



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 10, 2018 – 11:53 AM EST

PDB ID : 6CE9  
EMDB ID: : EMD-7462  
Title : Insulin Receptor ectodomain in complex with two insulin molecules  
Authors : Scapin, G.; Dandey, V.P.; Zhang, Z.; Strickland, C.; Potter, C.S.; Carragher, B.  
Deposited on : 2018-02-11  
Resolution : 4.30 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

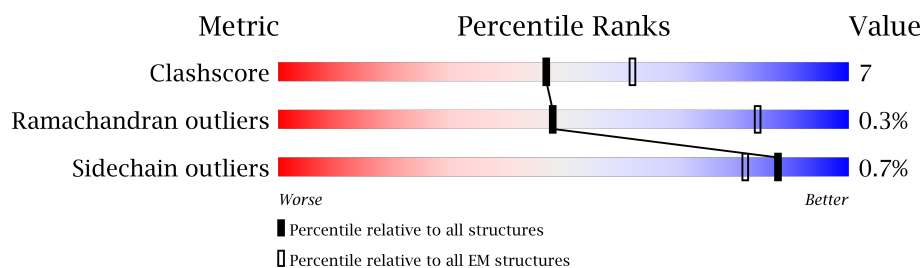
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	917	48% 13% 39%
1	B	917	49% 12% 39%
2	M	30	77% 20% .
2	P	30	77% 17% 7%
3	K	21	67% 29% 5%
3	N	21	76% 19% 5%
4	L	30	80% 17% .
4	O	30	83% 17%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10782 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Insulin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	562	Total	C	N	O	S	0	0
			4540	2882	785	833	40		
1	B	562	Total	C	N	O	S	0	0
			4540	2882	785	833	40		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	HIS	TYR	conflict	UNP P06213
B	144	HIS	TYR	conflict	UNP P06213

- Molecule 2 is a protein called Insulin receptor.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	M	30	Total	C	N	O	0	0
			253	164	42	47		
2	P	30	Total	C	N	O	0	0
			253	164	42	47		

- Molecule 3 is a protein called Insulin A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	21	Total	C	N	O	S	0	0
			163	99	25	35	4		
3	N	21	Total	C	N	O	S	0	0
			163	99	25	35	4		

- Molecule 4 is a protein called Insulin B chain.

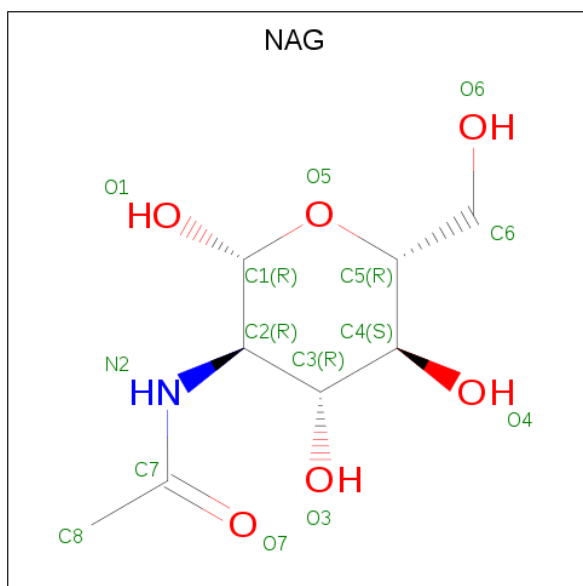
Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	30	Total	C	N	O	S	0	0
			240	157	40	41	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	30	Total	C	N	O	S	0	0
			240	157	40	41	2		

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



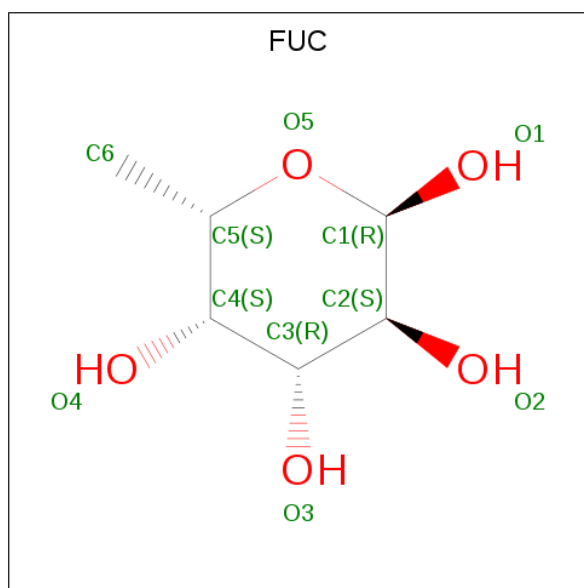
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O		0
			154	88	11	55		
5	A	1	Total	C	N	O		0
			154	88	11	55		
5	A	1	Total	C	N	O		0
			154	88	11	55		
5	A	1	Total	C	N	O		0
			154	88	11	55		
5	A	1	Total	C	N	O		0
			154	88	11	55		
5	A	1	Total	C	N	O		0
			154	88	11	55		
5	A	1	Total	C	N	O		0
			154	88	11	55		
5	A	1	Total	C	N	O		0
			154	88	11	55		

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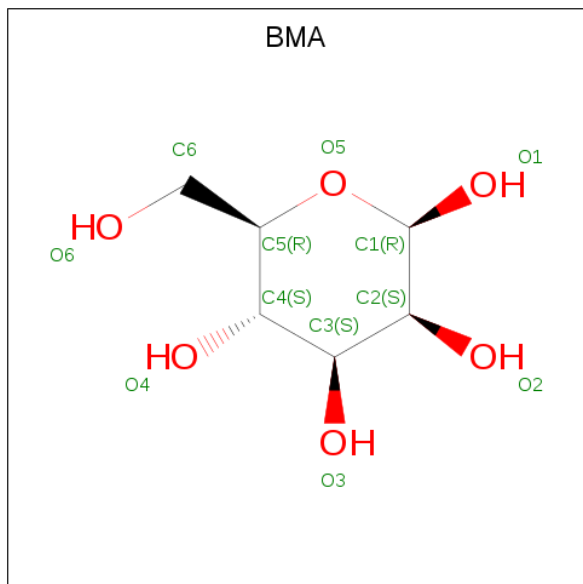
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			154	88	11	55	
5	B	1	Total	C	N	O	0
			154	88	11	55	
5	B	1	Total	C	N	O	0
			154	88	11	55	
5	B	1	Total	C	N	O	0
			154	88	11	55	
5	B	1	Total	C	N	O	0
			154	88	11	55	
5	B	1	Total	C	N	O	0
			154	88	11	55	
5	B	1	Total	C	N	O	0
			154	88	11	55	
5	B	1	Total	C	N	O	0
			154	88	11	55	
5	B	1	Total	C	N	O	0
			154	88	11	55	
5	B	1	Total	C	N	O	0
			154	88	11	55	

- Molecule 6 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			30	18	12	
6	A	1	Total	C	O	0
			30	18	12	
6	A	1	Total	C	O	0
			30	18	12	
6	B	1	Total	C	O	0
			30	18	12	
6	B	1	Total	C	O	0
			30	18	12	
6	B	1	Total	C	O	0
			30	18	12	

- Molecule 7 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).

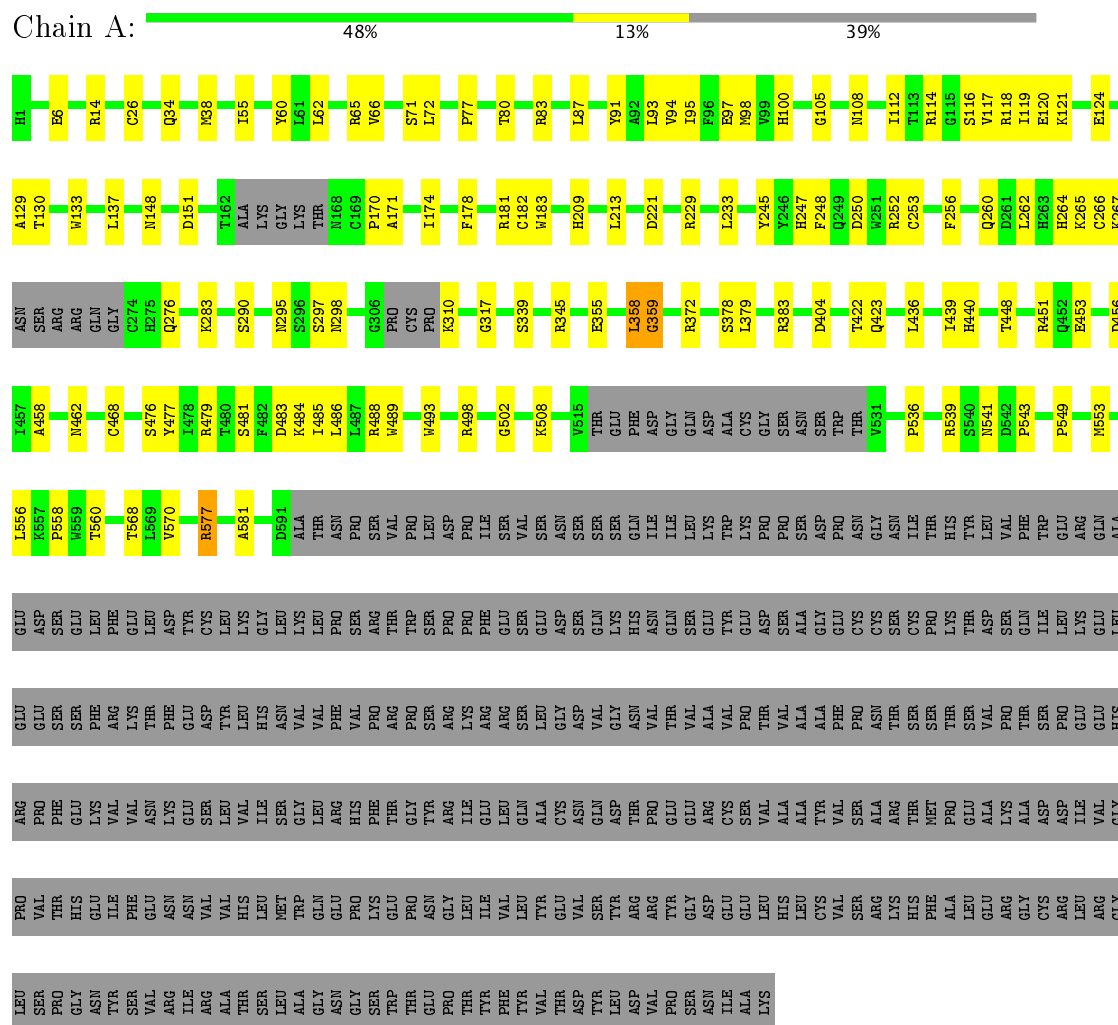


Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			11	6	5	
7	B	1	Total	C	O	0
			11	6	5	

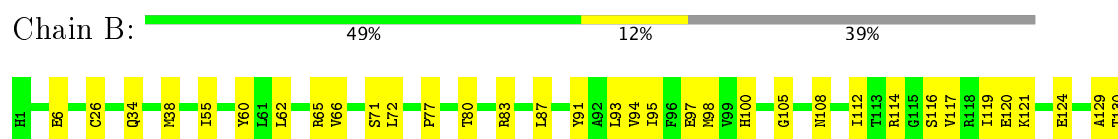
### 3 Residue-property plots

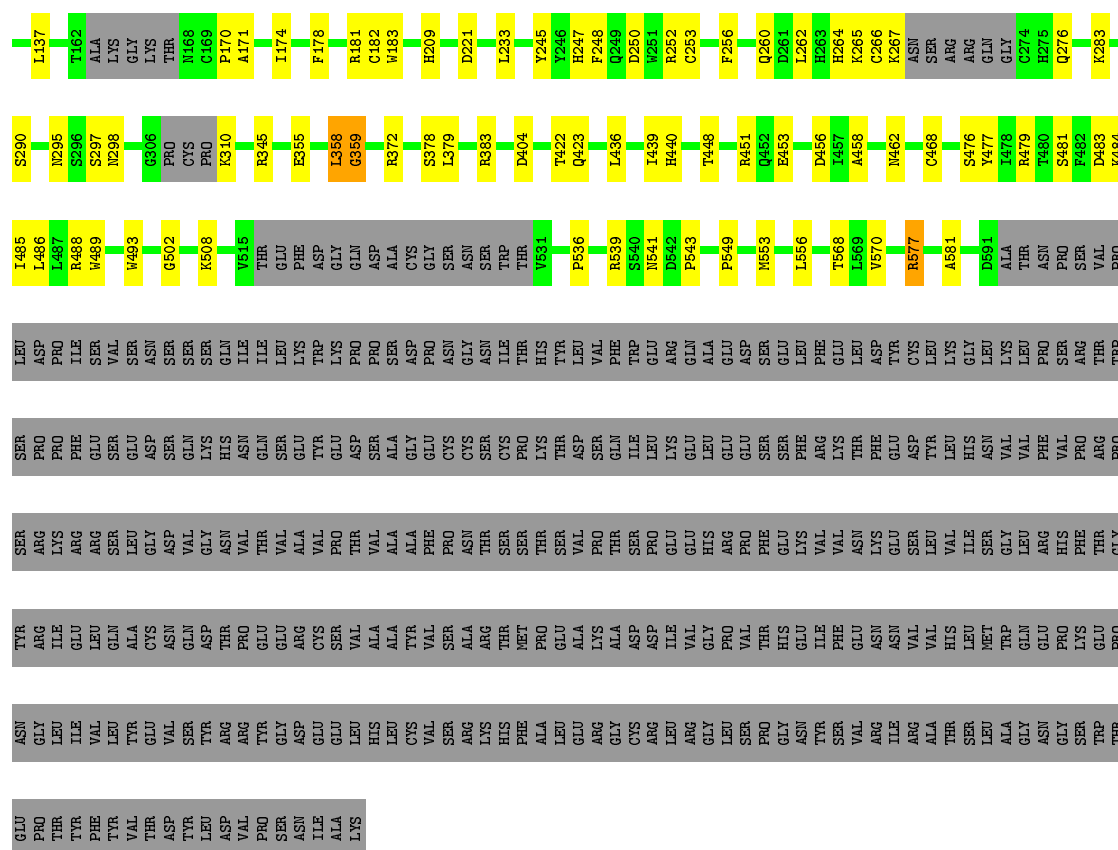
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

#### • Molecule 1: Insulin receptor



#### • Molecule 1: Insulin receptor





- Molecule 2: Insulin receptor

Chain M: 77% 20%



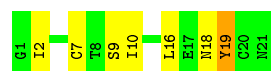
- Molecule 2: Insulin receptor

Chain P: 77% 17% 7%



- Molecule 3: Insulin A chain

Chain K: 67% 29% 5%



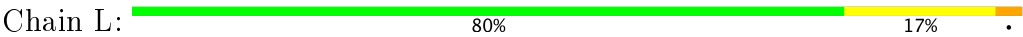
- Molecule 3: Insulin A chain

Chain N: 76% 19% 5%

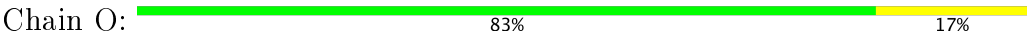




● Molecule 4: Insulin B chain



● Molecule 4: Insulin B chain



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	147436	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45.5	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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  >2	RMSZ	# Z  >2
1	A	0.41	0/4646	0.59	0/6290
1	B	0.41	0/4646	0.59	0/6290
2	M	0.48	0/259	0.62	0/349
2	P	0.48	0/259	0.62	0/349
3	K	0.47	0/164	0.61	0/220
3	N	0.48	0/164	0.61	0/220
4	L	0.40	0/247	0.61	0/332
4	O	0.40	0/247	0.61	0/332
All	All	0.42	0/10632	0.59	0/14382

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
2	M	0	1
2	P	0	1
3	K	0	1
3	N	0	1
4	L	0	1
4	O	0	1
All	All	0	10

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	358	LEU	Peptide
1	A	468	CYS	Peptide
1	B	358	LEU	Peptide
1	B	468	CYS	Peptide
3	K	19	TYR	Peptide
4	L	21	GLU	Peptide
2	M	715	VAL	Peptide
3	N	19	TYR	Peptide
4	O	21	GLU	Peptide
2	P	715	VAL	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4540	0	4423	72	0
1	B	4540	0	4423	64	0
2	M	253	0	245	6	0
2	P	253	0	245	8	0
3	K	163	0	151	6	0
3	N	163	0	151	3	0
4	L	240	0	232	4	0
4	O	240	0	232	2	0
5	A	154	0	135	0	0
5	B	154	0	135	0	0
6	A	30	0	30	0	0
6	B	30	0	30	0	0
7	A	11	0	10	0	0
7	B	11	0	10	0	0
All	All	10782	0	10452	156	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 7.

All (156) 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)
2:M:692:ILE:HG22	2:M:692:ILE:O	1.72	0.87
2:P:692:ILE:O	2:P:692:ILE:HG22	1.73	0.87
1:B:290:SER:HG	1:B:310:LYS:N	1.79	0.81
1:A:290:SER:HG	1:A:310:LYS:N	1.79	0.81
1:A:541:ASN:HB2	1:A:543:PRO:HD2	1.71	0.72
1:B:541:ASN:HB2	1:B:543:PRO:HD2	1.71	0.71
2:M:692:ILE:CG2	2:M:692:ILE:O	2.41	0.68
2:P:692:ILE:O	2:P:692:ILE:CG2	2.42	0.68
1:B:256:PHE:O	1:B:260:GLN:HB2	1.95	0.67
1:A:256:PHE:O	1:A:260:GLN:HB2	1.95	0.66
1:B:570:VAL:HG23	1:B:577:ARG:HH21	1.61	0.65
1:A:14:ARG:HH22	2:P:716:PRO:HG3	1.62	0.64
3:N:2:ILE:HD13	2:P:710:HIS:HB3	1.79	0.64
1:A:570:VAL:HG23	1:A:577:ARG:HH21	1.61	0.64
1:B:247:HIS:HB2	1:B:283:LYS:HG2	1.80	0.62
1:A:247:HIS:HB2	1:A:283:LYS:HG2	1.80	0.62
3:K:7:CYS:O	4:L:5:HIS:ND1	2.31	0.62
1:A:485:ILE:HG13	1:A:556:LEU:HD21	1.81	0.62
1:A:295:ASN:ND2	1:A:298:ASN:OD1	2.32	0.62
1:B:295:ASN:ND2	1:B:298:ASN:OD1	2.32	0.62
1:B:422:THR:HG22	1:B:423:GLN:HG3	1.83	0.61
1:B:83:ARG:NH2	1:B:250:ASP:O	2.34	0.60
1:A:422:THR:HG22	1:A:423:GLN:HG3	1.83	0.60
1:A:83:ARG:NH2	1:A:250:ASP:O	2.35	0.60
1:B:485:ILE:HG13	1:B:556:LEU:HD21	1.82	0.60
1:B:355:GLU:OE2	1:B:383:ARG:NH2	2.35	0.59
2:M:710:HIS:HB3	3:K:2:ILE:HD13	1.83	0.59
1:A:485:ILE:HB	1:A:553:MET:HB2	1.85	0.58
1:B:485:ILE:HB	1:B:553:MET:HB2	1.85	0.58
1:A:266:CYS:HB2	1:A:276:GLN:HE21	1.69	0.58
1:A:290:SER:OG	1:A:310:LYS:N	2.36	0.58
1:B:290:SER:OG	1:B:310:LYS:N	2.36	0.57
1:B:38:MET:HB2	1:B:66:VAL:HG13	1.86	0.57
1:B:266:CYS:HB2	1:B:276:GLN:HE21	1.69	0.57
1:A:355:GLU:OE2	1:A:383:ARG:NH2	2.35	0.57
1:A:498:ARG:HH21	4:L:8:GLY:HA3	1.69	0.57
1:A:87:LEU:HD11	1:A:114:ARG:HG2	1.87	0.57
1:B:87:LEU:HD11	1:B:114:ARG:HG2	1.87	0.56
1:A:38:MET:HB2	1:A:66:VAL:HG13	1.86	0.56
1:B:65:ARG:NE	1:B:97:GLU:OE1	2.40	0.55
1:A:65:ARG:NE	1:A:97:GLU:OE1	2.40	0.54
4:O:26:TYR:HA	2:P:716:PRO:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:PRO:O	1:A:108:ASN:ND2	2.33	0.54
1:B:378:SER:OG	1:B:379:LEU:N	2.40	0.53
1:A:378:SER:OG	1:A:379:LEU:N	2.40	0.53
3:K:16:LEU:HA	3:K:19:TYR:HD2	1.72	0.53
1:B:77:PRO:O	1:B:108:ASN:ND2	2.33	0.53
3:N:16:LEU:HA	3:N:19:TYR:HD2	1.73	0.53
1:B:502:GLY:HA2	1:B:536:PRO:HD3	1.91	0.52
1:A:479:ARG:HB3	1:A:486:LEU:HB3	1.91	0.52
1:B:479:ARG:HB3	1:B:486:LEU:HB3	1.91	0.52
1:A:502:GLY:HA2	1:A:536:PRO:HD3	1.92	0.52
1:B:453:GLU:N	1:B:456:ASP:OD2	2.42	0.52
1:B:493:TRP:CE2	1:B:539:ARG:HD3	2.45	0.52
4:L:25:PHE:HD2	4:L:27:THR:H	1.57	0.52
4:O:25:PHE:HD2	4:O:27:THR:H	1.57	0.51
1:B:436:LEU:HA	1:B:439:ILE:HD12	1.92	0.51
1:A:93:LEU:HB3	1:A:117:VAL:HG22	1.92	0.51
1:A:493:TRP:CE2	1:A:539:ARG:HD3	2.45	0.51
2:P:693:LEU:HA	2:P:696:LEU:HD23	1.92	0.51
1:A:458:ALA:O	1:A:462:ASN:ND2	2.44	0.51
1:B:458:ALA:O	1:B:462:ASN:ND2	2.44	0.51
2:M:693:LEU:HA	2:M:696:LEU:HD23	1.92	0.51
1:B:295:ASN:ND2	1:B:297:SER:OG	2.44	0.51
1:A:120:GLU:HG2	1:A:121:LYS:HG3	1.92	0.51
1:B:93:LEU:HB3	1:B:117:VAL:HG22	1.92	0.51
1:A:95:ILE:HB	1:A:119:ILE:HG12	1.93	0.51
1:B:264:HIS:HA	1:B:267:LYS:HE2	1.92	0.51
1:A:436:LEU:HA	1:A:439:ILE:HD12	1.92	0.50
1:A:295:ASN:ND2	1:A:297:SER:OG	2.44	0.50
1:B:120:GLU:HG2	1:B:121:LYS:HG3	1.92	0.50
1:A:264:HIS:HA	1:A:267:LYS:HE2	1.93	0.49
3:K:10:ILE:HG21	4:L:3:ASN:HD22	1.77	0.49
1:A:55:ILE:O	1:A:80:THR:N	2.40	0.49
1:B:95:ILE:HB	1:B:119:ILE:HG12	1.93	0.49
1:B:233:LEU:HD13	1:B:253:CYS:HB2	1.95	0.49
1:A:453:GLU:N	1:A:456:ASP:OD2	2.42	0.49
1:A:91:TYR:HA	1:A:116:SER:H	1.78	0.48
1:A:62:LEU:HA	1:A:94:VAL:HB	1.95	0.48
1:B:436:LEU:O	1:B:440:HIS:ND1	2.41	0.48
1:B:62:LEU:HA	1:B:94:VAL:HB	1.95	0.48
1:B:477:TYR:HB3	1:B:488:ARG:HB2	1.96	0.48
1:A:233:LEU:HD13	1:A:253:CYS:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ARG:HA	1:A:404:ASP:HB3	1.96	0.47
1:A:477:TYR:HB3	1:A:488:ARG:HB2	1.96	0.47
1:A:170:PRO:HG2	1:A:181:ARG:HB2	1.97	0.47
1:B:489:TRP:CE2	1:B:549:PRO:HG2	2.50	0.47
1:A:65:ARG:N	1:A:98:MET:SD	2.88	0.47
1:B:372:ARG:HA	1:B:404:ASP:HB3	1.96	0.47
1:B:91:TYR:HA	1:B:116:SER:H	1.78	0.47
1:B:65:ARG:N	1:B:98:MET:SD	2.88	0.47
1:A:436:LEU:O	1:A:440:HIS:ND1	2.41	0.47
1:B:256:PHE:O	1:B:260:GLN:CB	2.62	0.47
1:A:448:THR:HB	1:A:451:ARG:HD2	1.97	0.46
1:B:448:THR:HB	1:B:451:ARG:HD2	1.97	0.46
1:B:170:PRO:HG2	1:B:181:ARG:HB2	1.97	0.46
1:A:34:GLN:HE21	1:A:60:TYR:HE2	1.63	0.46
1:A:489:TRP:CE2	1:A:549:PRO:HG2	2.50	0.46
1:B:171:ALA:HB1	1:B:178:PHE:HB3	1.97	0.46
1:B:34:GLN:HG2	1:B:62:LEU:HB3	1.98	0.46
1:B:358:LEU:HB3	1:B:359:GLY:H	1.61	0.46
3:K:9:SER:OG	3:K:10:ILE:N	2.49	0.46
1:A:171:ALA:HB1	1:A:178:PHE:HB3	1.98	0.46
1:A:248:PHE:HD2	1:A:252:ARG:HE	1.64	0.46
1:A:256:PHE:O	1:A:260:GLN:CB	2.62	0.46
1:A:34:GLN:HG2	1:A:62:LEU:HB3	1.98	0.46
1:B:481:SER:HB2	1:B:484:LYS:H	1.81	0.46
1:B:34:GLN:HE21	1:B:60:TYR:HE2	1.63	0.45
1:A:129:ALA:O	1:A:181:ARG:NH1	2.50	0.45
1:A:476:SER:H	1:A:489:TRP:HA	1.81	0.45
1:B:476:SER:H	1:B:489:TRP:HA	1.81	0.45
1:B:245:TYR:HB3	1:B:253:CYS:HB3	1.99	0.45
1:A:262:LEU:HA	1:A:265:LYS:HE2	1.98	0.45
1:A:87:LEU:HD23	1:A:87:LEU:HA	1.83	0.45
1:B:129:ALA:O	1:B:181:ARG:NH1	2.50	0.45
1:A:481:SER:HB2	1:A:484:LYS:H	1.81	0.45
1:A:476:SER:N	1:A:488:ARG:O	2.50	0.45
1:B:476:SER:N	1:B:488:ARG:O	2.50	0.45
1:B:262:LEU:HA	1:B:265:LYS:HE2	1.99	0.44
1:A:209:HIS:HB2	1:A:221:ASP:N	2.32	0.44
1:B:130:THR:HB	1:B:182:CYS:H	1.82	0.44
3:N:9:SER:OG	3:N:10:ILE:N	2.49	0.44
1:A:130:THR:HB	1:A:182:CYS:H	1.82	0.44
1:B:209:HIS:HB2	1:B:221:ASP:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:PHE:HD2	1:B:252:ARG:HE	1.64	0.44
1:B:105:GLY:HA2	1:B:183:TRP:HB3	2.00	0.44
1:B:71:SER:OG	1:B:72:LEU:N	2.51	0.44
1:B:568:THR:OG1	1:B:581:ALA:N	2.50	0.44
1:A:105:GLY:HA2	1:A:183:TRP:HB3	2.00	0.44
2:M:715:VAL:HG13	2:M:718:PRO:HG2	2.00	0.44
2:P:715:VAL:HG13	2:P:718:PRO:HG2	2.00	0.43
1:A:245:TYR:HB3	1:A:253:CYS:HB3	1.99	0.43
1:A:358:LEU:HB3	1:A:359:GLY:H	1.61	0.43
1:B:55:ILE:O	1:B:80:THR:N	2.40	0.43
1:A:14:ARG:HH12	2:P:716:PRO:HG2	1.84	0.43
1:B:483:ASP:HA	1:B:556:LEU:HB2	2.01	0.43
1:A:483:ASP:HA	1:A:556:LEU:HB2	2.01	0.43
1:A:71:SER:OG	1:A:72:LEU:N	2.51	0.43
1:B:87:LEU:HD23	1:B:87:LEU:HA	1.83	0.42
1:A:100:HIS:HA	1:A:124:GLU:HG3	2.02	0.42
1:B:174:ILE:HG13	1:B:181:ARG:HH21	1.85	0.41
1:A:6:GLU:H	1:A:26:CYS:HA	1.85	0.41
1:B:100:HIS:HA	1:B:124:GLU:HG3	2.02	0.41
1:A:174:ILE:HG13	1:A:181:ARG:HH21	1.85	0.41
1:A:558:PRO:O	1:A:560:THR:OG1	2.31	0.41
1:B:6:GLU:H	1:B:26:CYS:HA	1.85	0.41
1:A:317:GLY:O	1:A:339:SER:N	2.47	0.41
1:B:112:ILE:HD12	1:B:137:LEU:HD11	2.02	0.41
1:A:568:THR:OG1	1:A:581:ALA:N	2.50	0.41
1:B:477:TYR:O	1:B:488:ARG:N	2.50	0.41
2:M:718:PRO:HB3	3:K:18:ASN:HB3	2.02	0.40
1:A:112:ILE:HD12	1:A:137:LEU:HD11	2.02	0.40
1:A:148:ASN:N	1:A:151:ASP:OD2	2.54	0.40
1:A:133:TRP:O	1:A:137:LEU:N	2.43	0.40
1:A:213:LEU:HB2	1:A:229:ARG:HA	2.04	0.40
1:A:91:TYR:CE1	1:A:118:ARG:HB2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM



entries.

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	552/917 (60%)	483 (88%)	68 (12%)	1 (0%)	51	85
1	B	552/917 (60%)	481 (87%)	70 (13%)	1 (0%)	51	85
2	M	28/30 (93%)	22 (79%)	5 (18%)	1 (4%)	4	35
2	P	28/30 (93%)	22 (79%)	5 (18%)	1 (4%)	4	35
3	K	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
3	N	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
4	L	28/30 (93%)	24 (86%)	4 (14%)	0	100	100
4	O	28/30 (93%)	24 (86%)	4 (14%)	0	100	100
All	All	1254/1996 (63%)	1092 (87%)	158 (13%)	4 (0%)	48	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	716	PRO
2	P	716	PRO
1	A	359	GLY
1	B	359	GLY

### 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 PDB entries followed by that with respect to all EM entries.

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	513/831 (62%)	510 (99%)	3 (1%)	89	94
1	B	513/831 (62%)	510 (99%)	3 (1%)	89	94
2	M	29/30 (97%)	29 (100%)	0	100	100
2	P	29/30 (97%)	29 (100%)	0	100	100
3	K	20/20 (100%)	20 (100%)	0	100	100
3	N	20/20 (100%)	20 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	25/25 (100%)	24 (96%)	1 (4%)	36	67
4	O	25/25 (100%)	24 (96%)	1 (4%)	36	67
All	All	1174/1812 (65%)	1166 (99%)	8 (1%)	87	93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	345	ARG
1	A	508	LYS
1	A	577	ARG
1	B	345	ARG
1	B	508	LYS
1	B	577	ARG
4	L	3	ASN
4	O	3	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	HIS
1	A	78	ASN
1	A	108	ASN
1	A	276	GLN
1	A	410	GLN
1	A	417	HIS
1	B	1	HIS
1	B	78	ASN
1	B	108	ASN
1	B	276	GLN
1	B	410	GLN
1	B	417	HIS
4	L	3	ASN
4	O	3	ASN
4	O	10	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

30 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	1001	1,5,6	14,14,15	0.31	0	15,19,21	0.91	1 (6%)
5	NAG	A	1002	5	14,14,15	0.34	0	15,19,21	0.42	0
6	FUC	A	1003	5	9,10,11	0.75	0	13,14,16	0.93	0
5	NAG	A	1004	1,5	14,14,15	0.19	0	15,19,21	1.06	1 (6%)
5	NAG	A	1005	5,7	14,14,15	0.43	0	15,19,21	0.74	1 (6%)
7	BMA	A	1006	5	11,11,12	0.85	0	13,15,17	0.88	1 (7%)
5	NAG	A	1007	1,5,6	14,14,15	0.23	0	15,19,21	0.60	0
5	NAG	A	1008	5	14,14,15	0.29	0	15,19,21	0.50	0
6	FUC	A	1009	5	9,10,11	0.76	0	13,14,16	0.76	0
5	NAG	A	1010	1,5	14,14,15	0.82	1 (7%)	15,19,21	0.81	0
5	NAG	A	1011	5	14,14,15	0.21	0	15,19,21	0.57	0
5	NAG	A	1012	1,6	14,14,15	0.32	0	15,19,21	0.69	0
6	FUC	A	1013	5	9,10,11	0.97	0	13,14,16	1.10	2 (15%)
5	NAG	A	1014	1	14,14,15	0.30	0	15,19,21	0.60	0
5	NAG	A	1015	-	14,14,15	0.38	0	15,19,21	0.46	0
5	NAG	B	1001	1,5,6	14,14,15	0.31	0	15,19,21	0.87	1 (6%)
5	NAG	B	1002	5	14,14,15	0.35	0	15,19,21	0.43	0
6	FUC	B	1003	5	9,10,11	0.76	0	13,14,16	0.89	0
5	NAG	B	1004	1,5	14,14,15	0.23	0	15,19,21	1.10	1 (6%)
5	NAG	B	1005	5,7	14,14,15	0.46	0	15,19,21	0.75	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BMA	B	1006	5	11,11,12	0.84	0	13,15,17	0.89	1 (7%)
5	NAG	B	1007	1,5,6	14,14,15	0.30	0	15,19,21	0.61	0
5	NAG	B	1008	5	14,14,15	0.27	0	15,19,21	0.51	0
6	FUC	B	1009	5	9,10,11	0.81	0	13,14,16	0.74	0
5	NAG	B	1010	1,5	14,14,15	0.78	1 (7%)	15,19,21	0.82	0
5	NAG	B	1011	5	14,14,15	0.21	0	15,19,21	0.58	0
5	NAG	B	1012	1,6	14,14,15	0.25	0	15,19,21	0.71	0
6	FUC	B	1013	5	9,10,11	0.96	0	13,14,16	1.14	3 (23%)
5	NAG	B	1014	1	14,14,15	0.23	0	15,19,21	0.62	0
5	NAG	B	1015	-	14,14,15	0.40	0	15,19,21	0.46	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	NAG	A	1001	1,5,6	-	0/6/23/26	0/1/1/1
5	NAG	A	1002	5	-	0/6/23/26	0/1/1/1
6	FUC	A	1003	5	-	0/0/17/20	0/1/1/1
5	NAG	A	1004	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1005	5,7	-	0/6/23/26	0/1/1/1
7	BMA	A	1006	5	-	0/2/19/22	0/1/1/1
5	NAG	A	1007	1,5,6	-	0/6/23/26	0/1/1/1
5	NAG	A	1008	5	-	0/6/23/26	0/1/1/1
6	FUC	A	1009	5	-	0/0/17/20	0/1/1/1
5	NAG	A	1010	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1011	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1012	1,6	-	0/6/23/26	0/1/1/1
6	FUC	A	1013	5	-	0/0/17/20	0/1/1/1
5	NAG	A	1014	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1015	-	-	0/6/23/26	0/1/1/1
5	NAG	B	1001	1,5,6	-	0/6/23/26	0/1/1/1
5	NAG	B	1002	5	-	0/6/23/26	0/1/1/1
6	FUC	B	1003	5	-	0/0/17/20	0/1/1/1
5	NAG	B	1004	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1005	5,7	-	0/6/23/26	0/1/1/1
7	BMA	B	1006	5	-	0/2/19/22	0/1/1/1
5	NAG	B	1007	1,5,6	-	0/6/23/26	0/1/1/1
5	NAG	B	1008	5	-	0/6/23/26	0/1/1/1
6	FUC	B	1009	5	-	0/0/17/20	0/1/1/1
5	NAG	B	1010	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1011	5	-	0/6/23/26	0/1/1/1
5	NAG	B	1012	1,6	-	0/6/23/26	0/1/1/1
6	FUC	B	1013	5	-	0/0/17/20	0/1/1/1
5	NAG	B	1014	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1015	-	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1010	NAG	O5-C1	-2.85	1.39	1.43
5	B	1010	NAG	O5-C1	-2.61	1.39	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1006	BMA	O2-C2-C3	-2.28	105.69	110.17
7	A	1006	BMA	O2-C2-C3	-2.28	105.70	110.17
6	B	1013	FUC	O5-C5-C4	2.02	112.95	109.62
6	A	1013	FUC	C1-O5-C5	2.08	116.99	112.39
6	B	1013	FUC	C1-O5-C5	2.15	117.14	112.39
5	A	1005	NAG	C1-O5-C5	2.24	115.25	112.17
6	A	1013	FUC	O2-C2-C1	2.24	113.74	109.18
5	B	1005	NAG	C1-O5-C5	2.31	115.35	112.17
6	B	1013	FUC	O2-C2-C1	2.32	113.89	109.18
5	B	1001	NAG	C1-O5-C5	2.91	116.17	112.17
5	A	1001	NAG	C1-O5-C5	3.04	116.35	112.17
5	A	1004	NAG	C1-O5-C5	3.12	116.47	112.17
5	B	1004	NAG	C1-O5-C5	3.22	116.60	112.17

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.