WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:53 PM GMT

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PDB ID	:	1R47
Title	:	Structure of human alpha-galactosidase
Authors	:	Garman, S.C.; Garboczi, D.N.
Deposited on	:	2003-10-03
Resolution	:	3.45 Å(reported)

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.45 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	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)

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 <=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	35% 56% 6% ··
1	B	398	% 37% 54% 7% ··

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		-	-
3	MAN	B	694	X		-	-
4	MAN	A	717	X		-	-
4	MAN	B	717	X		-	-
5	NAG	B	639	-		X	-
5	MAN	B	641	X		-	-
6	GAL	A	1101	X		-	-
6	GAL	B	1103	X		-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6602 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 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 (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		
3	B	5	Total	C	N	O	0	0
			61	34	2	25		
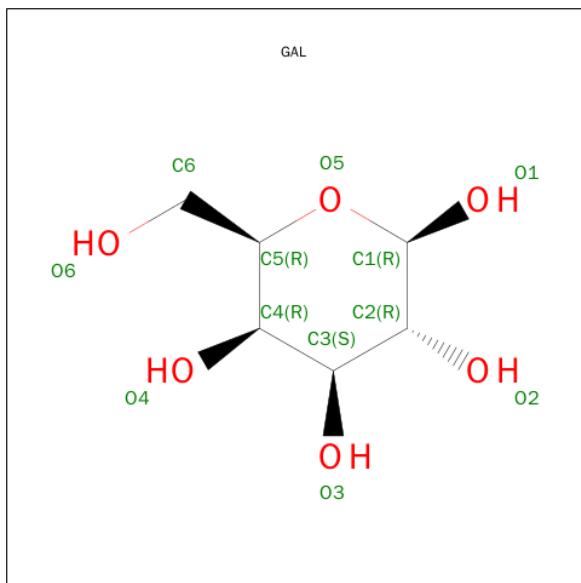
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is a polymer of unknown type called SUGAR (6-MER).
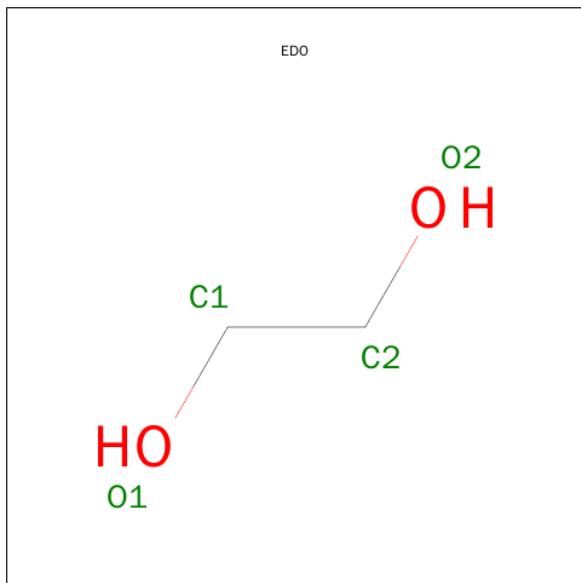
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	6	Total	C	N	O	0	0
			71	40	2	29		

• Molecule 6 is SUGAR (D-GALACTOSE) (three-letter code: GAL) (formula: $C_6H_{12}O_6$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 12	C 6	O 6	0	0
6	B	1	Total 12	C 6	O 6	0	0

• Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 4	C 2	O 2	0	0
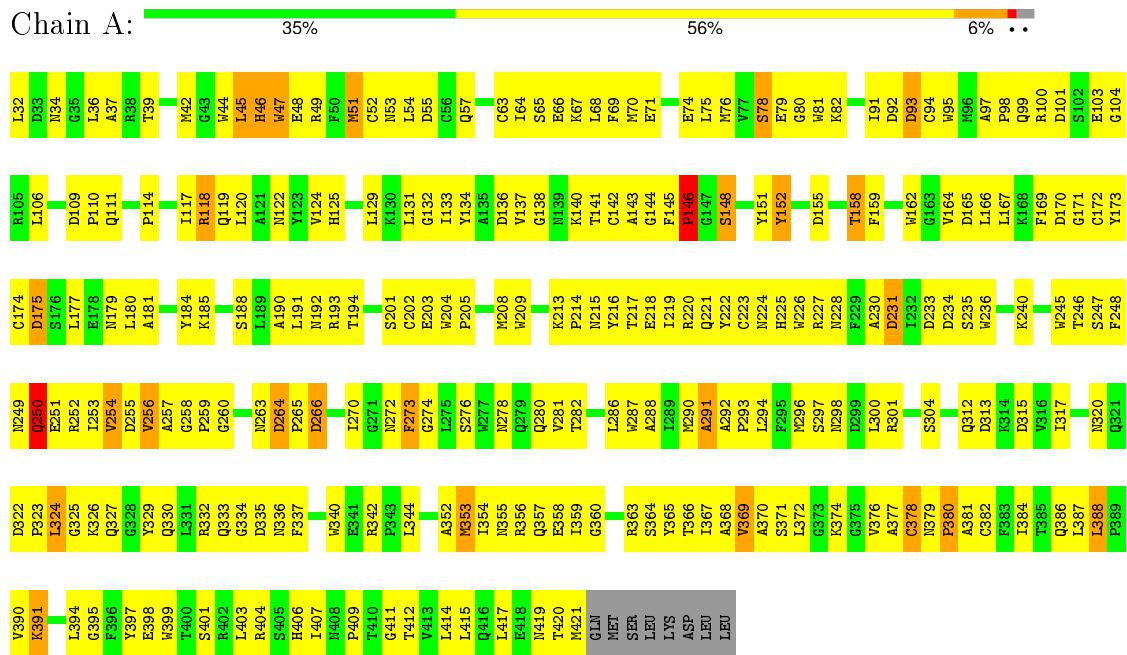
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	9	Total 9	O 9	0	0
8	B	9	Total 9	O 9	0	0
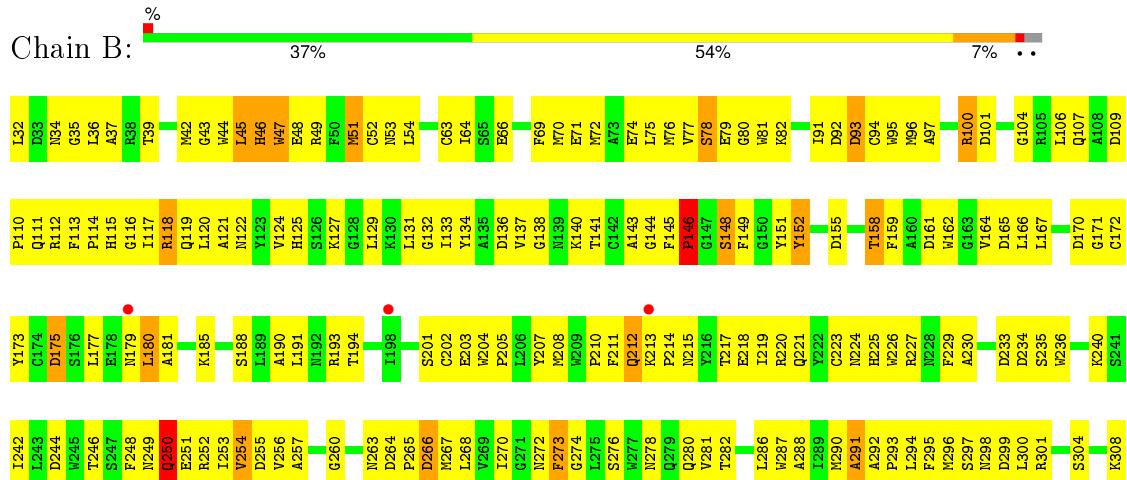
3 Residue-property plots ⓘ
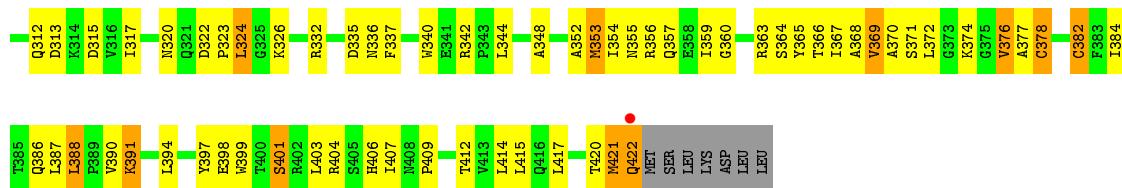
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Alpha-galactosidase A

Chain A:

- Molecule 1: Alpha-galactosidase A

Chain B:

Q312 D313 K314 D315 V316 I317 N320 Q321 D322 P323 L324 G325 K326 R332 D335 N336 F337 W340 E341 R342 P343 L344 A348 A352 M353 I354 N355 R356 Q357 E358 I359 G360 R363 S364 Y365 T366 I367 A368 V369 A370 S371 L372 G373 K374 G375 V376 A377 C378 C382 F383 I384

T385 Q386 L387 L388 P389 V390 K391 L394 Y397 E398 W399 T400 S401 R402 L403 R404 S405 H406 I407 N408 P409 T412 V413 L414 L415 Q416 L417 T420 M421 Q422 MET SER LEU LYS ASP LEU LEU

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	90.00Å 90.00Å 216.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.55 – 3.45 45.00 – 3.27	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.55-3.45) 99.5 (45.00-3.27)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 3.25Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.285 , 0.321 0.261 , 0.309	Depositor DCC
R_{free} test set	710 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	66.7	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 20.5	EDS
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 16031 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6602	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.42	0/3209	0.69	0/4358
1	B	0.41	0/3218	0.68	0/4370
All	All	0.42	0/6427	0.69	0/8728

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
3	B	1	0
4	A	1	0
4	B	1	0
5	B	1	0
All	All	5	0

There are no bond length outliers.

There are no bond angle outliers.

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	694	MAN	C1
4	A	717	MAN	C1
5	B	641	MAN	C1
3	B	694	MAN	C1
4	B	717	MAN	C1

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3122	0	2981	241	0
1	B	3131	0	2989	228	0
2	A	28	0	25	2	0
3	A	61	0	52	2	0
3	B	61	0	52	9	0
4	A	39	0	34	0	0
4	B	39	0	34	3	0
5	B	71	0	61	7	0
6	A	12	0	12	3	0
6	B	12	0	12	0	0
7	A	4	0	6	1	0
7	B	4	0	6	0	0
8	A	9	0	0	1	0
8	B	9	0	0	1	0
All	All	6602	0	6264	481	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 37.

All (481) 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:213:LYS:H	1:A:213:LYS:HD2	1.05	1.15
1:A:175:ASP:HB2	1:A:179:ASN:ND2	1.80	0.96
1:A:330:GLN:NE2	1:A:333:GLN:HE22	1.63	0.95
1:B:175:ASP:HB2	1:B:179:ASN:ND2	1.83	0.93
5:B:639:NAG:H62	5:B:644:FUC:O2	1.72	0.87
1:B:45:LEU:HD21	1:B:92:ASP:HB2	1.54	0.87
1:B:119:GLN:HA	1:B:122:ASN:HD22	1.40	0.87
1:B:127:LYS:HE2	1:B:127:LYS:HA	1.56	0.87
1:A:403:LEU:HD12	1:A:404:ARG:N	1.89	0.86
1:A:213:LYS:N	1:A:213:LYS:HD2	1.91	0.86
1:A:386:GLN:O	1:A:391:LYS:HA	1.76	0.85
1:A:45:LEU:HD21	1:A:92:ASP:HB2	1.55	0.85
1:B:386:GLN:O	1:B:391:LYS:HA	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:TRP:HB2	1:B:352:ALA:HB3	1.61	0.82
1:A:118:ARG:HH11	1:A:118:ARG:HB3	1.44	0.82
1:A:340:TRP:HB2	1:A:352:ALA:HB3	1.62	0.81
1:A:273:PHE:HB3	1:B:278:ASN:HD22	1.45	0.81
1:A:204:TRP:HB3	1:A:205:PRO:HD3	1.62	0.81
1:B:265:PRO:O	1:B:266:ASP:HB2	1.78	0.81
1:B:46:HIS:CD2	1:B:92:ASP:H	1.99	0.81
1:A:175:ASP:HB2	1:A:179:ASN:HD22	1.44	0.81
1:B:101:ASP:HB3	1:B:107:GLN:OE1	1.80	0.80
1:A:145:PHE:HB3	1:A:146:PRO:HD2	1.65	0.79
1:A:213:LYS:H	1:A:213:LYS:CD	1.86	0.78
1:B:204:TRP:HB3	1:B:205:PRO:HD3	1.63	0.78
1:A:265:PRO:O	1:A:266:ASP:HB2	1.82	0.78
1:A:324:LEU:HD12	1:A:344:LEU:O	1.84	0.77
1:B:49:ARG:HD3	1:B:272:ASN:HD21	1.49	0.77
1:B:175:ASP:HB2	1:B:179:ASN:HD22	1.47	0.77
3:B:694:MAN:H3	3:B:695:MAN:C5	2.15	0.76
1:B:324:LEU:HD12	1:B:344:LEU:O	1.86	0.75
1:B:140:LYS:HB2	1:B:173:TYR:CD2	2.20	0.75
1:B:138:GLY:HA3	1:B:173:TYR:O	1.86	0.75
4:B:716:NAG:H62	4:B:717:MAN:H2	1.68	0.74
1:B:315:ASP:CG	1:B:391:LYS:HE3	2.08	0.74
1:B:119:GLN:HA	1:B:122:ASN:ND2	2.03	0.73
1:B:177:LEU:HD11	1:B:211:PHE:CG	2.23	0.73
1:A:381:ALA:HB3	1:A:420:THR:HB	1.71	0.73
1:A:110:PRO:HB2	1:A:111:GLN:NE2	2.03	0.73
1:B:366:THR:HG22	1:B:404:ARG:HB2	1.71	0.73
1:A:330:GLN:HE22	1:A:333:GLN:HE22	1.34	0.73
1:B:224:ASN:HA	1:B:260:GLY:O	1.88	0.73
1:B:145:PHE:HB3	1:B:146:PRO:HD2	1.69	0.72
1:A:290:MET:O	1:A:291:ALA:C	2.28	0.72
1:B:72:MET:SD	1:B:300:LEU:HD13	2.30	0.72
1:A:377:ALA:O	1:A:378:CYS:HB2	1.88	0.72
5:B:639:NAG:C6	5:B:644:FUC:H3	2.20	0.71
1:A:366:THR:HG22	1:A:404:ARG:HB2	1.70	0.71
1:B:34:ASN:OD1	1:B:36:LEU:HB2	1.90	0.71
1:A:273:PHE:CD2	1:A:273:PHE:N	2.59	0.71
1:B:366:THR:HG22	1:B:404:ARG:CB	2.21	0.70
1:A:324:LEU:HD22	1:A:326:LYS:HG2	1.72	0.70
1:B:290:MET:O	1:B:291:ALA:C	2.29	0.70
1:B:324:LEU:HD22	1:B:326:LYS:HG2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:THR:HG22	1:A:404:ARG:CB	2.22	0.70
1:A:224:ASN:HA	1:A:260:GLY:O	1.92	0.70
1:B:273:PHE:CD2	1:B:273:PHE:N	2.60	0.69
1:A:333:GLN:HG3	1:A:334:GLY:H	1.57	0.69
1:A:138:GLY:HA3	1:A:173:TYR:O	1.92	0.69
1:B:46:HIS:HD2	1:B:92:ASP:H	1.40	0.69
1:A:273:PHE:HB3	1:B:278:ASN:ND2	2.07	0.69
1:B:49:ARG:HD3	1:B:272:ASN:ND2	2.08	0.68
3:B:694:MAN:H3	3:B:695:MAN:H5	1.76	0.68
1:A:34:ASN:OD1	1:A:36:LEU:HB2	1.94	0.68
4:B:715:NAG:H62	4:B:716:NAG:H82	1.76	0.68
3:B:693:NAG:O3	3:B:696:MAN:H5	1.93	0.68
1:B:208:MET:SD	1:B:214:PRO:HB3	2.34	0.68
1:B:110:PRO:HB2	1:B:111:GLN:NE2	2.09	0.68
1:B:136:ASP:O	1:B:148:SER:HB2	1.93	0.67
1:B:35:GLY:HA3	3:B:693:NAG:H61	1.75	0.67
1:B:296:MET:HB3	1:B:298:ASN:HD21	1.60	0.67
1:B:51:MET:O	1:B:64:ILE:HD11	1.94	0.67
1:B:45:LEU:HD22	1:B:47:TRP:H	1.60	0.67
1:B:288:ALA:HA	1:B:320:ASN:HB2	1.75	0.67
1:A:215:ASN:O	1:A:218:GLU:HB3	1.94	0.67
1:B:296:MET:HB3	1:B:298:ASN:ND2	2.10	0.67
1:A:118:ARG:NH1	1:A:118:ARG:CB	2.58	0.67
1:A:51:MET:O	1:A:64:ILE:HD11	1.94	0.67
1:A:386:GLN:HA	1:A:415:LEU:HD23	1.75	0.67
1:B:377:ALA:O	1:B:378:CYS:HB2	1.95	0.66
1:A:387:LEU:O	1:A:388:LEU:HD13	1.96	0.66
1:A:384:ILE:HG12	1:A:417:LEU:HG	1.78	0.66
1:B:75:LEU:HD21	1:B:301:ARG:HG2	1.77	0.66
1:A:136:ASP:O	1:A:148:SER:HB2	1.95	0.66
1:B:100:ARG:NH1	1:B:106:LEU:HG	2.11	0.66
1:A:118:ARG:NH1	1:A:118:ARG:HB3	2.10	0.66
1:A:46:HIS:CD2	1:A:92:ASP:H	2.14	0.65
1:B:398:GLU:N	1:B:401:SER:OG	2.30	0.65
1:B:270:ILE:HG23	1:B:280:GLN:OE1	1.97	0.65
1:A:296:MET:HB3	1:A:298:ASN:HD21	1.60	0.65
1:B:326:LYS:O	1:B:342:ARG:HG3	1.96	0.65
1:A:296:MET:HB3	1:A:298:ASN:ND2	2.11	0.65
1:A:381:ALA:HB3	1:A:420:THR:CB	2.26	0.65
1:B:386:GLN:HA	1:B:415:LEU:HD23	1.80	0.64
1:A:288:ALA:HA	1:A:320:ASN:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LEU:O	1:A:124:VAL:HG23	1.98	0.64
1:A:47:TRP:CZ2	6:A:1101:GAL:H62	2.33	0.64
1:B:69:PHE:CZ	1:B:91:ILE:HG12	2.33	0.63
1:A:140:LYS:HB2	1:A:173:TYR:CD2	2.34	0.63
1:B:46:HIS:NE2	1:B:92:ASP:HB3	2.13	0.63
1:B:282:THR:HG23	1:B:412:THR:OG1	1.99	0.63
1:A:205:PRO:HG3	1:A:219:ILE:HD13	1.81	0.62
1:A:118:ARG:HH11	1:A:118:ARG:CB	2.12	0.62
1:A:253:ILE:HG13	1:A:254:VAL:H	1.65	0.62
1:A:42:MET:HE3	1:A:317:ILE:HG23	1.82	0.62
1:A:250:GLN:O	1:A:254:VAL:HG12	2.00	0.61
1:B:253:ILE:HG13	1:B:254:VAL:H	1.64	0.61
1:B:315:ASP:OD2	1:B:391:LYS:HE3	2.00	0.61
1:A:247:SER:O	1:A:250:GLN:HG2	2.00	0.61
1:B:45:LEU:CD2	1:B:92:ASP:HB2	2.29	0.61
1:A:370:ALA:HB2	1:A:399:TRP:O	2.00	0.61
1:A:155:ASP:O	1:A:158:THR:HB	2.01	0.61
1:A:264:ASP:HB2	1:A:293:PRO:HG2	1.83	0.61
1:A:326:LYS:O	1:A:342:ARG:HG3	2.01	0.61
1:A:95:TRP:CD2	1:A:133:ILE:HD11	2.36	0.61
1:A:286:LEU:HD11	1:A:354:ILE:HD11	1.83	0.61
1:A:117:ILE:O	1:A:118:ARG:C	2.40	0.61
1:B:95:TRP:CD2	1:B:133:ILE:HD11	2.35	0.60
1:B:353:MET:HG2	1:B:407:ILE:HD11	1.82	0.60
1:A:216:TYR:HB3	1:A:256:VAL:HG21	1.84	0.60
1:A:45:LEU:HD22	1:A:47:TRP:H	1.65	0.60
1:B:81:TRP:HA	1:B:312:GLN:HE21	1.66	0.60
1:B:377:ALA:O	1:B:378:CYS:CB	2.50	0.60
1:A:92:ASP:HA	1:A:134:TYR:HB2	1.82	0.60
1:B:155:ASP:O	1:B:158:THR:HB	2.01	0.60
1:B:248:PHE:CG	1:B:248:PHE:O	2.55	0.60
1:A:170:ASP:OD1	1:A:171:GLY:N	2.35	0.60
1:B:387:LEU:O	1:B:388:LEU:HD13	2.01	0.60
1:A:330:GLN:NE2	1:A:333:GLN:NE2	2.43	0.60
1:B:276:SER:O	1:B:280:GLN:HG3	2.02	0.60
1:A:384:ILE:HD12	1:A:397:TYR:CD1	2.37	0.59
1:A:417:LEU:N	1:A:417:LEU:HD12	2.17	0.59
1:A:166:LEU:C	1:A:166:LEU:HD23	2.22	0.59
1:A:322:ASP:OD1	1:A:323:PRO:HD2	2.02	0.59
1:A:75:LEU:HD21	1:A:301:ARG:HG2	1.84	0.59
1:B:166:LEU:HD23	1:B:166:LEU:C	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:O	1:A:120:LEU:N	2.36	0.58
1:B:115:HIS:HB3	1:B:119:GLN:OE1	2.03	0.58
1:A:166:LEU:HD23	1:A:167:LEU:N	2.17	0.58
1:B:137:VAL:HG12	1:B:171:GLY:HA2	1.85	0.58
1:A:220:ARG:NH1	1:A:256:VAL:O	2.36	0.58
1:A:93:ASP:O	1:A:94:CYS:HB2	2.03	0.58
1:A:49:ARG:HD3	1:A:272:ASN:HD21	1.68	0.58
1:A:403:LEU:HD12	1:A:404:ARG:H	1.68	0.58
1:A:276:SER:O	1:A:280:GLN:HG3	2.04	0.58
1:B:322:ASP:OD1	1:B:323:PRO:HD2	2.04	0.58
1:B:166:LEU:HD23	1:B:167:LEU:N	2.18	0.57
1:A:353:MET:HG2	1:A:407:ILE:HD11	1.86	0.57
5:B:639:NAG:H62	5:B:644:FUC:C3	2.34	0.57
1:B:313:ASP:O	1:B:317:ILE:HG13	2.03	0.57
1:A:234:ASP:O	1:A:274:GLY:HA3	2.04	0.57
1:B:398:GLU:O	1:B:401:SER:HB2	2.03	0.57
1:A:282:THR:HG23	1:A:412:THR:OG1	2.05	0.57
1:B:170:ASP:OD1	1:B:171:GLY:N	2.37	0.57
5:B:639:NAG:H62	5:B:644:FUC:H3	1.86	0.57
1:A:377:ALA:O	1:A:378:CYS:CB	2.51	0.57
1:A:270:ILE:HG23	1:A:280:GLN:OE1	2.04	0.57
1:B:81:TRP:HA	1:B:312:GLN:NE2	2.20	0.57
1:B:121:ALA:O	1:B:125:HIS:CD2	2.58	0.57
3:A:694:MAN:H4	3:A:695:MAN:H2	1.87	0.57
1:A:357:GLN:NE2	1:A:363:ARG:HD3	2.20	0.57
1:B:97:ALA:HB2	1:B:109:ASP:HA	1.85	0.57
1:A:369:VAL:CG1	1:A:378:CYS:SG	2.92	0.57
1:A:365:TYR:CE2	1:A:367:ILE:HG23	2.40	0.57
1:A:66:GLU:O	1:A:70:MET:HB2	2.05	0.57
1:B:365:TYR:CE2	1:B:367:ILE:HG23	2.40	0.56
4:B:716:NAG:H62	4:B:717:MAN:C2	2.36	0.56
1:B:92:ASP:HA	1:B:134:TYR:HB2	1.87	0.56
1:B:417:LEU:N	1:B:417:LEU:HD12	2.19	0.56
1:A:332:ARG:HG3	1:A:332:ARG:HH11	1.70	0.56
1:B:422:GLN:HE21	1:B:422:GLN:H	1.53	0.56
1:B:34:ASN:HD21	1:B:224:ASN:HD21	1.54	0.56
1:B:264:ASP:HB2	1:B:293:PRO:HG2	1.87	0.56
1:B:202:CYS:O	1:B:226:TRP:HA	2.06	0.56
1:B:213:LYS:H	1:B:213:LYS:HD2	1.71	0.56
1:A:390:VAL:O	1:A:391:LYS:C	2.44	0.56
1:A:47:TRP:CH2	6:A:1101:GAL:H62	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:PRO:HG3	1:A:219:ILE:CD1	2.36	0.56
1:B:136:ASP:HB2	1:B:141:THR:HA	1.88	0.56
1:A:313:ASP:O	1:A:317:ILE:HG13	2.05	0.56
1:A:202:CYS:O	1:A:226:TRP:HA	2.05	0.56
1:A:388:LEU:HB2	1:A:414:LEU:HB3	1.88	0.56
1:B:357:GLN:NE2	1:B:363:ARG:HD3	2.21	0.56
1:A:191:LEU:O	1:A:192:ASN:C	2.44	0.55
1:A:359:ILE:HG12	1:A:360:GLY:N	2.22	0.55
1:B:388:LEU:HB2	1:B:414:LEU:HB3	1.88	0.55
1:B:250:GLN:O	1:B:254:VAL:HG12	2.06	0.55
1:A:177:LEU:HA	1:A:180:LEU:HB3	1.88	0.55
1:B:286:LEU:HD11	1:B:354:ILE:HD11	1.89	0.55
1:A:386:GLN:OE1	1:A:390:VAL:HG22	2.07	0.55
1:B:100:ARG:HH11	1:B:106:LEU:HG	1.70	0.55
1:B:386:GLN:OE1	1:B:390:VAL:HG22	2.07	0.55
1:A:300:LEU:HD12	1:A:300:LEU:N	2.22	0.55
1:A:276:SER:HA	1:B:276:SER:HA	1.89	0.55
1:B:372:LEU:O	1:B:374:LYS:N	2.38	0.54
1:B:208:MET:O	1:B:211:PHE:HB2	2.07	0.54
1:B:332:ARG:HH11	1:B:332:ARG:HG3	1.72	0.54
1:A:71:GLU:O	1:A:75:LEU:HD13	2.07	0.54
1:A:145:PHE:HB3	1:A:146:PRO:CD	2.37	0.54
1:B:54:LEU:HD12	1:B:54:LEU:N	2.23	0.54
1:B:355:ASN:ND2	1:B:409:PRO:HA	2.23	0.54
1:A:278:ASN:HD22	1:B:273:PHE:HB3	1.72	0.54
1:B:100:ARG:HD2	1:B:104:GLY:O	2.07	0.54
1:A:82:LYS:HD2	1:A:129:LEU:HD21	1.89	0.54
1:A:369:VAL:HG13	1:A:378:CYS:SG	2.47	0.54
1:B:299:ASP:CG	1:B:301:ARG:HE	2.11	0.54
1:A:372:LEU:O	1:A:374:LYS:N	2.39	0.54
1:B:215:ASN:O	1:B:218:GLU:HB3	2.08	0.54
1:A:119:GLN:HA	1:A:122:ASN:ND2	2.23	0.54
1:B:159:PHE:HB3	1:B:164:VAL:HG21	1.90	0.53
1:B:359:ILE:HG12	1:B:360:GLY:N	2.23	0.53
1:A:367:ILE:HD12	1:A:367:ILE:O	2.09	0.53
1:B:372:LEU:HD23	1:B:417:LEU:HD21	1.89	0.53
1:A:54:LEU:HD12	1:A:54:LEU:N	2.23	0.53
1:A:131:LEU:HD12	1:A:132:GLY:H	1.73	0.53
1:B:45:LEU:CD2	1:B:47:TRP:H	2.22	0.53
1:B:81:TRP:CZ2	1:B:308:LYS:HG3	2.44	0.53
1:B:42:MET:HE3	1:B:294:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:VAL:HB	1:A:401:SER:O	2.08	0.53
1:B:82:LYS:HD2	1:B:129:LEU:HD21	1.89	0.53
1:B:300:LEU:HD12	1:B:300:LEU:N	2.23	0.53
1:B:136:ASP:CB	1:B:141:THR:HA	2.40	0.52
1:B:253:ILE:HG13	1:B:254:VAL:N	2.23	0.52
1:A:370:ALA:O	1:A:372:LEU:N	2.37	0.52
1:A:101:ASP:OD1	1:A:103:GLU:HB3	2.09	0.52
1:A:259:PRO:HD3	1:A:325:GLY:HA3	1.91	0.52
1:B:93:ASP:O	1:B:94:CYS:HB2	2.09	0.52
1:A:66:GLU:OE2	1:A:114:PRO:HD2	2.10	0.52
1:B:390:VAL:O	1:B:391:LYS:C	2.48	0.52
1:A:253:ILE:HG13	1:A:254:VAL:N	2.24	0.52
1:B:382:CYS:N	1:B:397:TYR:O	2.42	0.52
1:B:384:ILE:HD13	1:B:403:LEU:HD22	1.92	0.52
1:A:46:HIS:HD2	1:A:92:ASP:H	1.56	0.52
1:A:164:VAL:HG12	1:A:165:ASP:N	2.25	0.52
1:B:91:ILE:HB	1:B:133:ILE:HD12	1.92	0.52
1:A:228:ASN:HB3	1:A:245:TRP:CH2	2.45	0.52
1:A:117:ILE:O	1:A:120:LEU:HB3	2.10	0.51
1:A:286:LEU:HD11	1:A:354:ILE:CD1	2.40	0.51
1:B:370:ALA:O	1:B:372:LEU:N	2.35	0.51
1:A:258:GLY:HA2	1:A:325:GLY:O	2.11	0.51
1:A:190:ALA:O	1:A:193:ARG:HB3	2.10	0.51
1:A:355:ASN:ND2	1:A:409:PRO:HA	2.26	0.51
1:B:217:THR:O	1:B:221:GLN:HG3	2.10	0.51
1:B:244:ASP:HA	8:B:10:HOH:O	2.09	0.51
1:B:149:PHE:CE2	5:B:639:NAG:H3	2.46	0.51
1:A:136:ASP:HB2	1:A:141:THR:HA	1.93	0.51
1:A:48:GLU:HB3	1:A:297:SER:OG	2.11	0.51
1:A:240:LYS:HE3	1:A:356:ARG:HH21	1.76	0.51
1:A:364:SER:HA	1:A:406:HIS:HA	1.92	0.51
1:B:177:LEU:HA	1:B:180:LEU:HB3	1.92	0.50
1:B:364:SER:HA	1:B:406:HIS:HA	1.94	0.50
1:A:117:ILE:HG13	1:A:162:TRP:CZ3	2.46	0.50
1:B:71:GLU:O	1:B:75:LEU:HD13	2.10	0.50
1:B:75:LEU:O	1:B:78:SER:N	2.45	0.50
1:B:112:ARG:HB2	1:B:112:ARG:NH1	2.26	0.50
1:B:66:GLU:HB3	1:B:113:PHE:HD1	1.77	0.50
1:A:95:TRP:CE2	1:A:133:ILE:HD11	2.46	0.50
1:A:137:VAL:HG12	1:A:171:GLY:HA2	1.92	0.50
1:A:217:THR:O	1:A:221:GLN:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:THR:CG2	1:A:420:THR:O	2.60	0.50
1:A:65:SER:OG	1:A:67:LYS:HB2	2.12	0.50
1:B:52:CYS:SG	1:B:54:LEU:HD11	2.52	0.50
1:A:227:ARG:NH2	1:A:231:ASP:HA	2.26	0.50
1:B:131:LEU:HD12	1:B:132:GLY:H	1.77	0.50
1:B:233:ASP:HB2	1:B:235:SER:OG	2.12	0.49
1:A:75:LEU:O	1:A:78:SER:N	2.45	0.49
1:B:234:ASP:O	1:B:274:GLY:HA3	2.11	0.49
1:A:300:LEU:HD12	1:A:300:LEU:H	1.76	0.49
1:B:164:VAL:HG12	1:B:165:ASP:N	2.26	0.49
1:B:112:ARG:HH11	1:B:112:ARG:HB2	1.78	0.49
1:A:263:ASN:HB2	1:A:327:GLN:HE22	1.77	0.49
1:A:97:ALA:HB2	1:A:109:ASP:HA	1.94	0.49
1:A:101:ASP:OD1	1:A:103:GLU:N	2.46	0.49
1:A:119:GLN:HA	1:A:122:ASN:HD22	1.77	0.49
1:B:420:THR:OG1	1:B:421:MET:N	2.45	0.49
1:A:34:ASN:HD21	1:A:224:ASN:HD21	1.61	0.49
1:B:367:ILE:HD12	1:B:367:ILE:O	2.12	0.49
1:A:380:PRO:CD	1:A:381:ALA:H	2.26	0.49
1:B:149:PHE:HE2	5:B:639:NAG:H3	1.78	0.49
1:B:75:LEU:O	1:B:76:MET:C	2.50	0.48
1:A:75:LEU:N	1:A:75:LEU:HD12	2.27	0.48
1:B:120:LEU:O	1:B:124:VAL:HG23	2.12	0.48
1:B:43:GLY:O	1:B:295:PHE:HA	2.13	0.48
1:A:49:ARG:HD3	1:A:272:ASN:ND2	2.28	0.48
1:A:44:TRP:CD1	1:A:300:LEU:HD11	2.48	0.48
1:B:203:GLU:HA	1:B:227:ARG:HB2	1.96	0.48
1:B:75:LEU:N	1:B:75:LEU:HD12	2.29	0.48
1:A:53:ASN:C	1:A:54:LEU:HD12	2.34	0.48
1:B:127:LYS:HA	1:B:127:LYS:CE	2.35	0.48
1:B:44:TRP:HE1	1:B:298:ASN:H	1.60	0.48
1:B:315:ASP:HB3	1:B:387:LEU:HD11	1.96	0.47
1:A:142:CYS:HB2	6:A:1101:GAL:O6	2.14	0.47
3:B:692:NAG:H61	3:B:693:NAG:C7	2.45	0.47
1:B:268:LEU:N	1:B:295:PHE:O	2.34	0.47
1:B:32:LEU:N	1:B:220:ARG:O	2.47	0.47
1:B:384:ILE:O	1:B:394:LEU:HB2	2.15	0.47
1:A:159:PHE:HB3	1:A:164:VAL:HG21	1.94	0.47
1:A:45:LEU:CD2	1:A:92:ASP:HB2	2.36	0.47
1:B:368:ALA:O	1:B:369:VAL:C	2.53	0.47
1:B:112:ARG:HH11	1:B:112:ARG:CB	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASP:HB2	1:A:235:SER:OG	2.14	0.47
1:A:91:ILE:HB	1:A:133:ILE:HD12	1.97	0.47
1:A:300:LEU:H	1:A:300:LEU:CD1	2.28	0.47
5:B:639:NAG:C6	5:B:644:FUC:O2	2.54	0.47
1:B:172:CYS:O	1:B:173:TYR:HB2	2.15	0.47
1:B:370:ALA:C	1:B:372:LEU:H	2.17	0.47
1:A:172:CYS:O	1:A:173:TYR:HB2	2.15	0.46
1:B:115:HIS:O	1:B:116:GLY:C	2.54	0.46
1:A:97:ALA:HB2	1:A:110:PRO:HD3	1.97	0.46
1:A:81:TRP:HA	1:A:312:GLN:HE21	1.78	0.46
1:A:278:ASN:O	1:A:411:GLY:HA2	2.16	0.46
1:A:384:ILE:O	1:A:394:LEU:HB2	2.15	0.46
1:B:133:ILE:HG13	1:B:134:TYR:N	2.30	0.46
1:B:71:GLU:OE2	1:B:301:ARG:NH1	2.43	0.46
1:B:253:ILE:HB	1:B:263:ASN:HD21	1.81	0.46
3:B:694:MAN:C3	3:B:695:MAN:C5	2.91	0.46
1:B:34:ASN:ND2	1:B:224:ASN:HD21	2.11	0.46
1:B:145:PHE:HB3	1:B:146:PRO:CD	2.40	0.46
1:B:53:ASN:C	1:B:54:LEU:HD12	2.35	0.46
1:B:37:ALA:C	1:B:39:THR:H	2.19	0.46
1:A:240:LYS:CE	1:A:356:ARG:HH21	2.28	0.46
1:B:300:LEU:HD12	1:B:300:LEU:H	1.81	0.46
1:A:335:ASP:O	1:A:336:ASN:C	2.53	0.46
1:B:335:ASP:O	1:B:336:ASN:HB2	2.14	0.46
1:A:185:LYS:O	1:A:188:SER:HB3	2.15	0.46
1:A:333:GLN:HA	1:A:333:GLN:NE2	2.31	0.45
3:B:692:NAG:H61	3:B:693:NAG:H82	1.98	0.45
1:B:42:MET:HE3	1:B:317:ILE:HG23	1.98	0.45
1:A:55:ASP:OD2	1:A:57:GLN:HB2	2.16	0.45
1:A:32:LEU:N	1:A:223:CYS:O	2.49	0.45
1:A:294:LEU:HD21	1:A:320:ASN:ND2	2.30	0.45
1:B:47:TRP:HB3	1:B:267:MET:SD	2.55	0.45
1:A:45:LEU:CD2	1:A:47:TRP:H	2.28	0.45
1:A:417:LEU:N	1:A:417:LEU:CD1	2.79	0.45
1:B:253:ILE:O	1:B:255:ASP:N	2.50	0.45
1:A:201:SER:HB2	1:A:225:HIS:CE1	2.51	0.45
1:A:93:ASP:OD1	1:A:94:CYS:N	2.50	0.45
1:A:276:SER:HB2	1:B:273:PHE:O	2.17	0.45
1:B:117:ILE:O	1:B:118:ARG:C	2.54	0.45
1:B:66:GLU:O	1:B:70:MET:HG3	2.15	0.45
1:A:203:GLU:HG3	1:A:227:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:TRP:CD1	1:B:240:LYS:HD2	2.51	0.45
1:B:286:LEU:HD11	1:B:354:ILE:CD1	2.46	0.45
1:B:190:ALA:O	1:B:193:ARG:HB3	2.16	0.45
1:A:205:PRO:O	1:A:209:TRP:HD1	1.99	0.45
1:A:381:ALA:HB3	1:A:420:THR:OG1	2.16	0.45
1:B:113:PHE:N	1:B:114:PRO:HD3	2.32	0.45
1:A:391:LYS:HB2	8:A:4:HOH:O	2.16	0.45
1:B:398:GLU:N	1:B:398:GLU:CD	2.70	0.45
1:A:75:LEU:O	1:A:76:MET:C	2.53	0.45
1:B:185:LYS:O	1:B:188:SER:HB3	2.16	0.45
1:B:132:GLY:HA2	1:B:166:LEU:O	2.17	0.45
1:A:133:ILE:HG13	1:A:134:TYR:N	2.30	0.45
1:B:422:GLN:HE21	1:B:422:GLN:N	2.13	0.45
1:A:137:VAL:HA	1:A:169:PHE:CZ	2.51	0.45
1:B:353:MET:O	1:B:412:THR:HA	2.17	0.45
1:A:395:GLY:HA2	7:A:1102:EDO:H12	1.99	0.45
1:A:37:ALA:C	1:A:39:THR:H	2.17	0.45
1:B:100:ARG:NH1	1:B:155:ASP:OD2	2.50	0.45
1:B:417:LEU:CD1	1:B:417:LEU:N	2.80	0.45
1:A:46:HIS:NE2	1:A:92:ASP:HB3	2.31	0.44
1:A:125:HIS:HE1	1:A:165:ASP:OD2	1.98	0.44
1:A:175:ASP:N	2:A:639:NAG:O7	2.38	0.44
1:A:403:LEU:HD12	1:A:403:LEU:C	2.38	0.44
1:A:100:ARG:CZ	1:A:106:LEU:HD21	2.47	0.44
1:A:118:ARG:NH1	1:A:118:ARG:HB2	2.32	0.44
1:A:140:LYS:HD3	1:A:144:GLY:HA2	1.98	0.44
1:B:77:VAL:HG21	1:B:127:LYS:HB3	1.99	0.44
1:A:379:ASN:HA	1:A:380:PRO:HA	1.82	0.44
1:B:369:VAL:HB	1:B:401:SER:O	2.16	0.44
1:B:348:ALA:HA	1:B:417:LEU:O	2.17	0.44
1:A:265:PRO:HD2	1:A:292:ALA:HB1	1.99	0.44
1:A:137:VAL:HG13	1:A:138:GLY:N	2.32	0.44
1:B:205:PRO:HG3	1:B:219:ILE:HD13	1.99	0.44
1:B:137:VAL:HG13	1:B:138:GLY:N	2.33	0.44
1:B:78:SER:C	1:B:80:GLY:H	2.20	0.44
1:B:253:ILE:HB	1:B:263:ASN:ND2	2.32	0.44
1:A:333:GLN:HG3	1:A:334:GLY:N	2.30	0.44
1:A:34:ASN:OD1	1:A:36:LEU:N	2.51	0.44
1:A:254:VAL:HG21	1:A:329:TYR:HB3	2.00	0.44
1:A:234:ASP:OD2	1:A:272:ASN:HB3	2.18	0.44
1:B:300:LEU:CD1	1:B:300:LEU:H	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:TRP:O	1:B:240:LYS:HG3	2.18	0.44
1:B:265:PRO:CD	1:B:292:ALA:HB1	2.48	0.44
1:A:255:ASP:C	1:A:257:ALA:H	2.21	0.44
1:A:398:GLU:O	1:A:401:SER:HB2	2.18	0.44
1:A:208:MET:HB2	1:A:214:PRO:HG3	1.99	0.44
1:B:140:LYS:HD3	1:B:144:GLY:HA2	2.00	0.43
1:B:255:ASP:C	1:B:257:ALA:H	2.21	0.43
1:A:52:CYS:SG	1:A:54:LEU:HD11	2.57	0.43
3:B:694:MAN:C3	3:B:695:MAN:H5	2.45	0.43
1:A:253:ILE:O	1:A:255:ASP:N	2.51	0.43
1:B:117:ILE:O	1:B:120:LEU:N	2.49	0.43
1:A:100:ARG:HD2	1:A:104:GLY:O	2.19	0.43
1:A:136:ASP:CB	1:A:141:THR:HA	2.48	0.43
1:B:378:CYS:O	1:B:399:TRP:HA	2.18	0.43
1:B:100:ARG:HD3	1:B:106:LEU:HD23	2.01	0.43
1:B:32:LEU:N	1:B:223:CYS:O	2.52	0.43
1:B:175:ASP:HB2	1:B:179:ASN:HD21	1.79	0.43
3:B:692:NAG:H61	3:B:693:NAG:C8	2.47	0.43
1:A:75:LEU:H	1:A:75:LEU:CD1	2.32	0.43
1:B:191:LEU:O	1:B:194:THR:N	2.52	0.43
1:B:229:PHE:CD2	1:B:242:ILE:HG12	2.54	0.43
1:A:100:ARG:HH22	1:A:148:SER:HA	1.84	0.43
1:A:368:ALA:O	1:A:369:VAL:C	2.57	0.43
1:B:397:TYR:CE2	1:B:403:LEU:HD13	2.54	0.43
1:A:141:THR:HG23	1:A:146:PRO:O	2.19	0.43
1:A:133:ILE:O	1:A:167:LEU:HD12	2.18	0.43
1:B:177:LEU:O	1:B:181:ALA:N	2.52	0.43
1:A:78:SER:C	1:A:80:GLY:H	2.22	0.43
1:B:91:ILE:HG21	1:B:95:TRP:HB3	2.01	0.42
1:B:290:MET:O	1:B:292:ALA:N	2.51	0.42
1:A:265:PRO:CD	1:A:292:ALA:HB1	2.49	0.42
1:A:185:LYS:HG2	1:A:222:TYR:CE2	2.54	0.42
1:A:69:PHE:CZ	1:A:91:ILE:HG12	2.54	0.42
1:A:281:VAL:CG2	1:A:282:THR:N	2.82	0.42
1:B:44:TRP:HD1	1:B:296:MET:HB2	1.84	0.42
1:A:236:TRP:CD1	1:A:240:LYS:HD2	2.55	0.42
1:B:201:SER:HB2	1:B:225:HIS:CE1	2.54	0.42
1:A:151:TYR:O	1:A:152:TYR:C	2.56	0.42
1:A:191:LEU:O	1:A:194:THR:N	2.52	0.42
1:B:151:TYR:O	1:B:152:TYR:C	2.58	0.42
1:B:252:ARG:NH1	1:B:252:ARG:HG3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ILE:HD12	1:A:397:TYR:CE1	2.55	0.42
1:B:95:TRP:CE2	1:B:133:ILE:HD11	2.54	0.42
1:A:34:ASN:ND2	1:A:224:ASN:HD21	2.16	0.42
1:B:141:THR:C	1:B:143:ALA:N	2.73	0.42
1:A:250:GLN:HG2	1:A:250:GLN:H	1.66	0.42
1:B:45:LEU:HD23	1:B:46:HIS:N	2.35	0.42
1:B:376:VAL:HG12	1:B:377:ALA:N	2.34	0.42
1:A:177:LEU:O	1:A:181:ALA:N	2.51	0.42
1:B:205:PRO:HG3	1:B:219:ILE:CD1	2.50	0.42
1:A:290:MET:O	1:A:292:ALA:N	2.53	0.42
1:A:358:GLU:O	1:B:234:ASP:HB3	2.20	0.42
1:B:133:ILE:O	1:B:167:LEU:HD12	2.20	0.41
1:B:281:VAL:CG2	1:B:282:THR:N	2.83	0.41
1:B:48:GLU:HB3	1:B:297:SER:OG	2.20	0.41
1:A:98:PRO:HB2	1:A:99:GLN:OE1	2.19	0.41
1:B:100:ARG:NH1	1:B:106:LEU:CG	2.81	0.41
1:A:44:TRP:HD1	1:A:296:MET:HB2	1.85	0.41
1:A:366:THR:HA	1:A:403:LEU:O	2.20	0.41
1:B:177:LEU:HD11	1:B:211:PHE:CD2	2.55	0.41
1:A:353:MET:O	1:A:412:THR:HA	2.21	0.41
1:B:91:ILE:CG2	1:B:95:TRP:HB3	2.50	0.41
1:A:378:CYS:O	1:A:380:PRO:O	2.39	0.41
1:A:141:THR:C	1:A:143:ALA:N	2.73	0.41
1:A:333:GLN:CA	1:A:333:GLN:HE21	2.32	0.41
1:B:205:PRO:C	1:B:207:TYR:N	2.73	0.41
1:B:211:PHE:C	1:B:212:GLN:HG2	2.41	0.41
1:A:81:TRP:HA	1:A:312:GLN:NE2	2.36	0.41
1:B:252:ARG:HH11	1:B:252:ARG:HG3	1.86	0.41
1:A:134:TYR:HE2	1:A:141:THR:HB	1.85	0.41
1:A:420:THR:HG22	1:A:420:THR:O	2.19	0.41
1:B:249:ASN:O	1:B:250:GLN:C	2.59	0.41
1:B:117:ILE:HG13	1:B:162:TRP:CZ3	2.56	0.41
1:B:234:ASP:OD2	1:B:273:PHE:HD2	2.04	0.41
1:A:315:ASP:HB3	1:A:387:LEU:HD21	2.03	0.41
1:B:384:ILE:HG12	1:B:417:LEU:HG	2.02	0.41
1:B:66:GLU:HG2	1:B:113:PHE:HA	2.03	0.41
1:A:174:CYS:HA	2:A:639:NAG:O7	2.21	0.41
1:B:180:LEU:O	1:B:181:ALA:C	2.58	0.41
1:A:336:ASN:O	1:A:363:ARG:NH2	2.54	0.41
1:A:252:ARG:NH1	1:A:252:ARG:HG3	2.36	0.41
1:A:204:TRP:HB3	1:A:205:PRO:CD	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ILE:HD12	1:A:367:ILE:C	2.42	0.40
3:A:692:NAG:O6	3:A:693:NAG:C7	2.69	0.40
1:B:95:TRP:NE1	1:B:96:MET:HE3	2.36	0.40
1:A:377:ALA:HA	1:A:419:ASN:HD22	1.86	0.40
1:A:249:ASN:O	1:A:250:GLN:C	2.59	0.40
1:B:75:LEU:H	1:B:75:LEU:CD1	2.34	0.40
1:A:180:LEU:O	1:A:181:ALA:C	2.60	0.40
1:A:92:ASP:OD1	1:A:93:ASP:N	2.54	0.40
1:B:208:MET:SD	1:B:214:PRO:HA	2.62	0.40
1:A:65:SER:O	1:A:68:LEU:N	2.54	0.40
1:A:184:TYR:CE2	1:A:204:TRP:HA	2.56	0.40
1:A:381:ALA:CB	1:A:420:THR:OG1	2.70	0.40
1:B:34:ASN:HD21	1:B:224:ASN:ND2	2.18	0.40
1:B:300:LEU:CD1	1:B:300:LEU:N	2.85	0.40
1:B:118:ARG:O	1:B:121:ALA:HB3	2.21	0.40
1:A:359:ILE:CG1	1:A:360:GLY:N	2.84	0.40
1:B:356:ARG:HA	1:B:356:ARG:HD2	1.87	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	388/398 (98%)	299 (77%)	65 (17%)	24 (6%)	2	19
1	B	389/398 (98%)	295 (76%)	67 (17%)	27 (7%)	1	16
All	All	777/796 (98%)	594 (76%)	132 (17%)	51 (7%)	1	18

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	TRP

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Mol	Chain	Res	Type
1	A	148	SER
1	A	175	ASP
1	A	266	ASP
1	B	118	ARG
1	B	148	SER
1	B	175	ASP
1	B	230	ALA
1	B	266	ASP
1	B	378	CYS
1	B	401	SER
1	A	78	SER
1	A	291	ALA
1	A	371	SER
1	A	378	CYS
1	B	47	TRP
1	B	78	SER
1	B	100	ARG
1	B	254	VAL
1	B	291	ALA
1	B	371	SER
1	B	376	VAL
1	A	51	MET
1	A	118	ARG
1	A	146	PRO
1	A	254	VAL
1	A	376	VAL
1	A	79	GLU
1	A	230	ALA
1	A	231	ASP
1	A	391	LYS
1	B	51	MET
1	B	93	ASP
1	B	146	PRO
1	B	256	VAL
1	B	391	LYS
1	A	93	ASP
1	A	152	TYR
1	A	248	PHE
1	A	250	GLN
1	B	79	GLU
1	B	180	LEU
1	A	158	THR

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Mol	Chain	Res	Type
1	A	256	VAL
1	B	152	TYR
1	B	158	THR
1	B	212	GLN
1	B	250	GLN
1	A	369	VAL
1	B	369	VAL
1	B	210	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/339 (98%)	312 (94%)	19 (6%)	25	65
1	B	332/339 (98%)	313 (94%)	19 (6%)	25	65
All	All	663/678 (98%)	625 (94%)	38 (6%)	25	65

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	46	HIS
1	A	63	CYS
1	A	74	GLU
1	A	146	PRO
1	A	246	THR
1	A	250	GLN
1	A	251	GLU
1	A	264	ASP
1	A	273	PHE
1	A	287	TRP
1	A	304	SER
1	A	324	LEU
1	A	337	PHE
1	A	353	MET

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Mol	Chain	Res	Type
1	A	380	PRO
1	A	382	CYS
1	A	388	LEU
1	A	421	MET
1	B	45	LEU
1	B	46	HIS
1	B	63	CYS
1	B	74	GLU
1	B	146	PRO
1	B	161	ASP
1	B	246	THR
1	B	250	GLN
1	B	251	GLU
1	B	273	PHE
1	B	287	TRP
1	B	304	SER
1	B	324	LEU
1	B	337	PHE
1	B	353	MET
1	B	382	CYS
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 (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	111	GLN
1	A	122	ASN
1	A	125	HIS
1	A	179	ASN
1	A	272	ASN
1	A	278	ASN
1	A	302	HIS
1	A	312	GLN
1	A	327	GLN
1	A	330	GLN
1	A	333	GLN
1	A	336	ASN
1	A	355	ASN
1	A	357	GLN

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Mol	Chain	Res	Type
1	B	46	HIS
1	B	57	GLN
1	B	111	GLN
1	B	115	HIS
1	B	122	ASN
1	B	179	ASN
1	B	221	GLN
1	B	272	ASN
1	B	312	GLN
1	B	355	ASN
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 ⓘ

24 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	639	1,2	14,14,15	0.91	0	15,19,21	0.81	0
2	NAG	A	640	2	14,14,15	0.77	0	15,19,21	0.80	1 (6%)
3	NAG	A	692	1,3	14,14,15	0.64	0	15,19,21	0.92	1 (6%)
3	NAG	A	693	3	14,14,15	0.65	0	15,19,21	0.63	0
3	MAN	A	694	3	11,11,12	0.65	0	14,15,17	0.60	0
3	MAN	A	695	3	11,11,12	0.55	0	14,15,17	0.71	0
3	MAN	A	696	3	11,11,12	0.46	0	14,15,17	0.79	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
4	NAG	A	715	1,4	14,14,15	0.54	0	15,19,21	0.72	1 (6%)
4	NAG	A	716	4	14,14,15	0.66	0	15,19,21	0.77	1 (6%)
4	MAN	A	717	4	11,11,12	0.89	0	14,15,17	0.42	0
5	NAG	B	639	1,5	14,14,15	0.50	0	15,19,21	0.94	1 (6%)
5	NAG	B	640	5	14,14,15	0.37	0	15,19,21	0.95	1 (6%)
5	MAN	B	641	5	11,11,12	0.66	0	14,15,17	1.86	3 (21%)
5	MAN	B	642	5	11,11,12	0.61	0	14,15,17	0.55	0
5	MAN	B	643	5	11,11,12	0.47	0	14,15,17	0.60	0
5	FUC	B	644	5	10,10,11	0.54	0	14,14,16	0.66	0
3	NAG	B	692	1,3	14,14,15	0.89	1 (7%)	15,19,21	0.92	1 (6%)
3	NAG	B	693	3	14,14,15	0.72	0	15,19,21	0.83	1 (6%)
3	MAN	B	694	3	11,11,12	0.51	0	14,15,17	1.14	1 (7%)
3	MAN	B	695	3	11,11,12	0.47	0	14,15,17	0.61	0
3	MAN	B	696	3	11,11,12	0.72	0	14,15,17	0.78	1 (7%)
4	NAG	B	715	1,4	14,14,15	0.53	0	15,19,21	1.05	1 (6%)
4	NAG	B	716	4	14,14,15	0.51	0	15,19,21	0.81	1 (6%)
4	MAN	B	717	4	11,11,12	0.90	0	14,15,17	0.91	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	639	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	640	2	-	0/6/23/26	0/1/1/1
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
4	MAN	A	717	4	1/1/4/5	0/2/19/22	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	692	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	693	3	-	0/6/23/26	0/1/1/1
3	MAN	B	694	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	B	695	3	-	0/2/19/22	0/1/1/1
3	MAN	B	696	3	-	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
4	MAN	B	717	4	1/1/4/5	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	692	NAG	C1-C2	2.56	1.56	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	694	MAN	C1-C2-C3	-3.45	105.46	109.54
3	A	692	NAG	C2-N2-C7	-2.81	119.43	123.04
4	B	716	NAG	C2-N2-C7	-2.69	119.59	123.04
2	A	640	NAG	C2-N2-C7	-2.52	119.80	123.04
5	B	639	NAG	C2-N2-C7	-2.41	119.94	123.04
3	B	693	NAG	C2-N2-C7	-2.29	120.10	123.04
5	B	641	MAN	O3-C3-C2	-2.26	105.91	110.00
4	A	716	NAG	C2-N2-C7	-2.22	120.19	123.04
3	B	692	NAG	C3-C4-C5	-2.21	106.35	110.20
5	B	640	NAG	C2-N2-C7	-2.10	120.34	123.04
4	A	715	NAG	C2-N2-C7	-2.03	120.44	123.04
3	B	696	MAN	C1-C2-C3	2.08	112.00	109.54
5	B	641	MAN	C2-C3-C4	2.24	114.85	111.04
4	B	715	NAG	C4-C3-C2	2.48	115.08	111.23
3	A	696	MAN	C1-O5-C5	2.49	115.41	112.25
4	B	717	MAN	C1-C2-C3	3.09	113.20	109.54
5	B	641	MAN	C1-C2-C3	5.64	116.21	109.54

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	641	MAN	C1
4	B	717	MAN	C1
3	B	694	MAN	C1
3	A	694	MAN	C1

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Mol	Chain	Res	Type	Atom
4	A	717	MAN	C1

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	639	NAG	2	0
3	A	692	NAG	1	0
3	A	693	NAG	1	0
3	A	694	MAN	1	0
3	A	695	MAN	1	0
5	B	639	NAG	7	0
5	B	644	FUC	5	0
3	B	692	NAG	3	0
3	B	693	NAG	5	0
3	B	694	MAN	4	0
3	B	695	MAN	4	0
3	B	696	MAN	1	0
4	B	715	NAG	1	0
4	B	716	NAG	3	0
4	B	717	MAN	2	0

5.6 Ligand geometry (i)

4 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
6	GAL	A	1101	-	12,12,12	0.28	0	17,17,17	0.72	1 (5%)
7	EDO	A	1102	-	3,3,3	0.66	0	2,2,2	0.29	0
6	GAL	B	1103	-	12,12,12	0.57	0	17,17,17	0.60	0
7	EDO	B	1104	-	3,3,3	0.53	0	2,2,2	0.43	0

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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	GAL	A	1101	-	1/1/5/5	0/2/22/22	0/1/1/1
7	EDO	A	1102	-	-	0/1/1/1	0/0/0/0
6	GAL	B	1103	-	1/1/5/5	0/2/22/22	0/1/1/1
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(^{o})	Ideal(^{o})
6	A	1101	GAL	C4-C3-C2	-2.45	106.22	110.79

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1101	GAL	C1
6	B	1103	GAL	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1101	GAL	3	0
7	A	1102	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%)	-0.34	0	100	100	7, 46, 85, 140	0
1	B	391/398 (98%)	-0.11	4 (1%)	84	78	12, 54, 96, 138	0
All	All	781/796 (98%)	-0.22	4 (0%)	91	89	7, 49, 91, 140	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	198	ILE	3.1
1	B	422	GLN	2.2
1	B	179	ASN	2.1
1	B	213	LYS	2.1

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
3	NAG	B	692	14/15	0.93	0.22	-0.50	73,89,101,102	0
3	NAG	A	692	14/15	0.94	0.17	-0.62	43,55,65,68	0
2	NAG	A	639	14/15	0.87	0.21	-0.72	70,94,114,133	0
5	NAG	B	639	14/15	0.86	0.18	-1.24	103,133,153,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	MAN	B	641	11/12	0.61	0.17	-	180,183,190,194	0
5	MAN	B	642	11/12	0.73	0.42	-	189,193,198,198	0
3	MAN	B	696	11/12	0.68	0.38	-	163,170,175,179	0
2	NAG	A	640	14/15	0.73	0.35	-	153,168,186,186	0
4	MAN	B	717	11/12	0.34	0.46	-	178,185,190,191	0
5	FUC	B	644	10/11	0.81	0.23	-	159,160,162,166	0
4	NAG	B	716	14/15	0.67	0.41	-	170,182,185,192	0
3	NAG	A	693	14/15	0.90	0.21	-	68,83,125,132	0
5	NAG	B	640	14/15	0.77	0.27	-	159,166,169,172	0
4	NAG	A	715	14/15	0.89	0.18	-	107,127,146,146	0
4	NAG	A	716	14/15	0.82	0.26	-	150,155,163,173	0
3	MAN	A	696	11/12	0.67	0.42	-	146,159,162,165	0
3	MAN	B	694	11/12	0.73	0.15	-	113,123,141,154	0
3	MAN	A	694	11/12	0.73	0.25	-	140,151,159,177	0
4	MAN	A	717	11/12	0.39	0.32	-	170,179,182,184	0
4	NAG	B	715	14/15	0.81	0.17	-	87,126,143,155	0
3	NAG	B	693	14/15	0.90	0.20	-	87,98,114,119	0
5	MAN	B	643	11/12	0.62	0.38	-	188,196,198,198	0
3	MAN	B	695	11/12	0.85	0.19	-	96,115,120,120	0
3	MAN	A	695	11/12	0.78	0.37	-	184,190,198,198	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(Å^2)	Q<0.9
6	GAL	B	1103	12/12	0.87	0.22	0.77	55,70,77,82	0
6	GAL	A	1101	12/12	0.91	0.20	0.72	47,60,66,69	0
7	EDO	A	1102	4/4	0.29	0.61	-	95,102,103,104	0
7	EDO	B	1104	4/4	0.68	0.49	-	103,105,106,108	0

6.5 Other polymers (i)

There are no such residues in this entry.