



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:22 AM GMT

PDB ID : 3I6S
Title : Crystal Structure of the plant subtilisin-like protease SBT3
Authors : Rose, R.; Ottmann, C.
Deposited on : 2009-07-07
Resolution : 2.50 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

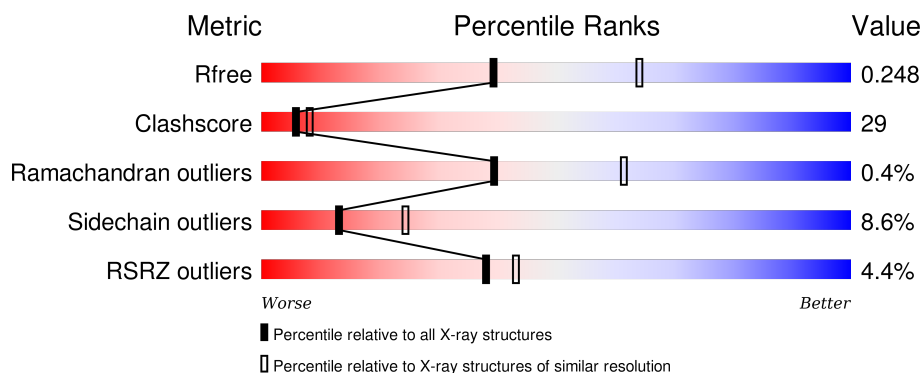
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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>5%</div> <div>59%</div> <div>34%</div> <div>5%</div> </div>
1	B	649	<div> <div>4%</div> <div>61%</div> <div>32%</div> <div>5%</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
5	NAG	B	1300	X	-	-	-
5	NAG	B	1400	-	-	X	-
6	NAG	B	1402	-	-	X	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10372 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	639	Total	C	N	O	S	0	0	0
			4822	3047	830	924	21			

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

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

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

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

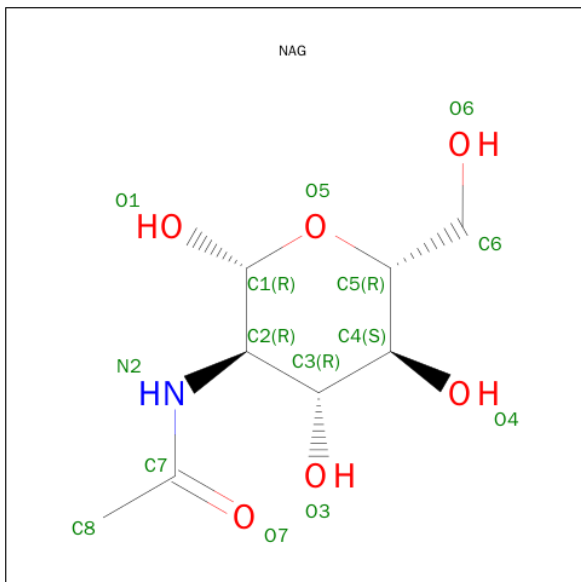
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

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 (2-MER).

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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

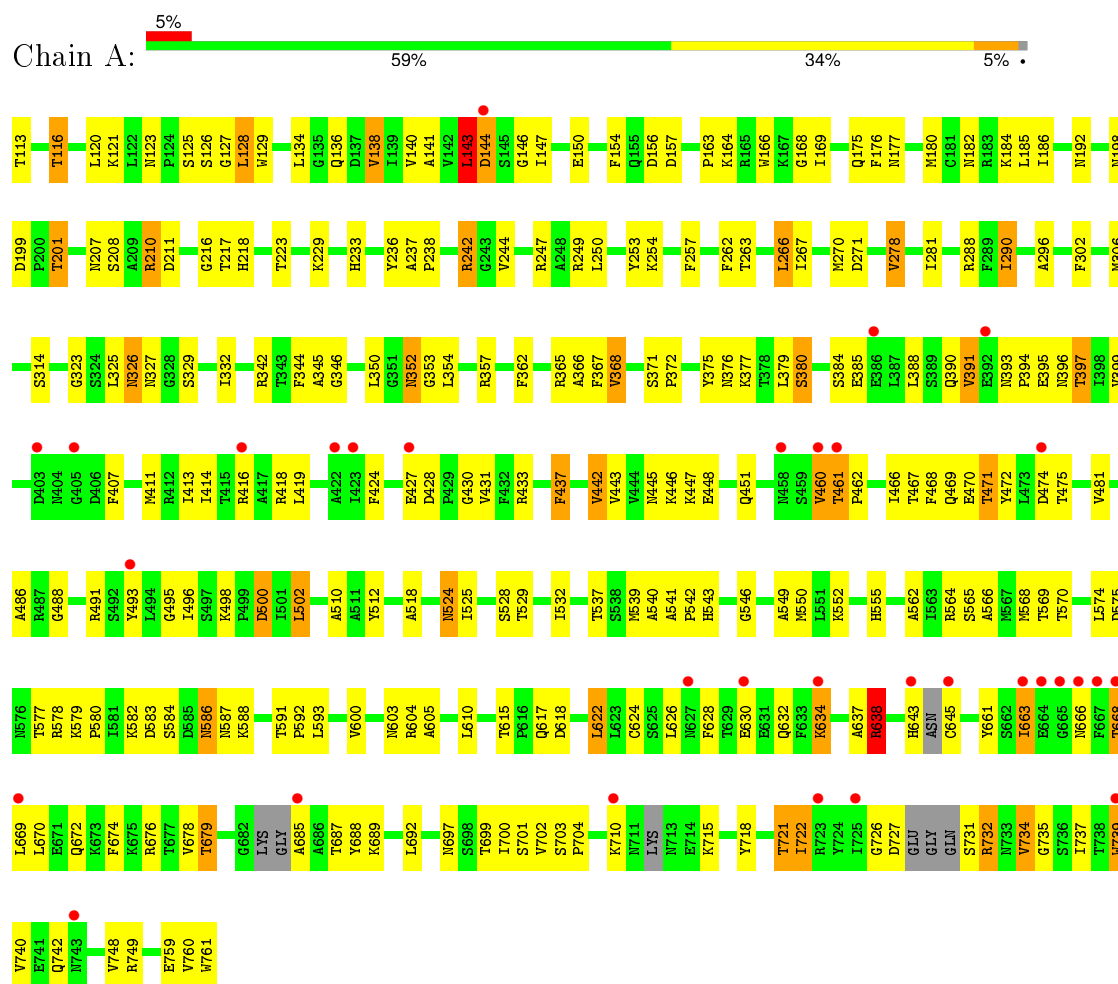
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	212	Total	O	0	0
			212	212		
7	B	290	Total	O	0	0
			290	290		

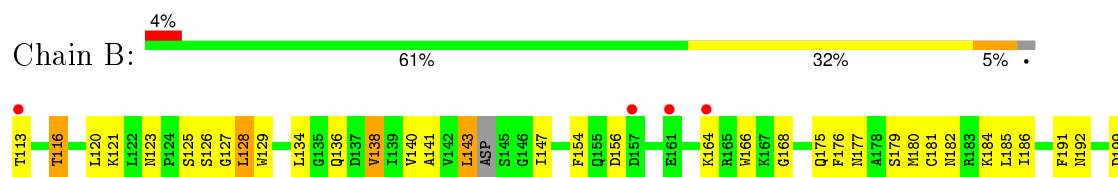
3 Residue-property plots

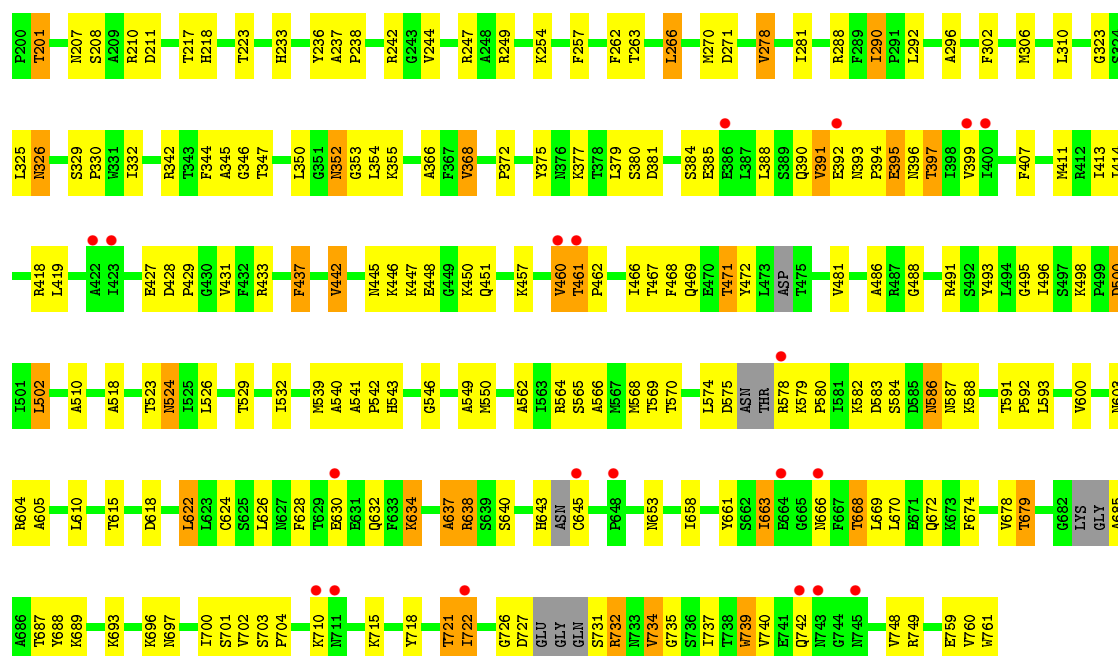
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Subtilisin-like protease



• Molecule 1: Subtilisin-like protease





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	143.89Å 143.89Å 195.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.50 19.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.50) 99.8 (19.99-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.249 , 0.283 0.247 , 0.248	Depositor DCC
R_{free} test set	3556 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 80262 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10372	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: NAG, 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	0.31	0/4951	0.47	0/6737
1	B	0.29	0/4927	0.46	0/6699
All	All	0.30	0/9878	0.46	0/13436

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
5	B	1	0
All	All	1	4

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1300	NAG	C1

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	LEU	Peptide
1	A	210	ARG	Sidechain
1	A	637	ALA	Peptide
1	B	637	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4844	0	4783	284	0
1	B	4822	0	4773	261	0
2	A	28	0	25	2	0
3	A	38	0	34	1	0
4	A	38	0	33	8	0
4	B	38	0	34	1	0
5	B	48	0	44	15	0
6	B	14	0	13	12	1
7	A	212	0	0	47	1
7	B	290	0	0	44	0
All	All	10372	0	9739	563	1

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 29.

All (563) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:THR:HA	7:A:781:HOH:O	1.35	1.25
1:A:475:THR:HA	7:A:908:HOH:O	1.35	1.22
1:B:395:GLU:HG3	7:B:9:HOH:O	1.40	1.18
1:A:591:THR:HG22	1:A:593:LEU:H	1.05	1.17
1:A:674:PHE:HE2	1:A:722:ILE:CD1	1.57	1.17
1:B:674:PHE:HE2	1:B:722:ILE:CD1	1.57	1.16
1:B:591:THR:HG22	1:B:593:LEU:H	1.05	1.15
1:B:674:PHE:CE2	1:B:722:ILE:HD11	1.82	1.14
1:B:591:THR:HG23	1:B:592:PRO:HD2	1.28	1.13
1:A:591:THR:HG23	1:A:592:PRO:HD2	1.22	1.13
1:A:674:PHE:CE2	1:A:722:ILE:HD11	1.84	1.12
1:B:143:LEU:HD21	1:B:270:MET:HG2	1.32	1.11
1:A:144:ASP:HB3	1:A:146:GLY:H	1.12	1.10
1:A:674:PHE:HE2	1:A:722:ILE:HD11	1.13	1.09
1:A:143:LEU:HD21	1:A:270:MET:HG2	1.31	1.09
1:A:433:ARG:HD2	7:A:854:HOH:O	1.53	1.08
1:B:674:PHE:HE2	1:B:722:ILE:HD11	1.10	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ILE:HG22	7:A:76:HOH:O	1.56	1.05
1:A:679:THR:HG22	7:A:52:HOH:O	1.55	1.04
1:A:674:PHE:CE2	1:A:722:ILE:CD1	2.39	1.03
1:B:674:PHE:CE2	1:B:722:ILE:CD1	2.38	1.03
1:B:393:ASN:O	1:B:397:THR:HG22	1.58	1.03
1:B:375:TYR:HD2	7:B:821:HOH:O	1.38	1.03
1:A:393:ASN:O	1:A:397:THR:HG22	1.59	1.02
1:B:693:LYS:HD2	7:B:977:HOH:O	1.58	1.01
1:A:689:LYS:HD2	1:A:742:GLN:CD	1.86	0.96
1:B:721:THR:HG22	7:B:784:HOH:O	1.64	0.95
1:B:689:LYS:HD2	1:B:742:GLN:CD	1.85	0.95
1:A:638:ARG:HD3	7:A:812:HOH:O	1.69	0.92
1:A:591:THR:CG2	1:A:592:PRO:HD2	2.00	0.92
1:A:591:THR:HG23	1:A:592:PRO:CD	2.00	0.92
1:A:672:GLN:HG2	1:A:674:PHE:CZ	2.05	0.92
1:A:555:HIS:CD2	7:A:878:HOH:O	2.23	0.91
1:B:461:THR:O	1:B:461:THR:HG22	1.70	0.91
5:B:1400:NAG:H62	6:B:1402:NAG:C1	2.00	0.91
5:B:1400:NAG:H62	6:B:1402:NAG:O7	1.69	0.90
1:A:175:GLN:O	1:A:210:ARG:NH1	2.04	0.90
1:B:591:THR:CG2	1:B:592:PRO:HD2	2.01	0.90
1:B:591:THR:HG22	1:B:593:LEU:N	1.88	0.89
1:B:262:PHE:HE1	7:B:835:HOH:O	1.55	0.89
1:A:591:THR:HG22	1:A:593:LEU:N	1.88	0.89
1:A:555:HIS:HD2	7:A:878:HOH:O	1.56	0.88
1:B:591:THR:HG23	1:B:592:PRO:CD	2.05	0.87
1:A:141:ALA:HB2	1:A:278:VAL:HG21	1.56	0.87
1:A:323:GLY:O	1:A:491:ARG:HD2	1.75	0.87
1:A:461:THR:HG22	1:A:461:THR:O	1.72	0.86
1:B:574:LEU:HD12	7:B:875:HOH:O	1.75	0.86
1:A:143:LEU:CD2	1:A:270:MET:HG2	2.06	0.85
1:B:181:CYS:HB3	7:B:98:HOH:O	1.76	0.85
1:B:175:GLN:O	1:B:210:ARG:NH1	2.11	0.84
1:A:471:THR:CG2	7:A:851:HOH:O	2.24	0.84
1:B:381:ASP:HB3	7:B:841:HOH:O	1.77	0.84
1:B:141:ALA:HB2	1:B:278:VAL:HG21	1.57	0.84
1:B:672:GLN:HG2	1:B:674:PHE:CZ	2.12	0.83
1:B:143:LEU:CD2	1:B:270:MET:HG2	2.07	0.83
1:A:674:PHE:HE2	1:A:722:ILE:HD13	1.44	0.83
1:B:447:LYS:CE	7:B:829:HOH:O	2.27	0.82
1:A:352:ASN:ND2	1:A:354:LEU:H	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:LYS:HB3	1:A:580:PRO:HD2	1.60	0.81
1:A:727:ASP:OD1	1:A:731:SER:HB3	1.81	0.81
1:A:144:ASP:HB3	1:A:146:GLY:N	1.94	0.80
1:B:323:GLY:O	1:B:491:ARG:HD2	1.81	0.80
1:B:523:THR:HG23	7:B:945:HOH:O	1.81	0.79
2:A:1000:NAG:O6	2:A:1001:NAG:C1	2.30	0.79
1:B:674:PHE:HE2	1:B:722:ILE:HD13	1.46	0.79
1:A:731:SER:HA	7:A:785:HOH:O	1.83	0.79
1:B:579:LYS:HB3	1:B:580:PRO:HD2	1.63	0.79
1:B:238:PRO:HD2	7:B:106:HOH:O	1.81	0.79
1:B:352:ASN:ND2	1:B:354:LEU:H	1.79	0.78
1:B:450:LYS:HG2	7:B:912:HOH:O	1.83	0.78
1:B:446:LYS:HD3	7:B:901:HOH:O	1.83	0.78
1:B:447:LYS:HE3	7:B:829:HOH:O	1.84	0.78
1:A:352:ASN:HD22	1:A:352:ASN:C	1.86	0.78
1:A:669:LEU:HD13	1:A:669:LEU:C	2.04	0.78
1:A:471:THR:HG22	7:A:851:HOH:O	1.83	0.77
1:B:388:LEU:O	1:B:391:VAL:HG12	1.85	0.77
1:A:591:THR:CG2	1:A:592:PRO:CD	2.61	0.76
1:A:388:LEU:O	1:A:391:VAL:HG12	1.84	0.76
1:A:346:GLY:HA2	1:A:467:THR:O	1.85	0.76
1:B:591:THR:CG2	1:B:592:PRO:CD	2.63	0.76
1:B:346:GLY:HA2	1:B:467:THR:O	1.86	0.76
1:B:727:ASP:OD1	1:B:731:SER:HB3	1.85	0.76
1:B:663:ILE:H	1:B:663:ILE:HD13	1.49	0.76
1:B:116:THR:HG21	1:B:543:HIS:NE2	2.01	0.76
1:B:352:ASN:C	1:B:352:ASN:HD22	1.90	0.75
1:A:663:ILE:HD13	1:A:663:ILE:H	1.50	0.75
1:B:493:TYR:CE1	7:B:845:HOH:O	2.39	0.75
1:A:552:LYS:CD	7:A:837:HOH:O	2.34	0.75
1:B:634:LYS:O	1:B:638:ARG:HA	1.85	0.74
5:B:1400:NAG:C4	6:B:1402:NAG:C1	2.66	0.74
1:A:116:THR:HG21	1:A:543:HIS:NE2	2.03	0.74
1:B:669:LEU:HD13	1:B:669:LEU:C	2.09	0.73
1:A:365:ARG:NE	7:A:913:HOH:O	2.20	0.73
5:B:1400:NAG:O4	6:B:1402:NAG:O5	2.07	0.73
1:B:381:ASP:CB	7:B:841:HOH:O	2.35	0.72
1:A:460:VAL:O	1:A:461:THR:HB	1.89	0.72
1:A:552:LYS:HD2	7:A:837:HOH:O	1.90	0.72
1:A:123:ASN:HD22	1:A:125:SER:H	1.38	0.72
1:A:393:ASN:O	1:A:397:THR:CG2	2.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:ASN:HD22	1:B:587:ASN:N	1.88	0.71
1:B:393:ASN:O	1:B:397:THR:CG2	2.37	0.71
1:B:460:VAL:O	1:B:461:THR:HB	1.90	0.71
1:A:472:TYR:HB3	7:A:782:HOH:O	1.91	0.71
1:A:577:THR:O	1:A:578:ARG:HB2	1.91	0.71
1:A:302:PHE:O	1:A:306:MET:HG2	1.92	0.70
1:B:450:LYS:CG	7:B:912:HOH:O	2.41	0.69
1:A:586:ASN:HD22	1:A:587:ASN:N	1.91	0.69
1:B:375:TYR:CD2	7:B:821:HOH:O	2.24	0.69
1:B:384:SER:O	1:B:388:LEU:HD23	1.93	0.69
1:B:177:ASN:H	1:B:180:MET:CE	2.06	0.69
1:A:384:SER:O	1:A:388:LEU:HD23	1.93	0.68
4:A:1201:NAG:H83	7:A:829:HOH:O	1.93	0.68
1:A:578:ARG:HA	1:A:578:ARG:HE	1.59	0.68
1:A:470:GLU:HA	7:A:10:HOH:O	1.93	0.68
5:B:1400:NAG:C6	6:B:1402:NAG:C1	2.72	0.68
1:B:218:HIS:CE1	1:B:510:ALA:HB3	2.29	0.68
1:A:570:THR:HG21	1:A:605:ALA:HB2	1.75	0.68
1:B:674:PHE:CE2	1:B:722:ILE:HD13	2.24	0.68
1:A:591:THR:HG22	1:A:592:PRO:N	2.09	0.67
1:A:578:ARG:NE	1:A:578:ARG:HA	2.09	0.67
1:A:129:TRP:CG	1:A:134:LEU:HD22	2.30	0.67
1:A:702:VAL:HG22	1:A:703:SER:N	2.10	0.67
1:B:591:THR:HG22	1:B:592:PRO:N	2.09	0.67
1:B:570:THR:HG21	1:B:605:ALA:HB2	1.75	0.67
1:B:123:ASN:HD21	1:B:126:SER:H	1.42	0.67
1:B:721:THR:CG2	7:B:784:HOH:O	2.29	0.67
1:B:302:PHE:O	1:B:306:MET:HG2	1.94	0.67
1:B:129:TRP:CG	1:B:134:LEU:HD22	2.30	0.67
1:A:199:ASP:OD1	1:A:201:THR:HB	1.94	0.66
1:B:199:ASP:OD1	1:B:201:THR:HB	1.95	0.66
1:A:634:LYS:O	1:A:638:ARG:HA	1.95	0.66
1:B:123:ASN:HD22	1:B:125:SER:H	1.41	0.66
1:B:433:ARG:NH2	7:B:101:HOH:O	2.28	0.66
5:B:1401:FUC:C6	6:B:1402:NAG:H2	2.26	0.66
1:A:460:VAL:HG22	7:A:863:HOH:O	1.96	0.66
1:B:702:VAL:HG22	1:B:703:SER:N	2.11	0.66
1:B:491:ARG:HG3	7:B:976:HOH:O	1.96	0.65
1:A:575:ASP:C	1:A:575:ASP:OD1	2.34	0.65
1:A:502:LEU:O	1:A:600:VAL:HG23	1.96	0.65
1:A:218:HIS:CE1	1:A:510:ALA:HB3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ALA:H	1:B:471:THR:HG21	1.60	0.65
1:B:128:LEU:HD22	1:B:550:MET:HB3	1.78	0.65
1:A:591:THR:CG2	1:A:592:PRO:N	2.60	0.65
1:B:177:ASN:H	1:B:180:MET:HE2	1.61	0.65
1:A:237:ALA:H	1:A:471:THR:HG21	1.60	0.65
1:A:177:ASN:HD22	2:A:1000:NAG:C1	2.01	0.64
1:B:502:LEU:O	1:B:600:VAL:HG23	1.98	0.64
1:A:674:PHE:CD2	1:A:722:ILE:HD11	2.31	0.64
1:B:461:THR:CG2	1:B:461:THR:O	2.44	0.64
1:A:123:ASN:HD21	1:A:126:SER:H	1.45	0.63
1:A:136:GLN:HA	1:A:247:ARG:O	1.98	0.63
1:B:674:PHE:CD2	1:B:722:ILE:HD11	2.31	0.63
1:A:177:ASN:H	1:A:180:MET:CE	2.11	0.62
6:B:1402:NAG:O7	6:B:1402:NAG:C1	2.47	0.62
1:A:352:ASN:ND2	1:A:352:ASN:C	2.52	0.62
1:B:136:GLN:HA	1:B:247:ARG:O	1.99	0.62
1:B:591:THR:CG2	1:B:592:PRO:N	2.63	0.62
1:B:583:ASP:HB3	1:B:586:ASN:HD21	1.64	0.62
1:A:583:ASP:HB3	1:A:586:ASN:HD21	1.65	0.62
1:B:375:TYR:OH	1:B:377:LYS:HE3	2.00	0.61
1:B:700:ILE:HG22	1:B:722:ILE:HG23	1.82	0.61
1:A:177:ASN:H	1:A:180:MET:HE2	1.65	0.61
1:A:524:ASN:H	1:A:524:ASN:HD22	1.48	0.61
1:A:129:TRP:HB3	1:A:134:LEU:CD2	2.30	0.61
1:A:375:TYR:OH	1:A:377:LYS:HE3	2.01	0.61
1:A:591:THR:CG2	1:A:593:LEU:H	1.97	0.60
1:B:181:CYS:CB	7:B:98:HOH:O	2.39	0.60
1:B:121:LYS:HD3	7:B:780:HOH:O	2.01	0.60
1:B:689:LYS:HD2	1:B:742:GLN:OE1	2.00	0.60
1:B:129:TRP:HB3	1:B:134:LEU:CD2	2.31	0.60
1:A:701:SER:OG	1:A:721:THR:HG23	2.00	0.60
1:A:674:PHE:CE2	1:A:722:ILE:HD13	2.23	0.60
1:A:700:ILE:HG22	1:A:722:ILE:HG23	1.82	0.60
1:B:175:GLN:NE2	7:B:897:HOH:O	2.35	0.60
1:A:428:ASP:OD1	1:A:428:ASP:C	2.39	0.60
1:A:345:ALA:HB3	1:A:472:TYR:HE1	1.66	0.60
1:B:457:LYS:HE3	7:B:821:HOH:O	2.01	0.60
1:A:689:LYS:HD2	1:A:742:GLN:OE1	2.02	0.60
1:B:610:LEU:HB3	1:B:678:VAL:HG22	1.83	0.59
1:B:266:LEU:O	1:B:266:LEU:HD12	2.02	0.59
1:B:352:ASN:ND2	1:B:352:ASN:C	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ARG:NH2	7:A:95:HOH:O	2.33	0.59
1:A:569:THR:HA	1:A:749:ARG:O	2.01	0.59
1:A:610:LEU:HB3	1:A:678:VAL:HG22	1.84	0.59
1:B:461:THR:N	1:B:462:PRO:CD	2.65	0.59
1:B:138:VAL:HG11	1:B:549:ALA:HB1	1.84	0.59
1:A:622:LEU:O	1:A:626:LEU:HD13	2.03	0.59
1:B:679:THR:HB	1:B:715:LYS:HG2	1.85	0.59
5:B:1300:NAG:H3	5:B:1301:FUC:H5	1.85	0.59
1:B:737:ILE:HD11	1:B:739:TRP:CZ3	2.37	0.59
1:B:566:ALA:O	1:B:570:THR:HG22	2.03	0.58
1:B:524:ASN:H	1:B:524:ASN:HD22	1.49	0.58
5:B:1400:NAG:C4	6:B:1402:NAG:O5	2.50	0.58
1:A:138:VAL:HG11	1:A:549:ALA:HB1	1.85	0.58
1:B:722:ILE:HD12	1:B:722:ILE:H	1.69	0.58
1:B:737:ILE:CD1	1:B:739:TRP:CZ3	2.86	0.58
1:B:388:LEU:O	1:B:391:VAL:CG1	2.52	0.58
1:A:679:THR:HB	1:A:715:LYS:HG2	1.83	0.58
1:B:701:SER:OG	1:B:721:THR:HG23	2.04	0.58
1:A:737:ILE:HD11	1:A:739:TRP:CZ3	2.39	0.58
1:B:345:ALA:HB3	1:B:472:TYR:HE1	1.68	0.58
1:A:461:THR:N	1:A:462:PRO:CD	2.67	0.58
1:A:737:ILE:CD1	1:A:739:TRP:CZ3	2.87	0.58
1:A:630:GLU:HB3	1:A:643:HIS:CD2	2.38	0.58
1:B:518:ALA:CB	1:B:529:THR:HG22	2.34	0.58
1:A:352:ASN:HD22	1:A:354:LEU:H	1.49	0.57
1:A:388:LEU:O	1:A:391:VAL:CG1	2.52	0.57
4:A:1201:NAG:C8	7:A:829:HOH:O	2.51	0.57
1:A:385:GLU:HG2	1:A:413:ILE:HD12	1.85	0.57
1:A:672:GLN:CG	1:A:674:PHE:CZ	2.86	0.57
1:B:570:THR:HG21	1:B:605:ALA:CB	2.35	0.57
1:A:564:ARG:O	1:A:568:MET:HG3	2.04	0.57
1:A:722:ILE:HD12	1:A:722:ILE:H	1.69	0.57
1:A:428:ASP:OD1	1:A:430:GLY:N	2.33	0.57
1:B:591:THR:CG2	1:B:593:LEU:H	1.97	0.57
1:A:570:THR:HG21	1:A:605:ALA:CB	2.35	0.57
1:B:290:ILE:H	1:B:290:ILE:HD13	1.69	0.56
1:B:123:ASN:ND2	1:B:126:SER:H	2.02	0.56
1:A:666:ASN:ND2	7:A:884:HOH:O	2.37	0.56
1:B:325:LEU:HA	1:B:486:ALA:HB1	1.88	0.56
1:A:128:LEU:HD22	1:A:550:MET:HB3	1.85	0.56
1:A:229:LYS:CG	7:A:94:HOH:O	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PHE:CE2	1:A:180:MET:HB3	2.41	0.56
1:A:702:VAL:HG22	1:A:703:SER:H	1.70	0.56
1:B:622:LEU:CD2	1:B:622:LEU:C	2.74	0.56
1:B:732:ARG:N	1:B:732:ARG:HD3	2.20	0.56
1:A:150:GLU:OE2	1:A:210:ARG:NH2	2.39	0.56
1:A:586:ASN:ND2	1:A:588:LYS:H	2.04	0.56
1:B:574:LEU:CD1	7:B:875:HOH:O	2.42	0.56
1:B:352:ASN:HD22	1:B:354:LEU:H	1.51	0.56
1:A:669:LEU:CD1	1:A:669:LEU:C	2.74	0.56
5:B:1401:FUC:H62	6:B:1402:NAG:H2	1.88	0.56
1:A:722:ILE:HD12	1:A:722:ILE:N	2.21	0.56
1:B:630:GLU:HB3	1:B:643:HIS:CD2	2.41	0.56
1:A:566:ALA:O	1:A:570:THR:HG22	2.06	0.56
1:B:569:THR:HA	1:B:749:ARG:O	2.06	0.56
1:B:486:ALA:HB2	7:B:796:HOH:O	2.05	0.56
1:A:176:PHE:HA	1:A:180:MET:HE2	1.87	0.55
1:B:201:THR:O	1:B:201:THR:CG2	2.55	0.55
1:A:737:ILE:HD11	1:A:739:TRP:CH2	2.41	0.55
1:A:493:TYR:CE2	1:A:495:GLY:HA3	2.40	0.55
1:A:266:LEU:HD12	1:A:266:LEU:O	2.06	0.55
1:A:461:THR:CG2	1:A:461:THR:O	2.46	0.55
1:A:123:ASN:HD22	1:A:125:SER:N	2.04	0.55
4:A:1202:NAG:O5	4:A:1203:FUC:H5	2.06	0.55
1:B:428:ASP:OD1	1:B:428:ASP:C	2.45	0.55
1:B:722:ILE:HD12	1:B:722:ILE:N	2.22	0.55
1:A:352:ASN:HD22	1:A:353:GLY:N	2.04	0.55
1:A:622:LEU:CD2	1:A:622:LEU:C	2.75	0.55
1:B:570:THR:HG21	1:B:605:ALA:CA	2.37	0.55
1:B:622:LEU:O	1:B:626:LEU:HD13	2.06	0.55
1:A:201:THR:O	1:A:201:THR:CG2	2.54	0.55
1:B:325:LEU:HD12	1:B:325:LEU:C	2.27	0.55
1:A:570:THR:HG21	1:A:605:ALA:CA	2.36	0.55
1:B:570:THR:OG1	1:B:604:ARG:HB3	2.07	0.55
1:B:385:GLU:HG2	1:B:413:ILE:HD12	1.88	0.55
1:B:737:ILE:HD11	1:B:739:TRP:CH2	2.41	0.55
1:A:518:ALA:CB	1:A:529:THR:HG22	2.36	0.55
1:A:144:ASP:OD1	1:A:216:GLY:HA2	2.07	0.55
1:A:290:ILE:H	1:A:290:ILE:HD13	1.72	0.55
1:B:123:ASN:HD22	1:B:125:SER:N	2.04	0.54
1:A:199:ASP:CG	7:A:872:HOH:O	2.45	0.54
1:A:325:LEU:HD12	1:A:325:LEU:C	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:VAL:CG1	1:A:761:TRP:N	2.70	0.54
1:A:390:GLN:HE22	4:A:1202:NAG:HN2	1.54	0.54
1:A:325:LEU:HA	1:A:486:ALA:HB1	1.89	0.54
1:A:579:LYS:HB2	7:A:950:HOH:O	2.07	0.54
1:A:460:VAL:CG2	7:A:863:HOH:O	2.54	0.54
1:B:760:VAL:CG1	1:B:761:TRP:N	2.70	0.54
1:B:179:SER:HB3	5:B:1300:NAG:H82	1.89	0.54
1:A:669:LEU:HD13	1:A:670:LEU:N	2.23	0.53
1:A:570:THR:OG1	1:A:604:ARG:HB3	2.06	0.53
1:B:697:ASN:ND2	7:B:970:HOH:O	2.41	0.53
1:B:760:VAL:HG12	1:B:761:TRP:N	2.23	0.53
1:B:586:ASN:ND2	1:B:588:LYS:H	2.07	0.53
1:B:679:THR:HG22	7:B:790:HOH:O	2.09	0.53
1:B:541:ALA:N	1:B:542:PRO:HD2	2.24	0.53
1:A:233:HIS:O	1:A:233:HIS:CD2	2.62	0.53
1:A:390:GLN:NE2	4:A:1201:NAG:O6	2.42	0.53
1:B:120:LEU:O	1:B:121:LYS:HB2	2.09	0.53
1:A:357:ARG:HH12	1:A:474:ASP:CG	2.11	0.53
1:A:661:TYR:CD2	1:A:726:GLY:HA3	2.44	0.53
1:A:760:VAL:HG12	1:A:761:TRP:N	2.24	0.53
1:A:688:TYR:CB	1:A:739:TRP:HD1	2.22	0.53
1:B:658:ILE:HG22	7:B:782:HOH:O	2.08	0.53
1:B:564:ARG:O	1:B:568:MET:HG3	2.09	0.53
1:A:610:LEU:HB2	1:A:748:VAL:HG21	1.90	0.53
1:A:288:ARG:HG3	1:A:326:ASN:HB3	1.91	0.53
1:B:352:ASN:HD22	1:B:353:GLY:N	2.07	0.53
1:A:123:ASN:ND2	1:A:126:SER:H	2.05	0.53
1:A:749:ARG:HB3	7:A:844:HOH:O	2.08	0.53
1:A:732:ARG:N	1:A:732:ARG:HD3	2.23	0.52
1:B:218:HIS:ND1	1:B:510:ALA:HB3	2.24	0.52
1:B:392:GLU:N	7:B:921:HOH:O	2.42	0.52
5:B:1400:NAG:H4	6:B:1402:NAG:O5	2.09	0.52
1:A:120:LEU:O	1:A:121:LYS:HB2	2.09	0.52
1:A:427:GLU:OE2	1:A:445:ASN:HB2	2.09	0.52
1:B:610:LEU:HB2	1:B:748:VAL:HG21	1.92	0.52
1:B:666:ASN:HB2	7:B:899:HOH:O	2.07	0.52
1:A:541:ALA:N	1:A:542:PRO:HD2	2.25	0.52
1:A:418:ARG:HG3	1:B:418:ARG:NH2	2.25	0.52
1:A:169:ILE:HG12	7:A:952:HOH:O	2.08	0.52
1:A:566:ALA:O	1:A:570:THR:CG2	2.58	0.52
1:B:702:VAL:HG22	1:B:703:SER:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:TYR:CZ	1:B:739:TRP:CZ3	2.98	0.52
1:B:266:LEU:HD12	1:B:266:LEU:C	2.30	0.51
1:B:688:TYR:CB	1:B:739:TRP:HD1	2.23	0.51
1:B:669:LEU:CD1	1:B:669:LEU:C	2.78	0.51
1:A:263:THR:HG23	1:A:296:ALA:HB2	1.92	0.51
1:A:345:ALA:CB	1:A:472:TYR:HE1	2.22	0.51
1:B:491:ARG:HH21	1:B:759:GLU:HB2	1.75	0.51
1:A:342:ARG:HD3	1:A:344:PHE:CE2	2.46	0.51
1:B:566:ALA:O	1:B:570:THR:CG2	2.58	0.51
1:B:610:LEU:HB3	1:B:678:VAL:CG2	2.40	0.51
1:A:718:TYR:CZ	1:A:739:TRP:CZ3	2.98	0.51
1:A:266:LEU:C	1:A:266:LEU:HD12	2.31	0.51
1:B:688:TYR:HB3	1:B:739:TRP:HD1	1.76	0.51
1:B:669:LEU:HD13	1:B:670:LEU:N	2.26	0.51
1:A:634:LYS:HB3	1:A:634:LYS:HZ3	1.76	0.50
1:B:288:ARG:HG3	1:B:326:ASN:HB3	1.92	0.50
1:A:689:LYS:NZ	7:A:862:HOH:O	2.39	0.50
1:A:540:ALA:O	1:A:543:HIS:HB2	2.11	0.50
1:A:610:LEU:HB3	1:A:678:VAL:CG2	2.40	0.50
1:A:352:ASN:HD21	1:A:354:LEU:CB	2.24	0.50
1:B:342:ARG:HD3	1:B:344:PHE:CE2	2.46	0.50
1:B:176:PHE:CE2	1:B:180:MET:HB3	2.47	0.50
1:B:366:ALA:HB3	1:B:468:PHE:CE1	2.46	0.50
1:B:368:VAL:O	1:B:368:VAL:HG22	2.12	0.50
1:B:637:ALA:O	1:B:640:SER:OG	2.26	0.50
1:B:427:GLU:OE2	1:B:445:ASN:HB2	2.11	0.50
1:B:661:TYR:CD2	1:B:726:GLY:HA3	2.47	0.50
1:A:562:ALA:O	1:A:565:SER:HB3	2.12	0.50
1:A:577:THR:O	1:A:578:ARG:CB	2.58	0.49
1:B:622:LEU:O	1:B:622:LEU:HD23	2.11	0.49
1:B:663:ILE:HD13	1:B:663:ILE:N	2.23	0.49
1:B:586:ASN:O	1:B:587:ASN:HB2	2.12	0.49
1:A:622:LEU:O	1:A:622:LEU:HD23	2.10	0.49
1:A:368:VAL:O	1:A:368:VAL:HG22	2.12	0.49
1:A:143:LEU:CD2	1:A:270:MET:CG	2.86	0.49
1:B:176:PHE:HA	1:B:180:MET:HE2	1.93	0.49
5:B:1401:FUC:H61	6:B:1402:NAG:H2	1.95	0.49
1:B:731:SER:N	7:B:960:HOH:O	2.44	0.49
3:A:1100:NAG:H61	3:A:1102:NAG:O7	2.13	0.49
1:A:346:GLY:O	1:A:442:VAL:HG11	2.13	0.49
1:A:512:TYR:HE1	7:A:773:HOH:O	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:ARG:HD2	7:B:51:HOH:O	2.11	0.49
1:A:418:ARG:NH2	1:B:418:ARG:HG3	2.28	0.49
1:B:448:GLU:HA	1:B:451:GLN:HE21	1.78	0.49
1:B:147:ILE:N	1:B:211:ASP:HB2	2.28	0.49
1:B:128:LEU:CD2	1:B:550:MET:HB3	2.42	0.49
1:A:357:ARG:NH1	1:A:474:ASP:OD2	2.40	0.49
1:B:562:ALA:O	1:B:565:SER:HB3	2.12	0.49
1:A:166:TRP:CZ2	1:A:168:GLY:HA3	2.48	0.49
1:B:129:TRP:CB	1:B:134:LEU:CD2	2.90	0.48
1:B:407:PHE:CD2	1:B:431:VAL:HG22	2.48	0.48
1:B:628:PHE:HB3	1:B:632:GLN:HB2	1.96	0.48
1:A:575:ASP:OD1	1:A:577:THR:N	2.34	0.48
1:A:129:TRP:CB	1:A:134:LEU:CD2	2.91	0.48
1:B:372:PRO:HD2	1:B:396:ASN:O	2.13	0.48
1:B:233:HIS:O	1:B:233:HIS:CD2	2.67	0.48
1:B:263:THR:HG23	1:B:296:ALA:HB2	1.95	0.48
1:B:447:LYS:HE2	7:B:829:HOH:O	2.03	0.48
1:A:688:TYR:HB3	1:A:739:TRP:HD1	1.78	0.48
4:A:1201:NAG:H61	4:A:1202:NAG:C7	2.44	0.48
1:B:166:TRP:CZ2	1:B:168:GLY:HA3	2.49	0.48
1:A:697:ASN:CG	7:A:857:HOH:O	2.51	0.48
1:A:689:LYS:HD2	1:A:742:GLN:NE2	2.29	0.48
1:B:129:TRP:HB3	1:B:134:LEU:HD21	1.95	0.48
1:B:290:ILE:N	1:B:290:ILE:HD13	2.28	0.48
1:A:617:GLN:CB	7:A:808:HOH:O	2.62	0.48
1:A:163:PRO:O	7:A:910:HOH:O	2.20	0.48
1:A:628:PHE:HB3	1:A:632:GLN:HB2	1.95	0.48
1:A:350:LEU:N	1:A:350:LEU:HD12	2.29	0.48
1:B:143:LEU:CD2	1:B:270:MET:CG	2.87	0.47
1:A:218:HIS:ND1	1:A:510:ALA:HB3	2.29	0.47
1:B:247:ARG:NE	7:B:62:HOH:O	2.43	0.47
1:A:366:ALA:HB3	1:A:468:PHE:CE1	2.48	0.47
1:B:685:ALA:HB2	1:B:710:LYS:O	2.14	0.47
1:B:672:GLN:CG	1:B:674:PHE:CZ	2.92	0.47
1:B:570:THR:HG21	1:B:605:ALA:HA	1.96	0.47
1:A:622:LEU:CD2	1:A:622:LEU:O	2.62	0.47
1:A:290:ILE:HD13	1:A:290:ILE:N	2.29	0.47
1:A:177:ASN:O	1:A:180:MET:HB2	2.13	0.47
1:B:493:TYR:CZ	7:B:845:HOH:O	2.65	0.47
1:A:208:SER:O	1:A:254:LYS:HD3	2.14	0.47
1:A:270:MET:HE3	1:A:281:ILE:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ARG:HH21	1:A:759:GLU:HB2	1.78	0.47
1:B:237:ALA:N	1:B:238:PRO:CD	2.78	0.47
1:A:702:VAL:CG2	1:A:703:SER:N	2.77	0.47
1:B:500:ASP:OD2	1:B:564:ARG:HD2	2.15	0.47
5:B:1400:NAG:O4	5:B:1401:FUC:H5	2.14	0.47
1:B:586:ASN:HD22	1:B:587:ASN:H	1.58	0.47
1:B:129:TRP:CG	1:B:134:LEU:CD2	2.98	0.47
1:A:357:ARG:NH2	1:A:474:ASP:OD2	2.45	0.47
1:B:326:ASN:HD22	1:B:326:ASN:C	2.18	0.47
1:A:367:PHE:N	1:B:526:LEU:O	2.44	0.47
1:B:199:ASP:C	1:B:199:ASP:OD1	2.54	0.47
1:B:622:LEU:CD2	1:B:622:LEU:O	2.63	0.47
1:A:491:ARG:O	1:A:760:VAL:HG13	2.15	0.47
1:B:352:ASN:HD21	1:B:354:LEU:CB	2.27	0.47
1:B:186:ILE:HD13	1:B:249:ARG:HB3	1.97	0.47
1:B:393:ASN:N	1:B:394:PRO:CD	2.77	0.46
1:A:689:LYS:HD3	7:A:862:HOH:O	2.14	0.46
1:A:399:VAL:CG1	1:A:419:LEU:HD13	2.44	0.46
1:A:393:ASN:N	1:A:394:PRO:CD	2.78	0.46
1:A:218:HIS:HE1	1:A:532:ILE:O	1.98	0.46
1:A:129:TRP:HB3	1:A:134:LEU:HD21	1.96	0.46
1:A:500:ASP:OD2	1:A:564:ARG:HD2	2.14	0.46
1:B:399:VAL:CG1	1:B:419:LEU:HD13	2.45	0.46
1:A:615:THR:O	1:A:618:ASP:HB2	2.15	0.46
1:A:176:PHE:HA	1:A:180:MET:CE	2.46	0.46
1:B:238:PRO:CD	7:B:106:HOH:O	2.53	0.46
1:B:177:ASN:O	1:B:180:MET:HB2	2.16	0.46
1:B:345:ALA:CB	1:B:472:TYR:HE1	2.28	0.46
1:B:678:VAL:O	1:B:678:VAL:HG13	2.15	0.46
1:A:154:PHE:HE1	1:A:217:THR:HG23	1.81	0.46
1:B:493:TYR:HE2	1:B:496:ILE:HG13	1.81	0.46
1:B:385:GLU:HG3	7:B:80:HOH:O	2.16	0.46
1:A:411:MET:HE3	1:A:437:PHE:CD1	2.51	0.46
1:B:540:ALA:O	1:B:543:HIS:HB2	2.16	0.46
1:A:325:LEU:HA	1:A:486:ALA:CB	2.46	0.46
1:B:491:ARG:O	1:B:760:VAL:HG13	2.16	0.45
1:A:663:ILE:HD13	1:A:663:ILE:N	2.24	0.45
1:B:493:TYR:CE2	1:B:495:GLY:HA3	2.50	0.45
1:A:407:PHE:CD2	1:A:431:VAL:HG22	2.50	0.45
1:B:329:SER:HB2	1:B:332:ILE:HD12	1.97	0.45
1:A:446:LYS:N	7:A:899:HOH:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ASN:HD22	1:A:587:ASN:H	1.63	0.45
5:B:1400:NAG:C6	6:B:1402:NAG:O7	2.53	0.45
1:A:229:LYS:CB	7:A:94:HOH:O	2.64	0.45
1:B:685:ALA:N	7:B:988:HOH:O	2.50	0.45
1:B:208:SER:O	1:B:254:LYS:HD3	2.16	0.45
1:A:147:ILE:N	1:A:211:ASP:HB2	2.31	0.45
1:A:578:ARG:CA	1:A:578:ARG:HE	2.29	0.45
1:B:350:LEU:N	1:B:350:LEU:HD12	2.31	0.45
1:B:310:LEU:O	7:B:102:HOH:O	2.21	0.45
1:A:390:GLN:NE2	4:A:1202:NAG:N2	2.63	0.45
1:A:570:THR:HG21	1:A:605:ALA:HA	1.97	0.45
1:A:727:ASP:OD1	1:A:731:SER:CB	2.60	0.45
1:A:327:ASN:HA	7:A:951:HOH:O	2.16	0.45
1:A:586:ASN:O	1:A:587:ASN:HB2	2.17	0.45
1:A:157:ASP:CG	7:A:909:HOH:O	2.54	0.45
1:A:129:TRP:CG	1:A:134:LEU:CD2	2.99	0.45
1:B:156:ASP:OD1	1:B:182:ASN:HB2	2.17	0.45
1:A:198:ASN:HB2	7:A:799:HOH:O	2.16	0.45
1:A:481:VAL:O	1:A:584:SER:HB3	2.17	0.45
1:B:127:GLY:HA3	1:B:603:ASN:OD1	2.16	0.44
1:B:689:LYS:HD2	1:B:742:GLN:NE2	2.29	0.44
1:A:237:ALA:N	1:A:238:PRO:CD	2.80	0.44
1:A:574:LEU:HD23	1:A:580:PRO:HA	1.98	0.44
1:B:218:HIS:HE1	1:B:532:ILE:O	2.01	0.44
1:A:271:ASP:OD2	1:A:638:ARG:NH2	2.50	0.44
1:B:702:VAL:CG2	1:B:703:SER:N	2.78	0.44
1:A:326:ASN:C	1:A:326:ASN:HD22	2.21	0.44
1:A:617:GLN:HB2	7:A:808:HOH:O	2.16	0.44
1:B:254:LYS:HE2	1:B:257:PHE:CD2	2.53	0.44
1:A:372:PRO:HD2	1:A:396:ASN:O	2.17	0.44
1:A:676:ARG:NH2	7:A:50:HOH:O	2.46	0.44
1:A:703:SER:HA	1:A:704:PRO:C	2.38	0.44
1:A:128:LEU:CD2	1:A:550:MET:HB3	2.48	0.44
1:A:314:SER:HB2	1:A:537:THR:HB	1.99	0.44
1:B:218:HIS:CG	1:B:510:ALA:HB3	2.53	0.44
1:A:129:TRP:CD2	1:A:134:LEU:HD22	2.52	0.44
1:A:448:GLU:HA	1:A:451:GLN:HE21	1.83	0.44
1:A:379:LEU:HD12	1:A:380:SER:N	2.33	0.44
1:A:244:VAL:CG1	1:A:546:GLY:HA3	2.48	0.44
1:A:143:LEU:HD12	1:A:253:TYR:HB2	1.98	0.44
1:B:734:VAL:CG2	1:B:735:GLY:N	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:TYR:CE1	1:A:469:GLN:HA	2.53	0.44
1:B:129:TRP:CD2	1:B:134:LEU:HD22	2.52	0.43
1:A:524:ASN:N	1:A:524:ASN:HD22	2.15	0.43
1:B:192:ASN:ND2	1:B:207:ASN:OD1	2.51	0.43
1:A:123:ASN:ND2	1:A:125:SER:HB2	2.33	0.43
1:B:325:LEU:HA	1:B:486:ALA:CB	2.47	0.43
1:B:379:LEU:HD12	1:B:380:SER:N	2.33	0.43
1:A:352:ASN:HD21	1:A:354:LEU:H	1.64	0.43
1:B:574:LEU:HD23	1:B:580:PRO:HA	2.00	0.43
1:A:329:SER:HB2	1:A:332:ILE:HD12	1.99	0.43
1:B:176:PHE:HA	1:B:180:MET:CE	2.48	0.43
1:A:718:TYR:CZ	1:A:739:TRP:CH2	3.07	0.43
1:A:685:ALA:HB2	1:A:710:LYS:O	2.18	0.43
1:A:488:GLY:HA3	1:A:498:LYS:O	2.18	0.43
1:B:696:LYS:HE3	1:B:696:LYS:HB2	1.86	0.43
1:A:692:LEU:HB3	1:A:700:ILE:HD11	2.00	0.43
1:B:271:ASP:OD2	1:B:638:ARG:NH2	2.52	0.43
1:A:528:SER:O	7:A:880:HOH:O	2.21	0.43
1:A:555:HIS:CB	7:A:878:HOH:O	2.66	0.43
5:B:1300:NAG:H3	5:B:1301:FUC:C5	2.48	0.43
1:B:578:ARG:HE	1:B:578:ARG:HA	1.84	0.43
1:B:481:VAL:O	1:B:584:SER:HB3	2.19	0.43
1:B:270:MET:HE3	1:B:281:ILE:HD13	2.01	0.43
1:B:123:ASN:ND2	1:B:125:SER:HB2	2.34	0.43
1:A:201:THR:HG23	7:A:915:HOH:O	2.18	0.43
1:B:518:ALA:HB2	1:B:529:THR:HG22	2.01	0.43
1:A:186:ILE:HD13	1:A:249:ARG:HB3	2.00	0.43
1:B:154:PHE:HE1	1:B:217:THR:HG23	1.84	0.43
1:B:663:ILE:CD1	1:B:663:ILE:H	2.26	0.42
1:B:177:ASN:H	1:B:180:MET:HE1	1.82	0.42
1:A:678:VAL:O	1:A:678:VAL:HG13	2.18	0.42
1:B:236:TYR:CE1	1:B:469:GLN:HA	2.54	0.42
1:A:263:THR:O	1:A:266:LEU:HB3	2.18	0.42
1:A:447:LYS:N	7:A:899:HOH:O	2.26	0.42
1:A:352:ASN:HD21	1:A:354:LEU:HB2	1.85	0.42
1:B:615:THR:O	1:B:618:ASP:HB2	2.19	0.42
1:A:192:ASN:ND2	1:A:207:ASN:OD1	2.53	0.42
1:B:346:GLY:O	1:B:442:VAL:HG11	2.19	0.42
1:B:347:THR:HG21	1:B:355:LYS:HE3	2.02	0.42
1:B:411:MET:HE3	1:B:437:PHE:CD1	2.55	0.42
1:A:218:HIS:CG	1:A:510:ALA:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ARG:HD3	1:B:344:PHE:CZ	2.54	0.42
1:B:661:TYR:CD2	1:B:661:TYR:O	2.73	0.42
1:B:703:SER:HA	1:B:704:PRO:C	2.40	0.42
1:A:254:LYS:HE2	1:A:257:PHE:CD2	2.55	0.42
1:A:424:PHE:HB2	1:A:443:VAL:HG22	2.02	0.42
1:A:113:THR:HA	1:A:116:THR:HB	2.02	0.42
1:B:586:ASN:C	1:B:586:ASN:HD22	2.21	0.42
1:A:199:ASP:OD1	1:A:199:ASP:C	2.57	0.42
1:A:493:TYR:HE2	1:A:496:ILE:HG13	1.85	0.42
1:A:661:TYR:O	1:A:661:TYR:CD2	2.72	0.42
1:A:342:ARG:HD3	1:A:344:PHE:CZ	2.54	0.42
1:B:446:LYS:HA	7:B:901:HOH:O	2.18	0.42
1:A:442:VAL:HG22	1:A:466:ILE:HD13	2.01	0.42
1:A:390:GLN:NE2	4:A:1202:NAG:HN2	2.17	0.42
1:A:734:VAL:CG2	1:A:735:GLY:N	2.82	0.42
1:B:575:ASP:OD1	1:B:575:ASP:C	2.58	0.42
1:A:127:GLY:HA3	1:A:603:ASN:OD1	2.19	0.42
1:A:156:ASP:OD1	1:A:182:ASN:HB2	2.20	0.42
1:A:399:VAL:HG12	1:A:419:LEU:HD13	2.02	0.41
1:B:237:ALA:N	1:B:471:THR:HG21	2.32	0.41
1:A:668:THR:O	1:A:669:LEU:C	2.58	0.41
1:B:113:THR:HA	1:B:116:THR:HB	2.02	0.41
1:B:177:ASN:N	1:B:180:MET:HE2	2.33	0.41
1:B:718:TYR:CZ	1:B:739:TRP:CH2	3.07	0.41
1:B:390:GLN:HE22	4:B:1501:NAG:HN2	1.69	0.41
1:B:460:VAL:O	1:B:461:THR:CB	2.60	0.41
1:B:442:VAL:HG22	1:B:466:ILE:HD13	2.02	0.41
1:B:394:PRO:HA	1:B:397:THR:HG23	2.03	0.41
1:A:270:MET:CE	1:A:281:ILE:HD13	2.51	0.41
1:A:702:VAL:CG2	1:A:703:SER:H	2.32	0.41
1:A:626:LEU:HD23	1:A:628:PHE:CE1	2.55	0.41
1:A:242:ARG:HD3	1:A:242:ARG:N	2.36	0.41
1:A:262:PHE:CE2	7:A:799:HOH:O	2.57	0.41
1:A:586:ASN:HD22	1:A:586:ASN:C	2.22	0.41
1:B:737:ILE:HG23	1:B:737:ILE:O	2.21	0.41
1:A:416:ARG:HD2	7:A:938:HOH:O	2.20	0.41
1:B:330:PRO:HB3	1:B:496:ILE:HD12	2.03	0.41
1:B:582:LYS:HD2	1:B:587:ASN:O	2.21	0.41
1:B:626:LEU:HD23	1:B:628:PHE:CE1	2.56	0.41
1:B:244:VAL:CG1	1:B:546:GLY:HA3	2.50	0.41
1:A:582:LYS:HD2	1:A:587:ASN:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:ASN:ND2	1:A:525:ILE:HG13	2.36	0.40
1:A:385:GLU:CG	1:A:413:ILE:HD12	2.51	0.40
1:B:237:ALA:N	1:B:238:PRO:HD3	2.37	0.40
1:B:668:THR:O	1:B:669:LEU:C	2.59	0.40
1:A:362:PHE:CE2	1:A:366:ALA:HB2	2.56	0.40
1:A:371:SER:HA	1:A:372:PRO:HD3	1.91	0.40
1:B:488:GLY:HA3	1:B:498:LYS:O	2.22	0.40
1:A:376:ASN:HB2	7:A:829:HOH:O	2.20	0.40
1:A:737:ILE:HG23	1:A:737:ILE:O	2.20	0.40
1:B:428:ASP:HA	1:B:429:PRO:HD2	1.92	0.40
1:B:191:PHE:HA	7:B:825:HOH:O	2.21	0.40
1:B:292:LEU:HG	7:B:913:HOH:O	2.21	0.40
1:A:250:LEU:HD23	1:A:250:LEU:HA	1.95	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1402:NAG:O3	7:A:820:HOH:O[6_555]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	597 (94%)	32 (5%)	3 (0%)	34	55
1	B	625/649 (96%)	589 (94%)	34 (5%)	2 (0%)	46	68
All	All	1257/1298 (97%)	1186 (94%)	66 (5%)	5 (0%)	39	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	638	ARG
1	B	653	ASN
1	A	380	SER
1	A	461	THR
1	B	461	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	528/533 (99%)	482 (91%)	46 (9%)	13	24
1	B	525/533 (98%)	480 (91%)	45 (9%)	13	24
All	All	1053/1066 (99%)	962 (91%)	91 (9%)	13	24

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	THR
1	A	128	LEU
1	A	138	VAL
1	A	140	VAL
1	A	143	LEU
1	A	144	ASP
1	A	164	LYS
1	A	184	LYS
1	A	185	LEU
1	A	201	THR
1	A	223	THR
1	A	242	ARG
1	A	266	LEU
1	A	278	VAL
1	A	290	ILE
1	A	326	ASN
1	A	352	ASN
1	A	368	VAL
1	A	391	VAL

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Mol	Chain	Res	Type
1	A	395	GLU
1	A	397	THR
1	A	414	ILE
1	A	437	PHE
1	A	442	VAL
1	A	460	VAL
1	A	471	THR
1	A	500	ASP
1	A	502	LEU
1	A	524	ASN
1	A	539	MET
1	A	586	ASN
1	A	622	LEU
1	A	624	CYS
1	A	634	LYS
1	A	638	ARG
1	A	645	CYS
1	A	663	ILE
1	A	668	THR
1	A	679	THR
1	A	687	THR
1	A	721	THR
1	A	722	ILE
1	A	732	ARG
1	A	734	VAL
1	A	739	TRP
1	A	740	VAL
1	B	116	THR
1	B	128	LEU
1	B	138	VAL
1	B	140	VAL
1	B	143	LEU
1	B	164	LYS
1	B	184	LYS
1	B	185	LEU
1	B	201	THR
1	B	223	THR
1	B	242	ARG
1	B	266	LEU
1	B	278	VAL
1	B	290	ILE
1	B	326	ASN

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Mol	Chain	Res	Type
1	B	352	ASN
1	B	368	VAL
1	B	391	VAL
1	B	395	GLU
1	B	397	THR
1	B	414	ILE
1	B	437	PHE
1	B	442	VAL
1	B	460	VAL
1	B	471	THR
1	B	500	ASP
1	B	502	LEU
1	B	524	ASN
1	B	539	MET
1	B	586	ASN
1	B	622	LEU
1	B	624	CYS
1	B	634	LYS
1	B	638	ARG
1	B	645	CYS
1	B	663	ILE
1	B	668	THR
1	B	679	THR
1	B	687	THR
1	B	721	THR
1	B	722	ILE
1	B	732	ARG
1	B	734	VAL
1	B	739	TRP
1	B	740	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	136	GLN
1	A	175	GLN
1	A	218	HIS
1	A	272	GLN
1	A	326	ASN
1	A	352	ASN
1	A	390	GLN

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Mol	Chain	Res	Type
1	A	451	GLN
1	A	524	ASN
1	A	555	HIS
1	A	586	ASN
1	A	617	GLN
1	B	123	ASN
1	B	136	GLN
1	B	175	GLN
1	B	218	HIS
1	B	326	ASN
1	B	352	ASN
1	B	390	GLN
1	B	451	GLN
1	B	524	ASN
1	B	555	HIS
1	B	586	ASN
1	B	617	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

15 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	$\# Z > 2$
2	NAG	A	1000	1,2	14,14,15	1.07	1 (7%)	15,19,21	1.78	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1001	2	14,14,15	0.79	0	15,19,21	1.73	3 (20%)
3	NAG	A	1100	1,3	14,14,15	0.58	0	15,19,21	0.74	0
3	FUC	A	1101	3	10,10,11	0.69	0	14,14,16	1.41	2 (14%)
3	NAG	A	1102	3	14,14,15	0.53	0	15,19,21	1.16	1 (6%)
4	NAG	A	1201	1,4	14,14,15	0.41	0	15,19,21	8.32	6 (40%)
4	NAG	A	1202	4	14,14,15	0.54	0	15,19,21	0.59	0
4	FUC	A	1203	4	10,10,11	0.63	0	14,14,16	0.77	1 (7%)
5	NAG	B	1300	1,5	14,14,15	0.42	0	15,19,21	0.92	0
5	FUC	B	1301	5	10,10,11	0.55	0	14,14,16	1.09	0
5	NAG	B	1400	1,5,6	14,14,15	0.53	0	15,19,21	0.58	0
5	FUC	B	1401	5	10,10,11	0.63	0	14,14,16	0.79	1 (7%)
4	NAG	B	1500	1,4	14,14,15	0.51	0	15,19,21	2.22	2 (13%)
4	NAG	B	1501	4	14,14,15	0.52	0	15,19,21	0.81	1 (6%)
4	FUC	B	1502	4	10,10,11	0.57	0	14,14,16	0.75	1 (7%)

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	NAG	A	1000	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1001	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1100	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	1101	3	-	0/0/17/20	0/1/1/1
3	NAG	A	1102	3	-	0/6/23/26	0/1/1/1
4	NAG	A	1201	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1202	4	-	0/6/23/26	0/1/1/1
4	FUC	A	1203	4	-	0/0/17/20	0/1/1/1
5	NAG	B	1300	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	FUC	B	1301	5	-	0/0/17/20	0/1/1/1
5	NAG	B	1400	1,5,6	-	0/6/23/26	0/1/1/1
5	FUC	B	1401	5	-	0/0/17/20	0/1/1/1
4	NAG	B	1500	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1501	4	-	0/6/23/26	0/1/1/1
4	FUC	B	1502	4	-	0/0/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	NAG	O5-C1	-2.25	1.40	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1201	NAG	O7-C7-C8	-18.68	87.78	122.06
4	A	1201	NAG	C4-C3-C2	-9.43	96.57	111.23
4	A	1201	NAG	C3-C2-N2	-7.35	92.95	110.56
4	B	1500	NAG	C4-C3-C2	-5.02	103.43	111.23
2	A	1001	NAG	C4-C3-C2	-4.35	104.46	111.23
2	A	1000	NAG	C4-C3-C2	-4.02	104.98	111.23
3	A	1102	NAG	C4-C3-C2	-3.17	106.31	111.23
2	A	1000	NAG	C2-N2-C7	-2.64	119.64	123.04
4	B	1501	NAG	C2-N2-C7	-2.55	119.76	123.04
2	A	1001	NAG	C2-N2-C7	-2.54	119.77	123.04
2	A	1000	NAG	O4-C4-C3	-2.45	104.81	110.34
2	A	1000	NAG	C3-C4-C5	-2.31	106.17	110.20
2	A	1000	NAG	O6-C6-C5	-2.23	103.96	111.33
5	B	1401	FUC	O5-C5-C6	2.03	109.48	106.13
4	A	1203	FUC	O5-C5-C6	2.07	109.54	106.13
4	B	1502	FUC	O5-C5-C6	2.25	109.84	106.13
3	A	1101	FUC	C3-C4-C5	2.38	113.72	109.72
2	A	1001	NAG	C1-O5-C5	2.77	115.76	112.25
3	A	1101	FUC	C1-C2-C3	3.21	113.33	109.54
4	B	1500	NAG	C1-O5-C5	6.40	120.37	112.25
4	A	1201	NAG	O3-C3-C2	9.11	127.16	109.11
4	A	1201	NAG	C1-O5-C5	14.26	130.35	112.25
4	A	1201	NAG	C8-C7-N2	16.01	146.75	116.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1300	NAG	C1

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	NAG	2	0
2	A	1001	NAG	1	0
3	A	1100	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	NAG	1	0
4	A	1201	NAG	4	0
4	A	1202	NAG	5	0
4	A	1203	FUC	1	0
5	B	1300	NAG	3	0
5	B	1301	FUC	2	0
5	B	1400	NAG	9	0
5	B	1401	FUC	4	0
4	B	1501	NAG	1	0

5.6 Ligand geometry

1 ligand is 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	$\# Z > 2$
6	NAG	B	1402	5	14,14,15	0.55	0	15,19,21	0.58	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
6	NAG	B	1402	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1402	NAG	12	1

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	642/649 (98%)	0.17	32 (4%) 32 37	33, 48, 65, 79	0
1	B	639/649 (98%)	0.15	24 (3%) 44 49	33, 48, 65, 79	0
All	All	1281/1298 (98%)	0.16	56 (4%) 38 43	33, 48, 65, 79	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	VAL	5.1
1	A	667	PHE	5.1
1	B	745	ASN	4.9
1	A	665	GLY	4.2
1	A	405	GLY	4.2
1	A	461	THR	3.8
1	A	725	ILE	3.7
1	A	663	ILE	3.6
1	B	664	GLU	3.5
1	A	668	THR	3.4
1	A	723	ARG	3.3
1	B	423	ILE	3.2
1	A	643	HIS	3.2
1	A	666	ASN	3.1
1	A	664	GLU	2.9
1	A	645	CYS	2.9
1	B	743	ASN	2.9
1	B	460	VAL	2.9
1	B	578	ARG	2.8
1	A	669	LEU	2.8
1	A	710	LYS	2.7
1	B	645	CYS	2.7
1	B	422	ALA	2.7
1	B	386	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	722	ILE	2.6
1	A	392	GLU	2.6
1	A	685	ALA	2.6
1	A	739	TRP	2.6
1	A	386	GLU	2.6
1	A	630	GLU	2.5
1	A	474	ASP	2.5
1	A	422	ALA	2.4
1	B	400	ILE	2.4
1	B	164	LYS	2.3
1	B	648	PRO	2.3
1	B	710	LYS	2.3
1	B	742	GLN	2.3
1	B	666	ASN	2.2
1	A	144	ASP	2.2
1	B	630	GLU	2.2
1	A	458	ASN	2.2
1	B	157	ASP	2.2
1	B	399	VAL	2.1
1	A	493	TYR	2.1
1	A	634	LYS	2.1
1	B	392	GLU	2.1
1	A	423	ILE	2.1
1	A	627	ASN	2.1
1	A	427	GLU	2.1
1	A	743	ASN	2.1
1	A	416	ARG	2.1
1	B	461	THR	2.1
1	B	711	ASN	2.0
1	B	113	THR	2.0
1	B	161	GLU	2.0
1	A	403	ASP	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. 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	NAG	A	1001	14/15	0.74	0.40	-	14,16,19,20	14
4	FUC	A	1203	10/11	0.95	0.33	-	79,79,79,79	0
4	NAG	B	1501	14/15	0.93	0.21	-	65,66,66,67	0
4	NAG	A	1202	14/15	0.89	0.24	-	78,78,79,79	0
5	NAG	B	1300	14/15	0.70	0.34	-	66,72,75,76	0
4	FUC	B	1502	10/11	0.93	0.29	-	64,65,65,66	0
3	NAG	A	1100	14/15	0.93	0.20	-	51,53,55,55	0
5	NAG	B	1400	14/15	0.85	0.17	-	51,53,54,55	0
3	FUC	A	1101	10/11	0.94	0.16	-	57,58,59,59	0
4	NAG	B	1500	14/15	0.87	0.14	-	60,62,64,64	0
5	FUC	B	1301	10/11	0.79	0.53	-	76,78,78,78	0
2	NAG	A	1000	14/15	0.85	0.27	-	13,14,16,18	14
3	NAG	A	1102	14/15	0.85	0.27	-	53,56,57,57	0
4	NAG	A	1201	14/15	0.90	0.14	-	75,76,78,78	0
5	FUC	B	1401	10/11	0.90	0.20	-	54,54,55,55	0

6.4 Ligands ⓘ

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
6	NAG	B	1402	14/15	0.79	0.33	8.10	55,55,57,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.