



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:08 PM GMT

PDB ID : 1JMJ  
Title : Crystal Structure of Native Heparin Cofactor II  
Authors : Baglin, T.P.; Carrell, R.W.; Church, F.C.; Huntington, J.A.  
Deposited on : 2001-07-18  
Resolution : 2.35 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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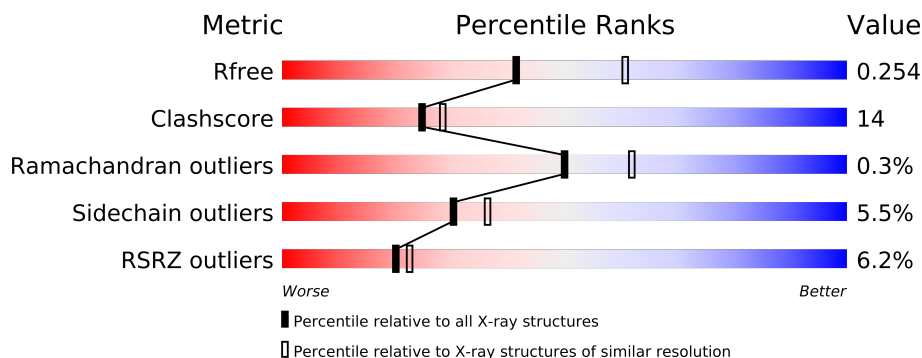
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	480	
1	B	480	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	B	481	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 6723 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

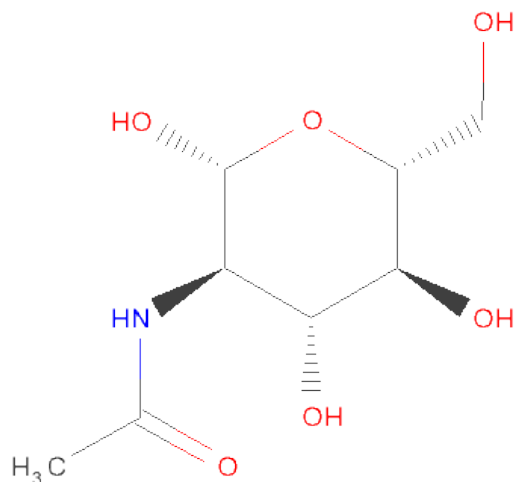
- Molecule 1 is a protein called HEPARIN COFACTOR II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	20	0	0
			3228	2069	560	579	20			
1	B	387	Total	C	N	O	S	14	0	0
			3144	2017	549	558	20			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0

- Molecule 5 is water.

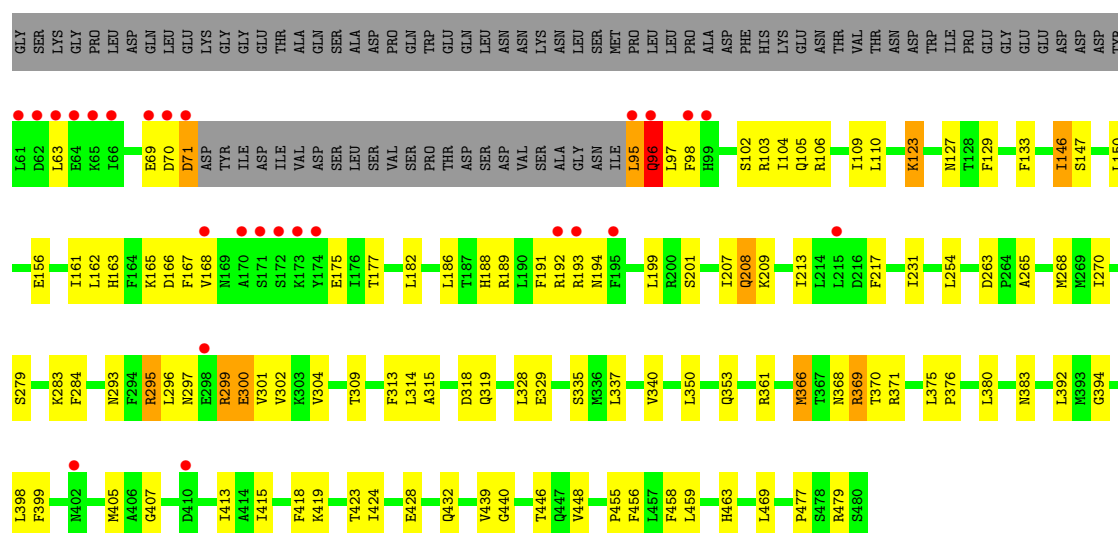
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	157	Total 157	O 157	0	0
5	B	140	Total 140	O 140	0	0

### 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.

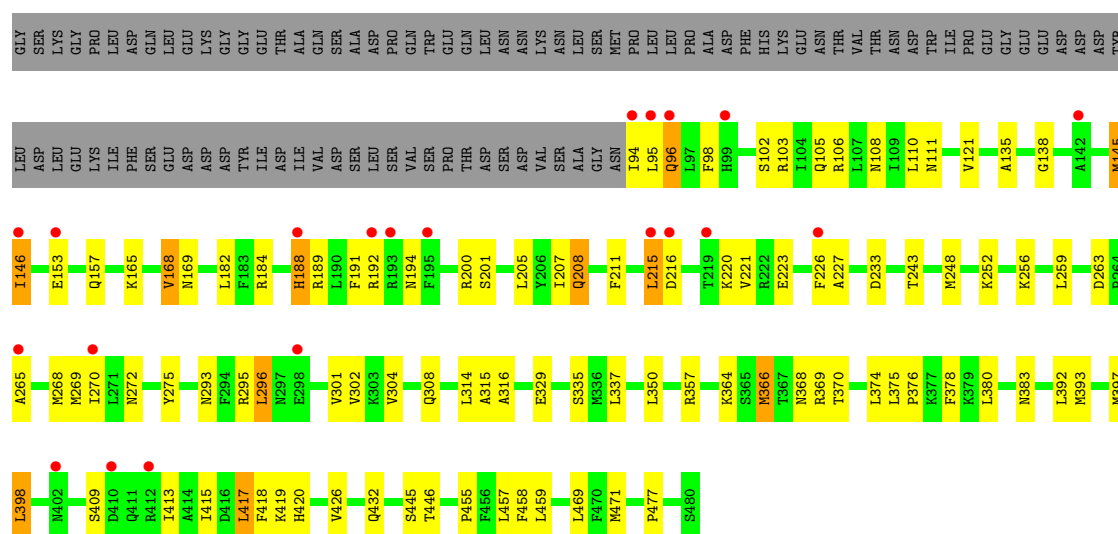
#### • Molecule 1: HEPARIN COFACTOR II

Chain A: 



#### • Molecule 1: HEPARIN COFACTOR II

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.73Å 80.00Å 92.24Å 90.00° 102.04° 90.00°	Depositor
Resolution (Å)	25.00 – 2.35 25.05 – 2.35	Depositor EDS
% Data completeness (in resolution range)	88.0 (25.00-2.35) 88.1 (25.05-2.35)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.36Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.208 , 0.255 0.208 , 0.254	Depositor DCC
$R_{free}$ test set	994 reflections (2.60%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 45.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 39171 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6723	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BMA, 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	A	0.36	0/3291	0.62	0/4431
1	B	0.35	0/3207	0.63	0/4320
All	All	0.36	0/6498	0.62	0/8751

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3228	0	3279	95	0
1	B	3144	0	3207	84	0
2	A	39	0	34	4	0
3	B	14	0	13	0	0
4	A	1	0	0	0	0
5	A	157	0	0	2	0
5	B	140	0	0	1	0
All	All	6723	0	6533	179	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 14.

All (179) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:314:LEU:HB3	1:A:366:MET:HG2	1.48	0.96
1:B:96:GLN:H	1:B:96:GLN:NE2	1.64	0.95
1:A:405:MET:HE1	1:A:413:ILE:HG13	1.52	0.92
1:A:110:LEU:HD12	1:A:167:PHE:HB2	1.59	0.84
2:A:482:NAG:H3	2:A:482:NAG:H82	1.61	0.83
1:A:329:GLU:OE1	1:A:335:SER:HB3	1.80	0.82
1:B:221:VAL:HG13	1:B:227:ALA:HB3	1.60	0.82
1:B:192:ARG:HG3	1:B:192:ARG:HH11	1.43	0.82
1:A:70:ASP:HB3	5:A:631:HOH:O	1.82	0.80
1:B:314:LEU:HB3	1:B:366:MET:HG2	1.65	0.78
1:B:135:ALA:H	1:B:420:HIS:CE1	2.03	0.77
1:A:95:LEU:O	1:A:96:GLN:HB3	1.87	0.73
1:B:398:LEU:HD11	1:B:415:ILE:HD12	1.70	0.73
1:A:370:THR:HG22	1:A:446:THR:HG22	1.69	0.72
1:B:329:GLU:OE2	1:B:335:SER:HB3	1.90	0.71
1:B:295:ARG:O	1:B:455:PRO:HD3	1.90	0.71
1:B:96:GLN:H	1:B:96:GLN:HE21	1.38	0.70
1:B:350:LEU:HD11	1:B:457:LEU:HD12	1.72	0.70
1:B:215:LEU:HD13	1:B:216:ASP:N	2.08	0.69
1:A:293:ASN:HB3	1:A:301:VAL:HG11	1.74	0.68
1:B:145:MET:HG2	1:B:221:VAL:HG22	1.75	0.67
1:B:304:VAL:HG11	1:B:477:PRO:HG2	1.77	0.67
1:A:63:LEU:HD22	1:A:63:LEU:H	1.63	0.64
1:A:375:LEU:HD12	1:A:376:PRO:HD2	1.79	0.64
1:A:95:LEU:HD22	1:A:98:PHE:CD1	2.32	0.64
1:B:216:ASP:OD1	1:B:220:LYS:HE2	1.98	0.63
1:B:207:ILE:HD13	1:B:268:MET:HG3	1.80	0.63
1:A:69:GLU:OE2	1:B:445:SER:HB2	1.98	0.63
1:A:95:LEU:O	1:A:96:GLN:CB	2.47	0.63
1:B:375:LEU:HD12	1:B:376:PRO:HD2	1.81	0.63
1:A:405:MET:HE1	1:A:413:ILE:CG1	2.26	0.62
1:B:146:ILE:HG13	1:B:270:ILE:HD11	1.80	0.62
1:B:138:GLY:C	1:B:272:ASN:HD21	2.03	0.62
1:B:98:PHE:CD2	1:B:106:ARG:HD3	2.34	0.62
1:B:252:LYS:HD2	1:B:275:TYR:OH	2.00	0.61
1:B:98:PHE:HZ	1:B:110:LEU:HD21	1.63	0.61
1:B:94:ILE:O	1:B:357:ARG:NH2	2.31	0.61
1:A:405:MET:CE	1:A:413:ILE:HG13	2.26	0.61
1:B:350:LEU:CD1	1:B:457:LEU:HD12	2.31	0.60
1:B:94:ILE:HG22	1:B:95:LEU:HG	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:153:GLU:O	1:B:157:GLN:HG3	2.03	0.59
1:B:135:ALA:H	1:B:420:HIS:HE1	1.46	0.58
1:A:96:GLN:HE21	1:A:96:GLN:HA	1.66	0.58
1:A:370:THR:CG2	1:A:446:THR:HG22	2.32	0.58
1:B:208:GLN:HA	1:B:208:GLN:OE1	2.03	0.58
1:B:192:ARG:CG	1:B:192:ARG:HH11	2.15	0.58
1:B:296:LEU:HD22	1:B:302:VAL:HG13	1.84	0.58
1:B:272:ASN:HD22	1:B:420:HIS:HD2	1.50	0.58
1:B:184:ARG:HG3	1:B:188:HIS:CE1	2.38	0.57
1:A:304:VAL:HG11	1:A:477:PRO:HG2	1.85	0.57
1:A:63:LEU:HD22	1:A:63:LEU:N	2.19	0.56
1:A:102:SER:OG	1:A:104:ILE:HG22	2.05	0.56
1:B:96:GLN:N	1:B:96:GLN:NE2	2.46	0.56
1:A:299:ARG:HB2	1:A:299:ARG:NH1	2.20	0.56
1:B:192:ARG:HG3	1:B:192:ARG:NH1	2.19	0.56
1:A:146:ILE:HG13	1:A:270:ILE:HD11	1.87	0.56
1:A:209:LYS:HB2	1:A:231:ILE:HD11	1.87	0.56
1:A:299:ARG:O	1:A:300:GLU:HB3	2.05	0.56
1:A:70:ASP:O	1:A:71:ASP:HB2	2.06	0.55
1:B:308:GLN:HG3	1:B:374:LEU:HG	1.88	0.55
1:A:405:MET:HE1	1:A:413:ILE:O	2.06	0.55
1:B:417:LEU:HD11	1:B:419:LYS:HB2	1.87	0.55
1:A:95:LEU:O	1:A:95:LEU:HG	2.05	0.55
1:B:95:LEU:HD22	1:B:98:PHE:CE1	2.41	0.55
1:A:192:ARG:HH11	1:A:192:ARG:HG3	1.73	0.54
1:A:188:HIS:O	1:A:192:ARG:HG2	2.08	0.54
1:A:168:VAL:HG13	1:A:175:GLU:HA	1.90	0.54
1:B:398:LEU:CD1	1:B:415:ILE:HD12	2.38	0.53
1:B:205:LEU:HD12	1:B:269:MET:O	2.09	0.53
1:B:370:THR:HG22	1:B:446:THR:HG22	1.91	0.53
1:A:147:SER:HA	1:A:150:LEU:HG	1.91	0.53
1:A:337:LEU:O	1:A:458:PHE:HA	2.09	0.53
1:A:398:LEU:HD13	1:A:398:LEU:O	2.09	0.53
1:A:368:ASN:HD22	2:A:481:NAG:H83	1.74	0.52
1:A:263:ASP:OD1	1:A:265:ALA:HB3	2.09	0.52
1:B:102:SER:O	1:B:106:ARG:HG3	2.10	0.52
1:A:110:LEU:CD1	1:A:167:PHE:HB2	2.37	0.51
1:A:405:MET:HE1	1:A:413:ILE:C	2.31	0.51
1:A:335:SER:OG	1:A:463:HIS:HE1	1.92	0.51
1:B:96:GLN:N	1:B:96:GLN:HE21	2.05	0.51
1:B:184:ARG:O	1:B:188:HIS:ND1	2.44	0.51
1:A:175:GLU:HG3	1:A:177:THR:CG2	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:94:ILE:HG22	1:B:95:LEU:N	2.26	0.50
1:A:295:ARG:O	1:A:455:PRO:HD3	2.11	0.50
1:A:208:GLN:HE21	1:A:208:GLN:CA	2.24	0.50
1:B:208:GLN:OE1	1:B:233:ASP:HA	2.11	0.50
1:A:69:GLU:CD	1:B:445:SER:HB2	2.32	0.50
1:A:209:LYS:CB	1:A:231:ILE:HD11	2.42	0.50
1:B:316:ALA:N	1:B:366:MET:HE2	2.27	0.49
1:B:184:ARG:HD3	1:B:223:GLU:O	2.11	0.49
1:A:299:ARG:HH11	1:A:299:ARG:CB	2.26	0.49
1:A:104:ILE:HG23	1:A:105:GLN:N	2.26	0.49
1:A:254:LEU:HD21	1:A:423:THR:HB	1.95	0.49
1:B:188:HIS:CE1	1:B:226:PHE:CZ	3.00	0.49
1:B:368:ASN:O	1:B:369:ARG:HD2	2.12	0.49
1:A:313:PHE:HB2	1:A:371:ARG:HD2	1.94	0.49
1:B:215:LEU:O	1:B:215:LEU:HD22	2.12	0.48
1:B:296:LEU:HD22	1:B:302:VAL:CG1	2.43	0.48
1:A:315:ALA:HB3	1:A:371:ARG:CZ	2.43	0.48
1:A:439:VAL:HG22	1:A:440:GLY:N	2.28	0.48
2:A:482:NAG:C3	2:A:482:NAG:H82	2.39	0.48
1:A:371:ARG:HG2	1:A:448:VAL:CG2	2.43	0.48
1:A:314:LEU:HD23	1:A:368:ASN:HA	1.96	0.48
2:A:482:NAG:H3	2:A:482:NAG:C8	2.39	0.48
1:A:279:SER:HB2	1:A:283:LYS:NZ	2.29	0.48
1:B:188:HIS:O	1:B:192:ARG:HG2	2.14	0.48
1:A:123:LYS:HD2	5:A:605:HOH:O	2.13	0.48
1:A:63:LEU:H	1:A:63:LEU:CD2	2.27	0.47
1:B:153:GLU:HB3	1:B:397:MET:CE	2.45	0.47
1:A:103:ARG:HG2	1:A:182:LEU:HD11	1.97	0.47
1:A:104:ILE:HD11	1:A:186:LEU:HB2	1.96	0.47
1:A:217:PHE:HB2	1:A:407:GLY:O	2.15	0.47
1:B:145:MET:HE1	1:B:146:ILE:HG12	1.96	0.46
1:B:383:ASN:HD21	1:B:419:LYS:HE3	1.80	0.46
1:A:318:ASP:OD2	1:A:361:ARG:NH2	2.40	0.46
1:A:192:ARG:NH1	1:A:194:ASN:OD1	2.48	0.46
1:A:127:ASN:HB3	1:A:129:PHE:CE1	2.50	0.46
1:A:405:MET:CE	1:A:413:ILE:O	2.64	0.46
1:A:268:MET:HG2	1:A:415:ILE:HD13	1.98	0.46
1:B:293:ASN:HB3	1:B:301:VAL:HG11	1.97	0.46
1:A:424:ILE:HA	1:A:432:GLN:HE22	1.80	0.46
1:A:368:ASN:O	1:A:369:ARG:HD3	2.16	0.45
1:A:162:LEU:O	1:A:163:HIS:HB2	2.16	0.45
1:A:297:ASN:ND2	1:A:300:GLU:HG2	2.31	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:248:MET:SD	1:B:256:LYS:HG2	2.56	0.45
1:A:207:ILE:HD12	1:A:213:ILE:HG12	1.97	0.45
1:A:192:ARG:CG	1:A:192:ARG:HH11	2.29	0.45
1:B:192:ARG:HH12	1:B:194:ASN:CG	2.19	0.45
1:B:357:ARG:HH11	1:B:357:ARG:HG2	1.82	0.45
1:A:268:MET:HE2	1:A:415:ILE:HD13	1.98	0.45
1:A:95:LEU:HD23	1:A:97:LEU:HB2	1.99	0.45
1:A:105:GLN:O	1:A:109:ILE:HG13	2.17	0.44
1:A:284:PHE:O	1:A:428:GLU:HB3	2.16	0.44
1:A:133:PHE:CZ	1:A:424:ILE:HB	2.52	0.44
1:A:156:GLU:OE1	1:A:165:LYS:NZ	2.40	0.44
1:A:370:THR:HG22	1:A:446:THR:HA	1.99	0.44
1:B:98:PHE:HZ	1:B:110:LEU:CD2	2.30	0.44
1:B:215:LEU:C	1:B:215:LEU:HD22	2.38	0.44
1:A:398:LEU:HD12	1:A:399:PHE:CE2	2.53	0.44
1:A:315:ALA:HB3	1:A:371:ARG:NH1	2.34	0.43
1:B:103:ARG:HG2	1:B:182:LEU:HD11	2.00	0.43
1:B:458:PHE:O	1:B:471:MET:HA	2.18	0.43
1:A:95:LEU:CD2	1:A:97:LEU:HB2	2.49	0.43
1:A:161:ILE:HD11	1:A:394:GLY:HA3	2.00	0.43
1:B:108:ASN:HA	1:B:111:ASN:HB2	2.00	0.43
1:B:102:SER:OG	1:B:105:GLN:HG3	2.19	0.43
1:A:301:VAL:HG12	1:A:302:VAL:N	2.32	0.43
1:B:378:PHE:CZ	1:B:426:VAL:HG21	2.53	0.43
1:B:200:ARG:NH2	1:B:252:LYS:HE3	2.34	0.42
1:A:340:VAL:HG22	1:A:456:PHE:HB3	2.01	0.42
1:A:299:ARG:HB2	1:A:299:ARG:HH11	1.82	0.42
1:B:191:PHE:CZ	1:B:201:SER:HB2	2.54	0.42
1:A:104:ILE:CG2	1:A:105:GLN:N	2.82	0.42
1:B:409:SER:HB3	1:B:413:ILE:HD11	2.02	0.42
1:B:315:ALA:C	1:B:366:MET:HG3	2.41	0.41
1:A:98:PHE:CD2	1:A:106:ARG:HD3	2.55	0.41
1:A:208:GLN:HA	1:A:208:GLN:NE2	2.35	0.41
1:A:129:PHE:HD2	1:A:479:ARG:NH1	2.18	0.41
1:A:191:PHE:CZ	1:A:201:SER:HB2	2.55	0.41
1:B:145:MET:HE1	1:B:146:ILE:HA	2.01	0.41
1:B:145:MET:CE	1:B:146:ILE:HA	2.51	0.41
1:A:284:PHE:HA	1:A:309:THR:HB	2.02	0.41
1:B:121:VAL:HG21	1:B:393:MET:HG2	2.03	0.41
1:B:263:ASP:OD1	1:B:265:ALA:HB3	2.20	0.41
1:B:337:LEU:O	1:B:458:PHE:HA	2.20	0.41
1:B:165:LYS:O	1:B:169:ASN:HB2	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:383:ASN:OD1	1:A:419:LYS:HE3	2.21	0.41
1:A:175:GLU:HG3	1:A:177:THR:HG23	2.02	0.41
1:B:243:THR:HG21	1:B:259:LEU:CD1	2.51	0.41
1:A:319:GLN:HG3	1:B:364:LYS:O	2.21	0.41
1:A:268:MET:CE	1:A:415:ILE:HD13	2.50	0.41
1:A:424:ILE:HG23	1:A:424:ILE:O	2.20	0.41
1:B:192:ARG:CG	1:B:192:ARG:NH1	2.74	0.40
1:A:192:ARG:O	1:A:193:ARG:C	2.59	0.40
1:B:168:VAL:CG2	1:B:169:ASN:N	2.84	0.40
1:A:370:THR:CG2	1:A:446:THR:HA	2.51	0.40
1:B:191:PHE:CE1	1:B:201:SER:HB2	2.56	0.40
1:B:211:PHE:CD1	1:B:211:PHE:N	2.89	0.40
1:B:189:ARG:HB2	5:B:576:HOH:O	2.22	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	393/480 (82%)	374 (95%)	17 (4%)	2 (0%)	38	45
1	B	385/480 (80%)	375 (97%)	10 (3%)	0	100	100
All	All	778/960 (81%)	749 (96%)	27 (4%)	2 (0%)	50	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	300	GLU

### 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	360/433 (83%)	338 (94%)	22 (6%)	26	31
1	B	350/433 (81%)	333 (95%)	17 (5%)	35	44
All	All	710/866 (82%)	671 (94%)	39 (6%)	30	36

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ASP
1	A	95	LEU
1	A	96	GLN
1	A	123	LYS
1	A	146	ILE
1	A	166	ASP
1	A	189	ARG
1	A	199	LEU
1	A	208	GLN
1	A	295	ARG
1	A	296	LEU
1	A	299	ARG
1	A	328	LEU
1	A	350	LEU
1	A	353	GLN
1	A	366	MET
1	A	369	ARG
1	A	380	LEU
1	A	392	LEU
1	A	418	PHE
1	A	459	LEU
1	A	469	LEU
1	B	96	GLN
1	B	145	MET
1	B	146	ILE
1	B	168	VAL
1	B	188	HIS
1	B	208	GLN
1	B	215	LEU
1	B	296	LEU
1	B	366	MET
1	B	380	LEU
1	B	392	LEU

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Mol	Chain	Res	Type
1	B	398	LEU
1	B	417	LEU
1	B	418	PHE
1	B	432	GLN
1	B	459	LEU
1	B	469	LEU

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

Mol	Chain	Res	Type
1	A	96	GLN
1	A	208	GLN
1	A	292	HIS
1	A	363	GLN
1	A	463	HIS
1	B	96	GLN
1	B	169	ASN
1	B	272	ASN
1	B	411	GLN
1	B	420	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

3 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
2	NAG	A	481	1,2	12,14,15	0.58	0	15,19,21	0.68	0
2	NAG	A	482	2	12,14,15	0.60	0	15,19,21	0.98	1 (6%)
2	BMA	A	483	2	10,11,12	0.40	0	11,15,17	0.29	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
2	NAG	A	481	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	482	2	-	2/6/23/26	0/1/1/1
2	BMA	A	483	2	-	0/2/19/22	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(°)	Ideal(°)
2	A	482	NAG	C3-C4-C5	2.25	114.23	110.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	482	NAG	O7-C7-N2-C2
2	A	482	NAG	C8-C7-N2-C2

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	B	481	1	12,14,15	0.49	0	15,19,21	0.60	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
3	NAG	B	481	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	481	NAG	O7-C7-N2-C2
3	B	481	NAG	C8-C7-N2-C2

There are no ring outliers.

## 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	A	397/480 (82%)	0.32	26 (6%) 18 21	19, 34, 69, 95	7 (1%)
1	B	387/480 (80%)	0.28	21 (5%) 25 28	17, 34, 60, 85	4 (1%)
All	All	784/960 (81%)	0.30	47 (5%) 20 24	17, 34, 62, 95	11 (1%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	LEU	7.0
1	B	94	ILE	6.2
1	B	215	LEU	5.8
1	A	62	ASP	5.6
1	A	70	ASP	5.4
1	A	193	ARG	5.3
1	A	172	SER	4.5
1	A	64	GLU	4.4
1	B	195	PHE	4.3
1	A	99	HIS	4.2
1	A	171	SER	4.0
1	A	65	LYS	4.0
1	A	215	LEU	3.9
1	B	193	ARG	3.8
1	A	96	GLN	3.7
1	A	195	PHE	3.7
1	A	402	ASN	3.7
1	A	71	ASP	3.5
1	A	173	LYS	3.4
1	B	402	ASN	3.3
1	B	226	PHE	3.3
1	A	66	ILE	3.1
1	B	96	GLN	3.0
1	A	98	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	412	ARG	3.0
1	B	188	HIS	2.9
1	A	410	ASP	2.9
1	B	298	GLU	2.9
1	A	95	LEU	2.8
1	B	216	ASP	2.7
1	B	410	ASP	2.7
1	A	170	ALA	2.7
1	B	99	HIS	2.6
1	A	298	GLU	2.6
1	A	168	VAL	2.6
1	A	192	ARG	2.6
1	A	174	TYR	2.5
1	B	265	ALA	2.5
1	B	270	ILE	2.5
1	A	63	LEU	2.4
1	B	219	THR	2.3
1	A	69	GLU	2.2
1	B	192	ARG	2.2
1	B	142	ALA	2.2
1	B	146	ILE	2.2
1	B	95	LEU	2.1
1	B	153	GLU	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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	481	14/15	0.35	11.42	61,65,71,80	0
2	BMA	A	483	11/12	0.61	-	96,97,97,97	0
2	NAG	A	482	14/15	0.64	-	86,90,93,95	0

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	B	481	14/15	0.34	5.23	51,56,58,59	0
4	CA	A	501	1/1	0.06	-3.61	44,44,44,44	0

## 6.5 Other polymers

There are no such residues in this entry.