



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:03 PM UTC

PDB ID : 3IDY / pdb_00003idy
Title : Crystal structure of HIV-gp120 core in complex with CD4-binding site antibody b13, space group C2221
Authors : Chen, L.; Kwon, Y.D.; Zhou, T.; Wu, X.; O'Dell, S.; Cavacini, L.; Hessel, A.J.; Pancera, M.; Tang, M.; Xu, L.; Yang, Z.Y.; Zhang, M.Y.; Arthos, J.; Burton, D.R.; Dimitrov, D.S.; Nabel, G.J.; Posner, M.; Sodroski, J.; Wyatt, R.; Mascola, J.R.; Kwong, P.D.
Deposited on : 2009-07-22
Resolution : 3.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

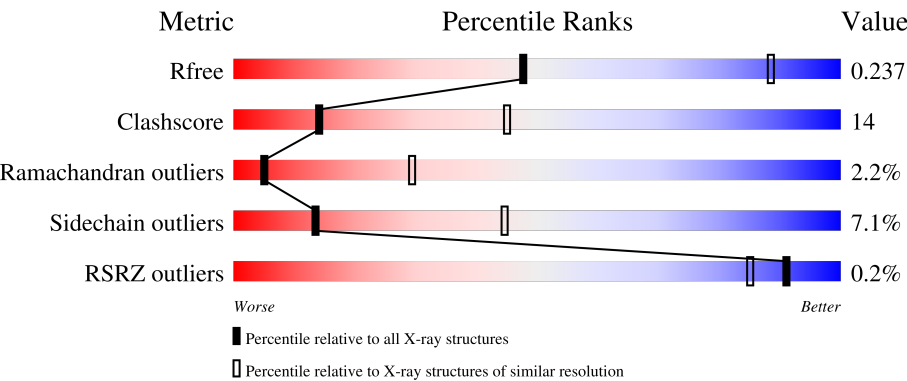
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	317	65%26%...
1	G	317	66%26%...
2	B	231	63%32%..
2	H	231	65%32%..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	215	% 72% 23% 5%
3	L	215	% 73% 22% 5%

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
4	NAG	G	588	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12038 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 HIV-1 HxBc2 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	306	Total	C	N	O	S	0	0	0
			2367	1483	412	448	24			
1	A	303	Total	C	N	O	S	0	0	0
			2354	1476	409	445	24			

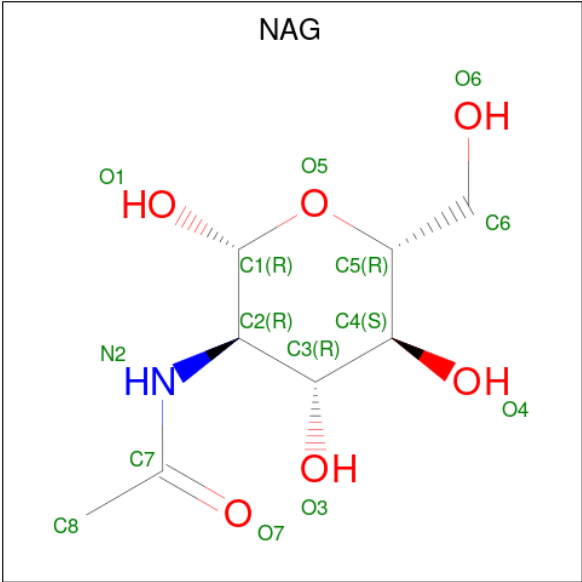
- Molecule 2 is a protein called Fab b13 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	229	Total	C	N	O	S	0	0	0
			1730	1092	297	334	7			
2	B	229	Total	C	N	O	S	0	0	0
			1730	1092	297	334	7			

- Molecule 3 is a protein called Fab b13 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1654	1028	284	337	5			
3	C	214	Total	C	N	O	S	0	0	0
			1654	1028	284	337	5			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



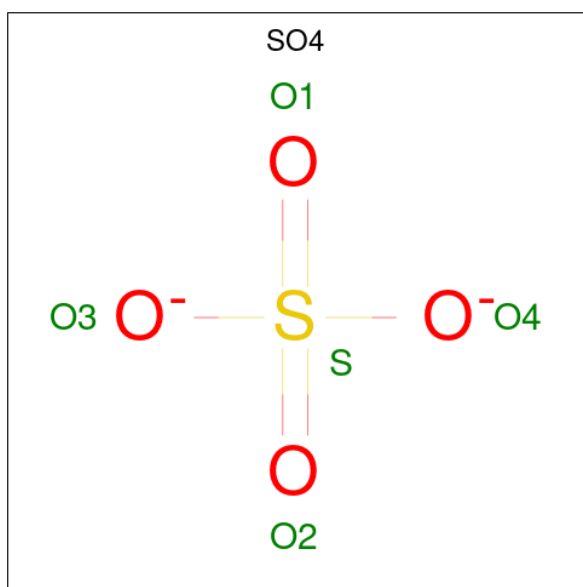
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	O	S	0	0
			5	4	1		

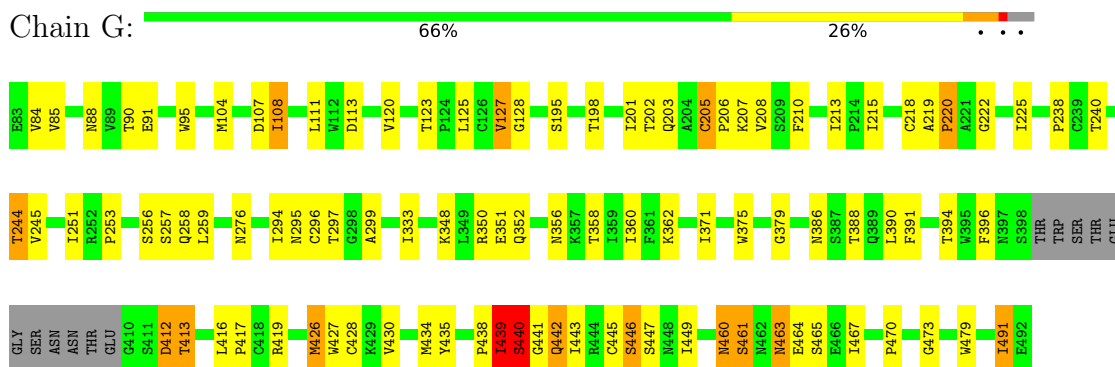
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	30	Total	O	0	0
			30	30		
6	H	12	Total	O	0	0
			12	12		
6	L	12	Total	O	0	0
			12	12		
6	A	41	Total	O	0	0
			41	41		
6	B	30	Total	O	0	0
			30	30		
6	C	27	Total	O	0	0
			27	27		

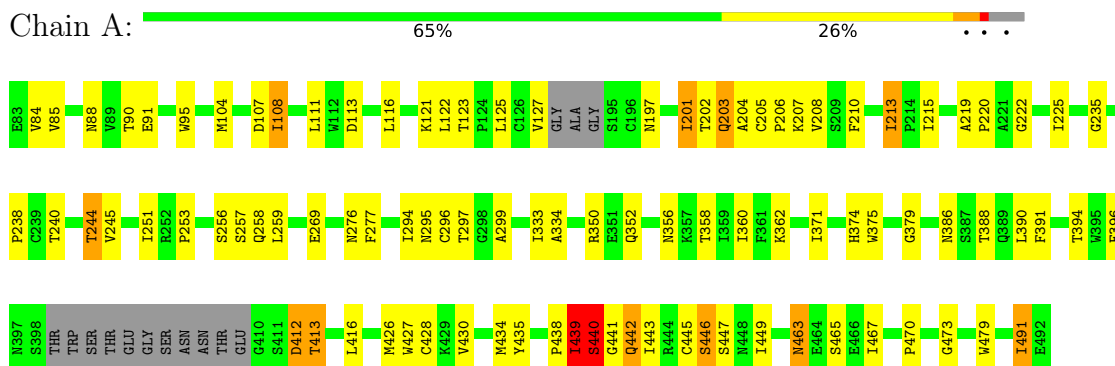
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

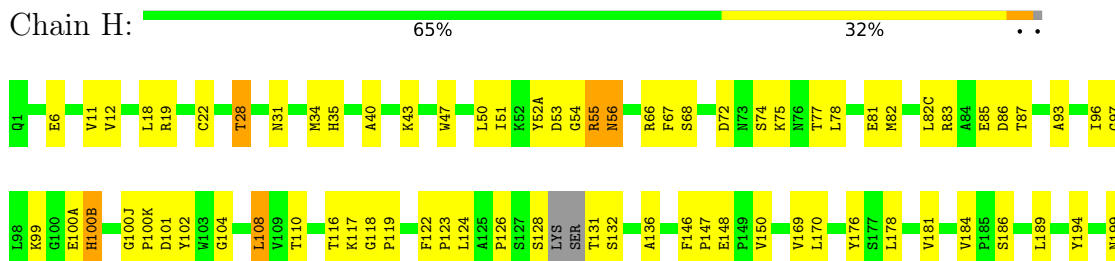
• Molecule 1: HIV-1 HxBc2 gp120 core



• Molecule 1: HIV-1 HxBc2 gp120 core



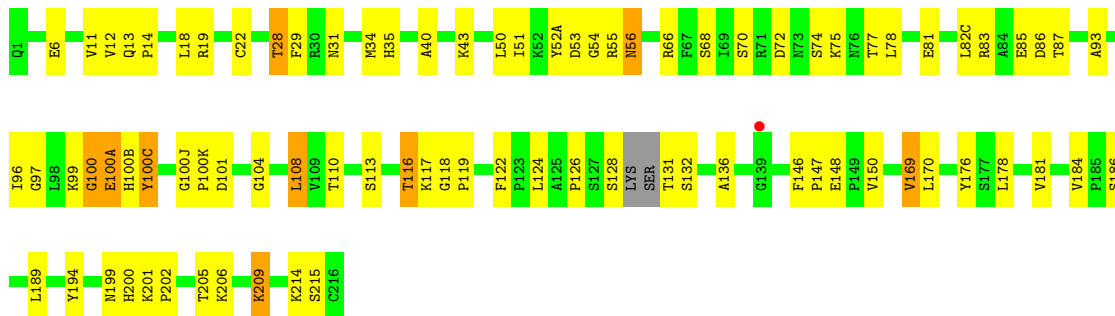
• Molecule 2: Fab b13 heavy chain





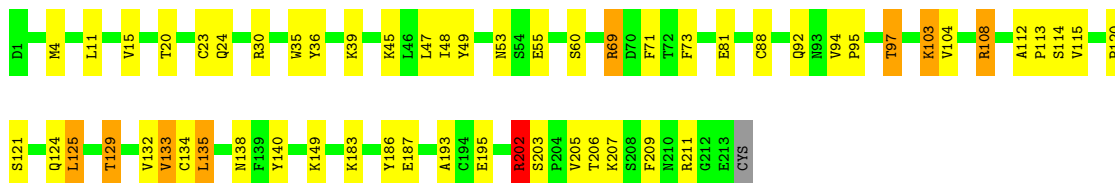
• Molecule 2: Fab b13 heavy chain

Chain B: 63% 32% ..



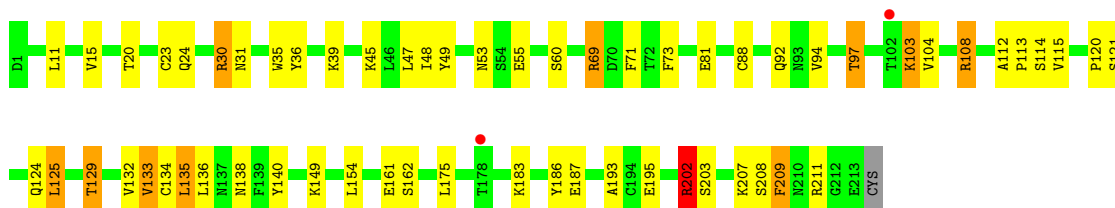
• Molecule 3: Fab b13 light chain

Chain L: 73% 22% .



• Molecule 3: Fab b13 light chain

Chain C: 72% 23% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	106.17Å 204.32Å 216.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.20 – 3.20 43.20 – 3.20	Depositor EDS
% Data completeness (in resolution range)	47.1 (43.20-3.20) 90.1 (43.20-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196 , 0.237 0.192 , 0.237	Depositor DCC
R_{free} test set	1900 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å ²)	92.9	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 111.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12038	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4

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	0.34	0/2401	0.76	5/3254 (0.2%)
1	G	0.33	0/2415	0.77	3/3274 (0.1%)
2	B	0.32	1/1771 (0.1%)	0.70	0/2407
2	H	0.39	2/1771 (0.1%)	0.72	2/2407 (0.1%)
3	C	0.29	0/1688	0.75	1/2291 (0.0%)
3	L	0.31	0/1688	0.74	0/2291
All	All	0.33	3/11734 (0.0%)	0.75	11/15924 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	100(B)	HIS	ND1-CE1	5.24	1.37	1.32
2	B	56	ASN	CG-OD1	5.22	1.33	1.23
2	H	56	ASN	CG-OD1	5.02	1.33	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	GLY	N-CA-C	-7.39	106.19	114.40
1	G	441	GLY	N-CA-C	-7.30	106.30	114.40
2	H	100(B)	HIS	CB-CG-CD2	-6.63	122.58	131.20
1	A	439	ILE	N-CA-C	6.42	117.05	110.82
1	G	439	ILE	N-CA-C	6.36	116.99	110.82
3	C	30	ARG	CB-CA-C	-6.08	109.55	116.54
2	H	100(B)	HIS	CB-CG-ND1	5.79	131.39	122.70
1	A	213	ILE	CA-C-N	5.21	125.46	119.83
1	A	213	ILE	C-N-CA	5.21	125.46	119.83
1	A	473	GLY	N-CA-C	-5.10	108.58	115.21
1	G	473	GLY	N-CA-C	-5.08	108.61	115.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2354	0	2285	67	0
1	G	2367	0	2298	69	0
2	B	1730	0	1696	72	0
2	H	1730	0	1696	63	0
3	C	1654	0	1602	36	0
3	L	1654	0	1602	41	0
4	A	196	0	181	10	0
4	G	196	0	182	7	0
5	G	5	0	0	1	0
6	A	41	0	0	2	0
6	B	30	0	0	9	0
6	C	27	0	0	3	0
6	G	30	0	0	2	0
6	H	12	0	0	0	0
6	L	12	0	0	0	0
All	All	12038	0	11542	334	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 14.

All (334) 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:H:100(A):GLU:HG2	3:L:53:ASN:ND2	1.85	0.92
2:H:100(A):GLU:HG2	3:L:53:ASN:HD21	1.35	0.90
1:G:461:SER:CA	4:G:963:NAG:H82	2.03	0.89
1:G:388:THR:HG21	4:G:886:NAG:H5	1.54	0.88
1:G:463:ASN:HD22	1:G:464:GLU:H	1.30	0.80
1:A:121:LYS:HE2	1:A:204:ALA:HB3	1.63	0.80
1:G:461:SER:HA	4:G:963:NAG:H82	1.63	0.79
1:A:269:GLU:HB3	4:A:789:NAG:H61	1.63	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:461:SER:CB	4:G:963:NAG:H82	2.13	0.77
1:A:439:ILE:HD12	1:A:439:ILE:H	1.52	0.75
1:A:113:ASP:HB2	1:A:213:ILE:HD11	1.69	0.74
2:B:118:GLY:HA2	6:B:220:HOH:O	1.89	0.73
1:G:296:CYS:H	1:G:446:SER:HB3	1.54	0.73
1:A:296:CYS:H	1:A:446:SER:HB3	1.55	0.72
2:B:119:PRO:HD3	6:B:220:HOH:O	1.90	0.71
1:G:439:ILE:HD12	1:G:439:ILE:H	1.55	0.71
1:G:113:ASP:HB2	1:G:213:ILE:HD11	1.72	0.70
2:H:209:LYS:HE3	2:H:209:LYS:HA	1.73	0.70
1:G:438:PRO:HB2	1:G:443:ILE:HG13	1.73	0.69
1:G:296:CYS:H	1:G:446:SER:CB	2.06	0.69
1:A:296:CYS:H	1:A:446:SER:CB	2.05	0.69
1:G:219:ALA:HB2	1:G:225:ILE:HG13	1.75	0.69
1:A:438:PRO:HB2	1:A:443:ILE:HG13	1.72	0.69
1:G:90:THR:HG22	1:G:240:THR:HA	1.73	0.69
1:A:90:THR:HG22	1:A:240:THR:HA	1.75	0.68
1:A:219:ALA:HB2	1:A:225:ILE:HG13	1.74	0.68
1:G:463:ASN:HD22	1:G:464:GLU:N	1.92	0.68
1:G:426:MET:HE3	2:H:55:ARG:NH1	2.09	0.67
2:B:209:LYS:HE3	2:B:209:LYS:HA	1.75	0.67
2:H:87:THR:HG23	2:H:110:THR:HA	1.76	0.67
2:B:87:THR:HG23	2:B:110:THR:HA	1.77	0.66
1:G:440:SER:C	1:G:442:GLN:N	2.53	0.65
2:H:100(A):GLU:CG	3:L:53:ASN:HD21	2.08	0.65
1:A:295:ASN:HA	1:A:446:SER:HB2	1.78	0.65
1:G:391:PHE:CG	1:G:470:PRO:HG3	2.31	0.65
1:A:104:MET:HE3	1:A:479:TRP:CZ3	2.31	0.65
1:A:391:PHE:CG	1:A:470:PRO:HG3	2.32	0.65
1:G:104:MET:HE3	1:G:479:TRP:CZ3	2.31	0.65
1:G:295:ASN:HA	1:G:446:SER:HB2	1.77	0.64
2:H:96:ILE:HG13	2:H:100(J):GLY:O	1.97	0.64
1:A:439:ILE:HD12	1:A:439:ILE:N	2.12	0.64
1:G:348:LYS:HE3	6:G:496:HOH:O	1.97	0.64
1:A:334:ALA:N	4:A:795:NAG:H81	2.12	0.64
1:G:362:LYS:HD2	1:G:467:ILE:HD13	1.78	0.64
3:C:92:GLN:O	3:C:92:GLN:HG3	1.97	0.64
2:H:68:SER:HB3	2:H:81:GLU:HG2	1.80	0.64
2:H:18:LEU:HD23	2:H:19:ARG:N	2.13	0.63
1:A:362:LYS:HD2	1:A:467:ILE:HD13	1.80	0.63
1:G:439:ILE:HD12	1:G:439:ILE:N	2.13	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100(K):PRO:HD2	3:C:36:TYR:OH	1.98	0.63
2:B:18:LEU:HD23	2:B:19:ARG:N	2.14	0.63
1:A:440:SER:C	1:A:442:GLN:N	2.55	0.63
2:B:96:ILE:HG13	2:B:100(J):GLY:O	2.00	0.62
1:G:440:SER:C	1:G:442:GLN:H	2.06	0.62
3:L:30:ARG:HB3	3:L:30:ARG:HH11	1.64	0.62
3:C:88:CYS:O	3:C:97:THR:HB	2.00	0.62
2:B:68:SER:HB3	2:B:81:GLU:HG2	1.81	0.61
2:B:199:ASN:HD21	2:B:206:LYS:HE2	1.65	0.61
1:A:439:ILE:HD13	1:A:442:GLN:NE2	2.15	0.61
3:C:161:GLU:HB2	6:C:231:HOH:O	2.00	0.61
1:A:391:PHE:CD1	1:A:470:PRO:HG3	2.36	0.61
1:A:440:SER:C	1:A:442:GLN:H	2.08	0.60
2:B:99:LYS:C	2:B:100(A):GLU:H	2.07	0.60
3:C:120:PRO:HD3	3:C:132:VAL:HG22	1.82	0.60
1:G:463:ASN:ND2	1:G:464:GLU:H	1.99	0.60
1:G:391:PHE:CD1	1:G:470:PRO:HG3	2.36	0.60
1:G:439:ILE:HD13	1:G:442:GLN:NE2	2.17	0.60
3:L:202:ARG:HD2	3:L:203:SER:N	2.17	0.60
2:H:199:ASN:HD21	2:H:206:LYS:HE2	1.67	0.59
3:L:88:CYS:O	3:L:97:THR:HB	2.02	0.59
1:A:374:HIS:HA	6:A:31:HOH:O	2.01	0.59
3:C:202:ARG:HD2	3:C:203:SER:N	2.17	0.59
2:B:34:MET:HB3	2:B:78:LEU:HD22	1.84	0.59
1:G:259:LEU:HD13	1:G:449:ILE:HD13	1.84	0.59
3:L:92:GLN:HG3	3:L:92:GLN:O	2.01	0.59
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.84	0.59
1:A:388:THR:HG21	4:A:886:NAG:H5	1.84	0.58
2:H:181:VAL:HG21	3:L:135:LEU:HD11	1.83	0.58
1:G:205:CYS:N	1:G:206:PRO:HD3	2.18	0.58
1:G:360:ILE:HB	1:G:467:ILE:HG12	1.85	0.58
1:A:360:ILE:HB	1:A:467:ILE:HG12	1.86	0.58
3:L:202:ARG:HD2	3:L:203:SER:H	1.68	0.58
3:C:202:ARG:HD2	3:C:203:SER:H	1.69	0.58
2:B:150:VAL:HG23	2:B:178:LEU:HD21	1.85	0.57
2:H:100(K):PRO:HD2	3:L:36:TYR:OH	2.04	0.57
3:L:125:LEU:O	3:L:183:LYS:HD2	2.05	0.56
1:A:259:LEU:HD13	1:A:449:ILE:HD13	1.87	0.56
3:C:125:LEU:O	3:C:183:LYS:HD2	2.05	0.56
2:H:108:LEU:HD11	2:H:148:GLU:HB2	1.87	0.56
2:H:136:ALA:HB3	2:H:189:LEU:HD11	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:VAL:HG13	1:G:128:GLY:H	1.71	0.55
2:B:136:ALA:HB3	2:B:189:LEU:HD11	1.87	0.55
1:A:210:PHE:CD2	1:A:442:GLN:HG3	2.42	0.55
3:C:24:GLN:HA	3:C:69:ARG:O	2.07	0.55
1:G:426:MET:HE3	2:H:55:ARG:HH12	1.71	0.55
2:H:34:MET:HB3	2:H:78:LEU:HD22	1.88	0.55
2:B:6:GLU:OE2	2:B:104:GLY:HA3	2.06	0.55
2:H:122:PHE:CD2	3:L:124:GLN:HB2	2.40	0.55
2:H:150:VAL:HG23	2:H:178:LEU:HD21	1.87	0.55
1:A:334:ALA:H	4:A:795:NAG:H81	1.70	0.55
1:A:350:ARG:HD3	1:A:396:PHE:CE2	2.41	0.55
1:G:440:SER:H	1:G:442:GLN:HB2	1.72	0.55
2:B:181:VAL:HG21	3:C:135:LEU:HD11	1.89	0.55
2:B:108:LEU:HD11	2:B:148:GLU:HB2	1.87	0.55
1:G:206:PRO:O	1:G:207:LYS:C	2.50	0.54
2:H:6:GLU:OE2	2:H:104:GLY:HA3	2.08	0.54
1:A:440:SER:H	1:A:442:GLN:HB2	1.71	0.54
3:L:47:LEU:C	3:L:48:ILE:HD12	2.32	0.54
2:B:99:LYS:O	2:B:100(A):GLU:N	2.37	0.54
1:G:350:ARG:HD3	1:G:396:PHE:CE2	2.41	0.54
1:A:201:ILE:C	1:A:201:ILE:HD13	2.33	0.54
2:H:200:HIS:HE1	2:H:202:PRO:HB2	1.72	0.54
2:B:51:ILE:HD11	2:B:54:GLY:HA2	1.89	0.54
1:A:205:CYS:N	1:A:206:PRO:HD3	2.23	0.54
2:B:184:VAL:HG11	2:B:194:TYR:CE1	2.43	0.54
1:A:84:VAL:HG23	1:A:244:THR:HB	1.89	0.53
3:L:108:ARG:HD2	3:L:140:TYR:CG	2.43	0.53
2:H:122:PHE:HB3	3:L:121:SER:OG	2.08	0.53
2:B:83:ARG:HD2	2:B:85:GLU:OE2	2.09	0.53
3:C:133:VAL:HG12	3:C:134:CYS:H	1.73	0.53
2:H:96:ILE:HG12	2:H:101:ASP:HB3	1.91	0.52
1:G:84:VAL:HG23	1:G:244:THR:HB	1.90	0.52
1:G:205:CYS:H	1:G:206:PRO:HD3	1.74	0.52
1:A:206:PRO:O	1:A:207:LYS:C	2.52	0.52
2:B:122:PHE:HB3	3:C:121:SER:OG	2.10	0.52
2:B:200:HIS:HE1	2:B:202:PRO:HB2	1.73	0.52
3:C:47:LEU:C	3:C:48:ILE:HD12	2.33	0.52
3:C:108:ARG:HD2	3:C:140:TYR:CG	2.44	0.52
2:H:184:VAL:HG11	2:H:194:TYR:CE1	2.43	0.52
3:L:133:VAL:HG12	3:L:134:CYS:H	1.74	0.52
2:H:51:ILE:HD11	2:H:54:GLY:HA2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:GLY:C	2:B:100(B):HIS:H	2.16	0.52
1:G:362:LYS:HD3	5:G:1003:SO4:O1	2.10	0.52
3:C:39:LYS:HE2	3:C:81:GLU:O	2.10	0.52
3:L:24:GLN:HA	3:L:69:ARG:O	2.09	0.52
2:H:83:ARG:HD2	2:H:85:GLU:OE2	2.09	0.52
1:A:447:SER:HB3	4:A:762:NAG:HN2	1.75	0.52
1:G:210:PHE:CD2	1:G:442:GLN:HG3	2.44	0.51
2:B:96:ILE:HG12	2:B:101:ASP:HB3	1.91	0.51
2:B:100(A):GLU:HG2	2:B:100(C):TYR:HB3	1.93	0.51
3:L:39:LYS:HE2	3:L:81:GLU:O	2.11	0.51
2:B:77:THR:N	6:B:229:HOH:O	2.43	0.51
3:C:175:LEU:HG	6:C:231:HOH:O	2.11	0.50
2:H:28:THR:HG21	2:H:31:ASN:ND2	2.27	0.50
1:A:204:ALA:C	1:A:206:PRO:HD3	2.36	0.50
2:B:119:PRO:HD2	2:B:205:THR:HG21	1.93	0.50
1:G:412:ASP:OD1	1:G:413:THR:HG22	2.12	0.50
2:H:68:SER:HB3	2:H:81:GLU:CG	2.42	0.50
3:L:108:ARG:HD2	3:L:140:TYR:CB	2.42	0.50
3:C:23:CYS:HB2	3:C:35:TRP:CH2	2.46	0.50
3:L:30:ARG:HB3	3:L:30:ARG:NH1	2.27	0.50
2:B:100:GLY:O	2:B:100(B):HIS:N	2.43	0.50
2:H:123:PRO:HD2	3:L:121:SER:CB	2.42	0.50
1:A:269:GLU:CB	4:A:789:NAG:H61	2.37	0.50
1:G:491:ILE:HD13	1:G:491:ILE:O	2.12	0.50
1:A:334:ALA:H	4:A:795:NAG:C8	2.25	0.49
2:H:178:LEU:HD12	2:H:178:LEU:C	2.37	0.49
2:B:113:SER:HB2	6:B:223:HOH:O	2.13	0.49
2:H:100(A):GLU:CG	3:L:53:ASN:ND2	2.68	0.49
2:B:136:ALA:CB	2:B:189:LEU:HD11	2.43	0.49
2:B:170:LEU:HD13	2:B:176:TYR:CE1	2.46	0.49
2:H:200:HIS:CE1	2:H:202:PRO:HB2	2.48	0.49
2:B:108:LEU:CD1	2:B:148:GLU:HB2	2.43	0.49
3:C:108:ARG:HD2	3:C:140:TYR:CB	2.43	0.49
1:A:107:ASP:O	1:A:108:ILE:HB	2.13	0.49
2:B:68:SER:HB3	2:B:81:GLU:CG	2.43	0.49
1:G:428:CYS:HB3	1:G:435:TYR:HB3	1.95	0.49
2:H:47:TRP:CZ3	3:L:95:PRO:HB3	2.48	0.49
2:H:119:PRO:HD2	2:H:205:THR:HG21	1.94	0.49
1:G:127:VAL:HG12	1:G:195:SER:O	2.13	0.48
2:H:108:LEU:CD1	2:H:148:GLU:HB2	2.42	0.48
2:H:170:LEU:HD13	2:H:176:TYR:CE1	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:TYR:O	3:C:53:ASN:HB2	2.13	0.48
2:H:93:ALA:HB1	2:H:100(K):PRO:HB3	1.96	0.48
1:A:412:ASP:OD1	1:A:413:THR:HG22	2.13	0.48
2:B:28:THR:HG21	2:B:31:ASN:ND2	2.29	0.48
1:G:218:CYS:N	6:G:500:HOH:O	2.42	0.48
2:H:136:ALA:CB	2:H:189:LEU:HD11	2.44	0.48
2:B:93:ALA:HB1	2:B:100(K):PRO:HB3	1.96	0.48
1:A:439:ILE:H	1:A:439:ILE:CD1	2.24	0.47
1:G:91:GLU:O	1:G:238:PRO:HA	2.14	0.47
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.95	0.47
3:C:115:VAL:HG13	3:C:207:LYS:HE3	1.96	0.47
3:L:49:TYR:O	3:L:53:ASN:HB2	2.14	0.47
1:A:428:CYS:HB3	1:A:435:TYR:HB3	1.97	0.47
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.96	0.47
2:B:178:LEU:C	2:B:178:LEU:HD12	2.40	0.47
1:A:251:ILE:O	1:A:253:PRO:HD3	2.14	0.47
1:G:386:ASN:O	1:G:416:LEU:HD22	2.15	0.47
1:G:352:GLN:O	1:G:352:GLN:HG3	2.15	0.47
1:A:386:ASN:O	1:A:416:LEU:HD22	2.14	0.47
1:G:107:ASP:O	1:G:108:ILE:HB	2.15	0.46
3:L:115:VAL:HG13	3:L:207:LYS:HE3	1.97	0.46
1:A:91:GLU:O	1:A:238:PRO:HA	2.14	0.46
3:L:124:GLN:HG2	3:L:129:THR:O	2.16	0.46
1:A:352:GLN:O	1:A:352:GLN:HG3	2.16	0.46
1:A:427:TRP:CE3	1:A:434:MET:HE3	2.51	0.46
2:B:200:HIS:CE1	2:B:202:PRO:HB2	2.49	0.46
3:C:124:GLN:HG2	3:C:129:THR:O	2.15	0.46
1:G:447:SER:HB3	4:G:762:NAG:N2	2.30	0.46
3:L:23:CYS:HB2	3:L:35:TRP:CH2	2.50	0.46
1:A:358:THR:HB	1:A:465:SER:HB3	1.98	0.46
2:H:12:VAL:HG11	2:H:82(C):LEU:HD13	1.98	0.46
2:H:99:LYS:H	2:H:100(B):HIS:CD2	2.34	0.46
2:H:201:LYS:N	2:H:202:PRO:CD	2.79	0.46
1:A:445:CYS:O	1:A:446:SER:CB	2.64	0.45
1:G:427:TRP:CE3	1:G:434:MET:HE3	2.51	0.45
1:A:197:ASN:HB2	6:A:494:HOH:O	2.15	0.45
1:A:491:ILE:HD13	1:A:491:ILE:O	2.15	0.45
1:G:208:VAL:O	1:G:208:VAL:HG13	2.16	0.45
1:G:445:CYS:O	1:G:446:SER:CB	2.64	0.45
2:B:100(C):TYR:CD1	2:B:100(C):TYR:C	2.94	0.45
2:B:116:THR:HB	6:B:230:HOH:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:251:ILE:O	1:G:253:PRO:HD3	2.17	0.45
2:H:72:ASP:C	2:H:74:SER:H	2.25	0.45
1:A:360:ILE:HG12	1:A:394:THR:HG23	1.99	0.45
2:B:169:VAL:HG22	3:C:162:SER:HB2	1.99	0.45
2:B:201:LYS:N	2:B:202:PRO:CD	2.80	0.45
3:L:112:ALA:HA	3:L:113:PRO:HD3	1.71	0.45
1:G:371:ILE:HD12	1:G:371:ILE:C	2.42	0.44
3:C:103:LYS:HB2	3:C:103:LYS:NZ	2.33	0.44
1:G:294:ILE:HG23	1:G:294:ILE:O	2.17	0.44
1:G:358:THR:HB	1:G:465:SER:HB3	1.99	0.44
2:H:101:ASP:OD2	2:H:102:TYR:N	2.47	0.44
2:B:12:VAL:HG11	2:B:82(C):LEU:HD13	1.99	0.44
2:B:35:HIS:CE1	2:B:50:LEU:HD13	2.53	0.44
2:H:128:SER:C	2:H:132:SER:HB2	2.42	0.44
1:A:296:CYS:H	1:A:446:SER:HB2	1.81	0.44
2:B:150:VAL:HG12	2:B:200:HIS:HB2	1.99	0.44
1:G:95:TRP:CD1	1:G:95:TRP:H	2.36	0.44
2:B:66:ARG:HG2	6:B:225:HOH:O	2.18	0.44
2:H:186:SER:HA	2:H:189:LEU:HG	1.99	0.43
2:H:199:ASN:ND2	2:H:206:LYS:HE2	2.33	0.43
3:C:120:PRO:HG2	3:C:186:TYR:CE1	2.53	0.43
2:B:75:LYS:O	2:B:77:THR:HG23	2.17	0.43
2:B:186:SER:HA	2:B:189:LEU:HG	1.99	0.43
2:B:199:ASN:ND2	2:B:206:LYS:HE2	2.32	0.43
2:H:83:ARG:HB2	2:H:85:GLU:HG2	2.00	0.43
3:L:149:LYS:HB2	3:L:193:ALA:HB3	2.01	0.43
3:C:187:GLU:HA	3:C:211:ARG:HH22	1.84	0.43
1:G:333:ILE:HD12	1:G:390:LEU:HD21	2.01	0.43
2:H:52(A):TYR:CG	2:H:53:ASP:N	2.87	0.43
1:A:95:TRP:H	1:A:95:TRP:CD1	2.36	0.43
1:A:222:GLY:O	1:A:491:ILE:HG22	2.18	0.43
2:B:72:ASP:C	2:B:74:SER:H	2.25	0.43
1:G:222:GLY:O	1:G:491:ILE:HG22	2.19	0.43
1:A:208:VAL:HG13	1:A:208:VAL:O	2.17	0.43
1:A:294:ILE:O	1:A:294:ILE:HG23	2.17	0.43
2:H:22:CYS:HB3	2:H:78:LEU:HB3	1.99	0.43
3:L:23:CYS:HB3	3:L:71:PHE:HB2	2.01	0.43
2:B:83:ARG:HB2	2:B:85:GLU:HG2	2.00	0.43
3:L:187:GLU:HA	3:L:211:ARG:HH22	1.84	0.43
2:B:29:PHE:CE2	6:B:229:HOH:O	2.57	0.43
2:B:202:PRO:HG2	6:B:231:HOH:O	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:23:CYS:HB3	3:C:71:PHE:HB2	2.00	0.43
3:L:11:LEU:HD12	3:L:11:LEU:O	2.19	0.43
2:B:128:SER:C	2:B:132:SER:HB2	2.43	0.43
2:H:150:VAL:HG12	2:H:200:HIS:HB2	2.01	0.43
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.78	0.43
1:G:460:ASN:ND2	4:G:963:NAG:H83	2.34	0.42
3:L:11:LEU:HD12	3:L:11:LEU:C	2.44	0.42
3:C:35:TRP:CD2	3:C:73:PHE:HB2	2.54	0.42
1:G:256:SER:HA	1:G:375:TRP:O	2.18	0.42
2:H:82:MET:HE3	2:H:82:MET:HB2	1.96	0.42
4:A:588:NAG:O7	4:A:588:NAG:C3	2.67	0.42
2:B:52(A):TYR:CG	2:B:53:ASP:N	2.87	0.42
3:C:149:LYS:HB2	3:C:193:ALA:HB3	2.01	0.42
2:H:146:PHE:HA	2:H:147:PRO:HA	1.86	0.42
1:A:439:ILE:HD13	1:A:442:GLN:HE21	1.85	0.42
2:H:75:LYS:O	2:H:77:THR:HG23	2.19	0.42
3:L:120:PRO:HG2	3:L:186:TYR:CE1	2.54	0.42
2:B:117:LYS:HD3	2:B:118:GLY:N	2.35	0.42
2:B:66:ARG:NH2	2:B:86:ASP:OD2	2.52	0.42
2:B:131:THR:HG22	2:B:132:SER:N	2.34	0.42
2:H:35:HIS:CE1	2:H:50:LEU:HD13	2.55	0.42
2:H:85:GLU:HG2	2:H:85:GLU:H	1.68	0.42
1:A:333:ILE:HD12	1:A:390:LEU:HD21	2.00	0.42
2:B:22:CYS:HB3	2:B:78:LEU:HB3	2.00	0.42
1:G:447:SER:HB3	4:G:762:NAG:HN2	1.84	0.42
3:L:103:LYS:NZ	3:L:103:LYS:HB2	2.34	0.42
3:L:149:LYS:HE3	3:L:195:GLU:OE1	2.20	0.42
2:B:50:LEU:HD12	2:B:51:ILE:H	1.84	0.42
1:G:360:ILE:HG12	1:G:394:THR:HG23	2.01	0.42
3:L:35:TRP:CD2	3:L:73:PHE:HB2	2.54	0.42
1:A:219:ALA:HA	1:A:220:PRO:HD3	1.91	0.42
2:B:117:LYS:HD3	2:B:118:GLY:O	2.20	0.42
1:G:219:ALA:HA	1:G:220:PRO:HD3	1.91	0.42
1:G:386:ASN:HB3	1:G:417:PRO:HD2	2.02	0.42
2:H:122:PHE:HA	2:H:123:PRO:HD3	1.82	0.42
4:A:588:NAG:O7	4:A:588:NAG:H3	2.20	0.42
2:B:100(J):GLY:HA2	2:B:100(K):PRO:HD3	1.89	0.42
2:H:55:ARG:HE	2:H:55:ARG:HB3	1.68	0.41
3:C:112:ALA:HA	3:C:113:PRO:HD3	1.72	0.41
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.52	0.41
2:H:117:LYS:HD3	2:H:118:GLY:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:THR:HG23	1:A:299:ALA:HB3	2.01	0.41
1:G:104:MET:HE3	1:G:479:TRP:HZ3	1.81	0.41
1:A:203:GLN:O	1:A:203:GLN:HG2	2.20	0.41
1:A:257:SER:O	1:A:258:GLN:HB2	2.20	0.41
1:A:277:PHE:HE1	4:A:734:NAG:H81	1.84	0.41
2:B:70:SER:O	2:B:78:LEU:HD12	2.20	0.41
1:A:256:SER:HA	1:A:375:TRP:O	2.21	0.41
2:B:85:GLU:HG2	2:B:85:GLU:H	1.68	0.41
2:B:214:LYS:HB3	2:B:215:SER:H	1.58	0.41
3:C:133:VAL:HG12	3:C:134:CYS:N	2.35	0.41
2:H:131:THR:HG22	2:H:132:SER:N	2.34	0.41
1:A:108:ILE:HG21	1:A:479:TRP:CH2	2.56	0.41
1:A:371:ILE:C	1:A:371:ILE:HD12	2.44	0.41
2:B:56:ASN:N	2:B:56:ASN:OD1	2.53	0.41
2:B:99:LYS:C	2:B:100(A):GLU:N	2.75	0.41
3:C:30:ARG:HB3	3:C:31:ASN:H	1.49	0.41
3:C:208:SER:O	3:C:209:PHE:HB3	2.21	0.41
1:G:257:SER:O	1:G:258:GLN:HB2	2.21	0.41
2:B:13:GLN:HA	2:B:14:PRO:HD3	1.95	0.41
1:G:125:LEU:HA	1:G:125:LEU:HD23	1.78	0.41
3:L:133:VAL:HG12	3:L:134:CYS:N	2.35	0.41
1:A:95:TRP:CD1	1:A:235:GLY:HA3	2.56	0.41
1:A:104:MET:HE3	1:A:479:TRP:HZ3	1.83	0.41
2:H:118:GLY:HA2	2:H:119:PRO:HD3	1.85	0.41
3:C:135:LEU:HD23	3:C:136:LEU:N	2.35	0.41
2:H:67:PHE:CE1	2:H:82:MET:HB3	2.57	0.40
2:B:100(B):HIS:HA	6:B:241:HOH:O	2.20	0.40
1:G:351:GLU:O	1:G:351:GLU:HG2	2.21	0.40
3:L:4:MET:HE3	3:L:23:CYS:SG	2.61	0.40
3:C:149:LYS:HE3	3:C:195:GLU:OE1	2.21	0.40
1:G:297:THR:HG23	1:G:299:ALA:HB3	2.02	0.40
2:H:56:ASN:N	2:H:56:ASN:OD1	2.54	0.40
2:B:100(A):GLU:C	2:B:100(C):TYR:H	2.30	0.40
3:C:11:LEU:HD12	3:C:11:LEU:C	2.46	0.40
1:G:371:ILE:HD12	1:G:371:ILE:O	2.21	0.40
3:L:205:VAL:HG12	3:L:206:THR:N	2.37	0.40
2:B:14:PRO:HA	2:B:82(C):LEU:O	2.22	0.40
2:B:146:PHE:HA	2:B:147:PRO:HA	1.85	0.40
3:C:154:LEU:HG	6:C:240:HOH:O	2.20	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	297/317 (94%)	258 (87%)	32 (11%)	7 (2%)	4	28
1	G	302/317 (95%)	260 (86%)	33 (11%)	9 (3%)	3	23
2	B	225/231 (97%)	183 (81%)	35 (16%)	7 (3%)	3	22
2	H	225/231 (97%)	189 (84%)	32 (14%)	4 (2%)	6	34
3	C	212/215 (99%)	185 (87%)	24 (11%)	3 (1%)	9	39
3	L	212/215 (99%)	183 (86%)	26 (12%)	3 (1%)	9	39
All	All	1473/1526 (96%)	1258 (85%)	182 (12%)	33 (2%)	5	29

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	440	SER
1	A	440	SER
2	B	100(A)	GLU
1	G	379	GLY
2	H	55	ARG
2	H	97	GLY
3	L	202	ARG
1	A	379	GLY
1	A	463	ASN
2	B	55	ARG
2	B	97	GLY
2	B	100(C)	TYR
3	C	202	ARG
1	G	111	LEU
2	H	28	THR
2	H	126	PRO
3	L	209	PHE
1	A	111	LEU
2	B	28	THR
2	B	126	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	209	PHE
1	G	276	ASN
1	G	446	SER
3	L	138	ASN
1	A	446	SER
3	C	138	ASN
1	G	108	ILE
1	A	108	ILE
1	A	276	ASN
2	B	100	GLY
1	G	460	ASN
1	G	205	CYS
1	G	220	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	271/281 (96%)	249 (92%)	22 (8%)	11	39
1	G	271/281 (96%)	247 (91%)	24 (9%)	9	34
2	B	189/191 (99%)	183 (97%)	6 (3%)	34	65
2	H	189/191 (99%)	183 (97%)	6 (3%)	34	65
3	C	189/190 (100%)	172 (91%)	17 (9%)	9	34
3	L	189/190 (100%)	172 (91%)	17 (9%)	9	34
All	All	1298/1324 (98%)	1206 (93%)	92 (7%)	13	44

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	85	VAL
1	G	88	ASN
1	G	120	VAL
1	G	123	THR
1	G	127	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	198	THR
1	G	201	ILE
1	G	202	THR
1	G	203	GLN
1	G	215	ILE
1	G	244	THR
1	G	245	VAL
1	G	356	ASN
1	G	412	ASP
1	G	413	THR
1	G	419	ARG
1	G	426	MET
1	G	430	VAL
1	G	439	ILE
1	G	440	SER
1	G	442	GLN
1	G	461	SER
1	G	463	ASN
1	G	491	ILE
2	H	11	VAL
2	H	108	LEU
2	H	116	THR
2	H	124	LEU
2	H	169	VAL
2	H	209	LYS
3	L	15	VAL
3	L	20	THR
3	L	45	LYS
3	L	55	GLU
3	L	60	SER
3	L	69	ARG
3	L	94	VAL
3	L	97	THR
3	L	103	LYS
3	L	104	VAL
3	L	108	ARG
3	L	114	SER
3	L	125	LEU
3	L	129	THR
3	L	133	VAL
3	L	135	LEU
3	L	202	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	85	VAL
1	A	88	ASN
1	A	122	LEU
1	A	123	THR
1	A	125	LEU
1	A	127	VAL
1	A	201	ILE
1	A	202	THR
1	A	203	GLN
1	A	215	ILE
1	A	244	THR
1	A	245	VAL
1	A	356	ASN
1	A	412	ASP
1	A	413	THR
1	A	426	MET
1	A	430	VAL
1	A	439	ILE
1	A	440	SER
1	A	442	GLN
1	A	463	ASN
1	A	491	ILE
2	B	11	VAL
2	B	108	LEU
2	B	116	THR
2	B	124	LEU
2	B	169	VAL
2	B	209	LYS
3	C	15	VAL
3	C	20	THR
3	C	45	LYS
3	C	55	GLU
3	C	60	SER
3	C	69	ARG
3	C	94	VAL
3	C	97	THR
3	C	103	LYS
3	C	104	VAL
3	C	108	ARG
3	C	114	SER
3	C	125	LEU
3	C	129	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	133	VAL
3	C	135	LEU
3	C	202	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	229	ASN
1	G	460	ASN
2	H	31	ASN
2	H	199	ASN
3	L	160	GLN
1	A	229	ASN
1	A	344	GLN
2	B	199	ASN
3	C	138	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

29 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
4	NAG	G	730	1	14,14,15	0.45	0	17,19,21	0.88	1 (5%)
4	NAG	A	730	1	14,14,15	0.53	0	17,19,21	0.95	1 (5%)
4	NAG	A	734	1	14,14,15	0.46	0	17,19,21	0.91	1 (5%)
4	NAG	G	741	1	14,14,15	0.42	0	17,19,21	0.95	1 (5%)
4	NAG	A	892	1	14,14,15	0.63	0	17,19,21	1.10	1 (5%)
4	NAG	G	588	1	14,14,15	0.53	0	17,19,21	0.83	1 (5%)
4	NAG	A	948	1	14,14,15	0.49	0	17,19,21	1.24	3 (17%)
4	NAG	A	588	1	14,14,15	0.60	0	17,19,21	1.49	2 (11%)
4	NAG	G	839	1	14,14,15	0.55	0	17,19,21	0.98	1 (5%)
4	NAG	A	839	1	14,14,15	0.54	0	17,19,21	1.02	1 (5%)
4	NAG	G	963	1	14,14,15	0.50	0	17,19,21	0.78	1 (5%)
4	NAG	A	776	1	14,14,15	1.26	1 (7%)	17,19,21	1.34	1 (5%)
4	NAG	A	789	1	14,14,15	0.50	0	17,19,21	0.74	0
4	NAG	G	795	1	14,14,15	0.50	0	17,19,21	0.66	0
4	NAG	A	886	1	14,14,15	0.63	0	17,19,21	0.70	0
4	NAG	A	963	1	14,14,15	0.59	0	17,19,21	1.06	2 (11%)
5	SO4	G	1003	-	4,4,4	0.23	0	6,6,6	0.10	0
4	NAG	G	762	1	14,14,15	0.62	0	17,19,21	1.29	2 (11%)
4	NAG	A	795	1	14,14,15	0.53	0	17,19,21	0.78	0
4	NAG	G	789	1	14,14,15	0.45	0	17,19,21	0.84	0
4	NAG	G	856	1	14,14,15	0.57	0	17,19,21	1.40	2 (11%)
4	NAG	G	886	1	14,14,15	0.64	0	17,19,21	1.12	1 (5%)
4	NAG	A	856	1	14,14,15	0.57	0	17,19,21	1.34	2 (11%)
4	NAG	A	762	1	14,14,15	0.53	0	17,19,21	0.98	1 (5%)
4	NAG	G	948	1	14,14,15	0.41	0	17,19,21	2.26	4 (23%)
4	NAG	G	892	1	14,14,15	0.57	0	17,19,21	0.94	1 (5%)
4	NAG	G	734	1	14,14,15	0.61	0	17,19,21	1.00	1 (5%)
4	NAG	G	776	1	14,14,15	0.46	0	17,19,21	1.00	1 (5%)
4	NAG	A	741	1	14,14,15	0.58	0	17,19,21	0.72	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
4	NAG	G	730	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	730	1	-	4/6/23/26	0/1/1/1
4	NAG	A	734	1	-	1/6/23/26	0/1/1/1
4	NAG	G	741	1	-	2/6/23/26	0/1/1/1
4	NAG	A	892	1	-	4/6/23/26	0/1/1/1
4	NAG	G	588	1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	A	948	1	-	0/6/23/26	0/1/1/1
4	NAG	A	588	1	-	1/6/23/26	0/1/1/1
4	NAG	G	839	1	-	3/6/23/26	0/1/1/1
4	NAG	A	839	1	-	2/6/23/26	0/1/1/1
4	NAG	G	963	1	-	0/6/23/26	0/1/1/1
4	NAG	A	776	1	-	2/6/23/26	0/1/1/1
4	NAG	A	789	1	-	1/6/23/26	0/1/1/1
4	NAG	G	795	1	-	3/6/23/26	0/1/1/1
4	NAG	A	886	1	-	0/6/23/26	0/1/1/1
4	NAG	A	963	1	-	2/6/23/26	0/1/1/1
4	NAG	G	762	1	-	2/6/23/26	0/1/1/1
4	NAG	A	795	1	-	4/6/23/26	0/1/1/1
4	NAG	G	789	1	-	3/6/23/26	0/1/1/1
4	NAG	G	856	1	-	2/6/23/26	0/1/1/1
4	NAG	G	886	1	-	2/6/23/26	0/1/1/1
4	NAG	A	856	1	-	2/6/23/26	0/1/1/1
4	NAG	A	762	1	-	2/6/23/26	0/1/1/1
4	NAG	G	948	1	-	0/6/23/26	0/1/1/1
4	NAG	G	892	1	-	0/6/23/26	0/1/1/1
4	NAG	G	734	1	-	1/6/23/26	0/1/1/1
4	NAG	G	776	1	-	0/6/23/26	0/1/1/1
4	NAG	A	741	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	776	NAG	C8-C7	-4.28	1.41	1.50

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	948	NAG	C1-O5-C5	6.99	121.56	112.19
4	A	856	NAG	C1-O5-C5	4.24	117.86	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	948	NAG	C4-C3-C2	-4.13	104.96	111.02
4	A	588	NAG	C2-N2-C7	3.78	127.97	122.90
4	A	776	NAG	C2-N2-C7	-3.75	117.88	122.90
4	G	856	NAG	O5-C1-C2	3.73	117.07	111.29
4	G	762	NAG	C1-O5-C5	3.66	117.09	112.19
4	G	856	NAG	C1-O5-C5	3.46	116.82	112.19
4	A	948	NAG	C1-O5-C5	3.42	116.76	112.19
4	G	948	NAG	O5-C1-C2	3.10	116.08	111.29
4	A	892	NAG	C4-C3-C2	2.99	115.40	111.02
4	G	741	NAG	C1-O5-C5	2.99	116.19	112.19
4	G	886	NAG	C4-C3-C2	2.94	115.33	111.02
4	A	734	NAG	C1-O5-C5	2.74	115.86	112.19
4	G	730	NAG	C1-O5-C5	2.72	115.83	112.19
4	G	776	NAG	C1-O5-C5	2.66	115.75	112.19
4	G	762	NAG	O5-C1-C2	2.62	115.35	111.29
4	G	839	NAG	O5-C1-C2	2.62	115.35	111.29
4	A	963	NAG	C1-O5-C5	2.56	115.61	112.19
4	A	839	NAG	O5-C1-C2	2.43	115.05	111.29
4	A	963	NAG	O5-C1-C2	2.40	115.01	111.29
4	A	730	NAG	O5-C1-C2	2.38	114.97	111.29
4	G	734	NAG	O5-C1-C2	2.38	114.97	111.29
4	A	948	NAG	C4-C3-C2	-2.28	107.68	111.02
4	G	948	NAG	C2-N2-C7	-2.28	119.85	122.90
4	G	588	NAG	C1-O5-C5	2.24	115.19	112.19
4	A	948	NAG	C2-N2-C7	-2.23	119.92	122.90
4	A	762	NAG	C2-N2-C7	-2.20	119.95	122.90
4	G	963	NAG	C1-O5-C5	2.17	115.09	112.19
4	A	588	NAG	O5-C1-C2	2.17	114.64	111.29
4	G	892	NAG	C4-C3-C2	2.13	114.14	111.02
4	A	856	NAG	O5-C1-C2	2.01	114.40	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	G	588	NAG	C1

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	588	NAG	C3-C2-N2-C7
4	G	588	NAG	C8-C7-N2-C2
4	G	588	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	741	NAG	C8-C7-N2-C2
4	G	741	NAG	O7-C7-N2-C2
4	G	795	NAG	C3-C2-N2-C7
4	G	795	NAG	C8-C7-N2-C2
4	G	795	NAG	O7-C7-N2-C2
4	G	839	NAG	C8-C7-N2-C2
4	G	839	NAG	O7-C7-N2-C2
4	G	856	NAG	C8-C7-N2-C2
4	G	856	NAG	O7-C7-N2-C2
4	A	588	NAG	C3-C2-N2-C7
4	A	741	NAG	C8-C7-N2-C2
4	A	741	NAG	O7-C7-N2-C2
4	A	839	NAG	C8-C7-N2-C2
4	A	839	NAG	O7-C7-N2-C2
4	A	856	NAG	C8-C7-N2-C2
4	A	856	NAG	O7-C7-N2-C2
4	A	730	NAG	C8-C7-N2-C2
4	A	892	NAG	C8-C7-N2-C2
4	A	730	NAG	O7-C7-N2-C2
4	A	795	NAG	C8-C7-N2-C2
4	A	892	NAG	O7-C7-N2-C2
4	A	963	NAG	C8-C7-N2-C2
4	A	762	NAG	C4-C5-C6-O6
4	G	886	NAG	C8-C7-N2-C2
4	A	762	NAG	O5-C5-C6-O6
4	A	734	NAG	O5-C5-C6-O6
4	A	892	NAG	O5-C5-C6-O6
4	A	795	NAG	O7-C7-N2-C2
4	A	776	NAG	C4-C5-C6-O6
4	A	795	NAG	C4-C5-C6-O6
4	A	776	NAG	O5-C5-C6-O6
4	A	892	NAG	C4-C5-C6-O6
4	A	963	NAG	O7-C7-N2-C2
4	G	886	NAG	O7-C7-N2-C2
4	A	795	NAG	O5-C5-C6-O6
4	G	789	NAG	C4-C5-C6-O6
4	G	762	NAG	O5-C5-C6-O6
4	G	762	NAG	C4-C5-C6-O6
4	A	789	NAG	C4-C5-C6-O6
4	G	588	NAG	C1-C2-N2-C7
4	G	734	NAG	C1-C2-N2-C7
4	G	839	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	730	NAG	C4-C5-C6-O6
4	A	741	NAG	O5-C5-C6-O6
4	G	789	NAG	C8-C7-N2-C2
4	A	730	NAG	O5-C5-C6-O6
4	G	789	NAG	O7-C7-N2-C2

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	734	NAG	1	0
4	A	588	NAG	2	0
4	G	963	NAG	4	0
4	A	789	NAG	2	0
4	A	886	NAG	1	0
5	G	1003	SO4	1	0
4	G	762	NAG	2	0
4	A	795	NAG	3	0
4	G	886	NAG	1	0
4	A	762	NAG	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	303/317 (95%)	-0.29	0 100 100	95, 125, 199, 271	0
1	G	306/317 (96%)	-0.32	0 100 100	92, 125, 205, 271	0
2	B	229/231 (99%)	-0.31	1 (0%) 88 79	100, 167, 237, 289	0
2	H	229/231 (99%)	-0.17	0 100 100	91, 165, 234, 288	0
3	C	214/215 (99%)	-0.21	2 (0%) 81 64	104, 151, 234, 303	0
3	L	214/215 (99%)	-0.23	0 100 100	93, 145, 232, 262	0
All	All	1495/1526 (97%)	-0.26	3 (0%) 91 85	91, 142, 231, 303	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	178	THR	2.3
3	C	102	THR	2.2
2	B	139	GLY	2.2

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](#)

There are no oligosaccharides in this entry.

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. 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	B-factors(Å ²)	Q<0.9
4	NAG	A	856	14/15	-0.11	0.17	170,250,287,291	0
4	NAG	G	856	14/15	-0.05	0.13	184,252,279,292	0
4	NAG	A	588	14/15	0.32	0.13	143,206,225,236	0
4	NAG	A	963	14/15	0.41	0.11	170,225,242,246	0
4	NAG	G	730	14/15	0.47	0.09	158,229,236,237	0
4	NAG	A	730	14/15	0.48	0.11	180,212,233,238	0
4	NAG	G	588	14/15	0.52	0.09	187,247,265,266	0
4	NAG	A	741	14/15	0.59	0.12	113,213,241,245	0
4	NAG	G	741	14/15	0.60	0.12	146,204,232,238	0
4	NAG	G	734	14/15	0.70	0.09	158,195,210,225	0
4	NAG	A	776	14/15	0.70	0.09	133,183,194,197	0
5	SO4	G	1003	5/5	0.73	0.09	162,173,190,220	0
4	NAG	A	734	14/15	0.74	0.10	165,188,209,216	0
4	NAG	A	892	14/15	0.74	0.11	132,192,205,212	0
4	NAG	A	839	14/15	0.75	0.10	131,213,220,222	0
4	NAG	G	776	14/15	0.81	0.08	151,175,183,195	0
4	NAG	G	892	14/15	0.83	0.08	118,177,197,209	0
4	NAG	G	839	14/15	0.84	0.10	153,188,211,216	0
4	NAG	G	795	14/15	0.85	0.10	124,161,166,195	0
4	NAG	G	963	14/15	0.85	0.07	211,229,239,241	0
4	NAG	A	795	14/15	0.86	0.09	120,152,170,189	0
4	NAG	A	789	14/15	0.86	0.09	112,128,141,152	0
4	NAG	G	948	14/15	0.87	0.08	86,148,198,201	0
4	NAG	A	948	14/15	0.88	0.08	117,140,165,165	0
4	NAG	G	789	14/15	0.89	0.10	108,146,178,179	0
4	NAG	A	886	14/15	0.92	0.10	113,154,172,179	0
4	NAG	G	886	14/15	0.94	0.08	109,142,159,171	0
4	NAG	G	762	14/15	0.96	0.07	76,96,128,130	0
4	NAG	A	762	14/15	0.96	0.08	77,94,125,144	0

6.5 Other polymers ⓘ

There are no such residues in this entry.