



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:14 PM GMT

PDB ID : 1EO8  
Title : INFLUENZA VIRUS HEMAGGLUTININ COMPLEXED WITH A NEUTRALIZING ANTIBODY  
Authors : Fleury, D.; Gigant, B.; Daniels, R.S.; Skehel, J.J.; Knossow, M.; Bizebard, T.  
Deposited on : 2000-03-22  
Resolution : 2.80 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

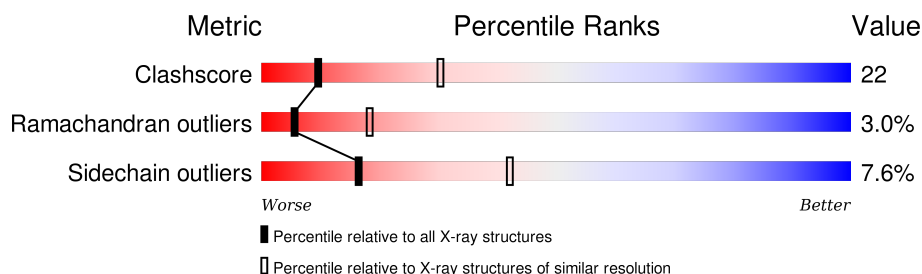
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	328	
2	B	175	
3	L	210	
4	H	217	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	B	410	X	-	-	-
6	MAN	A	452	X	-	-	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7357 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 HEMAGGLUTININ (HA1 CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2464	1543	433	475	13			

- Molecule 2 is a protein called HEMAGGLUTININ (HA2 CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1421	882	250	283	6			

- Molecule 3 is a protein called ANTIBODY (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1620	1009	270	332	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	40	SER	PRO	CONFLICT	GB 7159941

- Molecule 4 is a protein called ANTIBODY (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	217	Total	C	N	O	S	0	0	0
			1648	1046	272	323	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	64	LYS	ARG	CONFLICT	GB 7159939
H	187	PRO	THR	CONFLICT	GB 7159939

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Chain	Residue	Modelled	Actual	Comment	Reference
H	188	ARG	TRP	CONFLICT	GB 7159939

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 6 is a polymer of unknown type called SUGAR (NAG-NAG-MAN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is a polymer of unknown type called SUGAR (NAG-NAG).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is water.

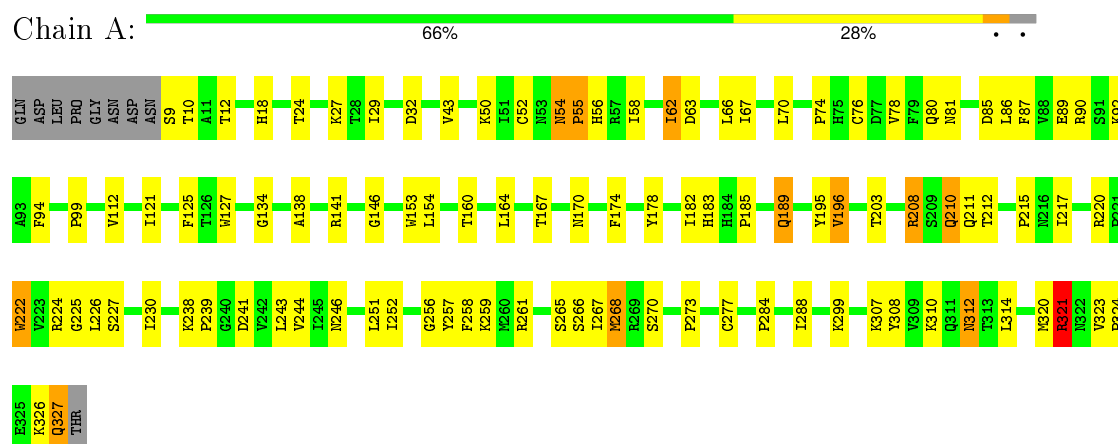
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	43	Total 43	O 43	0	0
8	B	44	Total 44	O 44	0	0
8	H	17	Total 17	O 17	0	0
8	L	5	Total 5	O 5	0	0

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

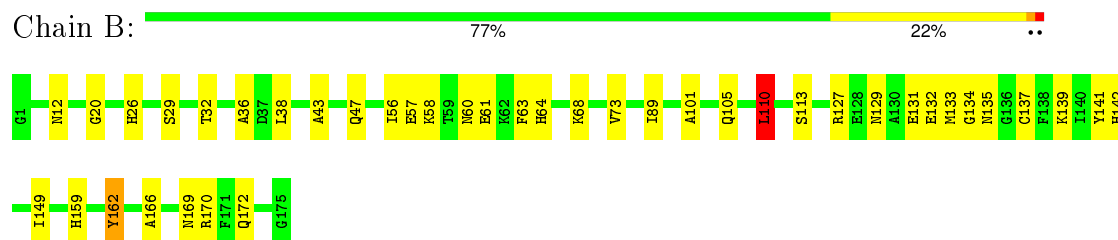
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

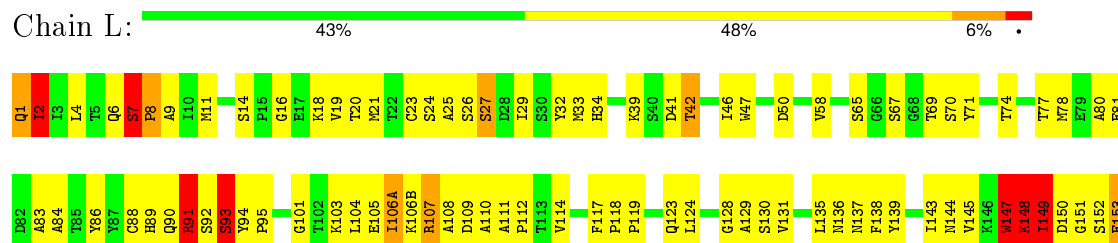
#### • Molecule 1: HEMAGGLUTININ (HA1 CHAIN)

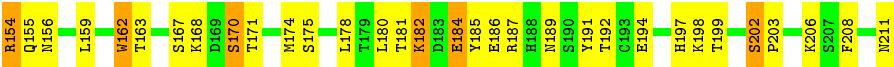


#### • Molecule 2: HEMAGGLUTININ (HA2 CHAIN)



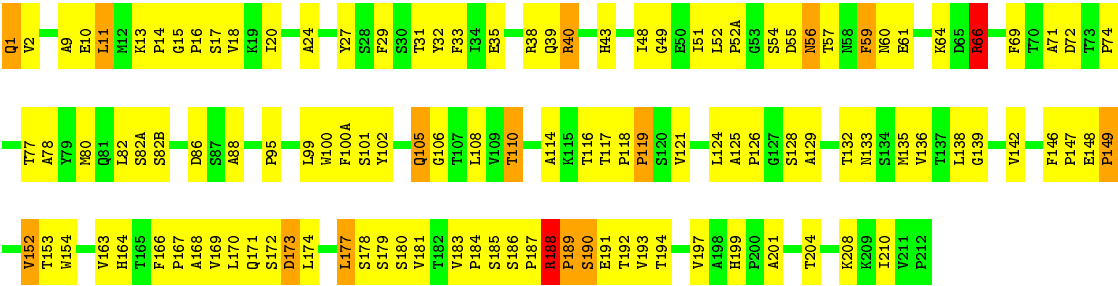
#### • Molecule 3: ANTIBODY (LIGHT CHAIN)





● Molecule 4: ANTIBODY (HEAVY CHAIN)

Chain H: 46% 47% 6% ●





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.15Å 138.15Å 129.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.80)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.196 , 0.298	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7357	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	A	0.60	0/2520	0.86	2/3433 (0.1%)
2	B	0.67	0/1445	0.84	2/1939 (0.1%)
3	L	0.59	0/1658	0.94	5/2249 (0.2%)
4	H	0.60	0/1695	0.87	3/2319 (0.1%)
All	All	0.61	0/7318	0.88	12/9940 (0.1%)

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
6	A	1	0

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	7	SER	N-CA-C	9.20	135.84	111.00
3	L	91	ARG	NE-CZ-NH2	7.17	123.89	120.30
3	L	8	PRO	N-CA-C	-7.07	93.73	112.10
2	B	110	LEU	CA-CB-CG	6.81	130.97	115.30
1	A	321	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	321	ARG	NE-CZ-NH2	-5.59	117.50	120.30
4	H	56	ASN	N-CA-C	-5.48	96.22	111.00
2	B	110	LEU	CB-CG-CD1	-5.32	101.96	111.00
4	H	60	ASN	N-CA-C	-5.29	96.70	111.00
4	H	11	LEU	CA-CB-CG	5.26	127.41	115.30
3	L	2	ILE	N-CA-C	-5.11	97.21	111.00
3	L	7	SER	C-N-CD	5.06	139.02	128.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	452	MAN	C1

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	A	2464	0	2415	93	0
2	B	1421	0	1344	32	0
3	L	1620	0	1557	109	0
4	H	1648	0	1608	105	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	39	0	34	1	0
7	A	28	0	25	0	0
8	A	43	0	0	3	0
8	B	44	0	0	2	0
8	H	17	0	0	0	0
8	L	5	0	0	0	0
All	All	7357	0	7009	319	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 22.

All (319) 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)
3:L:184:GLU:HA	3:L:187:ARG:HD2	1.34	1.06
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.23	1.02
3:L:6:GLN:HB2	3:L:88:CYS:SG	2.09	0.93
3:L:148:LYS:HB3	3:L:153:GLU:HA	1.52	0.89
4:H:17:SER:HB3	4:H:82(A):SER:HA	1.53	0.88
1:A:10:THR:HG22	2:B:141:TYR:HA	1.54	0.87
3:L:149:ILE:HD12	3:L:192:THR:H	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:184:PRO:HB2	4:H:187:PRO:HD2	1.62	0.82
1:A:312:ASN:HD22	1:A:312:ASN:H	1.30	0.80
3:L:1:GLN:O	3:L:2:ILE:HG13	1.82	0.79
1:A:141:ARG:HB2	1:A:146:GLY:HA3	1.65	0.77
3:L:143:ILE:HD12	3:L:197:HIS:HB2	1.69	0.74
3:L:6:GLN:HA	3:L:23:CYS:HA	1.70	0.74
3:L:80:ALA:HA	3:L:106(A):ILE:HD13	1.69	0.74
4:H:188:ARG:HB3	4:H:189:PRO:HD3	1.70	0.74
1:A:167:THR:HB	1:A:244:VAL:HG22	1.70	0.74
3:L:78:MET:SD	3:L:104:LEU:HD21	2.30	0.72
4:H:13:LYS:O	4:H:16:PRO:HD2	1.90	0.72
4:H:11:LEU:HA	4:H:110:THR:O	1.90	0.70
1:A:203:THR:HG23	1:A:212:THR:OG1	1.90	0.70
3:L:149:ILE:HD11	3:L:191:TYR:HD2	1.56	0.69
4:H:17:SER:HB3	4:H:82(A):SER:CA	2.23	0.69
3:L:159:LEU:HD13	4:H:169:VAL:HG11	1.74	0.69
4:H:105:GLN:HE21	4:H:105:GLN:H	1.42	0.68
3:L:106(A):ILE:HD12	3:L:170:SER:OG	1.93	0.67
3:L:107:ARG:HH12	3:L:110:ALA:HB2	1.59	0.66
1:A:326:LYS:HA	1:A:326:LYS:HE3	1.76	0.66
3:L:23:CYS:SG	3:L:33:MET:HE3	2.37	0.65
3:L:147:TRP:O	3:L:149:ILE:N	2.29	0.65
3:L:137:ASN:OD1	4:H:164:HIS:HE1	1.80	0.65
1:A:27:LYS:HG2	1:A:32:ASP:O	1.97	0.64
4:H:184:PRO:HB2	4:H:187:PRO:CD	2.28	0.63
1:A:321:ARG:NH1	1:A:321:ARG:HG2	2.00	0.63
4:H:138:LEU:HD11	4:H:188:ARG:HG3	1.80	0.63
4:H:105:GLN:NE2	4:H:105:GLN:H	1.96	0.63
4:H:199:HIS:CE1	4:H:201:ALA:HB3	2.33	0.63
3:L:119:PRO:HD3	3:L:131:VAL:HG22	1.81	0.62
1:A:182:ILE:HD11	1:A:215:PRO:HD3	1.80	0.62
1:A:312:ASN:HD22	1:A:312:ASN:N	1.95	0.62
1:A:134:GLY:O	1:A:153:TRP:HE3	1.82	0.62
4:H:51:ILE:HG13	4:H:57:THR:HG22	1.81	0.62
1:A:54:ASN:ND2	1:A:55:PRO:HA	2.15	0.61
1:A:62:ILE:HG22	1:A:63:ASP:N	2.14	0.61
1:A:312:ASN:H	1:A:312:ASN:ND2	1.99	0.61
2:B:141:TYR:O	2:B:166:ALA:HA	2.01	0.61
3:L:135:LEU:HD21	3:L:145:VAL:HG22	1.82	0.60
4:H:38:ARG:HH12	4:H:86:ASP:HA	1.66	0.60
3:L:191:TYR:HB2	3:L:208:PHE:CZ	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:48:ILE:HG22	4:H:69:PHE:HZ	1.66	0.59
3:L:186:GLU:HG2	3:L:211:ASN:OD1	2.02	0.59
1:A:67:ILE:O	1:A:70:LEU:HB3	2.02	0.59
4:H:95:PRO:HA	4:H:101:SER:HA	1.83	0.59
4:H:31:THR:CG2	4:H:32:TYR:CZ	2.86	0.59
2:B:61:GLU:HG2	2:B:63:PHE:CZ	2.38	0.58
1:A:62:ILE:HG22	1:A:63:ASP:H	1.67	0.58
4:H:1:GLN:N	4:H:1:GLN:OE1	2.36	0.58
1:A:208:ARG:HG3	1:A:208:ARG:O	2.04	0.57
3:L:16:GLY:HA2	3:L:77:THR:HB	1.85	0.57
1:A:86:LEU:HD21	1:A:268:MET:HE3	1.87	0.57
1:A:141:ARG:NH1	1:A:141:ARG:HG3	2.19	0.56
1:A:89:GLU:CD	1:A:267:ILE:HD11	2.25	0.56
3:L:4:LEU:HB3	3:L:23:CYS:SG	2.46	0.56
3:L:135:LEU:CD2	3:L:145:VAL:HG22	2.34	0.56
3:L:184:GLU:HA	3:L:187:ARG:CD	2.22	0.56
3:L:149:ILE:N	3:L:149:ILE:HD13	2.19	0.56
3:L:137:ASN:HA	3:L:171:THR:OG1	2.04	0.56
3:L:25:ALA:O	3:L:69:THR:HG23	2.06	0.56
4:H:31:THR:HG21	4:H:32:TYR:CZ	2.41	0.56
2:B:129:ASN:HA	2:B:166:ALA:HB1	1.87	0.56
3:L:93:SER:O	3:L:95:PRO:HD3	2.05	0.56
1:A:80:GLN:O	1:A:81:ASN:HB2	2.06	0.56
3:L:162:TRP:CE3	3:L:174:MET:HG3	2.41	0.56
4:H:168:ALA:HB2	4:H:177:LEU:HB2	1.88	0.56
4:H:125:ALA:HB2	4:H:210:ILE:HG22	1.88	0.56
2:B:131:GLU:HB2	2:B:141:TYR:HE1	1.71	0.56
3:L:194:GLU:CG	3:L:203:PRO:HB2	2.36	0.56
4:H:171:GLN:O	4:H:173:ASP:N	2.39	0.56
3:L:6:GLN:NE2	3:L:86:TYR:O	2.38	0.55
3:L:149:ILE:HD12	3:L:191:TYR:HA	1.87	0.55
3:L:159:LEU:HD13	4:H:169:VAL:CG1	2.35	0.55
1:A:288:ILE:HG13	1:A:288:ILE:O	2.05	0.55
3:L:83:ALA:HB2	3:L:106(A):ILE:HG12	1.88	0.55
2:B:141:TYR:CD1	2:B:170:ARG:HG2	2.42	0.55
3:L:162:TRP:N	3:L:162:TRP:CD1	2.72	0.55
4:H:59:PHE:HD2	4:H:64:LYS:HA	1.71	0.55
3:L:84:ALA:HB3	3:L:86:TYR:CE2	2.43	0.54
3:L:149:ILE:HD12	3:L:192:THR:N	2.18	0.54
4:H:124:LEU:HB2	4:H:139:GLY:O	2.06	0.54
4:H:55:ASP:O	4:H:57:THR:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:123:GLN:HG2	3:L:128:GLY:O	2.06	0.54
1:A:170:ASN:ND2	1:A:239:PRO:HA	2.22	0.54
4:H:188:ARG:O	4:H:190:SER:N	2.41	0.54
4:H:31:THR:CG2	4:H:32:TYR:CE1	2.90	0.54
4:H:114:ALA:HB3	4:H:146:PHE:CE2	2.43	0.54
4:H:38:ARG:NH1	4:H:86:ASP:HA	2.23	0.54
3:L:91:ARG:NH2	4:H:35:GLU:OE1	2.40	0.53
2:B:20:GLY:HA3	2:B:36:ALA:HB1	1.89	0.53
4:H:33:PHE:CZ	4:H:52:LEU:HB2	2.43	0.53
4:H:59:PHE:HD1	4:H:59:PHE:N	2.07	0.53
4:H:95:PRO:HB2	4:H:99:LEU:HD22	1.89	0.53
1:A:63:ASP:HB3	1:A:94:PHE:CE2	2.43	0.53
3:L:175:SER:HB3	4:H:166:PHE:CD1	2.44	0.53
3:L:41:ASP:O	3:L:42:THR:HG23	2.09	0.53
3:L:119:PRO:HG2	3:L:129:ALA:HB1	1.90	0.53
4:H:59:PHE:N	4:H:59:PHE:CD1	2.77	0.53
4:H:61:GLU:HA	4:H:64:LYS:HD2	1.91	0.53
3:L:117:PHE:O	3:L:131:VAL:HG13	2.08	0.52
4:H:133:ASN:HB2	4:H:185:SER:OG	2.09	0.52
1:A:141:ARG:HG3	1:A:141:ARG:HH11	1.73	0.52
1:A:99:PRO:HD2	1:A:226:LEU:HD12	1.92	0.52
3:L:181:THR:OG1	3:L:184:GLU:HB3	2.10	0.52
3:L:149:ILE:H	3:L:149:ILE:HD13	1.74	0.52
4:H:164:HIS:HB2	4:H:180:SER:OG	2.10	0.52
3:L:92:SER:O	3:L:93:SER:CB	2.57	0.52
1:A:222:TRP:CE3	1:A:225:GLY:HA2	2.44	0.52
1:A:174:PHE:HE1	1:A:257:TYR:CE1	2.28	0.52
3:L:135:LEU:HD12	3:L:135:LEU:N	2.25	0.51
4:H:31:THR:HG22	4:H:32:TYR:CD2	2.45	0.51
1:A:183:HIS:O	1:A:185:PRO:HD3	2.10	0.51
4:H:31:THR:HG22	4:H:32:TYR:CG	2.45	0.51
2:B:133:MET:HE2	2:B:137:CYS:HB2	1.92	0.51
3:L:33:MET:HG3	3:L:71:TYR:CG	2.46	0.51
4:H:1:GLN:CA	4:H:1:GLN:OE1	2.60	0.50
1:A:12:THR:O	2:B:26:HIS:HA	2.11	0.50
1:A:121:ILE:O	1:A:256:GLY:HA3	2.11	0.50
4:H:31:THR:HG22	4:H:32:TYR:CE2	2.47	0.50
4:H:54:SER:HB2	4:H:56:ASN:HD21	1.76	0.50
3:L:182:LYS:O	3:L:185:TYR:HB3	2.12	0.50
1:A:310:LYS:HD3	8:B:414:HOH:O	2.10	0.50
2:B:132:GLU:HG2	2:B:134:GLY:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:26:SER:O	3:L:27:SER:HB2	2.11	0.50
4:H:31:THR:HG22	4:H:32:TYR:CD1	2.46	0.50
4:H:72:ASP:OD2	4:H:74:PRO:HG2	2.12	0.50
3:L:34:HIS:HB2	3:L:89:HIS:HB3	1.94	0.49
1:A:326:LYS:HB3	1:A:327:GLN:OE1	2.13	0.49
4:H:189:PRO:O	4:H:190:SER:HB2	2.12	0.49
4:H:173:ASP:O	4:H:174:LEU:HD23	2.13	0.49
3:L:39:LYS:NZ	3:L:83:ALA:O	2.45	0.49
4:H:124:LEU:HB2	4:H:139:GLY:C	2.33	0.49
1:A:43:VAL:HG23	1:A:314:LEU:HB2	1.94	0.49
1:A:164:LEU:O	1:A:246:ASN:HA	2.12	0.49
4:H:24:ALA:HB1	4:H:27:TYR:CE2	2.46	0.49
1:A:141:ARG:CG	1:A:141:ARG:HH11	2.26	0.49
4:H:105:GLN:HG2	4:H:106:GLY:N	2.27	0.49
1:A:220:ARG:O	1:A:227:SER:HB2	2.12	0.49
1:A:50:LYS:HD2	1:A:273:PRO:HB2	1.94	0.49
1:A:299:LYS:HG2	8:A:497:HOH:O	2.13	0.49
1:A:70:LEU:HD12	1:A:258:PHE:CE2	2.48	0.49
4:H:31:THR:HG22	4:H:32:TYR:CE1	2.48	0.49
1:A:210:GLN:HG2	1:A:211:GLN:N	2.27	0.49
4:H:31:THR:HG22	4:H:32:TYR:CZ	2.48	0.49
1:A:238:LYS:O	1:A:241:ASP:HB2	2.13	0.49
3:L:20:THR:OG1	3:L:74:THR:HG23	2.13	0.49
1:A:321:ARG:CG	1:A:321:ARG:HH11	2.10	0.48
3:L:107:ARG:HD3	3:L:108:ALA:O	2.12	0.48
2:B:26:HIS:CD2	2:B:149:ILE:HG13	2.48	0.48
3:L:124:LEU:HD22	3:L:182:LYS:HG3	1.95	0.48
1:A:54:ASN:HD22	1:A:55:PRO:HA	1.78	0.48
1:A:320:MET:HG3	1:A:321:ARG:O	2.14	0.48
3:L:6:GLN:CB	3:L:88:CYS:SG	2.92	0.48
4:H:40:ARG:HB3	4:H:43:HIS:ND1	2.28	0.48
4:H:39:GLN:O	4:H:88:ALA:HB1	2.13	0.48
2:B:169:ASN:HA	2:B:172:GLN:HG3	1.95	0.48
1:A:121:ILE:HB	1:A:257:TYR:CE2	2.48	0.48
3:L:18:LYS:HE3	3:L:74:THR:CG2	2.44	0.48
1:A:29:ILE:HD13	2:B:101:ALA:HB1	1.95	0.48
3:L:147:TRP:HB3	3:L:148:LYS:H	1.50	0.48
1:A:312:ASN:ND2	1:A:312:ASN:N	2.61	0.48
3:L:143:ILE:HG13	3:L:144:ASN:N	2.29	0.48
1:A:78:VAL:HB	4:H:100:TRP:CD2	2.48	0.48
1:A:27:LYS:HA	1:A:32:ASP:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:TRP:HE3	8:A:490:HOH:O	1.96	0.47
3:L:150:ASP:HA	3:L:153:GLU:OE1	2.14	0.47
3:L:107:ARG:NH1	3:L:108:ALA:O	2.47	0.47
3:L:119:PRO:CG	3:L:129:ALA:HB1	2.45	0.47
3:L:103:LYS:HD2	3:L:105:GLU:HG3	1.95	0.47
4:H:66:ARG:HH22	4:H:86:ASP:CG	2.18	0.47
3:L:78:MET:CE	3:L:106(A):ILE:HG23	2.45	0.47
1:A:154:LEU:HD12	1:A:251:LEU:HD23	1.97	0.47
3:L:2:ILE:HG21	3:L:90:GLN:HG3	1.97	0.47
4:H:126:PRO:HD3	4:H:138:LEU:HD23	1.96	0.47
4:H:2:VAL:HG11	4:H:102:TYR:CG	2.50	0.46
1:A:308:TYR:CE2	2:B:89:ILE:HD13	2.50	0.46
1:A:58:ILE:HD13	1:A:58:ILE:N	2.30	0.46
2:B:56:ILE:HG23	2:B:57:GLU:HG3	1.98	0.46
1:A:125:PHE:HB3	1:A:127:TRP:CE2	2.50	0.46
4:H:17:SER:HB3	4:H:82(A):SER:CB	2.46	0.46
3:L:136:ASN:HB3	3:L:137:ASN:OD1	2.16	0.46
4:H:136:VAL:N	4:H:183:VAL:O	2.49	0.46
1:A:307:LYS:CE	2:B:60:ASN:ND2	2.79	0.46
4:H:117:THR:HG22	4:H:118:PRO:O	2.15	0.46
1:A:195:TYR:O	1:A:196:VAL:HB	2.16	0.46
3:L:83:ALA:HA	3:L:104:LEU:O	2.15	0.46
1:A:62:ILE:HD12	4:H:100(A):PHE:CD1	2.51	0.46
4:H:61:GLU:OE2	4:H:64:LYS:NZ	2.49	0.46
2:B:135:ASN:OD1	2:B:135:ASN:N	2.45	0.46
3:L:163:THR:HG23	4:H:166:PHE:CE2	2.51	0.45
3:L:86:TYR:O	3:L:101:GLY:HA2	2.17	0.45
3:L:148:LYS:O	3:L:153:GLU:HA	2.15	0.45
1:A:66:LEU:HD21	1:A:112:VAL:HG12	1.96	0.45
1:A:90:ARG:NH1	1:A:270:SER:O	2.44	0.45
4:H:108:LEU:HD21	4:H:148:GLU:HB2	1.98	0.45
1:A:76:CYS:O	1:A:78:VAL:N	2.49	0.45
2:B:162:TYR:CD2	2:B:162:TYR:N	2.85	0.45
4:H:105:GLN:HE21	4:H:105:GLN:N	2.10	0.45
4:H:119:PRO:HD2	4:H:204:THR:HG21	1.98	0.45
2:B:139:LYS:HD3	2:B:141:TYR:CZ	2.52	0.45
4:H:20:ILE:HD12	4:H:80:MET:CE	2.47	0.45
3:L:202:SER:HA	3:L:203:PRO:HD2	1.85	0.45
3:L:2:ILE:HD13	3:L:90:GLN:NE2	2.32	0.45
4:H:208:LYS:HA	4:H:208:LYS:HD3	1.78	0.45
3:L:162:TRP:CZ3	3:L:174:MET:SD	3.09	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:GLY:O	1:A:153:TRP:CE3	2.67	0.45
1:A:85:ASP:O	1:A:265:SER:HA	2.17	0.45
3:L:47:TRP:CD2	3:L:58:VAL:HG22	2.52	0.45
2:B:129:ASN:ND2	2:B:159:HIS:HB2	2.32	0.44
3:L:194:GLU:HG3	3:L:203:PRO:HB2	1.99	0.44
3:L:149:ILE:HD11	3:L:191:TYR:CD2	2.43	0.44
3:L:47:TRP:O	3:L:58:VAL:HG21	2.18	0.44
4:H:33:PHE:CE1	4:H:52:LEU:HB2	2.53	0.44
3:L:148:LYS:HB3	3:L:153:GLU:CA	2.36	0.44
3:L:185:TYR:CE2	3:L:211:ASN:OD1	2.71	0.44
1:A:230:ILE:HD12	1:A:252:ILE:HG13	2.00	0.44
4:H:163:VAL:HA	4:H:180:SER:O	2.17	0.44
3:L:19:VAL:O	3:L:74:THR:HG23	2.18	0.44
2:B:110:LEU:O	2:B:113:SER:HB3	2.18	0.44
4:H:29:PHE:CE2	4:H:52(A):PRO:HB3	2.52	0.44
1:A:29:ILE:HB	2:B:105:GLN:OE1	2.18	0.44
3:L:130:SER:HA	3:L:178:LEU:O	2.17	0.43
3:L:107:ARG:O	3:L:139:TYR:CE1	2.71	0.43
4:H:121:VAL:HG21	4:H:197:VAL:HB	2.00	0.43
3:L:106(B):LYS:HA	3:L:139:TYR:OH	2.18	0.43
4:H:194:THR:HG23	4:H:208:LYS:C	2.39	0.43
3:L:94:TYR:CE2	4:H:59:PHE:O	2.72	0.43
1:A:261:ARG:HG2	1:A:261:ARG:HH11	1.83	0.43
1:A:174:PHE:CE1	1:A:259:LYS:HG2	2.54	0.43
4:H:191:GLU:HB3	4:H:192:THR:H	1.62	0.43
1:A:67:ILE:HD13	1:A:67:ILE:HA	1.81	0.43
1:A:189:GLN:CD	1:A:189:GLN:N	2.72	0.43
3:L:4:LEU:HA	3:L:24:SER:O	2.19	0.43
1:A:74:PRO:HG3	1:A:141:ARG:CZ	2.49	0.43
4:H:170:LEU:HD11	4:H:173:ASP:HA	2.00	0.42
1:A:170:ASN:ND2	1:A:239:PRO:CA	2.82	0.42
1:A:174:PHE:CE1	1:A:257:TYR:CE1	3.06	0.42
1:A:323:VAL:CG1	2:B:12:ASN:HA	2.49	0.42
1:A:323:VAL:HG12	2:B:12:ASN:HA	2.01	0.42
3:L:182:LYS:O	3:L:186:GLU:HG3	2.19	0.42
1:A:266:SER:OG	1:A:267:ILE:N	2.52	0.42
3:L:20:THR:HA	3:L:74:THR:HA	2.01	0.42
4:H:152:VAL:HG21	4:H:179:SER:CB	2.49	0.42
1:A:167:THR:HG21	6:A:450:NAG:C6	2.50	0.42
1:A:86:LEU:HA	1:A:266:SER:O	2.19	0.42
4:H:142:VAL:O	4:H:142:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:HIS:HB2	1:A:58:ILE:HD11	2.01	0.42
3:L:119:PRO:HD2	3:L:185:TYR:CZ	2.54	0.42
3:L:191:TYR:HB2	3:L:208:PHE:CE1	2.55	0.42
4:H:166:PHE:HA	4:H:167:PRO:HD3	1.92	0.42
1:A:125:PHE:HB3	1:A:127:TRP:CZ2	2.54	0.42
2:B:43:ALA:O	2:B:47:GLN:HG3	2.20	0.42
1:A:67:ILE:HG12	8:A:488:HOH:O	2.19	0.42
4:H:31:THR:HG21	4:H:32:TYR:CE1	2.54	0.42
3:L:29:ILE:HD11	3:L:33:MET:HG2	2.01	0.42
3:L:162:TRP:CE3	3:L:174:MET:SD	3.13	0.42
2:B:58:LYS:HA	2:B:58:LYS:HD3	1.89	0.42
4:H:71:ALA:HA	4:H:78:ALA:HA	2.02	0.42
1:A:178:TYR:CD1	1:A:243:LEU:HD22	2.55	0.42
3:L:7:SER:O	3:L:9:ALA:N	2.53	0.41
4:H:163:VAL:HG22	4:H:181:VAL:HG23	2.02	0.41
4:H:49:GLY:HA3	4:H:69:PHE:CE2	2.55	0.41
3:L:91:ARG:HG2	3:L:91:ARG:HH11	1.85	0.41
3:L:33:MET:HG3	3:L:71:TYR:CB	2.51	0.41
1:A:138:ALA:CB	1:A:226:LEU:HD11	2.50	0.41
4:H:10:GLU:HG3	4:H:18:VAL:CG2	2.51	0.41
4:H:184:PRO:O	4:H:187:PRO:HD2	2.20	0.41
3:L:11:MET:HB3	3:L:104:LEU:HD12	2.02	0.41
4:H:154:TRP:CE2	4:H:181:VAL:HB	2.55	0.41
4:H:15:GLY:O	4:H:82(B):SER:HA	2.19	0.41
2:B:129:ASN:HA	2:B:166:ALA:CB	2.51	0.41
1:A:121:ILE:HG13	1:A:257:TYR:CZ	2.56	0.41
3:L:119:PRO:HD2	3:L:185:TYR:OH	2.20	0.41
1:A:89:GLU:HG3	1:A:267:ILE:HD11	2.03	0.41
1:A:174:PHE:CE1	1:A:257:TYR:HE1	2.39	0.41
4:H:99:LEU:N	4:H:99:LEU:HD23	2.36	0.41
4:H:188:ARG:HB3	4:H:189:PRO:CD	2.45	0.41
4:H:14:PRO:C	4:H:16:PRO:HD2	2.41	0.41
4:H:69:PHE:CE1	4:H:80:MET:HG3	2.56	0.41
4:H:142:VAL:HG22	4:H:177:LEU:HD22	2.02	0.41
1:A:138:ALA:HB1	1:A:224:ARG:HB3	2.03	0.41
3:L:124:LEU:HD11	3:L:185:TYR:HE2	1.86	0.41
3:L:131:VAL:HG12	3:L:147:TRP:HH2	1.86	0.41
3:L:151:GLY:N	3:L:153:GLU:HG2	2.36	0.41
4:H:13:LYS:C	4:H:16:PRO:HD2	2.40	0.41
4:H:51:ILE:HG13	4:H:57:THR:CG2	2.48	0.41
1:A:185:PRO:O	1:A:217:ILE:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:9:ALA:CB	4:H:108:LEU:HB3	2.51	0.41
3:L:152:SER:O	3:L:154:ARG:N	2.54	0.41
3:L:111:ALA:N	3:L:199:THR:HG21	2.35	0.41
3:L:8:PRO:HG2	3:L:21:MET:HA	2.02	0.41
3:L:114:VAL:HG12	3:L:206:LYS:HG3	2.03	0.41
3:L:131:VAL:N	3:L:178:LEU:O	2.51	0.41
4:H:142:VAL:O	4:H:142:VAL:CG2	2.68	0.41
1:A:308:TYR:CD2	2:B:89:ILE:HD13	2.55	0.41
1:A:324:PRO:C	1:A:326:LYS:H	2.23	0.40
3:L:46:ILE:HG12	4:H:99:LEU:O	2.20	0.40
2:B:68:LYS:HA	8:B:448:HOH:O	2.20	0.40
3:L:117:PHE:HA	3:L:118:PRO:HD3	1.84	0.40
1:A:266:SER:HB2	2:B:64:HIS:HB2	2.04	0.40
3:L:112:PRO:HA	3:L:138:PHE:HB3	2.03	0.40
3:L:78:MET:HE3	3:L:106(A):ILE:HG23	2.03	0.40
2:B:142:HIS:CE1	2:B:162:TYR:CD1	3.09	0.40
3:L:32:TYR:HB3	3:L:50:ASP:HA	2.02	0.40
1:A:52:CYS:HB3	1:A:277:CYS:O	2.20	0.40
4:H:177:LEU:HD23	4:H:178:SER:N	2.36	0.40
4:H:148:GLU:HA	4:H:149:PRO:HA	1.89	0.40
1:A:87:PHE:O	1:A:267:ILE:HA	2.21	0.40
4:H:142:VAL:CG2	4:H:177:LEU:HD22	2.51	0.40
4:H:135:MET:HA	4:H:185:SER:N	2.37	0.40
2:B:26:HIS:O	2:B:32:THR:HA	2.21	0.40
4:H:56:ASN:ND2	4:H:56:ASN:N	2.68	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	A	317/328 (97%)	292 (92%)	23 (7%)	2 (1%)	30 65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	173/175 (99%)	159 (92%)	13 (8%)	1 (1%)	30	65
3	L	208/210 (99%)	178 (86%)	17 (8%)	13 (6%)	2	4
4	H	215/217 (99%)	181 (84%)	23 (11%)	11 (5%)	2	8
All	All	913/930 (98%)	810 (89%)	76 (8%)	27 (3%)	5	18

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	27	SER
3	L	93	SER
3	L	148	LYS
3	L	153	GLU
3	L	182	LYS
3	L	189	ASN
4	H	172	SER
3	L	2	ILE
3	L	149	ILE
3	L	198	LYS
4	H	66	ARG
4	H	129	ALA
4	H	188	ARG
3	L	67	SER
4	H	128	SER
4	H	173	ASP
4	H	190	SER
4	H	193	VAL
3	L	170	SER
4	H	132	THR
4	H	189	PRO
1	A	62	ILE
3	L	147	TRP
2	B	127	ARG
3	L	7	SER
1	A	196	VAL
4	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	A	281/289 (97%)	265 (94%)	16 (6%)	25	58
2	B	149/149 (100%)	144 (97%)	5 (3%)	44	78
3	L	185/185 (100%)	161 (87%)	24 (13%)	5	15
4	H	187/187 (100%)	171 (91%)	16 (9%)	13	36
All	All	802/810 (99%)	741 (92%)	61 (8%)	16	42

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	18	HIS
1	A	24	THR
1	A	54	ASN
1	A	55	PRO
1	A	92	LYS
1	A	160	THR
1	A	189	GLN
1	A	208	ARG
1	A	210	GLN
1	A	222	TRP
1	A	268	MET
1	A	284	PRO
1	A	312	ASN
1	A	321	ARG
1	A	327	GLN
2	B	29	SER
2	B	38	LEU
2	B	73	VAL
2	B	110	LEU
2	B	162	TYR
3	L	1	GLN
3	L	7	SER
3	L	14	SER
3	L	42	THR
3	L	65	SER
3	L	70	SER
3	L	81	GLU
3	L	91	ARG
3	L	93	SER

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Mol	Chain	Res	Type
3	L	106(A)	ILE
3	L	107	ARG
3	L	109	ASP
3	L	147	TRP
3	L	148	LYS
3	L	149	ILE
3	L	154	ARG
3	L	155	GLN
3	L	156	ASN
3	L	162	TRP
3	L	167	SER
3	L	168	LYS
3	L	180	LEU
3	L	184	GLU
3	L	202	SER
4	H	1	GLN
4	H	40	ARG
4	H	59	PHE
4	H	66	ARG
4	H	77	THR
4	H	82	LEU
4	H	105	GLN
4	H	110	THR
4	H	116	THR
4	H	119	PRO
4	H	149	PRO
4	H	152	VAL
4	H	153	THR
4	H	177	LEU
4	H	186	SER
4	H	188	ARG

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

Mol	Chain	Res	Type
1	A	18	HIS
1	A	54	ASN
1	A	171	ASN
1	A	210	GLN
1	A	312	ASN
2	B	53	ASN
2	B	60	ASN

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Mol	Chain	Res	Type
3	L	38	GLN
3	L	156	ASN
4	H	39	GLN
4	H	56	ASN
4	H	105	GLN
4	H	133	ASN
4	H	164	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 ⓘ

5 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	A	450	1,6	14,14,15	1.86	5 (35%)	15,19,21	2.47	4 (26%)
6	NAG	A	451	6	14,14,15	1.23	1 (7%)	15,19,21	2.46	4 (26%)
6	MAN	A	452	6	11,11,12	1.65	2 (18%)	14,15,17	1.95	4 (28%)
7	NAG	A	460	1,7	14,14,15	1.15	2 (14%)	15,19,21	2.10	7 (46%)
7	NAG	A	461	7	14,14,15	2.12	4 (28%)	15,19,21	2.51	4 (26%)

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	A	450	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	451	6	-	0/6/23/26	0/1/1/1
6	MAN	A	452	6	1/1/4/5	0/2/19/22	0/1/1/1
7	NAG	A	460	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	461	7	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	450	NAG	C1-C2	-3.55	1.47	1.52
6	A	450	NAG	C4-C5	-2.93	1.46	1.53
6	A	451	NAG	C4-C5	-2.86	1.47	1.53
6	A	450	NAG	O5-C1	-2.43	1.39	1.43
6	A	450	NAG	C3-C2	-2.26	1.47	1.52
6	A	450	NAG	O3-C3	-2.11	1.37	1.43
6	A	452	MAN	C4-C3	2.07	1.57	1.52
7	A	461	NAG	C4-C3	2.10	1.57	1.52
7	A	460	NAG	C8-C7	2.10	1.54	1.50
7	A	460	NAG	C4-C5	2.15	1.57	1.53
7	A	461	NAG	O5-C5	2.40	1.48	1.43
7	A	461	NAG	C6-C5	2.62	1.61	1.51
6	A	452	MAN	C2-C3	4.75	1.59	1.52
7	A	461	NAG	C4-C5	6.02	1.65	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	450	NAG	C2-N2-C7	-7.06	113.97	123.04
6	A	451	NAG	C2-N2-C7	-6.57	114.59	123.04
6	A	450	NAG	O3-C3-C2	-4.12	100.94	109.11
6	A	451	NAG	O7-C7-C8	-4.06	114.61	122.06
6	A	452	MAN	O3-C3-C4	-3.68	102.05	110.34
7	A	461	NAG	C4-C3-C2	-3.47	105.83	111.23
7	A	460	NAG	O4-C4-C3	-3.22	103.10	110.34
6	A	451	NAG	O6-C6-C5	-3.16	100.90	111.33
7	A	460	NAG	O7-C7-C8	-3.10	116.38	122.06
6	A	452	MAN	O5-C1-C2	-2.50	106.80	110.86
7	A	461	NAG	O5-C5-C6	-2.35	102.27	107.35
7	A	461	NAG	C2-N2-C7	-2.09	120.35	123.04
6	A	450	NAG	O6-C6-C5	-2.02	104.65	111.33
6	A	452	MAN	C1-O5-C5	2.06	114.87	112.25
7	A	460	NAG	C2-N2-C7	2.21	125.88	123.04
7	A	460	NAG	C8-C7-N2	2.34	120.58	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	460	NAG	C1-O5-C5	2.46	115.37	112.25
7	A	460	NAG	O3-C3-C2	2.82	114.71	109.11
6	A	450	NAG	O4-C4-C3	2.95	116.98	110.34
6	A	451	NAG	C8-C7-N2	3.32	122.46	116.11
7	A	460	NAG	C6-C5-C4	3.45	121.52	113.02
6	A	452	MAN	C2-C3-C4	4.56	118.79	111.04
7	A	461	NAG	C1-O5-C5	7.63	121.93	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	452	MAN	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	450	NAG	1	0

## 5.6 Ligand geometry [i](#)

2 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	A	440	1	14,14,15	1.74	4 (28%)	15,19,21	2.00	6 (40%)
5	NAG	B	410	2	14,14,15	2.41	6 (42%)	15,19,21	3.69	6 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	440	1	-	0/6/23/26	0/1/1/1
5	NAG	B	410	2	1/1/5/7	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	440	NAG	C1-C2	-2.57	1.48	1.52
5	B	410	NAG	C3-C2	2.07	1.57	1.52
5	B	410	NAG	C4-C5	2.30	1.58	1.53
5	A	440	NAG	C6-C5	2.82	1.62	1.51
5	B	410	NAG	C8-C7	3.07	1.56	1.50
5	A	440	NAG	O5-C1	3.26	1.49	1.43
5	A	440	NAG	O5-C5	3.26	1.50	1.43
5	B	410	NAG	O5-C1	3.75	1.50	1.43
5	B	410	NAG	C1-C2	4.46	1.58	1.52
5	B	410	NAG	O5-C5	4.69	1.53	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	410	NAG	C3-C2-N2	-5.73	96.84	110.56
5	B	410	NAG	C4-C3-C2	-5.62	102.50	111.23
5	B	410	NAG	C2-N2-C7	-4.68	117.03	123.04
5	B	410	NAG	C3-C4-C5	-3.66	103.82	110.20
5	A	440	NAG	C3-C4-C5	-3.06	104.87	110.20
5	A	440	NAG	C2-N2-C7	-2.00	120.47	123.04
5	A	440	NAG	O6-C6-C5	2.60	119.91	111.33
5	A	440	NAG	O5-C5-C6	2.67	113.13	107.35
5	A	440	NAG	C1-O5-C5	2.74	115.72	112.25
5	A	440	NAG	C3-C2-N2	2.98	117.70	110.56
5	B	410	NAG	O3-C3-C2	5.86	120.73	109.11
5	B	410	NAG	C1-O5-C5	7.52	121.79	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	410	NAG	C1

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.