



wwPDB X-ray Structure Validation Summary Report

Feb 1, 2016 – 09:51 AM GMT

PDB ID : 3JWD
Title : Structure of HIV-1 gp120 with gp41-Interactive Region: Layered Architecture and Basis of Conformational Mobility
Authors : Pancera, M.; Majeed, S.; Ban, Y.A.; Chen, L.; Huang, C.C.; Kong, L.; Kwon, Y.D.; Stuckey, J.; Zhou, T.; Robinson, J.E.; Schief, W.R.; Sodroski, J.; Wyatt, R.; Kwong, P.D.
Deposited on : 2009-09-18
Resolution : 2.61 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the  symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

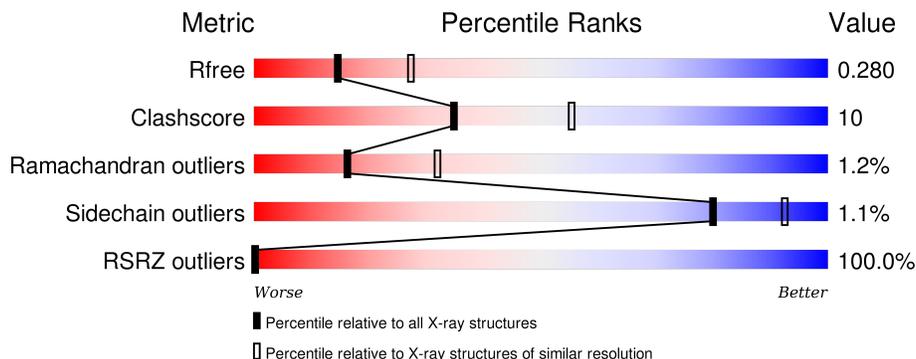
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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}	91344	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	379	 95% 69% 25% • 5%
1	B	379	 93% 69% 24% • 7%
2	C	184	 100% 74% 24% •
2	D	184	 99% 79% 20% ••
3	L	213	 100% 77% 23% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	O	213	<p>100% 83% 16%</p>
4	H	220	<p>100% 78% 21%</p>
4	P	220	<p>100% 73% 26%</p>

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
5	NAG	A	734	X	-	-	X
5	NAG	A	762	-	-	-	X
5	NAG	A	776	-	-	-	X
5	NAG	A	789	-	-	-	X
5	NAG	A	886	-	-	-	X
5	NAG	A	897	-	-	-	X
5	NAG	A	948	X	-	-	X
5	NAG	B	588	X	-	-	-
5	NAG	B	734	-	-	-	X
5	NAG	B	762	-	-	-	X
5	NAG	B	776	-	-	-	X
5	NAG	B	789	-	-	-	X
6	GOL	B	1	-	-	-	X
6	GOL	P	215	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 15697 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 GP120 ENVELOPE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	360	2800	1769	480	531	20	0	0	0
1	B	354	2756	1744	472	520	20	0	0	0

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	184	1432	896	250	281	5	0	0	0
2	D	183	1424	891	249	280	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1000	MET	-	INITIATING METHIONINE	UNP P01730
D	1000	MET	-	INITIATING METHIONINE	UNP P01730

- Molecule 3 is a protein called FAB 48D LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	213	1635	1022	274	333	6	0	0	0
3	O	212	1624	1017	272	330	5	0	0	0

- Molecule 4 is a protein called FAB 48D HEAVY CHAIN.

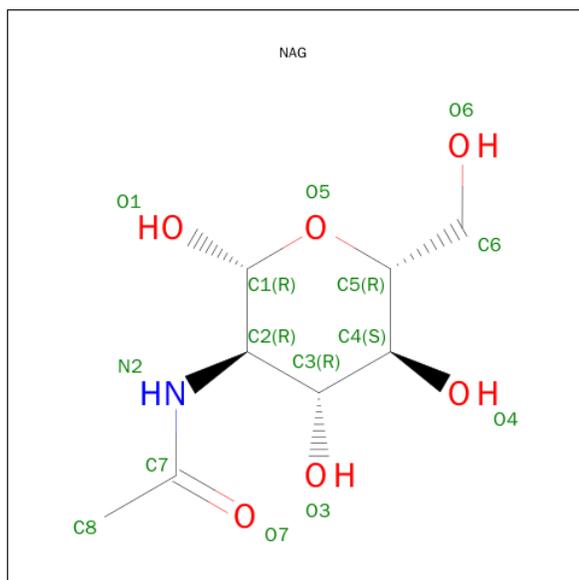
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	220	1654	1048	267	332	7	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	P	219	1644	1042	265	330	7	0	0	0

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



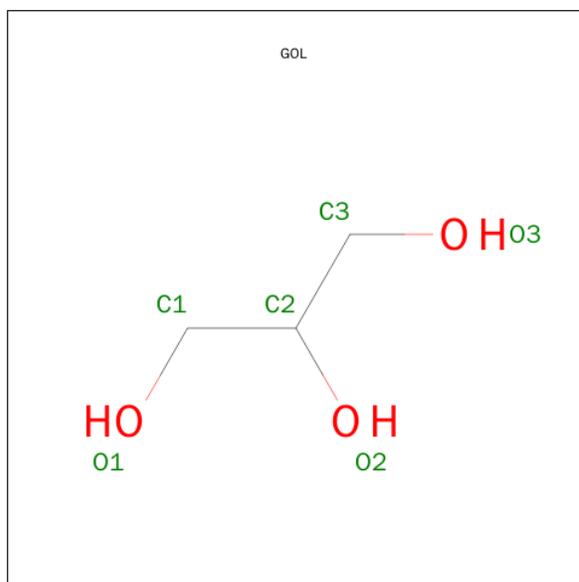
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	P	1	Total	C	O	0	0
			6	3	3		

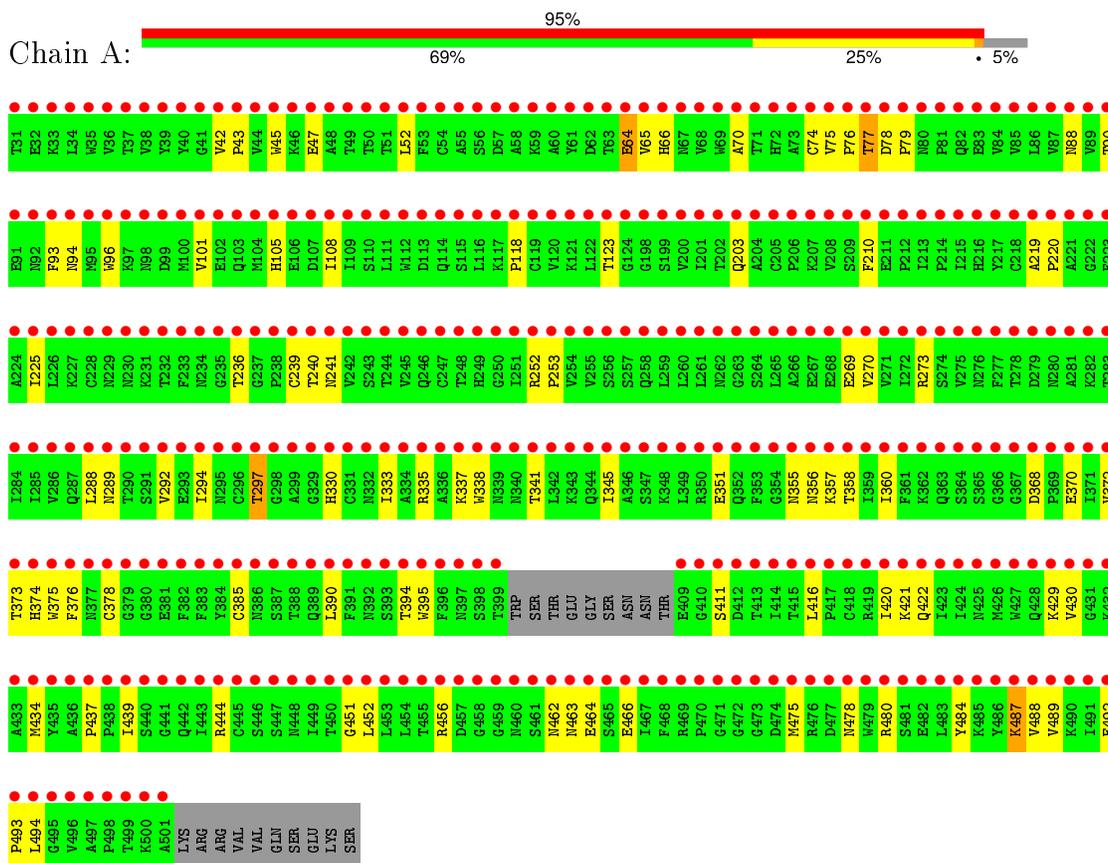
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	135	Total 135	O 135	0	0
7	C	50	Total 50	O 50	0	0
7	L	54	Total 54	O 54	0	0
7	H	47	Total 47	O 47	0	0
7	B	68	Total 68	O 68	0	0
7	D	34	Total 34	O 34	0	0
7	O	23	Total 23	O 23	0	0
7	P	39	Total 39	O 39	0	0

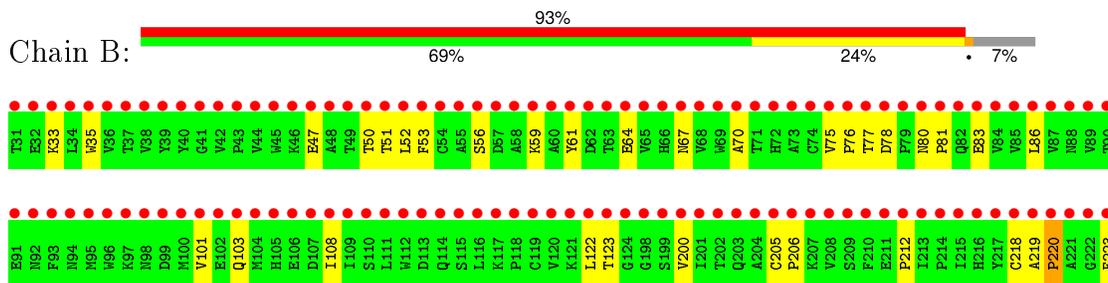
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 GP120 ENVELOPE GLYCOPROTEIN

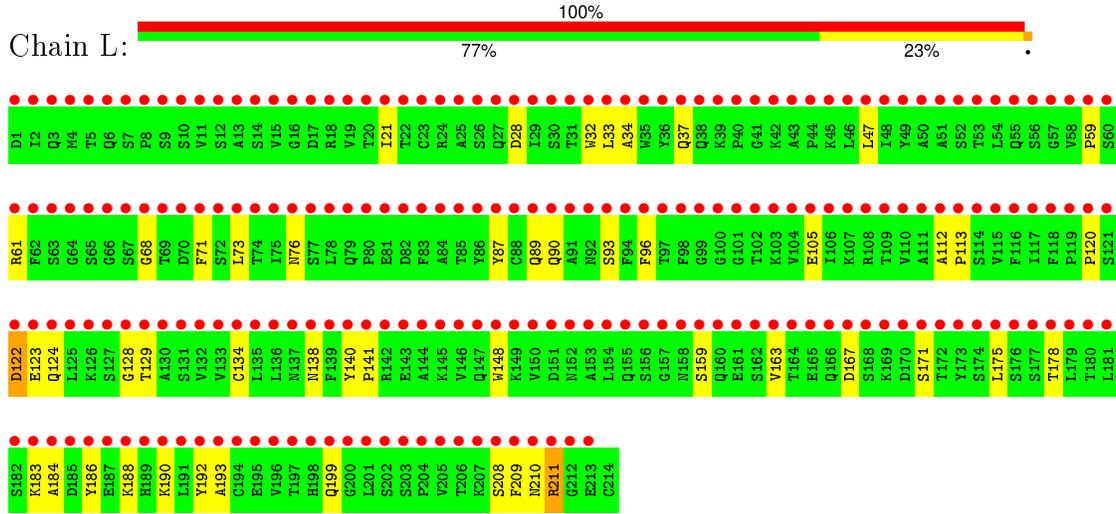


- Molecule 1: HIV-1 GP120 ENVELOPE GLYCOPROTEIN

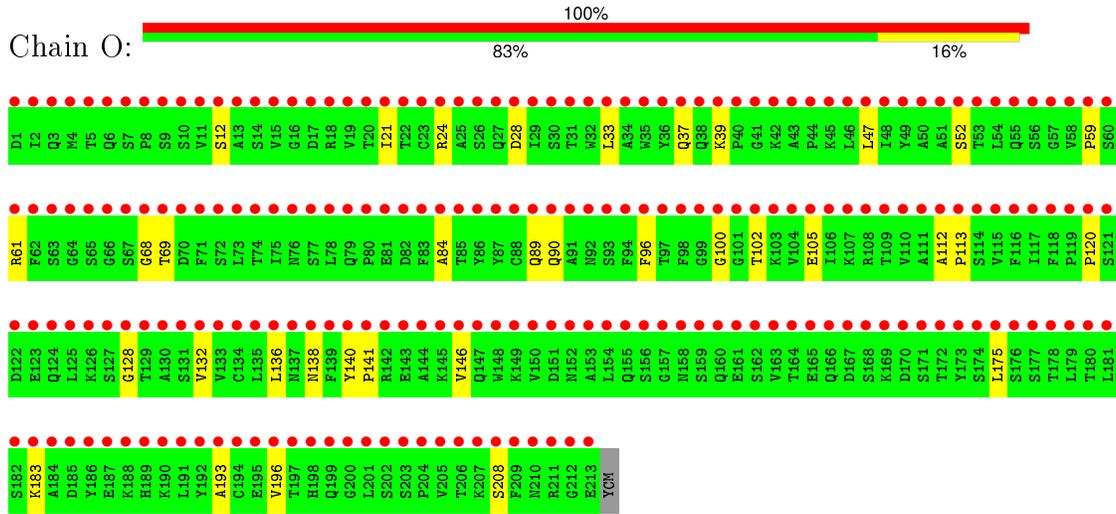


● Q1180
● K1181
● A1182
● S1183

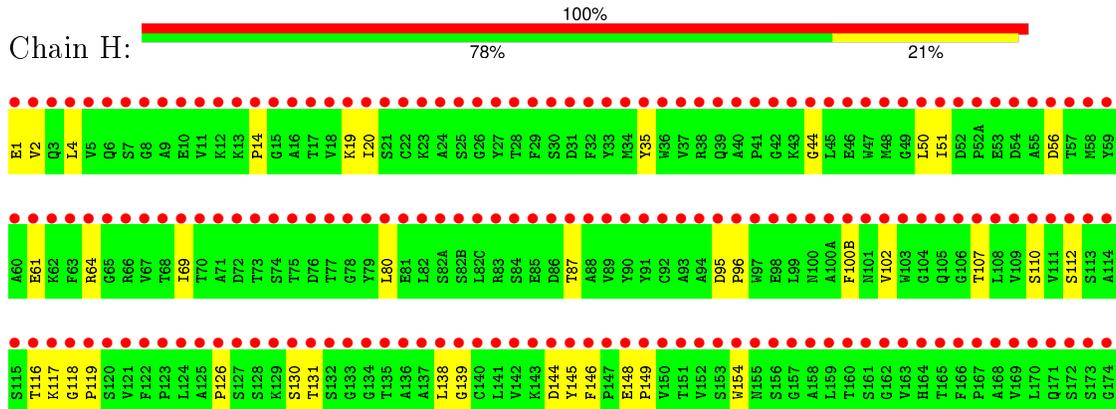
● Molecule 3: FAB 48D LIGHT CHAIN



● Molecule 3: FAB 48D LIGHT CHAIN



● Molecule 4: FAB 48D HEAVY CHAIN





• Molecule 4: FAB 48D HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.11Å 172.95Å 193.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.86 – 2.61 43.86 – 2.61	Depositor EDS
% Data completeness (in resolution range)	63.8 (43.86-2.61) 63.9 (43.86-2.61)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.04 (at 2.61Å)	Xtriage
Refinement program	PHENIX (CCI APPS 2007_04_06_1210)	Depositor
R, R_{free}	0.201 , 0.275 0.198 , 0.280	Depositor DCC
R_{free} test set	5577 reflections (10.14%)	DCC
Wilson B-factor (Å ²)	-10.7	Xtriage
Anisotropy	-7.799	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 62.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	23 of 59587 reflections (0.039%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15697	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, NAG, YCM

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	0.24	0/2865	0.42	0/3900
1	B	0.22	0/2821	0.39	0/3841
2	C	0.23	0/1452	0.43	0/1955
2	D	0.22	0/1444	0.38	0/1945
3	L	0.23	0/1659	0.40	0/2252
3	O	0.21	0/1659	0.38	0/2252
4	H	0.22	0/1695	0.42	0/2311
4	P	0.21	0/1685	0.39	0/2300
All	All	0.22	0/15280	0.40	0/20756

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	2800	0	2724	67	0
1	B	2756	0	2683	68	0
2	C	1432	0	1460	35	0
2	D	1424	0	1451	21	0
3	L	1635	0	1582	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	1624	0	1574	19	0
4	H	1654	0	1613	30	0
4	P	1644	0	1600	37	0
5	A	140	0	130	2	0
5	B	126	0	117	2	0
6	B	6	0	8	3	0
6	P	6	0	8	0	0
7	A	135	0	0	1	0
7	B	68	0	0	0	0
7	C	50	0	0	1	0
7	D	34	0	0	0	0
7	H	47	0	0	0	0
7	L	54	0	0	1	0
7	O	23	0	0	0	0
7	P	39	0	0	0	0
All	All	15697	0	14950	299	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 10.

The worst 5 of 299 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:B:254:VAL:HB	6:B:1:GOL:H11	1.43	1.00
1:A:492:GLU:HB2	1:A:493:PRO:HD2	1.55	0.88
4:H:126:PRO:HD3	4:H:138:LEU:HD13	1.54	0.88
2:C:1085:GLU:HG2	2:C:1090:LYS:HG3	1.57	0.84
1:B:342:LEU:HB3	1:B:395:TRP:HE1	1.42	0.84

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	A	356/379 (94%)	311 (87%)	40 (11%)	5 (1%)	14	26
1	B	350/379 (92%)	314 (90%)	31 (9%)	5 (1%)	14	26
2	C	182/184 (99%)	168 (92%)	13 (7%)	1 (0%)	34	58
2	D	181/184 (98%)	159 (88%)	22 (12%)	0	100	100
3	L	211/213 (99%)	194 (92%)	14 (7%)	3 (1%)	14	26
3	O	210/213 (99%)	181 (86%)	26 (12%)	3 (1%)	14	26
4	H	218/220 (99%)	193 (88%)	22 (10%)	3 (1%)	14	26
4	P	217/220 (99%)	194 (89%)	20 (9%)	3 (1%)	14	26
All	All	1925/1992 (97%)	1714 (89%)	188 (10%)	23 (1%)	16	32

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	76	ASN
3	L	138	ASN
1	B	439	ILE
1	B	440	SER
1	A	356	ASN

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	A	315/333 (95%)	310 (98%)	5 (2%)	70	88
1	B	310/333 (93%)	309 (100%)	1 (0%)	94	99
2	C	166/166 (100%)	161 (97%)	5 (3%)	48	75
2	D	165/166 (99%)	162 (98%)	3 (2%)	66	86
3	L	184/184 (100%)	180 (98%)	4 (2%)	60	83
3	O	184/184 (100%)	184 (100%)	0	100	100
4	H	185/185 (100%)	184 (100%)	1 (0%)	92	98
4	P	184/185 (100%)	184 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1693/1736 (98%)	1674 (99%)	19 (1%)	80 92

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	1106	THR
3	L	105	GLU
1	B	396	PHE
2	C	1059	ARG
2	D	1015	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	O	27	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](#)

1 non-standard protein/DNA/RNA residue is 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
3	YCM	L	214	3	7,10,10	1.30	2 (28%)	4,12,12	0.82	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
3	YCM	L	214	3	-	0/6/10/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	214	YCM	CB-SG	-2.37	1.76	1.81
3	L	214	YCM	CD-SG	-2.27	1.76	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

21 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	$\# Z > 2$
5	NAG	A	588	1	14,14,15	0.50	0	15,19,21	1.02	1 (6%)
5	NAG	A	734	1	14,14,15	0.51	0	15,19,21	0.75	0
5	NAG	A	741	1	14,14,15	0.46	0	15,19,21	0.98	1 (6%)
5	NAG	A	762	1	14,14,15	0.50	0	15,19,21	0.90	1 (6%)
5	NAG	A	776	1	14,14,15	0.47	0	15,19,21	0.92	1 (6%)
5	NAG	A	789	1	14,14,15	0.55	0	15,19,21	0.72	0
5	NAG	A	886	1	14,14,15	0.48	0	15,19,21	0.85	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	892	1	14,14,15	0.58	0	15,19,21	1.21	1 (6%)
5	NAG	A	897	1	14,14,15	0.53	0	15,19,21	0.74	0
5	NAG	A	948	1	14,14,15	0.52	0	15,19,21	0.75	0
6	GOL	B	1	-	5,5,5	0.38	0	5,5,5	0.20	0
5	NAG	B	588	1	14,14,15	0.48	0	15,19,21	0.80	1 (6%)
5	NAG	B	734	1	14,14,15	0.48	0	15,19,21	0.75	0
5	NAG	B	762	1	14,14,15	0.51	0	15,19,21	0.95	1 (6%)
5	NAG	B	776	1	14,14,15	0.47	0	15,19,21	0.88	1 (6%)
5	NAG	B	789	1	14,14,15	0.50	0	15,19,21	0.86	1 (6%)
5	NAG	B	795	1	14,14,15	0.45	0	15,19,21	0.88	1 (6%)
5	NAG	B	886	1	14,14,15	0.47	0	15,19,21	0.95	1 (6%)
5	NAG	B	892	1	14,14,15	0.51	0	15,19,21	0.70	0
5	NAG	B	948	1	14,14,15	0.49	0	15,19,21	0.70	0
6	GOL	P	215	-	5,5,5	0.38	0	5,5,5	0.24	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
5	NAG	A	588	1	-	0/6/23/26	0/1/1/1
5	NAG	A	734	1	1/1/5/7	1/6/23/26	0/1/1/1
5	NAG	A	741	1	-	0/6/23/26	0/1/1/1
5	NAG	A	762	1	-	0/6/23/26	0/1/1/1
5	NAG	A	776	1	-	0/6/23/26	0/1/1/1
5	NAG	A	789	1	-	1/6/23/26	0/1/1/1
5	NAG	A	886	1	-	0/6/23/26	0/1/1/1
5	NAG	A	892	1	-	0/6/23/26	0/1/1/1
5	NAG	A	897	1	-	0/6/23/26	0/1/1/1
5	NAG	A	948	1	1/1/5/7	0/6/23/26	0/1/1/1
6	GOL	B	1	-	-	0/4/4/4	0/0/0/0
5	NAG	B	588	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	B	734	1	-	1/6/23/26	0/1/1/1
5	NAG	B	762	1	-	0/6/23/26	0/1/1/1
5	NAG	B	776	1	-	0/6/23/26	0/1/1/1
5	NAG	B	789	1	-	0/6/23/26	0/1/1/1
5	NAG	B	795	1	-	0/6/23/26	0/1/1/1
5	NAG	B	886	1	-	0/6/23/26	0/1/1/1
5	NAG	B	892	1	-	1/6/23/26	0/1/1/1
5	NAG	B	948	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
6	GOL	P	215	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	789	NAG	C1-O5-C5	2.22	115.06	112.25
5	B	588	NAG	C1-O5-C5	2.27	115.13	112.25
5	B	776	NAG	C1-O5-C5	2.29	115.16	112.25
5	A	762	NAG	C1-O5-C5	2.29	115.16	112.25
5	B	795	NAG	C1-O5-C5	2.34	115.21	112.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	734	NAG	C1
5	B	588	NAG	C1
5	A	948	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	734	NAG	O7-C7-N2-C2
5	B	892	NAG	O7-C7-N2-C2
5	A	789	NAG	O7-C7-N2-C2
5	B	734	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	588	NAG	1	0
5	A	734	NAG	1	0
6	B	1	GOL	3	0
5	B	762	NAG	1	0
5	B	789	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	360/379 (94%)	13.52	360 (100%) 0 0	45, 78, 151, 254	0
1	B	354/379 (93%)	13.23	354 (100%) 0 0	66, 113, 190, 233	0
2	C	184/184 (100%)	13.79	184 (100%) 0 0	56, 83, 125, 144	0
2	D	183/184 (99%)	13.38	183 (100%) 0 0	74, 127, 165, 188	0
3	L	212/213 (99%)	14.03	212 (100%) 0 0	59, 101, 179, 240	0
3	O	212/213 (99%)	13.07	212 (100%) 0 0	91, 147, 189, 220	0
4	H	220/220 (100%)	14.19	220 (100%) 0 0	70, 121, 179, 251	0
4	P	219/220 (99%)	13.71	219 (100%) 0 0	66, 121, 195, 243	0
All	All	1944/1992 (97%)	13.58	1944 (100%) 0 0	45, 110, 180, 254	0

The worst 5 of 1944 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	41	GLY	27.1
4	H	88	ALA	24.9
1	B	385	CYS	24.6
4	P	26	GLY	24.2
1	A	228	CYS	23.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	YCM	L	214	11/11	-0.30	1.01	-	180,198,236,238	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	B	789	14/15	-0.11	1.22	1.40	139,187,198,202	0
5	NAG	A	789	14/15	-0.09	1.16	0.56	86,104,117,128	0
5	NAG	A	776	14/15	-0.22	1.19	0.52	80,95,117,119	0
5	NAG	B	734	14/15	-0.31	1.17	0.50	167,184,193,194	0
5	NAG	A	886	14/15	-0.13	1.29	0.16	70,97,131,139	0
5	NAG	A	897	14/15	-0.03	1.10	0.06	124,150,169,175	0
5	NAG	A	762	14/15	-0.10	1.09	-0.28	70,75,96,97	0
5	NAG	A	734	14/15	0.04	1.10	-0.29	113,130,148,153	0
5	NAG	B	762	14/15	0.01	1.01	-0.37	102,122,145,155	0
6	GOL	B	1	6/6	-0.05	0.87	-0.75	127,132,138,143	0
5	NAG	A	948	14/15	-0.14	1.04	-0.80	143,154,166,166	0
5	NAG	B	776	14/15	0.07	1.04	-1.09	118,135,157,161	0
6	GOL	P	215	6/6	0.26	0.82	-2.38	134,147,156,162	0
5	NAG	B	892	14/15	0.07	1.09	-	166,204,227,236	0
5	NAG	B	795	14/15	-0.14	1.04	-	169,190,203,209	0
5	NAG	A	892	14/15	-0.01	1.13	-	117,148,182,193	0
5	NAG	A	588	14/15	0.07	1.09	-	99,141,159,174	0
5	NAG	B	886	14/15	-0.20	1.05	-	105,122,143,147	0
5	NAG	B	948	14/15	-0.20	1.11	-	147,169,175,179	0
5	NAG	A	741	14/15	-0.02	1.01	-	141,160,164,166	0
5	NAG	B	588	14/15	-0.13	0.86	-	119,161,167,169	0

6.5 Other polymers [i](#)

There are no such residues in this entry.