



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:27 PM BST

PDB ID : 1J9C  
Title : Crystal Structure of tissue factor-factor VIIa complex  
Authors : Huang, M.; Ruf, W.; Edgington, T.S.; Wilson, I.A.  
Deposited on : 2001-05-24  
Resolution : 2.90 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.

---

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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

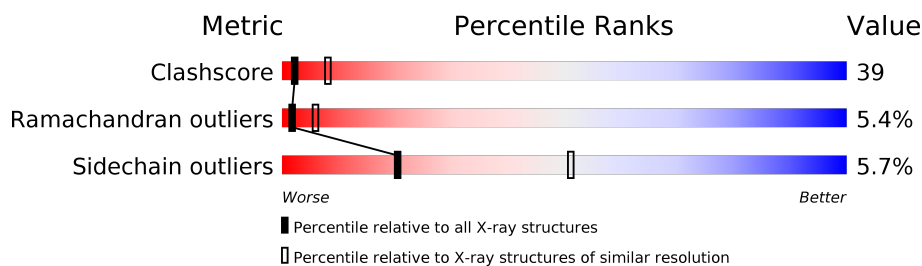
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	T	210	
2	L	95	
3	H	254	

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4559 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 Tissue factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	210	Total	C	N	O	S	0	0	0
			1673	1055	272	341	5			

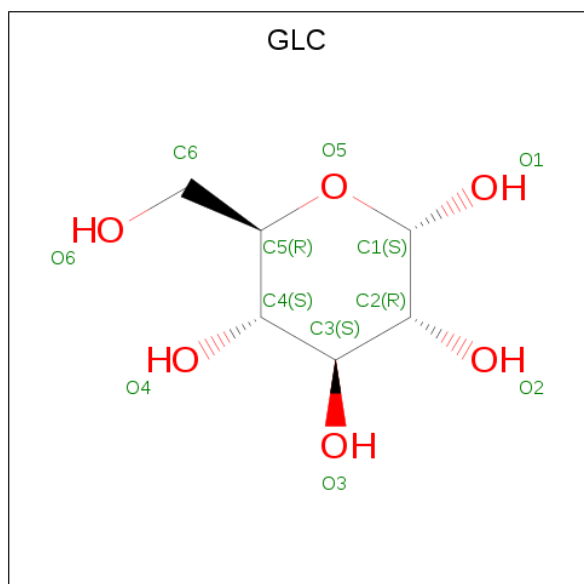
- Molecule 2 is a protein called factor VIIa light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	95	Total	C	N	O	S	0	0	0
			715	429	124	149	13			

- Molecule 3 is a protein called factor VIIa heavy chain.

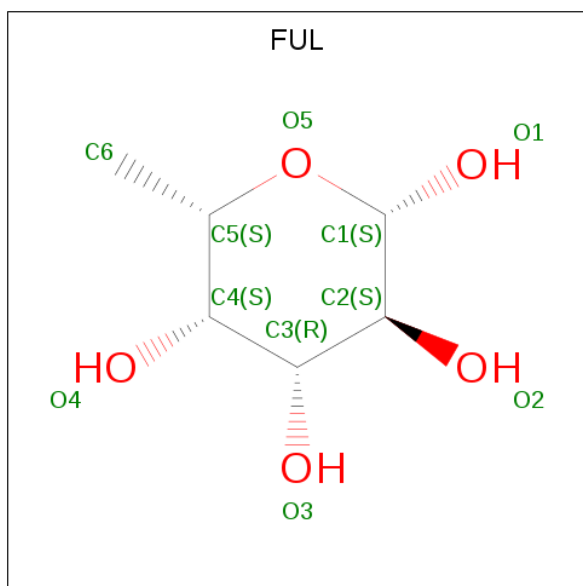
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	254	Total	C	N	O	S	0	0	0
			1974	1253	351	357	13			

- Molecule 4 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



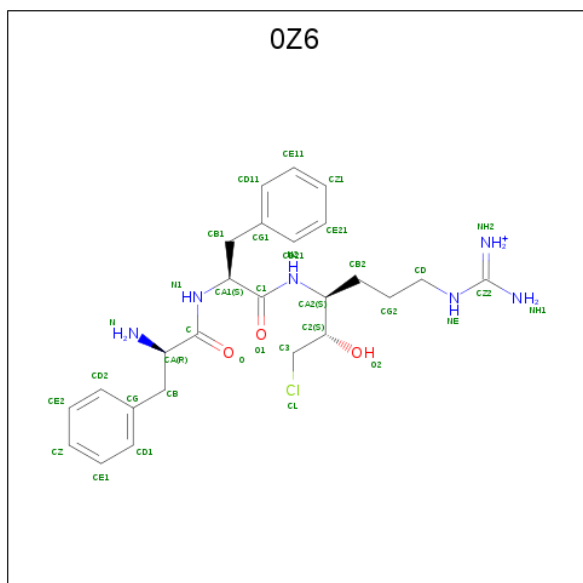
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is beta-L-fucopyranose (three-letter code: FUL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is D-phenylalanyl-N-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydroxyhexan-3-yl]-L-phenylalaninamide (three-letter code: OZ6) (formula: C<sub>25</sub>H<sub>36</sub>ClN<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	N	O	0	0
			34	25	6	3		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	1	Total	Ca	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	T	21	Total	O	0	0
			21	21		
9	L	31	Total	O	0	0
			31	31		
9	H	75	Total	O	0	0
			75	75		

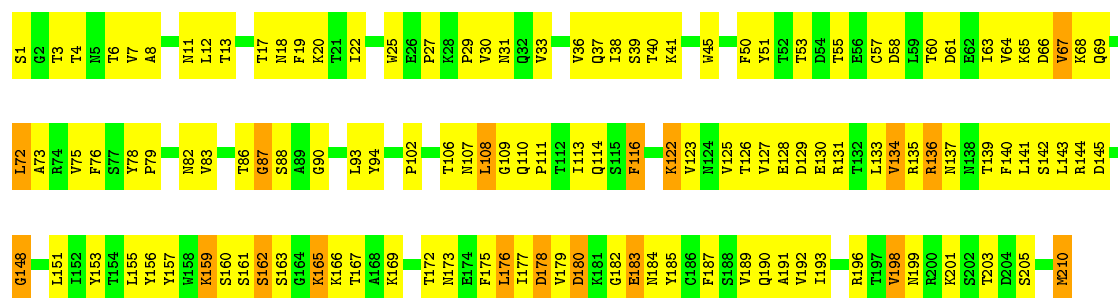
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

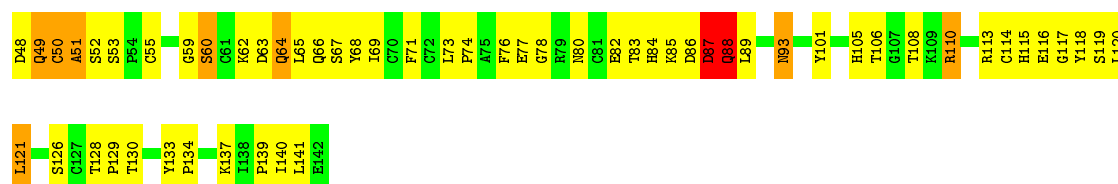
- Molecule 1: Tissue factor

Chain T: 



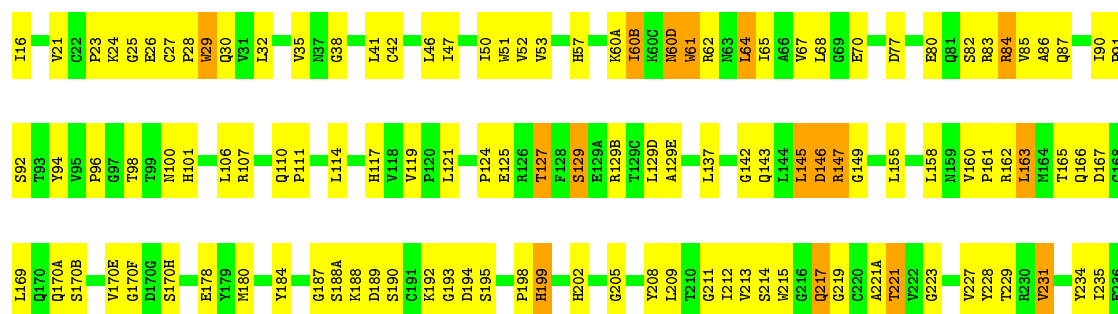
- Molecule 2: factor VIIa light chain

Chain L: 



- Molecule 3: factor VIIa heavy chain

Chain H: 



W237		M242		P246		G249		R253		A254
L238		R243		R247		V250		P255		P257
				P248		L251		F256		
						L252				

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.04Å 68.30Å 78.44Å 90.00° 92.12° 90.00°	Depositor
Resolution (Å)	53.94 – 2.90	Depositor
% Data completeness (in resolution range)	94.3 (53.94-2.90)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.221 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4559	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP



## 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: CA, GLC, NAG, FUL, 0Z6

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	T	0.36	0/1709	0.67	0/2325
2	L	0.36	0/728	0.65	0/982
3	H	0.41	0/2024	0.73	1/2755 (0.0%)
All	All	0.39	0/4461	0.70	1/6062 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	H	199	HIS	N-CA-C	-6.62	93.14	111.00

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	T	1673	0	1623	156	0
2	L	715	0	642	76	0
3	H	1974	0	1948	128	0
4	L	11	0	10	2	0
5	L	10	0	10	1	0
6	H	34	0	32	3	0
7	H	14	0	13	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1	0	0	0	0
9	H	75	0	0	8	0
9	L	31	0	0	1	0
9	T	21	0	0	3	0
All	All	4559	0	4278	341	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 39.

All (341) 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:T:159:LYS:HG2	1:T:162:SER:HA	1.46	0.96
1:T:198:VAL:HG13	1:T:199:ASN:H	1.28	0.95
1:T:111:PRO:HG2	1:T:205:SER:HB2	1.48	0.95
1:T:136:ARG:HB3	1:T:136:ARG:HH11	1.34	0.92
2:L:140:ILE:HD11	3:H:26:GLU:HG3	1.53	0.89
2:L:50:CYS:SG	2:L:63:ASP:HB3	2.12	0.89
3:H:247:ARG:HG3	3:H:248:PRO:HD2	1.54	0.89
1:T:135:ARG:HH12	2:L:74:PRO:HG3	1.38	0.89
3:H:247:ARG:CG	3:H:248:PRO:HD2	2.03	0.88
3:H:84:ARG:H	3:H:84:ARG:HE	1.21	0.88
1:T:1:SER:N	1:T:8:ALA:HB3	1.92	0.84
3:H:219:GLY:H	3:H:221:THR:HG21	1.44	0.81
3:H:124:PRO:O	3:H:235:ILE:HD13	1.81	0.81
1:T:22:ILE:HD13	1:T:58:ASP:HA	1.66	0.78
1:T:29:PRO:HG3	1:T:53:THR:O	1.84	0.78
1:T:135:ARG:HH22	2:L:74:PRO:HD3	1.49	0.77
1:T:177:ILE:HD11	1:T:187:PHE:HE1	1.48	0.77
3:H:247:ARG:CD	3:H:248:PRO:HD2	2.15	0.76
1:T:169:LYS:HA	1:T:175:PHE:HE1	1.51	0.74
3:H:121:LEU:HD23	3:H:209:LEU:HB2	1.69	0.74
1:T:1:SER:H1	1:T:8:ALA:HB3	1.50	0.74
1:T:136:ARG:HH11	1:T:141:LEU:HD21	1.53	0.73
2:L:63:ASP:HA	2:L:68:TYR:HA	1.69	0.72
2:L:88:GLN:HE21	2:L:88:GLN:HA	1.55	0.72
1:T:108:LEU:H	1:T:108:LEU:HD22	1.53	0.72
3:H:165:THR:O	3:H:169:LEU:HG	1.90	0.72
1:T:184:ASN:HA	1:T:210:MET:HE2	1.73	0.71
1:T:135:ARG:NH1	2:L:74:PRO:HG3	2.04	0.71
1:T:136:ARG:NH1	1:T:136:ARG:HB3	2.05	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:86:ASP:O	2:L:88:GLN:N	2.24	0.69
1:T:122:LYS:HB3	1:T:122:LYS:NZ	2.08	0.69
2:L:49:GLN:HE21	4:L:352:GLC:H5	1.57	0.68
1:T:18:ASN:ND2	1:T:109:GLY:H	1.91	0.68
3:H:213:VAL:HG13	9:H:383:HOH:O	1.92	0.68
1:T:1:SER:HA	1:T:8:ALA:H	1.59	0.68
1:T:110:GLN:H	2:L:64:GLN:HE22	1.43	0.67
1:T:67:VAL:HB	1:T:102:PRO:HB2	1.76	0.66
3:H:147:ARG:HG2	3:H:147:ARG:O	1.96	0.66
2:L:49:GLN:NE2	4:L:352:GLC:H5	2.10	0.66
3:H:189:ASP:OD2	3:H:190:SER:N	2.29	0.65
1:T:3:THR:HG22	1:T:4:THR:N	2.11	0.65
3:H:32:LEU:HD22	3:H:70:GLU:HG2	1.79	0.65
3:H:166:GLN:HG3	9:H:430:HOH:O	1.97	0.65
1:T:61:ASP:OD1	2:L:85:LYS:HE2	1.97	0.65
3:H:64:LEU:HD12	3:H:85:VAL:HG21	1.79	0.64
1:T:131:ARG:HH22	5:L:360:FUL:C1	2.09	0.64
1:T:198:VAL:HG13	1:T:199:ASN:N	2.06	0.64
2:L:121:LEU:HD12	2:L:126:SER:HB3	1.79	0.64
1:T:76:PHE:CD1	1:T:94:TYR:HB3	2.34	0.63
3:H:256:PHE:HA	3:H:257:PRO:C	2.19	0.63
1:T:110:GLN:HE22	2:L:65:LEU:HD22	1.64	0.63
1:T:108:LEU:N	1:T:108:LEU:HD22	2.13	0.62
1:T:142:SER:HB2	1:T:145:ASP:OD1	1.98	0.62
3:H:68:LEU:N	3:H:68:LEU:HD12	2.15	0.62
3:H:124:PRO:O	3:H:235:ILE:CD1	2.48	0.62
2:L:137:LYS:O	2:L:139:PRO:HD3	2.00	0.62
1:T:20:LYS:HD3	1:T:133:LEU:HG	1.82	0.62
2:L:121:LEU:HD21	2:L:128:THR:HB	1.80	0.62
1:T:18:ASN:HD21	1:T:109:GLY:H	1.48	0.61
1:T:50:PHE:CE1	2:L:93:ASN:HA	2.34	0.61
3:H:65:ILE:HD12	9:H:385:HOH:O	2.00	0.61
2:L:140:ILE:HG13	2:L:141:LEU:N	2.15	0.61
3:H:64:LEU:HD12	3:H:85:VAL:CG2	2.31	0.61
2:L:48:ASP:O	2:L:49:GLN:HB2	1.99	0.61
7:H:375:NAG:H3	7:H:375:NAG:H82	1.82	0.61
2:L:121:LEU:HD12	2:L:126:SER:CB	2.31	0.60
1:T:111:PRO:HG3	1:T:190:GLN:HA	1.83	0.60
3:H:163:LEU:N	3:H:163:LEU:HD12	2.17	0.60
3:H:219:GLY:N	3:H:221:THR:HG21	2.16	0.60
3:H:87:GLN:HE22	3:H:247:ARG:HB3	1.66	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:41:LEU:HD22	3:H:60(B):ILE:HD11	1.84	0.60
2:L:48:ASP:CG	2:L:49:GLN:H	2.05	0.60
1:T:3:THR:OG1	1:T:7:VAL:HA	2.01	0.60
1:T:114:GLN:HB2	1:T:128:GLU:N	2.17	0.60
1:T:122:LYS:NZ	1:T:178:ASP:HB3	2.17	0.60
1:T:156:TYR:CD1	1:T:167:THR:HG22	2.36	0.60
3:H:47:ILE:HD13	3:H:53:VAL:CG2	2.31	0.59
1:T:135:ARG:HH22	2:L:74:PRO:CD	2.14	0.59
1:T:159:LYS:HZ2	1:T:166:LYS:HE3	1.67	0.59
1:T:25:TRP:O	1:T:55:THR:HB	2.02	0.59
1:T:29:PRO:HG3	1:T:53:THR:C	2.21	0.59
2:L:126:SER:HB3	9:L:382:HOH:O	2.02	0.59
3:H:180:MET:HB2	3:H:227:VAL:CG1	2.32	0.59
2:L:89:LEU:HG	2:L:110:ARG:HG2	1.84	0.59
3:H:215:TRP:CZ2	3:H:227:VAL:HG21	2.37	0.59
3:H:219:GLY:H	3:H:221:THR:CG2	2.13	0.58
1:T:125:VAL:HB	1:T:175:PHE:HB2	1.83	0.58
3:H:187:GLY:HA2	3:H:221(A):ALA:O	2.03	0.58
3:H:247:ARG:HD2	3:H:248:PRO:HD2	1.86	0.58
3:H:110:GLN:HE21	3:H:111:PRO:HD2	1.69	0.57
1:T:40:THR:HG21	1:T:69:GLN:NE2	2.19	0.57
3:H:90:ILE:HD12	3:H:94:TYR:HD2	1.69	0.57
3:H:247:ARG:HG3	3:H:248:PRO:CD	2.31	0.57
1:T:63:ILE:HD12	1:T:64:VAL:N	2.19	0.57
2:L:140:ILE:HG13	2:L:141:LEU:H	1.68	0.57
3:H:107:ARG:HH12	3:H:246:PRO:HA	1.69	0.57
3:H:91:PRO:HG2	3:H:94:TYR:HB2	1.86	0.56
1:T:179:VAL:HG12	1:T:180:ASP:N	2.21	0.56
1:T:60:THR:O	1:T:64:VAL:HG22	2.05	0.56
3:H:41:LEU:O	3:H:42:CYS:SG	2.64	0.56
2:L:73:LEU:HB2	2:L:76:PHE:HD2	1.69	0.56
3:H:247:ARG:HG2	3:H:252:LEU:HD13	1.87	0.56
2:L:106:THR:O	2:L:108:THR:HG22	2.06	0.56
1:T:94:TYR:OH	3:H:166:GLN:HB2	2.06	0.56
3:H:27:CYS:N	3:H:28:PRO:CD	2.69	0.56
1:T:1:SER:H2	1:T:8:ALA:HB3	1.69	0.56
3:H:82:SER:O	3:H:83:ARG:HG2	2.06	0.55
3:H:92:SER:HB3	3:H:255:PRO:HA	1.88	0.55
1:T:192:VAL:C	1:T:193:ILE:HD12	2.26	0.55
1:T:122:LYS:HB3	1:T:122:LYS:HZ2	1.70	0.55
1:T:136:ARG:HB3	1:T:141:LEU:HD21	1.87	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:198:VAL:CG1	1:T:199:ASN:H	2.11	0.55
3:H:21:VAL:O	3:H:23:PRO:HD3	2.07	0.54
3:H:170(E):VAL:HB	3:H:170(H):SER:HB3	1.89	0.54
3:H:46:LEU:HD13	3:H:68:LEU:HD21	1.89	0.54
1:T:108:LEU:HD21	1:T:193:ILE:HD13	1.90	0.54
3:H:199:HIS:HB3	3:H:211:GLY:CA	2.38	0.54
2:L:105:HIS:HB3	2:L:108:THR:HG23	1.89	0.54
1:T:41:LYS:HE3	9:T:229:HOH:O	2.09	0.54
1:T:102:PRO:O	1:T:106:THR:HG22	2.07	0.53
1:T:110:GLN:OE1	2:L:65:LEU:HD13	2.08	0.53
1:T:3:THR:CG2	1:T:4:THR:N	2.71	0.53
3:H:127:THR:HG22	3:H:129(B):ARG:CZ	2.39	0.53
1:T:3:THR:HG1	1:T:7:VAL:HA	1.72	0.53
3:H:98:THR:O	6:H:10Z6:HE11	2.09	0.53
2:L:105:HIS:CB	2:L:108:THR:HG23	2.39	0.53
1:T:123:VAL:HG23	1:T:179:VAL:HG21	1.91	0.52
3:H:142:GLY:HA2	3:H:193:GLY:HA3	1.91	0.52
3:H:146:ASP:C	3:H:149:GLY:H	2.13	0.52
1:T:193:ILE:HD12	1:T:193:ILE:N	2.24	0.52
2:L:65:LEU:O	2:L:66:GLN:HB2	2.09	0.52
3:H:52:VAL:HB	3:H:106:LEU:HB2	1.92	0.52
1:T:8:ALA:HB2	1:T:93:LEU:HD11	1.91	0.52
1:T:11:ASN:O	1:T:13:THR:HG23	2.10	0.51
2:L:62:LYS:HB3	2:L:71:PHE:HE1	1.76	0.51
3:H:60(A):LYS:O	3:H:60(B):ILE:C	2.49	0.51
1:T:139:THR:HG22	1:T:140:PHE:N	2.26	0.51
1:T:140:PHE:O	1:T:141:LEU:HD23	2.10	0.51
3:H:60(D):ASN:C	3:H:62:ARG:H	2.13	0.51
1:T:63:ILE:HD12	1:T:64:VAL:HG13	1.92	0.51
3:H:247:ARG:HG2	3:H:252:LEU:CD1	2.40	0.51
1:T:130:GLU:HB2	1:T:143:LEU:CD1	2.41	0.50
1:T:136:ARG:HB2	1:T:141:LEU:HD11	1.93	0.50
3:H:124:PRO:HD3	3:H:208:TYR:HB3	1.93	0.50
1:T:190:GLN:O	1:T:190:GLN:HG3	2.12	0.50
1:T:193:ILE:CG2	1:T:196:ARG:HG3	2.41	0.50
3:H:178:GLU:N	3:H:178:GLU:OE1	2.37	0.50
1:T:6:THR:HG21	1:T:79:PRO:HD3	1.94	0.50
1:T:189:VAL:O	1:T:205:SER:N	2.34	0.50
3:H:84:ARG:H	3:H:84:ARG:NE	2.00	0.49
3:H:137:LEU:HA	3:H:158:LEU:O	2.12	0.49
1:T:135:ARG:HH12	2:L:74:PRO:CG	2.19	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:88:SER:C	1:T:90:GLY:H	2.14	0.49
3:H:83:ARG:HD2	3:H:110:GLN:O	2.13	0.49
3:H:143:GLN:NE2	3:H:146:ASP:O	2.46	0.49
3:H:28:PRO:HG2	3:H:29:TRP:CE3	2.48	0.49
1:T:156:TYR:HA	1:T:166:LYS:O	2.13	0.49
3:H:41:LEU:CD2	3:H:60(B):ILE:HD11	2.43	0.49
1:T:198:VAL:HG22	1:T:199:ASN:ND2	2.27	0.49
3:H:127:THR:CG2	3:H:129(B):ARG:CZ	2.91	0.49
2:L:120:LEU:HD12	2:L:126:SER:O	2.13	0.49
3:H:170(E):VAL:HG12	3:H:170(F):GLY:H	1.78	0.49
2:L:113:ARG:NH1	2:L:113:ARG:HB2	2.28	0.49
2:L:80:ASN:C	2:L:82:GLU:N	2.66	0.49
1:T:165:LYS:O	1:T:165:LYS:HD3	2.13	0.49
3:H:92:SER:CB	3:H:255:PRO:HA	2.42	0.48
1:T:108:LEU:H	1:T:108:LEU:CD2	2.24	0.48
1:T:114:GLN:HB2	1:T:128:GLU:CA	2.42	0.48
2:L:115:HIS:O	2:L:117:GLY:N	2.46	0.48
1:T:110:GLN:NE2	2:L:65:LEU:HD22	2.26	0.48
1:T:106:THR:HG23	1:T:106:THR:O	2.13	0.48
1:T:144:ARG:O	1:T:148:GLY:HA2	2.14	0.48
3:H:202:HIS:CE1	3:H:205:GLY:H	2.32	0.48
3:H:217:GLN:O	6:H:1:OZ6:N	2.47	0.48
2:L:110:ARG:HD2	2:L:110:ARG:C	2.34	0.48
1:T:133:LEU:O	1:T:135:ARG:N	2.46	0.48
1:T:159:LYS:CG	1:T:162:SER:HA	2.31	0.48
1:T:192:VAL:HG22	1:T:201:LYS:HG2	1.96	0.48
1:T:123:VAL:HG23	1:T:179:VAL:CG2	2.44	0.47
3:H:158:LEU:HD11	3:H:188:LYS:HB2	1.96	0.47
3:H:61:TRP:CZ2	3:H:251:LEU:HD22	2.48	0.47
2:L:101:TYR:OH	2:L:115:HIS:HD2	1.97	0.47
1:T:64:VAL:CG1	1:T:134:VAL:HA	2.44	0.47
1:T:136:ARG:NH1	1:T:136:ARG:O	2.47	0.47
1:T:51:TYR:CE1	1:T:83:VAL:HB	2.49	0.47
2:L:60:SER:HB2	2:L:71:PHE:HB2	1.96	0.47
1:T:66:ASP:C	1:T:68:LYS:H	2.18	0.47
1:T:139:THR:HG22	1:T:140:PHE:H	1.79	0.47
1:T:36:VAL:HG21	1:T:57:CYS:CB	2.45	0.47
1:T:37:GLN:HG2	1:T:45:TRP:HB3	1.97	0.47
1:T:144:ARG:NH1	1:T:151:LEU:O	2.44	0.47
1:T:160:SER:C	1:T:162:SER:H	2.17	0.47
3:H:167:ASP:O	3:H:170(A):GLN:HG3	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:182:GLY:O	1:T:183:GLU:C	2.52	0.47
3:H:194:ASP:O	3:H:195:SER:C	2.51	0.47
3:H:221:THR:HG23	9:H:409:HOH:O	2.14	0.47
2:L:82:GLU:HG2	2:L:83:THR:N	2.30	0.47
1:T:153:TYR:CD1	1:T:191:ALA:HA	2.49	0.47
1:T:86:THR:HG23	1:T:90:GLY:HA2	1.97	0.47
1:T:116:PHE:CB	1:T:125:VAL:HA	2.45	0.46
1:T:189:VAL:HG12	1:T:190:GLN:N	2.30	0.46
3:H:61:TRP:HB3	3:H:250:VAL:HG11	1.98	0.46
2:L:133:TYR:HB2	3:H:114:LEU:HD12	1.97	0.46
1:T:116:PHE:HB2	1:T:125:VAL:HA	1.98	0.46
1:T:72:LEU:HD13	1:T:73:ALA:N	2.30	0.46
3:H:129:SER:HA	3:H:129(D):LEU:HD12	1.97	0.46
2:L:64:GLN:O	2:L:67:SER:O	2.34	0.46
1:T:113:ILE:HG23	1:T:126:THR:O	2.15	0.46
1:T:30:VAL:O	1:T:31:ASN:HB2	2.15	0.46
1:T:179:VAL:HG12	1:T:180:ASP:H	1.79	0.46
2:L:49:GLN:C	2:L:51:ALA:H	2.17	0.46
1:T:22:ILE:HD13	1:T:58:ASP:CA	2.41	0.46
3:H:86:ALA:N	3:H:107:ARG:O	2.49	0.46
3:H:35:VAL:HG12	3:H:64:LEU:HD22	1.97	0.46
1:T:116:PHE:H	1:T:116:PHE:HD1	1.61	0.46
3:H:30:GLN:HG2	3:H:155:LEU:CD1	2.46	0.46
1:T:20:LYS:CD	1:T:133:LEU:HG	2.45	0.46
2:L:139:PRO:HG2	3:H:119:VAL:HG21	1.98	0.45
3:H:170(E):VAL:HG12	3:H:170(F):GLY:N	2.31	0.45
2:L:119:SER:HB2	2:L:130:THR:CG2	2.47	0.45
2:L:78:GLY:HA3	2:L:82:GLU:OE1	2.16	0.45
3:H:237:TRP:CD1	3:H:256:PHE:HD1	2.34	0.45
2:L:114:CYS:HB3	2:L:118:TYR:HB2	1.98	0.45
2:L:119:SER:HB2	2:L:130:THR:HG21	1.98	0.45
2:L:51:ALA:C	2:L:53:SER:H	2.20	0.45
1:T:19:PHE:HE1	1:T:67:VAL:HB	1.80	0.45
1:T:72:LEU:HD13	1:T:73:ALA:H	1.80	0.45
1:T:38:ILE:HG12	1:T:39:SER:N	2.32	0.45
3:H:50:ILE:CG2	3:H:111:PRO:HB3	2.46	0.45
3:H:212:ILE:HG13	3:H:231:VAL:CG2	2.46	0.45
3:H:101:HIS:HA	3:H:234:TYR:OH	2.17	0.45
1:T:63:ILE:CD1	1:T:64:VAL:HG13	2.47	0.45
1:T:136:ARG:NH1	1:T:141:LEU:HD21	2.27	0.45
3:H:161:PRO:HD3	3:H:184:TYR:CE1	2.52	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:94:TYR:CZ	3:H:96:PRO:HA	2.52	0.44
1:T:1:SER:N	1:T:8:ALA:CB	2.73	0.44
2:L:49:GLN:HB3	2:L:63:ASP:HB2	1.99	0.44
3:H:117:HIS:HD2	9:H:392:HOH:O	2.00	0.44
1:T:3:THR:CG2	1:T:4:THR:H	2.30	0.44
3:H:234:TYR:O	3:H:238:LEU:HG	2.17	0.44
3:H:47:ILE:HD13	3:H:53:VAL:HG21	1.99	0.44
2:L:64:GLN:HB3	2:L:64:GLN:HE21	1.58	0.44
1:T:50:PHE:CZ	2:L:93:ASN:HA	2.53	0.44
1:T:1:SER:H2	1:T:8:ALA:CB	2.30	0.44
3:H:243:ARG:NH1	9:H:431:HOH:O	2.50	0.44
2:L:129:PRO:HB3	2:L:134:PRO:HG3	1.99	0.44
1:T:189:VAL:HG12	1:T:190:GLN:H	1.81	0.44
3:H:147:ARG:CG	3:H:147:ARG:O	2.65	0.44
3:H:92:SER:N	3:H:254:ALA:O	2.50	0.44
1:T:193:ILE:HG21	1:T:196:ARG:HG3	1.99	0.44
3:H:170(E):VAL:HG21	3:H:217:GLN:NE2	2.32	0.44
1:T:160:SER:O	1:T:161:SER:HB3	2.17	0.44
2:L:101:TYR:CE2	3:H:125:GLU:HG3	2.53	0.44
2:L:62:LYS:HB3	2:L:71:PHE:CE1	2.53	0.44
1:T:122:LYS:HD3	1:T:176:LEU:HD22	2.00	0.44
3:H:67:VAL:C	3:H:68:LEU:HD12	2.38	0.43
2:L:140:ILE:HD13	3:H:25:GLY:HA3	2.00	0.43
3:H:51:TRP:CZ2	3:H:242:MET:HA	2.53	0.43
3:H:80:GLU:OE1	3:H:80:GLU:N	2.36	0.43
2:L:59:GLY:O	2:L:60:SER:O	2.36	0.43
1:T:17:THR:HG22	1:T:18:ASN:HD22	1.84	0.43
2:L:105:HIS:HB3	2:L:108:THR:CG2	2.48	0.43
2:L:80:ASN:C	2:L:82:GLU:H	2.21	0.43
1:T:129:ASP:CG	1:T:142:SER:HB3	2.38	0.43
3:H:68:LEU:C	3:H:70:GLU:H	2.22	0.43
2:L:76:PHE:HE1	2:L:84:HIS:ND1	2.16	0.43
3:H:237:TRP:CZ2	3:H:254:ALA:HB3	2.54	0.43
3:H:61:TRP:CH2	3:H:251:LEU:HD22	2.54	0.43
3:H:35:VAL:O	3:H:35:VAL:HG23	2.19	0.43
2:L:84:HIS:C	2:L:86:ASP:N	2.72	0.43
2:L:87:ASP:O	2:L:88:GLN:HG2	2.18	0.43
3:H:208:TYR:N	3:H:208:TYR:CD1	2.87	0.43
3:H:214:SER:OG	3:H:229:THR:OG1	2.36	0.43
3:H:23:PRO:O	3:H:24:LYS:C	2.57	0.43
1:T:127:VAL:HG21	1:T:189:VAL:HG11	1.99	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:33:VAL:HG23	1:T:78:TYR:HD2	1.84	0.43
1:T:130:GLU:HB2	1:T:143:LEU:HG	1.99	0.43
1:T:159:LYS:O	1:T:162:SER:N	2.52	0.43
1:T:60:THR:O	1:T:63:ILE:HG13	2.19	0.43
3:H:24:LYS:NZ	3:H:77:ASP:OD2	2.49	0.43
3:H:83:ARG:HD3	3:H:84:ARG:HH21	1.82	0.43
1:T:125:VAL:HG21	1:T:155:LEU:HD21	2.01	0.43
1:T:177:ILE:HD11	1:T:187:PHE:CE1	2.40	0.43
3:H:192:LYS:O	6:H:1:OZ6:O2	2.37	0.42
3:H:184:TYR:CD1	3:H:184:TYR:N	2.87	0.42
1:T:86:THR:O	1:T:87:GLY:O	2.36	0.42
1:T:66:ASP:OD1	1:T:68:LYS:HB2	2.19	0.42
1:T:75:VAL:O	1:T:94:TYR:HA	2.19	0.42
3:H:16:ILE:HD13	3:H:194:ASP:OD2	2.19	0.42
3:H:82:SER:O	3:H:83:ARG:NH1	2.37	0.42
1:T:82:ASN:OD1	1:T:82:ASN:O	2.37	0.42
2:L:121:LEU:HD12	2:L:126:SER:HB2	2.02	0.42
1:T:18:ASN:HD21	1:T:109:GLY:N	2.14	0.42
3:H:180:MET:HB2	3:H:227:VAL:HG13	2.01	0.42
3:H:46:LEU:HD22	3:H:68:LEU:CD2	2.50	0.42
1:T:140:PHE:CD2	1:T:140:PHE:N	2.87	0.42
3:H:107:ARG:HH12	3:H:246:PRO:CA	2.31	0.42
3:H:158:LEU:HG	3:H:160:VAL:HG13	2.02	0.42
2:L:113:ARG:HH11	2:L:113:ARG:CB	2.33	0.42
1:T:111:PRO:HD2	1:T:203:THR:O	2.20	0.42
1:T:18:ASN:ND2	1:T:109:GLY:N	2.64	0.42
1:T:30:VAL:HA	9:T:220:HOH:O	2.19	0.42
3:H:57:HIS:CE1	3:H:195:SER:OG	2.73	0.41
2:L:101:TYR:OH	3:H:124:PRO:HA	2.20	0.41
2:L:121:LEU:HB2	2:L:126:SER:HB2	2.02	0.41
2:L:87:ASP:O	2:L:88:GLN:CG	2.68	0.41
3:H:143:GLN:HB3	3:H:145:LEU:O	2.20	0.41
3:H:170(B):SER:HA	3:H:223:GLY:O	2.20	0.41
2:L:55:CYS:SG	2:L:60:SER:O	2.78	0.41
1:T:40:THR:O	1:T:41:LYS:C	2.57	0.41
2:L:77:GLU:O	2:L:83:THR:HB	2.20	0.41
3:H:92:SER:OG	3:H:255:PRO:HA	2.20	0.41
1:T:6:THR:CG2	1:T:79:PRO:HD3	2.51	0.41
3:H:192:LYS:NZ	9:H:398:HOH:O	2.53	0.41
1:T:155:LEU:O	1:T:167:THR:HA	2.21	0.41
3:H:198:PRO:HG2	9:H:400:HOH:O	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:47:ILE:HD13	3:H:53:VAL:HG23	2.01	0.41
2:L:66:GLN:O	2:L:67:SER:HB2	2.21	0.41
2:L:84:HIS:O	2:L:86:ASP:N	2.54	0.41
1:T:157:TYR:CZ	1:T:166:LYS:HB3	2.55	0.41
1:T:155:LEU:HD11	1:T:187:PHE:HB3	2.01	0.41
1:T:31:ASN:N	9:T:220:HOH:O	2.52	0.41
1:T:135:ARG:NE	1:T:140:PHE:CE2	2.89	0.41
1:T:179:VAL:HG13	1:T:185:TYR:CE1	2.56	0.41
3:H:180:MET:HA	3:H:228:TYR:O	2.20	0.41
2:L:69:ILE:O	2:L:69:ILE:HG22	2.20	0.41
1:T:114:GLN:HB2	1:T:128:GLU:HA	2.03	0.41
1:T:61:ASP:O	1:T:65:LYS:HG3	2.21	0.41
3:H:146:ASP:C	3:H:149:GLY:N	2.74	0.40
1:T:192:VAL:HG22	1:T:201:LYS:HA	2.03	0.40
3:H:35:VAL:C	3:H:38:GLY:H	2.24	0.40
3:H:90:ILE:HB	3:H:91:PRO:HD2	2.03	0.40
1:T:140:PHE:CE1	2:L:71:PHE:HD2	2.39	0.40
3:H:254:ALA:HA	3:H:255:PRO:HD3	1.81	0.40
2:L:87:ASP:C	2:L:88:GLN:HG2	2.41	0.40
1:T:155:LEU:HD22	1:T:175:PHE:CB	2.50	0.40
3:H:129(E):ALA:HA	3:H:162:ARG:NH1	2.35	0.40
1:T:12:LEU:HD21	1:T:75:VAL:HG23	2.04	0.40
1:T:122:LYS:HB3	1:T:178:ASP:HA	2.03	0.40
1:T:157:TYR:CE1	1:T:177:ILE:HG21	2.56	0.40
1:T:122:LYS:HZ2	1:T:178:ASP:HB3	1.86	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	T	208/210 (99%)	163 (78%)	34 (16%)	11 (5%)	<b>2</b> <b>6</b>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	93/95 (98%)	64 (69%)	19 (20%)	10 (11%)	0	1
3	H	252/254 (99%)	204 (81%)	39 (16%)	9 (4%)	3	14
All	All	553/559 (99%)	431 (78%)	92 (17%)	30 (5%)	2	6

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T	162	SER
1	T	172	THR
1	T	173	ASN
1	T	180	ASP
2	L	60	SER
2	L	87	ASP
2	L	116	GLU
3	H	60(B)	ILE
3	H	146	ASP
3	H	188(A)	SER
1	T	87	GLY
1	T	148	GLY
1	T	163	SER
1	T	198	VAL
2	L	49	GLN
2	L	93	ASN
2	L	121	LEU
3	H	248	PRO
1	T	183	GLU
3	H	61	TRP
1	T	134	VAL
2	L	88	GLN
3	H	217	GLN
3	H	249	GLY
2	L	52	SER
3	H	231	VAL
2	L	50	CYS
2	L	51	ALA
3	H	246	PRO
1	T	67	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	193/193 (100%)	180 (93%)	13 (7%)	16	43
2	L	83/83 (100%)	79 (95%)	4 (5%)	25	58
3	H	216/216 (100%)	205 (95%)	11 (5%)	24	56
All	All	492/492 (100%)	464 (94%)	28 (6%)	20	51

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	27	PRO
1	T	72	LEU
1	T	107	ASN
1	T	108	LEU
1	T	116	PHE
1	T	122	LYS
1	T	136	ARG
1	T	137	ASN
1	T	159	LYS
1	T	165	LYS
1	T	176	LEU
1	T	178	ASP
1	T	210	MET
2	L	64	GLN
2	L	87	ASP
2	L	88	GLN
2	L	110	ARG
3	H	29	TRP
3	H	60(D)	ASN
3	H	64	LEU
3	H	84	ARG
3	H	100	ASN
3	H	127	THR
3	H	129	SER
3	H	145	LEU
3	H	147	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	H	163	LEU
3	H	221	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	18	ASN
1	T	31	ASN
1	T	107	ASN
1	T	114	GLN
1	T	137	ASN
1	T	173	ASN
2	L	49	GLN
2	L	56	GLN
2	L	64	GLN
2	L	80	ASN
2	L	88	GLN
2	L	115	HIS
3	H	40	GLN
3	H	60(D)	ASN
3	H	87	GLN
3	H	100	ASN
3	H	110	GLN
3	H	117	HIS
3	H	166	GLN
3	H	202	HIS
3	H	217	GLN
3	H	224	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	FUL	L	360	2	10,10,11	0.59	0	14,14,16	0.51	0
6	0Z6	H	1	3	34,35,36	1.33	1 (2%)	41,45,46	0.51	0
4	GLC	L	352	2	11,11,12	0.41	0	15,15,17	0.66	0
7	NAG	H	375	3	14,14,15	0.65	0	17,19,21	0.61	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	FUL	L	360	2	-	-	0/1/1/1
6	0Z6	H	1	3	-	4/35/35/37	0/2/2/2
4	GLC	L	352	2	-	2/2/19/22	0/1/1/1
7	NAG	H	375	3	-	6/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	1	0Z6	O2-C2	-7.33	1.23	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	1	0Z6	O2-C2-CA2-CB2
7	H	375	NAG	C8-C7-N2-C2
7	H	375	NAG	O7-C7-N2-C2

*Continued on next page...*

*Continued from previous page...*

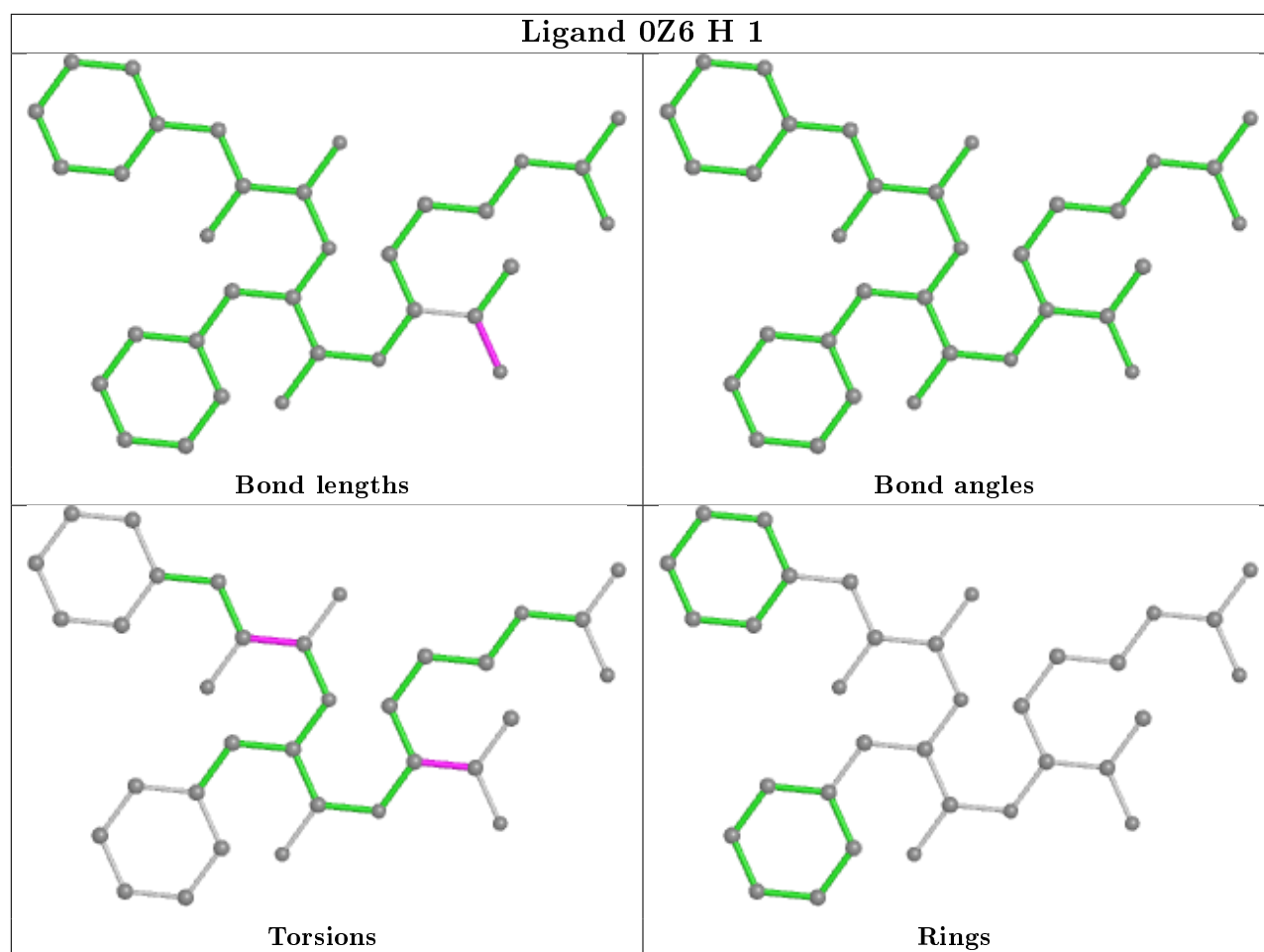
Mol	Chain	Res	Type	Atoms
7	H	375	NAG	C4-C5-C6-O6
4	L	352	GLC	O5-C5-C6-O6
7	H	375	NAG	O5-C5-C6-O6
4	L	352	GLC	C4-C5-C6-O6
6	H	1	0Z6	N1-C-CA-CB
7	H	375	NAG	C1-C2-N2-C7
6	H	1	0Z6	O-C-CA-CB
6	H	1	0Z6	O-C-CA-N
7	H	375	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	360	FUL	1	0
6	H	1	0Z6	3	0
4	L	352	GLC	2	0
7	H	375	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.