



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:09 PM GMT

PDB ID : 2GAM
Title : X-ray crystal structure of murine leukocyte-type Core 2 b1,6-N-acetylglucosaminyltransferase(C2GnT-L) in complex with Galb1,3GalNAc
Authors : Pak, J.E.; Rini, J.M.
Deposited on : 2006-03-09
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

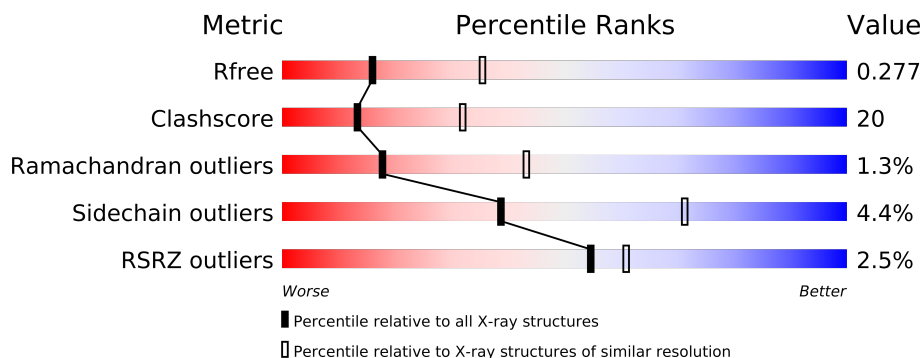
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	391	
1	B	391	
1	C	391	
1	D	391	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12285 atoms, of which 0 are hydrogen and 0 are deuterium.

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 beta-1,6-N-acetylglucosaminyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2966	1903	505	537	21			
1	B	359	Total	C	N	O	S	0	0	0
			2919	1871	499	528	21			
1	C	374	Total	C	N	O	S	0	0	0
			3050	1958	522	549	21			
1	D	368	Total	C	N	O	S	0	0	0
			2994	1921	510	542	21			

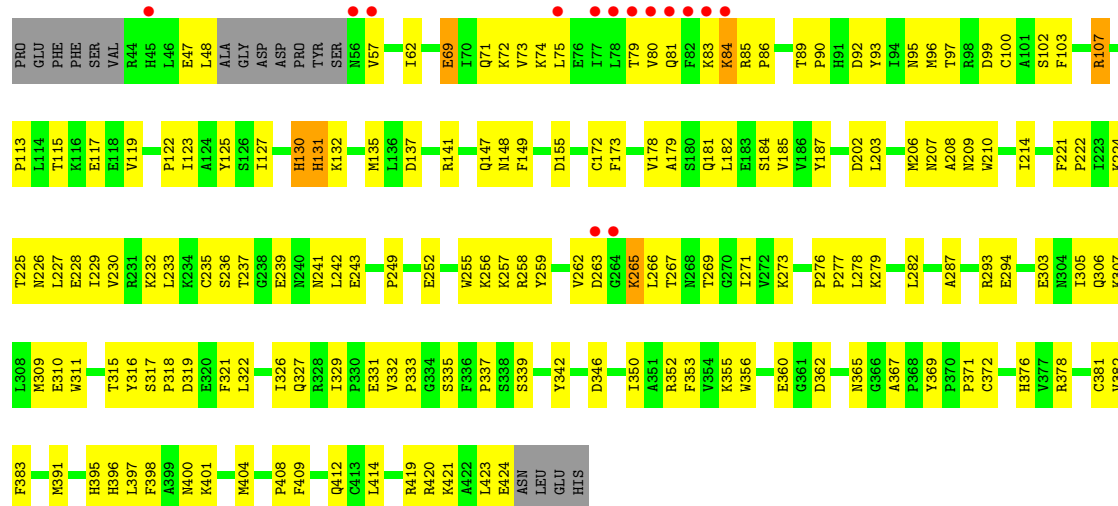
- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			26	14	1	11		
2	B	2	Total	C	N	O	0	0
			26	14	1	11		
2	C	2	Total	C	N	O	0	0
			26	14	1	11		
2	D	2	Total	C	N	O	0	0
			26	14	1	11		

- Molecule 3 is water.

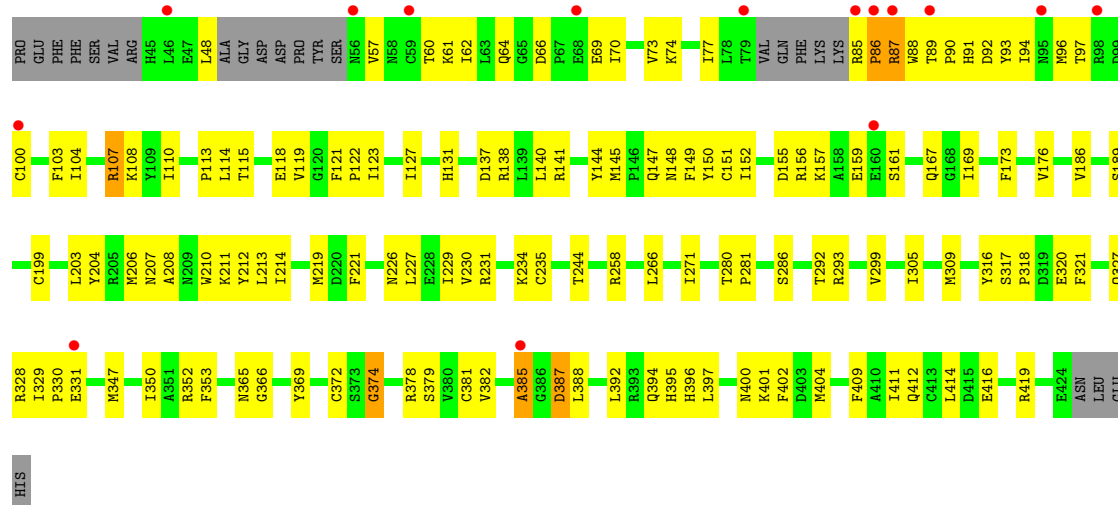
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	65	Total	O	0	0
			65	65		
3	B	85	Total	O	0	0
			85	85		
3	C	58	Total	O	0	0
			58	58		
3	D	44	Total	O	0	0
			44	44		

Chain C:



- Molecule 1: beta-1,6-N-acetylglucosaminyltransferase

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.50Å 80.58Å 102.33Å 73.61° 76.26° 64.56°	Depositor
Resolution (Å)	20.00 – 2.70 19.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.70) 97.2 (19.98-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.274 0.229 , 0.277	Depositor DCC
R_{free} test set	6847 reflections (11.26%)	DCC
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 67650 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12285	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, NGA

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	0.39	0/3042	0.61	0/4125
1	B	0.41	0/2995	0.63	0/4060
1	C	0.39	0/3128	0.61	0/4238
1	D	0.37	0/3070	0.57	0/4161
All	All	0.39	0/12235	0.61	0/16584

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the

Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2966	0	2937	103	0
1	B	2919	0	2882	115	0
1	C	3050	0	3028	149	0
1	D	2994	0	2962	117	0
2	A	26	0	24	0	0
2	B	26	0	24	1	0
2	C	26	0	24	0	0
2	D	26	0	24	1	0
3	A	65	0	0	4	0
3	B	85	0	0	3	0
3	C	58	0	0	2	0
3	D	44	0	0	3	0
All	All	12285	0	11905	476	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (476) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:151:CYS:HG	1:D:199:CYS:HG	1.10	0.96
1:D:372:CYS:HG	1:D:381:CYS:HG	0.98	0.95
1:A:372:CYS:HG	1:A:381:CYS:HG	1.10	0.95
1:C:79:THR:HG22	1:C:81:GLN:H	1.33	0.93
1:D:123:ILE:HD11	1:D:230:VAL:HG22	1.51	0.92
1:C:89:THR:HG22	1:C:92:ASP:OD2	1.70	0.92
1:C:372:CYS:HG	1:C:381:CYS:HG	1.08	0.91
1:C:276:PRO:HG2	1:C:282:LEU:HD11	1.57	0.86
1:D:122:PRO:HB2	1:D:210:TRP:HA	1.60	0.83
1:A:151:CYS:HG	1:A:199:CYS:HG	0.87	0.82
1:A:330:PRO:O	1:A:331:GLU:HB2	1.79	0.81
1:C:235:CYS:HG	1:D:235:CYS:HG	0.90	0.81
1:C:122:PRO:HB2	1:C:210:TRP:HA	1.62	0.81
1:A:138:ARG:NH2	1:A:412:GLN:HE22	1.79	0.80
1:B:114:LEU:HD13	1:B:145:MET:HE1	1.62	0.79
1:C:404:MET:O	1:C:408:PRO:HG3	1.83	0.79
1:A:99:ASP:OD2	1:A:102:SER:HB2	1.83	0.78
1:C:258:ARG:HG2	1:C:273:LYS:HG2	1.65	0.77
1:A:208:ALA:HA	1:A:293:ARG:NE	2.01	0.75
1:D:61:LYS:HB2	1:D:69:GLU:HG3	1.68	0.74
1:A:66:ASP:O	1:A:70:ILE:HG12	1.88	0.74
1:B:305:ILE:HD12	1:B:326:ILE:HD12	1.70	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:408:PRO:O	1:B:412:GLN:HG3	1.87	0.74
1:C:305:ILE:HD12	1:C:326:ILE:HD12	1.70	0.74
1:B:175:ASN:HD22	1:B:175:ASN:H	1.35	0.74
1:C:269:THR:OG1	1:C:271:ILE:HG12	1.89	0.73
1:C:83:LYS:HG3	1:C:84:LYS:HD3	1.72	0.72
1:C:135:MET:HE2	1:C:404:MET:HG3	1.70	0.71
1:B:123:ILE:H	1:B:148:ASN:ND2	1.89	0.71
1:B:132:LYS:HD2	1:B:135:MET:HE2	1.72	0.71
1:A:163:LEU:O	1:A:167:GLN:HG3	1.91	0.70
1:A:70:ILE:O	1:A:73:VAL:HG22	1.91	0.69
1:C:276:PRO:HG3	1:C:311:TRP:CZ2	2.27	0.69
1:B:92:ASP:O	1:B:96:MET:HG3	1.92	0.69
1:B:66:ASP:O	1:B:70:ILE:HG12	1.93	0.69
1:C:276:PRO:HG3	1:C:311:TRP:CH2	2.29	0.68
1:C:85:ARG:HG2	1:C:85:ARG:HH11	1.57	0.68
1:D:388:LEU:HD11	1:D:414:LEU:HD13	1.77	0.67
1:D:113:PRO:HB3	1:D:119:VAL:HG22	1.76	0.67
1:B:302:ASN:O	1:B:306:GLN:HG2	1.95	0.67
1:A:378:ARG:HH11	1:A:378:ARG:HB2	1.58	0.66
1:A:122:PRO:HB2	1:A:210:TRP:HA	1.77	0.66
1:B:151:CYS:HG	1:B:199:CYS:HG	0.68	0.66
1:C:259:TYR:HB3	1:C:266:LEU:HD11	1.78	0.65
1:B:276:PRO:HG3	1:B:311:TRP:CH2	2.32	0.65
1:C:47:GLU:OE2	1:C:420:ARG:HG3	1.97	0.65
1:B:70:ILE:HD12	1:B:386:GLY:HA2	1.78	0.64
1:D:73:VAL:O	1:D:77:ILE:HG13	1.97	0.64
1:A:92:ASP:HB3	1:A:96:MET:HE2	1.78	0.64
1:D:88:TRP:HZ3	1:D:96:MET:SD	2.22	0.63
1:B:156:ARG:HH11	1:B:156:ARG:HG3	1.64	0.63
1:A:138:ARG:NH2	1:A:412:GLN:NE2	2.45	0.63
1:C:322:LEU:O	1:C:326:ILE:HG12	1.99	0.63
1:C:103:PHE:CE1	1:C:107:ARG:HG3	2.33	0.63
1:D:204:TYR:HA	1:D:210:TRP:HZ2	1.64	0.63
1:A:231:ARG:O	1:A:235:CYS:SG	2.57	0.63
1:A:98:ARG:HG2	1:A:98:ARG:HH11	1.64	0.63
1:C:107:ARG:HD3	1:C:137:ASP:OD1	1.99	0.63
1:D:121:PHE:CD2	1:D:230:VAL:HG13	2.34	0.62
1:C:57:VAL:HA	1:C:72:LYS:NZ	2.14	0.62
1:B:93:TYR:HA	1:B:96:MET:HE3	1.81	0.62
1:D:123:ILE:CG2	1:D:214:ILE:HD13	2.30	0.61
1:B:175:ASN:ND2	1:B:175:ASN:H	1.98	0.61
1:C:294:GLU:N	1:C:294:GLU:OE1	2.33	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:48:LEU:HD23	1:D:108:LYS:HE2	1.82	0.61
1:B:132:LYS:HD2	1:B:135:MET:CE	2.31	0.61
1:C:131:HIS:CE1	1:C:132:LYS:HG3	2.36	0.61
1:A:372:CYS:CB	1:A:381:CYS:HG	2.12	0.60
1:D:122:PRO:HD2	1:D:211:LYS:HE2	1.83	0.60
1:A:92:ASP:O	1:A:96:MET:HG3	2.00	0.60
1:A:121:PHE:CD2	1:A:230:VAL:HG13	2.36	0.60
1:C:360:GLU:OE1	1:C:376:HIS:HE1	1.85	0.60
1:C:408:PRO:O	1:C:412:GLN:HB2	2.01	0.60
1:D:91:HIS:HA	1:D:94:ILE:CD1	2.32	0.60
1:C:225:THR:OG1	1:C:228:GLU:HG3	2.02	0.60
1:A:123:ILE:H	1:A:148:ASN:ND2	1.99	0.60
1:A:366:GLY:O	1:B:339:SER:HB2	2.01	0.60
1:C:372:CYS:CB	1:C:381:CYS:HG	2.15	0.59
1:D:61:LYS:CB	1:D:69:GLU:HG3	2.32	0.59
1:B:131:HIS:CE1	1:B:132:LYS:HG3	2.36	0.59
1:B:214:ILE:HD12	1:B:290:VAL:HG22	1.83	0.59
1:D:70:ILE:HG23	1:D:385:ALA:HB1	1.85	0.59
1:A:365:ASN:OD1	1:B:279:LYS:HE2	2.03	0.59
1:B:61:LYS:HB2	1:B:69:GLU:HG3	1.84	0.59
1:B:123:ILE:H	1:B:148:ASN:HD22	1.49	0.59
1:C:69:GLU:O	1:C:72:LYS:HB3	2.02	0.59
1:A:404:MET:O	1:A:408:PRO:HG3	2.03	0.59
1:A:139:LEU:HD13	1:A:220:ASP:O	2.03	0.59
1:D:404:MET:CG	1:D:411:ILE:HD12	2.33	0.59
1:C:229:ILE:O	1:C:233:LEU:HG	2.01	0.58
1:C:113:PRO:HB3	1:C:119:VAL:HG22	1.85	0.58
1:C:265:LYS:HZ2	1:C:265:LYS:HB3	1.68	0.58
1:C:100:CYS:HG	1:C:172:CYS:HG	1.16	0.58
1:C:331:GLU:CD	1:C:331:GLU:H	2.07	0.58
1:D:226:ASN:O	1:D:230:VAL:HG23	2.04	0.58
1:C:149:PHE:CD1	1:C:206:MET:HE3	2.39	0.58
1:A:404:MET:SD	1:A:411:ILE:HD12	2.43	0.58
1:D:48:LEU:HD11	1:D:419:ARG:HE	1.68	0.58
1:C:255:TRP:CZ3	1:C:256:LYS:HE3	2.38	0.58
1:B:135:MET:HE1	1:B:219:MET:HG2	1.85	0.58
1:A:100:CYS:HG	1:A:172:CYS:HG	1.51	0.57
1:D:85:ARG:HH11	1:D:85:ARG:HG3	1.68	0.57
1:C:135:MET:CE	1:C:404:MET:H	2.18	0.57
1:B:293:ARG:HG2	1:B:293:ARG:HH11	1.69	0.57
1:A:107:ARG:HD3	1:A:137:ASP:OD1	2.05	0.57
1:B:175:ASN:HD22	1:B:175:ASN:N	1.94	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:220:ASP:OD1	1:A:400:ASN:HB2	2.05	0.57
1:D:374:GLY:HA3	1:D:382:VAL:O	2.05	0.57
1:C:99:ASP:OD2	1:C:102:SER:HB2	2.05	0.57
1:B:293:ARG:NH1	1:B:293:ARG:HG2	2.20	0.56
1:C:400:ASN:OD1	1:C:401:LYS:HB3	2.05	0.56
1:A:202:ASP:O	1:A:206:MET:HB2	2.05	0.56
1:C:265:LYS:NZ	1:C:265:LYS:HB3	2.20	0.56
1:D:86:PRO:O	1:D:87:ARG:HB2	2.06	0.56
1:B:152:ILE:N	1:B:152:ILE:HD12	2.21	0.56
1:A:181:GLN:HB3	1:A:198:ASN:ND2	2.21	0.56
1:D:286:SER:HA	1:D:320:GLU:HG2	1.87	0.56
1:C:107:ARG:HE	1:C:107:ARG:HA	1.70	0.56
1:B:310:GLU:HA	1:B:313:GLN:HG3	1.88	0.56
1:C:79:THR:CG2	1:C:81:GLN:HB3	2.36	0.56
1:A:190:TRP:HA	1:A:318:PRO:HG3	1.87	0.56
1:D:123:ILE:HG23	1:D:214:ILE:HD13	1.88	0.56
1:C:276:PRO:CG	1:C:282:LEU:HD11	2.32	0.56
1:D:48:LEU:HD23	1:D:108:LYS:CE	2.35	0.56
1:B:372:CYS:HB3	1:B:376:HIS:HE1	1.71	0.55
1:A:232:LYS:HE2	1:A:395:HIS:O	2.07	0.55
1:C:262:VAL:O	1:C:263:ASP:HB2	2.06	0.55
1:B:87:ARG:NH2	1:B:404:MET:HB3	2.21	0.55
1:B:327:GLN:O	1:B:335:SER:HB2	2.07	0.55
1:B:241:ASN:CG	1:B:350:ILE:HG12	2.27	0.55
1:B:378:ARG:NH1	1:B:378:ARG:HB2	2.21	0.55
1:C:356:TRP:O	1:C:360:GLU:HG3	2.06	0.55
1:D:151:CYS:HG	1:D:199:CYS:CB	2.20	0.55
1:D:203:LEU:HA	1:D:206:MET:HG2	1.89	0.55
1:D:214:ILE:HD12	1:D:214:ILE:N	2.22	0.55
1:D:115:THR:OG1	1:D:118:GLU:HG3	2.06	0.55
1:A:388:LEU:HD22	1:A:414:LEU:HD13	1.89	0.55
1:A:235:CYS:CB	1:B:235:CYS:HG	2.18	0.55
1:B:330:PRO:HB2	1:B:331:GLU:OE2	2.07	0.55
1:B:360:GLU:OE2	1:B:372:CYS:N	2.39	0.54
1:A:310:GLU:HA	1:A:313:GLN:HG3	1.88	0.54
1:B:214:ILE:HD11	1:B:290:VAL:HG13	1.90	0.54
1:D:404:MET:HG2	1:D:411:ILE:HD12	1.88	0.54
1:C:83:LYS:HG3	1:C:84:LYS:CD	2.37	0.54
1:C:92:ASP:O	1:C:96:MET:HG3	2.08	0.54
1:C:135:MET:HE2	1:C:404:MET:CG	2.38	0.54
1:B:156:ARG:NH1	1:B:156:ARG:HG3	2.22	0.54
1:A:373:SER:HB2	1:A:387:ASP:OD1	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:213:LEU:C	1:D:214:ILE:HD12	2.28	0.54
1:C:48:LEU:HD13	1:C:141:ARG:NH2	2.22	0.54
1:C:327:GLN:NE2	1:C:335:SER:HA	2.23	0.54
1:C:339:SER:HB2	1:D:366:GLY:O	2.07	0.54
1:B:214:ILE:CD1	1:B:290:VAL:HG13	2.37	0.54
1:A:318:PRO:O	1:A:322:LEU:HB2	2.06	0.54
1:C:131:HIS:ND1	1:C:132:LYS:HG3	2.23	0.54
1:C:62:ILE:HD13	1:C:69:GLU:HB3	1.88	0.54
1:A:411:ILE:O	1:A:415:ASP:HB2	2.08	0.53
1:A:138:ARG:HH22	1:A:412:GLN:NE2	2.04	0.53
1:A:352:ARG:NH1	1:A:352:ARG:HB2	2.23	0.53
1:C:265:LYS:O	1:C:267:THR:HG23	2.08	0.53
1:D:123:ILE:H	1:D:148:ASN:ND2	2.06	0.53
1:C:85:ARG:NH1	1:C:85:ARG:HG2	2.22	0.53
1:C:226:ASN:O	1:C:230:VAL:HG23	2.09	0.53
1:B:258:ARG:HG3	1:B:314:ASP:OD2	2.09	0.53
1:D:88:TRP:CZ3	1:D:96:MET:SD	3.01	0.53
1:B:159:GLU:O	1:B:162:PHE:N	2.42	0.53
1:A:60:THR:O	1:A:64:GLN:HG3	2.08	0.53
1:D:140:LEU:O	1:D:144:TYR:HB2	2.09	0.53
1:D:62:ILE:HD12	1:D:70:ILE:HD13	1.90	0.53
1:B:87:ARG:HH22	1:B:404:MET:HB3	1.73	0.52
1:A:90:PRO:O	1:A:94:ILE:HG13	2.09	0.52
1:C:318:PRO:HA	1:C:321:PHE:CE2	2.44	0.52
1:C:187:TYR:HE1	1:C:378:ARG:NH1	2.07	0.52
1:A:208:ALA:HA	1:A:293:ARG:CZ	2.39	0.52
1:A:93:TYR:HA	1:A:96:MET:HE3	1.91	0.52
1:B:62:ILE:CD1	1:B:69:GLU:HB3	2.39	0.52
1:A:352:ARG:HB2	1:A:352:ARG:HH11	1.75	0.52
1:A:86:PRO:O	1:A:87:ARG:HD2	2.10	0.52
1:D:69:GLU:O	1:D:73:VAL:HG23	2.10	0.52
1:A:241:ASN:CG	1:A:350:ILE:HG12	2.31	0.52
1:A:278:LEU:HD21	1:A:308:LEU:HD22	1.92	0.52
1:D:212:TYR:CZ	1:D:292:THR:HG22	2.45	0.52
1:C:273:LYS:HB3	1:C:273:LYS:NZ	2.25	0.52
1:C:203:LEU:HD23	1:C:206:MET:HE2	1.92	0.52
1:C:147:GLN:N	1:C:147:GLN:OE1	2.32	0.52
1:A:293:ARG:HG2	1:A:293:ARG:HH11	1.74	0.51
1:C:187:TYR:CE1	1:C:378:ARG:NH1	2.78	0.51
1:C:262:VAL:O	1:C:265:LYS:HD2	2.11	0.51
1:A:374:GLY:HA3	1:A:382:VAL:O	2.11	0.51
1:A:299:VAL:HG12	1:A:305:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:79:THR:HG22	1:C:81:GLN:N	2.13	0.51
1:C:57:VAL:HA	1:C:72:LYS:HZ3	1.75	0.51
1:C:225:THR:O	1:C:229:ILE:HG12	2.09	0.51
1:A:273:LYS:HB2	3:A:503:HOH:O	2.10	0.51
1:D:186:VAL:O	1:D:189:SER:HB3	2.10	0.51
1:B:411:ILE:O	1:B:415:ASP:HB2	2.11	0.51
1:A:208:ALA:HA	1:A:293:ARG:HE	1.74	0.51
1:D:48:LEU:CD2	1:D:108:LYS:HE2	2.41	0.51
1:C:202:ASP:O	1:C:206:MET:HB2	2.11	0.51
1:A:104:ILE:HG21	1:A:111:VAL:HG11	1.92	0.51
1:D:280:THR:HG23	1:D:281:PRO:HD2	1.93	0.51
1:B:62:ILE:HD11	1:B:69:GLU:HB3	1.93	0.50
1:A:260:ALA:HA	3:A:564:HOH:O	2.10	0.50
1:C:135:MET:HE2	1:C:404:MET:CB	2.41	0.50
1:B:85:ARG:HH12	1:B:87:ARG:HH21	1.60	0.50
1:B:114:LEU:HD22	1:B:145:MET:HE2	1.93	0.50
1:C:259:TYR:HB3	1:C:266:LEU:CD1	2.40	0.50
1:C:409:PHE:HA	1:C:412:GLN:HB3	1.94	0.50
1:A:85:ARG:HB3	1:A:85:ARG:HH11	1.76	0.50
1:C:79:THR:HG21	1:C:81:GLN:HB3	1.92	0.50
1:C:278:LEU:HD21	1:C:329:ILE:HD11	1.93	0.50
1:B:372:CYS:HB3	1:B:376:HIS:CE1	2.47	0.50
1:C:222:PRO:HB3	1:C:398:PHE:CE2	2.46	0.50
1:B:99:ASP:OD2	1:B:102:SER:HB3	2.11	0.50
1:C:123:ILE:H	1:C:148:ASN:ND2	2.10	0.50
1:D:121:PHE:CD1	1:D:211:LYS:HG3	2.47	0.49
1:C:423:LEU:O	1:C:424:GLU:HG3	2.12	0.49
1:B:222:PRO:HB3	1:B:398:PHE:CE2	2.47	0.49
1:A:244:THR:HG23	1:A:244:THR:O	2.12	0.49
1:C:115:THR:O	1:C:119:VAL:HG23	2.12	0.49
1:D:107:ARG:HD3	1:D:137:ASP:OD2	2.13	0.49
1:D:48:LEU:CD1	1:D:419:ARG:HE	2.25	0.49
1:D:286:SER:HB2	3:D:523:HOH:O	2.12	0.49
1:D:229:ILE:HG23	1:D:397:LEU:HD13	1.94	0.49
1:B:346:ASP:OD2	2:B:503:GAL:H4	2.12	0.49
1:A:304:ASN:H	1:A:304:ASN:HD22	1.60	0.49
1:D:221:PHE:HB2	1:D:402:PHE:CD2	2.48	0.49
1:A:331:GLU:HA	1:A:331:GLU:OE1	2.12	0.49
1:B:378:ARG:HH11	1:B:378:ARG:CB	2.25	0.49
1:B:155:ASP:OD1	1:B:185:VAL:HB	2.13	0.49
1:C:355:LYS:HB2	1:C:381:CYS:HB3	1.94	0.49
1:B:208:ALA:HA	1:B:293:ARG:NE	2.28	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:80:VAL:HA	1:C:83:LYS:CD	2.42	0.48
1:D:73:VAL:HG13	1:D:409:PHE:CD1	2.48	0.48
1:B:257:LYS:HG3	1:B:268:ASN:HD21	1.78	0.48
1:B:103:PHE:HD2	1:B:104:ILE:HD12	1.78	0.48
1:C:360:GLU:HB3	1:C:371:PRO:HA	1.95	0.48
1:A:378:ARG:O	1:A:379:SER:HB2	2.13	0.48
1:D:91:HIS:HA	1:D:94:ILE:HD12	1.95	0.48
1:C:382:VAL:HG22	1:C:401:LYS:CG	2.43	0.48
1:B:113:PRO:HB3	1:B:119:VAL:CG2	2.44	0.48
1:B:315:THR:O	1:B:318:PRO:HD3	2.14	0.48
1:D:121:PHE:CE1	1:D:211:LYS:HG3	2.48	0.48
1:D:70:ILE:HG23	1:D:385:ALA:CB	2.43	0.48
1:C:173:PHE:HA	3:C:538:HOH:O	2.13	0.48
1:B:321:PHE:C	1:B:321:PHE:CD1	2.86	0.48
1:A:423:LEU:O	1:A:424:GLU:HB3	2.14	0.48
1:B:167:GLN:HE21	1:B:167:GLN:CA	2.26	0.48
1:D:320:GLU:OE2	2:D:508:NGA:H62	2.14	0.48
1:D:400:ASN:HA	1:D:401:LYS:HA	1.53	0.48
1:C:232:LYS:HA	1:C:235:CYS:SG	2.53	0.48
1:B:66:ASP:OD2	1:B:68:GLU:HB2	2.13	0.48
1:D:318:PRO:HA	1:D:321:PHE:CE2	2.49	0.48
1:B:360:GLU:HB3	1:B:371:PRO:HA	1.96	0.48
1:C:315:THR:OG1	1:C:318:PRO:HB3	2.14	0.48
1:D:400:ASN:CG	1:D:401:LYS:HB3	2.34	0.48
1:C:243:GLU:HG3	1:C:346:ASP:N	2.29	0.48
1:B:368:PRO:HB2	1:B:369:TYR:CD2	2.49	0.48
1:C:93:TYR:O	1:C:97:THR:HG23	2.13	0.47
1:A:283:PHE:O	1:A:321:PHE:HA	2.14	0.47
1:D:62:ILE:CD1	1:D:70:ILE:HD13	2.44	0.47
1:A:61:LYS:HD3	1:A:66:ASP:OD1	2.14	0.47
1:B:114:LEU:HD13	1:B:145:MET:CE	2.39	0.47
1:D:97:THR:HG21	1:D:169:ILE:N	2.29	0.47
1:D:91:HIS:HA	1:D:94:ILE:HG13	1.96	0.47
1:D:404:MET:HG3	1:D:411:ILE:HD12	1.96	0.47
1:D:219:MET:HB3	1:D:401:LYS:HB2	1.97	0.47
1:B:265:LYS:HD3	3:B:537:HOH:O	2.14	0.47
1:D:173:PHE:HB2	1:D:176:VAL:HB	1.96	0.47
1:C:181:GLN:O	1:C:182:LEU:HD23	2.14	0.47
1:D:66:ASP:O	1:D:70:ILE:HG12	2.15	0.47
1:C:278:LEU:HD11	1:C:329:ILE:CD1	2.45	0.47
1:A:138:ARG:HH22	1:A:412:GLN:CD	2.17	0.46
1:D:93:TYR:CD2	1:D:169:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:135:MET:HE2	1:C:404:MET:HB2	1.97	0.46
1:C:130:HIS:CD2	1:C:131:HIS:ND1	2.83	0.46
1:A:109:TYR:O	1:A:111:VAL:HG13	2.15	0.46
1:D:227:LEU:O	1:D:231:ARG:HG3	2.15	0.46
1:D:327:GLN:O	1:D:328:ARG:HD2	2.15	0.46
1:C:135:MET:HE2	1:C:404:MET:H	1.79	0.46
1:B:221:PHE:CD2	1:B:414:LEU:HD23	2.51	0.46
1:C:155:ASP:OD2	1:C:185:VAL:HB	2.15	0.46
1:C:73:VAL:HG23	1:C:74:LYS:N	2.30	0.46
1:B:298:TYR:CZ	1:B:302:ASN:ND2	2.83	0.46
1:C:329:ILE:HB	1:C:332:VAL:HG23	1.98	0.46
1:D:57:VAL:HG11	1:D:73:VAL:CG2	2.46	0.46
1:D:113:PRO:CB	1:D:119:VAL:HG22	2.44	0.46
1:C:353:PHE:CD2	1:C:391:MET:HG3	2.51	0.46
1:A:361:GLY:O	1:A:371:PRO:HD3	2.15	0.46
1:D:147:GLN:N	1:D:147:GLN:OE1	2.38	0.46
1:D:107:ARG:HE	1:D:107:ARG:HA	1.80	0.46
1:C:329:ILE:HB	1:C:332:VAL:CG2	2.46	0.46
1:B:107:ARG:NH2	1:B:141:ARG:HH12	2.13	0.46
1:D:89:THR:N	1:D:92:ASP:OD2	2.45	0.46
1:A:407:ASP:OD1	1:A:409:PHE:HB2	2.15	0.46
1:B:128:VAL:HG13	3:B:515:HOH:O	2.15	0.46
1:A:157:LYS:HD2	1:A:184:SER:OG	2.15	0.46
1:C:360:GLU:OE2	1:C:372:CYS:N	2.48	0.46
1:C:257:LYS:O	1:C:273:LYS:HD2	2.16	0.46
1:A:85:ARG:HB3	1:A:85:ARG:NH1	2.30	0.46
1:A:140:LEU:O	1:A:144:TYR:HB2	2.16	0.46
1:B:138:ARG:HH22	1:B:412:GLN:HG2	1.81	0.46
1:C:259:TYR:CE2	1:C:316:TYR:HB2	2.51	0.46
1:B:237:THR:HG22	1:B:237:THR:O	2.16	0.46
1:B:131:HIS:ND1	1:B:132:LYS:CG	2.79	0.45
1:C:221:PHE:HD2	1:C:414:LEU:HD23	1.81	0.45
1:B:348:ASN:O	1:B:395:HIS:HE1	1.99	0.45
1:B:174:ASP:N	1:B:174:ASP:OD1	2.49	0.45
1:B:212:TYR:CE2	1:B:292:THR:HG22	2.51	0.45
1:C:258:ARG:CG	1:C:273:LYS:HG2	2.40	0.45
1:B:123:ILE:HG22	1:B:124:ALA:N	2.31	0.45
1:C:382:VAL:HG22	1:C:401:LYS:HG3	1.97	0.45
1:D:208:ALA:HA	1:D:293:ARG:CZ	2.46	0.45
1:B:378:ARG:HH11	1:B:378:ARG:HB2	1.82	0.45
1:B:115:THR:OG1	1:B:118:GLU:HG3	2.16	0.45
1:D:57:VAL:HG13	1:D:69:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:326:ILE:HA	1:A:329:ILE:HD12	1.97	0.45
1:B:175:ASN:ND2	1:B:175:ASN:N	2.60	0.45
1:C:228:GLU:OE2	1:C:421:LYS:HE2	2.16	0.45
1:C:71:GLN:O	1:C:75:LEU:HG	2.17	0.45
1:C:273:LYS:HB3	1:C:273:LYS:HZ3	1.81	0.45
1:A:388:LEU:CD2	1:A:414:LEU:HD13	2.46	0.45
1:D:293:ARG:HG2	1:D:293:ARG:HH11	1.82	0.45
1:C:207:ASN:OD1	1:C:209:ASN:N	2.38	0.45
1:C:255:TRP:CH2	1:C:256:LYS:HE3	2.51	0.45
1:C:221:PHE:CG	1:C:222:PRO:HD2	2.52	0.45
1:B:60:THR:O	1:B:64:GLN:HG3	2.16	0.45
1:C:279:LYS:HA	1:C:279:LYS:HD2	1.87	0.45
1:D:353:PHE:HB2	1:D:396:HIS:CG	2.52	0.45
1:D:159:GLU:HA	1:D:159:GLU:OE1	2.17	0.45
1:C:259:TYR:CB	1:C:266:LEU:HD11	2.45	0.45
1:B:276:PRO:HG3	1:B:311:TRP:CZ2	2.52	0.45
1:B:327:GLN:NE2	1:B:335:SER:HA	2.31	0.45
1:D:100:CYS:O	1:D:104:ILE:HD13	2.17	0.45
1:B:100:CYS:O	1:B:104:ILE:HD13	2.17	0.45
1:D:103:PHE:CE1	1:D:107:ARG:HG3	2.52	0.44
1:D:60:THR:O	1:D:64:GLN:HG3	2.17	0.44
1:B:241:ASN:ND2	1:B:350:ILE:HG12	2.32	0.44
1:A:106:THR:O	1:A:108:LYS:HG3	2.16	0.44
1:A:219:MET:HG3	3:A:562:HOH:O	2.17	0.44
1:C:214:ILE:N	1:C:214:ILE:HD12	2.33	0.44
1:B:346:ASP:O	1:B:396:HIS:HE1	2.01	0.44
1:C:362:ASP:C	1:C:367:ALA:HB3	2.38	0.44
1:A:252:GLU:O	1:A:256:LYS:HG2	2.18	0.44
1:B:288:TYR:CG	1:B:352:ARG:NH2	2.85	0.44
1:C:409:PHE:HA	1:C:412:GLN:CB	2.47	0.44
1:B:167:GLN:HA	1:B:167:GLN:NE2	2.33	0.44
1:A:321:PHE:CD1	1:A:321:PHE:C	2.91	0.44
1:B:112:GLU:O	1:B:113:PRO:C	2.56	0.44
1:C:346:ASP:O	1:C:396:HIS:HE1	2.01	0.44
1:A:372:CYS:HB2	1:A:381:CYS:SG	2.58	0.44
1:C:208:ALA:HA	1:C:293:ARG:NE	2.33	0.44
1:A:59:CYS:SG	1:A:413:CYS:SG	3.03	0.44
1:A:219:MET:CE	1:A:401:LYS:HD3	2.48	0.44
1:B:103:PHE:CE1	1:B:107:ARG:HG3	2.53	0.44
1:D:90:PRO:HG3	3:D:532:HOH:O	2.18	0.44
1:D:155:ASP:OD2	1:D:157:LYS:HB2	2.17	0.43
1:B:420:ARG:O	1:B:424:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:150:TYR:N	1:D:150:TYR:CD2	2.85	0.43
1:A:200:MET:O	1:A:204:TYR:HB2	2.17	0.43
1:B:98:ARG:HD3	1:B:98:ARG:HA	1.72	0.43
1:A:258:ARG:HG2	1:A:314:ASP:OD2	2.18	0.43
1:A:131:HIS:HA	1:A:162:PHE:CE1	2.52	0.43
1:D:388:LEU:CD1	1:D:414:LEU:HD13	2.48	0.43
1:C:48:LEU:HG	1:C:419:ARG:HG2	2.00	0.43
1:C:321:PHE:C	1:C:321:PHE:CD1	2.92	0.43
1:D:221:PHE:HB3	1:D:402:PHE:CE2	2.53	0.43
1:D:387:ASP:HA	3:D:531:HOH:O	2.18	0.43
1:A:377:VAL:HG12	1:A:378:ARG:NH1	2.34	0.43
1:D:107:ARG:O	1:D:108:LYS:HB2	2.18	0.43
1:A:256:LYS:O	1:A:273:LYS:HG2	2.19	0.43
1:A:248:PRO:HA	1:A:249:PRO:HD3	1.87	0.43
1:D:258:ARG:HB3	1:D:271:ILE:HB	2.00	0.43
1:B:121:PHE:CE1	1:B:211:LYS:HG3	2.54	0.43
1:D:123:ILE:HD13	1:D:226:ASN:HD21	1.84	0.43
1:C:400:ASN:HA	1:C:401:LYS:HA	1.68	0.43
1:A:85:ARG:O	1:A:87:ARG:HG2	2.19	0.43
1:D:299:VAL:HG13	1:D:305:ILE:HG21	2.01	0.43
1:C:369:TYR:HE2	3:C:510:HOH:O	2.01	0.43
1:C:130:HIS:O	1:C:131:HIS:HB3	2.17	0.43
1:A:87:ARG:HH11	1:A:87:ARG:HG3	1.84	0.43
1:C:305:ILE:O	1:C:309:MET:HG3	2.18	0.43
1:B:178:VAL:O	1:B:179:ALA:C	2.57	0.43
1:B:304:ASN:ND2	3:B:588:HOH:O	2.51	0.43
1:D:145:MET:HG3	1:D:147:GLN:OE1	2.18	0.43
1:D:74:LYS:HA	1:D:77:ILE:HD12	2.01	0.42
1:A:247:MET:HA	1:A:248:PRO:HD3	1.90	0.42
1:D:230:VAL:O	1:D:234:LYS:HG3	2.20	0.42
1:A:248:PRO:HD3	1:A:284:SER:HB2	2.00	0.42
1:B:244:THR:O	1:B:244:THR:HG23	2.19	0.42
1:D:378:ARG:O	1:D:379:SER:HB2	2.20	0.42
1:B:136:LEU:HD23	1:B:166:VAL:HG22	2.02	0.42
1:B:328:ARG:HD2	1:B:336:PHE:HB2	2.01	0.42
1:C:276:PRO:HA	1:C:277:PRO:HD3	1.85	0.42
1:D:74:LYS:O	1:D:77:ILE:HB	2.19	0.42
1:C:332:VAL:HA	1:C:333:PRO:HD3	1.86	0.42
1:D:392:LEU:HA	1:D:392:LEU:HD23	1.93	0.42
1:C:241:ASN:ND2	1:C:350:ILE:HG13	2.34	0.42
1:D:151:CYS:SG	1:D:199:CYS:HA	2.60	0.42
1:B:130:HIS:O	1:B:131:HIS:HB3	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:355:LYS:HB2	1:B:381:CYS:HB3	2.00	0.42
1:C:117:GLU:OE1	1:C:227:LEU:HD11	2.19	0.42
1:B:400:ASN:HA	1:B:401:LYS:HA	1.64	0.42
1:D:416:GLU:O	1:D:419:ARG:HB3	2.18	0.42
1:D:208:ALA:HA	1:D:293:ARG:NE	2.35	0.42
1:C:208:ALA:HA	1:C:293:ARG:CZ	2.49	0.42
1:C:307:LYS:HA	1:C:310:GLU:CD	2.39	0.42
1:B:203:LEU:HA	1:B:206:MET:HG2	2.02	0.42
1:A:223:ILE:HG22	1:A:391:MET:HE3	2.02	0.42
1:A:298:TYR:CE1	1:A:332:VAL:HG22	2.54	0.42
1:B:417:HIS:CE1	1:B:421:LYS:HD2	2.55	0.42
1:B:131:HIS:ND1	1:B:132:LYS:HG3	2.34	0.42
1:B:221:PHE:CD2	1:B:222:PRO:HD2	2.55	0.42
1:C:178:VAL:O	1:C:179:ALA:C	2.58	0.42
1:A:266:LEU:HD12	1:A:266:LEU:HA	1.85	0.42
1:D:127:ILE:HD12	1:D:152:ILE:CD1	2.50	0.42
1:C:79:THR:HG22	1:C:81:GLN:HB3	2.02	0.42
1:A:226:ASN:O	1:A:230:VAL:HG23	2.20	0.42
1:C:252:GLU:O	1:C:256:LYS:HG2	2.19	0.42
1:D:85:ARG:NH1	1:D:85:ARG:HG3	2.35	0.42
1:B:160:GLU:HG3	1:B:161:SER:N	2.35	0.42
1:B:123:ILE:N	1:B:123:ILE:HD12	2.35	0.42
1:C:236:SER:O	1:C:239:GLU:HB2	2.20	0.42
1:C:125:TYR:HB3	1:C:127:ILE:HD11	2.02	0.42
1:B:212:TYR:CD1	1:B:233:LEU:HD22	2.55	0.41
1:A:113:PRO:HG3	1:A:146:PRO:HG2	2.02	0.41
1:C:360:GLU:HG2	1:C:369:TYR:CE1	2.55	0.41
1:A:408:PRO:O	1:A:412:GLN:HB2	2.19	0.41
1:B:61:LYS:CB	1:B:69:GLU:HG3	2.49	0.41
1:C:249:PRO:HA	1:C:252:GLU:OE1	2.19	0.41
1:B:204:TYR:CE1	1:B:293:ARG:NH1	2.88	0.41
1:D:138:ARG:HH22	1:D:412:GLN:HB2	1.86	0.41
1:D:330:PRO:O	1:D:331:GLU:HB2	2.20	0.41
1:A:347:MET:CE	1:B:342:TYR:OH	2.68	0.41
1:A:293:ARG:HG2	1:A:293:ARG:NH1	2.35	0.41
1:D:85:ARG:O	1:D:85:ARG:HG3	2.21	0.41
1:D:244:THR:HG23	1:D:244:THR:O	2.20	0.41
1:A:130:HIS:HD2	3:A:510:HOH:O	2.04	0.41
1:C:89:THR:OG1	1:C:90:PRO:HD2	2.20	0.41
1:B:110:ILE:HG21	1:B:114:LEU:HD11	2.02	0.41
1:C:303:GLU:H	1:C:303:GLU:CD	2.23	0.41
1:C:113:PRO:HB3	1:C:119:VAL:CG2	2.48	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:362:ASP:O	1:C:367:ALA:HB3	2.21	0.41
1:B:242:LEU:N	1:B:242:LEU:HD23	2.35	0.41
1:A:400:ASN:HA	1:A:401:LYS:HA	1.56	0.41
1:D:397:LEU:N	1:D:397:LEU:HD23	2.35	0.41
1:A:304:ASN:ND2	1:A:304:ASN:H	2.18	0.41
1:A:223:ILE:CG2	1:A:391:MET:HE3	2.50	0.41
1:D:57:VAL:HG11	1:D:73:VAL:HG22	2.02	0.41
1:D:91:HIS:HA	1:D:94:ILE:CG1	2.50	0.41
1:D:321:PHE:C	1:D:321:PHE:CD1	2.93	0.41
1:C:350:ILE:HD13	1:C:397:LEU:HG	2.03	0.41
1:D:280:THR:HB	1:D:329:ILE:CD1	2.51	0.41
1:C:278:LEU:HD11	1:C:329:ILE:HD11	2.03	0.41
1:B:222:PRO:O	1:B:418:LEU:HD11	2.20	0.41
1:D:350:ILE:O	1:D:397:LEU:HG	2.21	0.41
1:C:241:ASN:CG	1:C:350:ILE:HG13	2.41	0.41
1:C:337:PRO:HD2	1:C:342:TYR:CG	2.56	0.41
1:A:212:TYR:CZ	1:A:292:THR:HG22	2.56	0.41
1:D:149:PHE:CZ	1:D:207:ASN:ND2	2.89	0.41
1:D:266:LEU:HD23	1:D:316:TYR:CD1	2.56	0.41
1:A:257:LYS:HG3	1:A:268:ASN:HD21	1.86	0.41
1:C:79:THR:HG22	1:C:80:VAL:N	2.36	0.41
1:C:257:LYS:HA	1:C:271:ILE:O	2.20	0.41
1:C:342:TYR:OH	1:D:347:MET:CE	2.69	0.41
1:C:57:VAL:HA	1:C:72:LYS:HZ1	1.86	0.40
1:D:107:ARG:O	1:D:141:ARG:HD2	2.21	0.40
1:C:224:LYS:HB2	1:C:229:ILE:CD1	2.51	0.40
1:D:293:ARG:HG2	1:D:293:ARG:NH1	2.36	0.40
1:C:287:ALA:HB2	1:C:319:ASP:OD2	2.20	0.40
1:C:80:VAL:HG13	1:C:83:LYS:HD2	2.03	0.40
1:A:342:TYR:HE1	1:B:368:PRO:HA	1.86	0.40
1:D:394:GLN:HB3	1:D:396:HIS:HD2	1.86	0.40
1:B:121:PHE:CG	1:B:230:VAL:HG13	2.57	0.40
1:C:331:GLU:CD	1:C:331:GLU:N	2.75	0.40
1:C:318:PRO:HA	1:C:321:PHE:CD2	2.56	0.40

There are no symmetry-related clashes.

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	361/391 (92%)	341 (94%)	20 (6%)	0	100	100
1	B	355/391 (91%)	321 (90%)	27 (8%)	7 (2%)	11	28
1	C	370/391 (95%)	339 (92%)	27 (7%)	4 (1%)	21	49
1	D	362/391 (93%)	322 (89%)	32 (9%)	8 (2%)	10	25
All	All	1448/1564 (93%)	1323 (91%)	106 (7%)	19 (1%)	18	43

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	383	PHE
1	D	87	ARG
1	D	114	LEU
1	C	365	ASN
1	D	86	PRO
1	D	365	ASN
1	C	237	THR
1	D	385	ALA
1	B	383	PHE
1	D	387	ASP
1	B	156	ARG
1	B	351	ALA
1	B	113	PRO
1	B	179	ALA
1	B	365	ASN
1	C	86	PRO
1	D	110	ILE
1	D	374	GLY
1	B	73	VAL

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	327/351 (93%)	308 (94%)	19 (6%)	28	57
1	B	321/351 (92%)	305 (95%)	16 (5%)	34	66
1	C	336/351 (96%)	323 (96%)	13 (4%)	43	76
1	D	330/351 (94%)	320 (97%)	10 (3%)	53	84
All	All	1314/1404 (94%)	1256 (96%)	58 (4%)	39	71

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ARG
1	A	130	HIS
1	A	131	HIS
1	A	189	SER
1	A	217	CYS
1	A	242	LEU
1	A	265	LYS
1	A	273	LYS
1	A	286	SER
1	A	322	LEU
1	A	331	GLU
1	A	337	PRO
1	A	338	SER
1	A	352	ARG
1	A	369	TYR
1	A	372	CYS
1	A	378	ARG
1	A	395	HIS
1	A	404	MET
1	B	107	ARG
1	B	130	HIS
1	B	131	HIS
1	B	140	LEU
1	B	160	GLU
1	B	167	GLN
1	B	175	ASN
1	B	242	LEU
1	B	307	LYS
1	B	317	SER
1	B	321	PHE

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Mol	Chain	Res	Type
1	B	352	ARG
1	B	365	ASN
1	B	369	TYR
1	B	381	CYS
1	B	395	HIS
1	C	69	GLU
1	C	84	LYS
1	C	95	ASN
1	C	107	ARG
1	C	130	HIS
1	C	131	HIS
1	C	184	SER
1	C	242	LEU
1	C	265	LYS
1	C	306	GLN
1	C	317	SER
1	C	352	ARG
1	C	395	HIS
1	D	107	ARG
1	D	131	HIS
1	D	156	ARG
1	D	161	SER
1	D	167	GLN
1	D	309	MET
1	D	317	SER
1	D	352	ARG
1	D	369	TYR
1	D	395	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	148	ASN
1	A	181	GLN
1	A	226	ASN
1	A	304	ASN
1	A	340	ASN
1	A	376	HIS
1	A	396	HIS
1	B	148	ASN
1	B	167	GLN

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Mol	Chain	Res	Type
1	B	175	ASN
1	B	209	ASN
1	B	226	ASN
1	B	250	ASN
1	B	304	ASN
1	B	306	GLN
1	B	313	GLN
1	B	395	HIS
1	B	396	HIS
1	B	412	GLN
1	B	417	HIS
1	C	71	GLN
1	C	95	ASN
1	C	148	ASN
1	C	226	ASN
1	C	376	HIS
1	C	396	HIS
1	D	148	ASN
1	D	167	GLN
1	D	181	GLN
1	D	209	ASN
1	D	226	ASN
1	D	250	ASN
1	D	313	GLN
1	D	340	ASN
1	D	348	ASN
1	D	365	ASN
1	D	396	HIS
1	D	412	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

8 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	GAL	A	501	2	10,11,12	0.46	0	11,15,17	0.37	0
2	NGA	A	502	2	15,15,15	0.49	0	21,21,21	0.74	1 (4%)
2	GAL	B	503	2	10,11,12	0.38	0	11,15,17	0.40	0
2	NGA	B	504	2	15,15,15	0.47	0	21,21,21	0.55	0
2	GAL	C	505	2	10,11,12	0.39	0	11,15,17	0.49	0
2	NGA	C	506	2	15,15,15	0.40	0	21,21,21	0.69	0
2	GAL	D	507	2	10,11,12	0.37	0	11,15,17	0.41	0
2	NGA	D	508	2	15,15,15	0.41	0	21,21,21	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	A	501	2	-	0/2/19/22	0/1/1/1
2	NGA	A	502	2	-	0/6/26/26	0/1/1/1
2	GAL	B	503	2	-	0/2/19/22	0/1/1/1
2	NGA	B	504	2	-	0/6/26/26	0/1/1/1
2	GAL	C	505	2	-	0/2/19/22	0/1/1/1
2	NGA	C	506	2	-	0/6/26/26	0/1/1/1
2	GAL	D	507	2	-	0/2/19/22	0/1/1/1
2	NGA	D	508	2	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	502	NGA	C1-C2-C3	-2.08	107.61	110.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	365/391 (93%)	-0.16	5 (1%) 72 77	19, 41, 72, 107	0
1	B	359/391 (91%)	-0.29	3 (0%) 83 87	18, 36, 70, 87	0
1	C	374/391 (95%)	-0.09	14 (3%) 39 44	21, 41, 90, 114	0
1	D	368/391 (94%)	0.03	15 (4%) 35 40	15, 46, 93, 113	0
All	All	1466/1564 (93%)	-0.13	37 (2%) 54 61	15, 41, 84, 114	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	59	CYS	4.9
1	D	86	PRO	4.6
1	C	80	VAL	4.3
1	C	56	ASN	3.8
1	C	81	GLN	3.8
1	A	86	PRO	3.7
1	A	85	ARG	3.5
1	B	56	ASN	3.4
1	C	75	LEU	3.3
1	C	84	LYS	3.3
1	C	57	VAL	3.2
1	C	78	LEU	3.1
1	C	83	LYS	3.0
1	C	82	PHE	3.0
1	B	263	ASP	3.0
1	C	45	HIS	2.9
1	D	98	ARG	2.9
1	D	46	LEU	2.9
1	B	86	PRO	2.8
1	C	263	ASP	2.7
1	D	85	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	95	ASN	2.7
1	D	56	ASN	2.6
1	D	87	ARG	2.6
1	A	79	THR	2.5
1	C	79	THR	2.5
1	C	77	ILE	2.5
1	A	249	PRO	2.5
1	D	79	THR	2.3
1	C	264	GLY	2.3
1	D	68	GLU	2.3
1	D	331	GLU	2.3
1	A	420	ARG	2.1
1	D	160	GLU	2.1
1	D	89	THR	2.0
1	D	100	CYS	2.0
1	D	385	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GAL	C	505	11/12	0.13	0.17	41,43,44,45	0
2	NGA	A	502	15/15	0.14	0.11	25,31,35,38	0
2	NGA	C	506	15/15	0.14	-0.31	39,41,43,44	0
2	NGA	D	508	15/15	0.13	-0.56	29,32,33,37	0
2	NGA	B	504	15/15	0.10	-1.46	24,29,32,33	0
2	GAL	B	503	11/12	0.12	-1.64	27,30,31,32	0
2	GAL	D	507	11/12	0.08	-1.64	21,25,27,28	0
2	GAL	A	501	11/12	0.08	-1.88	19,23,24,24	0

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.