



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 05:04 PM BST

PDB ID : 3HI1
Title : Structure of HIV-1 gp120 (core with V3) in Complex with CD4-Binding-Site Antibody F105
Authors : Kwon, Y.D.; Chen, L.; Zhou, T.; Wu, X.; O'Dell, S.; Cavacini, L.; Hessel, A.J.; Pancera, M.; Tang, M.; Xu, L.; Yang, Z.; Zhang, M.-Y.; Arthos, J.; Burton, D.R.; Dimitrov, D.; Nabel, G.J.; Posner, M.; Sodroski, J.; Wyatt, R.; Mascola, J.R.; Kwong, P.D.
Deposited on : 2009-05-18
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

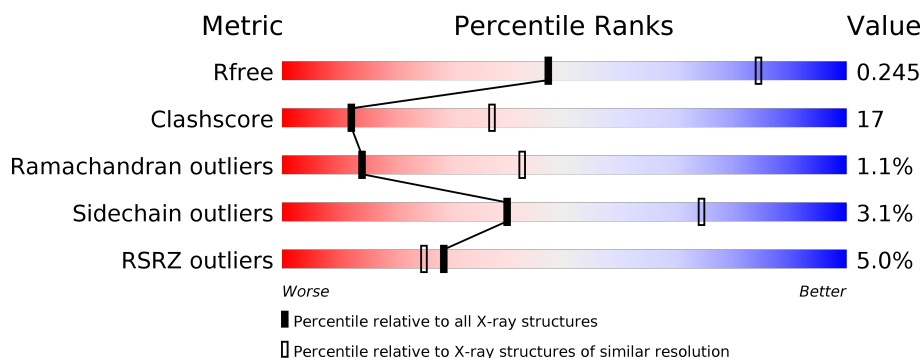
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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	G	321	<div> <div>7%</div> <div> <div></div> <div>59%</div> <div>28%</div> <div>•</div> <div>10%</div> </div> </div>
1	J	321	<div> <div>11%</div> <div> <div></div> <div>59%</div> <div>28%</div> <div>•</div> <div>10%</div> </div> </div>
2	A	215	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>•</div> </div> </div>
2	L	215	<div> <div></div> <div> <div></div> <div>77%</div> <div>21%</div> <div>•</div> </div> </div>
3	B	225	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>•</div> </div> </div>
3	H	225	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>27%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	G	801	-	-	-	X
4	NAG	G	856	-	-	-	X
4	NAG	G	894	-	-	-	X
4	NAG	G	963	-	-	-	X
4	NAG	J	801	X	-	-	X
4	NAG	J	894	X	-	-	-
4	NAG	J	913	X	-	-	X
4	NAG	J	963	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11670 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 Glycoprotein 120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	289	Total	C	N	O	S	0	0	0
			2276	1428	401	429	18			
1	J	289	Total	C	N	O	S	0	0	0
			2276	1428	401	429	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	124	GLY	-	linker	UNP P35961
G	198	GLY	-	linker	UNP P35961

- Molecule 2 is a protein called F105 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	0	0
			1651	1027	282	336	6			
2	A	215	Total	C	N	O	S	0	0	0
			1651	1027	282	336	6			

- Molecule 3 is a protein called F105 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	225	Total	C	N	O	S	0	0	0
			1680	1067	276	332	5			
3	B	225	Total	C	N	O	S	0	0	0
			1680	1067	276	332	5			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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	J	1	Total	C	N	O	0	0
			14	8	1	5		

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

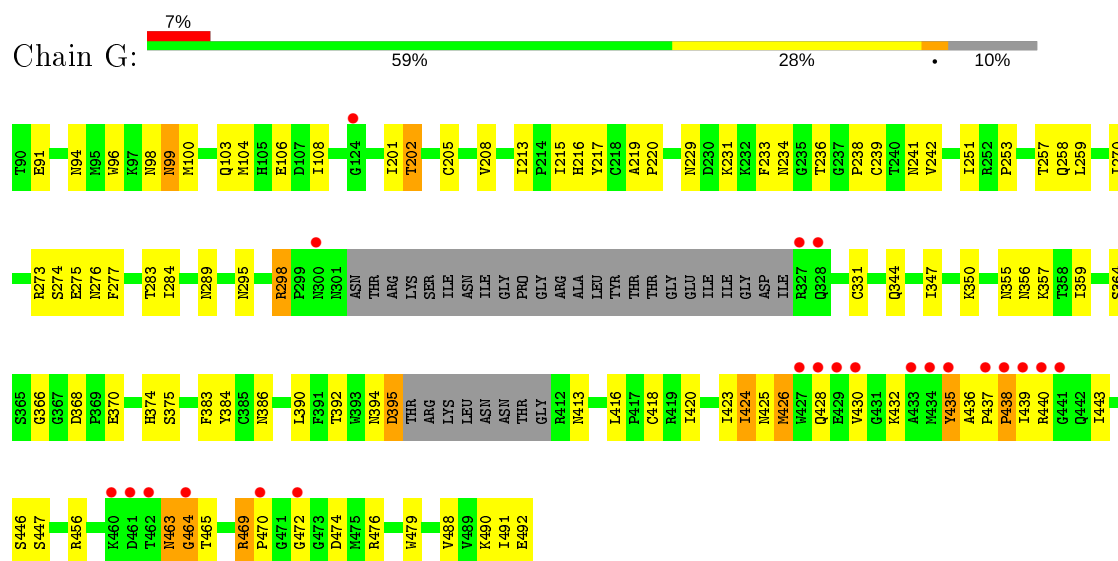
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	8	Total	O	0	0
			8	8		
5	L	22	Total	O	0	0
			22	22		
5	H	42	Total	O	0	0
			42	42		
5	J	2	Total	O	0	0
			2	2		
5	A	2	Total	O	0	0
			2	2		
5	B	2	Total	O	0	0
			2	2		

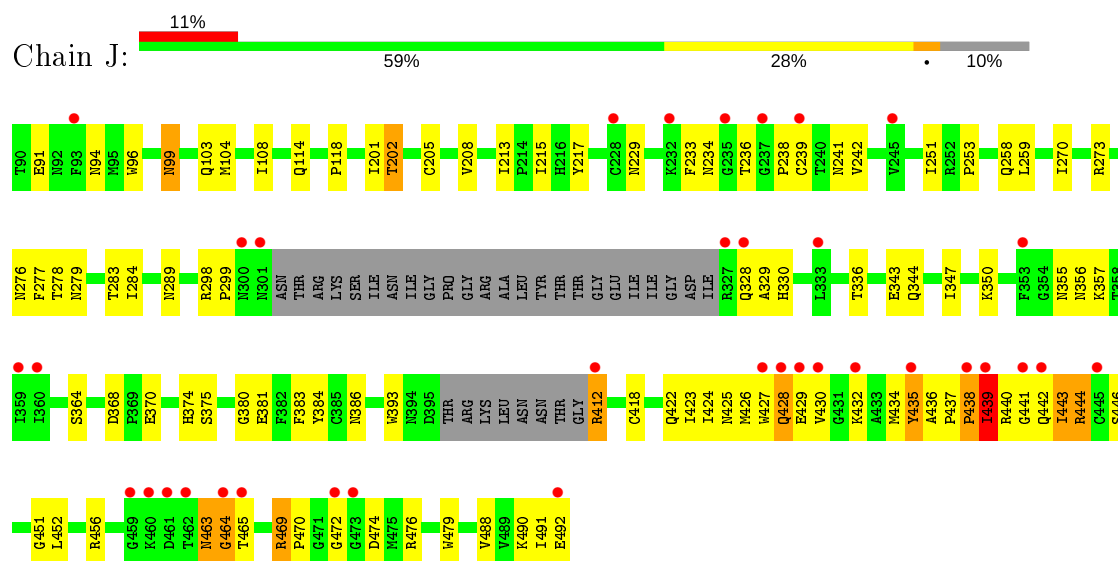
3 Residue-property plots [i](#)

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: Glycoprotein 120

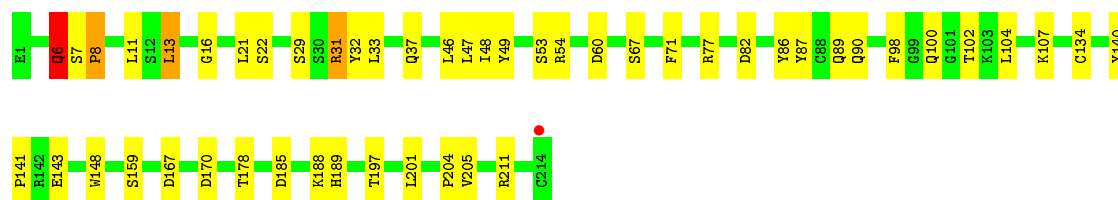


• Molecule 1: Glycoprotein 120




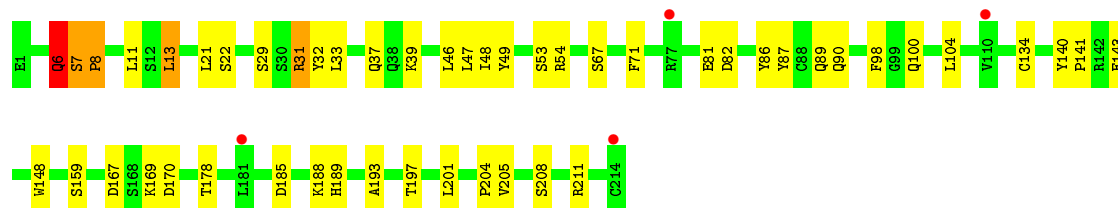
• Molecule 2: F105 Light Chain

Chain L:  77% 21% .



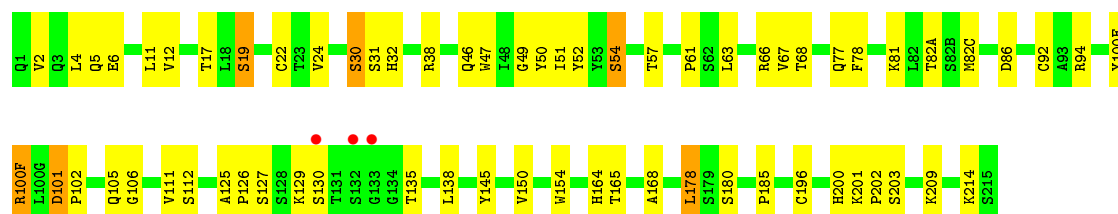
• Molecule 2: F105 Light Chain

Chain A:  77% 21% .



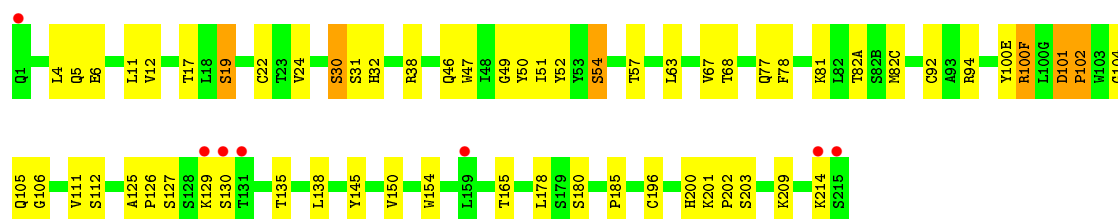
• Molecule 3: F105 Heavy Chain

Chain H:  71% 27% .



• Molecule 3: F105 Heavy Chain

Chain B:  73% 24% .



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	412.40Å 412.40Å 83.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.48 – 2.90 41.24 – 2.80	Depositor EDS
% Data completeness (in resolution range)	75.5 (43.48-2.90) 68.5 (41.24-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.243 0.208 , 0.245	Depositor DCC
R_{free} test set	2414 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	70.5	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11670	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: NAG

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	G	0.31	0/2321	0.49	0/3142
1	J	0.28	0/2321	0.48	1/3142 (0.0%)
2	A	0.30	0/1684	0.51	0/2283
2	L	0.34	0/1684	0.52	0/2283
3	B	0.30	0/1725	0.49	0/2357
3	H	0.37	0/1725	0.52	0/2357
All	All	0.32	0/11460	0.50	1/15564 (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	G	0	1
1	J	0	1
2	A	0	1
2	L	0	1
3	B	0	1
3	H	0	1
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	330	HIS	N-CA-CB	-5.04	101.53	110.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	6	GLN	Peptide
3	B	101	ASP	Peptide
1	G	469	ARG	Peptide
3	H	101	ASP	Peptide
1	J	469	ARG	Peptide
2	L	6	GLN	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	G	2276	0	2221	108	0
1	J	2276	0	2217	103	0
2	A	1651	0	1602	45	0
2	L	1651	0	1602	43	0
3	B	1680	0	1661	55	0
3	H	1680	0	1661	61	0
4	G	182	0	169	9	0
4	J	196	0	182	10	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	G	8	0	0	0	0
5	H	42	0	0	4	0
5	J	2	0	0	1	0
5	L	22	0	0	1	0
All	All	11670	0	11315	390	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 17.

All (390) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:426:MET:SD	2:A:32:TYR:OH	1.98	1.20
2:A:7:SER:HB3	2:A:8:PRO:HD3	1.32	1.07
2:A:7:SER:HB3	2:A:8:PRO:CD	1.87	1.04
2:A:7:SER:CB	2:A:8:PRO:HD3	1.87	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:ASN:HB2	1:J:202:THR:HG23	1.37	1.03
2:L:7:SER:CB	2:L:22:SER:H	1.71	1.02
1:G:469:ARG:HB3	1:G:470:PRO:CD	1.89	1.02
2:L:7:SER:HB2	2:L:22:SER:H	1.20	1.02
2:A:7:SER:HB2	2:A:22:SER:H	1.21	1.00
1:G:428:GLN:HE22	1:G:432:LYS:HG2	1.27	0.99
1:G:425:ASN:HB3	1:G:426:MET:HA	1.46	0.95
1:G:463:ASN:HB2	4:G:963:NAG:H2	1.47	0.95
1:G:202:THR:HG23	1:J:99:ASN:HB2	1.48	0.95
2:A:7:SER:CB	2:A:22:SER:H	1.79	0.95
1:G:425:ASN:CB	1:G:426:MET:HA	1.97	0.95
1:G:469:ARG:CB	1:G:470:PRO:HD3	1.96	0.93
1:J:441:GLY:H	1:J:442:GLN:HA	1.34	0.93
2:L:7:SER:HB2	2:L:22:SER:N	1.84	0.92
1:G:469:ARG:HB3	1:G:470:PRO:HD3	1.45	0.92
1:J:444:ARG:HD3	1:J:444:ARG:H	1.34	0.90
2:A:7:SER:HB2	2:A:22:SER:N	1.87	0.89
1:G:425:ASN:HB3	1:G:426:MET:CA	2.04	0.87
1:G:201:ILE:HG22	1:J:99:ASN:HB3	1.53	0.86
1:G:99:ASN:HB3	1:J:201:ILE:HG22	1.59	0.85
3:H:17:THR:HG22	5:H:243:HOH:O	1.78	0.84
1:J:441:GLY:N	1:J:442:GLN:HA	1.88	0.84
2:L:7:SER:HB3	2:L:8:PRO:HD2	1.57	0.84
1:G:368:ASP:H	3:H:32:HIS:HE1	1.25	0.84
1:G:436:ALA:HB1	1:G:437:PRO:CD	2.07	0.84
1:J:336:THR:OG1	1:J:412:ARG:HG2	1.78	0.83
2:L:189:HIS:O	2:L:211:ARG:NH1	2.11	0.82
2:A:189:HIS:O	2:A:211:ARG:NH1	2.13	0.82
1:G:435:TYR:HD2	1:G:436:ALA:H	1.25	0.82
2:L:31:ARG:NH2	3:H:100(E):TYR:HE1	1.78	0.82
1:G:216:HIS:CE1	1:J:440:ARG:HG2	2.15	0.81
3:H:38:ARG:HE	3:H:46:GLN:NE2	1.78	0.81
3:B:38:ARG:HE	3:B:46:GLN:NE2	1.79	0.80
1:G:428:GLN:NE2	1:G:432:LYS:HG2	1.96	0.80
1:J:429:GLU:HG2	1:J:430:VAL:H	1.46	0.80
2:L:7:SER:CB	2:L:8:PRO:CD	2.61	0.79
1:G:463:ASN:C	1:G:465:THR:H	1.86	0.78
1:G:436:ALA:HB1	1:G:437:PRO:HD2	1.65	0.77
1:G:274:SER:OG	1:G:276:ASN:O	2.03	0.76
1:J:463:ASN:C	1:J:465:THR:H	1.89	0.76
2:A:7:SER:CB	2:A:8:PRO:CD	2.54	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:435:TYR:HD2	1:J:436:ALA:H	1.33	0.75
2:L:7:SER:OG	2:L:8:PRO:HD3	1.87	0.75
3:H:17:THR:CG2	5:H:243:HOH:O	2.35	0.74
1:J:444:ARG:HD3	1:J:444:ARG:N	2.00	0.74
3:B:19:SER:HB3	3:B:81:LYS:NZ	2.02	0.74
2:A:33:LEU:HD22	2:A:71:PHE:CD2	2.23	0.73
1:G:216:HIS:HE1	1:J:440:ARG:HG2	1.51	0.73
1:G:469:ARG:CB	1:G:470:PRO:CD	2.57	0.71
2:A:33:LEU:HD22	2:A:71:PHE:CG	2.24	0.71
1:G:447:SER:HB3	4:G:762:NAG:HN2	1.55	0.71
1:G:94:ASN:HD22	1:G:236:THR:HG22	1.57	0.70
3:H:52:TYR:CD2	3:H:54:SER:HB3	2.27	0.70
1:J:469:ARG:HB3	1:J:470:PRO:HD2	1.74	0.70
3:H:19:SER:HB3	3:H:81:LYS:NZ	2.06	0.69
2:L:33:LEU:HD22	2:L:71:PHE:CG	2.27	0.69
2:L:67:SER:HA	2:L:71:PHE:CE2	2.27	0.69
2:L:31:ARG:NH2	3:H:100(E):TYR:CE1	2.60	0.69
1:J:469:ARG:HB3	1:J:470:PRO:CD	2.23	0.69
1:G:424:ILE:O	1:G:425:ASN:HB2	1.93	0.68
2:L:7:SER:HB3	2:L:8:PRO:CD	2.23	0.68
2:L:33:LEU:HD22	2:L:71:PHE:CD2	2.27	0.68
1:G:469:ARG:HB3	1:G:470:PRO:HD2	1.74	0.67
1:J:94:ASN:HD22	1:J:236:THR:HG22	1.60	0.67
3:B:126:PRO:HG3	3:B:138:LEU:HB3	1.78	0.66
1:G:277:PHE:O	1:G:456:ARG:NH2	2.29	0.66
3:B:52:TYR:CD2	3:B:54:SER:HB3	2.30	0.66
1:G:370:GLU:HG3	1:G:384:TYR:CE2	2.30	0.66
1:G:368:ASP:H	3:H:32:HIS:CE1	2.11	0.66
4:J:795:NAG:H62	4:J:913:NAG:H62	1.77	0.66
3:H:178:LEU:C	3:H:178:LEU:HD12	2.16	0.65
1:J:370:GLU:HG3	1:J:384:TYR:CE2	2.31	0.65
2:A:67:SER:HA	2:A:71:PHE:CE2	2.32	0.65
1:J:357:LYS:HB3	1:J:464:GLY:O	1.97	0.64
1:J:251:ILE:O	1:J:253:PRO:HD3	1.98	0.64
1:G:463:ASN:O	1:G:465:THR:N	2.31	0.64
1:G:99:ASN:CB	1:J:202:THR:HG23	2.21	0.64
3:H:126:PRO:HG3	3:H:138:LEU:HB3	1.79	0.63
1:G:463:ASN:C	1:G:465:THR:N	2.49	0.63
1:J:329:ALA:O	1:J:418:CYS:HB2	1.98	0.63
3:H:38:ARG:HE	3:H:46:GLN:HE21	1.47	0.63
2:L:197:THR:HG22	2:L:204:PRO:HG3	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:7:SER:HB2	2:L:22:SER:CA	2.28	0.63
3:B:178:LEU:C	3:B:178:LEU:HD12	2.19	0.62
1:J:463:ASN:C	1:J:465:THR:N	2.51	0.62
1:J:336:THR:HG1	1:J:412:ARG:HG2	1.63	0.62
3:B:19:SER:HB3	3:B:81:LYS:HZ3	1.63	0.62
1:J:299:PRO:HB3	1:J:328:GLN:HB2	1.80	0.62
1:G:357:LYS:HB3	1:G:464:GLY:O	2.00	0.62
3:B:68:THR:HB	3:B:81:LYS:HB3	1.82	0.62
1:G:463:ASN:CB	4:G:963:NAG:H2	2.27	0.61
2:A:31:ARG:NH2	3:B:100(E):TYR:HE1	1.98	0.61
2:A:197:THR:HG22	2:A:204:PRO:HG3	1.83	0.61
1:J:463:ASN:O	1:J:465:THR:N	2.34	0.61
2:A:7:SER:OG	2:A:8:PRO:HD3	2.01	0.60
3:H:19:SER:HB3	3:H:81:LYS:HZ2	1.66	0.60
1:J:380:GLY:O	1:J:423:ILE:HG13	2.01	0.60
3:B:17:THR:HG22	3:B:82(A):THR:HA	1.83	0.60
1:J:336:THR:H	1:J:412:ARG:HB3	1.65	0.60
1:J:364:SER:HB2	1:J:470:PRO:HG2	1.83	0.60
1:G:251:ILE:O	1:G:253:PRO:HD3	2.01	0.60
3:H:138:LEU:N	3:H:138:LEU:HD23	2.17	0.59
3:H:200:HIS:ND1	3:H:203:SER:OG	2.25	0.59
1:J:118:PRO:HG3	1:J:428:GLN:HG3	1.85	0.59
2:L:21:LEU:HD12	2:L:21:LEU:N	2.19	0.58
2:A:31:ARG:NH2	3:B:100(E):TYR:CE1	2.71	0.58
3:H:17:THR:HG22	3:H:82(A):THR:HA	1.85	0.58
1:G:474:ASP:OD2	1:G:476:ARG:HB2	2.03	0.58
1:J:239:CYS:SG	1:J:242:VAL:HG22	2.43	0.58
2:L:201:LEU:HD13	2:L:205:VAL:HG23	1.84	0.58
1:J:444:ARG:N	1:J:444:ARG:CD	2.67	0.57
3:B:47:TRP:CZ2	3:B:49:GLY:HA2	2.40	0.57
3:H:68:THR:HB	3:H:81:LYS:HB3	1.85	0.57
1:G:474:ASP:HB3	3:H:52:TYR:OH	2.04	0.57
1:J:424:ILE:O	1:J:425:ASN:C	2.42	0.57
3:B:38:ARG:HE	3:B:46:GLN:HE21	1.53	0.56
2:L:7:SER:OG	2:L:8:PRO:CD	2.53	0.56
1:J:476:ARG:HH22	3:B:54:SER:HB2	1.69	0.56
3:B:138:LEU:N	3:B:138:LEU:HD23	2.21	0.56
1:G:239:CYS:SG	1:G:242:VAL:HG22	2.46	0.56
1:J:350:LYS:HB3	1:J:355:ASN:HA	1.88	0.56
2:A:21:LEU:HD12	2:A:21:LEU:N	2.21	0.55
3:B:19:SER:HB3	3:B:81:LYS:HZ2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:427:TRP:O	1:J:428:GLN:HB2	2.06	0.55
2:A:48:ILE:HD13	2:A:54:ARG:HA	1.88	0.55
1:G:357:LYS:HZ3	4:G:856:NAG:HN2	1.55	0.55
1:J:344:GLN:OE1	4:J:789:NAG:H62	2.06	0.55
3:B:125:ALA:CB	3:B:214:LYS:HE3	2.37	0.55
1:J:96:TRP:CE3	1:J:236:THR:CG2	2.90	0.55
1:G:103:GLN:NE2	1:G:103:GLN:HA	2.21	0.54
4:J:795:NAG:H62	4:J:913:NAG:C6	2.37	0.54
1:J:103:GLN:NE2	1:J:103:GLN:HA	2.22	0.54
3:B:201:LYS:HB2	3:B:202:PRO:HD3	1.88	0.54
1:G:202:THR:HG23	1:J:99:ASN:CB	2.31	0.54
3:H:138:LEU:HD23	3:H:138:LEU:H	1.72	0.54
1:G:96:TRP:CE3	1:G:236:THR:HG21	2.43	0.54
1:G:99:ASN:HB2	1:J:202:THR:CG2	2.26	0.54
1:G:350:LYS:HB3	1:G:355:ASN:HA	1.90	0.54
1:G:96:TRP:CE3	1:G:236:THR:CG2	2.89	0.54
3:H:125:ALA:CB	3:H:214:LYS:HE3	2.38	0.54
3:H:201:LYS:HB2	3:H:202:PRO:HD3	1.90	0.53
1:G:344:GLN:HA	1:G:347:ILE:HD12	1.90	0.53
1:J:259:LEU:HB2	1:J:374:HIS:CE1	2.44	0.53
2:A:37:GLN:HG3	2:A:86:TYR:CE2	2.44	0.53
1:G:259:LEU:HB2	1:G:374:HIS:CE1	2.43	0.53
1:G:344:GLN:OE1	4:G:789:NAG:H61	2.09	0.53
1:G:108:ILE:HD13	1:G:479:TRP:CZ2	2.43	0.53
1:G:96:TRP:CZ3	1:G:236:THR:HG23	2.44	0.53
1:J:96:TRP:CE3	1:J:236:THR:HG21	2.44	0.53
1:G:283:THR:HG23	1:G:472:GLY:HA3	1.90	0.53
2:L:48:ILE:HD13	2:L:54:ARG:HA	1.90	0.53
1:J:430:VAL:HG12	1:J:430:VAL:O	2.09	0.52
1:J:276:ASN:HB3	1:J:279:ASN:HB3	1.91	0.52
3:H:47:TRP:CZ2	3:H:49:GLY:HA2	2.45	0.52
2:L:67:SER:HA	2:L:71:PHE:CZ	2.44	0.52
1:J:91:GLU:O	1:J:238:PRO:HA	2.10	0.52
1:J:370:GLU:HG3	1:J:384:TYR:HE2	1.73	0.52
1:J:474:ASP:OD2	1:J:476:ARG:HB2	2.09	0.52
1:G:104:MET:HA	1:G:217:TYR:OH	2.10	0.51
1:G:233:PHE:O	1:G:273:ARG:NH1	2.43	0.51
1:G:370:GLU:HG3	1:G:384:TYR:HE2	1.73	0.51
3:H:19:SER:HB3	3:H:81:LYS:HZ3	1.75	0.51
1:G:213:ILE:HD12	1:J:213:ILE:HD12	1.93	0.51
1:J:299:PRO:HD3	1:J:329:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:11:LEU:HD21	2:A:13:LEU:HD11	1.93	0.51
1:G:428:GLN:HE22	1:G:432:LYS:CG	2.11	0.51
1:J:233:PHE:O	1:J:273:ARG:NH1	2.44	0.51
1:G:295:ASN:HA	1:G:446:SER:HB3	1.93	0.50
1:G:491:ILE:O	1:G:492:GLU:HB3	2.10	0.50
1:G:96:TRP:HE3	1:G:236:THR:HG21	1.75	0.50
3:H:51:ILE:HG13	3:H:57:THR:HG22	1.93	0.50
1:J:491:ILE:O	1:J:492:GLU:HB3	2.11	0.50
2:L:37:GLN:HG3	2:L:86:TYR:CE2	2.46	0.50
1:G:91:GLU:O	1:G:238:PRO:HA	2.10	0.50
1:G:201:ILE:HD12	1:J:103:GLN:NE2	2.27	0.50
1:J:108:ILE:HD13	1:J:479:TRP:CZ2	2.47	0.50
1:G:384:TYR:O	1:G:418:CYS:HA	2.12	0.50
2:A:7:SER:HB3	2:A:8:PRO:HD2	1.87	0.50
2:L:11:LEU:HD21	2:L:13:LEU:HD11	1.92	0.50
3:H:11:LEU:HD11	3:H:112:SER:HB3	1.93	0.50
2:A:37:GLN:HB2	2:A:47:LEU:HD22	1.94	0.50
3:B:101:ASP:O	3:B:102:PRO:O	2.30	0.50
1:J:96:TRP:HE3	1:J:236:THR:HG21	1.76	0.50
1:J:96:TRP:CZ3	1:J:236:THR:HG23	2.46	0.50
3:B:22:CYS:O	3:B:77:GLN:HB2	2.12	0.49
1:G:298:ARG:HG3	1:G:443:ILE:HG13	1.94	0.49
3:H:4:LEU:HB3	3:H:22:CYS:SG	2.52	0.49
1:J:443:ILE:HG22	1:J:444:ARG:H	1.77	0.49
2:A:49:TYR:O	2:A:53:SER:HB2	2.12	0.49
1:G:463:ASN:N	1:G:463:ASN:OD1	2.43	0.49
1:J:104:MET:HA	1:J:217:TYR:OH	2.12	0.49
1:G:430:VAL:O	1:G:430:VAL:HG12	2.13	0.49
1:J:344:GLN:HA	1:J:347:ILE:HD12	1.93	0.49
1:J:463:ASN:OD1	1:J:463:ASN:N	2.46	0.49
2:L:89:GLN:HB2	2:L:98:PHE:CD2	2.47	0.49
3:B:30:SER:O	3:B:32:HIS:HD2	1.95	0.49
1:G:386:ASN:O	1:G:416:LEU:HD22	2.13	0.49
2:L:140:TYR:CG	2:L:141:PRO:HA	2.47	0.49
1:J:357:LYS:CB	1:J:464:GLY:O	2.60	0.49
2:L:37:GLN:HB2	2:L:47:LEU:HD22	1.94	0.49
3:H:94:ARG:HB3	3:H:101:ASP:O	2.13	0.49
3:H:178:LEU:O	3:H:178:LEU:HD12	2.13	0.49
1:J:258:GLN:HA	1:J:470:PRO:O	2.12	0.49
2:A:89:GLN:HB2	2:A:98:PHE:CD2	2.48	0.49
1:G:390:LEU:HD11	1:G:416:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:436:ALA:CB	1:G:437:PRO:CD	2.80	0.49
3:B:101:ASP:C	3:B:102:PRO:O	2.51	0.48
1:J:278:THR:HB	4:J:776:NAG:H5	1.95	0.48
3:B:12:VAL:O	3:B:111:VAL:HA	2.13	0.48
3:B:154:TRP:CZ3	3:B:196:CYS:HB3	2.48	0.48
1:G:420:ILE:HG22	1:G:420:ILE:O	2.13	0.48
1:G:270:ILE:HG12	4:G:789:NAG:H62	1.95	0.48
3:H:12:VAL:O	3:H:111:VAL:HA	2.12	0.48
3:B:200:HIS:ND1	3:B:203:SER:OG	2.30	0.48
1:G:234:ASN:HB2	4:G:734:NAG:C7	2.43	0.48
3:B:22:CYS:HB3	3:B:78:PHE:CE2	2.48	0.48
1:G:370:GLU:CD	1:G:370:GLU:H	2.17	0.48
2:L:167:ASP:HB3	2:L:170:ASP:OD1	2.13	0.48
3:H:178:LEU:C	3:H:178:LEU:CD1	2.81	0.48
3:H:30:SER:O	3:H:32:HIS:HD2	1.96	0.47
1:J:429:GLU:CG	1:J:430:VAL:H	2.22	0.47
2:A:140:TYR:CG	2:A:141:PRO:HA	2.48	0.47
3:H:30:SER:O	3:H:31:SER:HB2	2.14	0.47
1:G:94:ASN:HA	1:G:236:THR:HG22	1.96	0.47
1:J:370:GLU:CD	1:J:370:GLU:H	2.18	0.47
3:H:154:TRP:CZ3	3:H:196:CYS:HB3	2.50	0.47
2:L:143:GLU:CD	2:L:143:GLU:H	2.18	0.47
1:J:368:ASP:H	3:B:32:HIS:HE1	1.63	0.47
3:B:52:TYR:HD2	3:B:54:SER:HB3	1.77	0.47
1:G:96:TRP:CZ3	1:G:236:THR:CG2	2.98	0.47
1:J:229:ASN:HB2	1:J:241:ASN:O	2.15	0.47
2:L:170:ASP:OD1	2:L:170:ASP:C	2.52	0.47
3:H:22:CYS:O	3:H:77:GLN:HB2	2.14	0.47
2:L:6:GLN:HE21	2:L:6:GLN:HB3	1.52	0.47
2:A:67:SER:HA	2:A:71:PHE:CZ	2.49	0.47
1:G:357:LYS:CB	1:G:464:GLY:O	2.62	0.47
1:G:103:GLN:NE2	1:J:201:ILE:HD12	2.30	0.47
3:B:11:LEU:HD11	3:B:112:SER:HB3	1.96	0.47
3:B:138:LEU:H	3:B:138:LEU:HD23	1.78	0.47
1:G:375:SER:HA	1:G:383:PHE:O	2.15	0.47
1:G:438:PRO:HG2	1:G:439:ILE:H	1.78	0.47
1:J:234:ASN:HB2	4:J:734:NAG:C7	2.44	0.47
1:J:375:SER:HA	1:J:383:PHE:O	2.15	0.47
3:B:78:PHE:CZ	3:B:92:CYS:HB2	2.50	0.47
1:G:94:ASN:HD22	1:G:236:THR:CG2	2.27	0.47
1:J:429:GLU:HG2	1:J:430:VAL:N	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:143:GLU:CD	2:A:143:GLU:H	2.17	0.47
1:G:270:ILE:HD13	1:G:289:ASN:H	1.80	0.47
1:G:435:TYR:CD2	1:G:436:ALA:N	2.79	0.47
1:J:94:ASN:HA	1:J:236:THR:HG22	1.97	0.47
1:G:215:ILE:HG12	1:J:208:VAL:HG22	1.97	0.46
1:J:356:ASN:HB3	4:J:856:NAG:H83	1.97	0.46
1:G:423:ILE:HD11	1:G:440:ARG:HH22	1.81	0.46
2:A:201:LEU:HD13	2:A:205:VAL:HG23	1.97	0.46
3:B:30:SER:O	3:B:31:SER:HB2	2.16	0.46
1:J:386:ASN:OD1	4:J:886:NAG:H2	2.13	0.46
2:L:107:LYS:O	5:L:232:HOH:O	2.20	0.46
3:B:4:LEU:HB3	3:B:22:CYS:SG	2.54	0.46
1:G:298:ARG:HB2	1:G:443:ILE:H	1.81	0.46
3:H:135:THR:HG22	3:H:185:PRO:HA	1.98	0.46
1:J:94:ASN:HD22	1:J:236:THR:CG2	2.28	0.46
2:L:8:PRO:O	2:L:102:THR:HG23	2.15	0.46
1:G:295:ASN:O	1:G:331:CYS:HA	2.16	0.46
1:J:343:GLU:HG2	1:J:393:TRP:HZ2	1.81	0.46
3:B:51:ILE:HG13	3:B:57:THR:HG22	1.97	0.46
1:J:270:ILE:HD13	1:J:289:ASN:H	1.81	0.46
4:J:913:NAG:N2	4:J:913:NAG:H5	2.31	0.46
2:L:46:LEU:HD22	3:H:100(F):ARG:HG3	1.98	0.46
3:B:165:THR:HG23	3:B:180:SER:HB2	1.98	0.45
3:B:6:GLU:CD	3:B:106:GLY:H	2.19	0.45
3:B:6:GLU:OE2	3:B:105:GLN:N	2.47	0.45
1:G:364:SER:N	1:G:470:PRO:HG2	2.31	0.45
3:H:145:TYR:CE2	3:H:150:VAL:HG13	2.51	0.45
1:G:435:TYR:HD2	1:G:436:ALA:N	2.02	0.45
3:H:164:HIS:HD2	5:H:246:HOH:O	1.99	0.45
3:H:22:CYS:HB3	3:H:78:PHE:CE2	2.52	0.45
1:J:432:LYS:C	1:J:434:MET:H	2.20	0.45
1:J:96:TRP:HE3	1:J:236:THR:CG2	2.29	0.45
2:A:193:ALA:HA	2:A:208:SER:HB3	1.98	0.45
3:H:125:ALA:HA	3:H:126:PRO:HD3	1.82	0.45
2:L:49:TYR:O	2:L:53:SER:HB2	2.17	0.45
2:A:167:ASP:HB3	2:A:170:ASP:OD1	2.17	0.45
1:G:96:TRP:CE3	1:G:236:THR:HG23	2.52	0.45
1:J:277:PHE:O	1:J:456:ARG:NH2	2.50	0.45
3:B:94:ARG:HB3	3:B:101:ASP:O	2.15	0.45
1:G:229:ASN:HB2	1:G:241:ASN:O	2.16	0.45
3:B:63:LEU:O	3:B:67:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:96:TRP:CE3	1:J:236:THR:HG23	2.52	0.45
2:A:46:LEU:HD22	3:B:100(F):ARG:HG3	1.99	0.45
3:B:178:LEU:C	3:B:178:LEU:CD1	2.84	0.45
1:J:96:TRP:CZ3	1:J:236:THR:CG2	3.00	0.45
2:A:6:GLN:HB3	2:A:6:GLN:HE21	1.53	0.44
3:B:129:LYS:O	3:B:130:SER:C	2.56	0.44
3:H:125:ALA:HB3	3:H:214:LYS:HE3	1.97	0.44
2:A:29:SER:HB3	2:A:32:TYR:CD1	2.53	0.44
3:H:4:LEU:HD22	3:H:24:VAL:HG22	1.98	0.44
3:H:63:LEU:O	3:H:67:VAL:HG23	2.17	0.44
3:B:4:LEU:HD22	3:B:24:VAL:HG22	1.99	0.44
1:G:96:TRP:HE3	1:G:236:THR:CG2	2.29	0.44
1:G:356:ASN:OD1	4:G:856:NAG:O5	2.34	0.44
2:L:82:ASP:O	2:L:104:LEU:HD23	2.17	0.44
3:B:125:ALA:HB3	3:B:214:LYS:HE3	2.00	0.44
3:H:129:LYS:O	3:H:130:SER:C	2.56	0.44
3:H:154:TRP:CH2	3:H:196:CYS:HB3	2.53	0.44
2:L:185:ASP:O	2:L:188:LYS:HG2	2.17	0.44
2:A:82:ASP:O	2:A:104:LEU:HD23	2.18	0.44
2:A:32:TYR:O	2:A:90:GLN:HA	2.16	0.44
3:B:154:TRP:CH2	3:B:196:CYS:HB3	2.52	0.44
1:J:434:MET:O	1:J:435:TYR:CB	2.65	0.44
2:A:170:ASP:C	2:A:170:ASP:OD1	2.56	0.43
1:J:283:THR:HG22	1:J:284:ILE:N	2.33	0.43
2:A:134:CYS:HB2	2:A:148:TRP:CZ2	2.53	0.43
3:B:78:PHE:HZ	3:B:92:CYS:HB2	1.83	0.43
2:A:185:ASP:O	2:A:188:LYS:HG2	2.17	0.43
1:G:275:GLU:O	1:G:276:ASN:HB2	2.18	0.43
1:G:490:LYS:HG2	1:G:491:ILE:N	2.33	0.43
3:H:52:TYR:HD2	3:H:54:SER:HB3	1.78	0.43
3:H:61:PRO:HG2	5:H:236:HOH:O	2.18	0.43
1:G:216:HIS:CE1	1:J:440:ARG:CG	2.97	0.43
1:J:440:ARG:HA	1:J:441:GLY:HA2	1.67	0.43
3:B:50:TYR:CD2	3:B:50:TYR:C	2.91	0.43
1:G:103:GLN:O	1:G:106:GLU:HB2	2.19	0.43
1:G:283:THR:HG22	1:G:284:ILE:N	2.33	0.43
2:L:134:CYS:HB2	2:L:148:TRP:CZ2	2.54	0.43
1:J:276:ASN:HB3	1:J:279:ASN:CB	2.49	0.43
3:H:6:GLU:CD	3:H:106:GLY:H	2.22	0.43
1:G:258:GLN:HA	1:G:470:PRO:O	2.19	0.43
3:H:165:THR:HG23	3:H:180:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:6:GLN:OE1	2:L:87:TYR:HA	2.19	0.42
1:J:114:GLN:HA	5:J:63:HOH:O	2.18	0.42
2:A:29:SER:HB3	2:A:32:TYR:HD1	1.84	0.42
3:H:127:SER:HB2	3:H:130:SER:H	1.83	0.42
2:A:33:LEU:CD2	2:A:71:PHE:CD2	3.00	0.42
3:B:145:TYR:CE2	3:B:150:VAL:HG13	2.54	0.42
1:J:350:LYS:HB3	1:J:355:ASN:CB	2.49	0.42
3:B:135:THR:HG22	3:B:185:PRO:HA	2.01	0.42
1:G:219:ALA:HA	1:G:220:PRO:HD3	1.94	0.42
3:H:12:VAL:HG11	3:H:82(C):MET:HG3	2.02	0.42
1:J:439:ILE:HG13	1:J:439:ILE:H	1.55	0.42
1:G:350:LYS:HB3	1:G:355:ASN:CB	2.50	0.42
1:J:436:ALA:O	1:J:438:PRO:HD3	2.20	0.42
1:J:490:LYS:HG2	1:J:491:ILE:N	2.35	0.42
1:J:234:ASN:HB2	4:J:734:NAG:O7	2.19	0.42
1:G:395:ASP:N	1:G:395:ASP:OD1	2.53	0.42
3:H:5:GLN:HA	3:H:5:GLN:NE2	2.35	0.42
3:B:12:VAL:HG11	3:B:82(C):MET:HG3	2.02	0.42
3:H:6:GLU:OE2	3:H:105:GLN:N	2.50	0.42
1:J:463:ASN:H	1:J:465:THR:HG22	1.85	0.42
1:J:234:ASN:CB	4:J:734:NAG:H2	2.50	0.42
1:G:98:ASN:O	1:G:100:MET:N	2.53	0.41
1:G:436:ALA:HB1	1:G:437:PRO:HD3	1.99	0.41
2:L:16:GLY:HA2	2:L:77:ARG:HG2	2.02	0.41
3:B:6:GLU:OE2	3:B:104:GLY:HA3	2.20	0.41
1:J:381:GLU:HG2	1:J:422:GLN:HG2	2.01	0.41
2:L:60:ASP:N	2:L:60:ASP:OD1	2.53	0.41
2:A:159:SER:HA	2:A:178:THR:O	2.20	0.41
3:H:30:SER:O	3:H:31:SER:CB	2.69	0.41
3:H:50:TYR:CD2	3:H:50:TYR:C	2.93	0.41
2:L:140:TYR:CD1	2:L:141:PRO:HA	2.55	0.41
3:H:168:ALA:HA	3:H:178:LEU:HB3	2.03	0.41
1:G:208:VAL:HG22	1:J:215:ILE:HG12	2.03	0.41
3:B:30:SER:O	3:B:31:SER:CB	2.69	0.41
1:G:257:THR:O	1:G:259:LEU:N	2.49	0.41
3:H:138:LEU:N	3:H:138:LEU:CD2	2.84	0.41
1:J:283:THR:HG23	1:J:472:GLY:HA3	2.01	0.41
3:B:77:GLN:HE21	3:B:77:GLN:HB3	1.68	0.41
1:G:231:LYS:H	4:G:741:NAG:H83	1.85	0.41
1:G:366:GLY:HA3	3:H:2:VAL:CG2	2.51	0.41
3:H:78:PHE:CZ	3:H:92:CYS:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:125:ALA:HA	3:B:126:PRO:HD3	1.83	0.41
1:J:94:ASN:ND2	1:J:236:THR:HG22	2.33	0.41
2:A:167:ASP:OD2	2:A:169:LYS:N	2.53	0.41
2:A:6:GLN:OE1	2:A:87:TYR:HA	2.20	0.41
1:G:364:SER:H	1:G:470:PRO:HG2	1.86	0.41
2:L:159:SER:HA	2:L:178:THR:O	2.21	0.41
3:B:5:GLN:NE2	3:B:5:GLN:HA	2.35	0.40
3:H:38:ARG:HH21	3:H:46:GLN:HE22	1.68	0.40
2:A:39:LYS:HE3	2:A:81:GLU:O	2.21	0.40
3:B:127:SER:HB2	3:B:130:SER:H	1.86	0.40
1:J:451:GLY:C	1:J:452:LEU:HD12	2.41	0.40
2:L:32:TYR:O	2:L:90:GLN:HA	2.22	0.40
2:L:29:SER:HB3	2:L:32:TYR:CD1	2.55	0.40
2:A:47:LEU:HD12	2:A:47:LEU:HA	1.93	0.40
1:G:350:LYS:HG2	1:G:359:ILE:HD13	2.04	0.40
3:H:66:ARG:NH2	3:H:86:ASP:OD2	2.46	0.40
1:J:441:GLY:N	1:J:442:GLN:CA	2.72	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	G	283/321 (88%)	238 (84%)	41 (14%)	4 (1%)	11	36
1	J	283/321 (88%)	244 (86%)	32 (11%)	7 (2%)	5	21
2	A	213/215 (99%)	202 (95%)	9 (4%)	2 (1%)	17	48
2	L	213/215 (99%)	204 (96%)	8 (4%)	1 (0%)	29	61
3	B	223/225 (99%)	206 (92%)	16 (7%)	1 (0%)	34	66
3	H	223/225 (99%)	206 (92%)	16 (7%)	1 (0%)	34	66
All	All	1438/1522 (94%)	1300 (90%)	122 (8%)	16 (1%)	14	42

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	438	PRO
3	B	102	PRO
1	G	464	GLY
3	H	102	PRO
1	J	435	TYR
1	J	464	GLY
1	J	438	PRO
2	L	8	PRO
1	J	428	GLN
2	A	8	PRO
1	G	99	ASN
1	J	99	ASN
2	A	7	SER
1	J	437	PRO
1	G	424	ILE
1	J	439	ILE

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	G	258/284 (91%)	247 (96%)	11 (4%)	29	62
1	J	258/284 (91%)	248 (96%)	10 (4%)	32	66
2	A	186/186 (100%)	182 (98%)	4 (2%)	52	81
2	L	186/186 (100%)	182 (98%)	4 (2%)	52	81
3	B	193/193 (100%)	188 (97%)	5 (3%)	46	77
3	H	193/193 (100%)	187 (97%)	6 (3%)	40	74
All	All	1274/1326 (96%)	1234 (97%)	40 (3%)	40	74

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	202	THR

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Mol	Chain	Res	Type
1	G	205	CYS
1	G	298	ARG
1	G	392	THR
1	G	394	ASN
1	G	395	ASP
1	G	413	ASN
1	G	426	MET
1	G	435	TYR
1	G	463	ASN
1	G	488	VAL
2	L	6	GLN
2	L	13	LEU
2	L	31	ARG
2	L	100	GLN
3	H	19	SER
3	H	30	SER
3	H	54	SER
3	H	100(F)	ARG
3	H	178	LEU
3	H	209	LYS
1	J	202	THR
1	J	205	CYS
1	J	298	ARG
1	J	412	ARG
1	J	439	ILE
1	J	443	ILE
1	J	444	ARG
1	J	446	SER
1	J	463	ASN
1	J	488	VAL
2	A	6	GLN
2	A	13	LEU
2	A	31	ARG
2	A	100	GLN
3	B	19	SER
3	B	30	SER
3	B	54	SER
3	B	100(F)	ARG
3	B	209	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	94	ASN
1	G	103	GLN
1	G	216	HIS
1	G	330	HIS
1	G	337	GLN
1	G	352	GLN
1	G	442	GLN
2	L	138	ASN
2	L	199	GLN
3	H	5	GLN
3	H	32	HIS
3	H	46	GLN
3	H	77	GLN
3	H	164	HIS
1	J	94	ASN
1	J	103	GLN
1	J	337	GLN
1	J	352	GLN
1	J	442	GLN
2	A	100	GLN
2	A	199	GLN
3	B	5	GLN
3	B	32	HIS
3	B	46	GLN
3	B	77	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

27 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	832	1	14,14,15	0.54	0	17,19,21	0.78	0
4	NAG	G	789	1	14,14,15	0.51	0	17,19,21	0.97	1 (5%)
4	NAG	J	886	1	14,14,15	0.28	0	17,19,21	1.13	3 (17%)
4	NAG	J	795	1	14,14,15	0.53	0	17,19,21	0.83	0
4	NAG	G	776	1	14,14,15	0.54	0	17,19,21	0.78	0
4	NAG	G	734	1	14,14,15	0.68	0	17,19,21	0.70	0
4	NAG	J	894	1	14,14,15	0.51	0	17,19,21	0.86	1 (5%)
4	NAG	J	762	1	14,14,15	0.53	0	17,19,21	0.81	0
4	NAG	J	734	1	14,14,15	0.55	0	17,19,21	0.81	1 (5%)
4	NAG	G	963	1	14,14,15	1.52	2 (14%)	17,19,21	1.01	1 (5%)
4	NAG	G	762	1	14,14,15	0.63	0	17,19,21	0.95	0
4	NAG	J	801	1	14,14,15	0.46	0	17,19,21	1.13	1 (5%)
4	NAG	G	741	1	14,14,15	0.49	0	17,19,21	1.07	1 (5%)
4	NAG	G	948	1	14,14,15	0.65	0	17,19,21	1.12	1 (5%)
4	NAG	J	832	1	14,14,15	0.55	0	17,19,21	0.81	0
4	NAG	G	795	1	14,14,15	0.54	0	17,19,21	0.77	0
4	NAG	J	776	1	14,14,15	0.48	0	17,19,21	1.75	5 (29%)
4	NAG	J	963	1	14,14,15	0.58	0	17,19,21	1.14	1 (5%)
4	NAG	J	948	1	14,14,15	0.50	0	17,19,21	0.77	0
4	NAG	G	886	1	14,14,15	0.59	0	17,19,21	1.01	1 (5%)
4	NAG	G	801	1	14,14,15	0.59	0	17,19,21	0.76	0
4	NAG	J	741	1	14,14,15	0.58	0	17,19,21	1.24	2 (11%)
4	NAG	J	856	1	14,14,15	0.64	0	17,19,21	0.89	0
4	NAG	G	856	1	14,14,15	0.64	0	17,19,21	0.79	1 (5%)
4	NAG	J	789	1	14,14,15	0.61	0	17,19,21	1.69	4 (23%)
4	NAG	G	894	1	14,14,15	0.44	0	17,19,21	1.07	1 (5%)
4	NAG	J	913	1	14,14,15	0.56	0	17,19,21	0.92	1 (5%)

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	832	1	-	5/6/23/26	0/1/1/1
4	NAG	G	789	1	-	5/6/23/26	0/1/1/1
4	NAG	J	886	1	-	2/6/23/26	0/1/1/1
4	NAG	J	795	1	-	3/6/23/26	0/1/1/1
4	NAG	G	776	1	-	2/6/23/26	0/1/1/1
4	NAG	G	734	1	-	4/6/23/26	0/1/1/1
4	NAG	J	894	1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	J	762	1	-	2/6/23/26	0/1/1/1
4	NAG	J	734	1	-	2/6/23/26	0/1/1/1
4	NAG	G	963	1	-	5/6/23/26	0/1/1/1
4	NAG	G	762	1	-	0/6/23/26	0/1/1/1
4	NAG	J	801	1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	G	741	1	-	3/6/23/26	0/1/1/1
4	NAG	G	948	1	-	2/6/23/26	0/1/1/1
4	NAG	J	832	1	-	3/6/23/26	0/1/1/1
4	NAG	G	795	1	-	3/6/23/26	0/1/1/1
4	NAG	J	776	1	-	4/6/23/26	0/1/1/1
4	NAG	J	963	1	-	5/6/23/26	0/1/1/1
4	NAG	J	948	1	-	4/6/23/26	0/1/1/1
4	NAG	G	886	1	-	4/6/23/26	0/1/1/1
4	NAG	G	801	1	-	6/6/23/26	0/1/1/1
4	NAG	J	741	1	-	0/6/23/26	0/1/1/1
4	NAG	J	856	1	-	4/6/23/26	0/1/1/1
4	NAG	G	856	1	-	6/6/23/26	0/1/1/1
4	NAG	J	789	1	-	5/6/23/26	0/1/1/1
4	NAG	G	894	1	-	2/6/23/26	0/1/1/1
4	NAG	J	913	1	1/1/5/7	6/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	963	NAG	C1-C2	3.87	1.58	1.52
4	G	963	NAG	C3-C2	2.13	1.57	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	776	NAG	O5-C1-C2	-4.08	104.84	111.29
4	J	963	NAG	C1-O5-C5	3.91	117.49	112.19
4	J	789	NAG	O5-C1-C2	-3.82	105.26	111.29
4	G	894	NAG	C1-O5-C5	3.53	116.97	112.19
4	G	948	NAG	C4-C3-C2	3.44	116.05	111.02
4	J	741	NAG	C1-O5-C5	3.37	116.76	112.19
4	J	789	NAG	C1-C2-N2	2.95	115.53	110.49
4	G	886	NAG	C1-O5-C5	2.94	116.17	112.19
4	J	801	NAG	O5-C1-C2	-2.89	106.73	111.29
4	J	894	NAG	O5-C5-C6	2.80	111.60	107.20
4	G	789	NAG	O5-C5-C6	2.76	111.54	107.20
4	J	789	NAG	C1-O5-C5	2.60	115.71	112.19
4	J	776	NAG	C1-O5-C5	2.53	115.62	112.19
4	J	776	NAG	C1-C2-N2	2.51	114.78	110.49
4	J	776	NAG	C4-C3-C2	-2.50	107.35	111.02
4	J	741	NAG	O5-C1-C2	2.46	115.17	111.29
4	J	886	NAG	O5-C5-C6	2.45	111.04	107.20
4	G	741	NAG	O5-C1-C2	-2.43	107.44	111.29
4	J	789	NAG	C4-C3-C2	-2.36	107.56	111.02
4	G	963	NAG	O5-C1-C2	-2.27	107.70	111.29
4	J	776	NAG	C2-N2-C7	-2.24	119.71	122.90
4	J	886	NAG	C1-O5-C5	-2.22	109.18	112.19
4	J	734	NAG	C1-O5-C5	2.09	115.03	112.19
4	J	913	NAG	O5-C5-C6	2.07	110.45	107.20
4	J	886	NAG	C1-C2-N2	-2.06	106.97	110.49
4	G	856	NAG	C4-C3-C2	2.04	114.02	111.02

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	J	894	NAG	C1
4	J	801	NAG	C1
4	J	913	NAG	C1

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	832	NAG	C3-C2-N2-C7
4	G	832	NAG	C8-C7-N2-C2
4	G	832	NAG	O7-C7-N2-C2
4	G	789	NAG	C8-C7-N2-C2
4	G	789	NAG	O7-C7-N2-C2
4	J	795	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	J	795	NAG	C8-C7-N2-C2
4	J	795	NAG	O7-C7-N2-C2
4	J	894	NAG	C8-C7-N2-C2
4	J	894	NAG	O7-C7-N2-C2
4	J	734	NAG	C8-C7-N2-C2
4	J	734	NAG	O7-C7-N2-C2
4	G	963	NAG	C3-C2-N2-C7
4	G	963	NAG	C8-C7-N2-C2
4	G	963	NAG	O7-C7-N2-C2
4	J	801	NAG	C8-C7-N2-C2
4	J	801	NAG	O7-C7-N2-C2
4	G	741	NAG	C3-C2-N2-C7
4	G	741	NAG	C8-C7-N2-C2
4	G	741	NAG	O7-C7-N2-C2
4	J	832	NAG	C3-C2-N2-C7
4	J	832	NAG	C8-C7-N2-C2
4	J	832	NAG	O7-C7-N2-C2
4	J	776	NAG	C8-C7-N2-C2
4	J	776	NAG	O7-C7-N2-C2
4	J	963	NAG	C8-C7-N2-C2
4	J	963	NAG	O7-C7-N2-C2
4	J	948	NAG	C8-C7-N2-C2
4	J	948	NAG	O7-C7-N2-C2
4	G	886	NAG	O7-C7-N2-C2
4	G	801	NAG	C8-C7-N2-C2
4	G	801	NAG	O7-C7-N2-C2
4	G	856	NAG	C8-C7-N2-C2
4	G	856	NAG	O7-C7-N2-C2
4	J	789	NAG	C8-C7-N2-C2
4	J	789	NAG	O7-C7-N2-C2
4	J	913	NAG	C3-C2-N2-C7
4	J	913	NAG	C8-C7-N2-C2
4	J	913	NAG	O7-C7-N2-C2
4	J	762	NAG	C8-C7-N2-C2
4	J	762	NAG	O7-C7-N2-C2
4	G	886	NAG	C8-C7-N2-C2
4	J	856	NAG	C8-C7-N2-C2
4	G	886	NAG	O5-C5-C6-O6
4	G	734	NAG	O5-C5-C6-O6
4	J	948	NAG	O5-C5-C6-O6
4	J	801	NAG	C4-C5-C6-O6
4	J	801	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	G	734	NAG	C4-C5-C6-O6
4	J	856	NAG	O7-C7-N2-C2
4	J	948	NAG	C4-C5-C6-O6
4	G	801	NAG	C4-C5-C6-O6
4	J	856	NAG	C4-C5-C6-O6
4	J	776	NAG	C4-C5-C6-O6
4	J	963	NAG	C4-C5-C6-O6
4	J	894	NAG	O5-C5-C6-O6
4	J	894	NAG	C4-C5-C6-O6
4	J	886	NAG	O5-C5-C6-O6
4	G	886	NAG	C4-C5-C6-O6
4	J	789	NAG	O5-C5-C6-O6
4	G	894	NAG	O5-C5-C6-O6
4	G	776	NAG	C8-C7-N2-C2
4	G	776	NAG	O7-C7-N2-C2
4	G	948	NAG	C8-C7-N2-C2
4	J	856	NAG	O5-C5-C6-O6
4	G	832	NAG	O5-C5-C6-O6
4	J	776	NAG	O5-C5-C6-O6
4	G	801	NAG	O5-C5-C6-O6
4	G	948	NAG	O7-C7-N2-C2
4	J	963	NAG	O5-C5-C6-O6
4	G	832	NAG	C4-C5-C6-O6
4	J	886	NAG	C4-C5-C6-O6
4	G	789	NAG	C4-C5-C6-O6
4	G	795	NAG	C4-C5-C6-O6
4	G	789	NAG	O5-C5-C6-O6
4	G	856	NAG	C4-C5-C6-O6
4	G	963	NAG	C1-C2-N2-C7
4	G	801	NAG	C1-C2-N2-C7
4	G	734	NAG	C8-C7-N2-C2
4	G	856	NAG	C1-C2-N2-C7
4	J	913	NAG	C4-C5-C6-O6
4	J	789	NAG	C4-C5-C6-O6
4	G	856	NAG	O5-C5-C6-O6
4	G	795	NAG	O5-C5-C6-O6
4	G	795	NAG	C1-C2-N2-C7
4	G	734	NAG	O7-C7-N2-C2
4	G	894	NAG	C4-C5-C6-O6
4	G	963	NAG	O5-C5-C6-O6
4	J	913	NAG	C1-C2-N2-C7
4	G	789	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	J	789	NAG	C3-C2-N2-C7
4	J	913	NAG	O5-C5-C6-O6
4	J	963	NAG	C1-C2-N2-C7
4	G	801	NAG	C3-C2-N2-C7
4	G	856	NAG	C3-C2-N2-C7

There are no ring outliers.

13 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	789	NAG	2	0
4	J	886	NAG	1	0
4	J	795	NAG	2	0
4	G	734	NAG	1	0
4	J	734	NAG	3	0
4	G	963	NAG	2	0
4	G	762	NAG	1	0
4	G	741	NAG	1	0
4	J	776	NAG	1	0
4	J	856	NAG	1	0
4	G	856	NAG	2	0
4	J	789	NAG	1	0
4	J	913	NAG	3	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 ⓘ

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	G	289/321 (90%)	0.47	22 (7%) 13 10	55, 106, 187, 231	0
1	J	289/321 (90%)	0.64	36 (12%) 3 3	87, 137, 199, 252	0
2	A	215/215 (100%)	0.12	4 (1%) 66 65	83, 124, 165, 206	0
2	L	215/215 (100%)	-0.17	1 (0%) 91 91	48, 78, 105, 164	0
3	B	225/225 (100%)	0.15	7 (3%) 49 44	79, 115, 168, 213	0
3	H	225/225 (100%)	-0.12	3 (1%) 77 77	42, 60, 108, 178	0
All	All	1458/1522 (95%)	0.22	73 (5%) 28 25	42, 106, 179, 252	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	429	GLU	9.0
1	G	464	GLY	8.0
3	B	130	SER	7.5
1	J	435	TYR	6.8
1	G	427	TRP	6.6
1	J	430	VAL	6.5
3	H	130	SER	6.3
1	J	461	ASP	6.3
2	A	214	CYS	5.8
1	G	460	LYS	5.6
1	J	460	LYS	5.4
2	L	214	CYS	5.4
1	G	438	PRO	5.2
1	G	472	GLY	5.0
1	G	435	TYR	4.8
3	B	214	LYS	4.5
1	J	93	PHE	4.3
1	J	462	THR	4.3
1	G	433	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	439	ILE	4.3
1	G	430	VAL	4.2
1	J	327	ARG	4.1
1	G	429	GLU	4.0
1	G	300	ASN	3.7
1	J	353	PHE	3.7
1	G	461	ASP	3.7
1	J	438	PRO	3.6
3	B	129	LYS	3.5
1	G	440	ARG	3.5
1	G	434	MET	3.4
1	G	437	PRO	3.4
1	G	441	GLY	3.3
1	J	300	ASN	3.2
1	J	427	TRP	3.2
1	G	470	PRO	3.1
1	J	328	GLN	3.1
1	J	442	GLN	3.1
1	J	301	ASN	3.1
1	J	459	GLY	3.1
3	H	132	SER	3.0
1	G	327	ARG	3.0
3	B	131	THR	3.0
1	G	428	GLN	3.0
1	J	439	ILE	2.9
2	A	77	ARG	2.8
1	J	232	LYS	2.8
1	J	441	GLY	2.7
3	B	1	GLN	2.7
1	J	228	CYS	2.7
1	J	464	GLY	2.6
1	J	428	GLN	2.6
1	J	333	LEU	2.6
1	J	432	LYS	2.5
1	J	465	THR	2.5
1	J	492	GLU	2.5
1	G	328	GLN	2.5
2	A	181	LEU	2.5
1	J	235	GLY	2.5
2	A	110	VAL	2.4
1	G	124	GLY	2.4
1	J	237	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
3	B	159	LEU	2.4
1	G	462	THR	2.4
1	J	473	GLY	2.3
1	J	239	CYS	2.3
3	B	215	SER	2.3
1	J	359	ILE	2.3
1	J	412	ARG	2.2
3	H	133	GLY	2.1
1	J	445	CYS	2.1
1	J	360	ILE	2.1
1	J	245	VAL	2.1
1	J	472	GLY	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	J	963	14/15	0.31	0.69	169,170,170,170	0
4	NAG	J	913	14/15	0.62	0.62	143,144,144,144	0
4	NAG	G	801	14/15	0.63	0.53	159,159,159,159	0
4	NAG	J	801	14/15	0.64	0.75	155,155,155,155	0
4	NAG	J	856	14/15	0.70	0.34	179,180,180,180	0
4	NAG	G	734	14/15	0.72	0.26	164,165,165,165	0
4	NAG	J	741	14/15	0.72	0.35	166,167,167,167	0
4	NAG	G	894	14/15	0.74	0.45	151,152,152,152	0
4	NAG	G	963	14/15	0.75	0.48	168,168,168,168	0
4	NAG	G	856	14/15	0.75	0.41	180,180,180,180	0
4	NAG	J	795	14/15	0.76	0.27	138,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	J	948	14/15	0.82	0.24	129,129,130,130	0
4	NAG	G	741	14/15	0.83	0.34	166,166,166,166	0
4	NAG	J	894	14/15	0.83	0.40	144,144,144,144	0
4	NAG	J	734	14/15	0.83	0.41	166,166,166,166	0
4	NAG	G	789	14/15	0.87	0.24	130,130,131,131	0
4	NAG	J	886	14/15	0.88	0.34	42,53,62,65	0
4	NAG	J	789	14/15	0.88	0.28	129,130,130,131	0
4	NAG	J	776	14/15	0.88	0.26	114,115,115,115	0
4	NAG	G	886	14/15	0.88	0.21	110,110,111,111	0
4	NAG	G	795	14/15	0.90	0.14	134,135,135,135	0
4	NAG	G	832	14/15	0.92	0.16	139,140,140,140	0
4	NAG	G	948	14/15	0.92	0.15	124,124,124,124	0
4	NAG	J	832	14/15	0.92	0.32	142,142,142,142	0
4	NAG	J	762	14/15	0.93	0.14	99,99,100,100	0
4	NAG	G	776	14/15	0.94	0.14	118,118,118,118	0
4	NAG	G	762	14/15	0.95	0.20	96,96,97,97	0

6.5 Other polymers

There are no such residues in this entry.