



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:22 AM GMT

PDB ID : 3I74
Title : Crystal Structure of the plant subtilisin-like protease SBT3 in complex with a chloromethylketone inhibitor
Authors : Rose, R.; Ottmann, C.
Deposited on : 2009-07-08
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

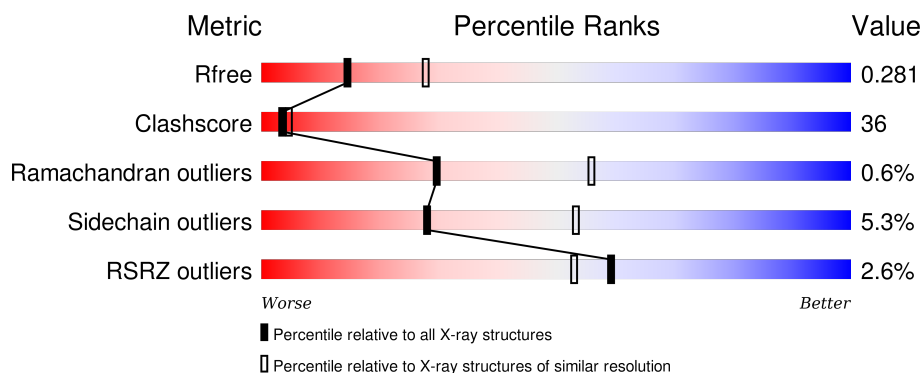
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	649	<div> <div>2%</div> <div>55%</div> <div>40%</div> <div>..</div> </div>
1	B	649	<div> <div>2%</div> <div>57%</div> <div>38%</div> <div>..</div> </div>
2	C	6	<div> <div>17%</div> <div>33%</div> <div>50%</div> <div>17%</div> </div>
2	D	6	<div> <div>17%</div> <div>50%</div> <div>33%</div> </div>

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
2	ALV	C	5	-	-	X	-
6	NAG	B	1300	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10391 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 Subtilisin-like protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			4844	3057	833	933	21			
1	B	640	Total	C	N	O	S	0	0	0
			4830	3051	831	927	21			

- Molecule 2 is a protein called ACE-PHE-GLU-LYS-ALA chloromethylketone INHIBITOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	1
			38	26	5	7			
2	D	6	Total	C	N	O	0	0	1
			38	26	5	7			

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			38	22	2	14		
4	B	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			38	22	2	14		

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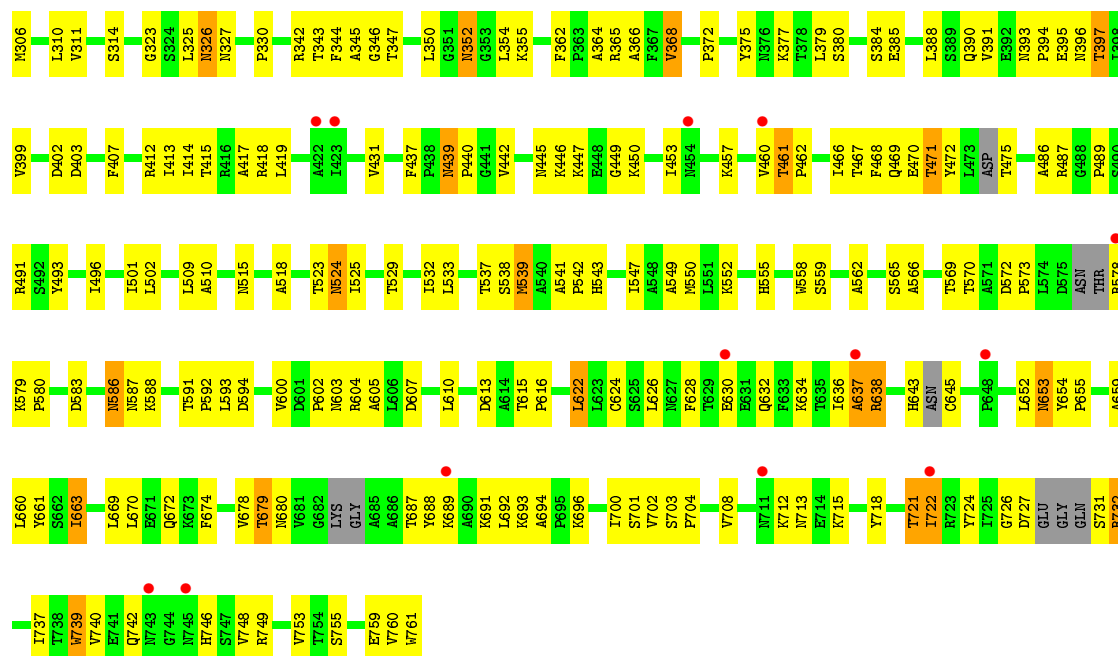
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 7 is water.

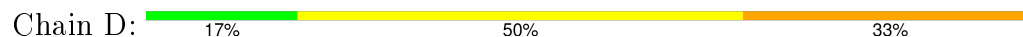
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	191	Total	O	0	0
			191	191		
7	C	1	Total	O	0	0
			1	1		
7	B	244	Total	O	0	0
			244	244		
7	D	1	Total	O	0	0
			1	1		



- Molecule 2: ACE-PHE-GLU-LYS-ALA chloromethylketone INHIBITOR



- Molecule 2: ACE-PHE-GLU-LYS-ALA chloromethylketone INHIBITOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	143.73 Å 143.73 Å 195.19 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.60 19.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.60) 99.8 (19.99-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.87 (at 2.59 Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.250 , 0.294 0.248 , 0.281	Depositor DCC
R_{free} test set	3155 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 63091 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10391	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ALV, NAG, 0QE, ACE, FUC

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	0.22	0/4951	0.41	0/6737
1	B	0.22	0/4936	0.40	0/6713
2	C	0.27	0/30	0.27	0/38
2	D	0.27	0/30	0.29	0/38
All	All	0.22	0/9947	0.40	0/13526

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	C	0	1
2	D	0	1
6	B	1	0
All	All	1	2

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	1300	NAG	C1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	4	LYS	Mainchain
2	D	4	LYS	Mainchain

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	4844	0	4783	369	0
1	B	4830	0	4778	316	0
2	C	38	0	35	20	0
2	D	38	0	35	20	0
3	A	28	0	25	1	0
4	A	38	0	34	3	0
4	B	38	0	34	4	0
5	A	38	0	34	7	0
5	B	38	0	34	8	0
6	B	24	0	22	4	0
7	A	191	0	0	32	0
7	B	244	0	0	26	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
All	All	10391	0	9814	712	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 36.

All (712) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:TYR:CE2	2:D:2:PHE:HB2	1.48	1.44
1:A:591:THR:CG2	1:A:592:PRO:HD2	1.67	1.23
1:A:538:SER:HG	2:C:5:ALV:C	1.53	1.18
1:A:237:ALA:H	1:A:471:THR:HG21	1.09	1.14
1:B:637:ALA:HB3	1:B:638:ARG:CA	1.77	1.13
1:B:637:ALA:CB	1:B:638:ARG:HA	1.73	1.11
1:B:591:THR:HG23	1:B:592:PRO:HD2	1.28	1.11
1:A:591:THR:HG23	1:A:592:PRO:CD	1.82	1.09
1:B:693:LYS:HD2	7:B:977:HOH:O	1.52	1.09
1:B:591:THR:CG2	1:B:592:PRO:HD2	1.81	1.09
1:B:175:GLN:O	1:B:210:ARG:NH1	1.85	1.08
1:A:175:GLN:O	1:A:210:ARG:NH1	1.88	1.07
1:A:638:ARG:CG	1:A:638:ARG:HH11	1.67	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LEU:HA	7:A:948:HOH:O	1.56	1.05
1:A:393:ASN:O	1:A:397:THR:HG22	1.57	1.04
1:B:674:PHE:HE2	1:B:722:ILE:CD1	1.71	1.04
1:A:591:THR:CG2	1:A:592:PRO:CD	2.36	1.03
1:A:638:ARG:HG3	1:A:638:ARG:NH1	1.60	1.03
1:B:287:TYR:CE2	2:D:2:PHE:CB	2.41	1.03
1:A:399:VAL:CG1	1:A:419:LEU:HD13	1.89	1.02
1:A:638:ARG:HH11	1:A:638:ARG:HG3	0.85	1.02
1:A:689:LYS:HD2	1:A:742:GLN:OE1	1.60	1.01
1:A:591:THR:HG23	1:A:592:PRO:HD2	1.05	1.01
1:B:393:ASN:O	1:B:397:THR:HG22	1.59	1.01
1:A:399:VAL:HG12	1:A:419:LEU:HD13	1.37	1.01
1:B:674:PHE:CE2	1:B:722:ILE:HD11	1.96	0.99
1:B:538:SER:OG	2:D:6:0QE:C1	2.09	0.99
1:B:116:THR:HG21	1:B:543:HIS:NE2	1.76	0.99
1:A:672:GLN:HG2	1:A:674:PHE:CZ	1.98	0.97
1:B:674:PHE:CE2	1:B:722:ILE:CD1	2.46	0.97
1:A:471:THR:HG23	7:A:851:HOH:O	1.64	0.97
1:B:566:ALA:O	1:B:570:THR:HG22	1.65	0.96
1:A:731:SER:HA	7:A:785:HOH:O	1.67	0.95
1:A:213:ASP:OD2	2:C:4:LYS:NZ	2.00	0.94
1:A:263:THR:HG23	1:A:296:ALA:HB2	1.50	0.93
2:D:2:PHE:CD1	2:D:3:GLU:N	2.36	0.93
1:B:591:THR:CG2	1:B:592:PRO:CD	2.47	0.93
1:A:493:TYR:CE2	1:A:495:GLY:HA3	2.04	0.93
1:B:637:ALA:HB3	1:B:638:ARG:HA	0.92	0.92
1:A:345:ALA:CB	1:A:472:TYR:HE1	1.84	0.91
1:B:385:GLU:HG3	7:B:80:HOH:O	1.71	0.89
1:B:123:ASN:HD22	1:B:125:SER:H	1.17	0.89
1:A:325:LEU:HA	1:A:486:ALA:HB1	1.54	0.89
1:B:285:TYR:CE2	2:D:4:LYS:HB3	2.07	0.89
1:B:591:THR:HG23	1:B:592:PRO:CD	2.01	0.89
1:A:352:ASN:ND2	1:A:354:LEU:H	1.71	0.88
1:B:610:LEU:HB3	1:B:678:VAL:CG2	2.04	0.88
1:B:287:TYR:HE2	2:D:2:PHE:HB2	1.39	0.88
1:B:384:SER:O	1:B:388:LEU:HD23	1.74	0.87
1:A:116:THR:HG21	1:A:543:HIS:NE2	1.89	0.87
1:B:388:LEU:O	1:B:391:VAL:HG12	1.73	0.87
1:A:461:THR:O	1:A:461:THR:HG22	1.73	0.87
1:B:213:ASP:OD2	2:D:4:LYS:NZ	2.08	0.86
1:A:287:TYR:CE2	2:C:2:PHE:CB	2.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ALA:N	1:A:471:THR:HG21	1.91	0.85
1:A:586:ASN:HD22	1:A:587:ASN:N	1.74	0.85
1:B:461:THR:O	1:B:461:THR:HG22	1.74	0.85
1:A:345:ALA:HB3	1:A:470:GLU:HB2	1.58	0.85
1:A:591:THR:HG22	1:A:593:LEU:H	1.42	0.83
1:B:674:PHE:HE2	1:B:722:ILE:HD13	1.43	0.83
1:B:287:TYR:CD2	2:D:2:PHE:HB2	2.13	0.82
1:A:460:VAL:O	1:A:461:THR:HB	1.78	0.82
1:B:460:VAL:O	1:B:461:THR:HB	1.79	0.82
1:A:502:LEU:O	1:A:600:VAL:HG23	1.80	0.82
1:A:566:ALA:O	1:A:570:THR:HG22	1.80	0.81
1:B:591:THR:HG22	1:B:593:LEU:H	1.46	0.81
1:B:450:LYS:HG2	7:B:912:HOH:O	1.81	0.80
1:A:323:GLY:O	1:A:491:ARG:HD2	1.79	0.80
1:A:352:ASN:HD22	1:A:352:ASN:C	1.85	0.80
1:B:583:ASP:HB3	1:B:586:ASN:HD21	1.47	0.80
1:B:721:THR:HG22	7:B:784:HOH:O	1.82	0.80
1:B:663:ILE:H	1:B:663:ILE:HD13	1.45	0.80
1:A:630:GLU:HB3	1:A:643:HIS:CD2	2.17	0.80
1:A:388:LEU:O	1:A:391:VAL:HG12	1.81	0.79
1:A:493:TYR:CZ	1:A:495:GLY:HA3	2.18	0.79
1:B:607:ASP:OD1	1:B:746:HIS:NE2	2.15	0.79
1:A:741:GLU:OE2	1:A:744:GLY:HA3	1.84	0.78
1:A:201:THR:HB	7:A:872:HOH:O	1.82	0.78
1:A:718:TYR:CE2	1:A:739:TRP:HH2	2.02	0.78
1:B:375:TYR:OH	1:B:377:LYS:HE3	1.83	0.78
1:A:538:SER:OG	2:C:6:0QE:C1	2.31	0.78
1:B:491:ARG:HG3	7:B:976:HOH:O	1.84	0.78
1:A:669:LEU:HD13	1:A:669:LEU:C	2.05	0.78
2:D:2:PHE:HD1	2:D:3:GLU:N	1.83	0.77
1:B:141:ALA:HB2	1:B:278:VAL:HG21	1.64	0.77
1:B:674:PHE:CE2	1:B:722:ILE:HD13	2.17	0.77
1:A:345:ALA:HB2	1:A:472:TYR:HE1	1.49	0.76
1:A:524:ASN:H	1:A:524:ASN:HD22	1.31	0.76
1:B:669:LEU:HD13	1:B:670:LEU:N	2.00	0.76
1:A:718:TYR:CZ	1:A:739:TRP:CH2	2.73	0.76
1:A:722:ILE:HD12	1:A:722:ILE:N	2.00	0.76
1:A:345:ALA:HB2	1:A:472:TYR:CE1	2.21	0.76
1:B:591:THR:HG22	1:B:592:PRO:HD2	1.68	0.76
1:A:674:PHE:HE2	1:A:722:ILE:HD13	1.50	0.76
1:A:461:THR:N	1:A:462:PRO:CD	2.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:GLU:OE2	1:A:445:ASN:HB2	1.85	0.75
1:A:263:THR:HG23	1:A:296:ALA:CB	2.16	0.75
1:A:566:ALA:O	1:A:570:THR:CG2	2.35	0.75
1:A:384:SER:O	1:A:388:LEU:HD23	1.86	0.75
1:B:138:VAL:HG11	1:B:549:ALA:HB1	1.68	0.75
1:B:238:PRO:HD2	7:B:106:HOH:O	1.86	0.75
1:B:737:ILE:HD11	1:B:739:TRP:CZ3	2.22	0.75
1:B:694:ALA:HB2	1:B:700:ILE:HG12	1.70	0.74
1:B:674:PHE:CD2	1:B:722:ILE:HD11	2.22	0.74
1:A:591:THR:HG22	1:A:592:PRO:CD	2.17	0.74
1:B:637:ALA:CB	1:B:638:ARG:CA	2.46	0.74
1:A:399:VAL:CG1	1:A:419:LEU:CD1	2.66	0.74
1:A:591:THR:HG22	1:A:592:PRO:N	2.02	0.73
1:A:693:LYS:NZ	1:A:693:LYS:HB2	2.03	0.73
1:A:169:ILE:HG12	7:A:952:HOH:O	1.89	0.73
3:A:1000:NAG:O6	3:A:1001:NAG:C1	2.36	0.73
1:A:287:TYR:HE2	2:C:2:PHE:HB3	1.53	0.73
1:A:622:LEU:O	1:A:626:LEU:CD1	2.36	0.73
1:A:491:ARG:O	1:A:760:VAL:HG13	1.89	0.72
1:B:501:ILE:CD1	1:B:600:VAL:HG22	2.19	0.72
1:A:742:GLN:NE2	1:A:742:GLN:HA	2.02	0.72
1:A:325:LEU:CA	1:A:486:ALA:HB1	2.20	0.72
1:B:722:ILE:HD12	1:B:722:ILE:H	1.55	0.71
1:A:287:TYR:CE2	2:C:2:PHE:HA	2.24	0.71
1:B:591:THR:HG22	1:B:592:PRO:CD	2.19	0.71
1:B:399:VAL:CG1	1:B:419:LEU:HD13	2.21	0.71
1:A:287:TYR:CE2	2:C:2:PHE:CA	2.73	0.71
1:B:524:ASN:H	1:B:524:ASN:HD22	1.37	0.71
1:A:697:ASN:CG	7:A:857:HOH:O	2.29	0.71
1:B:591:THR:HG22	1:B:592:PRO:N	2.06	0.70
1:A:399:VAL:HG11	1:A:419:LEU:CD1	2.20	0.70
1:A:622:LEU:O	1:A:622:LEU:HD23	1.91	0.70
1:A:418:ARG:HG3	1:B:418:ARG:NH2	2.07	0.70
1:A:579:LYS:HB3	1:A:580:PRO:CD	2.21	0.70
1:A:345:ALA:CB	1:A:472:TYR:CE1	2.72	0.70
1:B:722:ILE:HD12	1:B:722:ILE:N	2.06	0.70
1:B:467:THR:OG1	1:B:470:GLU:OE2	2.07	0.70
1:A:399:VAL:HG11	1:A:419:LEU:HD13	1.74	0.69
1:B:700:ILE:HG22	1:B:722:ILE:HG23	1.73	0.69
1:A:352:ASN:HD22	1:A:354:LEU:H	1.40	0.69
1:A:143:LEU:CD2	1:A:270:MET:HG2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:TYR:CD2	1:A:655:PRO:HD2	2.26	0.69
1:A:610:LEU:HB3	1:A:678:VAL:CG2	2.21	0.69
1:B:566:ALA:O	1:B:570:THR:CG2	2.41	0.69
1:A:691:LYS:C	1:A:692:LEU:HD12	2.13	0.69
1:A:703:SER:HA	1:A:704:PRO:C	2.12	0.69
1:B:177:ASN:H	1:B:180:MET:CE	2.07	0.68
1:B:136:GLN:HA	1:B:247:ARG:O	1.93	0.68
1:B:689:LYS:HD2	1:B:742:GLN:CD	2.13	0.68
1:A:591:THR:HG22	1:A:592:PRO:HD2	1.68	0.68
1:A:674:PHE:CE2	1:A:722:ILE:HD13	2.28	0.68
1:B:330:PRO:HB3	1:B:496:ILE:HD12	1.76	0.68
1:A:493:TYR:CE2	1:A:495:GLY:CA	2.76	0.68
1:A:552:LYS:HD3	1:A:552:LYS:O	1.94	0.68
1:A:311:VAL:N	7:A:948:HOH:O	2.26	0.68
1:B:570:THR:HG21	1:B:605:ALA:HA	1.76	0.68
1:B:737:ILE:CD1	1:B:739:TRP:CZ3	2.76	0.68
1:A:570:THR:HG21	1:A:605:ALA:HB2	1.76	0.67
1:A:287:TYR:CD2	2:C:2:PHE:HA	2.28	0.67
1:B:679:THR:HG22	7:B:790:HOH:O	1.94	0.67
1:A:570:THR:OG1	1:A:604:ARG:HB3	1.95	0.67
1:B:201:THR:CG2	1:B:201:THR:O	2.41	0.67
1:A:394:PRO:O	1:A:419:LEU:HA	1.95	0.67
1:A:158:GLY:C	7:A:877:HOH:O	2.32	0.67
1:B:143:LEU:HD21	1:B:270:MET:HG2	1.77	0.67
1:A:128:LEU:HD22	1:A:550:MET:HB3	1.76	0.67
2:D:2:PHE:C	2:D:2:PHE:CD1	2.69	0.66
1:B:323:GLY:O	1:B:491:ARG:HD2	1.95	0.66
1:B:123:ASN:HD22	1:B:125:SER:N	1.90	0.66
1:A:177:ASN:H	1:A:180:MET:HE2	1.60	0.66
1:A:136:GLN:HA	1:A:247:ARG:O	1.94	0.66
1:A:325:LEU:HA	1:A:486:ALA:CB	2.24	0.66
1:A:460:VAL:O	1:A:461:THR:CB	2.42	0.66
1:A:718:TYR:CE2	1:A:739:TRP:CH2	2.84	0.66
1:A:143:LEU:HD21	1:A:270:MET:HG2	1.76	0.66
1:A:167:LYS:HA	7:A:845:HOH:O	1.94	0.66
1:A:414:ILE:HG13	1:A:419:LEU:HD12	1.76	0.66
1:A:689:LYS:CD	1:A:742:GLN:OE1	2.42	0.66
1:A:634:LYS:HB3	1:A:634:LYS:NZ	2.10	0.66
1:B:731:SER:N	7:B:960:HOH:O	2.29	0.65
1:B:622:LEU:O	1:B:626:LEU:HD13	1.96	0.65
1:A:325:LEU:HD12	1:A:325:LEU:C	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ASN:O	1:B:397:THR:CG2	2.43	0.65
1:B:285:TYR:CE2	2:D:4:LYS:CB	2.80	0.65
1:A:654:TYR:CG	1:A:655:PRO:HD2	2.32	0.65
1:A:346:GLY:O	1:A:442:VAL:HG11	1.97	0.65
1:B:461:THR:N	1:B:462:PRO:CD	2.59	0.65
1:B:325:LEU:HA	1:B:486:ALA:HB1	1.78	0.65
1:B:674:PHE:HE2	1:B:722:ILE:HD11	1.36	0.65
1:B:399:VAL:HG12	1:B:419:LEU:HD13	1.79	0.65
1:A:586:ASN:ND2	1:A:588:LYS:H	1.94	0.65
1:A:586:ASN:O	1:A:587:ASN:HB2	1.96	0.65
1:B:491:ARG:HH21	1:B:759:GLU:HB2	1.62	0.65
1:A:287:TYR:CE2	2:C:2:PHE:HB3	2.30	0.65
1:A:326:ASN:HD22	1:A:326:ASN:C	2.01	0.64
1:B:570:THR:OG1	1:B:604:ARG:HB3	1.97	0.64
1:B:502:LEU:O	1:B:600:VAL:HG23	1.98	0.64
1:B:407:PHE:CD2	1:B:431:VAL:HG22	2.31	0.64
1:A:135:GLY:O	1:A:248:ALA:HA	1.97	0.64
1:A:123:ASN:HD22	1:A:125:SER:H	1.46	0.64
1:A:578:ARG:NE	1:A:578:ARG:HA	2.12	0.64
6:B:1300:NAG:H3	6:B:1301:FUC:H5	1.80	0.64
1:B:347:THR:HG21	1:B:355:LYS:HE3	1.80	0.63
1:B:732:ARG:N	1:B:732:ARG:HD3	2.13	0.63
1:A:352:ASN:HD22	1:A:353:GLY:N	1.96	0.63
1:B:215:HIS:CD2	2:D:6:0QE:C1	2.78	0.63
1:B:491:ARG:O	1:B:760:VAL:HG13	1.99	0.63
1:B:442:VAL:HG23	1:B:466:ILE:HD13	1.79	0.63
1:B:368:VAL:O	1:B:368:VAL:HG22	1.98	0.63
1:B:460:VAL:O	1:B:461:THR:CB	2.47	0.63
1:B:346:GLY:HA2	1:B:467:THR:O	1.99	0.63
1:A:591:THR:CG2	1:A:592:PRO:N	2.59	0.63
1:A:156:ASP:OD1	1:A:182:ASN:HB2	1.99	0.63
1:A:461:THR:H	1:A:462:PRO:HD2	1.64	0.62
1:B:439:ASN:ND2	1:B:440:PRO:HD2	2.15	0.62
1:B:447:LYS:HE3	7:B:829:HOH:O	1.99	0.62
1:A:672:GLN:CG	1:A:674:PHE:CZ	2.79	0.62
1:A:141:ALA:HB2	1:A:278:VAL:HG21	1.82	0.62
1:B:501:ILE:HD13	1:B:600:VAL:HG22	1.81	0.62
1:A:123:ASN:HD21	1:A:126:SER:H	1.46	0.62
1:B:302:PHE:O	1:B:306:MET:HG2	1.99	0.62
1:B:399:VAL:HG11	1:B:419:LEU:CD1	2.30	0.62
5:B:1501:NAG:O5	5:B:1502:FUC:H5	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:THR:HB	1:A:715:LYS:HG2	1.81	0.61
1:A:702:VAL:HG22	1:A:703:SER:N	2.15	0.61
1:B:610:LEU:HB3	1:B:678:VAL:HG22	1.82	0.61
1:B:669:LEU:HD13	1:B:669:LEU:C	2.20	0.61
1:B:610:LEU:HD23	1:B:680:ASN:HA	1.83	0.61
1:A:342:ARG:HD3	1:A:344:PHE:CE2	2.36	0.61
1:A:586:ASN:HD22	1:A:587:ASN:H	1.48	0.61
1:A:611:VAL:HG23	1:A:679:THR:HG23	1.83	0.61
1:B:395:GLU:HG3	7:B:9:HOH:O	2.00	0.61
1:A:610:LEU:HB2	1:A:748:VAL:HG21	1.81	0.61
1:B:345:ALA:HB3	1:B:472:TYR:HE1	1.66	0.61
1:B:143:LEU:CD2	1:B:270:MET:HG2	2.30	0.61
1:A:390:GLN:NE2	5:A:1201:NAG:O6	2.34	0.60
1:B:586:ASN:HD22	1:B:587:ASN:N	2.00	0.60
1:B:583:ASP:HB3	1:B:586:ASN:ND2	2.15	0.60
1:A:538:SER:OG	2:C:5:ALV:O	2.04	0.60
1:A:742:GLN:CA	1:A:742:GLN:NE2	2.64	0.60
1:A:199:ASP:OD1	1:A:201:THR:HB	2.00	0.60
1:B:493:TYR:CE1	7:B:845:HOH:O	2.51	0.60
1:A:129:TRP:CG	1:A:134:LEU:HD22	2.36	0.60
1:B:541:ALA:N	1:B:542:PRO:HD2	2.17	0.60
1:B:610:LEU:HB2	1:B:748:VAL:HG21	1.84	0.60
1:B:547:ILE:HD12	1:B:600:VAL:HG11	1.83	0.60
1:A:742:GLN:CA	1:A:742:GLN:HE21	2.15	0.60
1:A:302:PHE:O	1:A:306:MET:HG2	2.02	0.60
1:A:201:THR:O	1:A:201:THR:CG2	2.50	0.60
1:B:689:LYS:HD2	1:B:742:GLN:NE2	2.17	0.60
1:B:120:LEU:O	1:B:121:LYS:HB2	2.02	0.60
1:A:428:ASP:OD1	1:A:430:GLY:N	2.33	0.60
1:B:325:LEU:HD12	1:B:325:LEU:C	2.20	0.59
1:A:164:LYS:HD2	1:A:165:ARG:N	2.17	0.59
1:B:414:ILE:HD12	1:B:419:LEU:HD12	1.85	0.59
1:B:718:TYR:CZ	1:B:739:TRP:CZ3	2.90	0.59
1:B:449:GLY:O	1:B:453:ILE:HG13	2.03	0.59
1:A:718:TYR:CZ	1:A:739:TRP:CZ3	2.90	0.59
1:B:442:VAL:CG2	1:B:466:ILE:HD13	2.32	0.59
1:B:128:LEU:HD22	1:B:550:MET:HB3	1.84	0.59
1:B:634:LYS:O	1:B:638:ARG:HB3	2.03	0.59
1:A:461:THR:H	1:A:462:PRO:CD	2.15	0.59
1:A:287:TYR:CE2	2:C:2:PHE:HB2	2.38	0.59
1:B:372:PRO:HD2	1:B:396:ASN:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ASP:OD1	1:A:428:ASP:C	2.41	0.59
1:A:233:HIS:O	1:A:233:HIS:CD2	2.56	0.58
1:A:663:ILE:HD13	1:A:663:ILE:H	1.68	0.58
1:A:418:ARG:NH2	1:B:418:ARG:HG3	2.18	0.58
1:B:263:THR:HG23	1:B:296:ALA:HB2	1.85	0.58
1:B:199:ASP:OD1	1:B:201:THR:HB	2.03	0.58
1:A:541:ALA:N	1:A:542:PRO:HD2	2.19	0.58
1:A:350:LEU:N	1:A:350:LEU:HD12	2.19	0.58
1:B:290:ILE:H	1:B:290:ILE:HD13	1.69	0.58
1:A:669:LEU:CD1	1:A:669:LEU:C	2.71	0.58
1:B:325:LEU:HD12	1:B:325:LEU:O	2.04	0.58
1:A:263:THR:CG2	1:A:296:ALA:HB2	2.29	0.58
1:A:310:LEU:CA	7:A:948:HOH:O	2.30	0.58
1:B:128:LEU:HD13	1:B:550:MET:CE	2.33	0.58
1:A:138:VAL:HG22	1:A:139:ILE:N	2.19	0.57
1:A:143:LEU:CD2	1:A:270:MET:CG	2.82	0.57
1:B:295:ASP:O	1:B:299:ILE:HG13	2.04	0.57
1:A:123:ASN:ND2	1:A:126:SER:H	2.02	0.57
1:B:630:GLU:HB3	1:B:643:HIS:CD2	2.39	0.57
1:A:352:ASN:ND2	1:A:352:ASN:C	2.58	0.57
1:A:461:THR:CG2	1:A:461:THR:O	2.46	0.57
1:A:583:ASP:HB3	1:A:586:ASN:HD21	1.67	0.57
1:B:524:ASN:N	1:B:524:ASN:HD22	2.03	0.57
1:B:266:LEU:HD21	1:B:297:ILE:HG12	1.87	0.57
1:B:591:THR:CG2	1:B:592:PRO:N	2.66	0.57
1:B:538:SER:OG	2:D:5:ALV:O	2.15	0.57
1:A:689:LYS:HE2	1:A:742:GLN:HG3	1.87	0.57
1:B:399:VAL:CG1	1:B:419:LEU:CD1	2.83	0.57
1:B:701:SER:OG	1:B:721:THR:HG23	2.04	0.56
1:B:123:ASN:HD21	1:B:126:SER:H	1.51	0.56
1:B:718:TYR:CD2	1:B:739:TRP:HH2	2.23	0.56
1:B:266:LEU:HD12	1:B:266:LEU:O	2.05	0.56
1:B:652:LEU:HD13	1:B:653:ASN:N	2.19	0.56
1:A:693:LYS:HZ2	1:A:693:LYS:HB2	1.70	0.56
1:A:287:TYR:HE2	2:C:2:PHE:CB	2.08	0.56
1:B:201:THR:O	1:B:201:THR:HG22	2.05	0.56
1:B:442:VAL:HG22	1:B:466:ILE:HG21	1.86	0.55
1:B:538:SER:CB	1:B:539:MET:HE3	2.37	0.55
1:A:570:THR:HG21	1:A:605:ALA:CB	2.36	0.55
1:B:394:PRO:HA	1:B:397:THR:CG2	2.37	0.55
1:A:742:GLN:N	1:A:742:GLN:HE21	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:VAL:HG22	1:A:139:ILE:H	1.72	0.55
1:B:135:GLY:O	1:B:248:ALA:HA	2.06	0.55
1:B:688:TYR:CB	1:B:739:TRP:HD1	2.19	0.55
1:B:688:TYR:HB3	1:B:739:TRP:HD1	1.72	0.55
2:D:2:PHE:HD1	2:D:3:GLU:H	1.53	0.55
1:B:238:PRO:HD2	1:B:471:THR:HG21	1.89	0.55
1:A:718:TYR:CE1	1:A:739:TRP:CH2	2.95	0.55
1:B:218:HIS:CE1	1:B:510:ALA:HB3	2.40	0.55
1:B:579:LYS:HB3	1:B:580:PRO:HD2	1.89	0.55
1:B:515:ASN:HB3	7:B:953:HOH:O	2.07	0.55
1:B:493:TYR:HE2	1:B:496:ILE:HG13	1.72	0.54
1:B:123:ASN:ND2	1:B:125:SER:H	1.97	0.54
1:B:143:LEU:N	1:B:143:LEU:HD12	2.23	0.54
1:B:394:PRO:O	1:B:419:LEU:HA	2.07	0.54
1:A:128:LEU:CD2	1:A:550:MET:HB3	2.38	0.54
1:A:120:LEU:O	1:A:121:LYS:HB2	2.07	0.54
1:A:417:ALA:O	1:A:418:ARG:HB2	2.06	0.54
1:A:449:GLY:O	1:A:453:ILE:HG13	2.06	0.54
1:B:636:ILE:O	1:B:637:ALA:C	2.45	0.54
1:B:622:LEU:HD23	1:B:622:LEU:O	2.06	0.54
1:A:661:TYR:O	1:A:661:TYR:CD2	2.59	0.54
1:A:237:ALA:N	1:A:238:PRO:CD	2.71	0.54
1:A:579:LYS:HB3	1:A:580:PRO:HD2	1.89	0.54
1:A:352:ASN:HD21	1:A:354:LEU:CB	2.21	0.54
1:A:524:ASN:N	1:A:524:ASN:HD22	1.99	0.54
1:A:266:LEU:HD12	1:A:266:LEU:O	2.07	0.54
1:B:691:LYS:C	1:B:692:LEU:HD12	2.28	0.54
1:B:114:THR:HG23	1:B:509:LEU:HD23	1.90	0.54
2:D:2:PHE:O	2:D:3:GLU:CG	2.55	0.53
1:A:461:THR:N	1:A:462:PRO:HD2	2.22	0.53
1:B:659:ALA:HB1	1:B:724:TYR:CZ	2.42	0.53
5:B:1500:NAG:O7	5:B:1500:NAG:H3	2.07	0.53
1:A:570:THR:HG21	1:A:605:ALA:CA	2.38	0.53
1:A:693:LYS:NZ	1:A:693:LYS:CB	2.71	0.53
1:B:702:VAL:HG22	1:B:703:SER:N	2.24	0.53
1:B:663:ILE:HD13	1:B:663:ILE:N	2.19	0.53
1:A:532:ILE:HG12	1:A:533:LEU:N	2.24	0.53
1:A:630:GLU:CB	1:A:643:HIS:CD2	2.88	0.53
1:A:129:TRP:CG	1:A:134:LEU:CD2	2.91	0.53
5:A:1201:NAG:H61	5:A:1202:NAG:C7	2.39	0.53
1:A:393:ASN:O	1:A:397:THR:CG2	2.45	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:PHE:O	2:D:3:GLU:HG3	2.08	0.53
1:A:538:SER:HG	2:C:5:ALV:CA	2.21	0.53
1:A:326:ASN:HB2	7:A:809:HOH:O	2.08	0.53
1:A:177:ASN:H	1:A:180:MET:CE	2.21	0.53
1:A:487:ARG:HD2	1:A:594:ASP:OD1	2.09	0.53
4:B:1400:NAG:H62	4:B:1402:NAG:C1	2.39	0.53
1:A:661:TYR:CD2	1:A:726:GLY:HA3	2.44	0.53
1:A:218:HIS:CE1	1:A:510:ALA:HB3	2.44	0.53
1:A:742:GLN:HE21	1:A:742:GLN:HA	1.71	0.52
1:A:285:TYR:CE2	2:C:4:LYS:HB3	2.44	0.52
6:B:1300:NAG:C3	6:B:1301:FUC:H5	2.40	0.52
1:A:536:GLY:HA2	7:A:791:HOH:O	2.09	0.52
1:B:569:THR:HA	1:B:749:ARG:O	2.09	0.52
1:A:578:ARG:HA	1:A:578:ARG:HE	1.72	0.52
1:B:630:GLU:HG2	7:B:871:HOH:O	2.09	0.52
1:B:352:ASN:ND2	1:B:354:LEU:H	2.08	0.52
1:A:368:VAL:HG22	1:A:368:VAL:O	2.07	0.52
1:B:127:GLY:HA3	1:B:603:ASN:OD1	2.09	0.52
1:A:702:VAL:HG22	1:A:703:SER:H	1.73	0.52
1:B:570:THR:HG21	1:B:605:ALA:CA	2.39	0.52
1:A:418:ARG:HG3	1:B:418:ARG:HH21	1.73	0.52
1:B:164:LYS:HD2	1:B:165:ARG:N	2.23	0.52
1:B:663:ILE:CD1	1:B:663:ILE:H	2.20	0.52
1:B:610:LEU:HB3	1:B:678:VAL:HG21	1.88	0.52
1:A:737:ILE:HD11	1:A:739:TRP:CH2	2.45	0.52
1:A:278:VAL:CG1	1:A:280:MET:O	2.57	0.52
1:A:538:SER:C	1:A:539:MET:HE3	2.30	0.52
1:A:201:THR:CB	7:A:872:HOH:O	2.49	0.52
6:B:1300:NAG:H3	6:B:1301:FUC:C5	2.40	0.52
1:A:538:SER:HG	2:C:5:ALV:CB	2.24	0.51
1:B:221:SER:OG	1:B:510:ALA:HB1	2.09	0.51
1:A:674:PHE:HE2	1:A:722:ILE:CD1	2.21	0.51
1:B:292:LEU:HG	7:B:913:HOH:O	2.10	0.51
1:A:501:ILE:CD1	1:A:600:VAL:HG22	2.41	0.51
1:A:352:ASN:HD21	1:A:354:LEU:H	1.57	0.51
1:B:679:THR:HB	1:B:715:LYS:HG2	1.93	0.51
1:A:220:ALA:O	1:A:223:THR:HG22	2.10	0.51
1:A:592:PRO:HG2	1:A:753:VAL:HB	1.93	0.51
1:B:238:PRO:CD	1:B:471:THR:HG21	2.40	0.51
1:A:151:SER:HB3	1:A:154:PHE:CD1	2.46	0.51
1:A:287:TYR:CZ	2:C:2:PHE:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ARG:NE	7:B:62:HOH:O	2.43	0.51
1:B:727:ASP:OD1	1:B:731:SER:HB3	2.10	0.51
1:B:622:LEU:CD2	1:B:622:LEU:C	2.79	0.51
4:B:1401:FUC:C6	4:B:1402:NAG:H2	2.41	0.51
1:A:237:ALA:H	1:A:471:THR:CG2	2.01	0.50
1:A:674:PHE:CE2	1:A:722:ILE:CD1	2.95	0.50
5:A:1202:NAG:O5	5:A:1203:FUC:H5	2.11	0.50
1:A:622:LEU:O	1:A:626:LEU:HD13	2.09	0.50
1:A:362:PHE:CE2	1:A:366:ALA:HB2	2.46	0.50
1:A:668:THR:O	1:A:669:LEU:C	2.49	0.50
1:B:496:ILE:HB	7:B:995:HOH:O	2.11	0.50
1:A:266:LEU:HD21	1:A:297:ILE:HG12	1.94	0.50
1:B:712:LYS:O	1:B:713:ASN:HB2	2.11	0.50
4:B:1401:FUC:H62	4:B:1402:NAG:H2	1.93	0.50
1:A:460:VAL:HG22	7:A:863:HOH:O	2.12	0.50
1:A:555:HIS:HB3	1:A:558:TRP:CD1	2.47	0.50
1:B:457:LYS:HG2	7:B:821:HOH:O	2.10	0.50
1:B:123:ASN:ND2	1:B:126:SER:H	2.10	0.49
1:A:350:LEU:CD1	1:A:350:LEU:N	2.76	0.49
1:A:325:LEU:HD12	1:A:325:LEU:O	2.12	0.49
1:A:312:SER:N	7:A:57:HOH:O	2.44	0.49
1:A:613:ASP:OD1	1:A:614:ALA:N	2.42	0.49
1:B:266:LEU:HD21	1:B:297:ILE:CG1	2.42	0.49
1:B:460:VAL:HG23	1:B:460:VAL:O	2.12	0.49
1:A:129:TRP:CD2	1:A:134:LEU:HD22	2.47	0.49
1:B:652:LEU:HD13	1:B:652:LEU:C	2.32	0.49
1:B:412:ARG:NH2	1:B:413:ILE:HD11	2.27	0.49
1:A:391:VAL:HG13	1:A:391:VAL:O	2.12	0.49
1:A:622:LEU:CD2	1:A:622:LEU:C	2.81	0.49
5:A:1201:NAG:O4	5:A:1203:FUC:H5	2.13	0.49
1:B:326:ASN:HD22	1:B:326:ASN:C	2.15	0.49
1:B:123:ASN:ND2	1:B:125:SER:HB2	2.28	0.49
1:B:737:ILE:HD11	1:B:739:TRP:CH2	2.47	0.49
1:A:634:LYS:HB3	1:A:634:LYS:HZ3	1.77	0.49
5:A:1201:NAG:H61	5:A:1202:NAG:N2	2.27	0.49
1:A:536:GLY:CA	7:A:791:HOH:O	2.60	0.49
1:B:156:ASP:OD1	1:B:182:ASN:HB2	2.11	0.49
1:B:192:ASN:ND2	1:B:207:ASN:OD1	2.45	0.49
1:A:570:THR:HG23	7:A:814:HOH:O	2.11	0.49
1:A:290:ILE:H	1:A:290:ILE:HD13	1.77	0.49
1:B:247:ARG:HD2	7:B:62:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:LYS:HD3	7:B:901:HOH:O	2.13	0.49
1:B:737:ILE:HD13	1:B:739:TRP:CZ3	2.48	0.48
1:B:547:ILE:CD1	1:B:600:VAL:HG11	2.43	0.48
1:B:634:LYS:O	1:B:638:ARG:CB	2.60	0.48
1:A:586:ASN:ND2	1:A:587:ASN:N	2.55	0.48
1:B:669:LEU:CD1	1:B:669:LEU:C	2.82	0.48
1:A:123:ASN:HD22	1:A:125:SER:N	2.11	0.48
1:A:218:HIS:O	1:A:222:ILE:HG13	2.13	0.48
1:A:652:LEU:HD13	1:A:653:ASN:N	2.28	0.48
1:A:412:ARG:NH2	1:A:413:ILE:HD11	2.28	0.48
1:A:166:TRP:CZ2	1:A:168:GLY:HA3	2.48	0.48
1:B:148:TRP:CD1	1:B:150:GLU:HG2	2.49	0.48
1:A:582:LYS:HD2	1:A:587:ASN:O	2.13	0.48
1:A:626:LEU:HD12	1:A:626:LEU:N	2.27	0.48
1:B:143:LEU:CD2	1:B:270:MET:CG	2.91	0.48
1:A:129:TRP:HB3	1:A:134:LEU:CD2	2.43	0.48
1:A:539:MET:HE3	1:A:539:MET:N	2.29	0.48
1:B:238:PRO:CD	7:B:106:HOH:O	2.54	0.48
1:A:390:GLN:HE22	5:A:1202:NAG:HN2	1.60	0.48
1:A:231:VAL:HG11	1:A:531:TYR:CE1	2.49	0.48
1:B:287:TYR:CZ	2:D:2:PHE:HB2	2.32	0.48
1:A:144:ASP:O	1:A:254:LYS:HA	2.14	0.48
1:A:116:THR:HG21	1:A:543:HIS:CD2	2.48	0.48
1:B:123:ASN:ND2	1:B:125:SER:N	2.59	0.48
1:B:524:ASN:ND2	1:B:525:ILE:HG13	2.29	0.48
1:A:379:LEU:HD12	1:A:380:SER:N	2.29	0.48
1:A:337:SER:OG	1:A:505:GLY:HA3	2.14	0.48
1:B:538:SER:OG	2:D:5:ALV:CA	2.55	0.47
1:A:669:LEU:HD13	1:A:670:LEU:N	2.28	0.47
1:A:622:LEU:HA	1:A:649:SER:O	2.14	0.47
1:B:342:ARG:HD3	1:B:344:PHE:CE2	2.48	0.47
1:A:569:THR:HA	1:A:749:ARG:O	2.14	0.47
1:B:151:SER:HB3	1:B:154:PHE:CD1	2.48	0.47
1:A:201:THR:HG22	1:A:201:THR:O	2.14	0.47
1:B:760:VAL:HG12	1:B:761:TRP:N	2.29	0.47
1:A:386:GLU:O	1:A:390:GLN:HG3	2.15	0.47
1:B:138:VAL:CG1	1:B:139:ILE:N	2.77	0.47
5:B:1501:NAG:C1	5:B:1502:FUC:H5	2.44	0.47
1:A:379:LEU:HD12	1:A:379:LEU:C	2.34	0.47
1:B:532:ILE:HG12	1:B:533:LEU:N	2.30	0.47
1:B:393:ASN:N	1:B:394:PRO:CD	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:ALA:HB3	1:B:468:PHE:CE1	2.49	0.47
1:B:592:PRO:HG2	1:B:753:VAL:HB	1.97	0.47
1:A:461:THR:N	1:A:462:PRO:HD3	2.30	0.47
1:B:237:ALA:N	1:B:238:PRO:CD	2.78	0.47
5:B:1500:NAG:H61	5:B:1501:NAG:N2	2.30	0.47
1:B:148:TRP:NE1	1:B:150:GLU:HG2	2.29	0.47
1:A:518:ALA:CB	1:A:529:THR:HG22	2.44	0.47
1:B:689:LYS:HE2	1:B:742:GLN:HG3	1.95	0.47
1:A:259:GLU:OE2	1:A:259:GLU:N	2.48	0.47
1:B:461:THR:H	1:B:462:PRO:CD	2.28	0.47
1:B:586:ASN:O	1:B:587:ASN:HB2	2.15	0.47
1:A:703:SER:CA	1:A:704:PRO:O	2.63	0.47
1:A:589:ALA:HB1	7:A:946:HOH:O	2.14	0.47
1:B:394:PRO:HA	1:B:397:THR:HG23	1.96	0.47
1:A:701:SER:OG	1:A:721:THR:HG23	2.15	0.47
1:A:673:LYS:HG2	1:A:721:THR:HB	1.96	0.46
1:A:325:LEU:CD1	1:A:325:LEU:C	2.83	0.46
1:A:143:LEU:HD12	1:A:143:LEU:N	2.30	0.46
1:B:287:TYR:CD2	2:D:2:PHE:CB	2.87	0.46
1:A:583:ASP:HB3	1:A:586:ASN:ND2	2.30	0.46
1:A:622:LEU:CD2	1:A:622:LEU:O	2.61	0.46
1:B:380:SER:HG	1:B:402:ASP:CG	2.16	0.46
5:A:1202:NAG:C1	5:A:1203:FUC:H5	2.45	0.46
1:B:350:LEU:HD22	1:B:354:LEU:HD23	1.97	0.46
1:A:157:ASP:CG	7:A:909:HOH:O	2.53	0.46
1:B:461:THR:CG2	1:B:461:THR:O	2.47	0.46
1:B:233:HIS:O	1:B:233:HIS:CD2	2.69	0.46
1:A:637:ALA:O	1:A:638:ARG:C	2.54	0.46
1:A:472:TYR:HB3	7:A:782:HOH:O	2.14	0.46
1:B:128:LEU:HD13	1:B:550:MET:HE3	1.98	0.46
1:A:722:ILE:CD1	1:A:722:ILE:N	2.72	0.46
1:A:727:ASP:OD1	1:A:731:SER:CB	2.64	0.46
1:A:420:LYS:O	1:A:421:ALA:HB2	2.16	0.46
1:A:290:ILE:N	1:A:290:ILE:HD13	2.31	0.46
1:B:687:THR:HG22	1:B:708:VAL:HG13	1.98	0.46
1:A:586:ASN:HD22	1:A:586:ASN:C	2.12	0.45
1:B:586:ASN:ND2	1:B:588:LYS:H	2.14	0.45
1:A:176:PHE:CE2	1:A:180:MET:HB3	2.51	0.45
1:B:628:PHE:HB3	1:B:632:GLN:HB2	1.98	0.45
1:A:368:VAL:HG13	1:A:466:ILE:O	2.16	0.45
1:A:310:LEU:C	7:A:948:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:HD21	1:A:270:MET:CG	2.44	0.45
1:A:135:GLY:O	1:A:138:VAL:HG12	2.16	0.45
1:A:171:LYS:HA	1:A:172:PRO:HD3	1.77	0.45
1:A:330:PRO:HB3	1:A:496:ILE:HD12	1.98	0.45
1:A:524:ASN:ND2	1:A:525:ILE:HG13	2.32	0.45
1:B:689:LYS:CD	1:B:742:GLN:CD	2.83	0.45
1:B:442:VAL:CG2	1:B:466:ILE:HG21	2.46	0.45
1:B:380:SER:OG	1:B:402:ASP:OD2	2.31	0.45
1:A:476:LYS:NZ	7:A:800:HOH:O	2.50	0.45
1:A:727:ASP:OD1	1:A:731:SER:HB3	2.17	0.45
1:B:325:LEU:CA	1:B:486:ALA:HB1	2.43	0.45
1:B:129:TRP:CG	1:B:134:LEU:CD2	3.00	0.45
1:B:237:ALA:H	1:B:471:THR:HG21	1.81	0.45
1:A:580:PRO:O	1:A:582:LYS:NZ	2.44	0.45
1:B:208:SER:O	1:B:254:LYS:HD3	2.16	0.45
1:A:622:LEU:C	1:A:622:LEU:HD23	2.37	0.45
1:B:166:TRP:CZ2	1:B:168:GLY:HA3	2.52	0.45
1:B:165:ARG:HB3	1:B:165:ARG:HE	1.66	0.45
1:A:379:LEU:C	1:A:381:ASP:H	2.20	0.45
1:A:749:ARG:HB3	7:A:844:HOH:O	2.17	0.45
1:A:244:VAL:CG1	1:A:546:GLY:HA3	2.47	0.45
1:B:281:ILE:HB	1:B:311:VAL:HG22	1.98	0.45
1:A:678:VAL:O	1:A:678:VAL:HG13	2.17	0.45
1:A:342:ARG:HD3	1:A:344:PHE:CZ	2.52	0.45
1:A:379:LEU:C	1:A:381:ASP:N	2.70	0.45
1:B:672:GLN:HG2	1:B:674:PHE:CZ	2.52	0.44
1:A:283:ILE:HG23	1:A:283:ILE:O	2.17	0.44
1:B:552:LYS:O	1:B:552:LYS:HD3	2.17	0.44
1:A:460:VAL:O	1:A:460:VAL:HG23	2.17	0.44
1:A:161:GLU:HG2	1:A:183:ARG:NH1	2.33	0.44
1:B:365:ARG:O	1:B:365:ARG:HG2	2.18	0.44
1:B:461:THR:H	1:B:462:PRO:HD2	1.82	0.44
1:B:266:LEU:C	1:B:266:LEU:HD12	2.38	0.44
1:A:615:THR:HB	1:A:616:PRO:HD2	2.00	0.44
1:A:502:LEU:HD22	1:A:503:ALA:N	2.33	0.44
1:B:622:LEU:HD23	1:B:622:LEU:C	2.38	0.44
1:A:208:SER:O	1:A:254:LYS:HD3	2.18	0.44
1:A:266:LEU:HD12	1:A:266:LEU:C	2.38	0.44
1:B:417:ALA:O	1:B:418:ARG:HB2	2.18	0.44
1:A:502:LEU:CD2	1:A:503:ALA:H	2.30	0.44
1:A:394:PRO:HA	1:A:397:THR:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:THR:HA	1:A:116:THR:HB	2.00	0.44
1:B:280:MET:SD	1:B:310:LEU:HB3	2.58	0.44
1:A:693:LYS:HZ3	1:A:693:LYS:CB	2.31	0.44
1:A:610:LEU:HD23	1:A:680:ASN:HA	2.00	0.44
1:A:129:TRP:CB	1:A:134:LEU:CD2	2.95	0.44
1:A:679:THR:HG22	7:A:52:HOH:O	2.18	0.44
1:A:366:ALA:HB3	1:A:468:PHE:CE1	2.53	0.44
1:B:489:PRO:CB	7:B:823:HOH:O	2.64	0.44
1:A:697:ASN:O	1:A:698:SER:HB3	2.18	0.44
1:B:362:PHE:CE2	1:B:366:ALA:HB2	2.53	0.44
1:A:721:THR:C	1:A:722:ILE:HD12	2.39	0.43
1:B:290:ILE:HD13	1:B:290:ILE:N	2.31	0.43
1:B:615:THR:HB	1:B:616:PRO:HD2	2.00	0.43
1:B:578:ARG:HE	1:B:578:ARG:HA	1.83	0.43
1:A:439:ASN:ND2	1:A:440:PRO:HD2	2.33	0.43
1:A:538:SER:CB	2:C:5:ALV:O	2.66	0.43
5:B:1500:NAG:O7	5:B:1500:NAG:C3	2.65	0.43
1:B:390:GLN:HE22	5:B:1501:NAG:HN2	1.65	0.43
1:B:475:THR:HG21	7:B:852:HOH:O	2.18	0.43
1:A:215:HIS:CD2	2:C:6:0QE:C1	2.93	0.43
1:A:634:LYS:HB3	1:A:634:LYS:HZ2	1.82	0.43
1:A:577:THR:O	1:A:578:ARG:HB2	2.18	0.43
1:A:236:TYR:CE1	1:A:469:GLN:HA	2.54	0.43
1:B:278:VAL:CG1	1:B:280:MET:O	2.67	0.43
1:B:678:VAL:O	1:B:678:VAL:HG13	2.18	0.43
1:B:586:ASN:H	1:B:586:ASN:HD22	1.65	0.43
1:A:138:VAL:HG23	1:A:279:ASP:OD1	2.17	0.43
1:B:696:LYS:HB2	1:B:696:LYS:HE3	1.82	0.43
1:A:732:ARG:N	1:A:732:ARG:HD3	2.32	0.43
1:A:160:PRO:HG2	1:A:249:ARG:NH2	2.33	0.43
1:A:718:TYR:CD2	1:A:739:TRP:HH2	2.34	0.43
1:B:201:THR:O	1:B:201:THR:HG23	2.19	0.43
1:B:325:LEU:HA	1:B:486:ALA:CB	2.47	0.43
1:A:137:ASP:O	1:A:137:ASP:CG	2.57	0.43
1:B:487:ARG:HD2	1:B:594:ASP:OD1	2.18	0.43
1:B:718:TYR:CZ	1:B:739:TRP:CH2	3.07	0.43
1:A:610:LEU:HB3	1:A:678:VAL:HG21	1.97	0.43
1:B:518:ALA:CB	1:B:529:THR:HG22	2.48	0.43
1:B:661:TYR:CD2	1:B:726:GLY:HA3	2.54	0.43
1:B:403:ASP:OD1	1:B:403:ASP:C	2.57	0.43
1:B:718:TYR:CE1	1:B:739:TRP:CH2	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LEU:HB2	1:A:247:ARG:HG3	2.00	0.43
1:B:578:ARG:HA	1:B:578:ARG:NE	2.34	0.43
1:B:415:THR:HG22	1:B:523:THR:HG23	2.00	0.43
1:B:722:ILE:N	1:B:722:ILE:CD1	2.76	0.43
1:A:129:TRP:HB3	1:A:134:LEU:HD21	2.01	0.43
5:B:1500:NAG:O4	5:B:1502:FUC:H5	2.19	0.43
1:A:223:THR:CG2	1:A:224:ALA:N	2.81	0.43
1:A:652:LEU:HD13	1:A:652:LEU:C	2.39	0.43
1:B:538:SER:CB	2:D:6:OQE:C1	2.95	0.43
1:A:538:SER:OG	2:C:5:ALV:CA	2.60	0.43
1:A:501:ILE:HD13	1:A:600:VAL:HG22	2.01	0.43
1:A:623:LEU:O	1:A:626:LEU:HD13	2.19	0.43
1:A:126:SER:CA	1:A:130:PRO:HG3	2.49	0.43
1:B:242:ARG:N	1:B:242:ARG:HD3	2.33	0.43
1:A:175:GLN:NE2	7:A:92:HOH:O	2.29	0.42
1:A:638:ARG:HG2	7:A:812:HOH:O	2.17	0.42
1:B:116:THR:HG21	1:B:543:HIS:CD2	2.49	0.42
1:B:391:VAL:HG13	1:B:391:VAL:O	2.19	0.42
1:A:570:THR:HG21	1:A:605:ALA:HA	1.99	0.42
1:A:670:LEU:HD13	7:A:903:HOH:O	2.19	0.42
1:B:143:LEU:CD1	1:B:143:LEU:N	2.82	0.42
1:B:342:ARG:HG2	1:B:343:THR:N	2.34	0.42
1:B:663:ILE:CD1	1:B:663:ILE:N	2.80	0.42
1:A:270:MET:HE2	1:A:281:ILE:HD13	2.00	0.42
1:A:702:VAL:CG2	1:A:703:SER:N	2.82	0.42
1:B:150:GLU:CD	1:B:150:GLU:H	2.21	0.42
1:A:379:LEU:O	1:A:381:ASP:N	2.52	0.42
1:B:352:ASN:HD21	1:B:354:LEU:HB3	1.84	0.42
1:B:559:SER:OG	1:B:613:ASP:OD1	2.37	0.42
1:B:191:PHE:N	1:B:191:PHE:CD1	2.87	0.42
1:B:237:ALA:N	1:B:238:PRO:HD3	2.35	0.42
1:A:371:SER:HA	1:A:372:PRO:HD3	1.89	0.42
1:A:659:ALA:HB1	1:A:724:TYR:CE1	2.54	0.42
1:B:555:HIS:HB3	1:B:558:TRP:CD1	2.54	0.42
1:B:572:ASP:HA	1:B:573:PRO:HD3	1.80	0.42
1:B:327:ASN:HA	7:B:967:HOH:O	2.19	0.42
1:B:538:SER:O	1:B:542:PRO:CD	2.68	0.42
1:A:672:GLN:HG2	1:A:674:PHE:HZ	1.73	0.42
1:A:143:LEU:HD22	1:A:270:MET:HG2	2.01	0.42
1:A:288:ARG:HG3	1:A:326:ASN:HB3	2.01	0.42
1:A:288:ARG:O	1:A:289:PHE:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:THR:HG23	1:B:296:ALA:CB	2.49	0.42
1:B:626:LEU:HD23	1:B:628:PHE:CE1	2.54	0.42
1:B:236:TYR:CE1	1:B:469:GLN:HA	2.54	0.42
1:A:433:ARG:HD2	7:A:854:HOH:O	2.20	0.42
1:A:638:ARG:CG	1:A:638:ARG:NH1	2.39	0.42
1:A:703:SER:CA	1:A:704:PRO:C	2.85	0.42
1:B:628:PHE:HA	7:B:978:HOH:O	2.19	0.42
4:B:1400:NAG:H62	4:B:1402:NAG:O7	2.19	0.42
1:A:258:ASN:HB2	7:A:27:HOH:O	2.19	0.42
1:A:586:ASN:O	1:A:587:ASN:CB	2.66	0.42
1:B:622:LEU:CD2	1:B:626:LEU:HD11	2.50	0.42
4:A:1101:FUC:C6	4:A:1102:NAG:H2	2.49	0.42
1:A:150:GLU:H	1:A:150:GLU:CD	2.23	0.42
1:A:540:ALA:O	1:A:543:HIS:HB2	2.20	0.42
1:B:314:SER:HB2	1:B:537:THR:HB	2.02	0.42
1:A:415:THR:HG22	1:A:523:THR:HG22	2.02	0.42
1:B:689:LYS:HD2	1:B:742:GLN:OE1	2.20	0.42
1:A:610:LEU:HB3	1:A:678:VAL:HG22	1.99	0.41
1:B:247:ARG:CD	7:B:62:HOH:O	2.67	0.41
1:A:278:VAL:HG11	1:A:280:MET:O	2.19	0.41
5:B:1500:NAG:O7	5:B:1502:FUC:C1	2.68	0.41
1:A:663:ILE:HG21	1:A:756:PRO:HB3	2.02	0.41
1:B:122:LEU:HD21	1:B:602:PRO:HB2	2.00	0.41
1:B:138:VAL:CG1	1:B:549:ALA:HB1	2.45	0.41
1:B:737:ILE:HD13	1:B:739:TRP:HZ3	1.85	0.41
1:A:114:THR:HG23	1:A:509:LEU:HD23	2.01	0.41
1:A:242:ARG:HD3	1:A:242:ARG:N	2.34	0.41
1:A:538:SER:CB	2:C:5:ALV:C	2.92	0.41
1:A:345:ALA:HB3	1:A:472:TYR:HE1	1.79	0.41
1:A:615:THR:O	1:A:618:ASP:HB2	2.19	0.41
1:B:379:LEU:C	1:B:379:LEU:HD12	2.40	0.41
1:A:630:GLU:HB3	1:A:643:HIS:NE2	2.34	0.41
1:A:737:ILE:HG23	1:A:737:ILE:O	2.19	0.41
1:B:718:TYR:CD1	1:B:739:TRP:CH2	3.08	0.41
1:A:692:LEU:CD1	1:A:692:LEU:N	2.84	0.41
1:B:538:SER:C	1:B:539:MET:HE3	2.40	0.41
1:A:760:VAL:HG12	1:A:761:TRP:N	2.35	0.41
1:B:688:TYR:HB3	1:B:739:TRP:CD1	2.55	0.41
1:B:352:ASN:ND2	1:B:352:ASN:C	2.74	0.41
1:B:362:PHE:CE2	1:B:364:ALA:HB3	2.55	0.41
4:A:1100:NAG:H61	4:A:1102:NAG:C1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:TYR:CG	1:B:655:PRO:HD2	2.56	0.41
1:B:562:ALA:O	1:B:565:SER:HB3	2.21	0.41
1:B:760:VAL:CG1	1:B:761:TRP:N	2.84	0.41
1:B:325:LEU:C	1:B:325:LEU:CD1	2.88	0.41
1:B:218:HIS:O	1:B:222:ILE:HG13	2.21	0.41
1:A:685:ALA:N	7:A:929:HOH:O	2.53	0.41
1:A:660:LEU:HD23	1:A:755:SER:HB3	2.02	0.41
1:B:718:TYR:CE2	1:B:739:TRP:CH2	3.08	0.41
1:B:718:TYR:CE2	1:B:739:TRP:HH2	2.38	0.41
1:B:703:SER:HA	1:B:704:PRO:C	2.39	0.41
1:B:661:TYR:CD2	1:B:661:TYR:O	2.74	0.41
1:B:660:LEU:HA	1:B:755:SER:O	2.21	0.41
1:A:378:THR:O	1:A:387:LEU:HD13	2.20	0.41
1:B:445:ASN:OD1	1:B:445:ASN:C	2.59	0.41
1:B:213:ASP:HB2	7:B:881:HOH:O	2.21	0.41
1:A:622:LEU:CD2	1:A:626:LEU:HD11	2.51	0.41
1:A:288:ARG:O	1:A:289:PHE:CB	2.67	0.41
1:B:128:LEU:CD2	1:B:550:MET:HB3	2.50	0.41
1:A:488:GLY:HA3	1:A:498:LYS:O	2.21	0.41
1:A:192:ASN:ND2	1:A:207:ASN:OD1	2.53	0.41
1:A:579:LYS:HB3	1:A:580:PRO:HD3	2.02	0.41
1:A:737:ILE:CD1	1:A:739:TRP:CZ3	3.04	0.41
1:B:289:PHE:HA	1:B:761:TRP:CD1	2.57	0.41
1:B:352:ASN:HD21	1:B:354:LEU:CB	2.34	0.41
1:B:461:THR:N	1:B:462:PRO:HD2	2.36	0.40
1:A:610:LEU:HD13	1:A:678:VAL:HG21	2.03	0.40
1:A:703:SER:HA	1:A:704:PRO:O	2.20	0.40
1:A:129:TRP:N	1:A:130:PRO:HD2	2.36	0.40
1:A:438:PRO:HA	1:A:520:SER:O	2.21	0.40
1:A:719:THR:OG1	7:A:945:HOH:O	2.21	0.40
1:A:491:ARG:NH2	7:A:925:HOH:O	2.54	0.40
1:B:278:VAL:CG1	1:B:279:ASP:N	2.84	0.40
6:B:1300:NAG:C3	6:B:1301:FUC:C5	2.98	0.40
1:A:711:ASN:N	1:A:711:ASN:OD1	2.53	0.40
1:A:122:LEU:HD21	1:A:602:PRO:HB2	2.02	0.40
1:A:700:ILE:HG22	1:A:722:ILE:HG23	2.03	0.40
1:B:126:SER:CA	1:B:130:PRO:HG3	2.51	0.40
1:B:718:TYR:CE1	1:B:739:TRP:CZ3	3.09	0.40
1:A:221:SER:OG	1:A:510:ALA:HB1	2.21	0.40
1:B:352:ASN:C	1:B:352:ASN:HD22	2.25	0.40
1:B:288:ARG:HG3	1:B:326:ASN:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:ALA:HB1	1:A:724:TYR:CZ	2.57	0.40
4:A:1101:FUC:H62	4:A:1102:NAG:H2	2.02	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	632/649 (97%)	587 (93%)	42 (7%)	3 (0%)	34	60
1	B	628/649 (97%)	587 (94%)	37 (6%)	4 (1%)	30	56
2	C	3/6 (50%)	3 (100%)	0	0	100	100
2	D	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
All	All	1266/1310 (97%)	1179 (93%)	80 (6%)	7 (1%)	30	56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	461	THR
1	B	637	ALA
1	A	638	ARG
1	B	461	THR
1	B	178	ALA
1	A	669	LEU
1	B	653	ASN

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	528/533 (99%)	501 (95%)	27 (5%)	29	55
1	B	526/533 (99%)	498 (95%)	28 (5%)	28	53
2	C	3/3 (100%)	3 (100%)	0	100	100
2	D	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	1060/1072 (99%)	1004 (95%)	56 (5%)	28	53

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	LEU
1	A	164	LYS
1	A	184	LYS
1	A	185	LEU
1	A	242	ARG
1	A	290	ILE
1	A	326	ASN
1	A	352	ASN
1	A	368	VAL
1	A	395	GLU
1	A	397	THR
1	A	437	PHE
1	A	439	ASN
1	A	442	VAL
1	A	502	LEU
1	A	524	ASN
1	A	539	MET
1	A	586	ASN
1	A	622	LEU
1	A	638	ARG
1	A	663	ILE
1	A	679	THR
1	A	721	THR
1	A	734	VAL
1	A	739	TRP
1	A	740	VAL
1	A	742	GLN
1	B	128	LEU
1	B	140	VAL
1	B	164	LYS

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Mol	Chain	Res	Type
1	B	184	LYS
1	B	185	LEU
1	B	242	ARG
1	B	290	ILE
1	B	326	ASN
1	B	352	ASN
1	B	368	VAL
1	B	397	THR
1	B	437	PHE
1	B	439	ASN
1	B	471	THR
1	B	524	ASN
1	B	539	MET
1	B	586	ASN
1	B	622	LEU
1	B	624	CYS
1	B	638	ARG
1	B	645	CYS
1	B	663	ILE
1	B	679	THR
1	B	721	THR
1	B	722	ILE
1	B	732	ARG
1	B	739	TRP
1	B	740	VAL
2	D	2	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	136	GLN
1	A	218	HIS
1	A	272	GLN
1	A	326	ASN
1	A	352	ASN
1	A	390	GLN
1	A	439	ASN
1	A	524	ASN
1	A	586	ASN
1	A	617	GLN
1	A	643	HIS

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Mol	Chain	Res	Type
1	B	123	ASN
1	B	136	GLN
1	B	175	GLN
1	B	218	HIS
1	B	272	GLN
1	B	326	ASN
1	B	352	ASN
1	B	390	GLN
1	B	439	ASN
1	B	451	GLN
1	B	524	ASN
1	B	586	ASN
1	B	617	GLN
1	B	643	HIS
1	B	647	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ALV	C	5	1,2	4,4,5	2.47	1 (25%)	2,4,6	2.46	1 (50%)
2	ALV	D	5	1,2	4,4,5	2.47	1 (25%)	2,4,6	2.45	1 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ALV	C	5	1,2	-	0/2/2/4	0/0/0/0
2	ALV	D	5	1,2	-	0/2/2/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5	ALV	O-C	-4.59	1.22	1.42
2	C	5	ALV	O-C	-4.58	1.22	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5	ALV	O-C-CA	3.45	119.28	112.75
2	C	5	ALV	O-C-CA	3.47	119.31	112.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	5	ALV	7	0
2	D	5	ALV	2	0

5.5 Carbohydrates [i](#)

16 carbohydrates 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	A	1000	1,3	14,14,15	0.52	0	15,19,21	0.59	0
3	NAG	A	1001	3	14,14,15	0.51	0	15,19,21	0.61	0
4	NAG	A	1100	1,4	14,14,15	0.51	0	15,19,21	0.66	0
4	FUC	A	1101	4	10,10,11	0.72	0	14,14,16	1.70	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1102	4	14,14,15	0.50	0	15,19,21	0.82	0
5	NAG	A	1201	1,5	14,14,15	0.52	0	15,19,21	0.73	0
5	NAG	A	1202	5	14,14,15	0.51	0	15,19,21	0.69	0
5	FUC	A	1203	5	10,10,11	0.60	0	14,14,16	0.75	0
6	NAG	B	1300	1,6	14,14,15	0.42	0	15,19,21	0.92	0
6	FUC	B	1301	6	10,10,11	0.59	0	14,14,16	0.76	1 (7%)
4	NAG	B	1400	1,4	14,14,15	0.54	0	15,19,21	0.99	0
4	FUC	B	1401	4	10,10,11	0.62	0	14,14,16	0.80	1 (7%)
4	NAG	B	1402	4	14,14,15	0.49	0	15,19,21	0.81	1 (6%)
5	NAG	B	1500	1,5	14,14,15	0.52	0	15,19,21	0.99	1 (6%)
5	NAG	B	1501	5	14,14,15	0.54	0	15,19,21	0.59	0
5	FUC	B	1502	5	10,10,11	0.60	0	14,14,16	0.74	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	A	1000	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1001	3	-	0/6/23/26	0/1/1/1
4	NAG	A	1100	1,4	-	0/6/23/26	0/1/1/1
4	FUC	A	1101	4	-	0/0/17/20	0/1/1/1
4	NAG	A	1102	4	-	0/6/23/26	0/1/1/1
5	NAG	A	1201	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1202	5	-	0/6/23/26	0/1/1/1
5	FUC	A	1203	5	-	0/0/17/20	0/1/1/1
6	NAG	B	1300	1,6	1/1/5/7	0/6/23/26	0/1/1/1
6	FUC	B	1301	6	-	0/0/17/20	0/1/1/1
4	NAG	B	1400	1,4	-	0/6/23/26	0/1/1/1
4	FUC	B	1401	4	-	0/0/17/20	0/1/1/1
4	NAG	B	1402	4	-	0/6/23/26	0/1/1/1
5	NAG	B	1500	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1501	5	-	0/6/23/26	0/1/1/1
5	FUC	B	1502	5	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1500	NAG	C4-C3-C2	-2.51	107.32	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1402	NAG	C4-C3-C2	-2.15	107.88	111.23
6	B	1301	FUC	O5-C5-C6	2.01	109.45	106.13
4	B	1401	FUC	O5-C5-C6	2.03	109.49	106.13
4	A	1101	FUC	C2-C3-C4	2.73	115.67	111.04
4	A	1101	FUC	C3-C4-C5	3.02	114.80	109.72
4	A	1101	FUC	C1-C2-C3	3.53	113.72	109.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	1300	NAG	C1

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	NAG	1	0
3	A	1001	NAG	1	0
4	A	1100	NAG	1	0
4	A	1101	FUC	2	0
4	A	1102	NAG	3	0
5	A	1201	NAG	4	0
5	A	1202	NAG	5	0
5	A	1203	FUC	3	0
6	B	1300	NAG	4	0
6	B	1301	FUC	4	0
4	B	1400	NAG	2	0
4	B	1401	FUC	2	0
4	B	1402	NAG	4	0
5	B	1500	NAG	5	0
5	B	1501	NAG	4	0
5	B	1502	FUC	4	0

5.6 Ligand geometry

There are no ligands in this entry.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	642/649 (98%)	-0.08	16 (2%) 61 54	27, 37, 52, 61	0
1	B	640/649 (98%)	-0.13	16 (2%) 61 54	27, 37, 52, 61	0
2	C	3/6 (50%)	0.99	1 (33%) 0 0	65, 65, 66, 66	0
2	D	3/6 (50%)	1.22	0 100 100	65, 65, 66, 66	0
All	All	1288/1310 (98%)	-0.10	33 (2%) 59 53	27, 37, 53, 66	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	VAL	3.8
1	A	665	GLY	3.7
1	B	745	ASN	3.6
1	A	664	GLU	3.6
1	B	460	VAL	3.3
1	A	627	ASN	3.1
1	A	461	THR	3.0
1	A	666	ASN	2.8
1	B	722	ILE	2.8
1	A	630	GLU	2.6
1	B	423	ILE	2.6
1	A	645	CYS	2.6
1	A	667	PHE	2.6
1	B	689	LYS	2.6
1	B	637	ALA	2.5
1	B	164	LYS	2.5
1	A	663	ILE	2.4
2	C	2	PHE	2.4
1	B	157	ASP	2.3
1	A	447	LYS	2.3
1	A	725	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	710	LYS	2.3
1	B	578	ARG	2.3
1	B	648	PRO	2.2
1	B	630	GLU	2.1
1	B	229	LYS	2.1
1	B	422	ALA	2.1
1	B	743	ASN	2.1
1	B	454	ASN	2.1
1	B	711	ASN	2.1
1	A	669	LEU	2.1
1	A	668	THR	2.1
1	A	416	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ALV	D	5	5/6	0.88	0.17	-	54,55,55,55	0
2	ALV	C	5	5/6	0.90	0.23	-	55,55,55,55	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	1001	14/15	0.83	0.37	-	47,47,47,48	14
5	FUC	A	1203	10/11	0.93	0.31	-	52,52,52,53	0
5	NAG	B	1501	14/15	0.92	0.16	-	48,48,49,49	0
5	NAG	A	1202	14/15	0.83	0.27	-	52,52,53,53	0
4	FUC	B	1401	10/11	0.95	0.17	-	41,41,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	FUC	B	1502	10/11	0.91	0.31	-	48,49,49,49	0
4	NAG	A	1100	14/15	0.94	0.21	-	40,42,43,43	0
4	NAG	B	1400	14/15	0.91	0.19	-	39,40,41,42	0
4	FUC	A	1101	10/11	0.91	0.18	-	44,45,45,45	0
5	NAG	B	1500	14/15	0.85	0.19	-	46,47,48,48	0
6	FUC	B	1301	10/11	0.56	0.53	-	55,56,56,56	0
3	NAG	A	1000	14/15	0.81	0.20	-	45,46,46,47	14
6	NAG	B	1300	14/15	0.72	0.38	-	66,72,75,76	0
4	NAG	A	1102	14/15	0.81	0.32	-	43,44,45,45	0
4	NAG	B	1402	14/15	0.85	0.28	-	42,43,43,43	0
5	NAG	A	1201	14/15	0.93	0.17	-	49,50,51,51	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.