0.81	0
3	BGC	C	6	3	11,11,12	0.81	0	15,15,17	1.92	5 (33%)
3	BGC	C	7	3	11,11,12	0.74	0	15,15,17	1.81	3 (20%)
3	BGC	C	8	3	11,11,12	0.61	0	15,15,17	1.15	2 (13%)
3	BGC	C	9	3	11,11,12	0.55	0	15,15,17	1.55	3 (20%)

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	BGC	C	1	3	-	2/2/22/22	0/1/1/1
3	BGC	C	10	3	-	2/2/19/22	0/1/1/1
3	BGC	C	11	3	-	0/2/19/22	0/1/1/1
3	BGC	C	12	3	-	1/2/19/22	0/1/1/1
3	BGC	C	13	3	-	1/2/19/22	0/1/1/1
3	BGC	C	14	3	-	0/2/19/22	0/1/1/1
3	BGC	C	15	3	-	0/2/19/22	0/1/1/1
3	BGC	C	16	3	-	1/2/19/22	0/1/1/1
3	BGC	C	17	3	-	1/2/19/22	0/1/1/1
3	BGC	C	18	3	-	0/2/19/22	0/1/1/1
3	BGC	C	2	3	-	2/2/19/22	0/1/1/1
3	BGC	C	3	3	-	1/2/19/22	0/1/1/1
3	BGC	C	4	3	-	2/2/19/22	0/1/1/1
3	BGC	C	5	3	-	0/2/19/22	0/1/1/1
3	BGC	C	6	3	-	0/2/19/22	0/1/1/1
3	BGC	C	7	3	-	2/2/19/22	0/1/1/1
3	BGC	C	8	3	-	2/2/19/22	0/1/1/1
3	BGC	C	9	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	12	BGC	O5-C5	-2.02	1.39	1.43

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	17	BGC	C1-O5-C5	8.20	123.18	112.19
3	C	14	BGC	C1-O5-C5	6.97	121.52	112.19
3	C	2	BGC	C1-O5-C5	6.72	121.19	112.19
3	C	18	BGC	C1-C2-C3	5.67	117.90	109.64
3	C	1	BGC	O5-C5-C4	5.40	119.42	109.70
3	C	1	BGC	O5-C5-C6	4.43	117.41	106.44
3	C	7	BGC	C1-O5-C5	4.33	117.99	112.19
3	C	14	BGC	O4-C4-C5	-3.99	99.49	109.32
3	C	6	BGC	C1-C2-C3	3.96	115.41	109.64
3	C	11	BGC	O4-C4-C5	-3.89	99.74	109.32
3	C	12	BGC	C1-O5-C5	-3.76	107.15	112.19
3	C	14	BGC	C1-C2-C3	3.74	115.09	109.64
3	C	6	BGC	C2-C3-C4	3.71	117.39	110.86
3	C	13	BGC	C1-O5-C5	3.65	117.08	112.19
3	C	12	BGC	C1-C2-C3	3.55	114.81	109.64
3	C	7	BGC	C1-C2-C3	3.47	114.69	109.64
3	C	9	BGC	C1-C2-C3	3.46	114.69	109.64
3	C	12	BGC	O4-C4-C5	-3.41	100.93	109.32
3	C	17	BGC	O5-C5-C4	3.30	118.84	110.83
3	C	14	BGC	O5-C1-C2	3.22	118.48	110.79
3	C	14	BGC	O5-C5-C4	3.13	118.45	110.83
3	C	15	BGC	C1-O5-C5	-3.10	108.03	112.19
3	C	15	BGC	O4-C4-C3	-3.01	103.29	110.38
3	C	13	BGC	C2-C3-C4	-2.93	105.70	110.86
3	C	2	BGC	C3-C4-C5	2.88	115.45	110.23
3	C	6	BGC	C3-C4-C5	2.86	115.42	110.23
3	C	2	BGC	O5-C5-C4	2.70	117.39	110.83
3	C	16	BGC	C3-C4-C5	-2.69	105.36	110.23
3	C	17	BGC	O3-C3-C2	-2.68	104.58	110.05
3	C	18	BGC	C2-C3-C4	2.65	115.52	110.86
3	C	18	BGC	C1-O5-C5	2.65	115.74	112.19
3	C	17	BGC	O2-C2-C3	-2.63	104.71	110.15
3	C	16	BGC	O5-C1-C2	-2.56	104.68	110.79
3	C	7	BGC	O2-C2-C3	-2.38	105.22	110.15
3	C	11	BGC	C1-C2-C3	2.33	113.04	109.64
3	C	9	BGC	C2-C3-C4	2.32	114.94	110.86
3	C	14	BGC	O3-C3-C2	-2.32	105.33	110.05
3	C	17	BGC	O2-C2-C1	2.31	114.50	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	BGC	C6-C5-C4	2.30	118.68	113.02
3	C	10	BGC	O4-C4-C5	-2.26	103.75	109.32
3	C	16	BGC	O5-C5-C4	2.25	116.31	110.83
3	C	13	BGC	O5-C5-C6	2.15	111.85	107.66
3	C	8	BGC	C1-O5-C5	-2.13	109.33	112.19
3	C	9	BGC	C6-C5-C4	-2.10	107.86	113.02
3	C	13	BGC	C6-C5-C4	-2.09	107.88	113.02
3	C	8	BGC	C3-C4-C5	-2.09	106.44	110.23
3	C	6	BGC	O5-C5-C4	2.03	115.76	110.83
3	C	6	BGC	O4-C4-C3	-2.01	105.64	110.38

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	7	BGC	O5-C5-C6-O6
3	C	10	BGC	O5-C5-C6-O6
3	C	7	BGC	C4-C5-C6-O6
3	C	10	BGC	C4-C5-C6-O6
3	C	2	BGC	C4-C5-C6-O6
3	C	1	BGC	C4-C5-C6-O6
3	C	4	BGC	O5-C5-C6-O6
3	C	4	BGC	C4-C5-C6-O6
3	C	8	BGC	O5-C5-C6-O6
3	C	16	BGC	O5-C5-C6-O6
3	C	2	BGC	O5-C5-C6-O6
3	C	13	BGC	O5-C5-C6-O6
3	C	12	BGC	O5-C5-C6-O6
3	C	17	BGC	O5-C5-C6-O6
3	C	8	BGC	C4-C5-C6-O6
3	C	1	BGC	O5-C5-C6-O6
3	C	3	BGC	O5-C5-C6-O6

There are no ring outliers.

12 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	11	BGC	5	0
3	C	13	BGC	3	0
3	C	5	BGC	6	0
3	C	8	BGC	2	0

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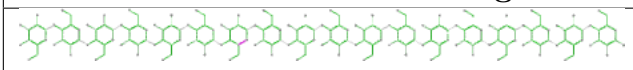
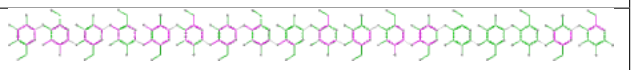
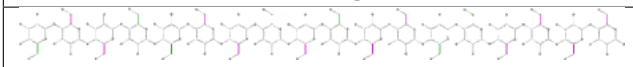
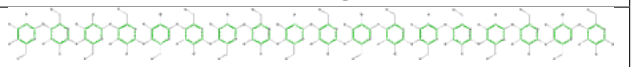
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	9	BGC	3	0
3	C	10	BGC	4	0
3	C	12	BGC	4	0
3	C	18	BGC	3	0
3	C	6	BGC	1	0
3	C	7	BGC	1	0
3	C	17	BGC	4	0
3	C	16	BGC	1	0

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

Oligosaccharide Chain C	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	LDA	A	921	-	13,15,15	2.14	2 (15%)	14,17,17	0.46	0
5	LDA	A	920	-	6,8,15	3.49	2 (33%)	7,10,17	0.43	0
4	UDP	A	919	-	25,26,26	0.97	1 (4%)	38,40,40	1.58	5 (13%)

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
5	LDA	A	921	-	-	4/13/13/13	-
5	LDA	A	920	-	-	3/6/6/13	-
4	UDP	A	919	-	-	10/16/32/32	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	920	LDA	O1-N1	-6.79	1.25	1.42
5	A	921	LDA	O1-N1	-6.30	1.26	1.42
5	A	920	LDA	C1-N1	-5.15	1.46	1.51
5	A	921	LDA	C1-N1	-4.30	1.47	1.51
4	A	919	UDP	C5-C4	-2.09	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	919	UDP	C4-N3-C2	-5.58	119.69	126.61
4	A	919	UDP	N3-C2-N1	4.19	120.35	114.89
4	A	919	UDP	C5-C4-N3	3.37	119.52	114.80
4	A	919	UDP	O4-C4-C5	-2.68	120.54	125.16
4	A	919	UDP	O2-C2-N1	-2.67	119.33	122.80

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	920	LDA	C2-C1-N1-O1
5	A	920	LDA	C2-C1-N1-CM1
5	A	920	LDA	C2-C1-N1-CM2
4	A	919	UDP	O4'-C4'-C5'-O5'
5	A	921	LDA	C11-C10-C9-C8
4	A	919	UDP	C3'-C4'-C5'-O5'
4	A	919	UDP	C2'-C1'-N1-C6
5	A	921	LDA	C4-C5-C6-C7
5	A	921	LDA	C1-C2-C3-C4
4	A	919	UDP	O4'-C1'-N1-C6
4	A	919	UDP	PA-O3A-PB-O1B
5	A	921	LDA	C9-C10-C11-C12
4	A	919	UDP	PA-O3A-PB-O2B
4	A	919	UDP	O4'-C1'-N1-C2
4	A	919	UDP	PB-O3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	A	919	UDP	C2'-C1'-N1-C2
4	A	919	UDP	PB-O3A-PA-O2A

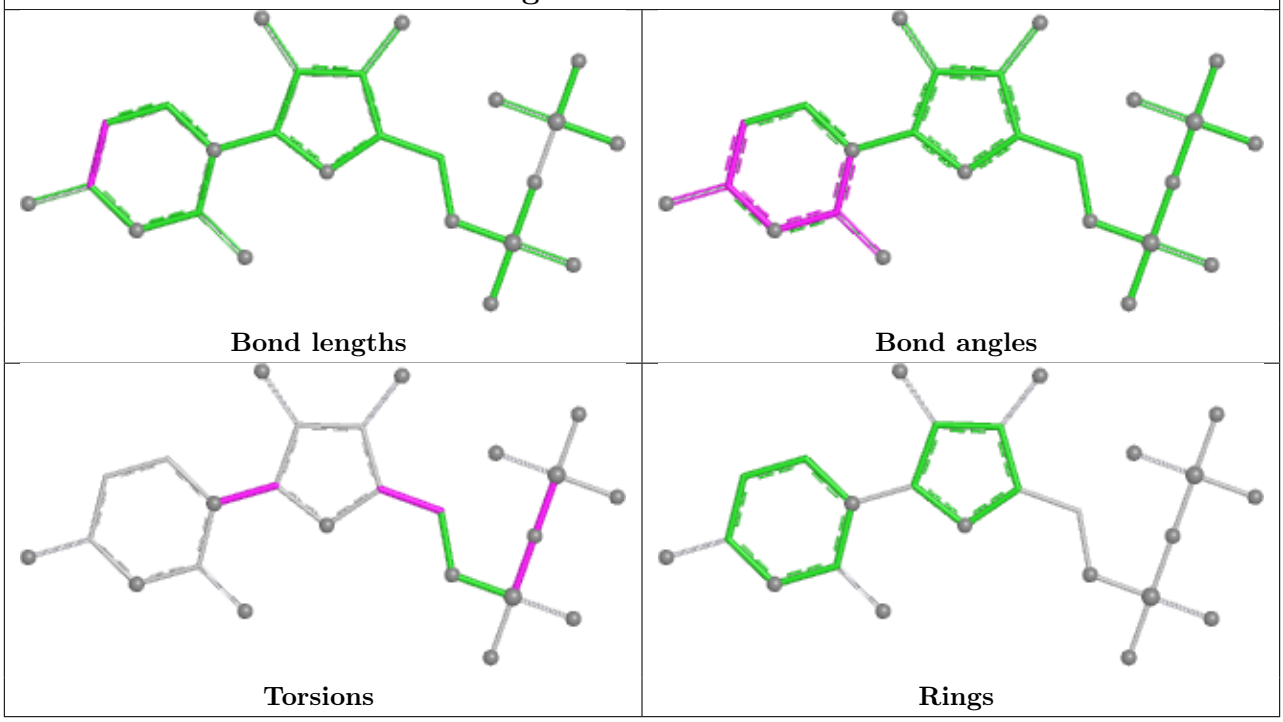
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	921	LDA	2	0
5	A	920	LDA	5	0
4	A	919	UDP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand UDP A 919



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	747/802 (93%)	-0.11	26 (3%)	44	40	77, 127, 205, 236	0
2	B	655/707 (92%)	-0.10	18 (2%)	54	51	82, 143, 210, 235	0
All	All	1402/1509 (92%)	-0.10	44 (3%)	49	47	77, 135, 208, 236	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	544	GLY	7.2
2	B	183	ALA	5.0
2	B	545	PRO	4.6
1	A	627	PRO	3.8
2	B	596	GLY	3.7
1	A	399	ARG	3.7
1	A	625	GLY	3.7
2	B	170	ASP	3.6
1	A	509	ASP	3.6
1	A	600	ASN	3.3
1	A	645	ASP	3.3
1	A	336	ALA	3.2
2	B	125	PHE	3.1
2	B	132	ALA	3.1
1	A	758	ASP	3.1
1	A	258	ARG	3.1
1	A	192	PRO	3.1
2	B	133	LEU	3.1
2	B	518	LEU	3.0
2	B	101	ARG	2.9
1	A	335	PHE	2.9
1	A	631	LEU	2.9
2	B	593	LEU	2.8
2	B	145	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	595	PRO	2.7
2	B	597	ASP	2.7
2	B	129	GLN	2.6
1	A	648	GLN	2.4
1	A	188	MET	2.4
1	A	626	ASP	2.4
1	A	629	PRO	2.3
1	A	362	ARG	2.3
1	A	187	CYS	2.3
1	A	672	ILE	2.3
1	A	510	GLU	2.2
1	A	630	ALA	2.2
1	A	601	ARG	2.2
2	B	718	ARG	2.2
1	A	502	ARG	2.1
2	B	510	THR	2.1
1	A	506	THR	2.0
2	B	112	GLN	2.0
1	A	624	VAL	2.0
1	A	507	ALA	2.0

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

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

6.3 Carbohydrates (i)

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	BGC	C	1	12/12	0.90	0.39	176,192,196,198	0
3	BGC	C	17	11/12	0.92	0.32	97,106,119,140	0
3	BGC	C	8	11/12	0.95	0.15	78,92,104,118	0
3	BGC	C	12	11/12	0.95	0.34	86,103,140,157	0
3	BGC	C	13	11/12	0.95	0.39	88,107,120,127	0
3	BGC	C	5	11/12	0.95	0.15	95,114,142,143	0
3	BGC	C	2	11/12	0.96	0.20	149,170,193,198	0
3	BGC	C	6	11/12	0.96	0.15	77,96,110,146	0

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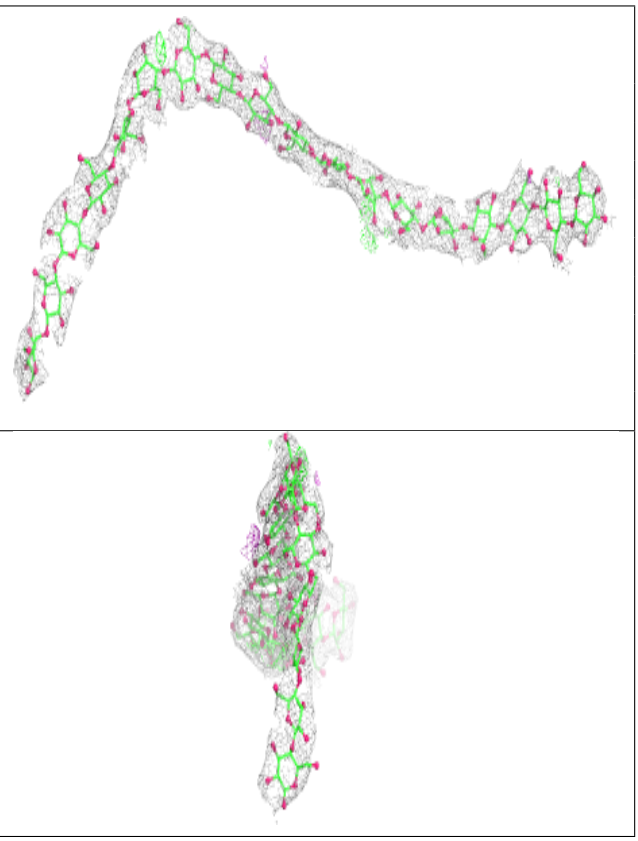
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BGC	C	18	11/12	0.96	0.28	116,121,136,142	0
3	BGC	C	4	11/12	0.97	0.11	97,115,128,142	0
3	BGC	C	15	11/12	0.97	0.33	108,116,170,173	0
3	BGC	C	16	11/12	0.97	0.26	90,104,129,158	0
3	BGC	C	10	11/12	0.97	0.17	82,97,109,114	0
3	BGC	C	7	11/12	0.97	0.17	79,109,137,143	0
3	BGC	C	3	11/12	0.98	0.09	100,112,144,154	0
3	BGC	C	14	11/12	0.98	0.32	97,114,126,129	0
3	BGC	C	11	11/12	0.99	0.22	83,93,108,111	0
3	BGC	C	9	11/12	0.99	0.18	70,96,103,127	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 C:

$2mF_o$-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)

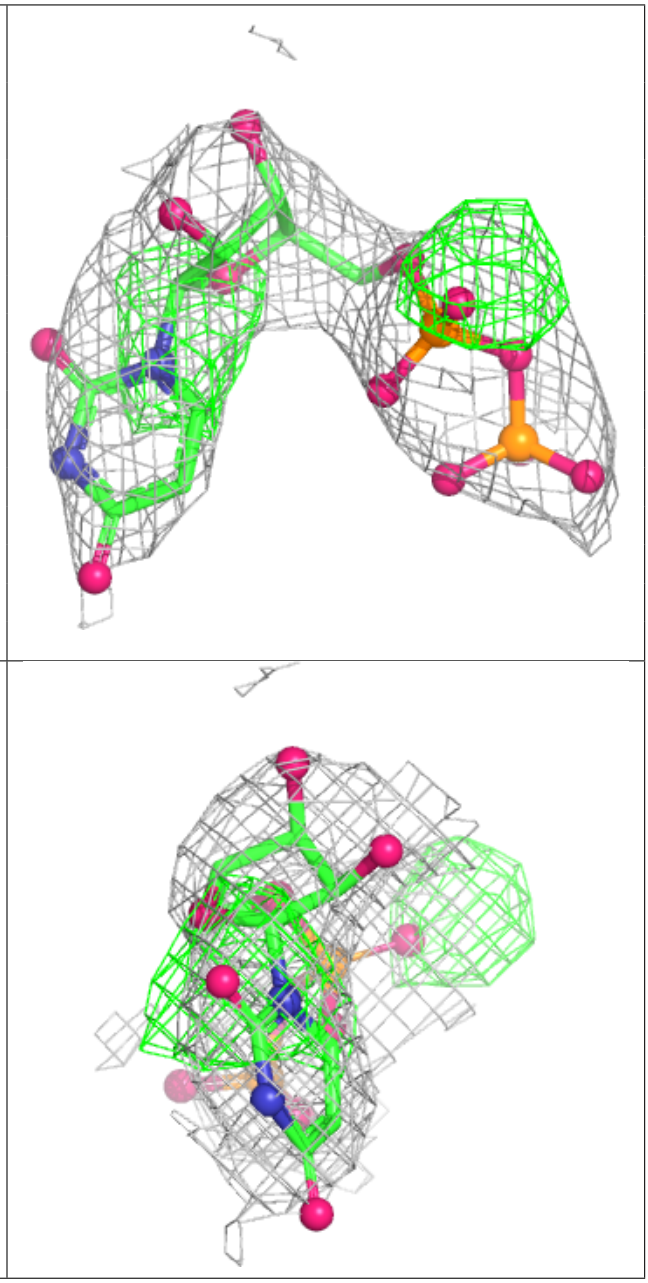
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	UDP	A	919	25/25	0.79	0.70	57,85,113,131	25
5	LDA	A	921	16/16	0.79	0.36	105,128,177,182	0
5	LDA	A	920	9/16	0.91	0.31	92,109,143,144	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UDP A 919:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.