



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 11:46 PM BST

PDB ID : 2B4C
Title : Crystal structure of HIV-1 JR-FL gp120 core protein containing the third variable region (V3) complexed with CD4 and the X5 antibody
Authors : Huang, C.; Tang, M.; Zhang, M.Y.; Majeed, S.; Montabana, E.; Stanfield, R.L.; Dimitrov, D.S.; Korber, B.; Sodroski, J.; Wilson, I.A.; Wyatt, R.; Kwong, P.D.
Deposited on : 2005-09-23
Resolution : 3.30 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 ⓘ 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

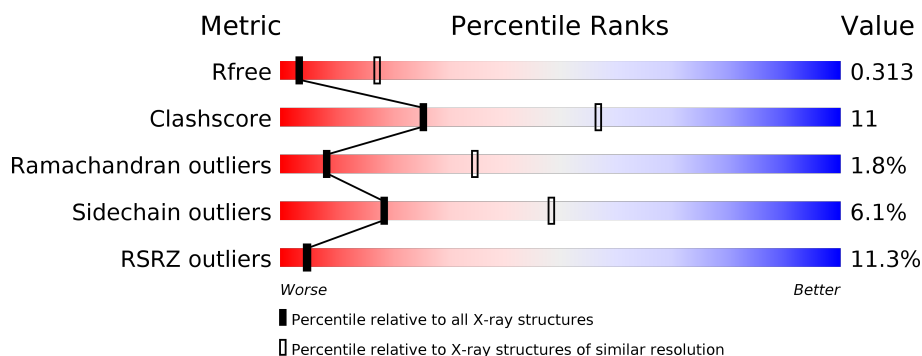
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	344	<div> <div>15%</div> <div>67%</div> <div>25%</div> <div>6%</div> </div>
2	C	181	<div> <div>14%</div> <div>78%</div> <div>18%</div> </div>
3	L	215	<div> <div>10%</div> <div>69%</div> <div>29%</div> </div>
4	H	235	<div> <div>6%</div> <div>83%</div> <div>15%</div> </div>
5	A	2	<div> <div>100%</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
5	NAG	A	1	X	-	-	X
6	NAG	G	832	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7543 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	339	Total	C	N	O	S	0	4	0
			2681	1674	477	509	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	175	Total	C	N	O	S	0	0	0
			1363	851	239	269	4			

- Molecule 3 is a protein called anti-HIV-1 gp120 immunoglobulin X5 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	0	0
			1636	1018	280	333	5			

- Molecule 4 is a protein called anti-HIV-1 gp120 immunoglobulin X5 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	233	Total	C	N	O	S	0	0	0
			1742	1098	290	346	8			

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



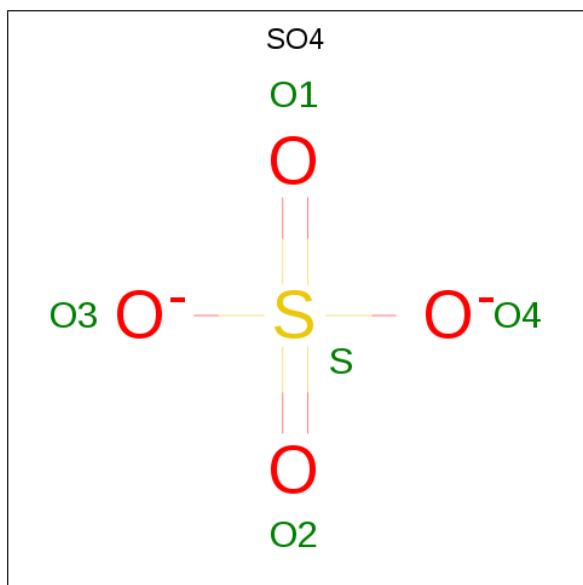
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	A	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



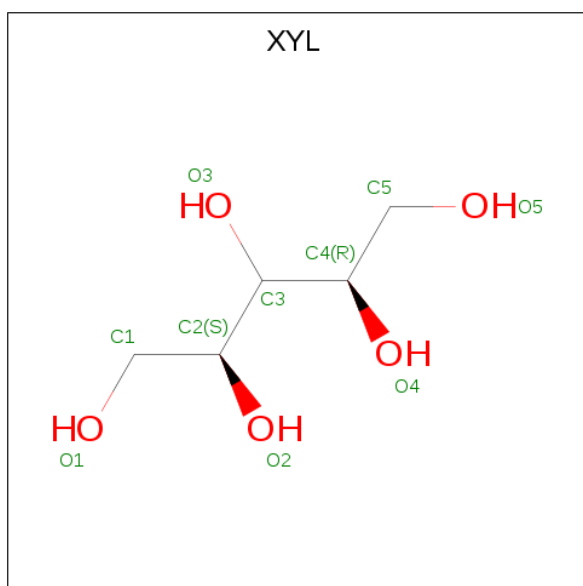
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

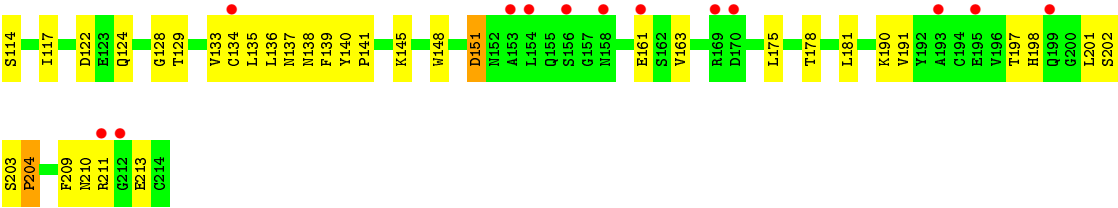


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total O S 5 4 1	0	0
7	L	1	Total O S 5 4 1	0	0
7	H	1	Total O S 5 4 1	0	0
7	H	1	Total O S 5 4 1	0	0
7	H	1	Total O S 5 4 1	0	0

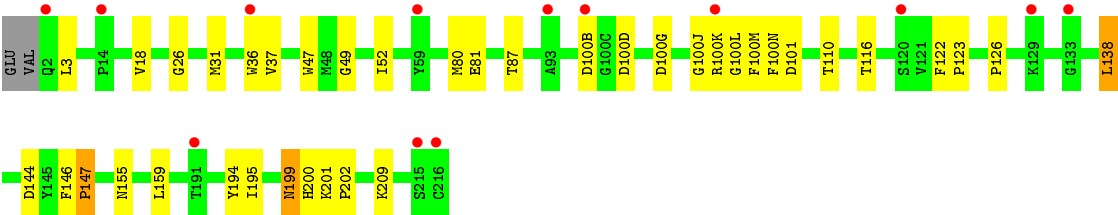
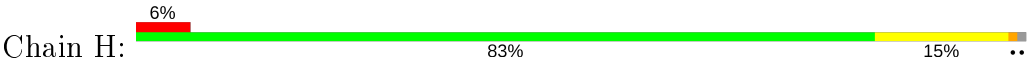
- Molecule 8 is Xylitol (three-letter code: XYL) (formula: $C_5H_{12}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total C O 10 5 5	0	0
8	H	1	Total C O 10 5 5	0	0
8	H	1	Total C O 10 5 5	0	0



● Molecule 4: anti-HIV-1 gp120 immunoglobulin X5 heavy chain



● Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, α , β , γ	225.99Å 225.99Å 97.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.30 19.88 – 3.31	Depositor EDS
% Data completeness (in resolution range)	86.2 (20.00-3.30) 86.3 (19.88-3.31)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.319 , 0.349 0.283 , 0.313	Depositor DCC
R_{free} test set	1928 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	134.8	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7543	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 2.02% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, XYL, SO4, 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	0.33	1/2734 (0.0%)	0.52	0/3701
2	C	0.26	0/1382	0.53	0/1863
3	L	0.28	0/1669	0.53	0/2264
4	H	0.28	0/1788	0.53	0/2432
All	All	0.30	1/7573 (0.0%)	0.53	0/10260

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	87	GLU	C-N	-7.20	1.17	1.34

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	G	2681	0	2628	79	0
2	C	1363	0	1389	28	0
3	L	1636	0	1591	38	0
4	H	1742	0	1662	22	0
5	A	24	0	22	0	0
6	G	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	5	0	0	0	0
7	H	15	0	0	0	0
7	L	5	0	0	0	0
8	H	30	0	36	0	0
All	All	7543	0	7367	158	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 11.

All (158) 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:G:326:ILE:HD13	1:G:326:ILE:H	1.35	0.92
4:H:126:PRO:HG3	4:H:138:LEU:HB3	1.52	0.91
1:G:371:ILE:HD13	2:C:45:THR:HG22	1.53	0.90
2:C:76:ILE:H	2:C:76:ILE:HD12	1.35	0.90
3:L:198:HIS:HB3	3:L:201:LEU:HB3	1.66	0.78
1:G:300:ASN:HD21	1:G:302:ASN:ND2	1.84	0.76
3:L:163:VAL:HG22	3:L:175:LEU:HD13	1.70	0.74
1:G:358:THR:HG23	1:G:396:ASN:HB3	1.70	0.73
1:G:371:ILE:HD11	2:C:43:PHE:HB3	1.71	0.72
1:G:251:ILE:HD12	1:G:482:GLU:HB3	1.72	0.71
1:G:491:ILE:O	1:G:491:ILE:HG23	1.93	0.68
3:L:90:GLN:HE21	3:L:97:THR:H	1.42	0.68
2:C:29:LYS:HB2	2:C:83:ILE:HD11	1.74	0.68
1:G:272:ILE:O	1:G:272:ILE:HD12	1.93	0.68
1:G:460:ILE:HD13	1:G:460:ILE:O	1.94	0.68
1:G:85:VAL:C	1:G:86:LEU:HD12	2.15	0.67
1:G:327:ARG:HH22	4:H:100(G):ASP:HB2	1.59	0.67
1:G:94:ASN:HD22	1:G:97:LYS:H	1.44	0.66
4:H:37:VAL:HG12	4:H:47:TRP:HA	1.78	0.66
1:G:327:ARG:NH2	4:H:100(G):ASP:HB2	2.10	0.66
1:G:300:ASN:HB3	1:G:442:GLN:CB	2.26	0.65
3:L:80:PRO:HA	3:L:106:ILE:HD13	1.77	0.65
3:L:135:LEU:HD23	3:L:136:LEU:N	2.11	0.65
1:G:279:ASN:HD22	1:G:282:LYS:HG2	1.61	0.64
2:C:51:LEU:HD23	2:C:71:ILE:HD12	1.79	0.64
1:G:120:VAL:HB	1:G:434:MET:HB3	1.81	0.63
3:L:108:ARG:HG2	3:L:109:THR:H	1.64	0.63
1:G:225:ILE:CD1	1:G:245:VAL:HG23	2.29	0.63
2:C:76:ILE:H	2:C:76:ILE:CD1	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:198:HIS:HB3	3:L:201:LEU:CB	2.28	0.62
1:G:300:ASN:HB3	1:G:442:GLN:HB2	1.81	0.61
2:C:83:ILE:HG22	2:C:92:GLU:HG2	1.83	0.60
2:C:76:ILE:N	2:C:76:ILE:HD12	2.12	0.60
1:G:371:ILE:HD13	2:C:45:THR:CG2	2.28	0.59
4:H:195:ILE:N	4:H:195:ILE:HD12	2.18	0.59
1:G:359:ILE:N	1:G:359:ILE:HD12	2.18	0.59
1:G:225:ILE:HD11	1:G:245:VAL:HG23	1.85	0.58
1:G:108:ILE:HD13	1:G:479:TRP:CE2	2.39	0.58
1:G:389:GLN:HE21	1:G:416:LEU:HD13	1.68	0.57
1:G:389:GLN:NE2	1:G:414:ILE:HG13	2.19	0.57
3:L:83:LEU:HD12	3:L:105:GLU:HA	1.89	0.55
1:G:94:ASN:ND2	1:G:97:LYS:H	2.04	0.55
2:C:74:LEU:HD13	2:C:75:LYS:N	2.22	0.55
1:G:334:SER:HB2	1:G:337:LYS:HB2	1.87	0.54
3:L:140:TYR:HB3	3:L:141:PRO:HD3	1.88	0.54
1:G:424:ILE:HD12	1:G:435:TYR:CD1	2.41	0.54
1:G:442:GLN:NE2	1:G:444:ARG:HH11	2.05	0.54
2:C:23:SER:HB3	2:C:63:ASP:HA	1.88	0.54
1:G:326:ILE:H	1:G:326:ILE:CD1	2.14	0.54
4:H:37:VAL:HG23	4:H:37:VAL:O	2.08	0.53
2:C:14:LEU:HB2	2:C:69:LEU:HB3	1.90	0.53
3:L:114:SER:OG	3:L:137:ASN:HB3	2.08	0.53
3:L:11:LEU:HG	3:L:13:LEU:HD13	1.91	0.53
3:L:134:CYS:HB2	3:L:148:TRP:CZ2	2.44	0.52
3:L:190:LYS:HA	3:L:211:ARG:HG2	1.91	0.52
2:C:30:ASN:HD21	2:C:34:ILE:HB	1.75	0.52
1:G:200:VAL:C	1:G:201:ILE:HD12	2.30	0.52
3:L:151:ASP:HA	3:L:191:VAL:HB	1.92	0.52
2:C:8:LYS:HA	2:C:74:LEU:HD12	1.92	0.52
1:G:234:ASN:HD22	1:G:234:ASN:H	1.59	0.51
2:C:70:ILE:O	2:C:71:ILE:HD13	2.10	0.51
3:L:161:GLU:HB2	3:L:175:LEU:HD11	1.93	0.51
2:C:14:LEU:HD12	2:C:69:LEU:HD12	1.93	0.51
1:G:442:GLN:HE22	1:G:444:ARG:HH11	1.59	0.50
1:G:126:CYS:HA	1:G:196:CYS:HB3	1.93	0.50
3:L:19:ALA:HB3	3:L:75:ILE:HB	1.93	0.50
2:C:157:TRP:HB2	2:C:172:ILE:HG13	1.93	0.50
3:L:38:GLN:HB3	3:L:85:VAL:HG23	1.93	0.50
1:G:390:LEU:HG	1:G:416:LEU:HD11	1.93	0.50
1:G:410:GLY:O	1:G:412:ASN:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:VAL:HG22	1:G:86:LEU:N	2.27	0.49
4:H:47:TRP:CZ2	4:H:49:GLY:HA2	2.47	0.49
1:G:405:SER:O	1:G:406:ASN:HB2	2.11	0.49
1:G:89:VAL:HG22	1:G:90:THR:N	2.27	0.49
1:G:365:SER:HB3	2:C:48:PRO:HG3	1.93	0.49
4:H:87:THR:HG23	4:H:110:THR:HA	1.95	0.49
1:G:420:ILE:HD12	1:G:420:ILE:N	2.28	0.49
1:G:385:CYS:N	1:G:418:CYS:SG	2.85	0.48
3:L:32:SER:HB2	3:L:91:TYR:CE2	2.49	0.48
1:G:412:ASN:OD1	1:G:413:THR:HG23	2.13	0.48
3:L:145:LYS:HB2	3:L:197:THR:HB	1.95	0.48
2:C:157:TRP:CE2	2:C:174:ILE:HD12	2.49	0.47
1:G:317:PHE:HB3	1:G:318:TYR:CD1	2.49	0.47
1:G:322(A):ILE:HG13	1:G:322(A):ILE:O	2.14	0.47
1:G:442:GLN:HE22	1:G:444:ARG:NH1	2.11	0.47
1:G:319:THR:HG22	1:G:319:THR:O	2.14	0.47
2:C:114:LEU:HB2	2:C:149:LEU:HD11	1.96	0.47
1:G:201:ILE:N	1:G:201:ILE:HD12	2.29	0.47
1:G:219:ALA:HA	1:G:220:PRO:HD3	1.82	0.47
1:G:331:CYS:SG	1:G:385:CYS:SG	3.12	0.47
2:C:83:ILE:HD12	2:C:83:ILE:C	2.35	0.47
3:L:91:TYR:HB2	4:H:100(L):GLY:HA3	1.97	0.46
4:H:36:TRP:CE2	4:H:80:MET:HB2	2.50	0.46
3:L:135:LEU:C	3:L:136:LEU:HD12	2.36	0.46
1:G:108:ILE:HD13	1:G:479:TRP:CZ2	2.50	0.46
3:L:136:LEU:HD22	3:L:175:LEU:HD23	1.97	0.46
3:L:190:LYS:HG2	3:L:211:ARG:HE	1.80	0.46
3:L:190:LYS:HE2	3:L:211:ARG:HH21	1.81	0.46
1:G:307:ILE:HG22	1:G:308:HIS:N	2.30	0.46
3:L:33:LEU:HD13	3:L:34:ALA:N	2.32	0.45
1:G:86:LEU:N	1:G:86:LEU:HD12	2.32	0.45
3:L:21:LEU:HD12	3:L:73:LEU:HD23	1.99	0.45
4:H:155:ASN:HD22	4:H:159:LEU:HB2	1.82	0.45
4:H:201:LYS:N	4:H:202:PRO:CD	2.80	0.45
1:G:128:GLY:O	1:G:129:ALA:C	2.55	0.44
1:G:292:VAL:HB	1:G:449:ILE:HB	1.98	0.44
3:L:112:ALA:HA	3:L:113:PRO:HD3	1.81	0.44
1:G:101:VAL:HG11	1:G:480:ARG:HG3	1.99	0.44
4:H:199:ASN:HD22	4:H:200:HIS:N	2.14	0.44
2:C:134:ARG:HG2	2:C:134:ARG:H	1.72	0.44
1:G:285:ILE:N	1:G:285:ILE:HD12	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:200:HIS:CE1	4:H:202:PRO:HB2	2.52	0.44
1:G:322(A):ILE:O	1:G:324:GLY:N	2.51	0.44
4:H:52:ILE:HD11	4:H:100(J):GLY:N	2.33	0.43
1:G:307:ILE:HG23	1:G:317:PHE:O	2.17	0.43
3:L:8:PRO:HG3	3:L:11:LEU:HD13	2.00	0.43
3:L:133:VAL:HG22	3:L:178:THR:HG22	2.01	0.43
3:L:117:ILE:HD13	3:L:209:PHE:HD2	1.84	0.43
4:H:194:TYR:C	4:H:195:ILE:HD12	2.38	0.43
1:G:272:ILE:HG22	1:G:286:VAL:HG22	2.00	0.43
3:L:113:PRO:HB3	3:L:139:PHE:CD1	2.54	0.43
1:G:338:TRP:O	1:G:342:LEU:HB2	2.19	0.43
1:G:90:THR:HG23	1:G:90:THR:O	2.18	0.43
3:L:32:SER:HB2	3:L:91:TYR:CZ	2.53	0.43
1:G:225:ILE:O	1:G:225:ILE:HD12	2.18	0.43
1:G:421:LYS:HD3	4:H:100(D):ASP:CG	2.39	0.43
1:G:130:GLY:O	1:G:195:SER:C	2.57	0.43
1:G:362:ASN:OD1	1:G:363:HIS:N	2.51	0.43
3:L:203:SER:HA	3:L:204:PRO:HD3	1.92	0.43
1:G:128:GLY:O	1:G:130:GLY:N	2.52	0.42
1:G:129:ALA:O	1:G:130:GLY:C	2.58	0.42
4:H:122:PHE:HA	4:H:123:PRO:HD3	1.80	0.42
2:C:93:VAL:O	2:C:93:VAL:HG13	2.20	0.42
1:G:296:CYS:HA	1:G:331:CYS:HA	2.01	0.42
3:L:124:GLN:HB3	3:L:124:GLN:HE21	1.67	0.42
1:G:326:ILE:N	1:G:326:ILE:HD13	2.17	0.41
2:C:11:THR:HG22	2:C:72:LYS:HA	2.02	0.41
2:C:12:VAL:HG22	2:C:13:GLU:N	2.35	0.41
1:G:477:ASP:HA	1:G:480:ARG:HB2	2.01	0.41
4:H:100(M):PHE:CD2	4:H:100(M):PHE:N	2.88	0.41
1:G:92:HIS:O	1:G:93:PHE:HD1	2.03	0.41
3:L:50:GLY:O	3:L:51:ALA:HB3	2.19	0.41
2:C:157:TRP:CD1	2:C:174:ILE:HD12	2.55	0.41
4:H:101:ASP:N	4:H:101:ASP:OD2	2.49	0.41
1:G:358:THR:HB	1:G:465:THR:HG22	2.02	0.41
1:G:386:ASN:O	1:G:416:LEU:HD12	2.20	0.41
3:L:210:ASN:HB2	3:L:213:GLU:HG3	2.03	0.41
1:G:251:ILE:CD1	1:G:482:GLU:HB3	2.45	0.41
4:H:146:PHE:HA	4:H:147:PRO:HA	1.74	0.41
1:G:437:PRO:HA	1:G:438:PRO:HD3	1.96	0.41
3:L:43:ALA:HA	3:L:44:PRO:HD3	1.97	0.41
2:C:13:GLU:HG3	2:C:70:ILE:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:18:VAL:O	4:H:81:GLU:HA	2.21	0.40
1:G:298:ARG:HA	1:G:299:PRO:HD3	1.97	0.40
1:G:220:PRO:HD2	1:G:223:PHE:HB2	2.03	0.40
1:G:280:ASN:HD22	2:C:35:LYS:HE2	1.87	0.40
3:L:108:ARG:HG2	3:L:109:THR:N	2.32	0.40
1:G:333:ILE:HD11	1:G:390:LEU:HD21	2.03	0.40

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	341/344 (99%)	290 (85%)	40 (12%)	11 (3%)	4	22
2	C	173/181 (96%)	158 (91%)	15 (9%)	0	100	100
3	L	213/215 (99%)	194 (91%)	14 (7%)	5 (2%)	6	29
4	H	231/235 (98%)	208 (90%)	21 (9%)	2 (1%)	17	48
All	All	958/975 (98%)	850 (89%)	90 (9%)	18 (2%)	8	34

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	129	ALA
1	G	299	PRO
1	G	323	ILE
1	G	412	ASN
3	L	202	SER
1	G	195	SER
1	G	322(A)	ILE
1	G	491	ILE
3	L	138	ASN

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Mol	Chain	Res	Type
1	G	406	ASN
3	L	204	PRO
4	H	26	GLY
1	G	397	ASN
3	L	68	GLY
4	H	144	ASP
3	L	128	GLY
1	G	313[A]	PRO
1	G	313[B]	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	302/303 (100%)	275 (91%)	27 (9%)	9	32
2	C	159/164 (97%)	154 (97%)	5 (3%)	40	67
3	L	182/182 (100%)	173 (95%)	9 (5%)	25	56
4	H	192/194 (99%)	182 (95%)	10 (5%)	23	54
All	All	835/843 (99%)	784 (94%)	51 (6%)	18	48

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	93	PHE
1	G	97	LYS
1	G	105	GLN
1	G	112	TRP
1	G	119	CYS
1	G	196	CYS
1	G	230	ASP
1	G	234	ASN
1	G	255	VAL
1	G	267	GLU
1	G	273	ARG
1	G	287	GLN

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Mol	Chain	Res	Type
1	G	289	LYS
1	G	326	ILE
1	G	340	ASP
1	G	342	LEU
1	G	352	GLN
1	G	386	ASN
1	G	397	ASN
1	G	418	CYS
1	G	434	MET
1	G	440	ARG
1	G	442	GLN
1	G	444	ARG
1	G	452	LEU
1	G	460	ILE
1	G	489	VAL
2	C	63	ASP
2	C	119	GLU
2	C	134	ARG
2	C	152	GLN
2	C	162	LEU
3	L	24	ARG
3	L	81	GLU
3	L	83	LEU
3	L	85	VAL
3	L	100	GLN
3	L	122	ASP
3	L	129	THR
3	L	151	ASP
3	L	181	LEU
4	H	3	LEU
4	H	31	MET
4	H	100(B)	ASP
4	H	100(K)	ARG
4	H	100(N)	PHE
4	H	116	THR
4	H	138	LEU
4	H	147	PRO
4	H	199	ASN
4	H	209	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	94	ASN
1	G	105	GLN
1	G	234	ASN
1	G	241	ASN
1	G	279	ASN
1	G	302	ASN
1	G	328	GLN
1	G	352	GLN
1	G	386	ASN
1	G	389	GLN
1	G	392	ASN
1	G	397	ASN
1	G	442	GLN
2	C	103	ASN
2	C	112	GLN
3	L	27	GLN
3	L	37	GLN
3	L	90	GLN
3	L	124	GLN
4	H	171	GLN
4	H	199	ASN

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 ⓘ

2 monosaccharides 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	1	1,5	14,14,15	0.74	0	17,19,21	0.62	0
5	FUC	A	2	5	10,10,11	0.70	0	14,14,16	0.70	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	1	1,5	1/1/5/7	4/6/23/26	0/1/1/1
5	FUC	A	2	5	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1	NAG	C3-C2-N2-C7
5	A	1	NAG	C8-C7-N2-C2
5	A	1	NAG	O7-C7-N2-C2
5	A	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry ⓘ

11 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	$\# Z > 2$
6	NAG	G	832	1	14,14,15	0.57	0	17,19,21	0.76	1 (5%)
7	SO4	H	221	-	4,4,4	0.29	0	6,6,6	0.04	0
8	XYL	H	217	-	9,9,9	1.26	1 (11%)	11,11,11	0.85	0
6	NAG	G	762	1	14,14,15	0.57	0	17,19,21	0.66	0
7	SO4	H	222	-	4,4,4	0.14	0	6,6,6	0.05	0
6	NAG	G	862	1	14,14,15	0.59	0	17,19,21	0.67	0
7	SO4	L	215	-	4,4,4	0.29	0	6,6,6	0.05	0
8	XYL	H	218	-	9,9,9	1.26	1 (11%)	11,11,11	0.83	0
7	SO4	G	5	-	4,4,4	0.14	0	6,6,6	0.04	0
7	SO4	H	220	-	4,4,4	0.29	0	6,6,6	0.04	0
8	XYL	H	219	-	9,9,9	1.27	1 (11%)	11,11,11	0.86	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
8	XYL	H	217	-	-	0/12/12/12	-
6	NAG	G	762	1	-	3/6/23/26	0/1/1/1
6	NAG	G	862	1	-	4/6/23/26	0/1/1/1
6	NAG	G	832	1	1/1/5/7	4/6/23/26	0/1/1/1
8	XYL	H	218	-	-	0/12/12/12	-
8	XYL	H	219	-	-	0/12/12/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	218	XYL	C4-C3	2.20	1.57	1.53
8	H	217	XYL	C4-C3	2.15	1.57	1.53
8	H	219	XYL	C4-C3	2.09	1.57	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	832	NAG	C2-N2-C7	-2.27	119.67	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	G	832	NAG	C1

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	832	NAG	C8-C7-N2-C2
6	G	832	NAG	O7-C7-N2-C2
6	G	762	NAG	C8-C7-N2-C2
6	G	762	NAG	O7-C7-N2-C2
6	G	862	NAG	C8-C7-N2-C2
6	G	862	NAG	O7-C7-N2-C2
6	G	832	NAG	O5-C5-C6-O6
6	G	832	NAG	C4-C5-C6-O6
6	G	862	NAG	O5-C5-C6-O6
6	G	862	NAG	C4-C5-C6-O6
6	G	762	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	87:GLU	C	88:ASN	N	1.17

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	339/344 (98%)	0.61	50 (14%) 2 2	58, 122, 148, 160	0
2	C	175/181 (96%)	0.68	25 (14%) 2 2	100, 139, 161, 166	0
3	L	215/215 (100%)	0.55	21 (9%) 7 7	65, 111, 141, 154	0
4	H	233/235 (99%)	0.28	13 (5%) 24 23	48, 83, 121, 150	0
All	All	962/975 (98%)	0.53	109 (11%) 5 5	48, 116, 154, 166	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	404	GLY	7.8
1	G	460	ILE	6.8
1	G	406	ASN	5.9
1	G	127	VAL	5.8
2	C	122	PRO	4.8
1	G	267	GLU	4.8
3	L	154	LEU	4.8
1	G	315[A]	ARG	4.8
1	G	355	ASN	4.7
1	G	321	GLY	4.6
1	G	403	GLU	4.6
1	G	405	SER	4.3
3	L	110	VAL	4.3
1	G	325	ASP	4.2
2	C	110	GLN	4.2
2	C	134	ARG	4.1
1	G	316	ALA	4.1
1	G	320	THR	4.1
1	G	408	THR	3.9
4	H	129	LYS	3.9
1	G	268	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
3	L	109	THR	3.8
1	G	324	GLY	3.7
3	L	169	ARG	3.7
1	G	462	GLU	3.6
1	G	302	ASN	3.6
1	G	407	ASN	3.6
4	H	216	CYS	3.6
2	C	109	LEU	3.5
1	G	461	ASN	3.4
1	G	322(A)	ILE	3.4
2	C	171	LYS	3.3
2	C	124	SER	3.3
1	G	319	THR	3.2
2	C	148	GLN	3.2
2	C	25	GLN	3.1
1	G	317	PHE	3.1
1	G	265	LEU	3.1
1	G	221	ALA	3.1
4	H	100(K)	ARG	3.1
1	G	322	GLU	3.0
1	G	459	GLY	3.0
3	L	3	VAL	3.0
4	H	215	SER	3.0
1	G	354	GLU	3.0
3	L	100	GLN	2.9
1	G	97	LYS	2.9
1	G	246	GLN	2.9
4	H	14	PRO	2.9
3	L	156	SER	2.9
1	G	236	LYS	2.8
3	L	212	GLY	2.8
4	H	191	THR	2.8
2	C	131	ARG	2.8
3	L	67	SER	2.8
1	G	446	SER	2.7
3	L	134	CYS	2.7
1	G	318	TYR	2.7
2	C	142	LYS	2.7
1	G	305	LYS	2.7
4	H	2	GLN	2.7
2	C	139	GLN	2.7
2	C	107	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
3	L	88	CYS	2.7
3	L	158	ASN	2.7
2	C	147	SER	2.6
1	G	396	ASN	2.6
3	L	211	ARG	2.6
3	L	161	GLU	2.6
1	G	412	ASN	2.6
4	H	36	TRP	2.5
1	G	413	THR	2.5
2	C	21	LYS	2.5
2	C	19	SER	2.5
2	C	135	GLY	2.4
2	C	73	ASN	2.4
2	C	141	GLY	2.4
1	G	409	GLU	2.4
3	L	199	GLN	2.4
2	C	22	LYS	2.3
3	L	34	ALA	2.3
1	G	401	ASN	2.3
1	G	323	ILE	2.3
2	C	72	LYS	2.3
1	G	306	SER	2.3
2	C	125	SER	2.2
3	L	170	ASP	2.2
1	G	297	THR	2.2
1	G	402	THR	2.2
2	C	137	ASN	2.2
1	G	308	HIS	2.2
3	L	193	ALA	2.2
4	H	133	GLY	2.2
4	H	59	TYR	2.2
2	C	28	TRP	2.2
2	C	13	GLU	2.2
4	H	120	SER	2.2
1	G	240	LYS	2.1
3	L	153	ALA	2.1
4	H	93	ALA	2.1
1	G	389	GLN	2.1
3	L	195	GLU	2.1
1	G	247	CYS	2.1
3	L	89	GLN	2.1
1	G	397	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	97	VAL	2.0
1	G	328	GLN	2.0
1	G	303	THR	2.0
4	H	100(B)	ASP	2.0

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](#)

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
5	NAG	A	1	14/15	0.72	0.41	138,139,140,141	0
5	FUC	A	2	10/11	0.80	0.35	141,142,143,143	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	XYL	H	217	10/10	0.53	0.31	145,150,150,150	0
8	XYL	H	219	10/10	0.63	0.28	153,155,156,157	0
7	SO4	H	220	5/5	0.70	0.18	161,161,161,161	0
7	SO4	H	221	5/5	0.71	0.24	189,189,190,190	0
6	NAG	G	862	14/15	0.77	0.35	135,138,140,140	0
8	XYL	H	218	10/10	0.77	0.20	134,136,137,137	0
6	NAG	G	832	14/15	0.82	0.28	141,144,147,147	0
7	SO4	L	215	5/5	0.83	0.14	186,187,187,187	0
6	NAG	G	762	14/15	0.91	0.37	105,108,110,110	0
7	SO4	G	5	5/5	0.92	0.15	163,163,164,164	5
7	SO4	H	222	5/5	0.96	0.15	143,143,143,143	5

6.5 Other polymers

There are no such residues in this entry.