WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 09:14 PM EDT

PDB ID	:	2NY7
Title	:	HIV-1 gp120 Envelope Glycoprotein Complexed with the Broadly Neutralizing CD4-Binding-Site Antibody b12
Authors	:	Zhou, T.; Xu, L.; Dey, B.; Hessell, A.J.; Van Ryk, D.; Xiang, S.H.; Yang, X.; Zhang, M.Y.; Zwick, M.B.; Arthos, J.; Burton, D.R.; Dimitrov, D.S.; Sodroski, J.; Wyatt, R.; Nabel, G.J.; Kwong, P.D.
Deposited on	:	2006-11-20
Resolution	:	2.30 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) 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)
Validation Pipeline (wwPDB-VP)	:	2.35
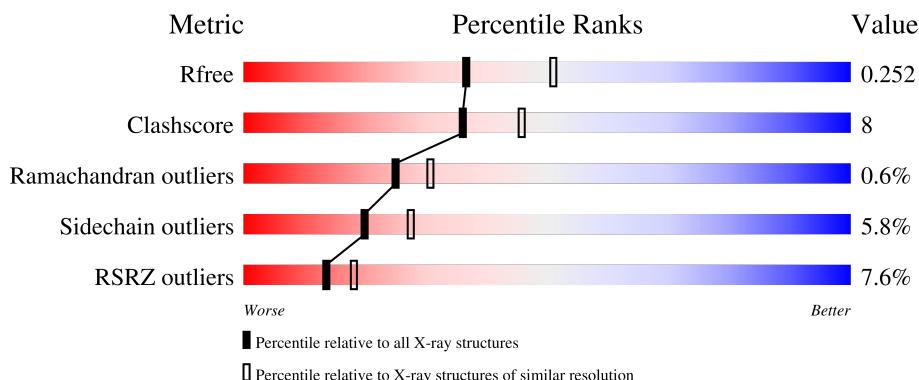
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
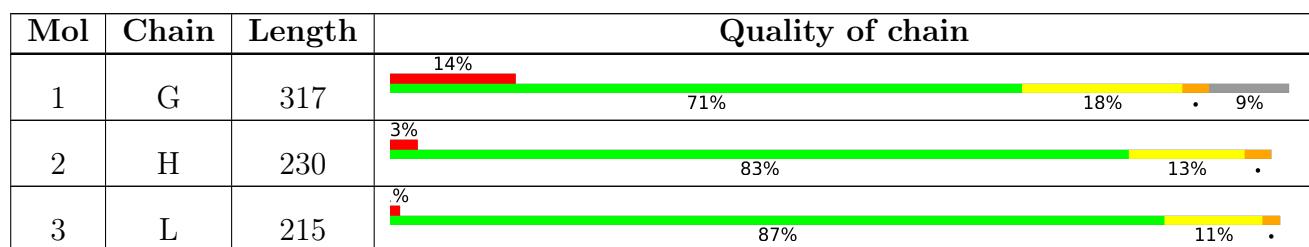
The reported resolution of this entry is 2.30 Å.

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	Percentile Ranks	Value
Rfree		0.252
Clashscore		8
Ramachandran outliers		0.6%
Sidechain outliers		5.8%
RSRZ outliers		7.6%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	317	14% 71% 18% • 9%
2	H	230	3% 83% 13% •
3	L	215	% 87% 11% •

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 6181 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 ENVELOPE GLYCOPROTEIN GP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	290	Total	C	N	O	S	0	0	0
			2266	1422	394	428	22			
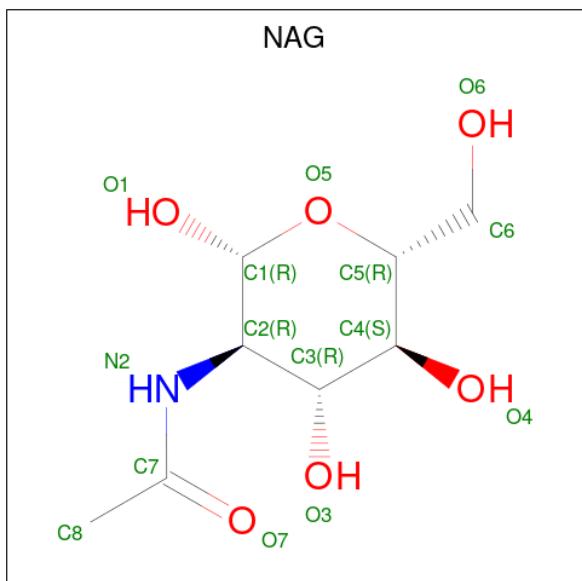
- Molecule 2 is a protein called ANTIBODY b12, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	230	Total	C	N	O	S	0	1	0
			1757	1109	300	340	8			

- Molecule 3 is a protein called ANTIBODY b12, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	0	0
			1668	1036	297	330	5			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
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		
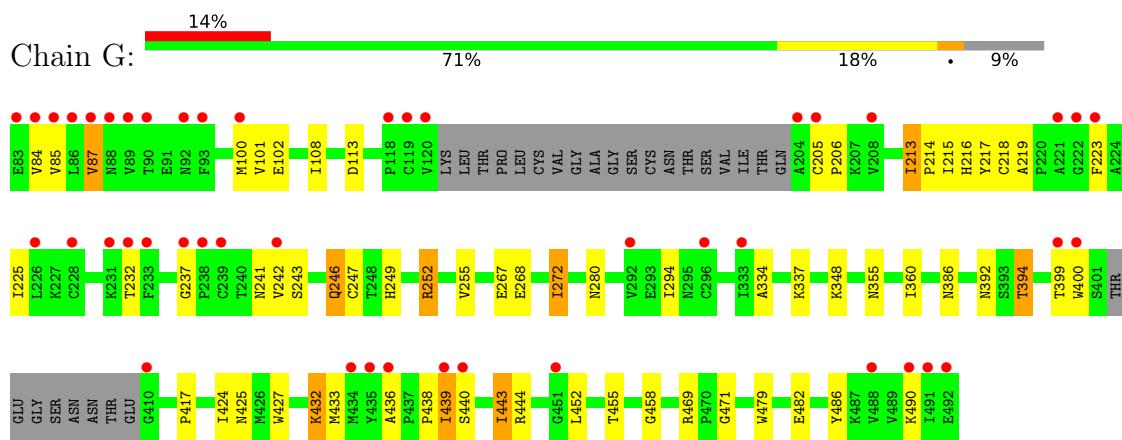
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	88	Total	O	0	0
			88	88		
5	H	123	Total	O	0	0
			123	123		
5	L	97	Total	O	0	0
			97	97		
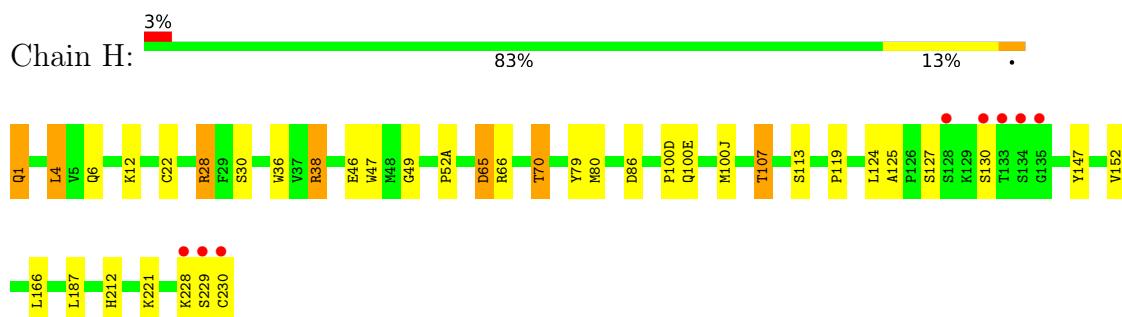
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
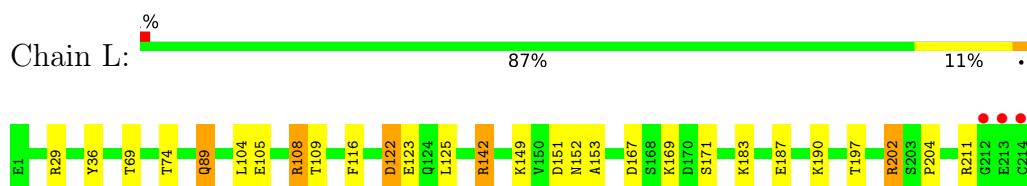
• Molecule 1: ENVELOPE GLYCOPROTEIN GP120

Chain G:

• Molecule 2: ANTIBODY b12, HEAVY CHAIN

Chain H:

• Molecule 3: ANTIBODY b12, LIGHT CHAIN

Chain L:

4 Data and refinement statistics (i)

| Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	101.95Å 101.95Å 298.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.45 – 2.30 49.43 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.45-2.30) 90.8 (49.43-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.193 , 0.255 0.191 , 0.252	Depositor DCC
R_{free} test set	1890 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	53.0	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 57.3	EDS
L-test for twinning[2]	$< \mid L \mid > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6181	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \mid L \mid >$, $< L^2 >$ 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	0.26	0/2314	0.43	0/3134
2	H	0.30	0/1812	0.48	0/2469
3	L	0.29	0/1704	0.47	0/2306
All	All	0.28	0/5830	0.45	0/7909

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 ⓘ

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	2266	0	2184	48	0
2	H	1757	0	1695	29	0
3	L	1668	0	1621	19	0
4	G	182	0	169	4	0
5	G	88	0	0	2	0
5	H	123	0	0	2	1
5	L	97	0	0	0	1
All	All	6181	0	5669	92	1

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 8.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:28[B]:ARG:NH2	5:H:353:HOH:O	1.79	1.11
3:L:142:ARG:HG2	3:L:142:ARG:HH21	1.07	1.08
3:L:142:ARG:HH21	3:L:142:ARG:CG	1.76	0.97
1:G:252:ARG:CG	1:G:252:ARG:HH11	1.78	0.96
2:H:70:THR:HG22	2:H:79:TYR:HB2	1.47	0.95
3:L:142:ARG:HG2	3:L:142:ARG:NH2	1.85	0.90
1:G:249:HIS:NE2	1:G:482:GLU:HG3	1.88	0.88
1:G:252:ARG:HH11	1:G:252:ARG:HG3	1.48	0.78
1:G:392:ASN:HD22	4:G:892:NAG:H83	1.49	0.77
1:G:469:ARG:HD2	2:H:28[B]:ARG:HH12	1.53	0.74
1:G:252:ARG:HH11	1:G:252:ARG:HG2	1.50	0.73
3:L:202:ARG:H	3:L:202:ARG:HE	1.37	0.71
3:L:183:LYS:O	3:L:187:GLU:HG2	1.94	0.68
1:G:113:ASP:HB2	5:G:980:HOH:O	1.94	0.66
1:G:280:ASN:O	2:H:28[A]:ARG:NH1	2.26	0.66
1:G:219:ALA:HB2	1:G:225:ILE:HG13	1.78	0.65
3:L:108:ARG:HD3	3:L:109:THR:O	1.97	0.65
2:H:30:SER:HA	2:H:52(A):PRO:HB2	1.80	0.63
3:L:202:ARG:H	3:L:202:ARG:NE	1.95	0.63
2:H:125:ALA:CB	2:H:228:LYS:HG2	2.29	0.61
1:G:85:VAL:HG11	4:G:741:NAG:H61	1.81	0.61
1:G:213:ILE:HD11	1:G:216:HIS:HE1	1.65	0.61
1:G:267:GLU:O	1:G:268:GLU:HG2	2.01	0.60
1:G:443:ILE:H	1:G:443:ILE:HD13	1.65	0.60
2:H:130:SER:HA	3:L:116:PHE:HD2	1.68	0.57
2:H:65:ASP:OD2	2:H:65:ASP:N	2.38	0.57
1:G:215:ILE:HG12	1:G:479:TRP:CZ2	2.40	0.56
1:G:438:PRO:C	1:G:440:SER:H	2.07	0.56
1:G:252:ARG:HG3	1:G:252:ARG:NH1	2.16	0.56
2:H:6:GLN:HE21	2:H:107:THR:HG23	1.70	0.56
3:L:36:TYR:HE1	3:L:89:GLN:HG2	1.72	0.55
2:H:6:GLN:HE21	2:H:107:THR:CG2	2.19	0.55
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.28	0.55
2:H:6:GLN:NE2	2:H:107:THR:HG23	2.22	0.53
2:H:28[B]:ARG:CZ	5:H:353:HOH:O	2.38	0.53
1:G:237:GLY:HA3	4:G:734:NAG:H62	1.92	0.52
1:G:272:ILE:HD12	1:G:348:LYS:HB3	1.90	0.52
2:H:228:LYS:O	2:H:230:CYS:N	2.42	0.52
3:L:122:ASP:OD1	3:L:122:ASP:N	2.35	0.52
2:H:36:TRP:CE2	2:H:80:MET:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.92	0.50
2:H:147:TYR:CE2	2:H:152:VAL:HG13	2.47	0.49
2:H:125:ALA:HB3	2:H:228:LYS:HG2	1.94	0.49
1:G:280:ASN:ND2	1:G:458:GLY:HA3	2.27	0.49
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.48	0.49
1:G:252:ARG:CG	1:G:252:ARG:NH1	2.49	0.49
1:G:355:ASN:HB2	4:G:856:NAG:H4	1.93	0.49
1:G:424:ILE:HD13	1:G:436:ALA:HB2	1.93	0.49
3:L:108:ARG:CD	3:L:109:THR:O	2.61	0.49
1:G:424:ILE:O	1:G:425:ASN:HB2	2.13	0.49
2:H:152:VAL:HG12	2:H:212:HIS:CD2	2.48	0.48
1:G:334:ALA:HB3	1:G:337:LYS:HD2	1.95	0.48
1:G:232:THR:O	5:G:1034:HOH:O	2.20	0.48
3:L:142:ARG:CG	3:L:142:ARG:NH2	2.48	0.47
1:G:213:ILE:HD12	1:G:214:PRO:HD2	1.95	0.47
1:G:242:VAL:HG12	1:G:243:SER:N	2.29	0.47
2:H:187:LEU:C	2:H:187:LEU:HD12	2.35	0.47
2:H:4:LEU:HG	2:H:22:CYS:SG	2.56	0.46
1:G:249:HIS:NE2	1:G:482:GLU:CG	2.71	0.46
2:H:130:SER:HA	3:L:116:PHE:CD2	2.50	0.46
1:G:439:ILE:HG22	1:G:439:ILE:O	2.15	0.46
1:G:84:VAL:HG22	1:G:85:VAL:H	1.82	0.45
1:G:217:TYR:O	1:G:247:CYS:HA	2.17	0.45
1:G:294:ILE:HG23	1:G:294:ILE:O	2.17	0.45
3:L:149:LYS:HA	3:L:153:ALA:O	2.16	0.45
2:H:1:GLN:CD	2:H:1:GLN:H3	2.21	0.45
1:G:108:ILE:HD11	1:G:433:MET:HG3	1.98	0.44
3:L:167:ASP:O	3:L:171:SER:HA	2.16	0.44
1:G:223:PHE:CE2	1:G:490:LYS:HG2	2.52	0.44
3:L:122:ASP:HA	3:L:125:LEU:HD12	1.99	0.44
1:G:213:ILE:HD11	1:G:216:HIS:CE1	2.50	0.44
2:H:1:GLN:CD	2:H:1:GLN:N	2.71	0.43
2:H:38:ARG:HD2	2:H:46:GLU:OE1	2.18	0.43
3:L:151:ASP:O	3:L:152:ASN:HB2	2.16	0.43
1:G:360:ILE:HG12	1:G:394:THR:HB	2.00	0.43
2:H:6:GLN:HB3	2:H:107:THR:HG22	2.01	0.43
1:G:218:CYS:HA	1:G:246:GLN:O	2.17	0.43
3:L:190:LYS:HA	3:L:211:ARG:HB2	1.99	0.42
3:L:197:THR:HG22	3:L:204:PRO:HB3	2.02	0.42
1:G:438:PRO:C	1:G:440:SER:N	2.72	0.42
1:G:443:ILE:HD13	1:G:443:ILE:N	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:399:THR:HG23	1:G:400:TRP:CD1	2.54	0.42
1:G:205:CYS:HA	1:G:206:PRO:HD3	1.96	0.42
1:G:386:ASN:HB3	1:G:417:PRO:HG2	2.01	0.41
1:G:455:THR:HG23	1:G:471:GLY:O	2.19	0.41
1:G:100:MET:SD	1:G:486:TYR:HB2	2.61	0.41
1:G:252:ARG:HG2	1:G:252:ARG:NH1	2.24	0.41
1:G:427:TRP:HD1	1:G:432:LYS:HB3	1.85	0.41
1:G:348:LYS:HA	1:G:348:LYS:HD3	1.91	0.41
2:H:36:TRP:CD2	2:H:80:MET:HB2	2.56	0.41
1:G:87:VAL:HG12	1:G:241:ASN:HA	2.03	0.41
2:H:100(D):PRO:O	2:H:100(E):GLN:HB2	2.20	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:342:HOH:O	5:L:303:HOH:O[12_566]	2.14	0.06

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	284/317 (90%)	262 (92%)	20 (7%)	2 (1%)	22	26
2	H	229/230 (100%)	221 (96%)	6 (3%)	2 (1%)	17	20
3	L	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
All	All	726/762 (95%)	690 (95%)	32 (4%)	4 (1%)	25	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	229	SER

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Mol	Chain	Res	Type
2	H	127	SER
1	G	439	ILE
1	G	87	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	258/281 (92%)	246 (95%)	12 (5%)	26	37
2	H	196/195 (100%)	182 (93%)	14 (7%)	14	19
3	L	187/187 (100%)	175 (94%)	12 (6%)	17	23
All	All	641/663 (97%)	603 (94%)	38 (6%)	20	27

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	101	VAL
1	G	102	GLU
1	G	213	ILE
1	G	246	GLN
1	G	252	ARG
1	G	255	VAL
1	G	272	ILE
1	G	394	THR
1	G	432	LYS
1	G	443	ILE
1	G	444	ARG
1	G	452	LEU
2	H	1	GLN
2	H	4	LEU
2	H	12	LYS
2	H	28[A]	ARG
2	H	28[B]	ARG
2	H	38	ARG
2	H	65	ASP

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Mol	Chain	Res	Type
2	H	70	THR
2	H	100(J)	MET
2	H	107	THR
2	H	113	SER
2	H	124	LEU
2	H	166	LEU
2	H	221	LYS
3	L	29	ARG
3	L	69	THR
3	L	74	THR
3	L	89	GLN
3	L	104	LEU
3	L	105	GLU
3	L	108	ARG
3	L	122	ASP
3	L	123	GLU
3	L	142	ARG
3	L	169	LYS
3	L	202	ARG

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

Mol	Chain	Res	Type
3	L	147	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

13 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	892	1	14,14,15	0.45	0	17,19,21	1.24	3 (17%)
4	NAG	G	734	1	14,14,15	0.52	0	17,19,21	0.63	0
4	NAG	G	789	1	14,14,15	0.48	0	17,19,21	1.27	3 (17%)
4	NAG	G	776	1	14,14,15	0.57	0	17,19,21	0.70	0
4	NAG	G	897	1	14,14,15	0.50	0	17,19,21	0.71	0
4	NAG	G	741	1	14,14,15	0.63	0	17,19,21	1.00	1 (5%)
4	NAG	G	886	1	14,14,15	0.27	0	17,19,21	1.13	3 (17%)
4	NAG	G	856	1	14,14,15	0.59	0	17,19,21	0.66	0
4	NAG	G	963	1	14,14,15	0.53	0	17,19,21	0.61	0
4	NAG	G	839	1	14,14,15	0.54	0	17,19,21	0.85	0
4	NAG	G	795	1	14,14,15	0.68	0	17,19,21	0.78	0
4	NAG	G	948	1	14,14,15	0.48	0	17,19,21	0.91	0
4	NAG	G	762	1	14,14,15	0.55	0	17,19,21	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	892	1	-	3/6/23/26	0/1/1/1
4	NAG	G	734	1	-	3/6/23/26	0/1/1/1
4	NAG	G	789	1	-	5/6/23/26	0/1/1/1
4	NAG	G	776	1	-	4/6/23/26	0/1/1/1
4	NAG	G	897	1	-	3/6/23/26	0/1/1/1
4	NAG	G	741	1	-	5/6/23/26	0/1/1/1
4	NAG	G	886	1	-	2/6/23/26	0/1/1/1
4	NAG	G	856	1	-	5/6/23/26	0/1/1/1
4	NAG	G	963	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	839	1	-	4/6/23/26	0/1/1/1
4	NAG	G	795	1	-	2/6/23/26	0/1/1/1
4	NAG	G	948	1	-	4/6/23/26	0/1/1/1
4	NAG	G	762	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	892	NAG	C4-C3-C2	-2.81	106.91	111.02
4	G	789	NAG	O5-C1-C2	-2.62	107.15	111.29
4	G	886	NAG	O5-C5-C6	2.40	110.96	107.20
4	G	789	NAG	C1-C2-N2	2.37	114.54	110.49
4	G	789	NAG	O5-C5-C6	2.36	110.91	107.20
4	G	886	NAG	C1-O5-C5	-2.30	109.08	112.19
4	G	892	NAG	O5-C1-C2	-2.15	107.89	111.29
4	G	741	NAG	C4-C3-C2	2.15	114.17	111.02
4	G	886	NAG	C1-C2-N2	-2.06	106.97	110.49
4	G	892	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	734	NAG	C8-C7-N2-C2
4	G	734	NAG	O7-C7-N2-C2
4	G	741	NAG	O7-C7-N2-C2
4	G	776	NAG	C8-C7-N2-C2
4	G	776	NAG	O7-C7-N2-C2
4	G	789	NAG	C8-C7-N2-C2
4	G	789	NAG	O7-C7-N2-C2
4	G	839	NAG	C8-C7-N2-C2
4	G	839	NAG	O7-C7-N2-C2
4	G	856	NAG	C3-C2-N2-C7
4	G	856	NAG	C8-C7-N2-C2
4	G	856	NAG	O7-C7-N2-C2
4	G	897	NAG	C3-C2-N2-C7
4	G	897	NAG	C8-C7-N2-C2
4	G	897	NAG	O7-C7-N2-C2
4	G	948	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	G	948	NAG	O7-C7-N2-C2
4	G	963	NAG	C8-C7-N2-C2
4	G	963	NAG	O7-C7-N2-C2
4	G	948	NAG	O5-C5-C6-O6
4	G	741	NAG	C8-C7-N2-C2
4	G	741	NAG	C1-C2-N2-C7
4	G	948	NAG	C4-C5-C6-O6
4	G	963	NAG	C4-C5-C6-O6
4	G	789	NAG	O5-C5-C6-O6
4	G	963	NAG	O5-C5-C6-O6
4	G	886	NAG	O5-C5-C6-O6
4	G	789	NAG	C4-C5-C6-O6
4	G	892	NAG	C8-C7-N2-C2
4	G	892	NAG	O7-C7-N2-C2
4	G	856	NAG	C4-C5-C6-O6
4	G	789	NAG	C1-C2-N2-C7
4	G	886	NAG	C4-C5-C6-O6
4	G	856	NAG	O5-C5-C6-O6
4	G	776	NAG	O5-C5-C6-O6
4	G	776	NAG	C4-C5-C6-O6
4	G	762	NAG	O5-C5-C6-O6
4	G	762	NAG	C4-C5-C6-O6
4	G	795	NAG	C4-C5-C6-O6
4	G	741	NAG	O5-C5-C6-O6
4	G	741	NAG	C3-C2-N2-C7
4	G	795	NAG	O5-C5-C6-O6
4	G	839	NAG	C4-C5-C6-O6
4	G	839	NAG	O5-C5-C6-O6
4	G	734	NAG	C4-C5-C6-O6
4	G	892	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	892	NAG	1	0
4	G	734	NAG	1	0
4	G	741	NAG	1	0
4	G	856	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	G	290/317 (91%)	0.93	45 (15%)	2	3	43, 88, 167, 231	0
2	H	230/230 (100%)	0.05	8 (3%)	44	51	36, 54, 101, 172	0
3	L	215/215 (100%)	-0.09	3 (1%)	75	80	36, 59, 122, 159	0
All	All	735/762 (96%)	0.36	56 (7%)	13	18	36, 63, 144, 231	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	84	VAL	11.8
1	G	83	GLU	10.4
1	G	85	VAL	8.1
1	G	492	GLU	7.5
2	H	230	CYS	7.5
1	G	118	PRO	7.0
1	G	87	VAL	6.6
1	G	120	VAL	6.1
1	G	222	GLY	5.7
2	H	229	SER	5.2
1	G	439	ILE	4.9
1	G	410	GLY	4.9
1	G	400	TRP	4.8
2	H	228	LYS	4.8
3	L	214	CYS	4.6
1	G	86	LEU	4.4
2	H	134	SER	4.4
1	G	440	SER	4.3
2	H	130	SER	4.0
1	G	238	PRO	4.0
1	G	242	VAL	3.9
1	G	90	THR	3.9
1	G	232	THR	3.6

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Mol	Chain	Res	Type	RSRZ
2	H	133	THR	3.5
3	L	212	GLY	3.4
2	H	135	GLY	3.4
1	G	89	VAL	3.3
1	G	88	ASN	3.3
1	G	491	ILE	3.3
1	G	204	ALA	3.2
1	G	228	CYS	3.2
1	G	451	GLY	3.2
1	G	488	VAL	3.1
2	H	128	SER	3.1
1	G	231	LYS	3.0
1	G	237	GLY	2.9
1	G	333	ILE	2.9
1	G	226	LEU	2.9
1	G	490	LYS	2.7
1	G	119	CYS	2.7
1	G	208	VAL	2.7
1	G	435	TYR	2.5
3	L	213	GLU	2.5
1	G	434	MET	2.4
1	G	93	PHE	2.4
1	G	436	ALA	2.4
1	G	221	ALA	2.4
1	G	399	THR	2.3
1	G	292	VAL	2.3
1	G	92	ASN	2.3
1	G	296	CYS	2.2
1	G	205	CYS	2.1
1	G	223	PHE	2.1
1	G	233	PHE	2.1
1	G	239	CYS	2.1
1	G	100	MET	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	G	897	14/15	0.55	0.29	105,116,121,125	0
4	NAG	G	963	14/15	0.60	0.37	123,136,146,149	0
4	NAG	G	734	14/15	0.69	0.34	136,142,155,155	0
4	NAG	G	741	14/15	0.80	0.33	186,201,209,220	0
4	NAG	G	856	14/15	0.81	0.34	154,162,176,177	0
4	NAG	G	948	14/15	0.82	0.30	120,131,137,139	0
4	NAG	G	839	14/15	0.82	0.27	122,138,148,150	0
4	NAG	G	795	14/15	0.83	0.27	103,127,142,144	0
4	NAG	G	892	14/15	0.87	0.19	76,93,103,112	0
4	NAG	G	789	14/15	0.89	0.21	110,114,136,138	0
4	NAG	G	762	14/15	0.90	0.17	74,94,103,107	0
4	NAG	G	886	14/15	0.95	0.11	42,53,62,65	0
4	NAG	G	776	14/15	0.96	0.13	73,81,88,89	0

6.5 Other polymers ⓘ

There are no such residues in this entry.