



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:32 am GMT

PDB ID : 1R46
Title : Structure of human alpha-galactosidase
Authors : Garman, S.C.; Garboczi, D.N.
Deposited on : 2003-10-03
Resolution : 3.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

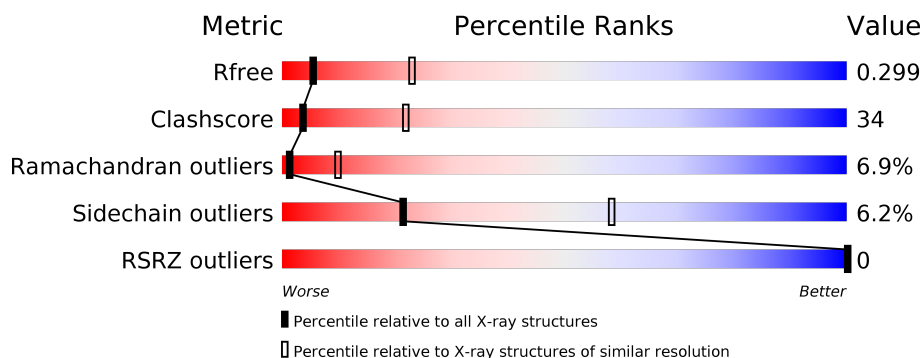
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1852 (3.32-3.20)
Clashscore	112137	2036 (3.32-3.20)
Ramachandran outliers	110173	2000 (3.32-3.20)
Sidechain outliers	110143	1998 (3.32-3.20)
RSRZ outliers	101464	1861 (3.32-3.20)

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	398	
1	B	398	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	A	694	X	-	-	-
5	NAG	B	639	-	-	X	-
5	MAN	B	641	X	-	-	-
6	MAN	B	694	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6539 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 Alpha-galactosidase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3122	1988	534	574	26			
1	B	391	Total	C	N	O	S	0	0	0
			3131	1993	536	576	26			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

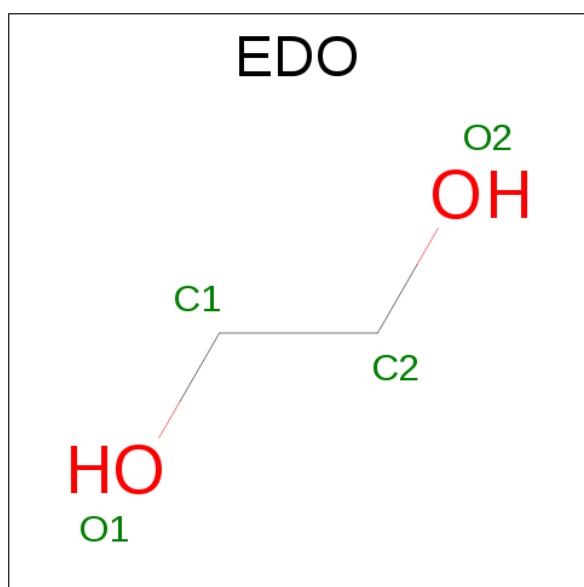
- Molecule 5 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

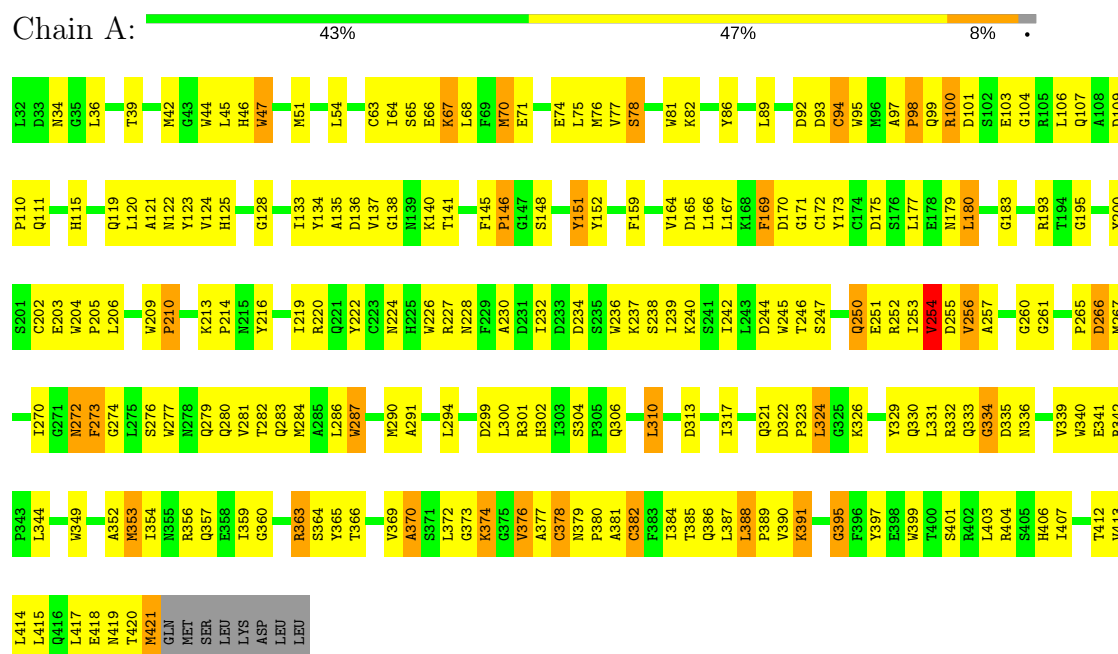
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	9	Total	O	0	0
			9	9		
8	B	9	Total	O	0	0
			9	9		

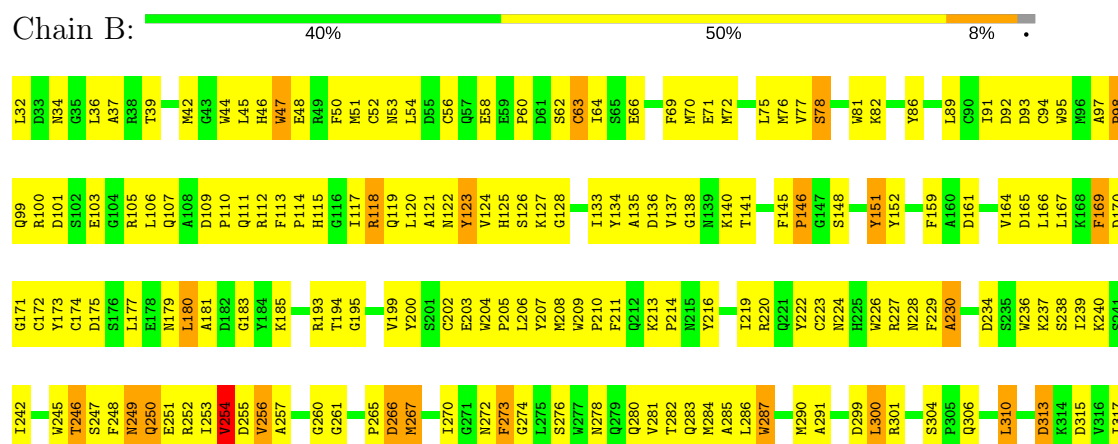
3 Residue-property plots

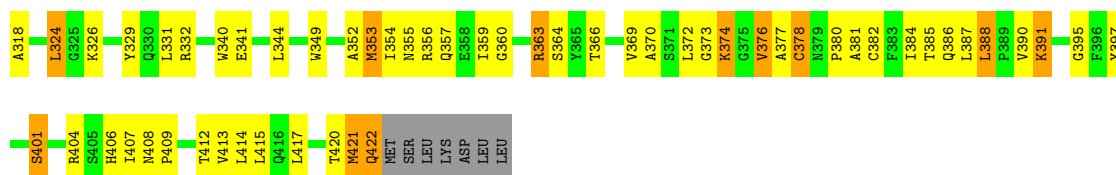
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: Alpha-galactosidase A



• Molecule 1: Alpha-galactosidase A





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.46Å 88.46Å 215.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.92 – 3.25 44.23 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.92-3.25) 99.6 (44.23-2.86)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.25	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.86Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.262 , 0.301 0.264 , 0.299	Depositor DCC
R_{free} test set	820 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	70.1	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6539	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, NAG, EDO, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/3209	0.69	0/4358
1	B	0.45	0/3218	0.70	1/4370 (0.0%)
All	All	0.45	0/6427	0.69	1/8728 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	TRP	N-CA-C	-6.42	93.66	111.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	694	MAN	C1
5	B	641	MAN	C1
6	B	694	MAN	C1

There are no planarity outliers.

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	3122	0	2981	195	0
1	B	3131	0	2989	230	1
2	A	14	0	13	0	0
3	A	61	0	52	0	0
4	A	28	0	25	0	0
4	B	28	0	25	3	0
5	B	71	0	61	14	0
6	B	50	0	43	5	0
7	A	8	0	12	1	0
7	B	8	0	12	1	0
8	A	9	0	0	1	0
8	B	9	0	0	2	0
All	All	6539	0	6213	437	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 34.

All (437) 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:386:GLN:HE21	1:A:390:VAL:HG22	1.22	1.05
1:B:386:GLN:HE21	1:B:390:VAL:HG22	1.22	1.04
1:A:213:LYS:H	1:A:213:LYS:HD2	1.20	1.03
1:A:286:LEU:HD11	1:A:354:ILE:HD11	1.51	0.91
1:B:286:LEU:HD11	1:B:354:ILE:HD11	1.54	0.87
1:A:366:THR:HG22	1:A:404:ARG:HB2	1.58	0.84
1:B:119:GLN:HA	1:B:122:ASN:HD22	1.40	0.84
1:A:240:LYS:CE	1:A:356:ARG:HH21	1.91	0.83
1:A:386:GLN:NE2	1:A:390:VAL:HG22	1.94	0.83
1:B:386:GLN:NE2	1:B:390:VAL:HG22	1.92	0.83
4:B:715:NAG:H62	4:B:716:NAG:H82	1.59	0.81
1:A:333:GLN:HG3	1:A:334:GLY:H	1.44	0.81
1:A:359:ILE:HG12	1:A:360:GLY:H	1.46	0.81
1:B:353:MET:HG2	1:B:407:ILE:HD11	1.63	0.81
1:A:213:LYS:CD	1:A:213:LYS:H	1.94	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLY:HA3	1:A:173:TYR:O	1.81	0.80
1:B:359:ILE:HG12	1:B:360:GLY:H	1.47	0.79
1:B:224:ASN:HA	1:B:260:GLY:O	1.81	0.79
1:B:177:LEU:H	1:B:177:LEU:HD12	1.46	0.79
1:A:359:ILE:HG12	1:A:360:GLY:N	1.98	0.79
1:B:120:LEU:O	1:B:124:VAL:HG23	1.83	0.79
1:B:359:ILE:HG12	1:B:360:GLY:N	1.98	0.78
5:B:639:NAG:H62	5:B:644:FUC:H3	1.63	0.78
1:B:366:THR:HG22	1:B:404:ARG:HB2	1.65	0.77
1:A:177:LEU:H	1:A:177:LEU:HD12	1.48	0.77
1:A:366:THR:HG22	1:A:404:ARG:CB	2.15	0.77
1:A:240:LYS:HE3	1:A:356:ARG:HH21	1.50	0.76
1:B:174:CYS:CB	5:B:639:NAG:H81	2.14	0.76
1:B:174:CYS:HA	5:B:639:NAG:H81	1.67	0.76
1:B:234:ASP:O	1:B:274:GLY:HA3	1.84	0.76
1:A:224:ASN:HA	1:A:260:GLY:O	1.86	0.75
1:A:100:ARG:HD2	1:A:104:GLY:O	1.87	0.75
1:A:286:LEU:HD11	1:A:354:ILE:CD1	2.16	0.75
1:B:265:PRO:O	1:B:266:ASP:HB2	1.86	0.74
1:B:46:HIS:CD2	1:B:92:ASP:H	2.05	0.74
1:B:135:ALA:HB2	1:B:167:LEU:HD11	1.70	0.74
1:A:377:ALA:O	1:A:378:CYS:HB2	1.86	0.74
1:B:138:GLY:HA3	1:B:173:TYR:O	1.88	0.74
1:A:353:MET:HG2	1:A:407:ILE:HD11	1.68	0.73
1:B:366:THR:HG22	1:B:404:ARG:CB	2.19	0.72
1:B:273:PHE:CD2	1:B:273:PHE:N	2.58	0.71
1:B:315:ASP:OD2	1:B:391:LYS:HE2	1.89	0.71
1:A:135:ALA:HB2	1:A:167:LEU:HD11	1.72	0.71
1:B:203:GLU:HG3	1:B:227:ARG:HG3	1.73	0.70
1:B:324:LEU:HD22	1:B:326:LYS:HG2	1.73	0.70
1:A:140:LYS:HB2	1:A:173:TYR:CD2	2.27	0.70
1:B:240:LYS:HE3	1:B:356:ARG:HH21	1.56	0.70
1:B:422:GLN:HE21	1:B:422:GLN:N	1.89	0.69
1:B:286:LEU:HD11	1:B:354:ILE:CD1	2.20	0.69
5:B:641:MAN:O4	5:B:642:MAN:H3	1.92	0.69
1:B:240:LYS:CE	1:B:356:ARG:HH21	2.06	0.69
1:B:363:ARG:HG2	1:B:363:ARG:HH11	1.55	0.69
1:A:45:LEU:HD21	1:A:92:ASP:HB2	1.75	0.69
1:B:276:SER:O	1:B:280:GLN:HG3	1.92	0.69
1:A:381:ALA:HB3	1:A:420:THR:HB	1.75	0.69
1:A:203:GLU:HG3	1:A:227:ARG:HG3	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:GLN:HA	1:B:122:ASN:ND2	2.08	0.68
1:A:234:ASP:O	1:A:274:GLY:HA3	1.94	0.68
1:B:224:ASN:O	1:B:261:GLY:HA2	1.94	0.68
1:A:265:PRO:O	1:A:266:ASP:HB2	1.93	0.68
1:A:369:VAL:HG12	1:A:378:CYS:SG	2.33	0.68
1:A:273:PHE:CD2	1:A:273:PHE:N	2.61	0.67
1:A:363:ARG:HG2	1:A:363:ARG:HH11	1.58	0.67
1:A:324:LEU:HD22	1:A:326:LYS:HG2	1.76	0.67
1:B:110:PRO:HB2	1:B:111:GLN:NE2	2.10	0.67
5:B:639:NAG:C6	5:B:644:FUC:H3	2.25	0.67
1:A:240:LYS:HE2	1:A:356:ARG:HH21	1.60	0.66
1:B:66:GLU:O	1:B:70:MET:HG3	1.95	0.66
1:B:101:ASP:HB3	1:B:107:GLN:OE1	1.95	0.66
1:A:110:PRO:HB2	1:A:111:GLN:NE2	2.10	0.66
1:A:224:ASN:O	1:A:261:GLY:HA2	1.96	0.65
1:B:127:LYS:HA	1:B:127:LYS:HE2	1.78	0.65
1:B:177:LEU:HD12	1:B:177:LEU:N	2.11	0.65
1:B:386:GLN:O	1:B:391:LYS:HA	1.96	0.65
1:B:69:PHE:CZ	1:B:91:ILE:HG23	2.32	0.65
1:B:140:LYS:HB2	1:B:173:TYR:CD2	2.29	0.65
1:A:177:LEU:N	1:A:177:LEU:HD12	2.11	0.65
1:A:369:VAL:CG1	1:A:378:CYS:SG	2.84	0.65
1:A:97:ALA:HB2	1:A:109:ASP:HA	1.78	0.64
1:A:46:HIS:CD2	1:A:92:ASP:H	2.14	0.64
1:B:300:LEU:HD12	1:B:300:LEU:H	1.62	0.64
1:B:369:VAL:HG12	1:B:378:CYS:SG	2.37	0.64
1:B:204:TRP:HB3	1:B:205:PRO:HD3	1.79	0.64
1:A:300:LEU:H	1:A:300:LEU:HD12	1.62	0.64
1:A:204:TRP:HB3	1:A:205:PRO:HD3	1.79	0.63
1:B:45:LEU:HD21	1:B:92:ASP:HB2	1.79	0.63
1:A:177:LEU:CD1	1:A:177:LEU:H	2.12	0.63
1:B:135:ALA:CB	1:B:167:LEU:HD11	2.27	0.63
1:B:177:LEU:H	1:B:177:LEU:CD1	2.11	0.63
1:B:174:CYS:CA	5:B:639:NAG:H81	2.27	0.63
1:A:145:PHE:HB3	1:A:146:PRO:HD2	1.81	0.63
1:A:386:GLN:O	1:A:391:LYS:HA	1.98	0.63
1:A:417:LEU:HD12	1:A:417:LEU:N	2.13	0.63
1:B:75:LEU:HD21	1:B:301:ARG:HG2	1.81	0.63
1:B:145:PHE:HB3	1:B:146:PRO:HD2	1.80	0.63
1:B:72:MET:O	1:B:76:MET:HG3	2.00	0.62
1:A:387:LEU:HD12	1:A:391:LYS:HG3	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:694:MAN:H3	6:B:695:MAN:C5	2.29	0.62
1:A:384:ILE:HD12	1:A:397:TYR:CD1	2.34	0.61
1:A:370:ALA:HB2	1:A:399:TRP:O	1.99	0.61
1:B:422:GLN:HE21	1:B:422:GLN:H	1.48	0.61
1:A:202:CYS:O	1:A:226:TRP:HA	2.00	0.61
1:B:208:MET:SD	1:B:214:PRO:HB3	2.40	0.61
1:B:377:ALA:O	1:B:378:CYS:HB2	2.01	0.61
1:A:93:ASP:O	1:A:94:CYS:HB2	1.98	0.61
1:B:359:ILE:CG1	1:B:360:GLY:H	2.12	0.61
1:A:381:ALA:HB1	1:A:420:THR:OG1	2.01	0.60
1:B:331:LEU:HD22	1:B:341:GLU:OE2	2.01	0.60
1:B:174:CYS:HA	5:B:639:NAG:O7	2.01	0.60
1:B:290:MET:O	1:B:291:ALA:C	2.40	0.60
1:A:359:ILE:CG1	1:A:360:GLY:H	2.14	0.60
1:A:403:LEU:HD12	1:A:404:ARG:N	2.17	0.60
1:A:228:ASN:HB3	1:A:245:TRP:CH2	2.36	0.60
1:A:34:ASN:OD1	1:A:36:LEU:HB2	2.02	0.60
1:A:330:GLN:NE2	1:A:333:GLN:HE22	1.99	0.59
1:A:384:ILE:HG12	1:A:417:LEU:HG	1.83	0.59
1:B:213:LYS:H	1:B:213:LYS:HD2	1.65	0.59
1:B:299:ASP:OD1	1:B:301:ARG:HB2	2.02	0.59
1:B:93:ASP:O	1:B:94:CYS:HB2	2.02	0.59
1:A:125:HIS:HE1	1:A:165:ASP:OD2	1.84	0.59
1:B:100:ARG:NH1	1:B:106:LEU:HG	2.18	0.59
1:A:135:ALA:HB3	1:A:169:PHE:HD1	1.68	0.59
1:A:254:VAL:HG21	1:A:329:TYR:HB3	1.84	0.59
1:B:417:LEU:N	1:B:417:LEU:HD12	2.18	0.59
1:A:290:MET:O	1:A:291:ALA:C	2.41	0.59
1:A:51:MET:O	1:A:64:ILE:HD11	2.04	0.58
1:A:44:TRP:CD1	1:A:300:LEU:HD11	2.38	0.58
1:B:205:PRO:HG3	1:B:219:ILE:HD13	1.84	0.58
1:B:387:LEU:HD12	1:B:391:LYS:HG3	1.85	0.58
4:B:715:NAG:H62	4:B:716:NAG:C8	2.32	0.58
1:B:118:ARG:O	1:B:121:ALA:HB3	2.03	0.58
1:A:138:GLY:CA	1:A:173:TYR:O	2.52	0.58
1:B:34:ASN:OD1	1:B:36:LEU:HB2	2.04	0.57
1:B:202:CYS:O	1:B:226:TRP:HA	2.04	0.57
1:B:359:ILE:CG1	1:B:360:GLY:N	2.66	0.57
1:B:253:ILE:HG13	1:B:254:VAL:N	2.19	0.57
1:B:384:ILE:HG12	1:B:417:LEU:HG	1.86	0.57
1:A:159:PHE:O	1:A:164:VAL:HG23	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ASP:CG	1:B:274:GLY:H	2.07	0.57
1:A:359:ILE:CG1	1:A:360:GLY:N	2.68	0.57
1:B:252:ARG:HH11	1:B:252:ARG:HG3	1.70	0.57
5:B:639:NAG:H62	5:B:644:FUC:C3	2.26	0.57
1:A:253:ILE:HG13	1:A:254:VAL:N	2.19	0.56
1:B:97:ALA:HB2	1:B:109:ASP:HA	1.87	0.56
1:B:136:ASP:OD2	1:B:141:THR:HA	2.05	0.56
1:B:278:ASN:OD1	1:B:408:ASN:HB2	2.05	0.56
1:A:331:LEU:HD22	1:A:341:GLU:OE2	2.06	0.56
1:B:208:MET:CE	1:B:214:PRO:HA	2.35	0.56
1:A:115:HIS:HB3	1:A:119:GLN:OE1	2.05	0.56
1:A:324:LEU:HD12	1:A:344:LEU:O	2.05	0.56
1:A:395:GLY:HA2	7:A:1102:EDO:H22	1.86	0.56
1:A:376:VAL:HG12	1:A:377:ALA:N	2.19	0.56
1:A:54:LEU:HD12	1:A:54:LEU:N	2.21	0.56
1:A:238:SER:O	1:A:242:ILE:HG13	2.06	0.56
1:B:159:PHE:O	1:B:164:VAL:HG23	2.06	0.56
5:B:639:NAG:H62	5:B:644:FUC:O2	2.06	0.56
1:B:238:SER:O	1:B:242:ILE:HG13	2.05	0.56
1:B:228:ASN:HB3	1:B:245:TRP:CH2	2.41	0.56
1:B:376:VAL:HG12	1:B:377:ALA:N	2.18	0.56
1:B:324:LEU:HD12	1:B:344:LEU:O	2.05	0.56
1:B:369:VAL:CG1	1:B:378:CYS:SG	2.94	0.56
1:A:234:ASP:CG	1:A:274:GLY:H	2.08	0.55
1:A:135:ALA:CB	1:A:167:LEU:HD11	2.35	0.55
1:A:66:GLU:O	1:A:70:MET:HB2	2.05	0.55
1:B:72:MET:SD	1:B:300:LEU:HD13	2.46	0.55
1:B:200:TYR:HD2	1:B:222:TYR:O	1.90	0.55
1:A:276:SER:O	1:A:280:GLN:HG3	2.06	0.55
1:A:372:LEU:O	1:A:374:LYS:N	2.40	0.55
1:A:71:GLU:O	1:A:75:LEU:HD13	2.06	0.55
1:B:51:MET:O	1:B:64:ILE:HD11	2.07	0.55
1:A:377:ALA:O	1:A:378:CYS:CB	2.52	0.55
1:A:417:LEU:CD1	1:A:417:LEU:N	2.69	0.55
1:A:101:ASP:HB3	1:A:107:GLN:OE1	2.07	0.55
1:B:54:LEU:HD12	1:B:54:LEU:N	2.22	0.54
1:B:366:THR:HG22	1:B:404:ARG:CG	2.38	0.54
1:B:252:ARG:NH1	1:B:252:ARG:HG3	2.23	0.54
1:B:340:TRP:HB2	1:B:352:ALA:HB3	1.89	0.54
1:B:278:ASN:O	1:B:281:VAL:HG22	2.07	0.54
1:A:359:ILE:HG13	1:B:48:GLU:OE2	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:VAL:HG21	1:B:127:LYS:HB3	1.90	0.54
1:B:386:GLN:HA	1:B:415:LEU:HD23	1.90	0.54
1:A:170:ASP:OD1	1:A:171:GLY:N	2.42	0.53
1:A:276:SER:H	1:A:279:GLN:HB2	1.74	0.53
1:B:248:PHE:CG	1:B:248:PHE:O	2.60	0.53
1:A:252:ARG:HG3	1:A:252:ARG:HH11	1.73	0.53
1:A:388:LEU:HB2	1:A:414:LEU:HB3	1.89	0.53
1:A:366:THR:HG22	1:A:404:ARG:CG	2.38	0.53
1:B:81:TRP:CD1	1:B:300:LEU:HD23	2.44	0.53
1:B:45:LEU:CD2	1:B:92:ASP:HB2	2.38	0.53
1:A:137:VAL:HG12	1:A:171:GLY:HA2	1.91	0.53
1:B:135:ALA:HB3	1:B:169:PHE:HD1	1.73	0.53
1:A:386:GLN:HA	1:A:415:LEU:HD23	1.91	0.52
1:B:112:ARG:NH2	8:B:18:HOH:O	2.41	0.52
1:B:174:CYS:HA	5:B:639:NAG:C8	2.39	0.52
1:B:229:PHE:CD2	1:B:242:ILE:HG12	2.43	0.52
1:B:44:TRP:CD1	1:B:300:LEU:HD11	2.44	0.52
1:B:377:ALA:O	1:B:378:CYS:CB	2.58	0.52
1:B:384:ILE:HD12	1:B:397:TYR:CD1	2.45	0.52
1:A:213:LYS:N	1:A:213:LYS:HD2	2.04	0.52
1:B:380:PRO:HG2	1:B:381:ALA:H	1.75	0.52
1:A:381:ALA:HB3	1:A:420:THR:CB	2.39	0.52
1:B:270:ILE:HG23	1:B:280:GLN:OE1	2.10	0.52
1:A:45:LEU:CD2	1:A:92:ASP:HB2	2.39	0.52
1:B:229:PHE:HD2	1:B:242:ILE:HG12	1.74	0.52
1:A:205:PRO:HG3	1:A:219:ILE:HD13	1.92	0.52
6:B:694:MAN:H3	6:B:695:MAN:H5	1.91	0.52
1:A:265:PRO:HB2	1:A:287:TRP:CZ2	2.45	0.51
1:B:179:ASN:HD22	1:B:179:ASN:N	2.08	0.51
1:A:340:TRP:HB2	1:A:352:ALA:HB3	1.93	0.51
1:A:100:ARG:NH1	1:A:106:LEU:HG	2.26	0.51
1:B:32:LEU:N	1:B:220:ARG:O	2.44	0.51
1:B:420:THR:OG1	1:B:421:MET:N	2.44	0.51
1:B:174:CYS:HB2	5:B:639:NAG:H81	1.88	0.51
1:A:119:GLN:O	1:A:122:ASN:HB3	2.11	0.51
1:A:270:ILE:HG23	1:A:280:GLN:OE1	2.10	0.51
1:B:387:LEU:O	1:B:388:LEU:HD13	2.11	0.51
1:A:333:GLN:HA	1:A:333:GLN:NE2	2.25	0.51
1:B:388:LEU:HB2	1:B:414:LEU:HB3	1.91	0.51
1:A:200:TYR:HD2	1:A:222:TYR:O	1.93	0.50
1:A:220:ARG:NH1	1:A:256:VAL:O	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ARG:HG3	1:A:332:ARG:HH11	1.75	0.50
1:A:252:ARG:NH1	1:A:252:ARG:HG3	2.27	0.50
1:B:123:TYR:O	1:B:126:SER:HB3	2.12	0.50
1:B:363:ARG:NH1	1:B:363:ARG:HG2	2.25	0.50
1:B:417:LEU:CD1	1:B:417:LEU:N	2.74	0.50
1:A:42:MET:HE3	1:A:317:ILE:HG23	1.92	0.50
1:B:220:ARG:NH1	1:B:256:VAL:O	2.44	0.50
1:B:113:PHE:N	1:B:114:PRO:HD3	2.26	0.50
1:B:117:ILE:O	1:B:119:GLN:N	2.45	0.50
1:A:214:PRO:HB2	1:A:219:ILE:HD11	1.93	0.49
1:A:277:TRP:HA	1:A:277:TRP:CE3	2.47	0.49
1:B:315:ASP:CG	1:B:391:LYS:HE2	2.33	0.49
1:B:353:MET:HG2	1:B:407:ILE:CD1	2.36	0.49
1:A:284:MET:HG2	1:A:310:LEU:CD2	2.42	0.49
1:B:172:CYS:O	1:B:173:TYR:HB2	2.12	0.49
1:A:44:TRP:NE1	1:A:300:LEU:HD11	2.27	0.49
1:B:373:GLY:O	1:B:376:VAL:N	2.44	0.49
1:A:205:PRO:O	1:A:209:TRP:HD1	1.96	0.49
1:A:97:ALA:HB2	1:A:110:PRO:HD3	1.95	0.49
1:B:304:SER:HB2	1:B:306:GLN:HG2	1.94	0.49
1:A:335:ASP:O	1:A:336:ASN:C	2.50	0.49
1:B:284:MET:HG2	1:B:310:LEU:CD2	2.43	0.49
5:B:641:MAN:O4	5:B:642:MAN:H2	2.12	0.49
1:A:179:ASN:N	1:A:179:ASN:HD22	2.10	0.49
1:A:236:TRP:NE1	1:A:240:LYS:HD2	2.27	0.49
1:A:388:LEU:HD22	1:A:414:LEU:HD23	1.95	0.49
1:A:387:LEU:O	1:A:388:LEU:HD13	2.13	0.48
1:A:381:ALA:CB	1:A:420:THR:OG1	2.60	0.48
1:B:164:VAL:HG12	1:B:166:LEU:H	1.78	0.48
1:B:313:ASP:O	1:B:317:ILE:HG13	2.12	0.48
1:A:151:TYR:O	1:A:152:TYR:C	2.51	0.48
1:A:332:ARG:HB2	1:A:339:VAL:HB	1.95	0.48
1:B:127:LYS:HA	1:B:127:LYS:CE	2.42	0.48
1:A:136:ASP:OD2	1:A:141:THR:HA	2.12	0.48
1:B:164:VAL:HG12	1:B:165:ASP:N	2.28	0.48
1:B:82:LYS:HE3	1:B:128:GLY:HA3	1.94	0.48
1:B:380:PRO:HG2	1:B:381:ALA:N	2.28	0.48
1:B:170:ASP:OD1	1:B:171:GLY:N	2.46	0.48
1:A:172:CYS:O	1:A:173:TYR:HB2	2.13	0.48
1:A:145:PHE:CB	1:A:146:PRO:HD2	2.44	0.47
1:B:93:ASP:OD1	1:B:94:CYS:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:TRP:CD1	1:B:377:ALA:HB2	2.50	0.47
1:A:45:LEU:CD2	1:A:47:TRP:H	2.27	0.47
1:B:136:ASP:O	1:B:148:SER:HB2	2.14	0.47
1:B:281:VAL:HG23	1:B:282:THR:N	2.29	0.47
1:B:332:ARG:HH11	1:B:332:ARG:HG3	1.79	0.47
1:B:45:LEU:CD2	1:B:47:TRP:H	2.27	0.47
1:B:412:THR:HG22	1:B:413:VAL:N	2.29	0.47
1:A:304:SER:HB2	1:A:306:GLN:HG2	1.95	0.47
1:B:151:TYR:O	1:B:152:TYR:C	2.52	0.47
1:B:95:TRP:CD2	1:B:133:ILE:HD11	2.50	0.47
1:B:315:ASP:O	1:B:318:ALA:HB3	2.15	0.47
1:B:205:PRO:O	1:B:207:TYR:N	2.48	0.47
1:B:64:ILE:O	1:B:112:ARG:NH1	2.47	0.47
1:B:299:ASP:C	1:B:301:ARG:H	2.17	0.47
1:B:353:MET:O	1:B:412:THR:HA	2.14	0.47
1:A:366:THR:CG2	1:A:404:ARG:HB2	2.37	0.46
1:B:71:GLU:O	1:B:75:LEU:HD13	2.16	0.46
1:A:216:TYR:HB3	1:A:256:VAL:HG21	1.98	0.46
1:A:244:ASP:HA	8:A:1:HOH:O	2.15	0.46
1:B:117:ILE:O	1:B:120:LEU:N	2.44	0.46
1:B:236:TRP:NE1	1:B:240:LYS:HD2	2.30	0.46
1:B:81:TRP:NE1	1:B:300:LEU:HD23	2.31	0.46
1:A:281:VAL:HG23	1:A:282:THR:N	2.31	0.46
1:B:270:ILE:HG13	1:B:283:GLN:OE1	2.15	0.46
1:A:364:SER:HB3	1:A:406:HIS:CE1	2.50	0.46
1:B:133:ILE:HG22	1:B:164:VAL:HG11	1.98	0.46
1:B:42:MET:HE3	1:B:317:ILE:HG23	1.98	0.46
1:B:372:LEU:O	1:B:374:LYS:N	2.42	0.46
1:B:369:VAL:HG23	1:B:401:SER:O	2.16	0.46
1:A:164:VAL:HG12	1:A:165:ASP:N	2.31	0.46
1:B:117:ILE:O	1:B:118:ARG:C	2.53	0.46
1:B:248:PHE:O	1:B:249:ASN:ND2	2.49	0.46
1:B:247:SER:O	1:B:250:GLN:HG2	2.15	0.46
1:B:60:PRO:O	1:B:63:CYS:HB3	2.15	0.46
1:B:101:ASP:OD1	1:B:103:GLU:HB3	2.16	0.45
1:A:270:ILE:HG13	1:A:283:GLN:OE1	2.16	0.45
1:A:373:GLY:O	1:A:376:VAL:N	2.49	0.45
1:A:379:ASN:HA	1:A:380:PRO:HA	1.66	0.45
1:A:166:LEU:C	1:A:166:LEU:HD23	2.37	0.45
1:A:92:ASP:HA	1:A:134:TYR:HB2	1.98	0.45
1:B:248:PHE:O	1:B:249:ASN:CG	2.54	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ASN:ND2	1:B:409:PRO:HA	2.31	0.45
6:B:694:MAN:HO4	6:B:695:MAN:C1	2.30	0.45
1:B:133:ILE:HG13	1:B:134:TYR:N	2.32	0.45
1:B:214:PRO:HB2	1:B:219:ILE:HD11	1.99	0.45
1:A:239:ILE:HD13	1:A:283:GLN:HB2	1.99	0.45
1:A:412:THR:HG22	1:A:413:VAL:N	2.32	0.45
1:A:120:LEU:O	1:A:121:ALA:C	2.54	0.45
1:B:253:ILE:CG1	1:B:254:VAL:N	2.80	0.45
1:B:366:THR:CG2	1:B:404:ARG:HB2	2.43	0.45
1:B:76:MET:SD	1:B:89:LEU:HD13	2.56	0.45
1:A:301:ARG:O	1:A:302:HIS:HD2	1.99	0.45
1:A:357:GLN:OE1	1:A:363:ARG:HD2	2.16	0.45
1:B:200:TYR:CD2	1:B:222:TYR:O	2.69	0.45
1:B:69:PHE:CZ	1:B:91:ILE:HG12	2.52	0.45
1:B:125:HIS:HE1	1:B:165:ASP:OD2	1.99	0.45
1:A:255:ASP:C	1:A:257:ALA:H	2.20	0.44
1:A:82:LYS:HA	1:A:86:TYR:O	2.18	0.44
1:B:166:LEU:C	1:B:166:LEU:HD23	2.37	0.44
1:A:299:ASP:OD1	1:A:301:ARG:HB2	2.18	0.44
1:B:240:LYS:HE2	1:B:356:ARG:HH21	1.79	0.44
1:A:95:TRP:CD2	1:A:133:ILE:HD11	2.52	0.44
1:A:228:ASN:HB3	1:A:245:TRP:CZ3	2.52	0.44
1:B:66:GLU:HB3	1:B:113:PHE:CD1	2.51	0.44
1:A:81:TRP:CD1	1:A:300:LEU:HD23	2.51	0.44
1:B:138:GLY:CA	1:B:173:TYR:O	2.63	0.44
1:B:281:VAL:CG2	1:B:282:THR:N	2.81	0.44
1:A:300:LEU:N	1:A:300:LEU:HD12	2.32	0.44
1:A:420:THR:O	1:A:421:MET:HG2	2.18	0.44
1:A:333:GLN:HG3	1:A:334:GLY:N	2.23	0.43
1:B:44:TRP:NE1	1:B:300:LEU:HD11	2.33	0.43
5:B:641:MAN:O4	5:B:642:MAN:C3	2.62	0.43
1:B:170:ASP:OD2	7:B:1103:EDO:H12	2.17	0.43
1:B:387:LEU:HA	1:B:391:LYS:HA	2.00	0.43
1:B:52:CYS:SG	1:B:54:LEU:HD11	2.58	0.43
1:A:404:ARG:NH2	1:B:58:GLU:O	2.50	0.43
1:A:164:VAL:HG12	1:A:166:LEU:H	1.83	0.43
1:A:322:ASP:OD1	1:A:323:PRO:HD2	2.18	0.43
1:A:363:ARG:NH1	1:A:363:ARG:HG2	2.27	0.43
1:B:315:ASP:HB3	1:B:387:LEU:HD11	1.99	0.43
1:B:193:ARG:O	1:B:195:GLY:N	2.51	0.43
4:B:715:NAG:H62	4:B:716:NAG:C7	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:TYR:HE2	1:B:141:THR:HB	1.82	0.43
1:A:281:VAL:HA	1:A:310:LEU:HD11	1.99	0.43
1:A:281:VAL:CG2	1:A:282:THR:N	2.81	0.43
1:B:254:VAL:HG21	1:B:329:TYR:HB3	2.01	0.43
1:B:255:ASP:C	1:B:257:ALA:H	2.22	0.43
1:A:101:ASP:OD1	1:A:103:GLU:N	2.52	0.43
1:B:179:ASN:ND2	1:B:179:ASN:N	2.67	0.43
1:B:234:ASP:OD2	1:B:273:PHE:HD2	2.00	0.43
1:A:136:ASP:O	1:A:148:SER:HB2	2.19	0.43
1:A:247:SER:O	1:A:250:GLN:HG2	2.19	0.43
1:A:123:TYR:O	1:A:124:VAL:C	2.57	0.43
1:A:213:LYS:CD	1:A:213:LYS:N	2.72	0.43
1:A:82:LYS:HE3	1:A:128:GLY:HA3	2.01	0.42
1:A:200:TYR:CD2	1:A:222:TYR:O	2.71	0.42
1:A:177:LEU:CD1	1:A:177:LEU:N	2.78	0.42
1:A:232:ILE:HG13	1:A:238:SER:OG	2.19	0.42
1:A:333:GLN:CG	1:A:334:GLY:H	2.22	0.42
1:A:381:ALA:O	1:A:419:ASN:HA	2.17	0.42
1:B:229:PHE:CG	1:B:230:ALA:N	2.87	0.42
1:B:364:SER:HA	1:B:406:HIS:HA	2.01	0.42
1:B:45:LEU:HD21	1:B:92:ASP:CB	2.49	0.42
1:A:75:LEU:O	1:A:78:SER:N	2.52	0.42
6:B:694:MAN:O4	6:B:695:MAN:C1	2.67	0.42
1:A:125:HIS:CE1	1:A:165:ASP:OD2	2.70	0.42
1:A:390:VAL:O	1:A:391:LYS:C	2.58	0.42
1:A:65:SER:O	1:A:68:LEU:N	2.52	0.42
1:B:422:GLN:HE21	1:B:422:GLN:CA	2.29	0.42
1:B:82:LYS:HA	1:B:86:TYR:O	2.18	0.42
1:A:177:LEU:HA	1:A:180:LEU:HB3	2.02	0.42
1:A:93:ASP:OD1	1:A:94:CYS:N	2.53	0.42
1:B:285:ALA:HB2	1:B:388:LEU:HD23	2.00	0.42
1:B:390:VAL:O	1:B:391:LYS:C	2.57	0.42
1:A:255:ASP:O	1:A:257:ALA:N	2.52	0.42
1:A:277:TRP:O	1:A:281:VAL:HG13	2.20	0.42
1:A:179:ASN:ND2	1:A:179:ASN:N	2.68	0.42
1:A:326:LYS:O	1:A:342:ARG:HG3	2.19	0.42
1:A:65:SER:C	1:A:67:LYS:N	2.74	0.42
1:B:101:ASP:OD2	1:B:105:ARG:HB2	2.20	0.42
1:B:180:LEU:O	1:B:183:GLY:N	2.52	0.42
1:B:208:MET:O	1:B:211:PHE:HB2	2.20	0.42
1:B:253:ILE:O	1:B:255:ASP:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:LEU:O	1:B:78:SER:N	2.53	0.42
1:A:239:ILE:CD1	1:A:283:GLN:HB2	2.49	0.42
1:B:388:LEU:HD22	1:B:414:LEU:HD23	2.02	0.42
1:B:97:ALA:HB2	1:B:110:PRO:HD3	2.02	0.41
1:B:137:VAL:HG12	1:B:171:GLY:HA2	2.02	0.41
1:A:99:GLN:N	1:A:99:GLN:OE1	2.53	0.41
1:B:32:LEU:HB2	1:B:223:CYS:N	2.35	0.41
1:B:93:ASP:O	1:B:94:CYS:CB	2.68	0.41
1:A:133:ILE:HG13	1:A:134:TYR:N	2.36	0.41
1:A:349:TRP:CD1	1:A:377:ALA:HB2	2.55	0.41
1:B:66:GLU:OE2	1:B:113:PHE:HA	2.20	0.41
1:A:193:ARG:O	1:A:195:GLY:N	2.53	0.41
1:A:237:LYS:HE3	1:B:237:LYS:HE3	2.01	0.41
1:A:332:ARG:HD3	1:A:365:TYR:OH	2.20	0.41
1:B:246:THR:HG22	1:B:247:SER:N	2.35	0.41
1:B:267:MET:H	1:B:267:MET:HG3	1.70	0.41
1:B:300:LEU:HD12	1:B:300:LEU:N	2.32	0.41
1:A:382:CYS:HA	1:A:418:GLU:O	2.21	0.41
1:A:75:LEU:C	1:A:77:VAL:N	2.73	0.41
1:A:387:LEU:HA	1:A:391:LYS:HA	2.03	0.41
1:B:265:PRO:HB2	1:B:287:TRP:CZ2	2.56	0.41
1:A:180:LEU:O	1:A:183:GLY:N	2.53	0.41
1:A:272:ASN:HB3	1:A:273:PHE:H	1.60	0.41
1:B:145:PHE:CB	1:B:146:PRO:HD2	2.44	0.41
1:B:56:CYS:HB2	8:B:11:HOH:O	2.20	0.41
1:B:115:HIS:HB3	1:B:119:GLN:OE1	2.21	0.41
1:B:216:TYR:HB3	1:B:256:VAL:HG21	2.03	0.41
1:B:199:VAL:HA	1:B:224:ASN:OD1	2.21	0.41
1:B:239:ILE:O	1:B:240:LYS:C	2.58	0.41
1:B:250:GLN:CB	1:B:254:VAL:HB	2.51	0.41
1:B:50:PHE:O	1:B:51:MET:C	2.60	0.41
1:B:53:ASN:HB3	1:B:62:SER:O	2.20	0.41
1:B:99:GLN:OE1	1:B:99:GLN:N	2.54	0.41
1:A:42:MET:HG2	1:A:294:LEU:HB2	2.03	0.41
1:A:353:MET:O	1:A:412:THR:HA	2.21	0.41
1:A:76:MET:SD	1:A:89:LEU:HD13	2.61	0.41
1:B:357:GLN:OE1	1:B:363:ARG:HD2	2.21	0.41
1:B:422:GLN:CG	1:B:422:GLN:O	2.68	0.41
6:B:692:NAG:H61	6:B:693:NAG:N2	2.36	0.41
1:A:39:THR:HB	1:A:321:GLN:OE1	2.21	0.40
1:B:205:PRO:C	1:B:207:TYR:N	2.75	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:SER:HB3	1:B:406:HIS:CE1	2.56	0.40
1:A:97:ALA:CB	1:A:110:PRO:HD3	2.51	0.40
1:A:209:TRP:HA	1:A:210:PRO:HA	1.91	0.40
1:B:388:LEU:HD12	1:B:388:LEU:HA	1.84	0.40
1:B:174:CYS:HA	5:B:639:NAG:C7	2.50	0.40
1:B:185:LYS:HG2	1:B:222:TYR:CE2	2.57	0.40
1:B:37:ALA:C	1:B:39:THR:H	2.25	0.40
1:B:60:PRO:HA	1:B:63:CYS:HB3	2.03	0.40
1:B:376:VAL:O	1:B:377:ALA:C	2.59	0.40
1:B:53:ASN:C	1:B:54:LEU:HD12	2.42	0.40
1:A:253:ILE:CG1	1:A:254:VAL:N	2.83	0.40
1:B:47:TRP:O	1:B:51:MET:N	2.41	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)
1:B:58:GLU:OE2	1:B:58:GLU:OE2[4_556]	1.96	0.24

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	388/398 (98%)	306 (79%)	56 (14%)	26 (7%)	1	11
1	B	389/398 (98%)	302 (78%)	59 (15%)	28 (7%)	1	9
All	All	777/796 (98%)	608 (78%)	115 (15%)	54 (7%)	1	10

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	376	VAL
1	B	118	ARG
1	B	376	VAL
1	B	378	CYS
1	B	401	SER
1	A	47	TRP
1	A	100	ARG
1	A	175	ASP
1	A	256	VAL
1	A	266	ASP
1	A	374	LYS
1	A	395	GLY
1	A	401	SER
1	B	47	TRP
1	B	175	ASP
1	B	180	LEU
1	B	266	ASP
1	B	374	LYS
1	B	395	GLY
1	A	180	LEU
1	A	313	ASP
1	B	206	LEU
1	B	249	ASN
1	B	267	MET
1	B	272	ASN
1	B	300	LEU
1	B	313	ASP
1	A	78	SER
1	A	151	TYR
1	A	210	PRO
1	A	267	MET
1	A	272	ASN
1	A	378	CYS
1	A	391	LYS
1	B	78	SER
1	B	151	TYR
1	B	256	VAL
1	A	94	CYS
1	A	146	PRO
1	A	370	ALA
1	B	146	PRO
1	B	230	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	391	LYS
1	A	98	PRO
1	A	206	LEU
1	B	181	ALA
1	B	194	THR
1	B	254	VAL
1	B	370	ALA
1	A	254	VAL
1	B	210	PRO
1	B	98	PRO
1	A	334	GLY

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	331/339 (98%)	310 (94%)	21 (6%)	21	58
1	B	332/339 (98%)	312 (94%)	20 (6%)	22	60
All	All	663/678 (98%)	622 (94%)	41 (6%)	21	58

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	CYS
1	A	67	LYS
1	A	70	MET
1	A	74	GLU
1	A	98	PRO
1	A	169	PHE
1	A	246	THR
1	A	250	GLN
1	A	251	GLU
1	A	254	VAL
1	A	273	PHE
1	A	287	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	310	LEU
1	A	324	LEU
1	A	353	MET
1	A	363	ARG
1	A	382	CYS
1	A	385	THR
1	A	388	LEU
1	A	389	PRO
1	A	421	MET
1	B	63	CYS
1	B	98	PRO
1	B	123	TYR
1	B	161	ASP
1	B	169	PHE
1	B	246	THR
1	B	250	GLN
1	B	251	GLU
1	B	254	VAL
1	B	273	PHE
1	B	287	TRP
1	B	310	LEU
1	B	324	LEU
1	B	353	MET
1	B	363	ARG
1	B	382	CYS
1	B	385	THR
1	B	388	LEU
1	B	421	MET
1	B	422	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	111	GLN
1	A	125	HIS
1	A	179	ASN
1	A	212	GLN
1	A	272	ASN
1	A	302	HIS
1	A	330	GLN
1	A	333	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	386	GLN
1	B	46	HIS
1	B	111	GLN
1	B	122	ASN
1	B	125	HIS
1	B	179	ASN
1	B	272	ASN
1	B	386	GLN
1	B	422	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 ⓘ

19 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	692	1,3	14,14,15	0.64	0	15,19,21	0.71	0
3	NAG	A	693	3	14,14,15	0.57	0	15,19,21	0.74	0
3	MAN	A	694	3	11,11,12	0.57	0	13,15,17	0.88	1 (7%)
3	MAN	A	695	3	11,11,12	0.88	1 (9%)	13,15,17	0.57	0
3	MAN	A	696	3	11,11,12	0.82	0	13,15,17	0.64	0
4	NAG	A	715	1,4	14,14,15	0.53	0	15,19,21	0.69	0
4	NAG	A	716	4	14,14,15	0.59	0	15,19,21	0.66	0
5	NAG	B	639	1,5	14,14,15	0.70	0	15,19,21	1.18	3 (20%)
5	NAG	B	640	5	14,14,15	0.58	0	15,19,21	0.88	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	B	641	5	11,11,12	0.77	0	13,15,17	1.66	2 (15%)
5	MAN	B	642	5	11,11,12	1.02	1 (9%)	13,15,17	1.15	2 (15%)
5	MAN	B	643	5	11,11,12	0.57	0	13,15,17	0.92	2 (15%)
5	FUC	B	644	5	9,10,11	0.76	0	13,14,16	0.53	0
6	NAG	B	692	1,6	14,14,15	0.70	0	15,19,21	0.73	0
6	NAG	B	693	6	14,14,15	0.56	0	15,19,21	0.89	1 (6%)
6	MAN	B	694	6	11,11,12	0.61	0	13,15,17	1.05	1 (7%)
6	MAN	B	695	6	11,11,12	0.54	0	13,15,17	1.02	1 (7%)
4	NAG	B	715	1,4	14,14,15	0.74	0	15,19,21	0.78	0
4	NAG	B	716	4	14,14,15	0.70	0	15,19,21	0.76	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	692	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	693	3	-	0/6/23/26	0/1/1/1
3	MAN	A	694	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	A	695	3	-	0/2/19/22	0/1/1/1
3	MAN	A	696	3	-	0/2/19/22	0/1/1/1
4	NAG	A	715	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	716	4	-	0/6/23/26	0/1/1/1
5	NAG	B	639	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	640	5	-	0/6/23/26	0/1/1/1
5	MAN	B	641	5	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	B	642	5	-	0/2/19/22	0/1/1/1
5	MAN	B	643	5	-	0/2/19/22	0/1/1/1
5	FUC	B	644	5	-	0/0/17/20	0/1/1/1
6	NAG	B	692	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	693	6	-	0/6/23/26	0/1/1/1
6	MAN	B	694	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	B	695	6	-	0/2/19/22	0/1/1/1
4	NAG	B	715	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	716	4	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	695	MAN	C2-C3	2.12	1.55	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	642	MAN	C2-C3	2.70	1.56	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	694	MAN	C1-C2-C3	-3.05	105.79	109.65
5	B	641	MAN	O3-C3-C2	-2.70	105.11	110.02
5	B	639	NAG	C2-N2-C7	-2.49	119.31	122.94
6	B	693	NAG	C2-N2-C7	-2.25	119.66	122.94
5	B	639	NAG	O5-C1-C2	-2.23	108.38	111.47
5	B	640	NAG	C2-N2-C7	-2.14	119.81	122.94
4	B	716	NAG	C2-N2-C7	-2.07	119.92	122.94
5	B	643	MAN	C1-O5-C5	2.06	115.01	112.17
3	A	694	MAN	O3-C3-C2	2.19	114.02	110.02
5	B	643	MAN	C1-C2-C3	2.24	112.49	109.65
5	B	639	NAG	C3-C4-C5	2.25	114.19	110.22
5	B	642	MAN	C6-C5-C4	2.39	118.60	113.00
5	B	642	MAN	C1-C2-C3	2.41	112.71	109.65
6	B	695	MAN	C1-C2-C3	2.58	112.93	109.65
5	B	641	MAN	C1-C2-C3	4.78	115.72	109.65

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	641	MAN	C1
6	B	694	MAN	C1
3	A	694	MAN	C1

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	639	NAG	11	0
5	B	641	MAN	3	0
5	B	642	MAN	3	0
5	B	644	FUC	4	0
6	B	692	NAG	1	0
6	B	693	NAG	1	0
6	B	694	MAN	4	0
6	B	695	MAN	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	715	NAG	3	0
4	B	716	NAG	3	0

5.6 Ligand geometry

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	EDO	A	1101	-	3,3,3	0.72	0	2,2,2	0.20	0
7	EDO	A	1102	-	3,3,3	0.85	0	2,2,2	0.05	0
2	NAG	A	639	1	14,14,15	0.86	0	15,19,21	0.87	1 (6%)
7	EDO	B	1103	-	3,3,3	0.36	0	2,2,2	0.66	0
7	EDO	B	1104	-	3,3,3	0.70	0	2,2,2	0.17	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
7	EDO	A	1101	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1102	-	-	0/1/1/1	0/0/0/0
2	NAG	A	639	1	-	0/6/23/26	0/1/1/1
7	EDO	B	1103	-	-	0/1/1/1	0/0/0/0
7	EDO	B	1104	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	639	NAG	C2-N2-C7	-2.08	119.91	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1102	EDO	1	0
7	B	1103	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	390/398 (97%)	-0.54	0 100 100	33, 58, 89, 119	0
1	B	391/398 (98%)	-0.54	0 100 100	35, 60, 94, 118	0
All	All	781/796 (98%)	-0.54	0 100 100	33, 59, 93, 119	0

There are no RSRZ outliers to report.

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
6	NAG	B	692	14/15	0.90	0.17	-0.25	58,76,91,94	0
5	NAG	B	639	14/15	0.87	0.16	-0.67	93,130,134,135	0
3	NAG	A	693	14/15	0.90	0.16	-0.90	65,73,84,96	0
3	NAG	A	692	14/15	0.95	0.17	-0.99	46,62,73,73	0
5	MAN	B	641	11/12	0.60	0.24	-	137,139,142,143	0
5	NAG	B	640	14/15	0.83	0.22	-	115,132,136,136	0
4	NAG	B	715	14/15	0.84	0.14	-	80,106,120,129	0
6	MAN	B	694	11/12	0.81	0.16	-	109,118,127,127	0
3	MAN	A	696	11/12	0.70	0.30	-	128,138,147,151	0
4	NAG	A	716	14/15	0.83	0.20	-	108,121,125,127	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	B	716	14/15	0.67	0.35	-	139,146,150,152	0
5	FUC	B	644	10/11	0.67	0.43	-	136,145,154,161	0
5	MAN	B	643	11/12	0.77	0.48	-	139,140,142,143	0
3	MAN	A	694	11/12	0.56	0.21	-	106,114,128,134	0
5	MAN	B	642	11/12	0.50	0.45	-	132,140,143,143	0
4	NAG	A	715	14/15	0.90	0.15	-	107,117,122,123	0
6	NAG	B	693	14/15	0.91	0.18	-	85,96,116,119	0
6	MAN	B	695	11/12	0.66	0.20	-	103,108,112,115	0
3	MAN	A	695	11/12	0.58	0.70	-	128,138,142,146	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
7	EDO	B	1103	4/4	0.71	0.26	1.87	24,29,39,42	0
2	NAG	A	639	14/15	0.75	0.20	0.03	67,81,95,98	0
7	EDO	A	1102	4/4	0.78	0.19	-0.26	31,47,50,57	0
7	EDO	A	1101	4/4	0.98	0.12	-1.06	25,31,32,46	0
7	EDO	B	1104	4/4	0.92	0.12	-3.58	40,41,44,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.