



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 06:46 AM BST

PDB ID : 6MG7  
Title : Crystal structure of the RV144 C1-C2 specific antibody CH54 Fab in complex with HIV-1 CLADE A/E GP120 and M48U1  
Authors : Van, V.; Tolbert, W.D.; Pazgier, M.  
Deposited on : 2018-09-13  
Resolution : 2.91 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](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.

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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 : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

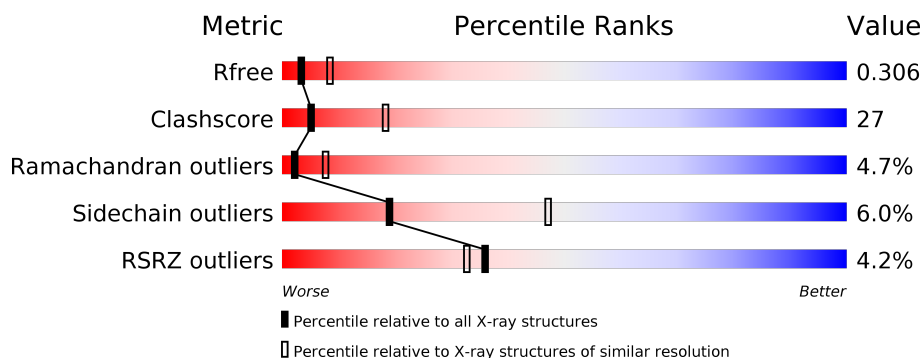
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	385	
2	N	28	
3	H	220	
4	L	210	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	G	606	-	-	X	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6167 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 clade A/E 93TH057 HIV-1 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	330	Total	C	N	O	S	0	0	0
			2591	1631	446	492	22			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	31	SER	-	expression tag	UNP A0A0M3KKW9
G	32	ASP	-	expression tag	UNP A0A0M3KKW9
G	33	ASN	-	expression tag	UNP A0A0M3KKW9
G	34	LEU	-	expression tag	UNP A0A0M3KKW9
G	35	TRP	-	expression tag	UNP A0A0M3KKW9
G	36	VAL	-	expression tag	UNP A0A0M3KKW9
G	37	THR	-	expression tag	UNP A0A0M3KKW9
G	38	VAL	-	expression tag	UNP A0A0M3KKW9
G	39	TYR	-	expression tag	UNP A0A0M3KKW9
G	40	TYR	-	expression tag	UNP A0A0M3KKW9
G	41	GLY	-	expression tag	UNP A0A0M3KKW9
G	42	VAL	-	expression tag	UNP A0A0M3KKW9
G	43	PRO	-	expression tag	UNP A0A0M3KKW9
G	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9
G	493	PRO	-	expression tag	UNP A0A0M3KKW9
G	494	LEU	-	expression tag	UNP A0A0M3KKW9
G	495	GLY	-	expression tag	UNP A0A0M3KKW9
G	496	ILE	-	expression tag	UNP A0A0M3KKW9
G	497	ALA	-	expression tag	UNP A0A0M3KKW9
G	498	PRO	-	expression tag	UNP A0A0M3KKW9
G	499	THR	-	expression tag	UNP A0A0M3KKW9
G	500	LYS	-	expression tag	UNP A0A0M3KKW9
G	501	ALA	-	expression tag	UNP A0A0M3KKW9
G	502	LYS	-	expression tag	UNP A0A0M3KKW9
G	503	ARG	-	expression tag	UNP A0A0M3KKW9
G	504	ARG	-	expression tag	UNP A0A0M3KKW9
G	505	VAL	-	expression tag	UNP A0A0M3KKW9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	506	VAL	-	expression tag	UNP A0A0M3KKW9
G	507	GLN	-	expression tag	UNP A0A0M3KKW9
G	508	ARG	-	expression tag	UNP A0A0M3KKW9
G	509	GLU	-	expression tag	UNP A0A0M3KKW9
G	510	LYS	-	expression tag	UNP A0A0M3KKW9
G	511	ARG	-	expression tag	UNP A0A0M3KKW9

- Molecule 2 is a protein called M48U1 CD4 mimetic peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			

- Molecule 3 is a protein called CH54 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	218	Total	C	N	O	S	0	0	0
			1635	1025	279	323	8			

- Molecule 4 is a protein called CH54 Fab light chain.

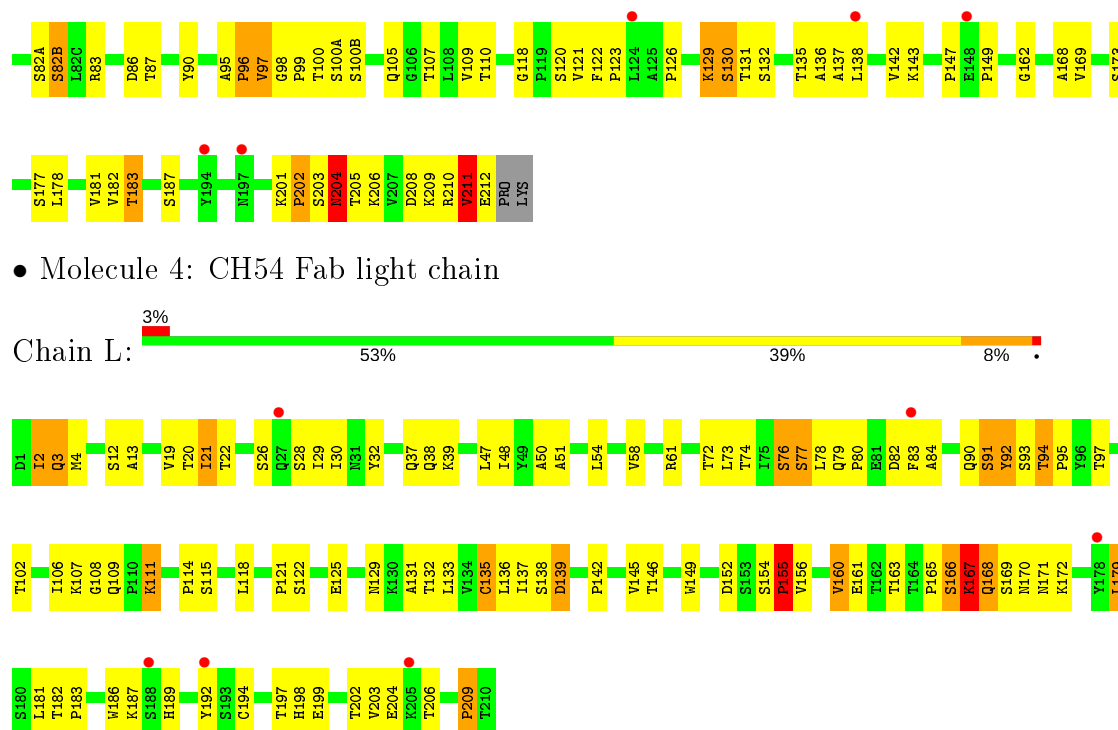
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	210	Total	C	N	O	S	0	0	0
			1592	1002	263	322	5			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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





• Molecule 4: CH54 Fab light chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.83Å 42.23Å 119.75Å 90.00° 115.24° 90.00°	Depositor
Resolution (Å)	39.68 – 2.91 39.65 – 2.91	Depositor EDS
% Data completeness (in resolution range)	94.5 (39.68-2.91) 94.6 (39.65-2.91)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, $R_{free}$	0.250 , 0.307 0.250 , 0.306	Depositor DCC
$R_{free}$ test set	807 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.4	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 52.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6167	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: MPT, NH2, U2X, DPR, 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	0.62	0/2645	0.75	1/3589 (0.0%)
2	N	0.61	0/176	0.69	0/231
3	H	0.65	0/1672	0.72	0/2278
4	L	0.65	0/1631	0.79	1/2225 (0.0%)
All	All	0.63	0/6124	0.75	2/8323 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	418	CYS	CA-CB-SG	-7.12	101.19	114.00
4	L	155	PRO	N-CA-CB	-5.08	97.01	102.60

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	2591	0	2529	156	1
2	N	209	0	212	6	0
3	H	1635	0	1616	83	0
4	L	1592	0	1558	111	0
5	G	140	0	130	16	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6167	0	6045	329	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 27.

All (329) 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)
4:L:94:THR:OG1	4:L:95:PRO:HD2	1.19	1.32
4:L:94:THR:OG1	4:L:95:PRO:CD	1.87	1.20
1:G:293:GLU:OE1	5:G:606:NAG:H83	1.48	1.11
1:G:293:GLU:CD	5:G:606:NAG:C8	2.22	1.08
1:G:59:LYS:HB2	1:G:62:GLU:HG3	1.36	1.04
1:G:360:ILE:HD11	1:G:465:ASN:HD22	1.20	1.02
1:G:492:GLU:HG2	1:G:494:LEU:CD1	1.90	1.02
3:H:97:VAL:HG23	3:H:98:GLY:H	1.25	1.00
4:L:79:GLN:HG3	4:L:80:PRO:HD2	1.42	0.99
1:G:293:GLU:CD	5:G:606:NAG:H83	1.83	0.98
4:L:94:THR:CB	4:L:95:PRO:CD	2.41	0.97
4:L:90:GLN:NE2	4:L:91:SER:O	1.97	0.96
1:G:117:GLN:NE2	1:G:206:PRO:HD2	1.81	0.95
1:G:116:LEU:H	1:G:208:ILE:HD11	1.32	0.95
1:G:92:ASN:ND2	1:G:238:PRO:HA	1.82	0.94
1:G:116:LEU:HD12	1:G:435:TYR:CE2	2.06	0.90
4:L:94:THR:CB	4:L:95:PRO:HD3	2.02	0.90
3:H:70:THR:HG23	3:H:79:TYR:HB2	1.53	0.88
1:G:96:TRP:HH2	1:G:285:ILE:HD12	1.37	0.88
1:G:293:GLU:OE1	5:G:606:NAG:C8	2.18	0.88
1:G:493:PRO:O	1:G:494:LEU:HD12	1.74	0.86
4:L:94:THR:HB	4:L:95:PRO:HD3	1.56	0.85
1:G:45:TRP:HA	1:G:490:GLN:O	1.78	0.84
1:G:116:LEU:HD12	1:G:435:TYR:HE2	1.40	0.84
1:G:492:GLU:HG2	1:G:494:LEU:HD11	1.59	0.84
1:G:360:ILE:HD11	1:G:465:ASN:ND2	1.93	0.83
3:H:87:THR:HG23	3:H:110:THR:HA	1.61	0.82
1:G:360:ILE:CD1	1:G:465:ASN:HB3	2.10	0.82
4:L:2:ILE:HG21	4:L:90:GLN:OE1	1.79	0.82
3:H:97:VAL:HG23	3:H:98:GLY:N	1.94	0.80
3:H:122:PHE:CG	4:L:125:GLU:HB2	2.16	0.80
3:H:39:GLN:HE22	4:L:38:GLN:HE22	1.30	0.80
3:H:181:VAL:HG21	4:L:136:LEU:HD11	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:ASN:HA	1:G:102:GLU:HG2	1.62	0.79
1:G:212:PRO:HG2	1:G:254:VAL:HG12	1.64	0.78
1:G:493:PRO:C	1:G:494:LEU:HD12	2.04	0.78
1:G:65:VAL:HG21	1:G:208:ILE:HD12	1.67	0.77
1:G:295:ASN:OD1	5:G:606:NAG:C7	2.33	0.76
3:H:131:THR:HG23	3:H:132:SER:H	1.50	0.76
3:H:122:PHE:CD2	4:L:125:GLU:HG3	2.21	0.76
1:G:293:GLU:CG	5:G:606:NAG:C8	2.64	0.75
4:L:166:SER:HB3	4:L:167:LYS:HD2	1.69	0.74
4:L:114:PRO:HB2	4:L:137:ILE:HG22	1.70	0.74
1:G:492:GLU:HG2	1:G:494:LEU:HD13	1.70	0.73
4:L:203:VAL:HG12	4:L:204:GLU:CG	2.18	0.73
3:H:82(B):SER:HB2	3:H:83:ARG:HH11	1.53	0.73
1:G:92:ASN:ND2	1:G:238:PRO:CA	2.52	0.72
4:L:139:ASP:C	4:L:172:LYS:HE2	2.09	0.72
1:G:84:ILE:HD11	3:H:52:VAL:HG21	1.71	0.71
3:H:4:LEU:HD23	3:H:24:ALA:HA	1.70	0.71
1:G:85:HIS:O	3:H:54:SER:OG	2.08	0.70
4:L:118:LEU:HD23	4:L:209:PRO:HD3	1.72	0.70
3:H:201:LYS:HB3	3:H:202:PRO:HD3	1.72	0.70
1:G:96:TRP:HH2	1:G:285:ILE:CD1	2.06	0.69
1:G:117:GLN:HE22	1:G:206:PRO:HD2	1.54	0.69
1:G:92:ASN:HD21	1:G:238:PRO:HB3	1.57	0.68
4:L:145:VAL:HG12	4:L:198:HIS:CD2	2.28	0.68
4:L:21:ILE:HG22	4:L:73:LEU:O	1.93	0.67
4:L:203:VAL:HG12	4:L:204:GLU:HG2	1.75	0.67
4:L:136:LEU:HD21	4:L:138:SER:HB2	1.75	0.67
4:L:167:LYS:CB	4:L:171:ASN:HA	2.24	0.67
1:G:229:ASN:HB2	1:G:241:ASN:O	1.94	0.67
4:L:32:TYR:HB3	4:L:91:SER:HB2	1.75	0.67
3:H:169:VAL:HG21	4:L:160:VAL:HG11	1.77	0.67
4:L:121:PRO:HD3	4:L:133:LEU:HG	1.77	0.67
4:L:121:PRO:HD2	4:L:186:TRP:CH2	2.29	0.67
4:L:167:LYS:O	4:L:169:SER:N	2.25	0.66
4:L:29:ILE:HG21	4:L:90:GLN:HG3	1.78	0.66
1:G:96:TRP:CH2	1:G:285:ILE:HD12	2.26	0.66
1:G:59:LYS:HB2	1:G:62:GLU:CG	2.20	0.66
4:L:22:THR:HG22	4:L:72:THR:HG22	1.79	0.65
1:G:95:MET:HE1	1:G:273:ARG:HD3	1.78	0.65
3:H:95:ALA:O	3:H:96:PRO:O	2.15	0.65
1:G:116:LEU:CD1	1:G:435:TYR:CE2	2.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:82(B):SER:HB2	3:H:83:ARG:NH1	2.12	0.64
2:N:5:PHE:CE2	2:N:9:ARG:HD2	2.32	0.64
1:G:293:GLU:CD	5:G:606:NAG:H82	2.17	0.64
4:L:2:ILE:C	4:L:3:GLN:HG2	2.18	0.64
1:G:295:ASN:OD1	5:G:606:NAG:N2	2.31	0.64
1:G:295:ASN:O	1:G:331:CYS:HA	1.98	0.63
1:G:339:ASN:O	1:G:343:LYS:HG3	1.98	0.63
4:L:167:LYS:HB2	4:L:171:ASN:HA	1.81	0.63
3:H:205:THR:HG23	3:H:205:THR:O	1.97	0.63
1:G:273:ARG:HH11	1:G:273:ARG:HG2	1.63	0.63
3:H:208:ASP:OD2	3:H:210:ARG:NH2	2.32	0.63
1:G:59:LYS:CB	1:G:62:GLU:HG3	2.22	0.63
3:H:122:PHE:CD1	4:L:125:GLU:HB2	2.34	0.63
1:G:293:GLU:HG2	5:G:606:NAG:C8	2.27	0.62
3:H:181:VAL:HG21	4:L:136:LEU:CD1	2.30	0.62
3:H:56:ASN:HD22	3:H:57:THR:N	1.97	0.62
1:G:116:LEU:O	1:G:116:LEU:HD12	1.99	0.62
1:G:117:GLN:HE21	1:G:205:CYS:HA	1.65	0.62
4:L:121:PRO:HD2	4:L:186:TRP:CZ2	2.34	0.61
1:G:293:GLU:CG	5:G:606:NAG:H81	2.30	0.61
4:L:203:VAL:HG12	4:L:204:GLU:HG3	1.83	0.60
1:G:210:PHE:O	1:G:379:ARG:HA	2.01	0.60
1:G:379:ARG:NH1	1:G:444:ASN:H	2.00	0.60
1:G:91:GLU:OE1	1:G:226:LEU:HD13	2.00	0.60
4:L:131:ALA:HB3	4:L:181:LEU:O	2.02	0.60
1:G:342:LEU:O	1:G:345:VAL:HG22	2.02	0.60
3:H:18:MET:HE1	3:H:20:ILE:HD12	1.84	0.59
4:L:139:ASP:HB3	4:L:172:LYS:HE2	1.85	0.59
1:G:492:GLU:CG	1:G:494:LEU:HD11	2.31	0.59
3:H:44:ARG:NH2	4:L:4:MET:O	2.36	0.59
3:H:126:PRO:HD2	3:H:211:VAL:O	2.03	0.59
1:G:201:ILE:O	1:G:201:ILE:HG23	2.03	0.58
1:G:67:ASN:O	1:G:71:THR:HB	2.03	0.58
4:L:20:THR:O	4:L:21:ILE:HG22	2.03	0.58
3:H:99:PRO:O	3:H:100:THR:HG22	2.04	0.58
4:L:114:PRO:CB	4:L:137:ILE:HG22	2.34	0.58
1:G:361:PHE:O	1:G:393:ASN:ND2	2.32	0.58
1:G:64:GLU:O	1:G:67:ASN:HB2	2.04	0.58
3:H:15:GLY:HA2	3:H:83:ARG:NH1	2.18	0.58
4:L:118:LEU:CD2	4:L:209:PRO:HD3	2.33	0.58
1:G:75:VAL:HG11	4:L:30:ILE:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:97:VAL:CG2	3:H:98:GLY:H	2.02	0.57
1:G:430:THR:HA	2:N:22:THR:CG2	2.34	0.57
1:G:341:VAL:O	1:G:344:GLN:HB2	2.04	0.57
4:L:21:ILE:HD11	4:L:102:THR:HB	1.85	0.57
1:G:224:VAL:HG23	1:G:491:ILE:HD11	1.86	0.57
1:G:273:ARG:NH1	1:G:273:ARG:HG2	2.20	0.57
4:L:3:GLN:HG3	4:L:26:SER:HB3	1.87	0.57
1:G:96:TRP:CH2	1:G:285:ILE:CD1	2.86	0.57
4:L:202:THR:HG22	4:L:203:VAL:CG2	2.35	0.57
1:G:370:GLU:OE2	1:G:384:TYR:OH	2.17	0.56
1:G:90:THR:OG1	1:G:240:LYS:HG3	2.05	0.56
1:G:343:LYS:HA	1:G:346:THR:HG22	1.87	0.56
1:G:241:ASN:OD1	5:G:603:NAG:H2	2.06	0.56
1:G:410:CYS:HB2	5:G:609:NAG:H61	1.87	0.56
3:H:143:LYS:HG2	3:H:177:SER:HB3	1.87	0.56
3:H:208:ASP:HB3	3:H:210:ARG:NH2	2.21	0.56
1:G:293:GLU:HG2	5:G:606:NAG:H82	1.87	0.55
3:H:33:THR:HG23	3:H:97:VAL:HA	1.87	0.55
3:H:56:ASN:HD22	3:H:57:THR:H	1.53	0.55
1:G:231:LYS:HB3	1:G:268:GLU:HB2	1.88	0.55
4:L:192:TYR:O	4:L:209:PRO:HD2	2.06	0.55
3:H:28:THR:HB	3:H:30:THR:HG22	1.88	0.55
4:L:146:THR:HB	4:L:197:THR:HG22	1.89	0.55
3:H:130:SER:OG	3:H:130:SER:O	2.25	0.55
3:H:143:LYS:NZ	4:L:132:THR:HG21	2.22	0.55
3:H:51:ILE:HB	3:H:69:ILE:HG22	1.89	0.55
1:G:298:ARG:HH11	1:G:298:ARG:HG2	1.72	0.54
1:G:270:ILE:HG13	1:G:289:ASN:HB2	1.89	0.54
1:G:95:MET:CE	1:G:273:ARG:HD3	2.37	0.54
4:L:79:GLN:CG	4:L:80:PRO:HD2	2.27	0.54
3:H:46:GLU:OE2	3:H:62:LYS:HE2	2.08	0.54
1:G:268:GLU:HG2	1:G:269:GLU:OE2	2.07	0.54
4:L:111:LYS:H	4:L:111:LYS:CE	2.20	0.54
3:H:169:VAL:HG21	4:L:160:VAL:CG1	2.38	0.53
4:L:167:LYS:HB3	4:L:171:ASN:HA	1.88	0.53
3:H:131:THR:HG23	3:H:132:SER:N	2.21	0.53
1:G:46:LYS:NZ	1:G:492:GLU:HB2	2.23	0.53
1:G:258:GLN:HE21	1:G:470:PRO:HB2	1.74	0.53
1:G:294:ILE:HG12	1:G:331:CYS:SG	2.49	0.53
1:G:295:ASN:O	1:G:331:CYS:SG	2.67	0.53
1:G:45:TRP:CD1	1:G:489:VAL:HG21	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:33:THR:CG2	3:H:97:VAL:HA	2.38	0.53
4:L:182:THR:HB	4:L:183:PRO:HD2	1.90	0.53
4:L:202:THR:HG22	4:L:203:VAL:HG22	1.91	0.53
1:G:223:TYR:CD2	1:G:490:GLN:HB3	2.44	0.53
4:L:129:ASN:O	4:L:183:PRO:HD3	2.09	0.53
4:L:12:SER:C	4:L:107:LYS:HB2	2.30	0.52
1:G:333:ILE:HD13	1:G:390:LEU:HD21	1.91	0.52
1:G:258:GLN:HE21	1:G:470:PRO:CB	2.23	0.52
4:L:142:PRO:HD2	4:L:198:HIS:NE2	2.24	0.52
1:G:293:GLU:CG	5:G:606:NAG:H82	2.40	0.51
1:G:358:THR:OG1	1:G:465:ASN:HA	2.11	0.51
4:L:106:ILE:HG22	4:L:108:GLY:H	1.75	0.51
1:G:264:SER:O	1:G:287:HIS:NE2	2.43	0.51
1:G:265:LEU:HD23	1:G:290:LYS:HA	1.93	0.51
1:G:59:LYS:HG2	1:G:62:GLU:OE2	2.11	0.51
3:H:181:VAL:HG11	4:L:136:LEU:CD1	2.40	0.51
1:G:490:GLN:HG3	1:G:490:GLN:O	2.09	0.51
3:H:129:LYS:H	3:H:129:LYS:HD2	1.76	0.51
3:H:4:LEU:HD23	3:H:24:ALA:CA	2.38	0.51
3:H:168:ALA:HB2	3:H:178:LEU:HD23	1.93	0.51
4:L:145:VAL:HG12	4:L:198:HIS:HD2	1.76	0.50
1:G:361:PHE:HB3	1:G:391:PHE:HB3	1.94	0.50
1:G:92:ASN:HD21	1:G:238:PRO:CB	2.23	0.50
1:G:430:THR:HA	2:N:22:THR:HG22	1.93	0.50
1:G:360:ILE:HD13	1:G:465:ASN:HB3	1.90	0.50
3:H:168:ALA:HA	3:H:178:LEU:HB3	1.93	0.50
4:L:78:LEU:HD21	4:L:83:PHE:CE1	2.46	0.50
1:G:430:THR:N	2:N:22:THR:HG23	2.27	0.50
2:N:4:HIS:O	2:N:8:LEU:HG	2.11	0.50
1:G:120:VAL:HB	1:G:434:MET:HE2	1.93	0.50
3:H:123:PRO:HA	3:H:210:ARG:HD2	1.93	0.50
4:L:54:LEU:HD11	4:L:58:VAL:CG1	2.41	0.50
3:H:37:VAL:HG12	3:H:45:LEU:HD22	1.93	0.50
3:H:137:ALA:HA	3:H:182:VAL:O	2.12	0.49
3:H:76:SER:OG	3:H:76:SER:O	2.24	0.49
1:G:463:THR:HG22	1:G:464:SER:H	1.77	0.49
1:G:52:LEU:HD21	1:G:488:VAL:HG21	1.94	0.49
1:G:333:ILE:HG21	1:G:390:LEU:HD21	1.95	0.49
4:L:20:THR:O	4:L:21:ILE:O	2.30	0.49
1:G:294:ILE:HG22	1:G:447:SER:O	2.12	0.49
1:G:286:VAL:HG22	1:G:452:ILE:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:100:THR:CG2	4:L:91:SER:HB3	2.43	0.49
1:G:360:ILE:CD1	1:G:465:ASN:HD22	2.10	0.49
1:G:91:GLU:HG3	1:G:92:ASN:N	2.28	0.48
4:L:170:ASN:ND2	4:L:172:LYS:HB2	2.29	0.48
1:G:296:CYS:SG	1:G:376:PHE:HZ	2.35	0.48
3:H:162:GLY:O	3:H:182:VAL:HA	2.14	0.48
3:H:136:ALA:O	3:H:183:THR:HA	2.13	0.48
1:G:257:THR:HG21	1:G:370:GLU:O	2.14	0.48
1:G:296:CYS:O	1:G:444:ASN:HA	2.13	0.48
1:G:223:TYR:HA	1:G:490:GLN:HA	1.95	0.48
1:G:225:ILE:HB	1:G:245:VAL:HG23	1.96	0.48
4:L:54:LEU:HD11	4:L:58:VAL:HG11	1.96	0.48
1:G:224:VAL:CG2	1:G:491:ILE:HD11	2.43	0.48
3:H:123:PRO:HG2	4:L:122:SER:HB2	1.96	0.48
4:L:189:HIS:HB2	4:L:192:TYR:OH	2.13	0.47
1:G:121:LYS:HB2	1:G:201:ILE:HG22	1.96	0.47
1:G:272:ILE:N	1:G:272:ILE:HD12	2.29	0.47
1:G:58:ALA:C	1:G:59:LYS:HD2	2.34	0.47
1:G:92:ASN:HD22	1:G:238:PRO:HA	1.70	0.47
4:L:161:GLU:N	4:L:161:GLU:OE1	2.46	0.47
1:G:82:GLN:HB2	3:H:99:PRO:HB3	1.96	0.47
1:G:389:GLN:HB2	1:G:416:LEU:HD21	1.97	0.47
1:G:202:LYS:HD3	1:G:202:LYS:C	2.34	0.47
1:G:205:CYS:SG	1:G:205:CYS:O	2.73	0.47
1:G:279:ASN:OD1	1:G:280:ASN:N	2.47	0.47
1:G:333:ILE:HG23	1:G:414:ILE:HB	1.97	0.47
4:L:167:LYS:C	4:L:168:GLN:OE1	2.53	0.47
1:G:116:LEU:N	1:G:208:ILE:HD11	2.15	0.47
4:L:92:TYR:CD2	4:L:93:SER:HB2	2.50	0.47
1:G:348:LYS:O	1:G:351:GLU:HB2	2.14	0.47
4:L:95:PRO:HG2	4:L:97:THR:HG23	1.97	0.47
1:G:117:GLN:HE22	1:G:206:PRO:CD	2.24	0.47
3:H:2:VAL:HA	3:H:26:GLY:HA3	1.96	0.46
4:L:145:VAL:CG1	4:L:198:HIS:CD2	2.97	0.46
1:G:457:ASP:HB3	1:G:467:THR:HB	1.97	0.46
1:G:69:TRP:O	1:G:73:ALA:HB3	2.15	0.46
1:G:221:ALA:HB2	4:L:32:TYR:CD1	2.50	0.46
4:L:136:LEU:CD2	4:L:138:SER:HB2	2.46	0.46
1:G:121:LYS:HB2	1:G:201:ILE:CG2	2.45	0.46
1:G:384:TYR:O	1:G:418:CYS:HA	2.15	0.46
1:G:457:ASP:OD2	1:G:469:ARG:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:66:ARG:NH2	3:H:86:ASP:OD2	2.49	0.46
4:L:168:GLN:HG2	4:L:169:SER:N	2.31	0.46
3:H:95:ALA:C	3:H:96:PRO:O	2.54	0.46
4:L:135:CYS:HB2	4:L:149:TRP:CZ2	2.52	0.46
3:H:90:TYR:CE1	3:H:109:VAL:CG1	2.99	0.45
4:L:78:LEU:HD21	4:L:83:PHE:CZ	2.51	0.45
1:G:336:THR:OG1	1:G:337:LYS:N	2.49	0.45
1:G:350:LYS:HG3	1:G:359:ILE:HD13	1.98	0.45
3:H:210:ARG:HD3	3:H:210:ARG:HA	1.73	0.45
1:G:219:THR:O	4:L:32:TYR:OH	2.27	0.45
3:H:100:THR:HG23	4:L:91:SER:HB3	1.99	0.45
3:H:118:GLY:HA3	3:H:204:ASN:HD22	1.82	0.45
3:H:122:PHE:CE2	4:L:125:GLU:HG3	2.51	0.45
3:H:122:PHE:HB3	4:L:125:GLU:HB2	1.99	0.45
3:H:48:ILE:HG21	3:H:80:MET:CE	2.48	0.45
1:G:293:GLU:HG2	5:G:606:NAG:H81	1.95	0.44
3:H:121:VAL:HG22	3:H:142:VAL:HG12	1.99	0.44
3:H:205:THR:O	3:H:205:THR:CG2	2.65	0.44
3:H:37:VAL:CG1	3:H:45:LEU:HD22	2.47	0.44
4:L:170:ASN:HD22	4:L:172:LYS:HB2	1.82	0.44
4:L:139:ASP:HB3	4:L:172:LYS:CE	2.47	0.44
4:L:61:ARG:NH2	4:L:82:ASP:OD1	2.51	0.44
1:G:360:ILE:HD12	1:G:465:ASN:HB3	1.93	0.44
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.97	0.44
4:L:76:SER:O	4:L:77:SER:HB3	2.18	0.44
1:G:64:GLU:HB2	1:G:67:ASN:HD22	1.83	0.44
3:H:123:PRO:HB3	3:H:210:ARG:CD	2.48	0.44
4:L:139:ASP:CB	4:L:172:LYS:HE2	2.48	0.44
1:G:258:GLN:OE1	1:G:374:HIS:N	2.50	0.44
3:H:72:ASP:C	3:H:72:ASP:OD2	2.56	0.44
4:L:132:THR:HA	4:L:179:LEU:O	2.17	0.44
3:H:122:PHE:CB	4:L:125:GLU:HB2	2.47	0.44
1:G:58:ALA:O	1:G:59:LYS:HD2	2.18	0.43
2:N:18:ARG:CG	2:N:19:CYS:N	2.80	0.43
4:L:111:LYS:H	4:L:111:LYS:CD	2.31	0.43
4:L:194:CYS:O	4:L:206:THR:HA	2.18	0.43
4:L:167:LYS:HG2	4:L:168:GLN:N	2.34	0.43
4:L:186:TRP:CD1	4:L:192:TYR:CZ	3.07	0.43
4:L:183:PRO:O	4:L:187:LYS:HG2	2.18	0.43
4:L:20:THR:O	4:L:73:LEU:O	2.36	0.43
1:G:43:PRO:O	1:G:492:GLU:OE1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:6:GLN:NE2	3:H:107:THR:OG1	2.48	0.43
1:G:116:LEU:CG	1:G:116:LEU:O	2.67	0.43
3:H:131:THR:HA	3:H:136:ALA:HA	2.00	0.43
1:G:343:LYS:O	1:G:347:GLU:HG2	2.19	0.42
1:G:379:ARG:HH12	1:G:444:ASN:H	1.66	0.42
1:G:46:LYS:HE3	1:G:492:GLU:HB2	2.02	0.42
3:H:120:SER:O	3:H:142:VAL:HA	2.19	0.42
1:G:203:GLN:OE1	1:G:204:ALA:N	2.51	0.42
3:H:10:GLU:O	3:H:109:VAL:HA	2.19	0.42
4:L:121:PRO:CD	4:L:133:LEU:HG	2.49	0.42
4:L:19:VAL:O	4:L:74:THR:HA	2.20	0.42
3:H:33:THR:HG23	3:H:96:PRO:O	2.19	0.42
1:G:279:ASN:OD1	1:G:281:ALA:N	2.46	0.42
4:L:48:ILE:HG13	4:L:73:LEU:HD12	2.02	0.42
4:L:13:ALA:N	4:L:107:LYS:HB2	2.34	0.42
4:L:125:GLU:OE2	4:L:131:ALA:HA	2.20	0.41
4:L:202:THR:HG22	4:L:203:VAL:HG23	2.00	0.41
1:G:112:TRP:O	1:G:115:SER:O	2.37	0.41
3:H:201:LYS:CB	3:H:202:PRO:HD3	2.45	0.41
3:H:209:LYS:HE2	3:H:211:VAL:HG11	2.01	0.41
1:G:272:ILE:HD11	1:G:348:LYS:CG	2.51	0.41
3:H:48:ILE:HG12	3:H:63:PHE:CE2	2.54	0.41
4:L:154:SER:HA	4:L:155:PRO:HD3	1.88	0.41
4:L:54:LEU:HD11	4:L:58:VAL:HB	2.02	0.41
4:L:139:ASP:CA	4:L:172:LYS:HE2	2.50	0.41
1:G:495:GLY:HA3	3:H:27:PHE:HB3	2.01	0.41
4:L:111:LYS:H	4:L:111:LYS:HE2	1.86	0.41
1:G:122:LEU:HD13	1:G:122:LEU:HA	1.97	0.41
1:G:120:VAL:HG12	1:G:122:LEU:HD22	2.03	0.41
1:G:119:CYS:CA	1:G:205:CYS:HB3	2.50	0.41
1:G:290:LYS:HD3	1:G:290:LYS:HA	1.90	0.41
3:H:1:GLN:HG2	3:H:3:GLN:HE21	1.85	0.41
3:H:51:ILE:HG23	3:H:51:ILE:O	2.20	0.41
4:L:37:GLN:OE1	4:L:39:LYS:HE3	2.20	0.41
4:L:90:GLN:NE2	4:L:93:SER:H	2.19	0.41
1:G:100:MET:SD	1:G:488:VAL:HG23	2.61	0.41
1:G:343:LYS:HA	1:G:346:THR:CG2	2.51	0.41
1:G:46:LYS:HZ2	1:G:492:GLU:HB2	1.85	0.41
3:H:149:PRO:HD2	3:H:201:LYS:HG3	2.02	0.41
4:L:121:PRO:HD3	4:L:133:LEU:CG	2.49	0.41
4:L:38:GLN:O	4:L:84:ALA:HB1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:265:LEU:N	1:G:265:LEU:HD12	2.36	0.40
1:G:348:LYS:HA	1:G:351:GLU:OE1	2.21	0.40
4:L:129:ASN:O	4:L:183:PRO:CD	2.68	0.40
1:G:379:ARG:NH1	1:G:444:ASN:O	2.53	0.40
1:G:256:SER:HB2	1:G:376:PHE:HB3	2.02	0.40
1:G:90:THR:HG23	1:G:239:CYS:O	2.21	0.40
1:G:241:ASN:OD1	5:G:603:NAG:C2	2.63	0.40
1:G:84:ILE:HD12	1:G:85:HIS:N	2.36	0.40
3:H:48:ILE:HG21	3:H:80:MET:HE2	2.03	0.40

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)
1:G:466:GLU:OE2	5:G:606:NAG:O4[1_565]	2.00	0.20

## 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	320/385 (83%)	282 (88%)	34 (11%)	4 (1%)	12	36
2	N	24/28 (86%)	20 (83%)	3 (12%)	1 (4%)	3	9
3	H	216/220 (98%)	183 (85%)	23 (11%)	10 (5%)	2	8
4	L	208/210 (99%)	158 (76%)	29 (14%)	21 (10%)	0	1
All	All	768/843 (91%)	643 (84%)	89 (12%)	36 (5%)	2	8

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	82(B)	SER

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Mol	Chain	Res	Type
3	H	96	PRO
4	L	3	GLN
4	L	94	THR
4	L	155	PRO
4	L	168	GLN
1	G	124	GLY
1	G	354	ASN
3	H	100(A)	SER
3	H	202	PRO
3	H	204	ASN
4	L	2	ILE
4	L	21	ILE
4	L	28	SER
4	L	51	ALA
4	L	77	SER
4	L	139	ASP
4	L	156	VAL
4	L	165	PRO
1	G	262	ASN
3	H	203	SER
3	H	211	VAL
4	L	50	ALA
4	L	76	SER
4	L	167	LYS
4	L	209	PRO
4	L	91	SER
4	L	166	SER
4	L	199	GLU
2	N	27	VAL
3	H	97	VAL
4	L	109	GLN
3	H	82(A)	SER
4	L	92	TYR
1	G	120	VAL
3	H	147	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	298/339 (88%)	287 (96%)	11 (4%)	34	66
2	N	20/20 (100%)	16 (80%)	4 (20%)	1	3
3	H	186/188 (99%)	168 (90%)	18 (10%)	8	24
4	L	181/181 (100%)	173 (96%)	8 (4%)	28	60
All	All	685/728 (94%)	644 (94%)	41 (6%)	19	47

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	46	LYS
1	G	47	ASP
1	G	116	LEU
1	G	231	LYS
1	G	241	ASN
1	G	252	LYS
1	G	378	CYS
1	G	410	CYS
1	G	463	THR
1	G	489	VAL
1	G	490	GLN
2	N	11	LYS
2	N	16	LEU
2	N	19	CYS
2	N	22	THR
3	H	18	MET
3	H	50	TRP
3	H	56	ASN
3	H	70	THR
3	H	71	ARG
3	H	100(B)	SER
3	H	105	GLN
3	H	129	LYS
3	H	130	SER
3	H	135	THR
3	H	138	LEU
3	H	173	SER
3	H	183	THR
3	H	187	SER
3	H	204	ASN
3	H	206	LYS

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Mol	Chain	Res	Type
3	H	211	VAL
3	H	212	GLU
4	L	111	LYS
4	L	115	SER
4	L	135	CYS
4	L	152	ASP
4	L	160	VAL
4	L	163	THR
4	L	167	LYS
4	L	179	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	92	ASN
1	G	117	GLN
3	H	39	GLN
3	H	43	GLN
3	H	56	ASN
3	H	61	GLN
4	L	79	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
2	U2X	N	23	2	19,20,21	1.15	1 (5%)	22,25,27	0.81	1 (4%)

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
2	U2X	N	23	2	-	4/10/19/21	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	23	U2X	OH-CZ	3.30	1.45	1.37

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	23	U2X	C7-OH-CZ	-2.09	113.48	117.93

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	23	U2X	CE1-CZ-OH-C7
2	N	23	U2X	CE2-CZ-OH-C7
2	N	23	U2X	C2-C3-C7-OH
2	N	23	U2X	C4-C3-C7-OH

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 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	G	605	1	14,14,15	0.36	0	17,19,21	0.75	0
5	NAG	G	601	1	14,14,15	0.31	0	17,19,21	1.34	4 (23%)
5	NAG	G	609	1	14,14,15	0.51	0	17,19,21	1.30	3 (17%)
5	NAG	G	607	1	14,14,15	0.62	0	17,19,21	1.47	1 (5%)
5	NAG	G	608	1	14,14,15	0.30	0	17,19,21	1.06	2 (11%)
5	NAG	G	603	1	14,14,15	1.44	2 (14%)	17,19,21	3.20	3 (17%)
5	NAG	G	604	1	14,14,15	0.40	0	17,19,21	0.55	0
5	NAG	G	610	1	14,14,15	0.36	0	17,19,21	0.65	0
5	NAG	G	606	1	14,14,15	0.86	1 (7%)	17,19,21	1.50	3 (17%)
5	NAG	G	602	1	14,14,15	0.36	0	17,19,21	0.81	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
5	NAG	G	605	1	-	0/6/23/26	0/1/1/1
5	NAG	G	601	1	-	1/6/23/26	0/1/1/1
5	NAG	G	609	1	-	2/6/23/26	0/1/1/1
5	NAG	G	607	1	-	2/6/23/26	0/1/1/1
5	NAG	G	608	1	-	0/6/23/26	0/1/1/1
5	NAG	G	603	1	-	0/6/23/26	0/1/1/1
5	NAG	G	604	1	-	2/6/23/26	0/1/1/1
5	NAG	G	610	1	-	2/6/23/26	0/1/1/1
5	NAG	G	606	1	-	2/6/23/26	0/1/1/1
5	NAG	G	602	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	603	NAG	C1-C2	4.29	1.58	1.52
5	G	603	NAG	O5-C1	2.54	1.47	1.43
5	G	606	NAG	C1-C2	-2.16	1.49	1.52

All (17) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	603	NAG	C1-O5-C5	9.37	124.88	112.19
5	G	603	NAG	O5-C1-C2	-8.26	98.24	111.29
5	G	607	NAG	O5-C1-C2	-5.19	103.09	111.29
5	G	606	NAG	O5-C1-C2	-4.04	104.92	111.29
5	G	603	NAG	C1-C2-N2	3.32	116.15	110.49
5	G	609	NAG	O5-C5-C6	3.02	111.94	107.20
5	G	601	NAG	C1-O5-C5	2.91	116.14	112.19
5	G	608	NAG	C1-O5-C5	2.88	116.09	112.19
5	G	609	NAG	C3-C4-C5	-2.70	105.43	110.24
5	G	601	NAG	C4-C3-C2	-2.57	107.25	111.02
5	G	601	NAG	O5-C1-C2	-2.56	107.24	111.29
5	G	606	NAG	C1-O5-C5	-2.53	108.77	112.19
5	G	609	NAG	O5-C5-C4	-2.40	104.99	110.83
5	G	602	NAG	C1-O5-C5	-2.34	109.02	112.19
5	G	601	NAG	C1-C2-N2	2.33	114.47	110.49
5	G	608	NAG	C4-C3-C2	-2.23	107.75	111.02
5	G	606	NAG	O5-C5-C4	-2.20	105.48	110.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	606	NAG	O5-C5-C6-O6
5	G	607	NAG	C4-C5-C6-O6
5	G	606	NAG	C4-C5-C6-O6
5	G	604	NAG	O5-C5-C6-O6
5	G	609	NAG	O5-C5-C6-O6
5	G	604	NAG	C4-C5-C6-O6
5	G	607	NAG	O5-C5-C6-O6
5	G	610	NAG	C4-C5-C6-O6
5	G	610	NAG	O5-C5-C6-O6
5	G	609	NAG	C4-C5-C6-O6
5	G	601	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	609	NAG	1	0
5	G	603	NAG	2	0
5	G	606	NAG	13	1

## 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, 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	330/385 (85%)	0.29	18 (5%) 25 22	61, 92, 126, 145	0
2	N	24/28 (85%)	0.03	3 (12%) 3 3	81, 97, 117, 124	0
3	H	218/220 (99%)	0.10	6 (2%) 53 50	57, 86, 110, 122	0
4	L	210/210 (100%)	-0.06	6 (2%) 51 48	54, 82, 115, 133	0
All	All	782/843 (92%)	0.13	33 (4%) 36 33	54, 87, 119, 145	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	414	ILE	4.7
3	H	197	ASN	4.4
1	G	209	SER	4.1
1	G	45	TRP	3.9
1	G	208	ILE	3.8
1	G	68	VAL	3.7
1	G	415	THR	3.4
4	L	178	TYR	3.3
1	G	65	VAL	3.2
2	N	8	LEU	3.1
1	G	123	THR	3.0
3	H	41	ARG	3.0
4	L	192	TYR	2.9
2	N	5	PHE	2.8
1	G	463	THR	2.8
1	G	60	ALA	2.7
1	G	353	PHE	2.7
3	H	194	TYR	2.7
4	L	27	GLN	2.6
3	H	138	LEU	2.5
1	G	277	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	H	148	GLU	2.5
1	G	269	GLU	2.4
2	N	4	HIS	2.4
3	H	124	LEU	2.4
1	G	464	SER	2.4
1	G	66	HIS	2.3
1	G	124	GLY	2.3
4	L	188	SER	2.2
4	L	83	PHE	2.2
1	G	64	GLU	2.2
4	L	205	LYS	2.2
1	G	434	MET	2.1

## 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. 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
2	DPR	N	21	7/8	0.95	0.21	80,90,93,93	0
2	U2X	N	23	19/20	0.96	0.19	70,73,77,77	0

## 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
5	NAG	G	606	14/15	0.69	0.41	104,109,113,116	0
5	NAG	G	605	14/15	0.82	0.23	91,102,111,112	0
5	NAG	G	610	14/15	0.83	0.26	93,110,124,124	0
5	NAG	G	609	14/15	0.86	0.25	97,106,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	G	608	14/15	0.86	0.23	107,121,130,138	0
5	NAG	G	603	14/15	0.88	0.20	84,91,104,106	0
5	NAG	G	601	14/15	0.89	0.21	93,106,117,121	0
5	NAG	G	607	14/15	0.90	0.17	96,113,117,117	0
5	NAG	G	602	14/15	0.92	0.16	82,94,113,121	0
5	NAG	G	604	14/15	0.95	0.18	67,77,87,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.