



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:44 am GMT

PDB ID : 4AYJ
Title : Molecular structure of a metal-independent bacterial glycosyltransferase that catalyzes the synthesis of histo-blood group A antigen
Authors : Thiagarajan, N.; Pham, T.T.K.; Stinson, B.; Sundriyal, A.; Tumbale, P.; Lizotte-Waniewskib, M.; Brewb, K.; Acharya, K.R.
Deposited on : 2012-06-21
Resolution : 3.00 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

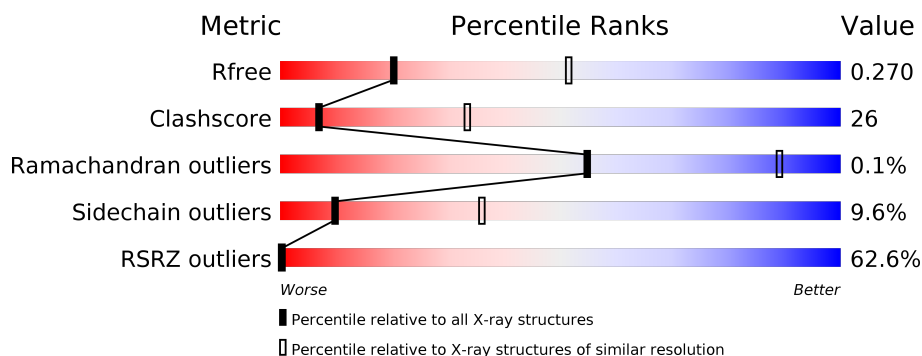
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	246	<div> <div>61%</div> <div> <div>52%</div> <div>38%</div> <div>6%</div> </div> </div>
1	B	246	<div> <div>59%</div> <div> <div>46%</div> <div>45%</div> <div>•</div> </div> </div>
1	C	246	<div> <div>60%</div> <div> <div>47%</div> <div>43%</div> <div>•</div> <div>5%</div> </div> </div>
1	D	246	<div> <div>59%</div> <div> <div>46%</div> <div>44%</div> <div>6%</div> <div>•</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BGC	A	1232	-	-	-	X
2	GAL	A	1233	-	-	-	X
2	BGC	B	1232	-	-	-	X
2	GAL	B	1233	-	-	-	X
2	FUC	B	1234	-	-	-	X
2	BGC	C	1232	-	-	X	-
2	FUC	C	1234	-	-	-	X
2	BGC	D	1232	-	-	-	X
2	GAL	D	1233	-	-	-	X
2	FUC	D	1234	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7939 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 BOGT - METAL-INDEPENDENT GLYCOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	4	0	0
			1928	1262	311	348	7			
1	B	235	Total	C	N	O	S	0	0	0
			1961	1282	318	354	7			
1	C	233	Total	C	N	O	S	4	0	0
			1945	1272	315	351	7			
1	D	236	Total	C	N	O	S	0	0	0
			1973	1291	319	356	7			

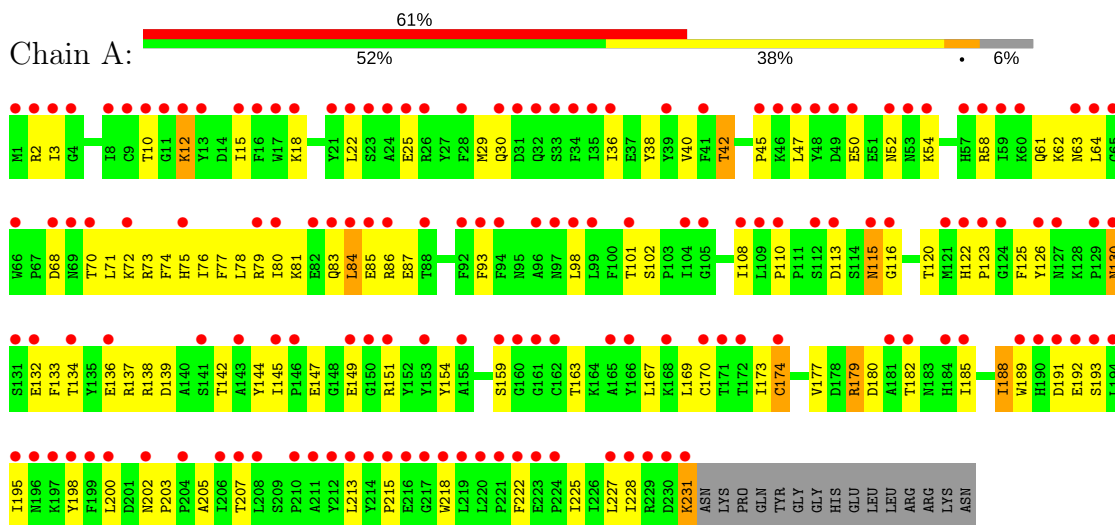
- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

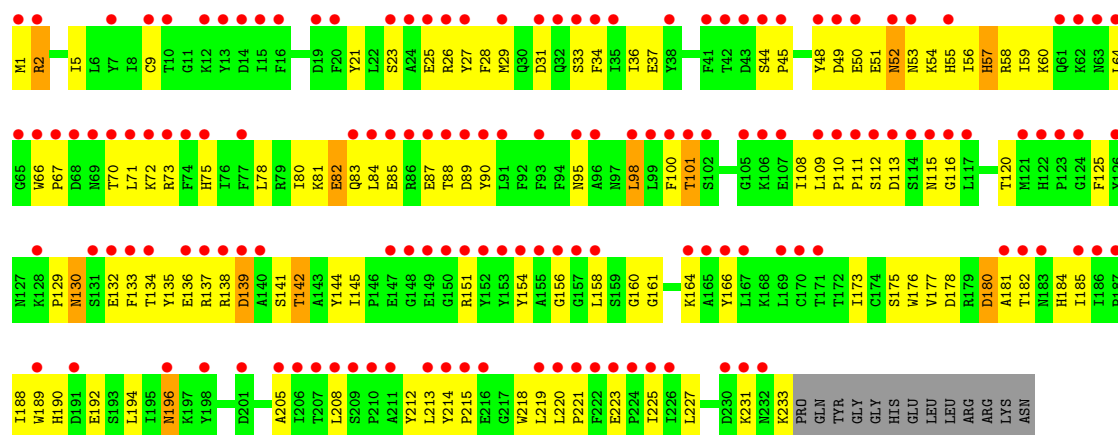
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	3	Total	C	O	0	0
			33	18	15		
2	B	3	Total	C	O	0	0
			33	18	15		
2	C	3	Total	C	O	0	0
			33	18	15		
2	D	3	Total	C	O	0	0
			33	18	15		

3 Residue-property plots

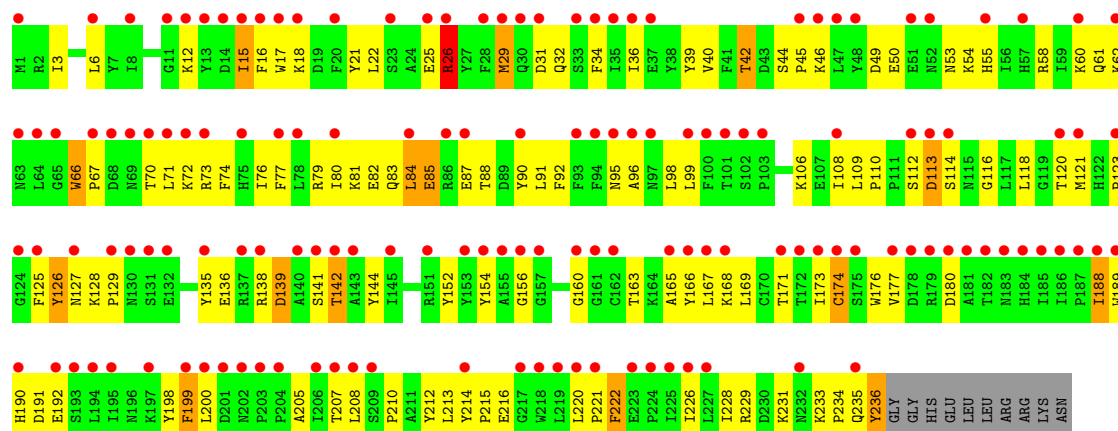
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: BOGT - METAL-INDEPENDENT GLYCOSYLTRANSFERASE





• Molecule 1: BOGT - METAL-INDEPENDENT GLYCOSYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.85Å 93.87Å 75.51Å 90.00° 93.82° 90.00°	Depositor
Resolution (Å)	70.69 – 3.00 70.69 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.7 (70.69-3.00) 93.7 (70.69-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.36 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.181 , 0.262 0.443 , 0.270	Depositor DCC
R_{free} test set	680 reflections (3.88%)	DCC
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.27$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.59	EDS
Total number of atoms	7939	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: BGC, GAL, 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	0.50	0/1991	0.72	0/2704
1	B	0.47	0/2025	0.68	1/2750 (0.0%)
1	C	0.47	0/2008	0.65	0/2726
1	D	0.47	0/2038	0.67	1/2768 (0.0%)
All	All	0.48	0/8062	0.68	2/10948 (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
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	26	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	B	220	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ASN	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	1928	0	1869	89	0
1	B	1961	0	1903	93	1
1	C	1945	0	1888	101	0
1	D	1973	0	1911	116	1
2	A	33	0	30	9	0
2	B	33	0	30	2	0
2	C	33	0	30	7	0
2	D	33	0	30	3	0
All	All	7939	0	7691	399	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 26.

All (399) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1232:BGC:O5	1:D:128:LYS:NZ	1.79	1.15
1:C:2:ARG:NH1	1:C:89:ASP:H	1.50	1.08
1:C:2:ARG:O	1:C:2:ARG:NH1	1.93	1.02
1:A:134:THR:HG21	1:A:189:TRP:HE1	1.28	0.98
1:B:229:ARG:HD3	1:C:223:GLU:OE2	1.64	0.97
2:A:1232:BGC:O5	1:B:128:LYS:NZ	2.00	0.93
1:D:80:ILE:HG13	1:D:84:LEU:HD22	1.51	0.91
2:C:1232:BGC:C1	1:D:128:LYS:HZ1	1.85	0.89
1:A:136:GLU:HA	1:A:188:ILE:HD11	1.56	0.88
1:B:232:ASN:OD1	1:B:233:LYS:N	2.07	0.87
1:B:208:LEU:HB3	1:B:212:TYR:HD2	1.40	0.86
1:C:2:ARG:NH2	1:C:87:GLU:O	2.09	0.85
1:B:208:LEU:HB3	1:B:212:TYR:CD2	2.12	0.85
1:C:2:ARG:CZ	1:C:88:THR:HA	2.07	0.84
1:D:50:GLU:OE2	1:D:58:ARG:NH1	2.10	0.83
1:C:51:GLU:HG2	1:C:52:ASN:OD1	1.79	0.81
1:D:165:ALA:HA	1:D:168:LYS:HE2	1.65	0.79
1:A:25:GLU:O	1:A:30:GLN:NE2	2.16	0.79
1:C:134:THR:HG21	1:C:189:TRP:CD1	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:TRP:CG	1:D:67:PRO:HA	2.20	0.77
1:D:83:GLN:O	1:D:87:GLU:HG3	1.83	0.77
1:B:158:LEU:HD23	1:B:159:SER:N	2.00	0.76
1:A:80:ILE:HG13	1:A:84:LEU:HD22	1.66	0.76
1:A:134:THR:CG2	1:A:189:TRP:HE1	1.98	0.76
1:C:134:THR:HG22	1:C:134:THR:O	1.85	0.75
1:C:2:ARG:HH11	1:C:89:ASP:H	1.33	0.75
1:D:138:ARG:O	1:D:144:TYR:HB2	1.86	0.74
1:D:188:ILE:HD13	1:D:189:TRP:H	1.51	0.74
1:A:72:LYS:HD2	1:A:75:HIS:ND1	2.03	0.74
1:C:82:GLU:HA	1:C:85:GLU:HG3	1.70	0.73
1:D:121:MET:HE2	1:D:126:TYR:HB2	1.70	0.73
1:D:74:PHE:HA	1:D:77:PHE:HD2	1.52	0.73
1:D:92:PHE:CD1	1:D:160:GLY:HA3	2.23	0.73
1:C:1:MET:O	1:C:34:PHE:HA	1.90	0.72
1:A:81:LYS:O	1:A:85:GLU:HG3	1.90	0.71
1:B:86:ARG:HG2	1:B:87:GLU:HG3	1.72	0.71
1:C:84:LEU:O	1:C:88:THR:OG1	2.06	0.71
1:A:198:TYR:O	1:A:202:ASN:HB2	1.89	0.71
1:B:75:HIS:CD2	1:B:174:CYS:SG	2.84	0.71
1:C:80:ILE:HG13	1:C:84:LEU:HD11	1.72	0.70
1:D:12:LYS:O	1:D:15:ILE:HG12	1.91	0.70
1:C:134:THR:CG2	1:C:189:TRP:CD1	2.75	0.70
1:D:26:ARG:HH11	1:D:26:ARG:CB	2.05	0.70
1:A:231:LYS:HD3	1:A:231:LYS:H	1.58	0.69
1:C:2:ARG:NH1	1:C:89:ASP:N	2.34	0.69
1:C:48:TYR:CD1	1:C:49:ASP:HB2	2.29	0.68
1:A:125:PHE:HE2	2:A:1233:GAL:H61	1.59	0.68
1:D:118:LEU:HD11	1:D:208:LEU:HD11	1.75	0.68
1:D:169:LEU:O	1:D:173:ILE:HG13	1.94	0.68
1:D:31:ASP:O	1:D:32:GLN:HG2	1.94	0.68
1:B:134:THR:HG21	1:B:189:TRP:HE1	1.59	0.68
1:A:62:LYS:HG2	1:A:63:ASN:N	2.09	0.67
1:A:70:THR:O	1:A:73:ARG:HG3	1.93	0.67
1:C:180:ASP:HB3	1:C:185:ILE:O	1.95	0.67
2:C:1232:BGC:C1	1:D:128:LYS:NZ	2.49	0.67
2:C:1232:BGC:O3	2:C:1233:GAL:O5	2.04	0.66
1:B:130:ASN:HD21	1:B:148:GLY:HA2	1.61	0.66
1:D:215:PRO:HA	1:D:228:ILE:HB	1.77	0.66
1:B:29:MET:HB2	1:B:36:ILE:HD11	1.76	0.66
1:A:136:GLU:O	1:A:144:TYR:HA	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:TYR:CE1	1:C:49:ASP:HB2	2.32	0.65
1:C:50:GLU:OE2	1:C:58:ARG:NH1	2.29	0.65
1:D:6:LEU:HB3	1:D:77:PHE:HE1	1.62	0.65
1:D:233:LYS:O	1:D:236:TYR:HB2	1.97	0.64
1:A:179:ARG:O	1:A:182:THR:OG1	2.13	0.64
1:D:26:ARG:HB2	1:D:26:ARG:HH11	1.62	0.64
1:D:90:TYR:O	1:D:91:LEU:HD23	1.98	0.64
1:D:126:TYR:OH	1:D:221:PRO:HG3	1.97	0.64
1:D:50:GLU:CD	1:D:58:ARG:HH11	2.01	0.64
1:D:114:SER:HB2	1:D:205:ALA:HB2	1.80	0.64
1:D:6:LEU:HB3	1:D:77:PHE:CE1	2.33	0.64
1:D:82:GLU:HA	1:D:85:GLU:HG3	1.81	0.63
1:A:122:HIS:HE2	2:A:1233:GAL:HO4	1.45	0.62
1:D:53:ASN:OD1	1:D:55:HIS:N	2.20	0.62
1:D:3:ILE:HD11	1:D:34:PHE:CE1	2.34	0.62
1:D:73:ARG:NH1	1:D:191:ASP:CG	2.52	0.62
1:C:136:GLU:HG2	1:C:141:SER:OG	2.00	0.62
1:C:139:ASP:OD1	1:C:139:ASP:N	2.28	0.62
1:A:120:THR:HG21	1:A:213:LEU:HD12	1.81	0.62
1:D:73:ARG:NH1	1:D:191:ASP:OD2	2.33	0.61
1:B:121:MET:HB2	1:B:210:PRO:HD3	1.81	0.61
1:D:126:TYR:OH	1:D:221:PRO:CG	2.49	0.61
1:A:79:ARG:HH11	1:A:79:ARG:HB3	1.66	0.61
1:A:120:THR:CG2	1:A:213:LEU:HD12	2.31	0.61
1:C:2:ARG:NH2	1:C:88:THR:HA	2.15	0.61
1:C:2:ARG:HB2	1:C:2:ARG:CZ	2.27	0.61
1:A:101:THR:OG1	1:A:225:ILE:O	2.17	0.60
1:C:2:ARG:CZ	1:C:87:GLU:O	2.49	0.60
1:B:143:ALA:HB2	1:B:194:LEU:HG	1.82	0.60
1:A:134:THR:HG21	1:A:189:TRP:NE1	2.09	0.60
1:D:73:ARG:HB3	1:D:77:PHE:HE2	1.66	0.60
1:A:145:ILE:HD13	1:A:200:LEU:HD22	1.83	0.60
1:B:92:PHE:CD1	1:B:160:GLY:HA3	2.37	0.60
1:A:180:ASP:HB3	1:A:185:ILE:O	2.02	0.60
1:C:181:ALA:O	1:C:184:HIS:N	2.26	0.59
1:C:134:THR:HG21	1:C:189:TRP:NE1	2.17	0.59
1:C:90:TYR:CZ	1:C:109:LEU:HD22	2.36	0.59
1:B:60:LYS:O	1:B:79:ARG:NH1	2.31	0.59
1:C:173:ILE:O	1:C:177:VAL:HG23	2.02	0.59
1:D:80:ILE:CG1	1:D:84:LEU:HD22	2.27	0.59
1:D:188:ILE:HD13	1:D:189:TRP:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:LEU:HD22	1:B:212:TYR:CE2	2.38	0.59
2:A:1232:BGC:O1	1:B:128:LYS:HE2	2.02	0.59
1:D:73:ARG:HH11	1:D:191:ASP:CG	2.06	0.59
1:D:26:ARG:HH11	1:D:26:ARG:CG	2.15	0.59
1:B:15:ILE:CD1	1:B:235:GLN:H	2.16	0.58
1:B:28:PHE:O	1:B:30:GLN:NE2	2.34	0.58
1:C:134:THR:HG22	1:C:189:TRP:HD1	1.68	0.58
1:C:115:ASN:OD1	1:C:205:ALA:HB2	2.03	0.58
1:C:142:THR:OG1	1:C:180:ASP:OD1	2.14	0.58
1:C:90:TYR:CE2	1:C:109:LEU:HD22	2.38	0.58
1:D:73:ARG:NH1	1:D:191:ASP:OD1	2.37	0.58
1:D:212:TYR:O	1:D:226:ILE:HB	2.04	0.58
1:C:214:TYR:CE2	1:C:220:LEU:HB2	2.38	0.57
1:A:215:PRO:HA	1:A:228:ILE:HB	1.87	0.57
1:B:215:PRO:HB2	1:B:218:TRP:CG	2.39	0.57
1:D:135:TYR:OH	1:D:152:TYR:O	2.21	0.57
1:A:68:ASP:HA	1:A:71:LEU:HB3	1.87	0.56
1:A:123:PRO:O	1:A:126:TYR:HD1	1.87	0.56
1:D:66:TRP:CD1	1:D:67:PRO:N	2.73	0.56
1:B:122:HIS:NE2	2:B:1233:GAL:O4	2.31	0.56
1:A:138:ARG:O	1:A:144:TYR:HB2	2.05	0.56
1:C:160:GLY:HA2	1:C:166:TYR:CD2	2.41	0.56
1:D:66:TRP:CD1	1:D:67:PRO:HA	2.40	0.56
1:A:154:TYR:HE1	1:A:207:THR:HG23	1.70	0.56
1:B:233:LYS:HB2	1:B:234:PRO:HD2	1.87	0.56
1:C:134:THR:CG2	1:C:189:TRP:HD1	2.19	0.56
1:A:79:ARG:HB3	1:A:79:ARG:NH1	2.21	0.55
1:A:74:PHE:O	1:A:78:LEU:HG	2.07	0.55
1:D:67:PRO:O	1:D:70:THR:HG22	2.05	0.55
1:B:138:ARG:O	1:B:144:TYR:HB2	2.07	0.55
1:C:25:GLU:HA	1:C:25:GLU:OE1	2.06	0.55
1:D:83:GLN:HG3	1:D:87:GLU:OE2	2.07	0.55
1:B:15:ILE:HD13	1:B:235:GLN:H	1.72	0.55
1:D:73:ARG:O	1:D:76:ILE:HB	2.07	0.55
1:B:215:PRO:HB2	1:B:218:TRP:CD2	2.41	0.55
1:C:101:THR:HG23	1:C:225:ILE:O	2.07	0.55
1:A:134:THR:CG2	1:A:189:TRP:NE1	2.69	0.55
1:A:29:MET:HE2	1:A:108:ILE:HD11	1.88	0.55
1:B:48:TYR:CD1	1:B:49:ASP:HB2	2.42	0.55
1:A:83:GLN:O	1:A:87:GLU:HG3	2.06	0.54
1:B:114:SER:HB2	1:B:116:GLY:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:O	1:A:215:PRO:HD3	2.07	0.54
1:B:126:TYR:CE1	1:B:127:ASN:HB3	2.41	0.54
1:D:139:ASP:N	1:D:139:ASP:OD1	2.36	0.54
1:D:6:LEU:HD13	1:D:77:PHE:CD1	2.42	0.54
1:A:222:PHE:HA	1:D:216:GLU:HG3	1.89	0.54
1:B:59:ILE:HG21	1:B:80:ILE:HG21	1.90	0.54
1:A:122:HIS:NE2	2:A:1233:GAL:O4	2.33	0.54
1:C:51:GLU:OE1	1:C:51:GLU:N	2.34	0.54
1:A:231:LYS:HD3	1:A:231:LYS:N	2.21	0.54
1:C:233:LYS:HE3	1:C:233:LYS:HA	1.90	0.54
1:C:129:PRO:HG2	1:C:132:GLU:HG2	1.88	0.54
1:C:134:THR:CG2	1:C:134:THR:O	2.55	0.54
1:C:2:ARG:NH1	1:C:88:THR:HA	2.23	0.54
1:B:197:LYS:O	1:B:200:LEU:HB3	2.07	0.53
1:B:212:TYR:O	1:B:226:ILE:HB	2.08	0.53
1:D:70:THR:HG23	1:D:71:LEU:N	2.24	0.53
1:B:135:TYR:CD1	1:B:145:ILE:HD12	2.44	0.53
1:C:142:THR:HG21	1:C:176:TRP:CD1	2.43	0.53
1:D:15:ILE:HD12	1:D:236:TYR:HA	1.91	0.53
1:C:67:PRO:HB2	1:C:190:HIS:CD2	2.44	0.53
1:D:169:LEU:HD23	1:D:173:ILE:HG13	1.90	0.52
1:A:130:ASN:HB2	1:A:133:PHE:CD2	2.44	0.52
1:A:145:ILE:HG22	1:A:149:GLU:HB3	1.91	0.52
1:B:135:TYR:CG	1:B:145:ILE:HD12	2.44	0.52
1:B:53:ASN:C	1:B:54:LYS:HE2	2.29	0.52
1:C:136:GLU:OE1	1:C:137:ARG:N	2.42	0.52
1:A:139:ASP:HA	1:A:144:TYR:CG	2.45	0.51
1:A:80:ILE:CG1	1:A:84:LEU:HD22	2.37	0.51
1:B:156:GLY:N	1:B:192:GLU:HG3	2.25	0.51
1:C:26:ARG:HG2	1:C:27:TYR:CE2	2.45	0.51
1:C:80:ILE:HG13	1:C:84:LEU:CD1	2.40	0.51
1:B:173:ILE:O	1:B:177:VAL:HG23	2.11	0.51
1:D:61:GLN:HG3	1:D:62:LYS:O	2.11	0.51
1:C:78:LEU:HD22	1:C:81:LYS:HD2	1.93	0.51
1:D:136:GLU:HG2	1:D:141:SER:OG	2.11	0.51
1:B:206:ILE:CG2	1:B:207:THR:N	2.74	0.51
1:C:156:GLY:N	1:C:192:GLU:HG3	2.26	0.51
1:D:166:TYR:O	1:D:169:LEU:HB3	2.11	0.51
1:D:66:TRP:CD1	1:D:67:PRO:CA	2.94	0.51
1:A:115:ASN:OD1	1:A:205:ALA:HB2	2.11	0.50
1:C:130:ASN:HB2	1:C:133:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ASP:N	1:D:113:ASP:OD1	2.42	0.50
1:D:163:THR:HG22	1:D:167:LEU:HD12	1.92	0.50
1:B:211:ALA:HB2	1:B:222:PHE:HB3	1.94	0.50
1:C:75:HIS:HE1	1:C:177:VAL:HG11	1.77	0.50
1:B:104:ILE:HG21	1:B:108:ILE:HD13	1.92	0.50
1:D:106:LYS:O	1:D:109:LEU:HD12	2.12	0.50
1:C:83:GLN:O	1:C:87:GLU:HG3	2.12	0.50
1:D:66:TRP:CD1	1:D:66:TRP:C	2.85	0.50
1:A:61:GLN:OE1	1:A:64:LEU:HD11	2.10	0.50
1:D:213:LEU:O	1:D:215:PRO:HD3	2.12	0.50
1:D:95:ASN:CB	1:D:98:LEU:HD13	2.41	0.50
1:B:134:THR:HG21	1:B:189:TRP:NE1	2.23	0.50
1:A:145:ILE:CG2	1:A:149:GLU:HB3	2.42	0.49
1:C:57:HIS:N	1:C:57:HIS:CD2	2.80	0.49
1:B:104:ILE:CG2	1:B:108:ILE:HD13	2.42	0.49
1:C:70:THR:O	1:C:73:ARG:HG3	2.12	0.49
1:D:91:LEU:O	1:D:160:GLY:HA2	2.13	0.49
2:A:1232:BGC:C1	1:B:128:LYS:NZ	2.75	0.49
1:A:80:ILE:HG13	1:A:84:LEU:CD2	2.40	0.49
1:C:158:LEU:HB2	1:C:213:LEU:HD21	1.95	0.49
1:A:136:GLU:OE1	1:A:137:ARG:N	2.45	0.49
1:D:142:THR:HG21	1:D:176:TRP:CG	2.48	0.49
2:A:1232:BGC:C1	1:B:128:LYS:HZ3	2.20	0.48
1:D:110:PRO:HB2	1:D:116:GLY:HA2	1.95	0.48
1:C:135:TYR:CG	1:C:145:ILE:HD12	2.49	0.48
1:C:2:ARG:NH1	1:C:2:ARG:C	2.66	0.48
1:B:115:ASN:OD1	1:B:205:ALA:HB2	2.13	0.48
1:D:40:VAL:HG12	1:D:42:THR:HG22	1.95	0.48
1:A:163:THR:O	1:A:167:LEU:HD12	2.13	0.48
1:C:178:ASP:O	1:C:182:THR:HG23	2.13	0.48
1:C:72:LYS:HD2	1:C:75:HIS:ND1	2.29	0.48
1:A:50:GLU:HG2	1:A:50:GLU:O	2.12	0.48
1:B:97:ASN:ND2	1:B:228:ILE:CG2	2.77	0.48
1:A:40:VAL:O	1:A:42:THR:HG22	2.14	0.48
1:C:26:ARG:HG2	1:C:27:TYR:CD2	2.49	0.48
1:D:81:LYS:O	1:D:84:LEU:HB2	2.13	0.48
1:A:29:MET:HE2	1:A:108:ILE:CD1	2.44	0.48
1:A:70:THR:OG1	1:A:191:ASP:OD2	2.31	0.48
1:C:164:LYS:HB3	1:C:164:LYS:HE2	1.68	0.48
1:C:215:PRO:HB2	1:C:218:TRP:CG	2.49	0.48
1:D:95:ASN:HB3	1:D:98:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:PRO:HG2	1:B:194:LEU:HD11	1.96	0.47
1:C:208:LEU:HB3	1:C:212:TYR:CD2	2.49	0.47
1:B:225:ILE:HG22	1:B:226:ILE:HG13	1.95	0.47
1:A:192:GLU:HA	1:A:195:ILE:HG22	1.97	0.47
1:D:12:LYS:O	1:D:15:ILE:CG1	2.62	0.47
1:A:173:ILE:O	1:A:177:VAL:HG23	2.15	0.47
1:D:156:GLY:N	1:D:192:GLU:HG3	2.30	0.47
1:B:159:SER:HB2	1:B:166:TYR:HE1	1.79	0.47
1:B:72:LYS:HD3	1:B:75:HIS:ND1	2.30	0.47
1:C:36:ILE:N	1:C:36:ILE:HD12	2.30	0.47
1:D:99:LEU:HD22	1:D:229:ARG:HD3	1.97	0.47
1:A:125:PHE:CE2	2:A:1233:GAL:H61	2.46	0.47
1:B:141:SER:HB2	1:B:185:ILE:HG21	1.97	0.47
1:C:138:ARG:O	1:C:144:TYR:HB2	2.14	0.47
1:C:120:THR:HG23	1:C:208:LEU:HB2	1.97	0.46
1:D:173:ILE:O	1:D:177:VAL:HG23	2.15	0.46
1:C:52:ASN:N	1:C:52:ASN:OD1	2.47	0.46
1:D:114:SER:HB2	1:D:205:ALA:CB	2.46	0.46
1:D:234:PRO:HA	1:D:235:GLN:HA	1.42	0.46
1:B:7:TYR:CE1	1:B:96:ALA:HA	2.51	0.46
1:A:189:TRP:HB2	1:A:193:SER:OG	2.15	0.46
1:B:36:ILE:N	1:B:36:ILE:HD12	2.30	0.46
1:D:26:ARG:HB2	1:D:26:ARG:NH1	2.30	0.46
1:A:36:ILE:HG22	1:A:38:TYR:CE1	2.51	0.46
1:D:39:TYR:N	1:D:39:TYR:CD1	2.83	0.46
1:C:31:ASP:OD2	1:C:33:SER:OG	2.27	0.46
1:A:18:LYS:O	1:A:22:LEU:HG	2.16	0.45
1:B:72:LYS:CD	1:B:75:HIS:ND1	2.79	0.45
1:C:215:PRO:HB2	1:C:218:TRP:CD2	2.51	0.45
1:A:202:ASN:O	1:A:203:PRO:C	2.53	0.45
1:B:158:LEU:HD23	1:B:158:LEU:C	2.35	0.45
1:C:44:SER:HA	1:C:45:PRO:HD3	1.70	0.45
1:A:98:LEU:N	1:A:98:LEU:CD1	2.79	0.45
1:C:54:LYS:O	1:C:54:LYS:HG2	2.16	0.45
1:D:198:TYR:CD1	1:D:198:TYR:O	2.70	0.45
1:A:123:PRO:O	1:A:126:TYR:CD1	2.69	0.45
1:B:134:THR:O	1:B:134:THR:HG22	2.17	0.45
1:A:77:PHE:HZ	1:A:93:PHE:CD1	2.35	0.45
1:C:21:TYR:CE1	1:C:56:ILE:HD11	2.51	0.45
1:D:25:GLU:HA	1:D:25:GLU:OE1	2.16	0.45
1:C:71:LEU:HD13	1:C:190:HIS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:PHE:HD1	1:B:160:GLY:HA3	1.80	0.45
1:D:36:ILE:N	1:D:36:ILE:HD12	2.32	0.45
1:D:66:TRP:CZ2	1:D:190:HIS:CE1	3.05	0.45
1:D:72:LYS:O	1:D:73:ARG:C	2.55	0.45
1:D:29:MET:HE1	1:D:108:ILE:HG12	1.97	0.45
1:A:47:LEU:HB2	1:A:50:GLU:HB2	2.00	0.44
1:C:176:TRP:HE3	1:C:194:LEU:HD22	1.82	0.44
1:C:23:SER:HB2	1:C:100:PHE:HB2	1.99	0.44
1:C:5:ILE:HD11	1:C:28:PHE:CE2	2.52	0.44
1:D:74:PHE:HA	1:D:77:PHE:CD2	2.42	0.44
1:B:178:ASP:O	1:B:181:ALA:HB3	2.16	0.44
2:D:1232:BGC:O6	2:D:1234:FUC:H3	2.17	0.44
1:B:50:GLU:OE2	1:B:58:ARG:NH1	2.50	0.44
1:A:12:LYS:O	1:A:15:ILE:HG12	2.18	0.44
1:C:136:GLU:O	1:C:144:TYR:HA	2.18	0.44
1:D:154:TYR:OH	1:D:207:THR:OG1	2.21	0.44
1:B:130:ASN:HA	1:B:133:PHE:CE2	2.52	0.44
1:B:75:HIS:HD2	1:B:174:CYS:SG	2.38	0.44
1:B:189:TRP:HB2	1:B:193:SER:OG	2.17	0.44
1:B:32:GLN:HG2	1:B:32:GLN:H	1.66	0.44
1:C:59:ILE:O	1:C:60:LYS:C	2.55	0.44
1:C:2:ARG:HH22	1:C:88:THR:HG22	1.82	0.44
1:B:122:HIS:HA	1:B:155:ALA:HB2	1.99	0.44
2:A:1232:BGC:O1	1:B:128:LYS:CE	2.64	0.44
1:B:113:ASP:OD1	1:B:113:ASP:N	2.50	0.44
1:D:189:TRP:NE1	2:D:1233:GAL:H62	2.33	0.44
1:B:121:MET:HE1	1:B:126:TYR:HB2	1.99	0.44
1:D:214:TYR:HE2	1:D:222:PHE:O	2.00	0.44
1:D:84:LEU:O	1:D:88:THR:OG1	2.29	0.44
1:A:72:LYS:O	1:A:75:HIS:HB2	2.18	0.44
1:B:122:HIS:ND1	1:B:123:PRO:HD2	2.33	0.43
1:B:2:ARG:HG2	1:B:35:ILE:HD12	2.00	0.43
1:D:66:TRP:HA	1:D:67:PRO:C	2.38	0.43
1:C:116:GLY:O	1:C:161:GLY:HA3	2.18	0.43
1:C:28:PHE:CE1	1:C:29:MET:HG2	2.54	0.43
1:A:45:PRO:O	1:A:58:ARG:CZ	2.67	0.43
1:B:206:ILE:HG22	1:B:207:THR:N	2.32	0.43
1:B:77:PHE:HZ	1:B:93:PHE:CD2	2.36	0.43
1:A:75:HIS:CD2	1:A:174:CYS:SG	3.11	0.43
1:C:139:ASP:HA	1:C:144:TYR:CG	2.53	0.43
1:D:73:ARG:HB3	1:D:77:PHE:CE2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LYS:HD2	1:A:75:HIS:CE1	2.54	0.43
1:A:98:LEU:N	1:A:98:LEU:HD12	2.32	0.43
1:D:17:TRP:CZ2	1:D:21:TYR:HB2	2.53	0.43
1:D:53:ASN:OD1	1:D:54:LYS:N	2.52	0.43
1:A:169:LEU:HD23	1:A:169:LEU:C	2.39	0.43
1:C:219:LEU:HD23	1:C:219:LEU:HA	1.81	0.43
1:D:125:PHE:HZ	2:D:1233:GAL:HO6	1.63	0.43
1:A:189:TRP:HA	1:A:189:TRP:CE3	2.54	0.43
1:B:84:LEU:HA	1:B:84:LEU:HD12	1.89	0.43
1:B:80:ILE:HG13	1:B:84:LEU:HD22	1.99	0.43
1:B:229:ARG:CD	1:C:223:GLU:OE2	2.52	0.43
1:B:168:LYS:O	1:B:168:LYS:HD2	2.19	0.43
1:B:231:LYS:H	1:B:231:LYS:HG3	1.58	0.43
1:D:189:TRP:HA	1:D:189:TRP:CE3	2.53	0.43
1:A:167:LEU:O	1:A:170:CYS:N	2.51	0.43
1:A:188:ILE:H	1:A:188:ILE:HG12	1.54	0.43
1:A:10:THR:HG22	1:A:42:THR:HA	2.01	0.42
1:C:189:TRP:CD1	2:C:1233:GAL:H62	2.54	0.42
1:D:128:LYS:HB3	1:D:129:PRO:CD	2.49	0.42
1:B:111:PRO:HB2	1:B:114:SER:OG	2.19	0.42
1:B:189:TRP:CZ2	2:B:1233:GAL:H5	2.54	0.42
1:C:82:GLU:H	1:C:82:GLU:HG2	1.63	0.42
1:D:44:SER:HA	1:D:45:PRO:HD3	1.74	0.42
1:C:130:ASN:HB2	1:C:133:PHE:CD2	2.54	0.42
1:A:61:GLN:NE2	1:A:76:ILE:HG23	2.35	0.42
2:C:1232:BGC:HC	2:C:1233:GAL:HO6	1.62	0.42
1:B:214:TYR:CE1	1:C:221:PRO:HB3	2.54	0.42
1:A:225:ILE:N	1:A:225:ILE:HD13	2.33	0.42
1:A:110:PRO:HB3	1:A:116:GLY:CA	2.50	0.42
1:A:137:ARG:NH1	1:A:147:GLU:HA	2.34	0.42
1:C:125:PHE:CD1	1:C:125:PHE:N	2.87	0.42
1:D:128:LYS:CB	1:D:129:PRO:CD	2.98	0.42
1:D:26:ARG:NH1	1:D:26:ARG:CG	2.80	0.42
1:A:110:PRO:HB3	1:A:116:GLY:HA3	2.02	0.42
1:D:127:ASN:OD1	1:D:127:ASN:N	2.51	0.42
1:A:174:CYS:O	1:A:177:VAL:HB	2.20	0.42
1:B:139:ASP:N	1:B:139:ASP:OD1	2.52	0.42
1:B:9:CYS:HB2	1:B:14:ASP:HB3	2.01	0.42
1:B:12:LYS:O	1:B:15:ILE:HG13	2.19	0.42
1:A:130:ASN:HB2	1:A:133:PHE:CE2	2.55	0.41
1:B:53:ASN:O	1:B:54:LYS:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:PRO:HA	1:C:111:PRO:HD3	1.97	0.41
1:D:60:LYS:O	1:D:79:ARG:NH2	2.54	0.41
1:B:105:GLY:H	1:B:107:GLU:CD	2.20	0.41
1:B:166:TYR:O	1:B:169:LEU:HB3	2.20	0.41
2:C:1232:BGC:O3	2:C:1233:GAL:O6	2.27	0.41
1:A:231:LYS:H	1:A:231:LYS:CD	2.26	0.41
1:B:29:MET:CB	1:B:36:ILE:HD11	2.45	0.41
1:C:26:ARG:HG2	1:C:27:TYR:CZ	2.56	0.41
1:C:5:ILE:HD11	1:C:28:PHE:CD2	2.55	0.41
1:D:110:PRO:CB	1:D:116:GLY:HA2	2.50	0.41
1:C:95:ASN:N	1:C:98:LEU:HD22	2.36	0.41
1:D:213:LEU:HA	1:D:213:LEU:HD23	1.85	0.41
1:A:75:HIS:HD2	1:A:174:CYS:SG	2.43	0.41
1:C:233:LYS:HA	1:C:233:LYS:CE	2.46	0.41
1:A:2:ARG:NH1	1:A:86:ARG:O	2.53	0.41
1:B:233:LYS:HB2	1:B:234:PRO:CD	2.50	0.41
1:B:89:ASP:C	1:B:163:THR:OG1	2.59	0.41
1:C:72:LYS:HD2	1:C:75:HIS:CE1	2.56	0.41
1:D:17:TRP:O	1:D:18:LYS:C	2.58	0.41
1:D:46:LYS:HB3	1:D:46:LYS:HE2	1.82	0.41
1:A:3:ILE:HB	1:A:36:ILE:HG13	2.02	0.41
1:B:144:TYR:CE2	1:B:146:PRO:HG3	2.56	0.41
1:C:133:PHE:HD2	1:C:135:TYR:HH	1.68	0.41
1:C:66:TRP:CG	1:C:67:PRO:HA	2.56	0.41
1:A:215:PRO:HB2	1:A:218:TRP:CG	2.56	0.41
1:B:223:GLU:HB2	1:B:225:ILE:CD1	2.51	0.41
1:D:173:ILE:O	1:D:174:CYS:C	2.59	0.41
1:D:220:LEU:HD23	1:D:222:PHE:CE1	2.56	0.41
1:B:44:SER:OG	1:B:45:PRO:HD2	2.21	0.41
1:C:37:GLU:OE1	1:C:57:HIS:NE2	2.50	0.41
1:D:16:PHE:HB3	1:D:96:ALA:O	2.21	0.41
1:A:213:LEU:O	1:A:228:ILE:CD1	2.69	0.41
1:C:154:TYR:O	1:C:196:ASN:ND2	2.54	0.41
1:C:53:ASN:OD1	1:C:55:HIS:HB2	2.21	0.41
1:D:120:THR:HG23	1:D:208:LEU:HB2	2.03	0.41
1:A:74:PHE:CE1	1:A:173:ILE:HG21	2.56	0.40
1:A:192:GLU:O	1:A:195:ILE:HG22	2.21	0.40
1:B:135:TYR:O	1:B:137:ARG:HG2	2.21	0.40
1:C:156:GLY:H	1:C:192:GLU:HG3	1.87	0.40
1:D:66:TRP:CG	1:D:67:PRO:CA	3.00	0.40
1:A:110:PRO:CB	1:A:116:GLY:HA3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:LEU:O	1:D:160:GLY:CA	2.69	0.40
1:D:199:PHE:HA	1:D:199:PHE:HD1	1.75	0.40
1:D:22:LEU:HA	1:D:22:LEU:HD12	1.92	0.40
1:D:31:ASP:HB2	1:D:34:PHE:HD2	1.85	0.40
1:D:84:LEU:HG	1:D:91:LEU:HD11	2.03	0.40
1:B:57:HIS:CD2	1:B:57:HIS:N	2.89	0.40
1:B:136:GLU:HG2	1:B:141:SER:HB3	2.04	0.40
1:D:123:PRO:CA	1:D:210:PRO:HB3	2.51	0.40
1:D:70:THR:CG2	1:D:71:LEU:N	2.84	0.40
1:A:74:PHE:HD2	1:A:170:CYS:SG	2.45	0.40
1:D:80:ILE:O	1:D:81:LYS:C	2.60	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:12:LYS:NZ	1:D:200:LEU:O[2_645]	2.18	0.02

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	229/246 (93%)	225 (98%)	4 (2%)	0	100	100
1	B	233/246 (95%)	221 (95%)	11 (5%)	1 (0%)	38	78
1	C	231/246 (94%)	219 (95%)	12 (5%)	0	100	100
1	D	234/246 (95%)	223 (95%)	11 (5%)	0	100	100
All	All	927/984 (94%)	888 (96%)	38 (4%)	1 (0%)	55	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	234	PRO

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	208/221 (94%)	191 (92%)	17 (8%)	13	44
1	B	212/221 (96%)	190 (90%)	22 (10%)	8	31
1	C	210/221 (95%)	189 (90%)	21 (10%)	9	33
1	D	213/221 (96%)	192 (90%)	21 (10%)	9	34
All	All	843/884 (95%)	762 (90%)	81 (10%)	10	36

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	42	THR
1	A	52	ASN
1	A	54	LYS
1	A	84	LEU
1	A	102	SER
1	A	113	ASP
1	A	130	ASN
1	A	132	GLU
1	A	142	THR
1	A	151	ARG
1	A	159	SER
1	A	174	CYS
1	A	179	ARG
1	A	188	ILE
1	A	227	LEU
1	A	231	LYS
1	B	9	CYS
1	B	15	ILE
1	B	31	ASP
1	B	33	SER

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Mol	Chain	Res	Type
1	B	49	ASP
1	B	62	LYS
1	B	68	ASP
1	B	70	THR
1	B	84	LEU
1	B	86	ARG
1	B	98	LEU
1	B	112	SER
1	B	113	ASP
1	B	114	SER
1	B	130	ASN
1	B	142	THR
1	B	151	ARG
1	B	159	SER
1	B	180	ASP
1	B	188	ILE
1	B	219	LEU
1	B	220	LEU
1	C	2	ARG
1	C	9	CYS
1	C	52	ASN
1	C	57	HIS
1	C	64	LEU
1	C	82	GLU
1	C	98	LEU
1	C	101	THR
1	C	108	ILE
1	C	112	SER
1	C	113	ASP
1	C	130	ASN
1	C	139	ASP
1	C	142	THR
1	C	151	ARG
1	C	175	SER
1	C	180	ASP
1	C	188	ILE
1	C	196	ASN
1	C	227	LEU
1	C	231	LYS
1	D	15	ILE
1	D	26	ARG
1	D	29	MET

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Mol	Chain	Res	Type
1	D	42	THR
1	D	49	ASP
1	D	66	TRP
1	D	84	LEU
1	D	85	GLU
1	D	112	SER
1	D	113	ASP
1	D	126	TYR
1	D	139	ASP
1	D	142	THR
1	D	171	THR
1	D	174	CYS
1	D	180	ASP
1	D	188	ILE
1	D	199	PHE
1	D	222	PHE
1	D	231	LYS
1	D	236	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	75	HIS
1	B	75	HIS
1	B	130	ASN
1	C	75	HIS
1	C	196	ASN
1	D	75	HIS
1	D	190	HIS

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

12 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	BGC	A	1232	2	12,12,12	1.42	2 (16%)	17,17,17	1.49	3 (17%)
2	GAL	A	1233	2	11,11,12	2.03	1 (9%)	13,15,17	1.65	3 (23%)
2	FUC	A	1234	2	9,10,11	1.94	3 (33%)	13,14,16	2.35	4 (30%)
2	BGC	B	1232	2	12,12,12	1.37	2 (16%)	17,17,17	1.56	3 (17%)
2	GAL	B	1233	2	11,11,12	1.96	1 (9%)	13,15,17	1.95	3 (23%)
2	FUC	B	1234	2	9,10,11	2.25	4 (44%)	13,14,16	2.46	3 (23%)
2	BGC	C	1232	2	12,12,12	1.18	2 (16%)	17,17,17	2.04	5 (29%)
2	GAL	C	1233	2	11,11,12	1.95	1 (9%)	13,15,17	1.91	5 (38%)
2	FUC	C	1234	2	9,10,11	2.00	4 (44%)	13,14,16	2.67	5 (38%)
2	BGC	D	1232	2	12,12,12	1.60	2 (16%)	17,17,17	1.02	1 (5%)
2	GAL	D	1233	2	11,11,12	2.40	1 (9%)	13,15,17	2.15	3 (23%)
2	FUC	D	1234	2	9,10,11	2.39	4 (44%)	13,14,16	2.43	2 (15%)

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	BGC	A	1232	2	-	0/2/22/22	0/1/1/1
2	GAL	A	1233	2	-	0/2/19/22	0/1/1/1
2	FUC	A	1234	2	-	0/0/17/20	0/1/1/1
2	BGC	B	1232	2	-	0/2/22/22	0/1/1/1
2	GAL	B	1233	2	-	0/2/19/22	0/1/1/1
2	FUC	B	1234	2	-	0/0/17/20	0/1/1/1
2	BGC	C	1232	2	-	0/2/22/22	0/1/1/1
2	GAL	C	1233	2	-	0/2/19/22	0/1/1/1
2	FUC	C	1234	2	-	0/0/17/20	0/1/1/1
2	BGC	D	1232	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	D	1233	2	-	0/2/19/22	0/1/1/1
2	FUC	D	1234	2	-	0/0/17/20	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1232	BGC	O4-C4	2.27	1.48	1.43
2	C	1234	FUC	C4-C3	2.35	1.58	1.52
2	D	1234	FUC	C4-C3	2.56	1.58	1.52
2	B	1232	BGC	O4-C4	2.59	1.48	1.43
2	A	1232	BGC	O5-C1	2.61	1.47	1.43
2	B	1234	FUC	C4-C3	2.66	1.59	1.52
2	A	1234	FUC	C6-C5	2.67	1.57	1.51
2	B	1234	FUC	C6-C5	2.78	1.58	1.51
2	A	1234	FUC	O5-C1	2.83	1.48	1.43
2	C	1232	BGC	O5-C1	2.85	1.48	1.43
2	C	1234	FUC	C6-C5	2.87	1.58	1.51
2	C	1234	FUC	O5-C1	2.94	1.48	1.43
2	A	1234	FUC	C2-C3	3.04	1.56	1.52
2	D	1234	FUC	C6-C5	3.05	1.58	1.51
2	D	1234	FUC	O5-C1	3.05	1.48	1.43
2	B	1232	BGC	O5-C1	3.07	1.48	1.43
2	C	1234	FUC	C2-C3	3.13	1.56	1.52
2	B	1234	FUC	O5-C1	3.16	1.48	1.43
2	D	1232	BGC	O4-C4	3.38	1.50	1.43
2	A	1232	BGC	O4-C4	3.48	1.51	1.43
2	D	1232	BGC	O5-C1	3.48	1.49	1.43
2	B	1234	FUC	C2-C3	4.05	1.58	1.52
2	D	1234	FUC	C2-C3	4.41	1.58	1.52
2	B	1233	GAL	C2-C3	5.67	1.60	1.52
2	C	1233	GAL	C2-C3	5.85	1.60	1.52
2	A	1233	GAL	C2-C3	6.25	1.61	1.52
2	D	1233	GAL	C2-C3	7.32	1.62	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1233	GAL	C1-C2-C3	-6.48	101.43	109.65
2	C	1232	BGC	C1-C2-C3	-5.63	100.49	110.65
2	B	1233	GAL	C1-C2-C3	-4.62	103.80	109.65
2	A	1232	BGC	C1-C2-C3	-3.98	103.46	110.65
2	A	1233	GAL	C1-C2-C3	-3.93	104.67	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1232	BGC	O5-C1-C2	-3.54	104.16	110.04
2	C	1233	GAL	C1-C2-C3	-3.03	105.82	109.65
2	A	1232	BGC	O5-C1-C2	-2.82	105.36	110.04
2	C	1233	GAL	C2-C3-C4	-2.68	106.20	110.88
2	C	1233	GAL	C3-C4-C5	-2.62	105.60	110.22
2	C	1233	GAL	O2-C2-C1	-2.61	103.87	109.18
2	D	1233	GAL	O2-C2-C1	-2.60	103.88	109.18
2	A	1233	GAL	C3-C4-C5	-2.45	105.90	110.22
2	C	1234	FUC	O3-C3-C2	-2.43	105.60	110.02
2	C	1232	BGC	C4-C3-C2	-2.35	106.69	110.84
2	B	1233	GAL	O3-C3-C2	-2.27	105.89	110.02
2	A	1233	GAL	O6-C6-C5	-2.22	103.88	111.34
2	A	1234	FUC	O3-C3-C2	-2.20	106.03	110.02
2	C	1232	BGC	O4-C4-C5	-2.16	103.83	109.28
2	B	1232	BGC	O2-C2-C3	-2.15	105.67	110.36
2	B	1234	FUC	O5-C1-C2	2.05	114.00	110.79
2	C	1234	FUC	C1-O5-C5	2.06	116.95	112.39
2	A	1232	BGC	C3-C4-C5	2.08	113.88	110.22
2	D	1233	GAL	O2-C2-C3	2.10	114.30	110.17
2	D	1232	BGC	C1-O5-C5	2.19	117.34	113.39
2	B	1232	BGC	O2-C2-C1	2.28	114.50	109.75
2	B	1233	GAL	O5-C1-C2	2.48	114.67	110.79
2	A	1234	FUC	O2-C2-C1	2.49	114.24	109.18
2	C	1234	FUC	O5-C1-C2	2.55	114.79	110.79
2	C	1233	GAL	O5-C1-C2	3.04	115.56	110.79
2	C	1232	BGC	O2-C2-C1	3.14	116.28	109.75
2	C	1234	FUC	O2-C2-C3	3.47	116.99	110.17
2	A	1234	FUC	O2-C2-C3	3.52	117.08	110.17
2	D	1234	FUC	O2-C2-C3	3.79	117.62	110.17
2	B	1232	BGC	C3-C4-C5	4.05	117.35	110.22
2	B	1234	FUC	O2-C2-C3	4.08	118.19	110.17
2	A	1234	FUC	C1-C2-C3	6.22	117.53	109.65
2	B	1234	FUC	C1-C2-C3	6.64	118.07	109.65
2	D	1234	FUC	C1-C2-C3	7.08	118.62	109.65
2	C	1234	FUC	C1-C2-C3	7.40	119.03	109.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1232	BGC	5	0
2	A	1233	GAL	4	0
2	B	1233	GAL	2	0
2	C	1232	BGC	6	0
2	C	1233	GAL	4	0
2	D	1232	BGC	1	0
2	D	1233	GAL	2	0
2	D	1234	FUC	1	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	231/246 (93%)	2.85	150 (64%) 0 0	16, 28, 50, 67	1 (0%)
1	B	235/246 (95%)	2.71	144 (61%) 0 0	17, 34, 60, 74	0
1	C	233/246 (94%)	2.73	147 (63%) 0 0	18, 41, 63, 96	1 (0%)
1	D	236/246 (95%)	2.82	144 (61%) 0 0	20, 37, 60, 83	0
All	All	935/984 (95%)	2.78	585 (62%) 0 0	16, 34, 60, 96	2 (0%)

All (585) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	174	CYS	10.8
1	B	166	TYR	9.9
1	C	116	GLY	9.8
1	B	108	ILE	9.5
1	A	85	GLU	9.4
1	C	73	ARG	9.0
1	D	203	PRO	8.8
1	D	70	THR	8.8
1	D	72	LYS	8.5
1	A	98	LEU	8.5
1	D	31	ASP	8.3
1	C	88	THR	8.0
1	A	123	PRO	7.8
1	A	9	CYS	7.7
1	C	61	GLN	7.7
1	A	216	GLU	7.6
1	B	232	ASN	7.6
1	A	83	GLN	7.6
1	C	98	LEU	7.6
1	C	49	ASP	7.4
1	B	15	ILE	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	171	THR	7.1
1	A	166	TYR	7.0
1	D	52	ASN	7.0
1	D	78	LEU	6.9
1	D	35	ILE	6.9
1	A	33	SER	6.8
1	B	207	THR	6.8
1	A	11	GLY	6.8
1	C	171	THR	6.7
1	D	225	ILE	6.7
1	B	33	SER	6.7
1	A	124	GLY	6.6
1	A	75	HIS	6.6
1	D	102	SER	6.5
1	C	34	PHE	6.5
1	C	95	ASN	6.4
1	D	186	ILE	6.4
1	C	157	GLY	6.4
1	D	182	THR	6.4
1	A	121	MET	6.4
1	B	41	PHE	6.4
1	D	123	PRO	6.4
1	D	51	GLU	6.3
1	B	17	TRP	6.2
1	B	109	LEU	6.2
1	C	77	PHE	6.2
1	B	209	SER	6.2
1	D	143	ALA	6.1
1	A	219	LEU	6.0
1	D	178	ASP	6.0
1	A	82	GLU	5.9
1	A	15	ILE	5.9
1	A	50	GLU	5.9
1	A	222	PHE	5.9
1	B	101	THR	5.8
1	A	21	TYR	5.8
1	A	231	LYS	5.8
1	C	156	GLY	5.8
1	B	230	ASP	5.8
1	A	220	LEU	5.8
1	D	55	HIS	5.7
1	D	36	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	86	ARG	5.7
1	A	230	ASP	5.7
1	B	75	HIS	5.7
1	A	113	ASP	5.7
1	B	164	LYS	5.7
1	D	37	GLU	5.6
1	A	65	GLY	5.6
1	A	54	LYS	5.6
1	A	229	ARG	5.6
1	C	31	ASP	5.5
1	C	19	ASP	5.5
1	A	213	LEU	5.5
1	D	130	ASN	5.4
1	D	14	ASP	5.4
1	A	212	TYR	5.4
1	B	66	TRP	5.4
1	D	68	ASP	5.4
1	B	1	MET	5.4
1	A	184	HIS	5.4
1	D	202	ASN	5.3
1	B	187	PRO	5.3
1	B	148	GLY	5.3
1	C	186	ILE	5.3
1	C	112	SER	5.3
1	C	74	PHE	5.2
1	B	9	CYS	5.2
1	B	233	LYS	5.2
1	B	7	TYR	5.2
1	C	71	LEU	5.2
1	D	161	GLY	5.2
1	D	94	PHE	5.1
1	B	97	ASN	5.1
1	A	31	ASP	5.1
1	D	185	ILE	5.1
1	A	80	ILE	5.1
1	C	155	ALA	5.1
1	B	208	LEU	5.1
1	B	70	THR	5.0
1	A	69	ASN	5.0
1	D	84	LEU	5.0
1	D	165	ALA	5.0
1	D	226	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	46	LYS	4.9
1	A	4	GLY	4.9
1	D	45	PRO	4.9
1	C	26	ARG	4.9
1	A	221	PRO	4.8
1	D	46	LYS	4.8
1	B	224	PRO	4.8
1	C	66	TRP	4.8
1	C	86	ARG	4.8
1	B	100	PHE	4.7
1	A	84	LEU	4.7
1	B	106	LYS	4.7
1	D	69	ASN	4.7
1	B	136	GLU	4.7
1	B	53	ASN	4.7
1	B	40	VAL	4.7
1	B	58	ARG	4.7
1	B	184	HIS	4.7
1	C	1	MET	4.6
1	B	95	ASN	4.6
1	D	124	GLY	4.6
1	C	85	GLU	4.6
1	D	101	THR	4.6
1	A	109	LEU	4.6
1	A	168	LYS	4.5
1	A	185	ILE	4.5
1	B	78	LEU	4.5
1	A	12	LYS	4.5
1	C	62	LYS	4.5
1	C	164	LYS	4.5
1	C	138	ARG	4.4
1	C	149	GLU	4.4
1	C	2	ARG	4.4
1	D	218	TRP	4.4
1	D	13	TYR	4.4
1	A	64	LEU	4.4
1	B	85	GLU	4.4
1	D	160	GLY	4.4
1	B	10	THR	4.4
1	D	188	ILE	4.4
1	B	235	GLN	4.4
1	D	30	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	219	LEU	4.4
1	D	97	ASN	4.4
1	C	24	ALA	4.4
1	D	23	SER	4.3
1	C	89	ASP	4.3
1	B	115	ASN	4.3
1	B	163	THR	4.3
1	B	112	SER	4.3
1	D	220	LEU	4.3
1	B	222	PHE	4.3
1	C	231	LYS	4.3
1	C	70	THR	4.3
1	A	228	ILE	4.2
1	A	165	ALA	4.2
1	D	180	ASP	4.2
1	C	91	LEU	4.2
1	D	232	ASN	4.2
1	B	18	LYS	4.2
1	B	45	PRO	4.2
1	A	60	LYS	4.2
1	D	201	ASP	4.1
1	B	46	LYS	4.1
1	D	73	ARG	4.1
1	B	44	SER	4.1
1	C	170	CYS	4.1
1	A	108	ILE	4.1
1	C	50	GLU	4.1
1	D	177	VAL	4.1
1	D	12	LYS	4.1
1	D	157	GLY	4.1
1	C	32	GLN	4.1
1	A	217	GLY	4.1
1	B	182	THR	4.1
1	D	184	HIS	4.1
1	D	172	THR	4.1
1	D	108	ILE	4.1
1	A	215	PRO	4.1
1	D	190	HIS	4.0
1	A	207	THR	4.0
1	A	48	TYR	4.0
1	B	131	SER	4.0
1	C	166	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	65	GLY	4.0
1	D	217	GLY	4.0
1	D	132	GLU	4.0
1	A	53	ASN	4.0
1	D	175	SER	4.0
1	A	202	ASN	4.0
1	C	198	TYR	4.0
1	A	45	PRO	3.9
1	B	68	ASP	3.9
1	D	95	ASN	3.9
1	B	171	THR	3.9
1	A	191	ASP	3.9
1	A	198	TYR	3.9
1	C	14	ASP	3.9
1	D	214	TYR	3.9
1	D	129	PRO	3.9
1	A	1	MET	3.9
1	A	196	ASN	3.9
1	A	192	GLU	3.9
1	B	111	PRO	3.9
1	A	3	ILE	3.9
1	A	32	GLN	3.9
1	D	208	LEU	3.9
1	A	47	LEU	3.9
1	C	210	PRO	3.9
1	C	42	THR	3.8
1	D	11	GLY	3.8
1	B	196	ASN	3.8
1	C	10	THR	3.8
1	C	167	LEU	3.8
1	B	60	LYS	3.8
1	C	189	TRP	3.8
1	A	132	GLU	3.8
1	A	10	THR	3.8
1	D	162	CYS	3.8
1	D	199	PHE	3.8
1	D	189	TRP	3.7
1	A	204	PRO	3.7
1	B	221	PRO	3.7
1	C	33	SER	3.7
1	C	35	ILE	3.7
1	C	84	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	221	PRO	3.7
1	B	140	ALA	3.7
1	D	223	GLU	3.7
1	D	62	LYS	3.6
1	C	55	HIS	3.6
1	C	136	GLU	3.6
1	D	127	ASN	3.6
1	D	224	PRO	3.6
1	A	131	SER	3.6
1	B	98	LEU	3.6
1	B	48	TYR	3.6
1	A	79	ARG	3.6
1	A	39	TYR	3.6
1	B	59	ILE	3.6
1	C	211	ALA	3.6
1	C	67	PRO	3.6
1	B	189	TRP	3.5
1	B	13	TYR	3.5
1	B	105	GLY	3.5
1	C	64	LEU	3.5
1	C	38	TYR	3.5
1	D	167	LEU	3.5
1	C	7	TYR	3.5
1	B	19	ASP	3.5
1	B	30	GLN	3.5
1	C	48	TYR	3.5
1	D	77	PHE	3.5
1	D	8	ILE	3.5
1	D	141	SER	3.5
1	A	99	LEU	3.4
1	C	115	ASN	3.4
1	B	142	THR	3.4
1	C	122	HIS	3.4
1	C	226	ILE	3.4
1	B	153	TYR	3.4
1	A	68	ASP	3.4
1	D	156	GLY	3.4
1	B	149	GLU	3.4
1	D	209	SER	3.4
1	C	187	PRO	3.4
1	D	29	MET	3.4
1	A	151	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	14	ASP	3.4
1	D	28	PHE	3.4
1	B	6	LEU	3.3
1	D	121	MET	3.3
1	B	12	LYS	3.3
1	A	88	THR	3.3
1	C	126	TYR	3.3
1	A	41	PHE	3.3
1	A	189	TRP	3.3
1	B	137	ARG	3.3
1	D	60	LYS	3.3
1	B	36	ILE	3.3
1	C	68	ASP	3.3
1	A	214	TYR	3.3
1	B	139	ASP	3.3
1	B	62	LYS	3.3
1	A	97	ASN	3.2
1	A	49	ASP	3.2
1	B	122	HIS	3.2
1	C	223	GLU	3.2
1	C	83	GLN	3.2
1	D	187	PRO	3.2
1	D	114	SER	3.2
1	B	154	TYR	3.2
1	D	235	GLN	3.2
1	D	207	THR	3.2
1	A	25	GLU	3.2
1	D	112	SER	3.2
1	C	137	ARG	3.2
1	C	140	ALA	3.2
1	A	17	TRP	3.1
1	D	26	ARG	3.1
1	A	110	PRO	3.1
1	B	86	ARG	3.1
1	C	185	ILE	3.1
1	D	181	ALA	3.1
1	D	193	SER	3.1
1	A	160	GLY	3.1
1	D	145	ILE	3.1
1	D	153	TYR	3.1
1	D	179	ARG	3.1
1	A	116	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	109	LEU	3.1
1	B	210	PRO	3.1
1	D	90	TYR	3.1
1	B	203	PRO	3.1
1	B	215	PRO	3.1
1	A	13	TYR	3.1
1	B	147	GLU	3.1
1	A	96	ALA	3.1
1	A	145	ILE	3.1
1	B	71	LEU	3.1
1	A	112	SER	3.1
1	C	139	ASP	3.1
1	A	59	ILE	3.1
1	D	17	TRP	3.1
1	D	120	THR	3.1
1	A	58	ARG	3.1
1	B	150	GLY	3.0
1	B	34	PHE	3.0
1	B	123	PRO	3.0
1	C	111	PRO	3.0
1	C	72	LYS	3.0
1	B	217	GLY	3.0
1	A	208	LEU	3.0
1	C	63	ASN	3.0
1	A	2	ARG	3.0
1	D	67	PRO	3.0
1	A	150	GLY	3.0
1	A	8	ILE	3.0
1	B	125	PHE	3.0
1	C	123	PRO	3.0
1	D	168	LYS	2.9
1	C	13	TYR	2.9
1	A	63	ASN	2.9
1	C	69	ASN	2.9
1	C	208	LEU	2.9
1	C	20	PHE	2.9
1	C	183	ASN	2.9
1	C	213	LEU	2.9
1	C	222	PHE	2.9
1	C	106	LYS	2.9
1	B	94	PHE	2.9
1	A	134	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	197	LYS	2.9
1	A	93	PHE	2.9
1	A	193	SER	2.9
1	C	99	LEU	2.9
1	C	206	ILE	2.9
1	C	220	LEU	2.9
1	C	133	PHE	2.9
1	B	31	ASP	2.9
1	B	92	PHE	2.8
1	B	197	LYS	2.8
1	D	155	ALA	2.8
1	C	181	ALA	2.8
1	A	101	THR	2.8
1	D	75	HIS	2.8
1	C	232	ASN	2.8
1	B	3	ILE	2.8
1	A	26	ARG	2.8
1	C	147	GLU	2.8
1	A	129	PRO	2.8
1	C	158	LEU	2.8
1	A	174	CYS	2.8
1	C	9	CYS	2.8
1	C	196	ASN	2.8
1	B	51	GLU	2.8
1	B	52	ASN	2.8
1	C	27	TYR	2.8
1	A	22	LEU	2.7
1	B	199	PHE	2.7
1	B	212	TYR	2.7
1	D	183	ASN	2.7
1	C	132	GLU	2.7
1	C	128	LYS	2.7
1	C	107	GLU	2.7
1	B	195	ILE	2.7
1	D	71	LEU	2.7
1	C	113	ASP	2.7
1	A	86	ARG	2.7
1	C	154	TYR	2.7
1	A	170	CYS	2.7
1	D	47	LEU	2.7
1	D	227	LEU	2.7
1	C	148	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	120	THR	2.7
1	A	16	PHE	2.7
1	D	34	PHE	2.7
1	B	165	ALA	2.7
1	A	141	SER	2.7
1	A	70	THR	2.7
1	C	230	ASP	2.7
1	A	159	SER	2.7
1	A	218	TRP	2.7
1	D	166	TYR	2.7
1	C	12	LYS	2.7
1	A	92	PHE	2.7
1	C	29	MET	2.7
1	C	15	ILE	2.6
1	C	205	ALA	2.6
1	A	172	THR	2.6
1	C	207	THR	2.6
1	D	142	THR	2.6
1	B	146	PRO	2.6
1	C	90	TYR	2.6
1	A	195	ILE	2.6
1	A	211	ALA	2.6
1	C	153	TYR	2.6
1	B	83	GLN	2.6
1	C	152	TYR	2.6
1	A	105	GLY	2.6
1	A	223	GLU	2.6
1	D	6	LEU	2.6
1	B	47	LEU	2.6
1	D	113	ASP	2.6
1	C	110	PRO	2.6
1	C	44	SER	2.6
1	D	25	GLU	2.6
1	B	72	LYS	2.6
1	D	87	GLU	2.6
1	C	165	ALA	2.6
1	C	87	GLU	2.6
1	C	117	LEU	2.6
1	B	25	GLU	2.5
1	C	43	ASP	2.5
1	B	234	PRO	2.5
1	C	121	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	103	PRO	2.5
1	B	5	ILE	2.5
1	B	204	PRO	2.5
1	C	100	PHE	2.5
1	A	30	GLN	2.5
1	B	107	GLU	2.5
1	B	172	THR	2.5
1	C	131	SER	2.5
1	A	115	ASN	2.5
1	A	122	HIS	2.5
1	A	130	ASN	2.5
1	B	132	GLU	2.5
1	D	15	ILE	2.5
1	C	75	HIS	2.5
1	B	229	ARG	2.5
1	A	143	ALA	2.5
1	D	195	ILE	2.5
1	B	213	LEU	2.5
1	D	219	LEU	2.5
1	D	221	PRO	2.5
1	B	152	TYR	2.5
1	D	33	SER	2.5
1	C	96	ALA	2.5
1	D	48	TYR	2.5
1	D	99	LEU	2.4
1	A	206	ILE	2.4
1	B	32	GLN	2.4
1	D	131	SER	2.4
1	A	52	ASN	2.4
1	C	215	PRO	2.4
1	A	127	ASN	2.4
1	B	201	ASP	2.4
1	D	151	ARG	2.4
1	A	34	PHE	2.4
1	A	126	TYR	2.4
1	C	53	ASN	2.4
1	B	102	SER	2.4
1	B	223	GLU	2.4
1	B	141	SER	2.4
1	C	25	GLU	2.4
1	A	18	LYS	2.4
1	D	65	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	214	TYR	2.4
1	A	181	ALA	2.4
1	B	69	ASN	2.4
1	B	214	TYR	2.4
1	A	136	GLU	2.3
1	D	80	ILE	2.3
1	A	72	LYS	2.3
1	B	61	GLN	2.3
1	B	27	TYR	2.3
1	A	200	LEU	2.3
1	C	45	PRO	2.3
1	C	150	GLY	2.3
1	A	104	ILE	2.3
1	A	182	THR	2.3
1	B	87	GLU	2.3
1	D	64	LEU	2.3
1	D	18	LYS	2.3
1	B	11	GLY	2.3
1	D	140	ALA	2.3
1	D	16	PHE	2.3
1	D	20	PHE	2.3
1	B	80	ILE	2.3
1	B	128	LYS	2.3
1	A	24	ALA	2.3
1	B	185	ILE	2.3
1	C	16	PHE	2.3
1	C	182	THR	2.3
1	D	138	ARG	2.3
1	C	114	SER	2.3
1	A	36	ILE	2.3
1	B	67	PRO	2.3
1	D	154	TYR	2.2
1	D	125	PHE	2.2
1	D	57	HIS	2.2
1	A	57	HIS	2.2
1	B	226	ILE	2.2
1	C	201	ASP	2.2
1	A	153	TYR	2.2
1	C	41	PHE	2.2
1	A	224	PRO	2.2
1	B	55	HIS	2.2
1	D	1	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	204	PRO	2.2
1	C	102	SER	2.2
1	D	194	LEU	2.2
1	B	77	PHE	2.2
1	D	63	ASN	2.2
1	B	161	GLY	2.2
1	B	227	LEU	2.2
1	A	28	PHE	2.2
1	C	101	THR	2.2
1	D	192	GLU	2.2
1	D	200	LEU	2.2
1	A	149	GLU	2.2
1	D	173	ILE	2.2
1	B	160	GLY	2.2
1	D	137	ARG	2.2
1	A	194	LEU	2.1
1	B	186	ILE	2.1
1	B	200	LEU	2.1
1	A	155	ALA	2.1
1	C	209	SER	2.1
1	B	220	LEU	2.1
1	B	194	LEU	2.1
1	D	171	THR	2.1
1	C	105	GLY	2.1
1	A	66	TRP	2.1
1	D	206	ILE	2.1
1	B	116	GLY	2.1
1	D	100	PHE	2.1
1	B	29	MET	2.1
1	C	124	GLY	2.1
1	A	161	GLY	2.1
1	C	151	ARG	2.1
1	A	227	LEU	2.1
1	B	183	ASN	2.1
1	C	216	GLU	2.1
1	D	197	LYS	2.1
1	C	23	SER	2.1
1	A	190	HIS	2.1
1	B	162	CYS	2.1
1	A	94	PHE	2.1
1	C	225	ILE	2.1
1	B	218	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	93	PHE	2.0
1	A	162	CYS	2.0
1	C	134	THR	2.0
1	C	169	LEU	2.0
1	A	199	PHE	2.0
1	A	35	ILE	2.0
1	A	210	PRO	2.0
1	A	23	SER	2.0
1	B	170	CYS	2.0
1	C	52	ASN	2.0
1	D	96	ALA	2.0
1	D	135	TYR	2.0
1	A	146	PRO	2.0
1	C	224	PRO	2.0
1	B	121	MET	2.0
1	C	191	ASP	2.0
1	D	93	PHE	2.0
1	B	84	LEU	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	BGC	D	1232	12/12	0.30	0.84	2.46	42,53,59,60	0
2	GAL	D	1233	11/12	0.28	0.66	1.74	44,47,58,62	0
2	GAL	B	1233	11/12	0.31	0.69	1.49	27,29,30,32	0
2	BGC	B	1232	12/12	0.34	0.59	0.82	26,29,33,33	0
2	BGC	A	1232	12/12	0.44	0.57	0.28	25,28,32,36	0
2	FUC	B	1234	10/11	0.51	0.52	0.16	26,35,41,41	0
2	FUC	D	1234	10/11	0.54	0.57	0.07	48,54,62,64	0
2	GAL	A	1233	11/12	0.44	0.44	-0.81	21,23,26,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FUC	C	1234	10/11	0.55	0.41	-0.95	23,31,36,41	0
2	BGC	C	1232	12/12	0.45	0.38	-1.14	28,33,39,46	0
2	FUC	A	1234	10/11	0.51	0.37	-1.58	13,19,30,33	0
2	GAL	C	1233	11/12	0.55	0.33	-2.54	31,33,39,43	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.