



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 04:13 PM BST

PDB ID : 6BCK  
Title : Crystal Structure of Broadly Neutralizing Antibody N49P7 in Complex with HIV-1 Clade AE strain 93TH057 gp120 core.  
Authors : Tolbert, W.D.; Gohain, N.; Pazgier, M.  
Deposited on : 2017-10-20  
Resolution : 2.70 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

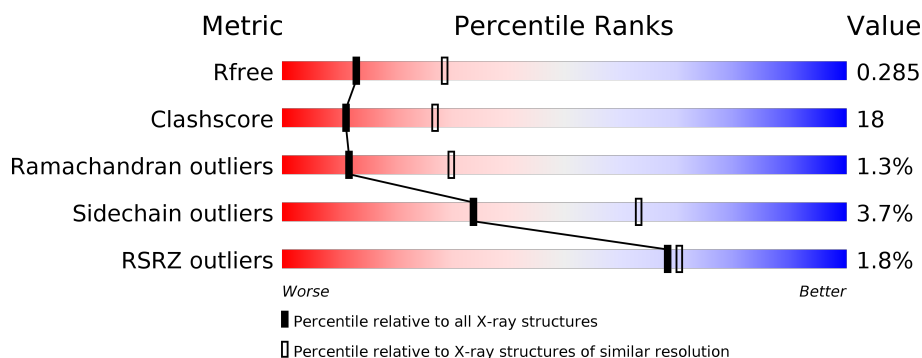
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	353	<div> <div>2%</div> <div>66% 27% 5%</div> </div>
2	H	228	<div> <div>2%</div> <div>61% 35% 4%</div> </div>
3	L	205	<div> <div>2%</div> <div>57% 35% 8%</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	MPD	H	301	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6019 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	337	Total	C	N	O	S	0	0	0
			2639	1658	457	502	22			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9

- Molecule 2 is a protein called N49P7 Fab heavy chain of N29P7 IgG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1697	1071	297	321	8			

- Molecule 3 is a protein called N49P7 Fab light chain from N49P7 IgG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	199	Total	C	N	O	S	0	0	0
			1486	931	252	298	5			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			8	6	2		
5	H	1	Total	C	O	0	0
			8	6	2		

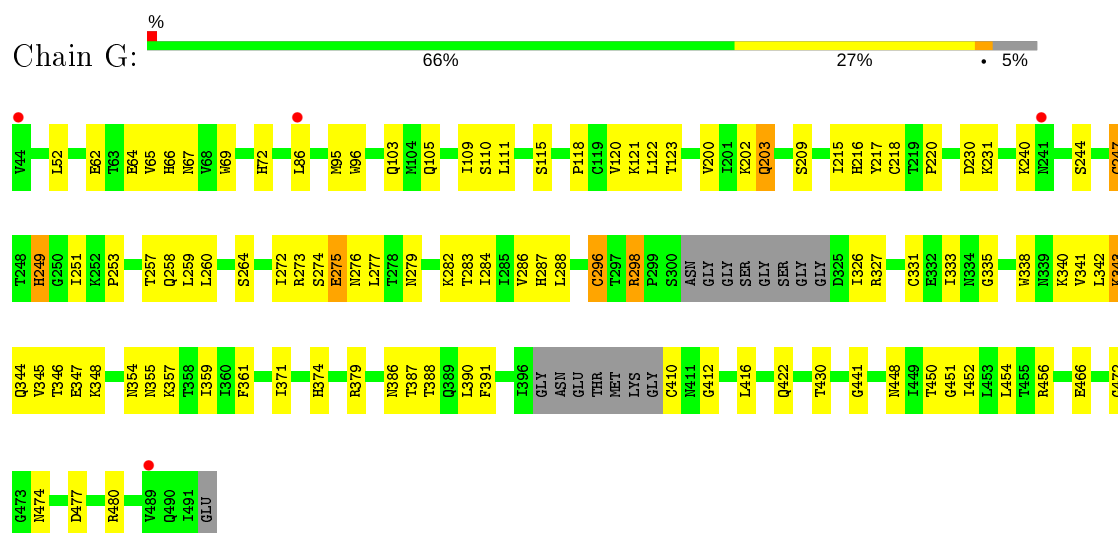
- Molecule 6 is water.

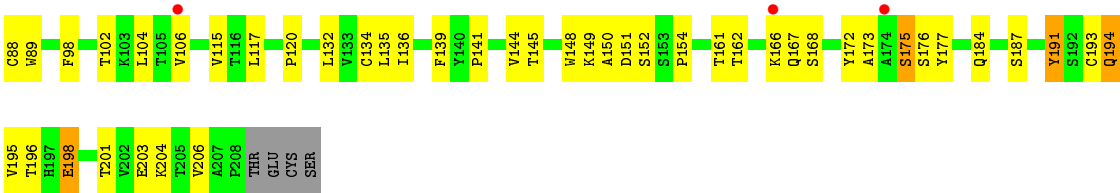
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	11	Total	O	0	0
			11	11		
6	H	12	Total	O	0	0
			12	12		
6	L	4	Total	O	0	0
			4	4		

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

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

- Molecule 1: clade A/E 93TH057 HIV-1 gp120 core







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.44Å 63.87Å 255.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.26 – 2.70 44.26 – 2.60	Depositor EDS
% Data completeness (in resolution range)	63.1 (44.26-2.70) 59.2 (44.26-2.60)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.12 _2829, REFMAC	Depositor
R, $R_{free}$	0.225 , 0.285 0.225 , 0.285	Depositor DCC
$R_{free}$ test set	957 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.044 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6019	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, 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	0.34	0/2694	0.54	0/3658
2	H	0.36	1/1741 (0.1%)	0.59	1/2368 (0.0%)
3	L	0.32	0/1525	0.56	0/2083
All	All	0.34	1/5960 (0.0%)	0.56	1/8109 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
2	H	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	196	CYS	CB-SG	-5.43	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	H	140	CYS	CA-CB-SG	-7.37	100.73	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	275	GLU	Peptide
2	H	139	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2639	0	2578	87	0
2	H	1697	0	1654	69	0
3	L	1486	0	1433	61	0
4	G	154	0	143	11	0
5	G	8	0	14	0	0
5	H	8	0	14	5	0
6	G	11	0	0	1	0
6	H	12	0	0	1	0
6	L	4	0	0	2	0
All	All	6019	0	5836	209	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 18.

All (209) 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:276:ASN:HD22	4:G:504:NAG:C1	1.28	1.47
1:G:276:ASN:ND2	4:G:504:NAG:C1	1.96	1.24
2:H:47:TRP:HB3	5:H:301:MPD:HM3	1.35	1.06
3:L:6:GLN:NE2	3:L:23:CYS:SG	2.38	0.95
1:G:410:CYS:N	4:G:509:NAG:HO6	1.65	0.94
1:G:276:ASN:HB3	4:G:504:NAG:C1	2.02	0.90
2:H:37:ILE:HD11	2:H:91:TYR:HB2	1.57	0.86
2:H:195:ILE:HG22	2:H:210:ARG:HG3	1.61	0.83
1:G:218:CYS:HG	1:G:247:CYS:HG	0.91	0.83
2:H:94:ARG:HH12	2:H:96:ARG:HD3	1.46	0.79
1:G:118:PRO:O	1:G:203:GLN:NE2	2.16	0.79
1:G:258:GLN:OE1	1:G:387:THR:HG21	1.84	0.78
1:G:276:ASN:CB	4:G:504:NAG:C1	2.64	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:THR:HG23	2:H:110:THR:HA	1.68	0.75
1:G:276:ASN:OD1	1:G:279:ASN:HB2	1.84	0.75
1:G:298:ARG:NH2	1:G:441:GLY:O	2.22	0.72
3:L:117:LEU:HD13	3:L:134:CYS:HB2	1.70	0.71
2:H:193:THR:HG21	2:H:210:ARG:HD3	1.72	0.70
1:G:218:CYS:HG	1:G:247:CYS:CB	2.05	0.69
2:H:2:ALA:HA	2:H:25:GLN:O	1.93	0.68
1:G:276:ASN:CG	4:G:504:NAG:C1	2.62	0.68
1:G:371:ILE:HD11	2:H:54:GLY:HA3	1.76	0.67
2:H:105:ARG:HH12	3:L:42:ARG:HA	1.61	0.66
1:G:276:ASN:OD1	1:G:279:ASN:CB	2.43	0.66
1:G:66:HIS:HD2	1:G:111:LEU:HD21	1.61	0.65
3:L:32:LEU:HD12	3:L:32:LEU:H	1.62	0.65
3:L:36:CYS:HB2	3:L:89:TRP:HZ3	1.61	0.65
3:L:5:THR:OG1	3:L:6:GLN:N	2.29	0.64
3:L:42:ARG:HB3	3:L:42:ARG:HH11	1.61	0.64
2:H:17:SER:HB3	2:H:82(A):ARG:HA	1.79	0.64
2:H:32:TYR:HB3	2:H:95:ASP:O	1.98	0.63
1:G:474:ASN:ND2	2:H:53:MET:HG2	2.14	0.62
1:G:282:LYS:HE2	2:H:98:ASN:ND2	2.14	0.62
1:G:342:LEU:O	1:G:345:VAL:HG12	2.00	0.62
2:H:98:ASN:HA	2:H:100(C):ARG:HD3	1.82	0.62
3:L:46:LEU:HD12	3:L:55:PRO:HG2	1.81	0.62
2:H:94:ARG:NH1	2:H:96:ARG:HD3	2.15	0.61
2:H:28:ARG:HD2	2:H:31:ASP:CG	2.20	0.61
1:G:357:LYS:HE2	1:G:466:GLU:HG2	1.83	0.60
2:H:144:ASP:OD1	2:H:171:GLN:NE2	2.27	0.60
2:H:15:GLY:O	2:H:82(C):LEU:N	2.33	0.59
1:G:354:ASN:C	1:G:357:LYS:H	2.06	0.59
2:H:47:TRP:H	5:H:301:MPD:H13	1.67	0.59
1:G:259:LEU:HD12	1:G:374:HIS:CG	2.37	0.59
2:H:105:ARG:NH1	3:L:42:ARG:HA	2.18	0.59
3:L:149:LYS:HG2	3:L:154:PRO:HA	1.84	0.58
3:L:167:GLN:NE2	3:L:173:ALA:HB2	2.19	0.58
1:G:354:ASN:O	1:G:357:LYS:N	2.36	0.58
2:H:90:TYR:HE1	2:H:109:VAL:HG22	1.68	0.58
3:L:194:GLN:NE2	3:L:203:GLU:OE1	2.36	0.58
1:G:64:GLU:HA	1:G:209:SER:HB3	1.85	0.57
1:G:216:HIS:HB3	1:G:247:CYS:SG	2.45	0.56
1:G:326:ILE:HG13	1:G:327:ARG:HD2	1.87	0.56
1:G:448:ASN:HD22	4:G:510:NAG:H83	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:11:VAL:HG23	3:L:104:LEU:HA	1.87	0.56
2:H:47:TRP:HE3	5:H:301:MPD:CM	2.19	0.56
1:G:388:THR:HG21	4:G:508:NAG:O4	2.06	0.56
2:H:37:ILE:CD1	2:H:91:TYR:HB2	2.33	0.56
1:G:386:ASN:O	1:G:416:LEU:HG	2.05	0.55
2:H:153:SER:O	2:H:197:ASN:HB2	2.06	0.55
2:H:47:TRP:HE3	5:H:301:MPD:HM1	1.71	0.55
1:G:123:THR:HG22	1:G:430:THR:HG22	1.87	0.55
3:L:42:ARG:HB3	3:L:42:ARG:NH1	2.21	0.55
3:L:141:PRO:HD2	3:L:198:GLU:OE1	2.07	0.55
3:L:184:GLN:HA	3:L:187:SER:HB3	1.89	0.55
3:L:69:GLY:N	6:L:301:HOH:O	2.39	0.55
1:G:348:LYS:NZ	4:G:505:NAG:O6	2.40	0.54
2:H:63:PHE:O	2:H:67:VAL:HG12	2.06	0.54
3:L:19:VAL:HG22	3:L:75:ILE:HG12	1.89	0.54
2:H:199:ASN:OD1	2:H:206:LYS:HD2	2.08	0.54
2:H:61:TRP:HA	2:H:64:GLN:HG2	1.89	0.53
3:L:11:VAL:HG11	3:L:21:ILE:HG12	1.89	0.53
2:H:195:ILE:CG2	2:H:210:ARG:HG3	2.35	0.53
3:L:150:ALA:O	3:L:152:SER:N	2.41	0.53
1:G:69:TRP:HA	1:G:72:HIS:CE1	2.43	0.53
3:L:14:SER:O	3:L:16:GLY:N	2.42	0.53
2:H:105:ARG:HG2	2:H:105:ARG:HH11	1.73	0.53
1:G:64:GLU:OE2	1:G:67:ASN:ND2	2.24	0.53
3:L:33:VAL:HA	3:L:89:TRP:O	2.09	0.53
1:G:216:HIS:CB	1:G:247:CYS:SG	2.97	0.53
3:L:61:ARG:NH1	3:L:82:ASP:OD2	2.33	0.53
1:G:52:LEU:HD12	1:G:103:GLN:OE1	2.09	0.52
1:G:333:ILE:HD13	1:G:390:LEU:HD21	1.92	0.52
1:G:335:GLY:N	1:G:412:GLY:O	2.37	0.52
2:H:166:PHE:CD1	3:L:135:LEU:HD22	2.44	0.52
3:L:70:THR:N	6:L:301:HOH:O	2.11	0.52
1:G:123:THR:CG2	1:G:430:THR:HG22	2.40	0.52
3:L:166:LYS:HG2	3:L:172:TYR:CE2	2.45	0.52
3:L:7:PRO:O	3:L:102:THR:OG1	2.20	0.52
3:L:161:THR:HG22	3:L:162:THR:H	1.75	0.51
2:H:67:VAL:HA	2:H:81:ASP:O	2.11	0.51
1:G:277:LEU:O	1:G:456:ARG:NH2	2.43	0.51
3:L:37:GLN:HE22	3:L:39:GLN:HE21	1.57	0.51
3:L:35:TRP:CD1	3:L:48:ILE:HD11	2.45	0.51
2:H:59:ILE:HD11	2:H:69:MET:SD	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:26:THR:HG22	3:L:27:HIS:H	1.76	0.51
3:L:32:LEU:HD12	3:L:32:LEU:N	2.25	0.50
1:G:361:PHE:HB3	1:G:391:PHE:HB3	1.94	0.50
1:G:286:VAL:HG22	1:G:452:ILE:HB	1.94	0.50
1:G:284:ILE:HG23	1:G:454:LEU:HB2	1.92	0.50
1:G:272:ILE:HD13	1:G:286:VAL:HG12	1.94	0.50
1:G:249:HIS:CD2	1:G:251:ILE:HG13	2.46	0.50
1:G:379:ARG:N	1:G:379:ARG:HD3	2.27	0.50
2:H:61:TRP:O	2:H:63:PHE:N	2.45	0.50
3:L:145:THR:HB	3:L:196:THR:HB	1.93	0.49
1:G:342:LEU:O	1:G:346:THR:HG23	2.11	0.49
1:G:259:LEU:HD12	1:G:374:HIS:CD2	2.48	0.49
3:L:36:CYS:HB2	3:L:89:TRP:CZ3	2.45	0.49
1:G:288:LEU:HD12	1:G:288:LEU:H	1.78	0.49
2:H:61:TRP:O	2:H:64:GLN:HG2	2.13	0.49
2:H:32:TYR:HA	2:H:98:ASN:O	2.12	0.49
1:G:249:HIS:HD2	1:G:251:ILE:HG13	1.78	0.48
1:G:111:LEU:O	1:G:115:SER:HB2	2.12	0.48
2:H:155:ASN:OD1	2:H:195:ILE:HG12	2.12	0.48
1:G:343:LYS:O	1:G:347:GLU:HG3	2.13	0.48
3:L:13:ALA:HB1	3:L:17:GLN:HG3	1.95	0.48
1:G:257:THR:O	1:G:259:LEU:N	2.44	0.48
1:G:272:ILE:CG2	1:G:284:ILE:HD11	2.44	0.47
3:L:167:GLN:HE21	3:L:173:ALA:HB2	1.78	0.47
1:G:86:LEU:HD11	1:G:244:SER:HB2	1.96	0.47
2:H:144:ASP:HB3	2:H:175:LEU:HD13	1.97	0.47
2:H:37:ILE:HG22	2:H:47:TRP:HA	1.95	0.47
1:G:259:LEU:HD12	1:G:374:HIS:CE1	2.49	0.47
2:H:119:PRO:HB3	2:H:142:VAL:HG13	1.95	0.47
1:G:340:LYS:O	1:G:344:GLN:HG3	2.15	0.47
2:H:100(D):PHE:O	2:H:100(E):GLU:HB2	2.15	0.47
3:L:117:LEU:HG	3:L:206:VAL:HG23	1.95	0.47
1:G:296:CYS:HA	1:G:331:CYS:HA	1.98	0.46
5:H:301:MPD:H4	5:H:301:MPD:HM1	1.67	0.46
1:G:260:LEU:HD12	1:G:451:GLY:HA3	1.96	0.46
3:L:59:PRO:HB2	3:L:61:ARG:HG2	1.98	0.46
1:G:264:SER:O	1:G:287:HIS:NE2	2.44	0.46
1:G:284:ILE:CG2	1:G:454:LEU:HB2	2.46	0.46
2:H:105:ARG:HG2	2:H:105:ARG:NH1	2.31	0.46
2:H:169:VAL:HG21	3:L:177:TYR:CE1	2.51	0.46
2:H:94:ARG:HE	2:H:102:LEU:HD12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:196:THR:HG23	3:L:201:THR:HG22	1.97	0.45
1:G:260:LEU:HB2	1:G:451:GLY:HA3	1.97	0.45
3:L:82:ASP:O	3:L:104:LEU:HD22	2.17	0.45
1:G:386:ASN:OD1	1:G:388:THR:HG23	2.17	0.45
2:H:166:PHE:CG	3:L:135:LEU:HD22	2.52	0.45
3:L:37:GLN:HE21	3:L:39:GLN:HG3	1.80	0.45
2:H:24:ALA:HB1	2:H:27:TYR:CE1	2.52	0.45
1:G:230:ASP:CG	1:G:240:LYS:H	2.20	0.45
2:H:119:PRO:HD2	2:H:205:THR:HG21	1.98	0.45
2:H:61:TRP:HA	2:H:64:GLN:CG	2.47	0.45
3:L:150:ALA:HA	3:L:191:TYR:CE1	2.51	0.45
1:G:66:HIS:CD2	1:G:111:LEU:HD21	2.46	0.44
2:H:100(K):LEU:HA	2:H:100(K):LEU:HD13	1.71	0.44
2:H:45:PRO:HB2	3:L:98:PHE:CD1	2.52	0.44
2:H:146:PHE:HA	2:H:147:PRO:HA	1.86	0.44
3:L:83:ASP:HB2	3:L:106:VAL:HG22	1.98	0.44
1:G:277:LEU:HD11	4:G:501:NAG:H81	2.00	0.44
4:G:504:NAG:H2	6:H:401:HOH:O	2.18	0.44
3:L:38:HIS:O	3:L:84:ALA:HB1	2.17	0.44
1:G:346:THR:HA	1:G:359:ILE:HD11	1.99	0.44
2:H:193:THR:CG2	2:H:210:ARG:HD3	2.44	0.44
1:G:283:THR:HG23	1:G:472:GLY:HA3	2.00	0.44
1:G:379:ARG:H	1:G:379:ARG:HD3	1.83	0.43
3:L:37:GLN:NE2	3:L:39:GLN:HE21	2.15	0.43
2:H:33:ILE:HA	2:H:52(A):PRO:HD3	1.99	0.43
2:H:112:GLN:C	2:H:114:ALA:H	2.21	0.43
2:H:196:CYS:O	2:H:208:ASP:HA	2.18	0.43
3:L:7:PRO:HD2	3:L:22:SER:O	2.18	0.43
1:G:105:GLN:O	1:G:109:ILE:HG13	2.19	0.43
1:G:477:ASP:O	1:G:480:ARG:HB2	2.19	0.43
3:L:65:SER:OG	3:L:66:GLY:N	2.51	0.43
2:H:121:VAL:HA	2:H:141:LEU:O	2.19	0.43
1:G:288:LEU:HD12	1:G:288:LEU:N	2.34	0.43
2:H:140:CYS:SG	2:H:154:TRP:CH2	3.11	0.43
2:H:127:SER:OG	2:H:128:SER:N	2.52	0.42
1:G:120:VAL:HG22	1:G:202:LYS:HG3	2.00	0.42
1:G:338:TRP:CZ2	1:G:390:LEU:HB3	2.54	0.42
1:G:95:MET:HG3	1:G:96:TRP:CD1	2.54	0.42
1:G:121:LYS:O	1:G:200:VAL:HA	2.20	0.42
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.54	0.42
3:L:135:LEU:HD23	3:L:175:SER:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:115:VAL:O	3:L:204:LYS:HE3	2.19	0.42
1:G:215:ILE:HD12	1:G:253:PRO:HG3	2.02	0.42
1:G:231:LYS:N	1:G:231:LYS:HD2	2.35	0.42
3:L:148:TRP:HE1	3:L:176:SER:HG	1.68	0.42
1:G:122:LEU:HG	1:G:200:VAL:CG2	2.50	0.42
1:G:218:CYS:N	1:G:247:CYS:SG	2.93	0.41
2:H:166:PHE:CZ	3:L:135:LEU:HB3	2.55	0.41
3:L:33:VAL:CG1	3:L:88:CYS:HB2	2.50	0.41
2:H:36:TRP:CG	2:H:80:LEU:HD13	2.56	0.41
1:G:276:ASN:OD1	1:G:279:ASN:HB3	2.20	0.41
1:G:326:ILE:HD11	1:G:327:ARG:NH1	2.36	0.41
2:H:31:ASP:HB3	2:H:100:SER:O	2.20	0.41
2:H:82:LEU:HD12	2:H:82:LEU:HA	1.95	0.41
2:H:35:HIS:NE2	2:H:95:ASP:OD2	2.53	0.41
1:G:217:TYR:C	1:G:247:CYS:SG	2.99	0.41
3:L:120:PRO:HD3	3:L:132:LEU:CD2	2.50	0.41
1:G:274:SER:HB2	1:G:284:ILE:HD12	2.02	0.41
1:G:288:LEU:HD13	1:G:450:THR:HA	2.03	0.41
2:H:196:CYS:SG	2:H:209:LYS:HB3	2.61	0.41
3:L:136:ILE:HG12	3:L:195:VAL:HG21	2.03	0.41
1:G:65:VAL:HG22	6:G:602:HOH:O	2.20	0.41
2:H:59:ILE:HD13	2:H:67:VAL:HG13	2.03	0.41
2:H:29:PHE:CD1	2:H:76:GLU:HA	2.55	0.41
1:G:273:ARG:O	1:G:284:ILE:HD12	2.22	0.40
3:L:139:PHE:CE2	3:L:172:TYR:HB2	2.55	0.40
1:G:343:LYS:O	1:G:346:THR:OG1	2.28	0.40
3:L:61:ARG:HG2	3:L:61:ARG:H	1.51	0.40
1:G:288:LEU:HD23	1:G:341:VAL:HG11	2.03	0.40
2:H:121:VAL:CG1	2:H:207:VAL:HG11	2.52	0.40
3:L:144:VAL:CG1	3:L:195:VAL:HG13	2.52	0.40
2:H:210:ARG:HD2	2:H:210:ARG:HH11	1.75	0.40
3:L:34:SER:HB2	3:L:89:TRP:CZ2	2.57	0.40

There are no symmetry-related clashes.

## 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	331/353 (94%)	303 (92%)	26 (8%)	2 (1%)	25	50
2	H	218/228 (96%)	192 (88%)	24 (11%)	2 (1%)	17	40
3	L	197/205 (96%)	169 (86%)	22 (11%)	6 (3%)	4	10
All	All	746/786 (95%)	664 (89%)	72 (10%)	10 (1%)	12	30

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	15	PRO
2	H	62	LYS
3	L	5	THR
3	L	151	ASP
3	L	198	GLU
1	G	355	ASN
2	H	32	TYR
3	L	6	GLN
3	L	55	PRO
1	G	220	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	302/311 (97%)	292 (97%)	10 (3%)	38	67
2	H	187/193 (97%)	181 (97%)	6 (3%)	39	68
3	L	165/171 (96%)	157 (95%)	8 (5%)	25	53
All	All	654/675 (97%)	630 (96%)	24 (4%)	34	63

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	62	GLU
1	G	110	SER
1	G	203	GLN
1	G	247	CYS
1	G	249	HIS
1	G	275	GLU
1	G	296	CYS
1	G	298	ARG
1	G	343	LYS
1	G	422	GLN
2	H	22	CYS
2	H	71	ARG
2	H	95	ASP
2	H	100(G)	SER
2	H	101	ASP
2	H	206	LYS
3	L	22	SER
3	L	42	ARG
3	L	61	ARG
3	L	168	SER
3	L	175	SER
3	L	191	TYR
3	L	193	CYS
3	L	194	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	216	HIS
1	G	249	HIS
1	G	276	ASN
1	G	474	ASN
2	H	98	ASN
3	L	37	GLN
3	L	79	GLN
3	L	167	GLN
3	L	170	ASN
3	L	194	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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$
5	MPD	H	301	-	7,7,7	0.38	0	9,10,10	0.61	0
4	NAG	G	508	1	14,14,15	2.09	1 (7%)	17,19,21	1.07	1 (5%)
4	NAG	G	503	1	14,14,15	0.42	0	17,19,21	0.60	0
4	NAG	G	507	1	14,14,15	0.39	0	17,19,21	0.40	0
5	MPD	G	512	-	7,7,7	0.27	0	9,10,10	0.38	0
4	NAG	G	509	1	14,14,15	0.29	0	17,19,21	1.30	2 (11%)
4	NAG	G	502	1	14,14,15	0.80	1 (7%)	17,19,21	0.82	1 (5%)
4	NAG	G	511	1	14,14,15	0.90	1 (7%)	17,19,21	1.13	2 (11%)
4	NAG	G	501	1	14,14,15	0.70	0	17,19,21	1.12	2 (11%)
4	NAG	G	505	1	14,14,15	0.50	0	17,19,21	0.96	1 (5%)
4	NAG	G	510	1	14,14,15	0.24	0	17,19,21	0.38	0
4	NAG	G	506	1	14,14,15	0.41	0	17,19,21	0.41	0
4	NAG	G	504	-	14,14,15	0.43	0	17,19,21	0.97	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	MPD	H	301	-	-	2/5/5/5	-
4	NAG	G	508	1	-	4/6/23/26	0/1/1/1
4	NAG	G	503	1	-	0/6/23/26	0/1/1/1
4	NAG	G	507	1	-	2/6/23/26	0/1/1/1
5	MPD	G	512	-	-	0/5/5/5	-
4	NAG	G	509	1	-	4/6/23/26	0/1/1/1
4	NAG	G	502	1	-	2/6/23/26	0/1/1/1
4	NAG	G	511	1	-	3/6/23/26	0/1/1/1
4	NAG	G	501	1	-	0/6/23/26	0/1/1/1
4	NAG	G	505	1	-	2/6/23/26	0/1/1/1
4	NAG	G	510	1	-	4/6/23/26	0/1/1/1
4	NAG	G	506	1	-	2/6/23/26	0/1/1/1
4	NAG	G	504	-	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	508	NAG	O5-C1	-7.64	1.31	1.43
4	G	511	NAG	O5-C1	-3.00	1.38	1.43
4	G	502	NAG	C1-C2	2.52	1.56	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	508	NAG	C1-O5-C5	3.37	116.76	112.19
4	G	509	NAG	C1-O5-C5	3.33	116.70	112.19
4	G	509	NAG	C3-C4-C5	3.06	115.70	110.24
4	G	511	NAG	C3-C4-C5	2.87	115.36	110.24
4	G	511	NAG	C1-O5-C5	-2.67	108.57	112.19
4	G	501	NAG	C1-O5-C5	2.57	115.68	112.19
4	G	502	NAG	C1-O5-C5	2.55	115.65	112.19
4	G	505	NAG	O5-C1-C2	-2.48	107.37	111.29
4	G	501	NAG	O5-C1-C2	-2.07	108.02	111.29
4	G	504	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	301	MPD	CM-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	G	505	NAG	O5-C5-C6-O6
4	G	509	NAG	O5-C5-C6-O6
4	G	507	NAG	O5-C5-C6-O6
4	G	506	NAG	O5-C5-C6-O6
4	G	502	NAG	O5-C5-C6-O6
4	G	507	NAG	C4-C5-C6-O6
4	G	505	NAG	C4-C5-C6-O6
4	G	510	NAG	C4-C5-C6-O6
4	G	510	NAG	O5-C5-C6-O6
4	G	511	NAG	C1-C2-N2-C7
4	G	506	NAG	C4-C5-C6-O6
4	G	508	NAG	C8-C7-N2-C2
4	G	508	NAG	O7-C7-N2-C2
4	G	509	NAG	C8-C7-N2-C2
4	G	509	NAG	O7-C7-N2-C2
4	G	510	NAG	C8-C7-N2-C2
4	G	510	NAG	O7-C7-N2-C2
4	G	509	NAG	C4-C5-C6-O6
4	G	502	NAG	C4-C5-C6-O6
4	G	508	NAG	O5-C5-C6-O6
4	G	508	NAG	C4-C5-C6-O6
4	G	504	NAG	O5-C5-C6-O6
5	H	301	MPD	C1-C2-C3-C4
4	G	511	NAG	C3-C2-N2-C7
4	G	511	NAG	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	301	MPD	5	0
4	G	508	NAG	1	0
4	G	509	NAG	1	0
4	G	501	NAG	1	0
4	G	505	NAG	1	0
4	G	510	NAG	1	0
4	G	504	NAG	6	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, 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	337/353 (95%)	-0.26	4 (1%) 79 80	12, 39, 70, 97	0
2	H	222/228 (97%)	-0.06	5 (2%) 60 62	13, 53, 82, 95	0
3	L	199/205 (97%)	-0.03	5 (2%) 57 59	32, 66, 87, 101	0
All	All	758/786 (96%)	-0.14	14 (1%) 68 70	12, 49, 83, 101	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	86	LEU	3.5
3	L	166	LYS	3.3
3	L	106	VAL	3.0
3	L	80	ASP	2.9
3	L	174	ALA	2.6
2	H	117	LYS	2.4
2	H	196	CYS	2.4
2	H	116	THR	2.3
1	G	489	VAL	2.2
2	H	127	SER	2.2
3	L	81	ASP	2.2
2	H	153	SER	2.2
1	G	44	VAL	2.2
1	G	241	ASN	2.1

### 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, 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	MPD	H	301	8/8	0.73	0.45	68,83,108,120	0
4	NAG	G	510	14/15	0.83	0.17	56,68,76,76	0
5	MPD	G	512	8/8	0.84	0.25	32,62,68,85	0
4	NAG	G	509	14/15	0.85	0.21	75,85,99,100	0
4	NAG	G	504	14/15	0.85	0.18	56,78,82,91	0
4	NAG	G	502	14/15	0.86	0.28	50,70,86,91	0
4	NAG	G	507	14/15	0.87	0.29	51,74,86,91	0
4	NAG	G	501	14/15	0.88	0.24	56,65,88,91	0
4	NAG	G	508	14/15	0.88	0.22	35,46,62,82	0
4	NAG	G	511	14/15	0.88	0.18	71,86,96,100	0
4	NAG	G	506	14/15	0.90	0.16	24,46,71,83	0
4	NAG	G	505	14/15	0.90	0.18	50,68,84,89	0
4	NAG	G	503	14/15	0.96	0.17	21,28,41,41	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.