



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:12 PM UTC

PDB ID : 1F45 / pdb_00001f45
Title : HUMAN INTERLEUKIN-12
Authors : Yoon, C.; Johnston, S.C.; Tang, J.; Tobin, J.F.; Somers, W.S.
Deposited on : 2000-06-07
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

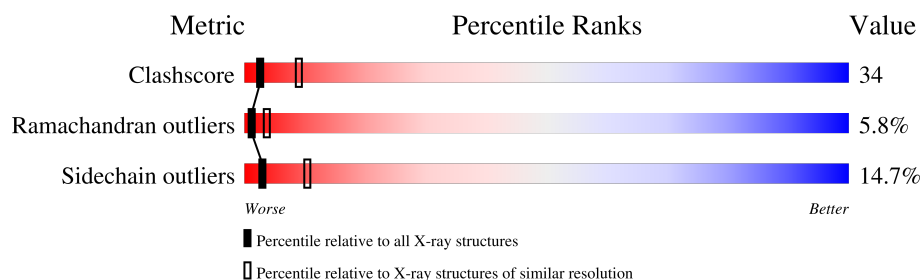
1 Overall quality at a glance

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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	306	
2	B	197	
3	C	3	

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
3	MAN	C	3	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3348 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 INTERLEUKIN-12 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2226	1411	357	446	12			

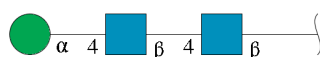
- Molecule 2 is a protein called INTERLEUKIN-12 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1062	679	176	193	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	191	MET	THR	engineered mutation	UNP P29459

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 is water.

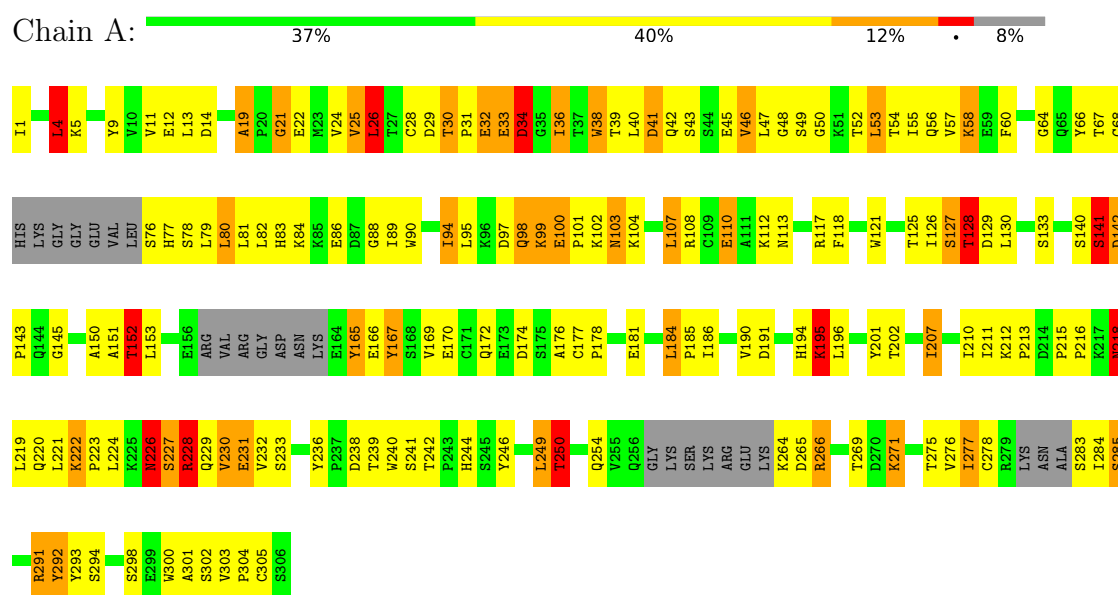
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		
4	B	7	Total	O	0	0
			7	7		

3 Residue-property plots

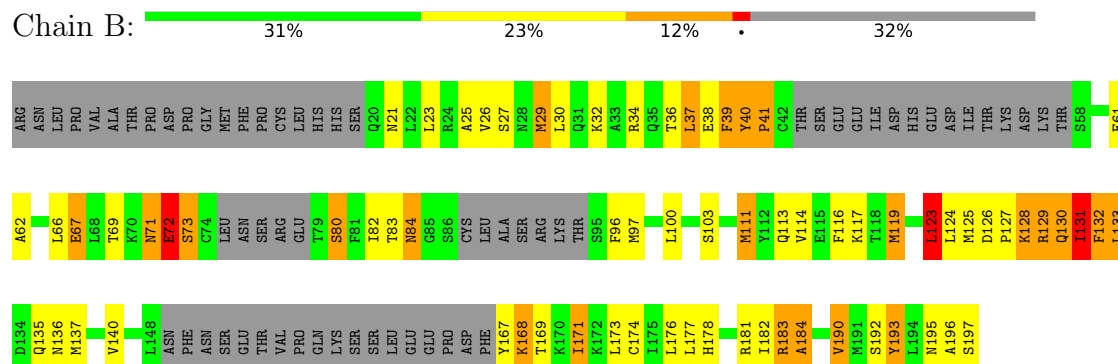
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: INTERLEUKIN-12 BETA CHAIN



• Molecule 2: INTERLEUKIN-12 ALPHA CHAIN



• Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
MAG3

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	112.90Å 154.20Å 101.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3348	wwPDB-VP
Average B, all atoms (Å ²)	64.0	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	0.98	2/2280 (0.1%)	1.44	43/3104 (1.4%)
2	B	1.24	5/1072 (0.5%)	1.50	22/1435 (1.5%)
All	All	1.07	7/3352 (0.2%)	1.46	65/4539 (1.4%)

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	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	111	MET	SD-CE	9.56	2.03	1.79
2	B	119	MET	SD-CE	7.26	1.97	1.79
2	B	171	ILE	CA-CB	6.64	1.62	1.54
2	B	190	VAL	CA-CB	6.01	1.62	1.54
1	A	293	TYR	CA-C	-5.54	1.49	1.52
2	B	114	VAL	CA-CB	5.46	1.60	1.54
1	A	94	ILE	CA-CB	-5.21	1.46	1.54

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	GLY	N-CA-C	11.65	127.39	111.54
2	B	40	TYR	CA-C-N	11.38	134.07	119.84
2	B	40	TYR	C-N-CA	11.38	134.07	119.84
1	A	228	ARG	N-CA-C	-10.73	99.64	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ALA	N-CA-C	10.31	125.01	108.41
1	A	88	GLY	CA-C-N	-8.87	110.82	123.06
1	A	88	GLY	C-N-CA	-8.87	110.82	123.06
1	A	292	TYR	N-CA-C	8.84	125.01	114.04
2	B	96	PHE	N-CA-C	-8.56	101.17	111.69
1	A	21	GLY	N-CA-C	-8.00	101.15	112.60
1	A	212	LYS	CA-C-N	-7.64	112.33	120.66
1	A	212	LYS	C-N-CA	-7.64	112.33	120.66
2	B	80	SER	N-CA-C	7.63	119.79	110.41
1	A	14	ASP	N-CA-C	-7.43	98.67	109.59
1	A	278	CYS	N-CA-C	7.34	120.45	110.55
1	A	19	ALA	CA-C-N	7.32	127.35	119.89
1	A	19	ALA	C-N-CA	7.32	127.35	119.89
2	B	21	ASN	N-CA-C	-7.09	104.10	112.89
1	A	152	THR	N-CA-C	6.94	119.07	108.52
1	A	184	LEU	CA-C-N	-6.94	113.65	120.52
1	A	184	LEU	C-N-CA	-6.94	113.65	120.52
1	A	190	VAL	N-CA-C	6.93	117.81	108.11
1	A	36	ILE	N-CA-C	6.91	118.43	108.48
1	A	226	ASN	N-CA-C	-6.75	103.01	110.91
2	B	36	THR	N-CA-C	6.41	121.25	113.17
1	A	174	ASP	N-CA-C	6.29	124.19	110.80
1	A	222	LYS	CA-C-N	6.21	126.23	119.89
1	A	222	LYS	C-N-CA	6.21	126.23	119.89
2	B	131	ILE	N-CA-C	-6.12	96.62	109.34
1	A	41	ASP	CB-CA-C	-6.10	109.53	116.54
2	B	195	ASN	N-CA-C	-6.03	97.95	110.80
2	B	73	SER	N-CA-C	5.99	123.56	110.80
1	A	25	VAL	N-CA-C	5.97	117.24	106.61
2	B	177	LEU	N-CA-C	-5.94	104.80	111.28
1	A	26	LEU	N-CA-C	5.90	118.83	108.56
1	A	150	ALA	N-CA-C	5.88	118.69	108.76
1	A	53	LEU	N-CA-C	-5.84	102.78	110.43
2	B	131	ILE	CA-C-N	-5.81	110.44	121.54
2	B	131	ILE	C-N-CA	-5.81	110.44	121.54
2	B	184	ALA	N-CA-C	-5.80	104.95	111.28
1	A	39	THR	N-CA-C	5.79	118.50	109.52
1	A	250	THR	N-CA-C	-5.78	100.29	109.59
2	B	128	LYS	N-CA-C	-5.77	105.40	113.37
1	A	4	LEU	N-CA-C	-5.76	98.52	110.80
1	A	125	THR	N-CA-C	-5.76	106.29	113.38
1	A	38	TRP	N-CA-C	5.73	117.72	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	GLU	N-CA-C	5.70	118.07	107.99
1	A	238	ASP	N-CA-C	5.68	118.24	111.71
2	B	168	LYS	N-CA-C	-5.68	104.30	111.11
1	A	215	PRO	N-CA-C	5.59	117.52	110.70
1	A	249	LEU	N-CA-C	-5.53	100.87	109.72
2	B	29	MET	N-CA-C	-5.47	105.39	111.36
2	B	132	PHE	N-CA-C	5.44	122.39	110.80
2	B	193	TYR	N-CA-C	-5.43	105.44	111.36
1	A	118	PHE	N-CA-C	5.40	117.29	108.76
1	A	185	PRO	N-CA-C	5.37	119.13	111.13
1	A	41	ASP	N-CA-C	5.35	116.44	108.31
2	B	37	LEU	N-CA-C	5.31	118.86	112.38
2	B	25	ALA	N-CA-C	-5.29	105.52	111.28
2	B	27	SER	N-CA-C	5.27	117.03	111.28
1	A	293	TYR	O-C-N	5.12	124.62	120.83
1	A	94	ILE	N-CA-C	5.06	118.16	111.17
1	A	216	PRO	N-CA-C	-5.06	103.16	111.15
2	B	123	LEU	N-CA-C	5.05	121.57	110.80
1	A	218	ASN	N-CA-C	5.04	121.53	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246	TYR	Sidechain

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	2226	0	2102	166	0
2	B	1062	0	1095	56	0
3	C	39	0	34	6	0
4	A	14	0	0	1	0
4	B	7	0	0	1	0
All	All	3348	0	3231	224	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 34.

All (224) 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:B:111:MET:SD	2:B:111:MET:CE	2.03	1.46
2:B:80:SER:HA	2:B:97:MET:HE2	1.32	1.09
2:B:130:GLN:OE1	2:B:130:GLN:HA	1.53	1.06
1:A:36:ILE:HB	1:A:50:GLY:O	1.67	0.92
2:B:130:GLN:NE2	2:B:131:ILE:HG12	1.85	0.91
1:A:108:ARG:HD2	1:A:121:TRP:CZ2	2.12	0.85
2:B:71:ASN:C	2:B:71:ASN:HD22	1.86	0.83
1:A:40:LEU:O	1:A:43:SER:HB3	1.78	0.83
1:A:46:VAL:HG12	1:A:46:VAL:O	1.79	0.82
1:A:227:SER:OG	1:A:229:GLN:HB3	1.79	0.82
2:B:80:SER:CA	2:B:97:MET:HE2	2.09	0.82
3:C:2:NAG:O3	3:C:2:NAG:H83	1.80	0.81
1:A:133:SER:HB3	1:A:191:ASP:HB2	1.64	0.80
1:A:221:LEU:HD13	1:A:303:VAL:HG11	1.63	0.79
1:A:219:LEU:O	1:A:220:GLN:HG2	1.83	0.78
2:B:123:LEU:HD21	2:B:173:LEU:HD22	1.64	0.78
2:B:80:SER:HA	2:B:97:MET:CE	2.12	0.78
1:A:29:ASP:O	1:A:76:SER:HB2	1.86	0.75
1:A:219:LEU:C	1:A:220:GLN:HG2	2.12	0.74
1:A:236:TYR:CE2	1:A:249:LEU:HD12	2.22	0.74
1:A:22:GLU:O	1:A:57:VAL:HG22	1.88	0.74
1:A:22:GLU:H	1:A:57:VAL:HG23	1.54	0.73
2:B:127:PRO:C	2:B:129:ARG:H	1.94	0.72
1:A:128:THR:OG1	1:A:129:ASP:N	2.19	0.72
1:A:79:LEU:O	1:A:80:LEU:HD23	1.90	0.70
1:A:33:GLU:O	1:A:34:ASP:O	2.09	0.70
2:B:39:PHE:HD1	2:B:39:PHE:H	1.40	0.69
1:A:141:SER:O	1:A:142:ASP:HB3	1.91	0.69
1:A:97:ASP:C	1:A:99:LYS:H	1.99	0.69
1:A:250:THR:HG22	1:A:291:ARG:HA	1.75	0.69
2:B:126:ASP:OD1	2:B:128:LYS:HD3	1.92	0.69
1:A:81:LEU:HD22	1:A:196:LEU:HA	1.74	0.68
2:B:39:PHE:CD1	2:B:39:PHE:N	2.60	0.68
1:A:140:SER:O	1:A:143:PRO:HD3	1.93	0.68
2:B:130:GLN:HE22	2:B:131:ILE:HG12	1.59	0.67
1:A:303:VAL:HG13	1:A:304:PRO:HD2	1.76	0.67
1:A:152:THR:O	1:A:167:TYR:HA	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ASP:O	1:A:36:ILE:HG13	1.95	0.66
1:A:40:LEU:HD13	1:A:66:TYR:CE2	2.31	0.66
2:B:71:ASN:HD22	2:B:72:GLU:N	1.93	0.66
1:A:25:VAL:HG13	1:A:52:THR:HG23	1.78	0.65
1:A:221:LEU:HD12	1:A:221:LEU:N	2.10	0.65
1:A:117:ARG:HB2	1:A:172:GLN:NE2	2.12	0.65
1:A:222:LYS:HE2	1:A:231:GLU:OE1	1.97	0.65
1:A:226:ASN:O	1:A:227:SER:HB2	1.96	0.64
1:A:103:ASN:O	1:A:104:LYS:HB2	1.97	0.64
1:A:54:THR:O	1:A:55:ILE:HG23	1.98	0.64
1:A:221:LEU:CD1	1:A:303:VAL:HG11	2.28	0.64
1:A:108:ARG:HD2	1:A:121:TRP:CH2	2.32	0.64
1:A:213:PRO:O	1:A:298:SER:HB2	1.97	0.63
1:A:101:PRO:HD3	1:A:108:ARG:NH2	2.13	0.63
1:A:11:VAL:HG13	1:A:22:GLU:OE1	1.99	0.62
1:A:40:LEU:HD13	1:A:66:TYR:HE2	1.65	0.62
2:B:67:GLU:H	2:B:67:GLU:CD	2.05	0.62
1:A:220:GLN:C	1:A:221:LEU:HD12	2.25	0.61
1:A:223:PRO:O	1:A:224:LEU:HD23	2.01	0.61
2:B:130:GLN:HE22	2:B:131:ILE:CG1	2.14	0.60
1:A:12:GLU:HG2	1:A:90:TRP:CH2	2.36	0.60
1:A:79:LEU:HD12	1:A:80:LEU:H	1.67	0.60
3:C:2:NAG:H4	3:C:3:MAN:O2	2.02	0.60
1:A:167:TYR:CD1	1:A:167:TYR:N	2.68	0.60
1:A:30:THR:O	1:A:32:GLU:N	2.35	0.59
1:A:228:ARG:HG3	1:A:228:ARG:HH11	1.66	0.59
1:A:285:SER:HB2	1:A:300:TRP:CE3	2.37	0.59
1:A:81:LEU:CD2	1:A:196:LEU:HA	2.32	0.59
1:A:9:TYR:HB2	1:A:80:LEU:CD2	2.32	0.59
1:A:1:ILE:HG23	1:A:1:ILE:O	2.00	0.59
1:A:264:LYS:HG3	1:A:265:ASP:H	1.68	0.58
1:A:55:ILE:CD1	1:A:66:TYR:HE1	2.17	0.58
1:A:100:GLU:CB	1:A:101:PRO:HD3	2.34	0.58
2:B:127:PRO:C	2:B:129:ARG:N	2.62	0.58
2:B:136:ASN:O	2:B:140:VAL:HG23	2.04	0.58
1:A:19:ALA:O	1:A:58:LYS:NZ	2.35	0.57
1:A:264:LYS:CG	1:A:265:ASP:H	2.17	0.57
1:A:167:TYR:N	1:A:167:TYR:HD1	2.00	0.57
2:B:130:GLN:HB3	2:B:135:GLN:OE1	2.04	0.57
2:B:196:ALA:O	2:B:197:SER:HB3	2.04	0.57
1:A:52:THR:O	1:A:52:THR:HG22	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ARG:HB2	1:A:172:GLN:HE22	1.68	0.57
1:A:283:SER:HB3	1:A:303:VAL:O	2.05	0.57
1:A:46:VAL:HG13	1:A:48:GLY:O	2.04	0.57
1:A:128:THR:HG1	1:A:129:ASP:H	1.49	0.57
1:A:126:ILE:N	1:A:126:ILE:HD12	2.19	0.56
2:B:126:ASP:OD1	2:B:126:ASP:C	2.47	0.56
1:A:213:PRO:O	1:A:298:SER:CB	2.53	0.56
1:A:292:TYR:O	2:B:34:ARG:HD3	2.05	0.56
1:A:9:TYR:HB2	1:A:80:LEU:HD22	1.88	0.56
1:A:97:ASP:C	1:A:99:LYS:N	2.63	0.56
1:A:79:LEU:HD12	1:A:80:LEU:N	2.21	0.55
1:A:32:GLU:O	1:A:32:GLU:HG2	2.06	0.55
1:A:219:LEU:H	1:A:219:LEU:HD12	1.72	0.55
1:A:221:LEU:HD21	1:A:284:ILE:HD12	1.90	0.55
1:A:29:ASP:C	1:A:76:SER:HB2	2.32	0.54
2:B:131:ILE:O	2:B:135:GLN:NE2	2.40	0.54
2:B:174:CYS:O	2:B:178:HIS:HD2	1.89	0.54
1:A:41:ASP:OD1	1:A:42:GLN:HG2	2.07	0.54
1:A:28:CYS:SG	1:A:30:THR:CG2	2.96	0.54
1:A:29:ASP:HB3	1:A:76:SER:OG	2.08	0.53
1:A:221:LEU:N	1:A:221:LEU:CD1	2.72	0.53
1:A:227:SER:HG	1:A:229:GLN:HB3	1.73	0.53
1:A:55:ILE:CD1	1:A:66:TYR:CE1	2.91	0.53
1:A:26:LEU:N	1:A:26:LEU:HD23	2.24	0.53
1:A:169:VAL:HG22	1:A:170:GLU:N	2.24	0.52
1:A:38:TRP:CZ3	1:A:68:CYS:HB3	2.45	0.52
2:B:130:GLN:HE22	2:B:131:ILE:CD1	2.23	0.52
1:A:83:HIS:HD2	3:C:1:NAG:O6	1.93	0.52
1:A:25:VAL:CG1	1:A:52:THR:HG23	2.40	0.52
1:A:117:ARG:HE	1:A:172:GLN:HE21	1.56	0.52
1:A:141:SER:O	1:A:142:ASP:CB	2.59	0.51
1:A:38:TRP:HB2	1:A:48:GLY:O	2.11	0.51
1:A:113:ASN:ND2	1:A:239:THR:O	2.42	0.50
1:A:21:GLY:HA3	1:A:57:VAL:O	2.11	0.50
1:A:186:ILE:HD12	1:A:207:ILE:CD1	2.41	0.50
1:A:55:ILE:HD11	1:A:66:TYR:HE1	1.76	0.50
1:A:38:TRP:CE3	1:A:68:CYS:HB3	2.46	0.50
1:A:55:ILE:HD11	1:A:66:TYR:CE1	2.47	0.50
1:A:117:ARG:HE	1:A:172:GLN:NE2	2.09	0.50
1:A:165:TYR:CD1	1:A:165:TYR:N	2.80	0.49
1:A:126:ILE:HG21	1:A:130:LEU:HG	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLU:OE1	2:B:183:ARG:NH1	2.46	0.49
2:B:126:ASP:O	2:B:129:ARG:N	2.45	0.49
1:A:38:TRP:CE2	1:A:53:LEU:HB2	2.47	0.49
1:A:83:HIS:CD2	3:C:1:NAG:O6	2.66	0.49
1:A:140:SER:O	1:A:142:ASP:N	2.46	0.49
1:A:236:TYR:CD2	1:A:249:LEU:HD12	2.47	0.49
1:A:98:GLN:O	1:A:100:GLU:N	2.45	0.48
1:A:11:VAL:HA	4:A:516:HOH:O	2.12	0.48
1:A:201:TYR:N	1:A:201:TYR:CD1	2.81	0.48
3:C:1:NAG:H83	3:C:1:NAG:O3	2.13	0.48
2:B:71:ASN:C	2:B:71:ASN:ND2	2.57	0.48
1:A:38:TRP:HB3	1:A:53:LEU:HD13	1.95	0.48
1:A:121:TRP:CD1	1:A:121:TRP:N	2.82	0.48
2:B:124:LEU:HB3	2:B:125:MET:HE2	1.95	0.48
3:C:2:NAG:C4	3:C:3:MAN:O2	2.61	0.48
2:B:83:THR:HG22	2:B:84:ASN:H	1.77	0.48
1:A:64:GLY:HA2	1:A:196:LEU:HD21	1.96	0.47
2:B:131:ILE:C	2:B:132:PHE:CD1	2.92	0.47
1:A:55:ILE:HD13	1:A:66:TYR:CE1	2.50	0.47
1:A:55:ILE:HD13	1:A:66:TYR:OH	2.15	0.47
1:A:110:GLU:C	1:A:210:ILE:HD12	2.40	0.47
2:B:128:LYS:HD2	2:B:128:LYS:N	2.29	0.47
1:A:166:GLU:C	1:A:167:TYR:CD1	2.93	0.47
1:A:227:SER:OG	1:A:229:GLN:CB	2.59	0.47
2:B:26:VAL:HG22	2:B:140:VAL:CG1	2.45	0.47
2:B:167:TYR:O	2:B:168:LYS:C	2.58	0.47
2:B:126:ASP:OD1	2:B:128:LYS:HB2	2.14	0.46
1:A:186:ILE:HD12	1:A:207:ILE:HD12	1.97	0.46
2:B:82:ILE:HG13	2:B:193:TYR:HE2	1.80	0.46
2:B:83:THR:HG22	2:B:84:ASN:N	2.29	0.46
1:A:4:LEU:HD23	1:A:5:LYS:HE3	1.98	0.46
1:A:126:ILE:CG2	1:A:127:SER:N	2.78	0.46
1:A:97:ASP:CG	1:A:104:LYS:H	2.23	0.46
1:A:223:PRO:HA	1:A:230:VAL:HG13	1.98	0.46
1:A:242:THR:HG22	1:A:244:HIS:CE1	2.50	0.46
1:A:28:CYS:SG	1:A:30:THR:HG22	2.55	0.45
1:A:229:GLN:HG2	1:A:275:THR:CG2	2.45	0.45
1:A:207:ILE:O	1:A:211:ILE:HG13	2.17	0.45
1:A:97:ASP:O	1:A:99:LYS:N	2.49	0.45
1:A:26:LEU:HD11	1:A:66:TYR:CD1	2.51	0.45
1:A:79:LEU:C	1:A:80:LEU:HD23	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:LEU:HD13	2:B:137:MET:HE3	1.97	0.45
2:B:82:ILE:HG13	2:B:193:TYR:CE2	2.52	0.45
1:A:126:ILE:N	1:A:126:ILE:CD1	2.80	0.45
2:B:131:ILE:O	2:B:132:PHE:CG	2.70	0.45
1:A:218:ASN:CG	1:A:218:ASN:O	2.60	0.44
1:A:40:LEU:O	1:A:41:ASP:OD1	2.35	0.44
1:A:48:GLY:O	1:A:49:SER:OG	2.35	0.44
1:A:94:ILE:O	1:A:94:ILE:HG22	2.17	0.44
1:A:194:HIS:O	1:A:195:LYS:HB2	2.17	0.44
2:B:100:LEU:HA	2:B:100:LEU:HD23	1.73	0.44
1:A:169:VAL:CG2	1:A:170:GLU:N	2.80	0.44
1:A:219:LEU:HD12	1:A:219:LEU:N	2.32	0.44
1:A:219:LEU:HB2	1:A:303:VAL:HG21	1.99	0.44
1:A:64:GLY:HA2	1:A:196:LEU:CD2	2.48	0.44
1:A:165:TYR:N	1:A:165:TYR:HD1	2.15	0.44
2:B:38:GLU:C	2:B:40:TYR:H	2.26	0.44
1:A:45:GLU:O	1:A:47:LEU:N	2.51	0.44
2:B:126:ASP:O	2:B:128:LYS:N	2.51	0.44
2:B:32:LYS:HB2	2:B:32:LYS:HE2	1.71	0.43
1:A:4:LEU:CD2	1:A:5:LYS:HE3	2.47	0.43
1:A:38:TRP:CG	1:A:53:LEU:HD13	2.53	0.43
1:A:195:LYS:HB3	1:A:196:LEU:H	1.42	0.43
1:A:229:GLN:HA	1:A:276:VAL:O	2.18	0.43
1:A:223:PRO:CA	1:A:230:VAL:HG13	2.49	0.43
1:A:26:LEU:CD1	1:A:66:TYR:HD1	2.32	0.43
1:A:26:LEU:CD1	1:A:66:TYR:CD1	3.02	0.43
1:A:38:TRP:CB	1:A:53:LEU:HD13	2.49	0.43
2:B:196:ALA:O	2:B:197:SER:CB	2.66	0.43
1:A:166:GLU:C	1:A:167:TYR:HD1	2.26	0.42
1:A:219:LEU:HD22	1:A:303:VAL:HG23	2.01	0.42
1:A:240:TRP:CG	1:A:241:SER:N	2.87	0.42
2:B:61:GLU:O	2:B:62:ALA:C	2.63	0.42
1:A:84:LYS:O	1:A:90:TRP:HE3	2.03	0.42
2:B:30:LEU:HD21	2:B:184:ALA:HB3	2.00	0.42
2:B:126:ASP:OD1	2:B:128:LYS:CD	2.64	0.42
2:B:29:MET:HE3	2:B:29:MET:HB3	1.90	0.42
2:B:37:LEU:HD23	2:B:37:LEU:HA	1.89	0.42
1:A:152:THR:HG23	1:A:153:LEU:N	2.35	0.42
1:A:107:LEU:N	1:A:107:LEU:CD1	2.83	0.41
1:A:211:ILE:O	1:A:294:SER:OG	2.29	0.41
1:A:95:LEU:HD12	1:A:201:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:HG22	1:A:127:SER:N	2.34	0.41
1:A:285:SER:HA	1:A:301:ALA:O	2.20	0.41
2:B:66:LEU:O	2:B:69:THR:HB	2.19	0.41
1:A:24:VAL:HG23	1:A:57:VAL:HG22	2.02	0.41
1:A:254:GLN:OE1	1:A:266:ARG:NH1	2.54	0.41
1:A:28:CYS:SG	1:A:30:THR:HG21	2.60	0.41
1:A:32:GLU:O	1:A:34:ASP:N	2.54	0.41
2:B:113:GLN:O	2:B:117:LYS:HG3	2.20	0.41
1:A:104:LYS:HD3	1:A:104:LYS:HA	1.86	0.41
2:B:130:GLN:HE22	2:B:131:ILE:HD11	1.85	0.41
1:A:60:PHE:CD1	1:A:82:LEU:HD12	2.56	0.41
1:A:25:VAL:HG13	1:A:52:THR:CG2	2.50	0.40
1:A:177:CYS:HA	1:A:178:PRO:HD3	1.94	0.40
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.91	0.40
1:A:302:SER:O	1:A:303:VAL:HG23	2.21	0.40
1:A:269:THR:OG1	1:A:271:LYS:HG3	2.21	0.40
2:B:181:ARG:HB3	4:B:202:HOH:O	2.22	0.40
1:A:40:LEU:HD11	1:A:64:GLY:HA3	2.03	0.40
1:A:194:HIS:O	1:A:195:LYS:CB	2.68	0.40
1:A:277:ILE:O	1:A:277:ILE:HG22	2.21	0.40
1:A:219:LEU:HA	1:A:233:SER:O	2.21	0.40
2:B:116:PHE:CE2	2:B:176:LEU:HD23	2.56	0.40
2:B:123:LEU:HD12	2:B:123:LEU:HA	1.81	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	A	272/306 (89%)	224 (82%)	31 (11%)	17 (6%)	1	3
2	B	123/197 (62%)	107 (87%)	10 (8%)	6 (5%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	395/503 (78%)	331 (84%)	41 (10%)	23 (6%)	1 4

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	PRO
1	A	33	GLU
1	A	34	ASP
1	A	100	GLU
1	A	142	ASP
2	B	41	PRO
1	A	58	LYS
1	A	78	SER
1	A	99	LYS
1	A	102	LYS
1	A	103	ASN
1	A	151	ALA
1	A	227	SER
2	B	123	LEU
2	B	131	ILE
1	A	98	GLN
1	A	128	THR
1	A	195	LYS
2	B	84	ASN
2	B	72	GLU
1	A	4	LEU
1	A	141	SER
2	B	73	SER

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	252/277 (91%)	216 (86%)	36 (14%)	3 11
2	B	121/183 (66%)	102 (84%)	19 (16%)	2 9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	373/460 (81%)	318 (85%)	55 (15%)	3 10

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	26	LEU
1	A	30	THR
1	A	32	GLU
1	A	34	ASP
1	A	46	VAL
1	A	56	GLN
1	A	67	THR
1	A	77	HIS
1	A	80	LEU
1	A	89	ILE
1	A	107	LEU
1	A	110	GLU
1	A	112	LYS
1	A	127	SER
1	A	128	THR
1	A	141	SER
1	A	152	THR
1	A	165	TYR
1	A	167	TYR
1	A	195	LYS
1	A	202	THR
1	A	207	ILE
1	A	218	ASN
1	A	226	ASN
1	A	228	ARG
1	A	230	VAL
1	A	231	GLU
1	A	232	VAL
1	A	250	THR
1	A	266	ARG
1	A	271	LYS
1	A	277	ILE
1	A	285	SER
1	A	291	ARG
1	A	305	CYS
2	B	23	LEU

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Mol	Chain	Res	Type
2	B	39	PHE
2	B	41	PRO
2	B	67	GLU
2	B	71	ASN
2	B	72	GLU
2	B	103	SER
2	B	119	MET
2	B	123	LEU
2	B	129	ARG
2	B	130	GLN
2	B	131	ILE
2	B	133	LEU
2	B	169	THR
2	B	171	ILE
2	B	182	ILE
2	B	183	ARG
2	B	190	VAL
2	B	192	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	83	HIS
1	A	172	GLN
1	A	226	ASN
1	A	229	GLN
2	B	20	GLN
2	B	21	ASN
2	B	31	GLN
2	B	71	ASN
2	B	120	ASN
2	B	130	GLN
2	B	135	GLN
2	B	178	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 ⓘ

3 monosaccharides 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	$\# Z > 2$
3	NAG	C	1	3,1	14,14,15	0.78	0	17,19,21	1.06	1 (5%)
3	NAG	C	2	3	14,14,15	1.11	1 (7%)	17,19,21	1.20	1 (5%)
3	MAN	C	3	3	11,11,12	0.78	0	15,15,17	1.08	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
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	MAN	C	3	3	1/1/4/5	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	C1-C2	-2.36	1.49	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C2-N2-C7	-3.41	118.32	122.90
3	C	3	MAN	C1-C2-C3	2.80	113.72	109.64
3	C	1	NAG	C2-N2-C7	-2.26	119.88	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	3	MAN	C1

All (6) torsion outliers are listed below:

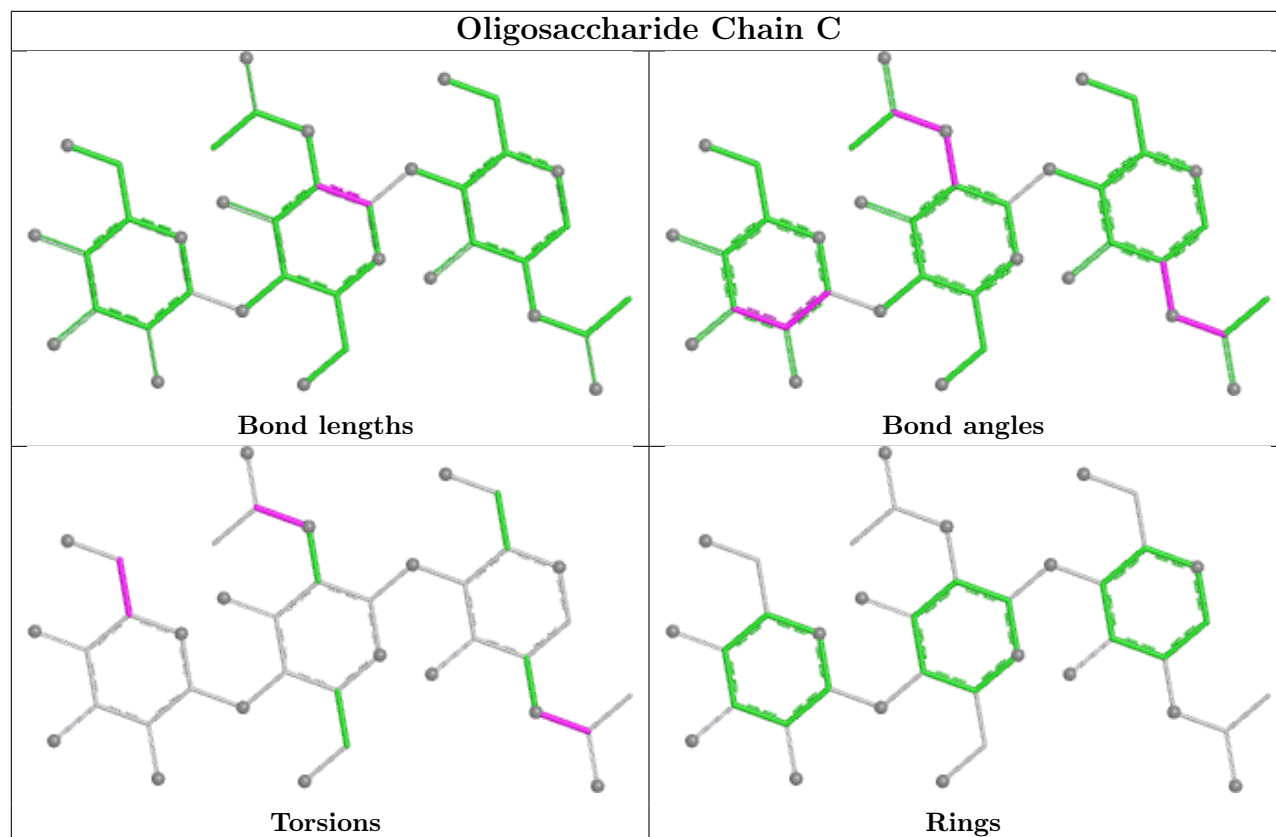
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	3	MAN	O5-C5-C6-O6
3	C	3	MAN	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	3	0
3	C	2	NAG	3	0
3	C	3	MAN	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.