Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2023 – 09:01 AM EST

PDB ID	:	1IGR
Title	:	Type 1 Insulin-like growth factor receptor (DOMAINS 1-3)
Authors	:	Garrett, T.P.J.; Mckern, N.M.; Lou, M.; Frenkel, M.J.; Bentley, J.D.; Lovrecz, G.O.; Elleman, T.C.; Cosgrove, L.J.; Ward, C.W.
Deposited on	:	1998-09-28
Resolution	:	2.60 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:

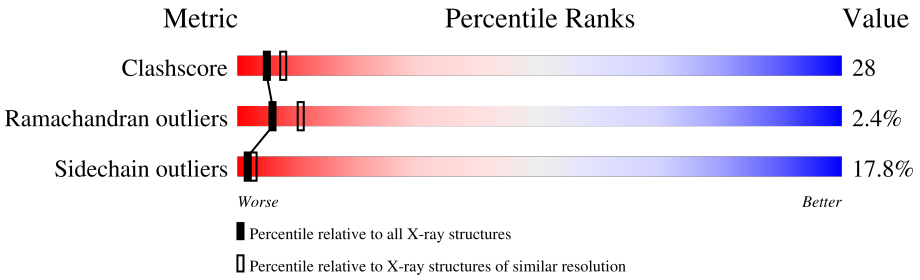
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	478	40% 41% 15%
2	B	3	100%
3	C	5	80% 20%

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
2	NAG	B	2	-	-	X	-
2	FUC	B	3	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	2	X	-	-	-
4	NAG	A	479(A)	X	-	-	-
5	SO4	A	493	-	-	X	-
5	SO4	A	497	-	-	X	-

2 Entry composition

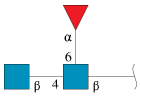
There are 6 unique types of molecules in this entry. The entry contains 3900 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 INSULIN-LIKE GROWTH FACTOR RECEPTOR 1.

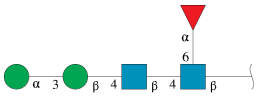
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	471	3686	2312	633	701	40	0	0	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



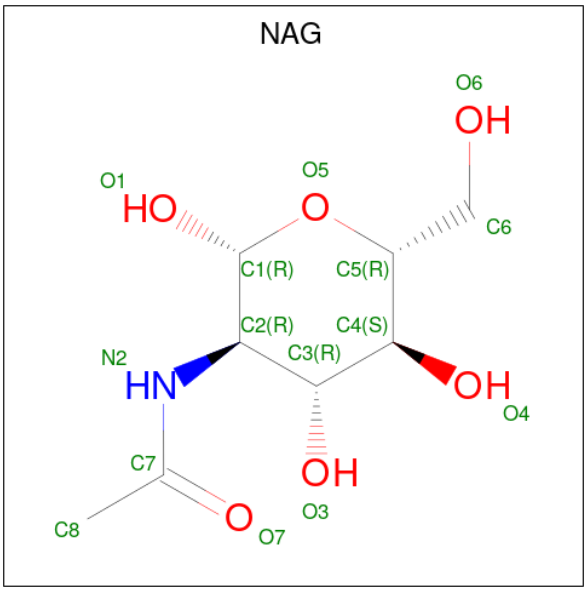
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	38	22	2	14	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



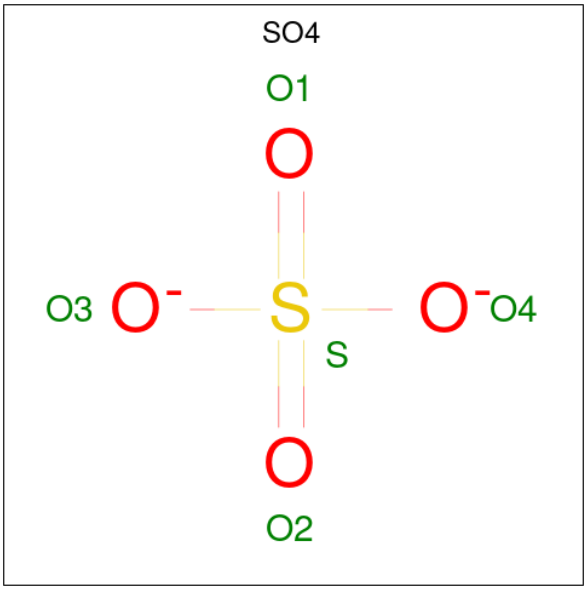
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	5	60	34	2	24	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	48	Total O 48 48	0	0

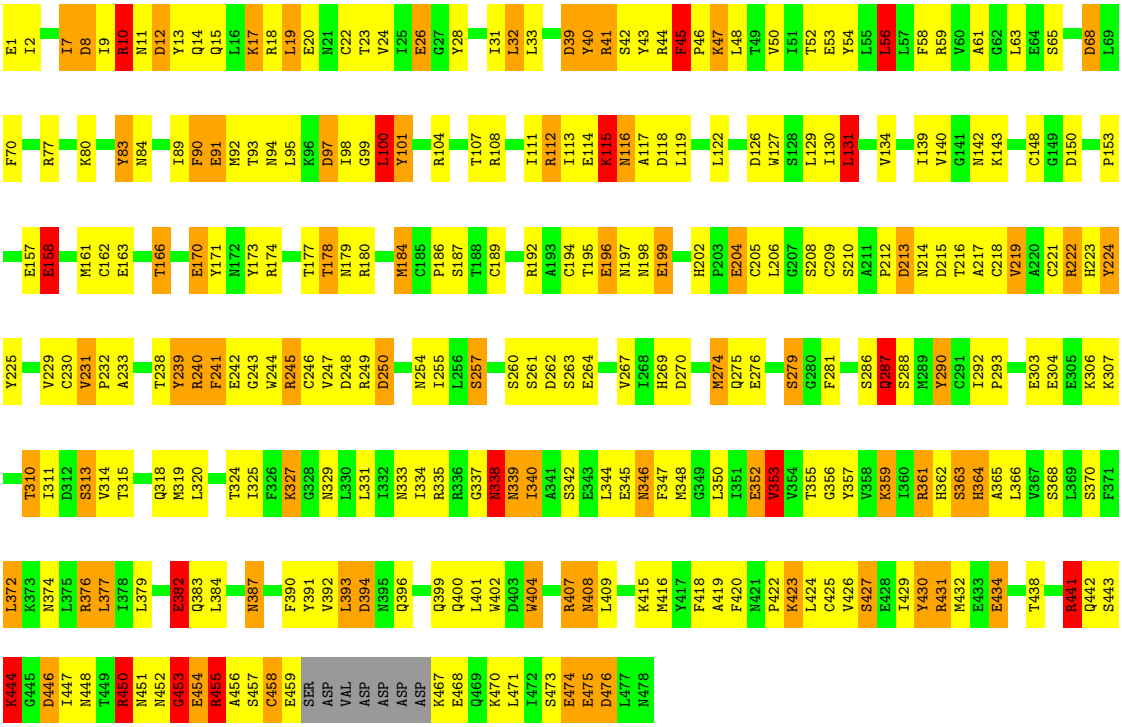
3 Residue-property plots (i)

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: INSULIN-LIKE GROWTH FACTOR RECEPTOR 1

Chain A:

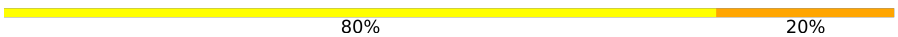


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

• Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:




NAG1
NAG2
BMA3
MAN4
FUC5

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.39Å 99.72Å 120.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.60	Depositor
% Data completeness (in resolution range)	97.0 (7.00-2.60)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.237 , 0.304	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3900	wwPDB-VP
Average B, all atoms (Å^2)	53.0	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: SO4, BMA, FUC, MAN, 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	0.85	0/3756	2.05	129/5082 (2.5%)

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	17

There are no bond length outliers.

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	431	ARG	NE-CZ-NH2	18.01	129.31	120.30
1	A	77	ARG	NE-CZ-NH1	17.56	129.08	120.30
1	A	112	ARG	NE-CZ-NH2	-16.58	112.01	120.30
1	A	97	ASP	CB-CG-OD1	16.50	133.15	118.30
1	A	245	ARG	NE-CZ-NH2	15.89	128.25	120.30
1	A	450	ARG	NE-CZ-NH1	-15.67	112.46	120.30
1	A	222	ARG	NE-CZ-NH2	15.21	127.90	120.30
1	A	250	ASP	CB-CG-OD1	15.20	131.98	118.30
1	A	249	ARG	NE-CZ-NH2	-14.02	113.29	120.30
1	A	248	ASP	CB-CG-OD2	13.68	130.61	118.30
1	A	222	ARG	NE-CZ-NH1	-13.51	113.55	120.30
1	A	131	LEU	CA-CB-CG	13.45	146.23	115.30
1	A	91	GLU	OE1-CD-OE2	13.25	139.20	123.30
1	A	192	ARG	NE-CZ-NH1	-12.35	114.12	120.30
1	A	59	ARG	CD-NE-CZ	11.62	139.87	123.60
1	A	431	ARG	NE-CZ-NH1	-11.07	114.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	476	ASP	CB-CG-OD1	11.04	128.24	118.30
1	A	270	ASP	CB-CG-OD2	10.88	128.09	118.30
1	A	26	GLU	OE1-CD-OE2	-10.75	110.40	123.30
1	A	10	ARG	NE-CZ-NH2	10.66	125.63	120.30
1	A	104	ARG	NE-CZ-NH2	-10.29	115.16	120.30
1	A	173	TYR	CB-CG-CD1	-10.02	114.99	121.00
1	A	174	ARG	NE-CZ-NH2	-9.96	115.32	120.30
1	A	126	ASP	CB-CG-OD1	9.88	127.19	118.30
1	A	174	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	A	361	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	A	357	TYR	CB-CG-CD1	8.69	126.21	121.00
1	A	118	ASP	CB-CG-OD1	-8.66	110.51	118.30
1	A	10	ARG	NH1-CZ-NH2	-8.30	110.27	119.40
1	A	18	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	112	ARG	NH1-CZ-NH2	8.18	128.40	119.40
1	A	231	VAL	CG1-CB-CG2	-8.12	97.91	110.90
1	A	173	TYR	CB-CG-CD2	7.95	125.77	121.00
1	A	140	VAL	CA-CB-CG1	7.95	122.82	110.90
1	A	26	GLU	CG-CD-OE2	7.83	133.95	118.30
1	A	10	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	A	267	VAL	CA-CB-CG1	7.36	121.94	110.90
1	A	224	TYR	CB-CG-CD1	-7.26	116.64	121.00
1	A	250	ASP	OD1-CG-OD2	-7.22	109.58	123.30
1	A	219	VAL	CG1-CB-CG2	-7.02	99.67	110.90
1	A	77	ARG	NH1-CZ-NH2	-6.95	111.75	119.40
1	A	222	ARG	CD-NE-CZ	6.89	133.25	123.60
1	A	357	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	A	247	VAL	CG1-CB-CG2	6.80	121.78	110.90
1	A	407	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	A	370	SER	O-C-N	-6.78	111.85	122.70
1	A	12	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	262	ASP	CB-CG-OD1	6.60	124.24	118.30
1	A	279	SER	C-N-CA	-6.57	108.51	122.30
1	A	225	TYR	CB-CG-CD2	-6.53	117.08	121.00
1	A	390	PHE	CB-CG-CD1	-6.48	116.26	120.80
1	A	184	MET	CA-CB-CG	6.46	124.28	113.30
1	A	394	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	446	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	248	ASP	CB-CG-OD1	-6.41	112.53	118.30
1	A	446	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	231	VAL	CA-CB-CG2	-6.24	101.53	110.90
1	A	250	ASP	N-CA-CB	6.22	121.81	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	353	VAL	CA-CB-CG1	6.15	120.12	110.90
1	A	8	ASP	C-N-CA	6.13	137.04	121.70
1	A	112	ARG	CD-NE-CZ	6.13	132.18	123.60
1	A	18	ARG	NH1-CZ-NH2	6.11	126.12	119.40
1	A	53	GLU	O-C-N	6.11	132.47	122.70
1	A	90	PHE	CB-CG-CD1	-6.11	116.53	120.80
1	A	77	ARG	CD-NE-CZ	-6.10	115.06	123.60
1	A	224	TYR	CB-CG-CD2	6.08	124.65	121.00
1	A	267	VAL	CA-CB-CG2	-6.07	101.80	110.90
1	A	108	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	A	12	ASP	CB-CG-OD1	-6.03	112.88	118.30
1	A	391	TYR	CB-CG-CD1	-5.99	117.40	121.00
1	A	446	ASP	OD1-CG-OD2	-5.98	111.95	123.30
1	A	83	TYR	O-C-N	-5.92	113.22	122.70
1	A	275	GLN	N-CA-CB	-5.78	100.20	110.60
1	A	287	GLN	CB-CG-CD	5.77	126.61	111.60
1	A	441	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	382	GLU	OE1-CD-OE2	-5.75	116.39	123.30
1	A	286	SER	O-C-N	-5.73	113.53	122.70
1	A	116	ASN	CB-CG-OD1	-5.63	110.34	121.60
1	A	387	ASN	OD1-CG-ND2	-5.58	109.07	121.90
1	A	453	GLY	O-C-N	-5.57	113.78	122.70
1	A	68	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	241	PHE	CB-CG-CD2	-5.57	116.90	120.80
1	A	240	ARG	CD-NE-CZ	-5.56	115.82	123.60
1	A	346	ASN	O-C-N	-5.55	113.81	122.70
1	A	204	GLU	CG-CD-OE1	5.55	129.39	118.30
1	A	274	MET	O-C-N	-5.54	113.84	122.70
1	A	383	GLN	CG-CD-OE1	-5.52	110.55	121.60
1	A	345	GLU	OE1-CD-OE2	-5.49	116.72	123.30
1	A	19	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	97	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	A	255	ILE	CG1-CB-CG2	-5.44	99.44	111.40
1	A	279	SER	CA-CB-OG	-5.43	96.53	111.20
1	A	474	GLU	CG-CD-OE2	5.38	129.06	118.30
1	A	54	TYR	CB-CG-CD2	5.38	124.22	121.00
1	A	134	VAL	CB-CA-C	-5.37	101.20	111.40
1	A	372	LEU	N-CA-CB	5.37	121.14	110.40
1	A	245	ARG	NH1-CZ-NH2	-5.36	113.51	119.40
1	A	240	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	A	376	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	45	PHE	CB-CG-CD1	5.34	124.54	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	91	GLU	CG-CD-OE2	-5.30	107.69	118.30
1	A	270	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	A	101	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	A	290	TYR	CB-CG-CD2	5.26	124.16	121.00
1	A	216	THR	CA-CB-CG2	5.25	119.75	112.40
1	A	451	ASN	OD1-CG-ND2	5.23	133.92	121.90
1	A	427	SER	CA-CB-OG	-5.22	97.10	111.20
1	A	18	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	A	276	GLU	OE1-CD-OE2	5.22	129.56	123.30
1	A	10	ARG	O-C-N	-5.21	114.37	122.70
1	A	455	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	97	ASP	OD1-CG-OD2	-5.18	113.45	123.30
1	A	243	GLY	CA-C-N	5.15	128.54	117.20
1	A	100	LEU	O-C-N	-5.15	114.46	122.70
1	A	335	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	A	77	ARG	CB-CA-C	5.15	120.70	110.40
1	A	108	ARG	CD-NE-CZ	5.10	130.74	123.60
1	A	249	ARG	NH1-CZ-NH2	5.10	125.01	119.40
1	A	450	ARG	NH1-CZ-NH2	5.10	125.01	119.40
1	A	366	LEU	CA-CB-CG	5.08	126.99	115.30
1	A	213	ASP	N-CA-CB	-5.08	101.45	110.60
1	A	213	ASP	O-C-N	-5.07	114.58	122.70
1	A	63	LEU	CB-CG-CD2	-5.05	102.41	111.00
1	A	77	ARG	O-C-N	-5.05	114.62	123.20
1	A	104	ARG	NH1-CZ-NH2	5.04	124.95	119.40
1	A	430	TYR	CB-CG-CD1	5.03	124.02	121.00
1	A	56	LEU	CA-CB-CG	5.01	126.83	115.30
1	A	239	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	A	420	PHE	CB-CG-CD2	-5.00	117.30	120.80

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	LEU	Mainchain
1	A	129	LEU	Mainchain
1	A	19	LEU	Mainchain
1	A	205	CYS	Mainchain
1	A	219	VAL	Mainchain
1	A	238	THR	Mainchain
1	A	287	GLN	Mainchain
1	A	288	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	A	292	ILE	Mainchain
1	A	346	ASN	Mainchain
1	A	364	HIS	Mainchain
1	A	382	GLU	Mainchain
1	A	444	LYS	Mainchain
1	A	45	PHE	Mainchain
1	A	453	GLY	Mainchain
1	A	50	VAL	Mainchain
1	A	8	ASP	Mainchain

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	3686	0	3544	191	0
2	B	38	0	34	23	0
3	C	60	0	50	1	0
4	A	28	0	26	1	0
5	A	40	0	0	5	0
6	A	48	0	0	5	0
All	All	3900	0	3654	205	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 28.

All (205) 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)
1:A:222:ARG:HD3	2:B:3:FUC:H61	1.36	1.07
2:B:2:NAG:H3	2:B:3:FUC:H3	1.39	1.02
1:A:143:LYS:HG2	1:A:148:CYS:SG	2.07	0.94
2:B:2:NAG:N2	2:B:3:FUC:H3	1.88	0.89
2:B:2:NAG:HN2	2:B:3:FUC:H3	1.39	0.86
1:A:166:THR:HG22	1:A:171:TYR:HD1	1.41	0.85
1:A:157:GLU:O	1:A:158:GLU:HB2	1.74	0.84
2:B:2:NAG:N2	2:B:3:FUC:O2	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ILE:HD11	1:A:365:ALA:HB1	1.58	0.83
2:B:2:NAG:C3	2:B:3:FUC:H3	2.10	0.81
1:A:310:THR:HB	1:A:331:LEU:HD23	1.62	0.80
1:A:92:MET:HG2	1:A:95:LEU:HD22	1.62	0.79
2:B:2:NAG:H3	2:B:3:FUC:C3	2.14	0.78
2:B:2:NAG:HN2	2:B:3:FUC:C3	1.95	0.78
1:A:222:ARG:HD3	2:B:3:FUC:C6	2.13	0.77
1:A:117:ALA:O	1:A:143:LYS:HB2	1.85	0.77
1:A:177:THR:HG22	1:A:178:THR:N	2.00	0.76
1:A:32:LEU:HB2	1:A:33:LEU:HG	1.67	0.75
1:A:431:ARG:O	1:A:434:GLU:HG3	1.86	0.75
1:A:17:LYS:O	1:A:20:GLU:HG2	1.87	0.75
2:B:2:NAG:HN2	2:B:3:FUC:C2	1.98	0.74
1:A:318:GLN:HA	1:A:347:PHE:CE2	2.22	0.73
1:A:311:ILE:HD11	1:A:320:LEU:HD11	1.70	0.73
1:A:92:MET:HA	1:A:92:MET:HE2	1.71	0.72
1:A:166:THR:HG22	1:A:171:TYR:CD1	2.25	0.71
1:A:422:PRO:HB2	1:A:455:ARG:HG3	1.71	0.71
1:A:180:ARG:HH11	1:A:180:ARG:HG2	1.55	0.71
1:A:450:ARG:HH12	1:A:476:ASP:CG	1.96	0.68
1:A:32:LEU:HD23	1:A:32:LEU:N	2.09	0.68
1:A:377:LEU:HD11	1:A:379:LEU:CD2	2.24	0.68
1:A:361:ARG:O	1:A:362:HIS:HB2	1.94	0.68
1:A:90:PHE:CE2	1:A:91:GLU:HG3	2.30	0.67
1:A:337:GLY:HA2	1:A:340:ILE:HD12	1.77	0.66
1:A:222:ARG:CD	2:B:3:FUC:H61	2.22	0.66
1:A:93:THR:O	1:A:94:ASN:HB2	1.97	0.65
1:A:318:GLN:HA	1:A:347:PHE:CD2	2.31	0.65
1:A:334:ILE:HG22	1:A:365:ALA:HB3	1.80	0.64
1:A:222:ARG:CG	2:B:3:FUC:O5	2.45	0.64
1:A:311:ILE:HD11	1:A:320:LEU:CD1	2.27	0.63
1:A:229:VAL:O	1:A:231:VAL:HG23	1.99	0.62
1:A:377:LEU:HD11	1:A:379:LEU:HD23	1.81	0.62
1:A:98:ILE:HD11	1:A:113:ILE:HD13	1.80	0.62
1:A:221:CYS:HB3	6:A:502:HOH:O	1.99	0.61
1:A:424:LEU:HD23	1:A:429:ILE:HD11	1.82	0.61
1:A:368:SER:HA	1:A:400:GLN:O	2.00	0.61
1:A:224:TYR:CZ	1:A:240:ARG:HD2	2.36	0.61
2:B:2:NAG:C2	2:B:3:FUC:H3	2.30	0.61
1:A:32:LEU:HD23	1:A:32:LEU:H	1.64	0.60
1:A:340:ILE:HG12	1:A:340:ILE:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ASN:OD1	1:A:356:GLY:HA3	2.02	0.60
1:A:177:THR:HG22	1:A:178:THR:H	1.67	0.60
1:A:327:LYS:HG2	1:A:355:THR:HG21	1.85	0.59
1:A:352:GLU:HG2	1:A:376:ARG:HD3	1.85	0.59
1:A:10:ARG:O	1:A:11:ASN:HB2	2.03	0.59
1:A:44:ARG:NH2	5:A:497:SO4:O3	2.36	0.59
1:A:438:THR:O	1:A:441:ARG:HG3	2.03	0.59
1:A:210:SER:OG	1:A:217:ALA:HB1	2.04	0.58
1:A:119:LEU:O	1:A:143:LYS:HB3	2.04	0.58
1:A:212:PRO:O	1:A:214:ASN:N	2.37	0.58
1:A:97:ASP:HA	1:A:119:LEU:HD12	1.86	0.57
1:A:404:TRP:HA	1:A:404:TRP:CE3	2.40	0.57
1:A:222:ARG:NH1	2:B:1:NAG:H62	2.19	0.57
1:A:222:ARG:HG2	1:A:223:HIS:CE1	2.40	0.57
1:A:48:LEU:HD23	1:A:70:PHE:CD2	2.40	0.56
2:B:2:NAG:H3	2:B:3:FUC:H4	1.87	0.56
1:A:90:PHE:CD2	1:A:91:GLU:HG3	2.40	0.56
1:A:202:HIS:CD2	1:A:215:ASP:HB3	2.41	0.56
1:A:350:LEU:HB2	6:A:534:HOH:O	2.05	0.56
1:A:40:TYR:HD2	1:A:41:ARG:N	2.04	0.56
1:A:99:GLY:O	1:A:101:TYR:N	2.38	0.56
1:A:450:ARG:NH1	1:A:476:ASP:OD2	2.38	0.56
1:A:231:VAL:CG1	1:A:233:ALA:O	2.54	0.55
1:A:1:GLU:H2	1:A:23:THR:HG23	1.70	0.55
1:A:98:ILE:HG22	1:A:100:LEU:HG	1.87	0.55
1:A:443:SER:N	1:A:446:ASP:OD2	2.40	0.55
1:A:222:ARG:HG3	2:B:3:FUC:C1	2.37	0.54
1:A:153:PRO:HD2	1:A:162:CYS:SG	2.47	0.54
1:A:222:ARG:HG2	2:B:3:FUC:O5	2.06	0.54
1:A:426:VAL:HB	1:A:430:TYR:CE1	2.42	0.54
1:A:269:HIS:HB3	1:A:274:MET:CE	2.38	0.54
1:A:334:ILE:O	1:A:363:SER:HA	2.08	0.54
1:A:423:LYS:HA	1:A:456:ALA:HB2	1.89	0.54
1:A:404:TRP:HA	1:A:404:TRP:HE3	1.72	0.54
1:A:450:ARG:HE	1:A:467:LYS:HA	1.73	0.53
1:A:422:PRO:CB	1:A:455:ARG:HG3	2.37	0.53
1:A:158:GLU:HA	1:A:158:GLU:OE1	2.09	0.53
1:A:204:GLU:OE2	1:A:232:PRO:HB3	2.08	0.53
1:A:231:VAL:HG12	1:A:233:ALA:O	2.09	0.53
1:A:350:LEU:HD23	1:A:374:ASN:OD1	2.09	0.52
1:A:281:PHE:CE1	1:A:293:PRO:HG3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ILE:HG23	1:A:131:LEU:HD11	1.91	0.52
1:A:166:THR:HA	1:A:170:GLU:O	2.09	0.52
1:A:84:ASN:ND2	6:A:529:HOH:O	2.43	0.52
1:A:307:LYS:NZ	1:A:382:GLU:OE2	2.41	0.52
1:A:333:ASN:ND2	1:A:361:ARG:HH21	2.07	0.52
2:B:2:NAG:H3	2:B:3:FUC:C4	2.40	0.51
1:A:177:THR:CG2	1:A:178:THR:N	2.72	0.51
1:A:2:ILE:HA	1:A:24:VAL:O	2.11	0.51
1:A:448:ASN:O	1:A:452:ASN:HB2	2.11	0.51
1:A:450:ARG:NH2	1:A:475:GLU:HG2	2.26	0.51
2:B:2:NAG:C8	2:B:3:FUC:O2	2.59	0.50
1:A:331:LEU:CD1	1:A:359:LYS:HG2	2.42	0.50
1:A:186:PRO:HG2	1:A:189:CYS:SG	2.52	0.50
1:A:377:LEU:HD11	1:A:379:LEU:HD21	1.94	0.50
1:A:393:LEU:HA	1:A:419:ALA:O	2.12	0.50
1:A:314:VAL:HG22	1:A:344:LEU:HD23	1.93	0.50
1:A:404:TRP:CB	1:A:431:ARG:HG2	2.41	0.50
1:A:443:SER:O	1:A:444:LYS:HE2	2.12	0.50
1:A:311:ILE:HD13	1:A:348:MET:SD	2.52	0.49
1:A:12:ASP:O	1:A:13:TYR:C	2.50	0.49
1:A:231:VAL:HG12	1:A:232:PRO:HD2	1.94	0.49
1:A:23:THR:HA	1:A:47:LYS:O	2.12	0.49
1:A:114:GLU:HG2	1:A:115:LYS:HG2	1.94	0.49
1:A:224:TYR:OH	1:A:240:ARG:HD2	2.13	0.49
1:A:431:ARG:NE	1:A:434:GLU:OE1	2.45	0.49
1:A:14:GLN:HA	1:A:43:TYR:OH	2.13	0.49
1:A:20:GLU:OE1	4:A:479(A):NAG:H3	2.13	0.49
1:A:340:ILE:CD1	1:A:365:ALA:HB1	2.36	0.49
1:A:56:LEU:HD12	1:A:56:LEU:C	2.33	0.49
1:A:402:TRP:HB2	1:A:404:TRP:CH2	2.47	0.49
1:A:92:MET:HE2	1:A:92:MET:CA	2.41	0.48
1:A:116:ASN:HB2	1:A:142:ASN:OD1	2.13	0.48
1:A:148:CYS:HB3	1:A:150:ASP:OD1	2.13	0.48
1:A:179:ASN:HB2	5:A:493:SO4:O4	2.13	0.48
1:A:1:GLU:O	1:A:22:CYS:HA	2.13	0.48
1:A:254:ASN:O	1:A:257:SER:HB3	2.13	0.48
1:A:264:GLU:HA	1:A:287:GLN:NE2	2.28	0.48
1:A:194:CYS:HA	1:A:199:GLU:O	2.13	0.48
1:A:364:HIS:CE1	1:A:396:GLN:H	2.32	0.48
2:B:2:NAG:H82	2:B:3:FUC:O2	2.13	0.48
1:A:93:THR:O	1:A:94:ASN:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:GLN:NE2	1:A:347:PHE:HE2	2.11	0.48
1:A:9:ILE:O	1:A:10:ARG:HB3	2.14	0.47
1:A:44:ARG:NH2	5:A:497:SO4:S	2.88	0.47
1:A:12:ASP:O	1:A:15:GLN:HB2	2.14	0.47
1:A:206:LEU:HB2	1:A:222:ARG:N	2.29	0.47
1:A:425:CYS:HB2	6:A:519:HOH:O	2.14	0.47
1:A:112:ARG:NH2	1:A:114:GLU:OE1	2.36	0.47
1:A:364:HIS:ND1	1:A:396:GLN:HB2	2.29	0.47
1:A:52:THR:HG21	1:A:244:TRP:CD1	2.49	0.47
1:A:26:GLU:CG	1:A:242:GLU:HG3	2.45	0.47
1:A:101:TYR:CG	1:A:180:ARG:HD3	2.50	0.47
1:A:127:TRP:O	1:A:131:LEU:N	2.39	0.47
1:A:426:VAL:O	1:A:430:TYR:CD1	2.68	0.47
1:A:44:ARG:NH2	5:A:497:SO4:O2	2.48	0.46
1:A:352:GLU:HG2	1:A:376:ARG:CD	2.45	0.46
1:A:325:ILE:HG12	1:A:353:VAL:HG13	1.97	0.46
1:A:392:VAL:HG21	1:A:418:PHE:CE2	2.50	0.46
1:A:404:TRP:HB3	1:A:431:ARG:HG2	1.98	0.46
1:A:362:HIS:HD2	1:A:394:ASP:HB3	1.79	0.46
1:A:47:LYS:HE2	1:A:47:LYS:HB3	1.80	0.46
1:A:61:ALA:HA	1:A:93:THR:O	2.16	0.46
1:A:180:ARG:HH11	1:A:180:ARG:CG	2.25	0.46
1:A:44:ARG:HG3	1:A:46:PRO:HD3	1.98	0.46
1:A:130:ILE:C	2:B:1:NAG:H82	2.36	0.46
1:A:337:GLY:HA2	1:A:340:ILE:CD1	2.43	0.46
1:A:401:LEU:HD13	1:A:432:MET:SD	2.56	0.46
1:A:352:GLU:HA	1:A:374:ASN:O	2.16	0.45
1:A:101:TYR:CD2	1:A:180:ARG:HD3	2.52	0.45
1:A:377:LEU:CD1	1:A:379:LEU:HD23	2.45	0.45
1:A:195:THR:HG22	1:A:196:GLU:H	1.82	0.45
1:A:408:ASN:HD22	1:A:409:LEU:N	2.14	0.44
1:A:215:ASP:OD2	1:A:215:ASP:C	2.54	0.44
1:A:281:PHE:HE1	1:A:293:PRO:HG3	1.82	0.44
1:A:41:ARG:HB3	1:A:42:SER:H	1.68	0.44
1:A:269:HIS:HB3	1:A:274:MET:HE1	1.99	0.44
1:A:269:HIS:HB3	1:A:274:MET:HE2	1.99	0.44
1:A:44:ARG:CG	1:A:46:PRO:HD3	2.48	0.44
1:A:208:SER:OG	1:A:209:CYS:N	2.51	0.43
1:A:429:ILE:HG21	1:A:447:ILE:HG23	1.99	0.43
1:A:111:ILE:CG2	1:A:131:LEU:HD11	2.48	0.43
1:A:2:ILE:HD13	1:A:245:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:GLN:O	1:A:423:LYS:HG3	2.19	0.43
1:A:338:ASN:HB2	1:A:339:ASN:H	1.48	0.43
1:A:230:CYS:HB3	6:A:502:HOH:O	2.17	0.43
1:A:89:ILE:CD1	1:A:98:ILE:HD13	2.49	0.43
1:A:197:ASN:O	1:A:198:ASN:C	2.55	0.43
1:A:458:CYS:HB3	1:A:459:GLU:H	1.54	0.42
1:A:218:CYS:SG	1:A:230:CYS:SG	3.17	0.42
1:A:348:MET:CE	1:A:372:LEU:HD21	2.50	0.42
2:B:2:NAG:C7	2:B:3:FUC:O2	2.65	0.42
1:A:114:GLU:O	1:A:116:ASN:ND2	2.53	0.42
1:A:340:ILE:HD11	1:A:365:ALA:CB	2.38	0.42
1:A:26:GLU:CD	1:A:242:GLU:HG3	2.40	0.42
1:A:313:SER:OG	1:A:314:VAL:N	2.52	0.42
1:A:180:ARG:CG	1:A:180:ARG:NH1	2.83	0.42
1:A:1:GLU:N	1:A:23:THR:HG23	2.35	0.42
1:A:92:MET:CA	1:A:92:MET:CE	2.96	0.42
1:A:241:PHE:O	1:A:242:GLU:HB2	2.20	0.42
1:A:231:VAL:CG1	1:A:232:PRO:HD2	2.50	0.42
1:A:65:SER:O	1:A:68:ASP:HB2	2.19	0.41
1:A:101:TYR:CD1	1:A:101:TYR:C	2.93	0.41
1:A:239:TYR:O	1:A:246:CYS:HA	2.20	0.41
1:A:111:ILE:HD13	1:A:111:ILE:HG21	1.87	0.41
1:A:179:ASN:ND2	5:A:493:SO4:O4	2.37	0.41
1:A:45:PHE:CD2	1:A:45:PHE:N	2.88	0.41
1:A:7:ILE:HG22	1:A:9:ILE:HG12	2.03	0.41
1:A:290:TYR:CD2	3:C:1:NAG:H62	2.56	0.41
1:A:222:ARG:CG	2:B:3:FUC:C1	2.99	0.40
1:A:333:ASN:ND2	1:A:362:HIS:HB2	2.37	0.40
1:A:20:GLU:O	1:A:47:LYS:HD3	2.21	0.40
1:A:31:ILE:HD13	1:A:31:ILE:HG21	1.89	0.40
1:A:426:VAL:O	1:A:430:TYR:HD1	2.03	0.40
1:A:28:TYR:CD1	1:A:28:TYR:C	2.95	0.40
1:A:453:GLY:O	1:A:454:GLU:C	2.58	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	467/478 (98%)	396 (85%)	60 (13%)	11 (2%)	6 10

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	158	GLU
1	A	213	ASP
1	A	41	ARG
1	A	338	ASN
1	A	404	TRP
1	A	39	ASP
1	A	115	LYS
1	A	387	ASN
1	A	468	GLU
1	A	83	TYR

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	405/426 (95%)	333 (82%)	72 (18%)	2 3

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	10	ARG
1	A	17	LYS
1	A	32	LEU
1	A	39	ASP
1	A	40	TYR
1	A	47	LYS
1	A	56	LEU
1	A	58	PHE
1	A	80	LYS
1	A	107	THR
1	A	115	LYS
1	A	122	LEU
1	A	131	LEU
1	A	139	ILE
1	A	158	GLU
1	A	161	MET
1	A	163	GLU
1	A	166	THR
1	A	170	GLU
1	A	178	THR
1	A	184	MET
1	A	187	SER
1	A	196	GLU
1	A	199	GLU
1	A	250	ASP
1	A	257	SER
1	A	260	SER
1	A	261	SER
1	A	263	SER
1	A	279	SER
1	A	303	GLU
1	A	304	GLU
1	A	306	LYS
1	A	310	THR
1	A	313	SER
1	A	315	THR
1	A	319	MET
1	A	324	THR
1	A	327	LYS
1	A	338	ASN
1	A	339	ASN
1	A	340	ILE

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Mol	Chain	Res	Type
1	A	342	SER
1	A	352	GLU
1	A	353	VAL
1	A	359	LYS
1	A	363	SER
1	A	377	LEU
1	A	384	LEU
1	A	393	LEU
1	A	399	GLN
1	A	407	ARG
1	A	408	ASN
1	A	415	LYS
1	A	416	MET
1	A	423	LYS
1	A	427	SER
1	A	434	GLU
1	A	441	ARG
1	A	442	GLN
1	A	444	LYS
1	A	450	ARG
1	A	454	GLU
1	A	455	ARG
1	A	457	SER
1	A	458	CYS
1	A	470	LYS
1	A	471	LEU
1	A	473	SER
1	A	474	GLU
1	A	475	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	237	ASN
1	A	318	GLN
1	A	333	ASN
1	A	362	HIS
1	A	400	GLN
1	A	408	ASN

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

8 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	$\#\|Z\| > 2$
2	NAG	B	1	1,2	14,14,15	2.37	6 (42%)	17,19,21	2.82	7 (41%)
2	NAG	B	2	2	14,14,15	2.03	3 (21%)	17,19,21	1.82	2 (11%)
2	FUC	B	3	2	10,10,11	1.25	1 (10%)	14,14,16	2.46	5 (35%)
3	NAG	C	1	1,3	14,14,15	1.41	1 (7%)	17,19,21	1.64	4 (23%)
3	NAG	C	2	3	14,14,15	1.83	4 (28%)	17,19,21	2.94	6 (35%)
3	BMA	C	3	3	11,11,12	1.74	2 (18%)	15,15,17	1.68	3 (20%)
3	MAN	C	4	3	11,11,12	1.02	1 (9%)	15,15,17	1.47	2 (13%)
3	FUC	C	5	3	10,10,11	0.65	0	14,14,16	1.25	2 (14%)

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	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1
2	FUC	B	3	2	-	-	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	1/1/5/7	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	FUC	C	5	3	-	-	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	5.83	1.61	1.52
2	B	2	NAG	C1-C2	-4.91	1.45	1.52
3	C	2	NAG	C1-C2	-4.59	1.45	1.52
3	C	3	BMA	C4-C5	-4.51	1.43	1.53
2	B	2	NAG	O5-C1	-4.47	1.36	1.43
3	C	1	NAG	C4-C5	-3.59	1.45	1.53
2	B	1	NAG	C4-C5	3.18	1.59	1.53
2	B	1	NAG	O7-C7	-3.16	1.16	1.23
2	B	2	NAG	C2-N2	-2.70	1.41	1.46
2	B	1	NAG	C8-C7	2.63	1.56	1.50
2	B	3	FUC	C2-C3	2.61	1.56	1.52
2	B	1	NAG	O5-C5	2.57	1.48	1.43
3	C	2	NAG	C7-N2	-2.32	1.26	1.34
3	C	4	MAN	O5-C1	-2.22	1.40	1.43
3	C	2	NAG	C8-C7	2.14	1.55	1.50
2	B	1	NAG	C3-C2	-2.09	1.48	1.52
3	C	3	BMA	O4-C4	-2.05	1.38	1.43
3	C	2	NAG	O7-C7	-2.01	1.18	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2	NAG	C1-C2-N2	7.52	123.33	110.49
2	B	3	FUC	C1-C2-C3	6.14	117.21	109.67
2	B	1	NAG	C8-C7-N2	6.10	126.42	116.10
2	B	1	NAG	C1-O5-C5	5.82	120.08	112.19
3	C	2	NAG	O5-C5-C6	-4.95	99.45	107.20
2	B	2	NAG	C2-N2-C7	-4.53	116.45	122.90
3	C	2	NAG	O5-C1-C2	-4.41	104.33	111.29
3	C	4	MAN	C6-C5-C4	4.23	122.90	113.00
2	B	1	NAG	O7-C7-C8	-4.19	114.28	122.06
2	B	3	FUC	C6-C5-C4	3.79	120.08	113.07
3	C	1	NAG	C8-C7-N2	3.73	122.42	116.10
2	B	1	NAG	C4-C3-C2	3.69	116.42	111.02
3	C	2	NAG	C4-C3-C2	-3.54	105.83	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	FUC	C2-C3-C4	3.45	116.87	110.89
3	C	2	NAG	C2-N2-C7	3.16	127.40	122.90
2	B	2	NAG	C1-C2-N2	-3.03	105.31	110.49
3	C	2	NAG	C8-C7-N2	-2.99	111.03	116.10
3	C	5	FUC	C6-C5-C4	2.81	118.27	113.07
3	C	3	BMA	C1-O5-C5	-2.75	108.47	112.19
3	C	1	NAG	C1-C2-N2	-2.75	105.79	110.49
2	B	1	NAG	O5-C5-C6	-2.68	103.00	107.20
2	B	3	FUC	C3-C4-C5	2.64	113.89	109.77
3	C	5	FUC	C3-C4-C5	-2.55	105.80	109.77
2	B	1	NAG	C6-C5-C4	2.53	118.93	113.00
3	C	3	BMA	O5-C5-C6	2.51	111.13	107.20
2	B	3	FUC	O5-C1-C2	-2.48	106.94	110.77
3	C	1	NAG	C3-C4-C5	-2.35	106.05	110.24
3	C	1	NAG	O7-C7-C8	-2.35	117.70	122.06
3	C	3	BMA	C1-C2-C3	2.24	112.42	109.67
2	B	1	NAG	C3-C4-C5	2.15	114.08	110.24
3	C	4	MAN	C3-C4-C5	-2.03	106.61	110.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	2	NAG	C2

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6

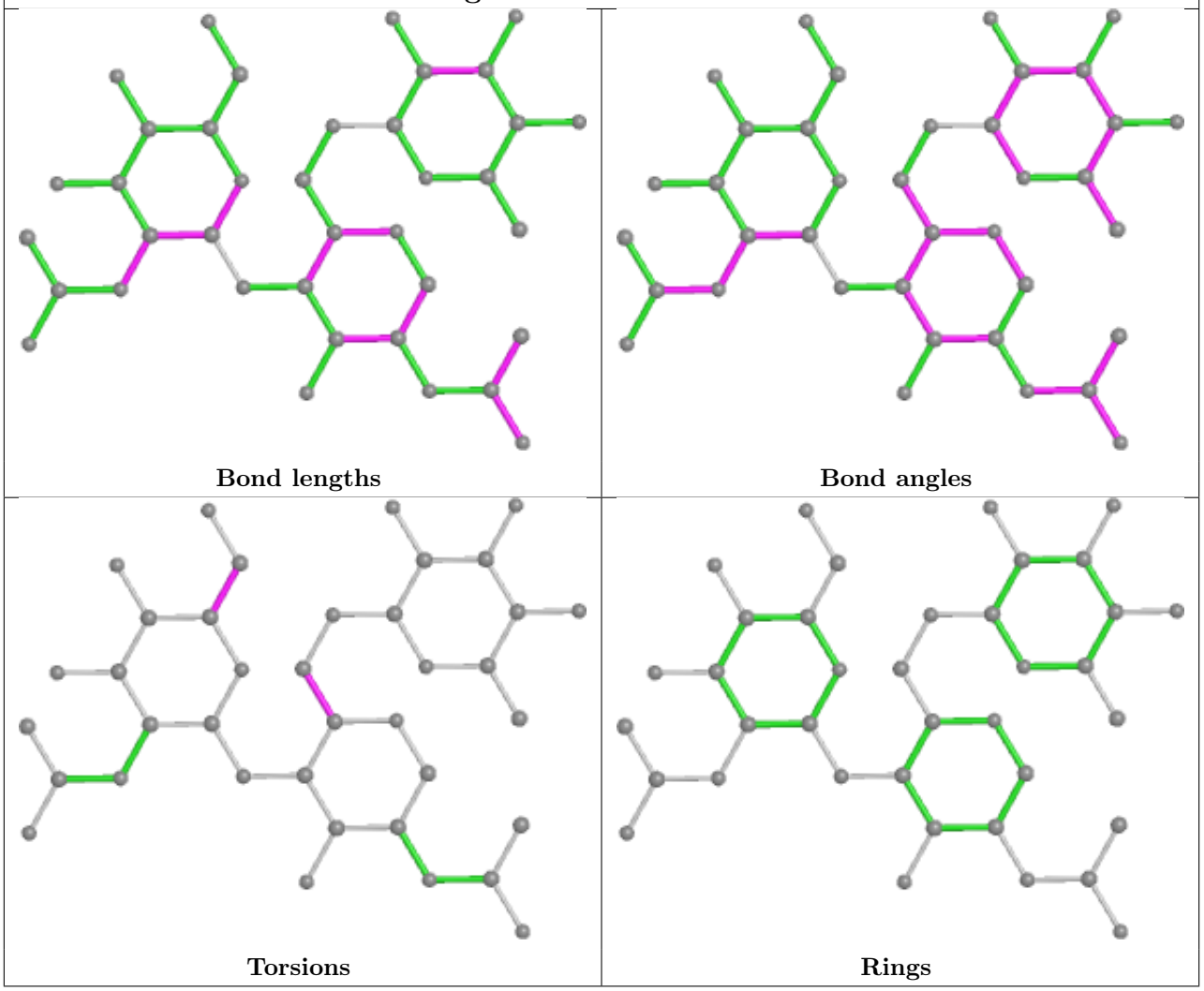
There are no ring outliers.

4 monomers are involved in 24 short contacts:

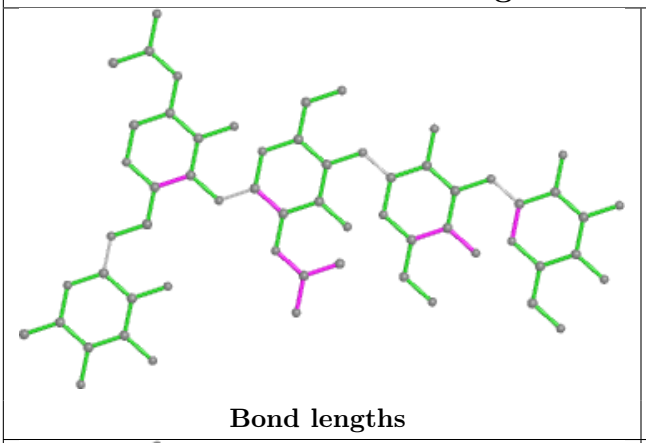
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
2	B	2	NAG	14	0
2	B	3	FUC	21	0
2	B	1	NAG	2	0

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

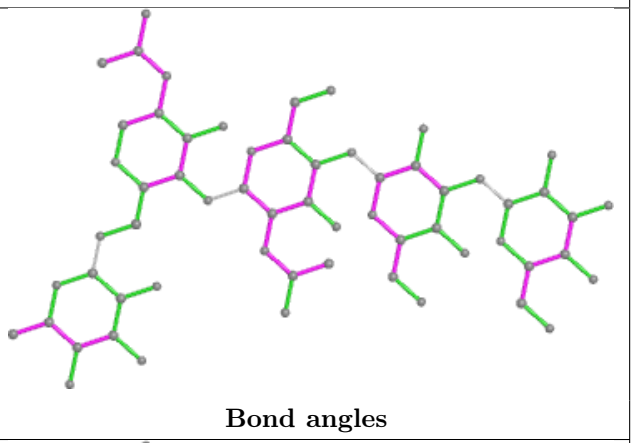
Oligosaccharide Chain B



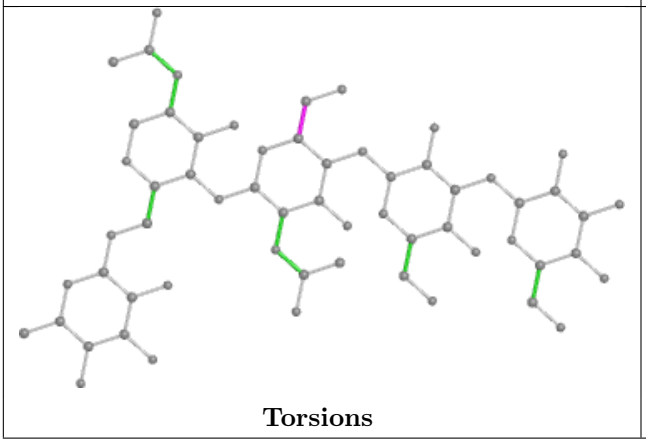
Oligosaccharide Chain C



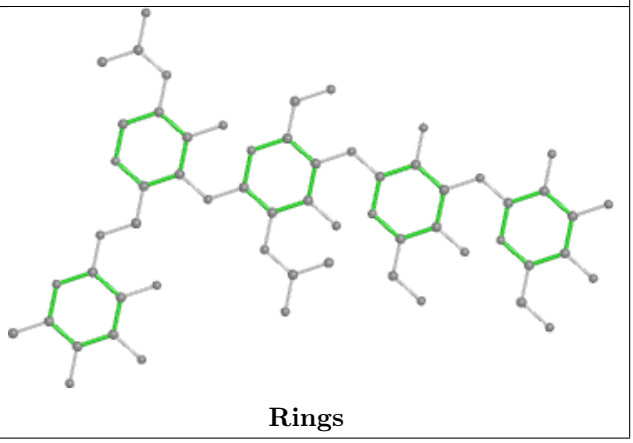
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

10 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	SO4	A	498	-	4,4,4	0.48	0	6,6,6	1.33	1 (16%)
5	SO4	A	497	-	4,4,4	0.50	0	6,6,6	0.87	0
5	SO4	A	494	-	4,4,4	0.65	0	6,6,6	0.43	0
5	SO4	A	496	-	4,4,4	0.67	0	6,6,6	1.44	1 (16%)
5	SO4	A	495	-	4,4,4	0.74	0	6,6,6	0.72	0
5	SO4	A	499	-	4,4,4	0.64	0	6,6,6	0.53	0
4	NAG	A	483(A)	1	14,14,15	1.33	1 (7%)	17,19,21	2.11	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SO4	A	493	-	4,4,4	0.61	0	6,6,6	0.66	0
4	NAG	A	479(A)	1	14,14,15	1.45	2 (14%)	17,19,21	2.29	6 (35%)
5	SO4	A	500	-	4,4,4	0.45	0	6,6,6	0.69	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
4	NAG	A	483(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	A	479(A)	1	1/1/5/7	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	483(A)	NAG	O7-C7	-3.66	1.14	1.23
4	A	479(A)	NAG	O7-C7	-3.37	1.15	1.23
4	A	479(A)	NAG	C2-N2	2.18	1.50	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	479(A)	NAG	C2-N2-C7	-6.27	113.97	122.90
4	A	483(A)	NAG	C4-C3-C2	-5.37	103.15	111.02
4	A	483(A)	NAG	C2-N2-C7	-3.94	117.30	122.90
4	A	479(A)	NAG	O3-C3-C4	-3.02	103.36	110.35
4	A	479(A)	NAG	C1-O5-C5	2.88	116.10	112.19
4	A	479(A)	NAG	C4-C3-C2	-2.75	106.99	111.02
5	A	498	SO4	O4-S-O3	-2.49	98.44	109.06
4	A	479(A)	NAG	O5-C1-C2	2.34	114.98	111.29
4	A	483(A)	NAG	C1-O5-C5	2.26	115.25	112.19
5	A	496	SO4	O4-S-O1	-2.21	97.77	109.31
4	A	479(A)	NAG	C8-C7-N2	-2.12	112.50	116.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	479(A)	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	479(A)	NAG	O5-C5-C6-O6
4	A	483(A)	NAG	O5-C5-C6-O6
4	A	479(A)	NAG	C4-C5-C6-O6
4	A	483(A)	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	497	SO4	3	0
5	A	493	SO4	2	0
4	A	479(A)	NAG	1	0

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.