



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:52 PM GMT

PDB ID : 1VIT  
Title : THROMBIN:HIRUDIN 51-65 COMPLEX  
Authors : Vitali, J.; Edwards, B.F.P.  
Deposited on : 1996-01-31  
Resolution : 3.20 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

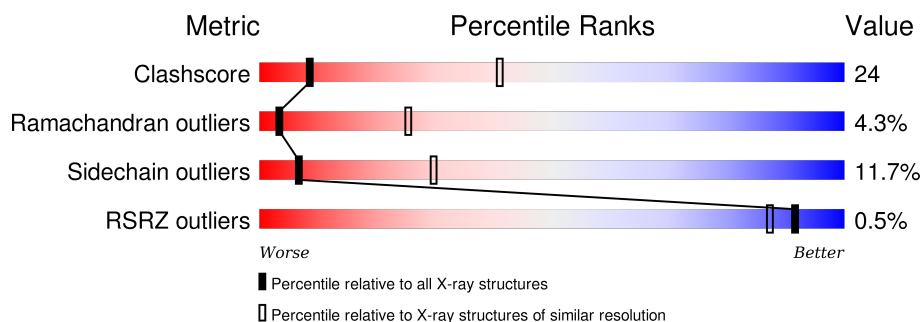
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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. 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	L	49	<div> <div>2%</div> <div>47%</div> <div>22%</div> <div>•</div> <div>27%</div> </div>
1	M	49	<div> <div>35%</div> <div>35%</div> <div>•</div> <div>27%</div> </div>
2	H	259	<div> <div>51%</div> <div>41%</div> <div>8%</div> </div>
3	I	15	<div> <div>33%</div> <div>53%</div> <div>13%</div> </div>
3	J	15	<div> <div>53%</div> <div>33%</div> <div>13%</div> </div>
4	F	150	<div> <div>40%</div> <div>49%</div> <div>11%</div> </div>
5	G	109	<div> <div>%</div> <div>49%</div> <div>41%</div> <div>8%</div> <div>•</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5071 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 EPSILON THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	36	Total	C	N	O	S	0	0	0
			290	181	48	60	1			
1	M	36	Total	C	N	O	S	0	0	0
			290	181	48	60	1			

- Molecule 2 is a protein called ALPHA THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	259	Total	C	N	O	S	0	0	0
			2094	1337	376	369	12			

- Molecule 3 is a protein called HIRUDIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	15	Total	C	N	O	0	0	0
			130	80	19	31			
3	J	15	Total	C	N	O	0	0	0
			130	80	19	31			

- Molecule 4 is a protein called EPSILON THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	150	Total	C	N	O	S	0	0	0
			1235	793	222	215	5			

- Molecule 5 is a protein called EPSILON THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	109	Total	C	N	O	S	0	0	0
			860	544	154	155	7			

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

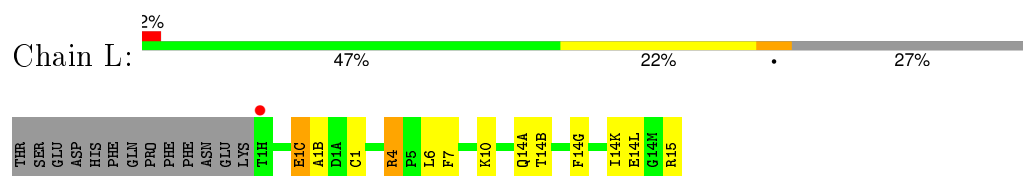


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	F	1	Total	C	N	O	0	0
			14	8	1	5		

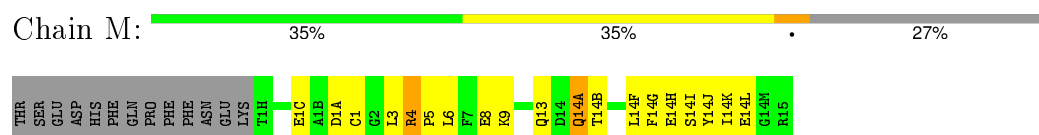
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

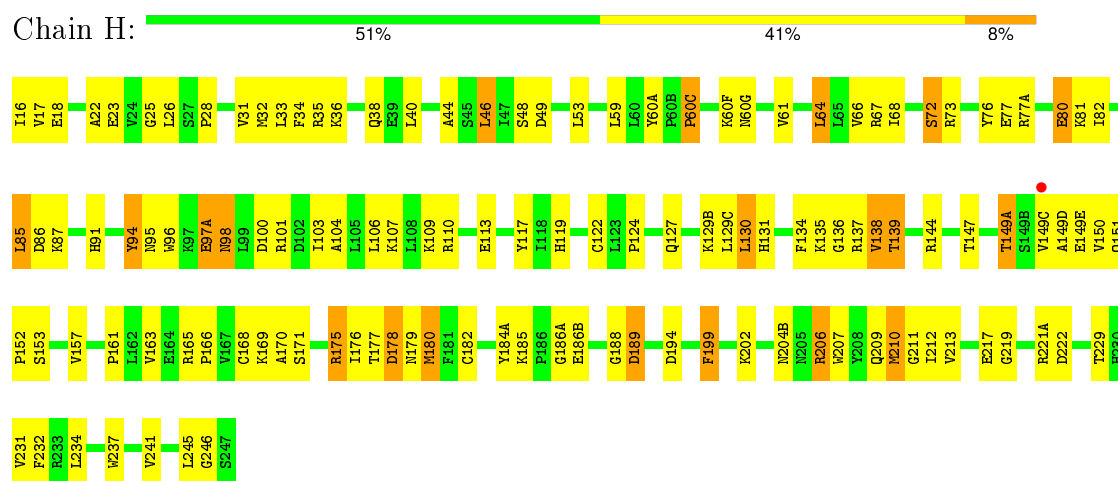
- Molecule 1: EPSILON THROMBIN



- Molecule 1: EPSILON THROMBIN



- Molecule 2: ALPHA THROMBIN

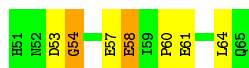


- Molecule 3: HIRUDIN



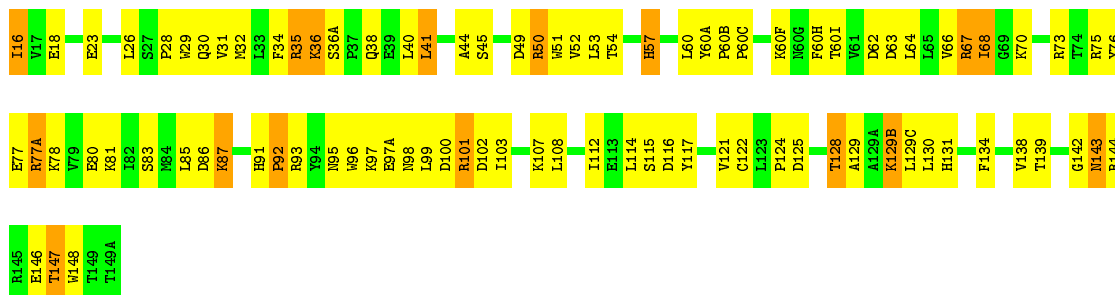
- Molecule 3: HIRUDIN

Chain J:  53% 33% 13%



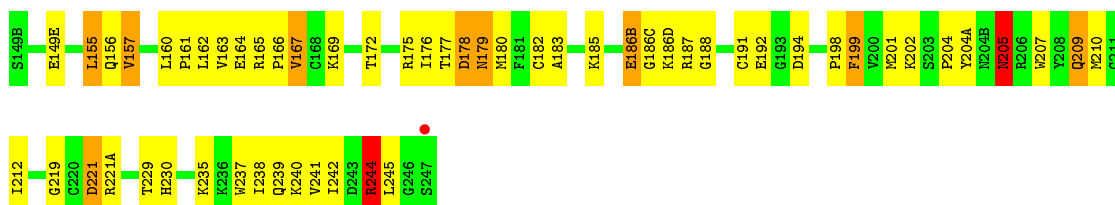
• Molecule 4: EPSILON THROMBIN

Chain F:  40% 49% 11%



• Molecule 5: EPSILON THROMBIN

Chain G:  49% 41% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.40 Å   116.40 Å   200.60 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	7.00 – 3.20 7.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	69.8 (7.00-3.20) 70.0 (7.00-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 3.19 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.192 , (Not available) 0.190 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	39.2	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.18 , 81.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 8659 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	5071	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	L	0.50	0/294	0.72	0/390
1	M	0.49	0/294	0.74	0/390
2	H	0.43	0/2148	0.79	5/2905 (0.2%)
3	I	0.69	0/133	1.30	2/178 (1.1%)
3	J	0.53	0/133	0.86	0/178
4	F	0.42	0/1267	0.82	1/1716 (0.1%)
5	G	0.45	0/881	0.76	2/1186 (0.2%)
All	All	0.45	0/5150	0.81	10/6943 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	54	GLY	N-CA-C	-8.00	93.10	113.10
5	G	205	ASN	N-CA-C	5.97	127.12	111.00
2	H	149(C)	VAL	N-CA-C	5.88	126.87	111.00
5	G	199	PHE	N-CA-C	-5.68	95.67	111.00
2	H	186(A)	GLY	N-CA-C	-5.65	98.98	113.10
4	F	64	LEU	N-CA-C	5.62	126.18	111.00
2	H	199	PHE	N-CA-C	-5.53	96.08	111.00
3	I	61	GLU	N-CA-C	5.40	125.58	111.00
2	H	64	LEU	N-CA-C	5.33	125.38	111.00
2	H	149(D)	ALA	N-CA-C	-5.12	97.17	111.00

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	290	0	276	13	0
1	M	290	0	276	14	0
2	H	2094	0	2096	97	0
3	I	130	0	102	4	0
3	J	130	0	102	6	0
4	F	1235	0	1250	88	0
5	G	860	0	844	57	0
6	H	28	0	25	1	0
7	F	14	0	13	0	0
All	All	5071	0	4984	239	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 24.

All (239) 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:F:36:LYS:HG2	3:J:64:LEU:HD13	1.49	0.92
1:L:6:LEU:HD12	2:H:25:GLY:HA3	1.52	0.91
4:F:91:HIS:HD2	4:F:92:PRO:HD2	1.32	0.90
4:F:31:VAL:HB	4:F:44:ALA:HB3	1.57	0.85
4:F:139:THR:HG22	5:G:157:VAL:HG12	1.58	0.85
4:F:53:LEU:HG	5:G:212:ILE:HD11	1.60	0.82
2:H:85:LEU:H	2:H:85:LEU:HD12	1.45	0.81
2:H:81:LYS:HE3	2:H:113:GLU:HB3	1.63	0.80
2:H:219:GLY:HA3	2:H:221(A):ARG:HD2	1.64	0.79
4:F:32:MET:HG3	4:F:40:LEU:HD13	1.65	0.78
2:H:204(B):ASN:HD21	2:H:206:ARG:HD2	1.50	0.77
4:F:68:ILE:HD12	4:F:81:LYS:O	1.85	0.77
2:H:18:GLU:HB2	2:H:188:GLY:HA2	1.67	0.76
2:H:139:THR:HG23	2:H:157:VAL:HG22	1.69	0.74
2:H:33:LEU:HD11	2:H:44:ALA:HB2	1.69	0.74
2:H:204(B):ASN:ND2	2:H:206:ARG:HD2	2.03	0.73
4:F:73:ARG:HH22	3:J:54:GLY:HA2	1.53	0.73
3:I:65:GLN:HA	3:I:65:GLN:HE21	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:168:CYS:O	2:H:171:SER:HB3	1.90	0.72
4:F:91:HIS:CD2	4:F:92:PRO:HD2	2.20	0.72
5:G:202:LYS:HE3	5:G:205:ASN:O	1.92	0.70
2:H:31:VAL:HB	2:H:44:ALA:HB3	1.74	0.69
4:F:124:PRO:HB2	4:F:129:ALA:HB2	1.74	0.69
4:F:77:GLU:HB2	4:F:80:GLU:HG2	1.75	0.69
1:L:1(C):GLU:HG3	1:L:1(B):ALA:H	1.58	0.68
5:G:163:VAL:HG11	5:G:167:VAL:HG22	1.76	0.67
2:H:130:LEU:HD12	2:H:210:MET:HG3	1.77	0.67
4:F:128:THR:HG22	4:F:129(C):LEU:HD22	1.77	0.66
2:H:188:GLY:O	2:H:189:ASP:HB2	1.95	0.65
2:H:219:GLY:HA3	2:H:221(A):ARG:CD	2.26	0.65
4:F:86:ASP:O	4:F:87:LYS:HB2	1.96	0.65
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.32	0.64
2:H:34:PHE:CZ	2:H:38:GLN:HB2	2.33	0.64
5:G:201:MET:SD	5:G:210:MET:HG3	2.38	0.63
2:H:16:ILE:HG13	2:H:194:ASP:OD2	1.99	0.62
1:M:5:PRO:HA	1:M:9:LYS:CG	2.29	0.62
4:F:98:ASN:OD1	4:F:100:ASP:HB2	2.00	0.61
2:H:85:LEU:N	2:H:85:LEU:HD12	2.14	0.61
2:H:139:THR:CG2	2:H:157:VAL:HG22	2.30	0.61
4:F:129(C):LEU:HB3	5:G:210:MET:HE2	1.82	0.61
4:F:30:GLN:HG2	5:G:155:LEU:HD11	1.83	0.61
1:M:5:PRO:HA	1:M:9:LYS:HG2	1.83	0.60
1:L:14(A):GLN:HG2	2:H:23:GLU:OE1	2.01	0.60
5:G:237:TRP:O	5:G:241:VAL:HG22	2.01	0.60
2:H:147:THR:OG1	2:H:149(A):THR:HG22	2.02	0.60
4:F:41:LEU:HD11	4:F:60(H):PHE:CE2	2.37	0.60
4:F:131:HIS:HB2	4:F:134:PHE:CD2	2.37	0.59
6:H:401:NAG:H4	6:H:402:NAG:N2	2.17	0.59
2:H:184(A):TYR:HB3	2:H:186(B):GLU:HG2	1.83	0.59
2:H:98:ASN:OD1	2:H:100:ASP:HB2	2.02	0.59
4:F:97:LYS:HG3	4:F:97(A):GLU:H	1.67	0.59
4:F:18:GLU:HB2	5:G:188:GLY:HA2	1.85	0.59
2:H:206:ARG:HB3	2:H:206:ARG:NH1	2.18	0.59
4:F:51:TRP:CZ3	4:F:107:LYS:HB2	2.37	0.59
4:F:31:VAL:HB	4:F:44:ALA:CB	2.32	0.59
5:G:163:VAL:HG12	5:G:164:GLU:N	2.18	0.59
4:F:147:THR:HG22	4:F:148:TRP:N	2.18	0.59
2:H:16:ILE:HD11	2:H:138:VAL:HG22	1.83	0.58
4:F:96:TRP:CZ3	4:F:97:LYS:HB3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:31:VAL:CB	4:F:44:ALA:HB3	2.31	0.58
4:F:143:ASN:CG	5:G:192:GLU:HB2	2.23	0.58
5:G:162:LEU:HD21	5:G:199:PHE:HE2	1.67	0.58
2:H:163:VAL:HG13	2:H:185:LYS:HE3	1.83	0.58
2:H:135:LYS:HA	2:H:161:PRO:HA	1.86	0.57
4:F:49:ASP:HA	4:F:112:ILE:HD11	1.86	0.57
2:H:217:GLU:O	2:H:221(A):ARG:HD3	2.05	0.57
4:F:35:ARG:O	4:F:38:GLN:HA	2.05	0.57
2:H:127:GLN:O	2:H:129(B):LYS:HG3	2.03	0.57
4:F:91:HIS:CE1	4:F:101:ARG:HG2	2.39	0.57
5:G:163:VAL:HG23	5:G:183:ALA:HA	1.85	0.57
2:H:59:LEU:HD21	2:H:64:LEU:HD11	1.87	0.57
2:H:17:VAL:O	2:H:188:GLY:HA2	2.04	0.56
4:F:129(B):LYS:HA	4:F:129(B):LYS:HE2	1.88	0.56
2:H:206:ARG:HB3	2:H:206:ARG:HH11	1.70	0.56
2:H:33:LEU:CD1	2:H:44:ALA:HB2	2.35	0.55
4:F:101:ARG:HG3	5:G:179:ASN:OD1	2.05	0.55
5:G:165:ARG:HG2	5:G:169:LYS:HE2	1.88	0.55
4:F:125:ASP:HB2	4:F:128:THR:OG1	2.06	0.55
2:H:53:LEU:HD11	2:H:103:ILE:HD11	1.88	0.55
4:F:103:ILE:HG22	5:G:212:ILE:HD12	1.87	0.55
2:H:165:ARG:NH2	2:H:180:MET:O	2.40	0.55
5:G:187:ARG:HG2	5:G:188:GLY:H	1.71	0.55
4:F:41:LEU:HD11	4:F:60(H):PHE:CZ	2.42	0.55
4:F:131:HIS:HB2	4:F:134:PHE:CE2	2.42	0.55
5:G:162:LEU:HD21	5:G:199:PHE:CE2	2.42	0.55
4:F:147:THR:HG22	4:F:148:TRP:H	1.72	0.55
2:H:59:LEU:HD11	2:H:106:LEU:HD21	1.88	0.54
4:F:143:ASN:HB3	5:G:191:CYS:SG	2.48	0.54
2:H:165:ARG:N	2:H:166:PRO:HD2	2.23	0.54
5:G:235:LYS:HE3	5:G:239:GLN:HE22	1.71	0.54
4:F:66:VAL:HG23	4:F:85:LEU:HD21	1.90	0.54
4:F:57:HIS:HA	4:F:60:LEU:O	2.07	0.54
2:H:94:TYR:CZ	2:H:96:TRP:HB3	2.43	0.53
1:M:4:ARG:HB3	4:F:28:PRO:HG2	1.90	0.53
5:G:235:LYS:HA	5:G:238:ILE:HD12	1.89	0.53
5:G:235:LYS:HA	5:G:238:ILE:CD1	2.38	0.53
2:H:85:LEU:H	2:H:85:LEU:CD1	2.18	0.53
4:F:67:ARG:HG2	4:F:70:LYS:NZ	2.24	0.52
1:L:1(C):GLU:HG3	1:L:1(B):ALA:N	2.22	0.52
2:H:170:ALA:HB2	5:G:185:LYS:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:99:LEU:O	4:F:102:ASP:HB2	2.10	0.52
5:G:235:LYS:HE3	5:G:239:GLN:NE2	2.24	0.52
4:F:139:THR:HG22	5:G:157:VAL:CG1	2.35	0.52
5:G:185:LYS:HB2	5:G:186(B):GLU:HG3	1.92	0.52
5:G:163:VAL:HG12	5:G:164:GLU:H	1.75	0.52
4:F:16:ILE:N	4:F:142:GLY:O	2.43	0.52
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.44	0.52
3:I:59:ILE:HD12	3:I:63:TYR:HD2	1.75	0.52
2:H:46:LEU:HD11	2:H:68:ILE:HD13	1.92	0.52
4:F:67:ARG:HG2	4:F:70:LYS:HZ3	1.75	0.52
3:J:57:GLU:HG2	3:J:58:GLU:N	2.26	0.51
4:F:31:VAL:HG13	4:F:66:VAL:HG13	1.93	0.51
4:F:85:LEU:N	4:F:85:LEU:HD22	2.26	0.51
2:H:87:LYS:HG2	2:H:107:LYS:HE2	1.93	0.51
4:F:143:ASN:OD1	5:G:192:GLU:HB2	2.12	0.50
2:H:28:PRO:HB2	2:H:119:HIS:HB3	1.93	0.50
2:H:46:LEU:CD2	2:H:48:SER:O	2.60	0.50
4:F:23:GLU:HB2	4:F:26:LEU:HB2	1.94	0.50
1:M:6:LEU:HD23	4:F:116:ASP:O	2.11	0.50
4:F:32:MET:HG3	4:F:40:LEU:CD1	2.38	0.50
2:H:209:GLN:NE2	2:H:212:ILE:HG22	2.26	0.50
2:H:131:HIS:HB2	2:H:134:PHE:CD2	2.47	0.50
4:F:95:ASN:HD21	4:F:97(A):GLU:HB3	1.76	0.50
2:H:144:ARG:HD3	2:H:152:PRO:HB3	1.92	0.50
2:H:60(A):TYR:CD1	2:H:60(C):PRO:HD2	2.47	0.49
4:F:138:VAL:HG22	5:G:199:PHE:HD1	1.77	0.49
5:G:187:ARG:HG2	5:G:221:ASP:OD2	2.13	0.49
1:M:14(A):GLN:O	1:M:14(A):GLN:HG2	2.12	0.49
2:H:22:ALA:HB2	2:H:157:VAL:HG23	1.95	0.49
1:M:5:PRO:HA	1:M:9:LYS:HG3	1.94	0.49
2:H:86:ASP:OD2	2:H:109:LYS:HA	2.13	0.49
4:F:129(B):LYS:HB3	5:G:204(A):TYR:CE2	2.48	0.49
3:J:57:GLU:HG2	3:J:58:GLU:H	1.78	0.49
1:L:14(B):THR:HG22	1:L:14(B):THR:O	2.13	0.49
2:H:31:VAL:HG13	2:H:66:VAL:HG13	1.95	0.48
3:I:65:GLN:HA	3:I:65:GLN:NE2	2.25	0.48
5:G:202:LYS:HB2	5:G:207:TRP:CZ2	2.48	0.48
4:F:144:ARG:HD3	5:G:149(E):GLU:O	2.14	0.48
2:H:73:ARG:HD2	2:H:151:GLN:HE21	1.78	0.48
4:F:68:ILE:HD13	4:F:112:ILE:HG21	1.94	0.48
4:F:91:HIS:ND1	4:F:101:ARG:HB3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:31:VAL:HG22	2:H:68:ILE:HG12	1.96	0.48
5:G:240:LYS:HG2	5:G:245:LEU:HD22	1.96	0.48
4:F:45:SER:O	4:F:52:VAL:HA	2.13	0.48
2:H:72:SER:HB2	2:H:77:GLU:OE2	2.15	0.47
2:H:149(A):THR:OG1	3:I:52:ASN:ND2	2.47	0.47
4:F:129(C):LEU:HD11	5:G:204:PRO:HD2	1.97	0.47
2:H:95:ASN:HB3	2:H:100:ASP:H	1.80	0.47
4:F:50:ARG:O	4:F:108:LEU:HG	2.14	0.47
4:F:93:ARG:O	4:F:101:ARG:HD3	2.15	0.47
2:H:212:ILE:HG12	2:H:229:THR:HB	1.96	0.47
2:H:73:ARG:HD3	2:H:152:PRO:O	2.15	0.47
2:H:61:VAL:HG13	2:H:85:LEU:HB2	1.97	0.47
2:H:77:GLU:HB2	2:H:80:GLU:HG2	1.97	0.47
4:F:139:THR:HA	5:G:156:GLN:O	2.15	0.46
2:H:67:ARG:HD3	2:H:82:ILE:HG12	1.97	0.46
2:H:46:LEU:HD23	2:H:48:SER:O	2.14	0.46
2:H:35:ARG:O	2:H:38:GLN:HA	2.16	0.46
4:F:34:PHE:CE2	4:F:38:GLN:HB2	2.50	0.46
4:F:73:ARG:NH2	3:J:54:GLY:HA2	2.28	0.46
5:G:163:VAL:CG1	5:G:167:VAL:HG22	2.46	0.46
2:H:169:LYS:HD2	2:H:176:ILE:HB	1.98	0.46
4:F:129(B):LYS:HB3	5:G:204(A):TYR:HE2	1.81	0.46
1:L:14(K):ILE:HG22	1:L:14(L):GLU:N	2.31	0.46
4:F:60(B):PRO:HB2	4:F:60(C):PRO:HD3	1.98	0.46
2:H:129(C):LEU:O	2:H:134:PHE:HD2	1.99	0.46
4:F:143:ASN:CB	5:G:191:CYS:SG	3.04	0.45
5:G:177:THR:H	5:G:180:MET:HE3	1.81	0.45
2:H:32:MET:HB2	2:H:40:LEU:CD1	2.46	0.45
2:H:137:ARG:HH21	2:H:207:TRP:HH2	1.64	0.45
2:H:25:GLY:O	2:H:28:PRO:HD3	2.17	0.45
5:G:165:ARG:N	5:G:166:PRO:HD2	2.31	0.45
2:H:137:ARG:HH11	2:H:157:VAL:HG11	1.82	0.45
2:H:61:VAL:HG11	2:H:86:ASP:O	2.15	0.45
4:F:129(C):LEU:HB3	5:G:210:MET:CE	2.45	0.45
2:H:165:ARG:NH2	2:H:178:ASP:HA	2.31	0.45
2:H:131:HIS:HB2	2:H:134:PHE:CE2	2.51	0.45
1:L:14(G):PHE:CZ	2:H:202:LYS:HD3	2.51	0.45
2:H:31:VAL:CG1	2:H:66:VAL:HG13	2.46	0.45
4:F:34:PHE:HE2	4:F:38:GLN:HB2	1.82	0.44
2:H:150:VAL:HG23	2:H:151:GLN:N	2.32	0.44
2:H:23:GLU:HB2	2:H:26:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1(C):GLU:O	1:M:1(A):ASP:N	2.50	0.44
4:F:128:THR:O	4:F:129(C):LEU:HB2	2.17	0.44
4:F:36:LYS:HE3	4:F:36:LYS:HB2	1.84	0.44
4:F:76:TYR:HB3	3:J:57:GLU:OE2	2.17	0.44
2:H:103:ILE:HG21	2:H:234:LEU:HD13	1.99	0.44
4:F:60(A):TYR:HB3	4:F:60(F):LYS:HB2	2.00	0.44
1:M:3:LEU:HA	1:M:8:GLU:HG3	2.00	0.44
1:L:10:LYS:HG2	1:L:10:LYS:O	2.18	0.44
2:H:60(A):TYR:HB3	2:H:60(F):LYS:HB2	2.00	0.43
2:H:32:MET:SD	2:H:40:LEU:HD13	2.58	0.43
2:H:124:PRO:HB2	2:H:232:PHE:CD1	2.52	0.43
2:H:36:LYS:HE3	2:H:64:LEU:O	2.19	0.43
2:H:144:ARG:HG3	2:H:150:VAL:O	2.19	0.43
2:H:237:TRP:O	2:H:241:VAL:HG23	2.18	0.43
2:H:33:LEU:N	2:H:33:LEU:HD12	2.33	0.43
4:F:121:VAL:HG11	5:G:209:GLN:NE2	2.34	0.43
2:H:33:LEU:H	2:H:33:LEU:HD12	1.82	0.43
4:F:31:VAL:CG1	4:F:44:ALA:HB3	2.48	0.43
4:F:130:LEU:HG	5:G:210:MET:HE3	2.00	0.43
4:F:16:ILE:HD11	4:F:138:VAL:HG12	2.01	0.43
1:L:4:ARG:NH2	2:H:207:TRP:CZ2	2.87	0.43
5:G:238:ILE:O	5:G:242:ILE:HG13	2.17	0.43
2:H:122:CYS:SG	2:H:206:ARG:HG3	2.59	0.43
4:F:78:LYS:HE2	4:F:78:LYS:HB2	1.83	0.42
2:H:97(A):GLU:OE2	2:H:175:ARG:HD2	2.19	0.42
4:F:115:SER:C	4:F:117:TYR:H	2.23	0.42
1:L:1:CYS:C	2:H:122:CYS:SG	2.98	0.42
5:G:244:ARG:HG3	5:G:244:ARG:O	2.18	0.42
2:H:76:TYR:HE2	2:H:77(A):ARG:HD3	1.85	0.42
4:F:129(B):LYS:HA	4:F:129(B):LYS:CE	2.50	0.42
5:G:209:GLN:HB2	5:G:209:GLN:HE21	1.59	0.42
1:M:14(G):PHE:HA	1:M:14(J):TYR:HD2	1.83	0.42
1:M:14(H):GLU:O	1:M:14(K):ILE:HB	2.20	0.42
4:F:96:TRP:CE3	4:F:97:LYS:HB3	2.55	0.42
1:M:14(F):LEU:CD1	5:G:207:TRP:HH2	2.32	0.42
5:G:198:PRO:HB3	5:G:209:GLN:NE2	2.35	0.42
4:F:146:GLU:OE1	5:G:221(A):ARG:NH1	2.53	0.42
2:H:53:LEU:HD12	2:H:104:ALA:O	2.19	0.41
5:G:172:THR:HG21	5:G:176:ILE:HD11	2.02	0.41
1:M:1:CYS:O	4:F:122:CYS:SG	2.77	0.41
1:M:4:ARG:HA	1:M:5:PRO:HD3	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:18:GLU:HB2	5:G:188:GLY:CA	2.51	0.41
4:F:77(A):ARG:NH2	4:F:78:LYS:HD3	2.36	0.41
2:H:130:LEU:CD1	2:H:210:MET:HG3	2.47	0.41
4:F:134:PHE:O	5:G:162:LEU:HG	2.20	0.41
5:G:160:LEU:HA	5:G:161:PRO:HD3	1.89	0.41
5:G:161:PRO:O	5:G:183:ALA:HB1	2.20	0.41
4:F:36:LYS:HB3	4:F:36(A):SER:H	1.76	0.41
1:L:4:ARG:HD3	2:H:28:PRO:HD2	2.03	0.41
1:L:6:LEU:HD11	2:H:117:TYR:CE1	2.56	0.41
1:M:14(I):SER:HA	1:M:14(L):GLU:HG2	2.02	0.41
2:H:18:GLU:HB2	2:H:188:GLY:CA	2.45	0.41
5:G:204:PRO:HG2	5:G:204(A):TYR:CD1	2.56	0.41
5:G:178:ASP:N	5:G:178:ASP:OD1	2.54	0.41
2:H:211:GLY:HA2	2:H:231:VAL:HG23	2.03	0.41
1:L:4:ARG:HH11	1:L:7:PHE:HB2	1.86	0.40
4:F:60(I):THR:O	4:F:63:ASP:N	2.49	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	34/49 (69%)	27 (79%)	6 (18%)	1 (3%)	6	36
1	M	34/49 (69%)	25 (74%)	9 (26%)	0	100	100
2	H	257/259 (99%)	214 (83%)	36 (14%)	7 (3%)	6	39
3	I	13/15 (87%)	8 (62%)	2 (15%)	3 (23%)	0	0
3	J	13/15 (87%)	8 (62%)	3 (23%)	2 (15%)	0	1
4	F	148/150 (99%)	120 (81%)	21 (14%)	7 (5%)	3	22
5	G	107/109 (98%)	85 (79%)	16 (15%)	6 (6%)	2	18
All	All	606/646 (94%)	487 (80%)	93 (15%)	26 (4%)	3	25

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1(C)	GLU
2	H	149(A)	THR
2	H	213	VAL
3	I	55	ASP
4	F	77(A)	ARG
4	F	143	ASN
4	F	147	THR
5	G	186(B)	GLU
5	G	205	ASN
2	H	98	ASN
3	I	61	GLU
4	F	36	LYS
4	F	57	HIS
2	H	189	ASP
2	H	246	GLY
5	G	244	ARG
3	J	53	ASP
2	H	60(G)	ASN
2	H	149(E)	GLU
4	F	87	LYS
5	G	194	ASP
5	G	186(C)	GLY
3	I	60	PRO
5	G	219	GLY
3	J	54	GLY
4	F	92	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	L	30/43 (70%)	28 (93%)	2 (7%)	20	60
1	M	30/43 (70%)	26 (87%)	4 (13%)	5	23
2	H	226/226 (100%)	203 (90%)	23 (10%)	9	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	14/14 (100%)	11 (79%)	3 (21%)	1	6
3	J	14/14 (100%)	11 (79%)	3 (21%)	1	6
4	F	134/134 (100%)	119 (89%)	15 (11%)	7	32
5	G	92/92 (100%)	79 (86%)	13 (14%)	4	20
All	All	540/566 (95%)	477 (88%)	63 (12%)	7	30

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	ARG
1	L	15	ARG
2	H	46	LEU
2	H	49	ASP
2	H	60(C)	PRO
2	H	72	SER
2	H	80	GLU
2	H	85	LEU
2	H	94	TYR
2	H	97(A)	GLU
2	H	110	ARG
2	H	130	LEU
2	H	138	VAL
2	H	139	THR
2	H	153	SER
2	H	175	ARG
2	H	177	THR
2	H	178	ASP
2	H	179	ASN
2	H	180	MET
2	H	182	CYS
2	H	206	ARG
2	H	210	MET
2	H	222	ASP
2	H	245	LEU
3	I	58	GLU
3	I	62	GLU
3	I	65	GLN
1	M	4	ARG
1	M	13	GLN
1	M	14(A)	GLN
1	M	14(B)	THR

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Mol	Chain	Res	Type
4	F	16	ILE
4	F	29	TRP
4	F	35	ARG
4	F	41	LEU
4	F	50	ARG
4	F	54	THR
4	F	62	ASP
4	F	67	ARG
4	F	68	ILE
4	F	75	ARG
4	F	83	SER
4	F	101	ARG
4	F	114	LEU
4	F	128	THR
4	F	129(B)	LYS
5	G	155	LEU
5	G	157	VAL
5	G	167	VAL
5	G	175	ARG
5	G	178	ASP
5	G	179	ASN
5	G	182	CYS
5	G	186(D)	LYS
5	G	209	GLN
5	G	221	ASP
5	G	229	THR
5	G	230	HIS
5	G	244	ARG
3	J	58	GLU
3	J	60	PRO
3	J	61	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	20	GLN
2	H	30	GLN
2	H	71	HIS
2	H	119	HIS
2	H	151	GLN
3	I	52	ASN
3	I	65	GLN

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Mol	Chain	Res	Type
1	M	14(A)	GLN
4	F	91	HIS
5	G	205	ASN
5	G	209	GLN
5	G	230	HIS
5	G	239	GLN
3	J	65	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

2 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	NAG	H	401	2,6	14,14,15	0.54	0	15,19,21	0.60	0
6	NAG	H	402	6	14,14,15	0.62	1 (7%)	15,19,21	0.62	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
6	NAG	H	401	2,6	-	0/6/23/26	0/1/1/1
6	NAG	H	402	6	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	402	NAG	C1-C2	2.06	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	401	NAG	1	0
6	H	402	NAG	1	0

## 5.6 Ligand geometry

1 ligand is 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	$\# Z  > 2$
7	NAG	F	501	4	14,14,15	0.42	0	15,19,21	0.72	1 (6%)

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
7	NAG	F	501	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
7	F	501	NAG	C2-N2-C7	-2.37	120.00	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	L	36/49 (73%)	-0.66	1 (2%) 56 42	2, 12, 71, 106	0
1	M	36/49 (73%)	-0.82	0 100 100	2, 11, 82, 113	0
2	H	259/259 (100%)	-0.95	1 (0%) 93 90	2, 13, 67, 129	0
3	I	15/15 (100%)	-0.16	0 100 100	17, 52, 88, 94	0
3	J	15/15 (100%)	0.34	0 100 100	49, 70, 101, 104	0
4	F	150/150 (100%)	-0.78	0 100 100	2, 27, 61, 91	0
5	G	109/109 (100%)	-0.92	1 (0%) 85 78	2, 8, 65, 117	0
All	All	620/646 (95%)	-0.83	3 (0%) 91 87	2, 16, 71, 129	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	1(H)	THR	3.0
5	G	247	SER	3.0
2	H	149(C)	VAL	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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	H	402	14/15	0.90	0.32	-	5,5,5,5	0
6	NAG	H	401	14/15	0.94	0.23	-	5,5,5,5	0

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	F	501	14/15	0.87	0.33	-	8,8,8,8	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.