



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 27, 2023 – 02:46 PM EDT

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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 : 2.35  
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)

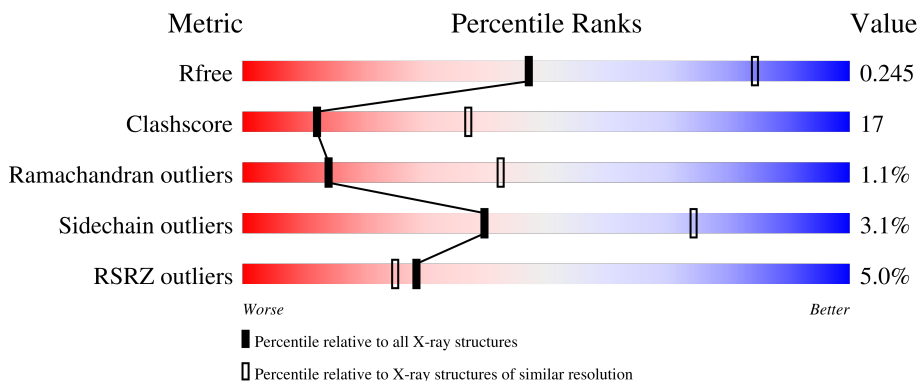
# 1 Overall quality at a glance

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 7% 59% 28% 10%
1	J	321	 11% 59% 28% 10%
2	A	215	 2% 77% 21%
2	L	215	 77% 21%

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Mol	Chain	Length	Quality of chain
3	B	225	
3	H	225	

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
			Total	C	N	O	S			
1	G	289	2276	1428	401	429	18	0	0	0
1	J	289	2276	1428	401	429	18	0	0	0

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
			Total	C	N	O	S			
2	L	215	1651	1027	282	336	6	0	0	0
2	A	215	1651	1027	282	336	6	0	0	0

- Molecule 3 is a protein called F105 Heavy Chain.

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
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		

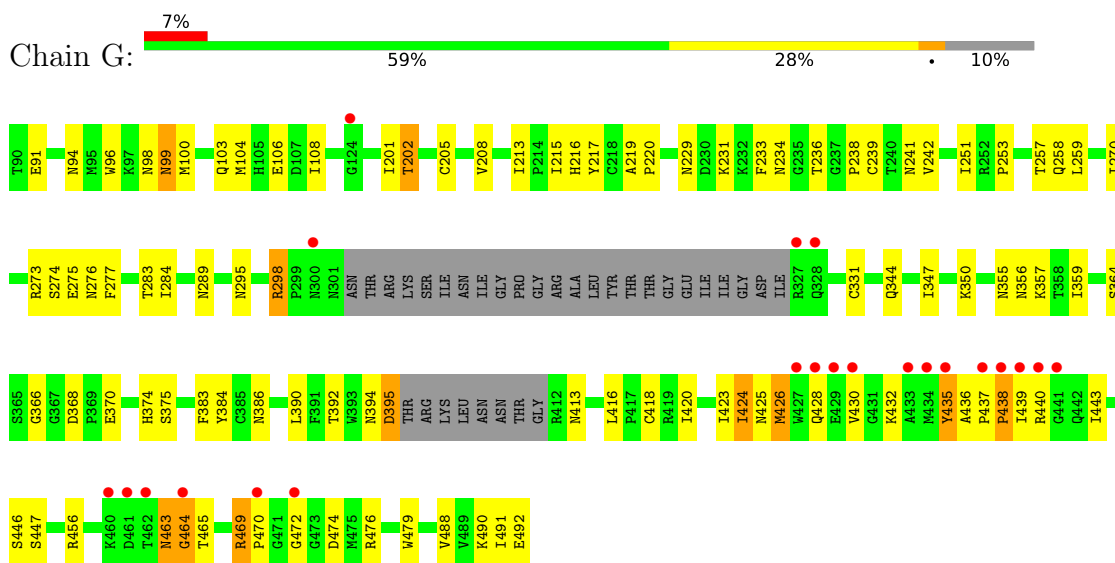
- Molecule 5 is water.

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		

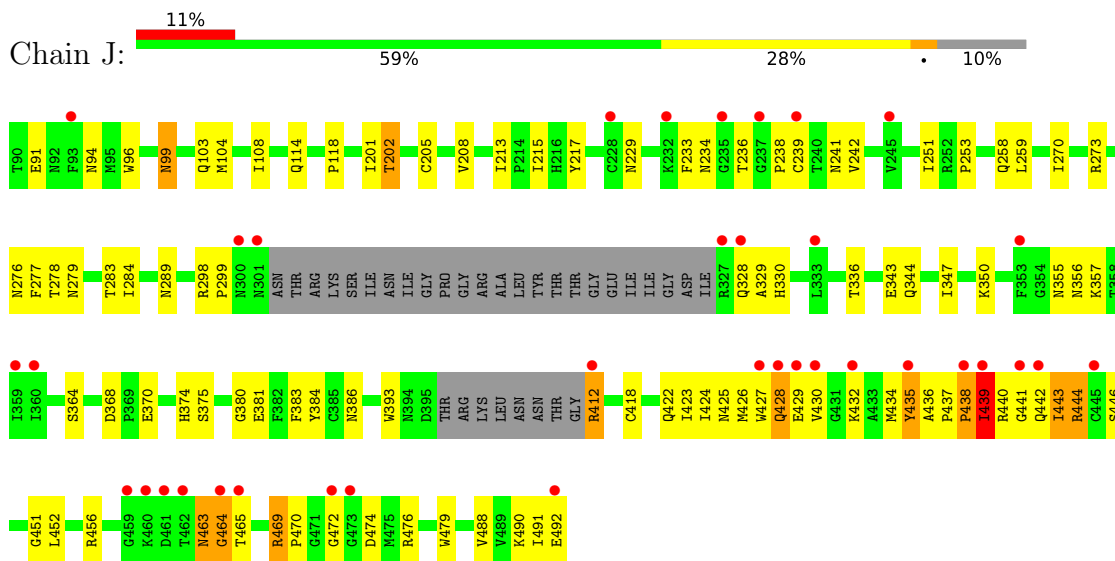
### 3 Residue-property plots [i](#)

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

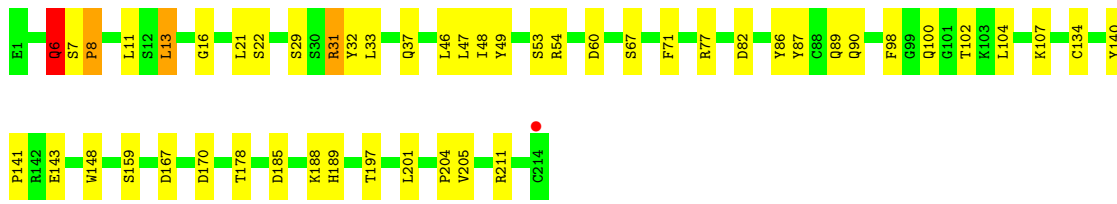


- Molecule 1: Glycoprotein 120




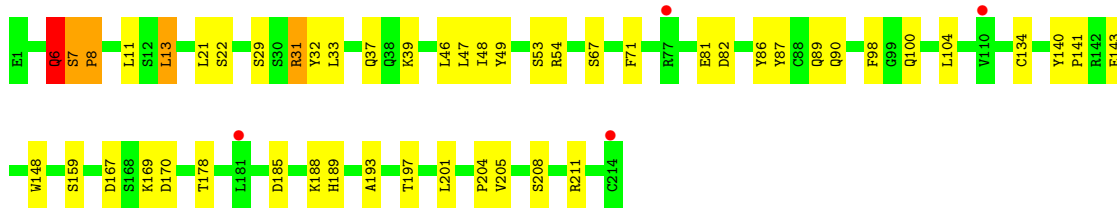
- Molecule 2: F105 Light Chain

Chain L:  77% 21% .



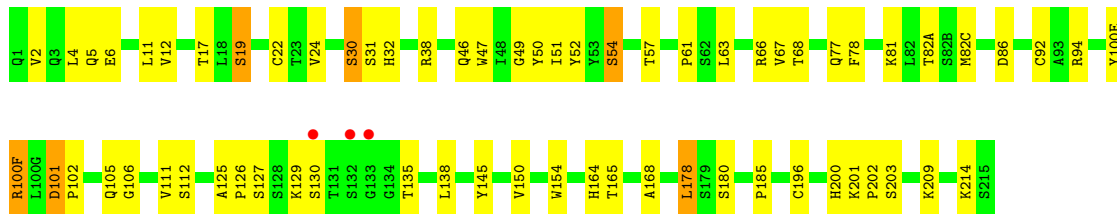
• Molecule 2: F105 Light Chain

Chain A:  77% 21% .




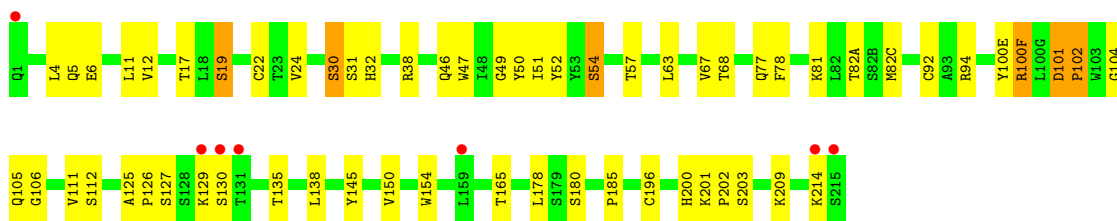
• Molecule 3: F105 Heavy Chain

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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.81Å)	Xtrriage
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 <sup>2</sup> )	70.5	Xtrriage
Anisotropy	0.312	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 56.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11670	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	109.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	6	GLN	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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.

The worst 5 of 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
1:G:99:ASN:HB2	1:J:202:THR:HG23	1.37	1.03

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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

5 of 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

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	258/284 (91%)	247 (96%)	11 (4%)	29	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	446	SER
3	B	19	SER
1	J	463	ASN
2	A	13	LEU
3	B	54	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	94	ASN
1	J	352	GLN
3	B	77	GLN
1	J	337	GLN
1	J	442	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

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	795	1	14,14,15	0.54	0	17,19,21	0.77	0
4	NAG	J	795	1	14,14,15	0.53	0	17,19,21	0.83	0
4	NAG	J	894	1	14,14,15	0.51	0	17,19,21	0.86	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	886	1	14,14,15	0.28	0	17,19,21	1.13	3 (17%)
4	NAG	G	789	1	14,14,15	0.51	0	17,19,21	0.97	1 (5%)
4	NAG	G	734	1	14,14,15	0.68	0	17,19,21	0.70	0
4	NAG	G	856	1	14,14,15	0.64	0	17,19,21	0.79	1 (5%)
4	NAG	G	801	1	14,14,15	0.59	0	17,19,21	0.76	0
4	NAG	J	832	1	14,14,15	0.55	0	17,19,21	0.81	0
4	NAG	J	741	1	14,14,15	0.58	0	17,19,21	1.24	2 (11%)
4	NAG	J	948	1	14,14,15	0.50	0	17,19,21	0.77	0
4	NAG	J	913	1	14,14,15	0.56	0	17,19,21	0.92	1 (5%)
4	NAG	J	762	1	14,14,15	0.53	0	17,19,21	0.81	0
4	NAG	G	741	1	14,14,15	0.49	0	17,19,21	1.07	1 (5%)
4	NAG	G	832	1	14,14,15	0.54	0	17,19,21	0.78	0
4	NAG	G	762	1	14,14,15	0.63	0	17,19,21	0.95	0
4	NAG	G	886	1	14,14,15	0.59	0	17,19,21	1.01	1 (5%)
4	NAG	J	734	1	14,14,15	0.55	0	17,19,21	0.81	1 (5%)
4	NAG	J	963	1	14,14,15	0.58	0	17,19,21	1.14	1 (5%)
4	NAG	G	948	1	14,14,15	0.65	0	17,19,21	1.12	1 (5%)
4	NAG	J	856	1	14,14,15	0.64	0	17,19,21	0.89	0
4	NAG	G	776	1	14,14,15	0.54	0	17,19,21	0.78	0
4	NAG	G	963	1	14,14,15	1.52	2 (14%)	17,19,21	1.01	1 (5%)
4	NAG	J	776	1	14,14,15	0.48	0	17,19,21	1.75	5 (29%)
4	NAG	J	801	1	14,14,15	0.46	0	17,19,21	1.13	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	795	1	-	3/6/23/26	0/1/1/1
4	NAG	J	795	1	-	3/6/23/26	0/1/1/1
4	NAG	J	894	1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	J	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	886	1	-	2/6/23/26	0/1/1/1
4	NAG	G	789	1	-	5/6/23/26	0/1/1/1
4	NAG	G	734	1	-	4/6/23/26	0/1/1/1
4	NAG	G	856	1	-	6/6/23/26	0/1/1/1
4	NAG	G	801	1	-	6/6/23/26	0/1/1/1
4	NAG	J	832	1	-	3/6/23/26	0/1/1/1
4	NAG	J	741	1	-	0/6/23/26	0/1/1/1
4	NAG	J	948	1	-	4/6/23/26	0/1/1/1
4	NAG	J	913	1	1/1/5/7	6/6/23/26	0/1/1/1
4	NAG	J	762	1	-	2/6/23/26	0/1/1/1
4	NAG	G	741	1	-	3/6/23/26	0/1/1/1
4	NAG	G	832	1	-	5/6/23/26	0/1/1/1
4	NAG	G	762	1	-	0/6/23/26	0/1/1/1
4	NAG	G	886	1	-	4/6/23/26	0/1/1/1
4	NAG	J	734	1	-	2/6/23/26	0/1/1/1
4	NAG	J	963	1	-	5/6/23/26	0/1/1/1
4	NAG	G	948	1	-	2/6/23/26	0/1/1/1
4	NAG	J	856	1	-	4/6/23/26	0/1/1/1
4	NAG	G	776	1	-	2/6/23/26	0/1/1/1
4	NAG	G	963	1	-	5/6/23/26	0/1/1/1
4	NAG	J	776	1	-	4/6/23/26	0/1/1/1
4	NAG	J	801	1	1/1/5/7	4/6/23/26	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

The worst 5 of 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

All (3) chirality outliers are listed below:

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

5 of 95 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	G	789	NAG	C8-C7-N2-C2
4	G	789	NAG	O7-C7-N2-C2

There are no ring outliers.

13 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	795	NAG	2	0
4	J	789	NAG	1	0
4	J	886	NAG	1	0
4	G	789	NAG	2	0
4	G	734	NAG	1	0
4	G	856	NAG	2	0
4	J	913	NAG	3	0
4	G	741	NAG	1	0
4	G	762	NAG	1	0
4	J	734	NAG	3	0
4	J	856	NAG	1	0
4	G	963	NAG	2	0
4	J	776	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, 95<sup>th</sup> 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 <sup>2</sup> )	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	78, 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

The worst 5 of 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

### 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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	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
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	734	14/15	0.83	0.41	166,166,166,166	0
4	NAG	J	894	14/15	0.83	0.40	144,144,144,144	0
4	NAG	G	789	14/15	0.87	0.24	130,130,131,131	0
4	NAG	G	886	14/15	0.88	0.21	110,110,111,111	0
4	NAG	J	776	14/15	0.88	0.26	114,115,115,115	0
4	NAG	J	789	14/15	0.88	0.28	129,130,130,131	0
4	NAG	J	886	14/15	0.88	0.34	42,53,62,65	0
4	NAG	G	795	14/15	0.90	0.14	134,135,135,135	0
4	NAG	G	948	14/15	0.92	0.15	124,124,124,124	0
4	NAG	G	832	14/15	0.92	0.16	139,140,140,140	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 [i](#)

There are no such residues in this entry.