



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 08:11 AM EDT

PDB ID : 3SI1 / pdb_00003si1
Title : Structure of glycosylated murine glutaminyl cyclase
Authors : Dambe, T.; Carrillo, D.; Parthier, C.; Stubbs, M.T.
Deposited on : 2011-06-17
Resolution : 2.90 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

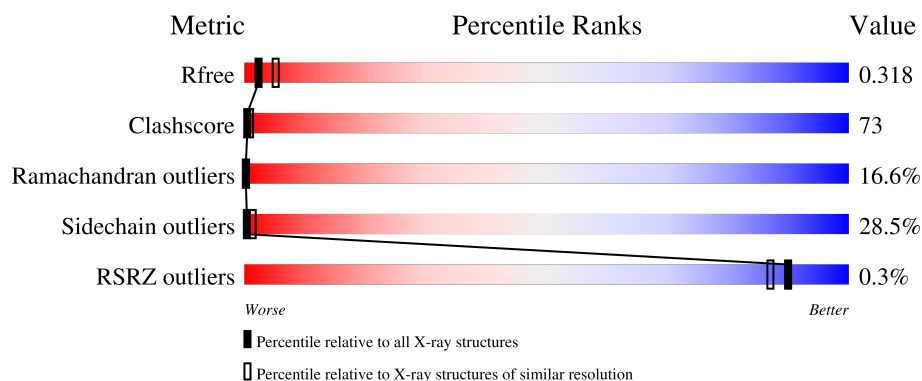
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

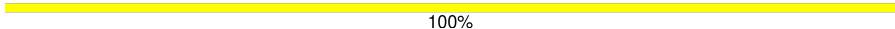
The reported resolution of this entry is 2.90 Å.

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	327	
2	B	2	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2712 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 Glutaminyl-peptide cyclotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2631	1682	462	478	9			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

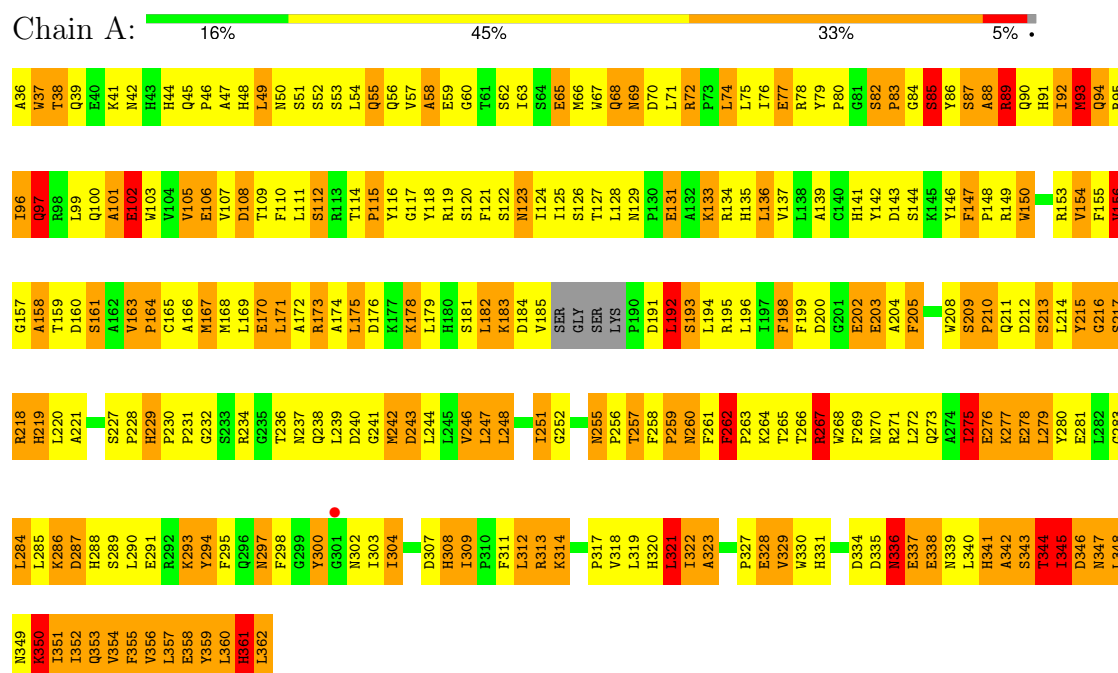
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		

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 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: Glutaminyl-peptide cyclotransferase



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.24Å 86.87Å 97.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.75 – 2.90 19.75 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.75-2.90) 99.3 (19.75-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.83Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.245 , 0.301 0.245 , 0.318	Depositor DCC
R_{free} test set	452 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	2712	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.15	7/2707 (0.3%)	1.36	39/3675 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	VAL	CA-CB	-10.98	1.48	1.54
1	A	275	ILE	CA-CB	6.57	1.63	1.54
1	A	198	PHE	CA-C	-6.42	1.45	1.52
1	A	246	VAL	CA-CB	-6.37	1.46	1.53
1	A	247	LEU	CA-C	-6.11	1.45	1.52
1	A	336	ASN	CA-C	6.05	1.59	1.53
1	A	298	PHE	N-CA	5.20	1.52	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ALA	N-CA-C	-11.61	98.62	113.72
1	A	117	GLY	N-CA-C	7.09	118.59	111.21
1	A	163	VAL	CB-CA-C	-6.69	107.34	113.70
1	A	262	PHE	CA-C-N	6.62	128.12	119.84
1	A	262	PHE	C-N-CA	6.62	128.12	119.84
1	A	122	SER	N-CA-C	6.40	121.77	108.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ASN	N-CA-C	6.20	119.29	107.75
1	A	102	GLU	N-CA-C	6.18	120.59	111.87
1	A	209	SER	CA-C-N	6.12	127.48	119.84
1	A	209	SER	C-N-CA	6.12	127.48	119.84
1	A	123	ASN	N-CA-C	5.89	118.90	110.24
1	A	300	TYR	N-CA-C	5.87	119.09	109.76
1	A	309	ILE	CA-C-N	-5.87	113.94	120.45
1	A	309	ILE	C-N-CA	-5.87	113.94	120.45
1	A	59	GLU	N-CA-C	-5.77	106.10	114.12
1	A	314	LYS	N-CA-C	-5.75	103.53	110.88
1	A	336	ASN	N-CA-C	5.72	119.24	108.65
1	A	112	SER	N-CA-C	5.55	115.61	108.34
1	A	105	VAL	N-CA-C	5.51	115.79	107.80
1	A	163	VAL	O-C-N	5.47	123.92	120.42
1	A	353	GLN	N-CA-C	-5.45	106.33	112.87
1	A	172	ALA	N-CA-C	-5.43	106.52	114.39
1	A	129	ASN	CA-C-N	5.37	125.19	119.28
1	A	129	ASN	C-N-CA	5.37	125.19	119.28
1	A	158	ALA	CA-C-N	5.37	127.47	120.28
1	A	158	ALA	C-N-CA	5.37	127.47	120.28
1	A	321	LEU	N-CA-C	5.36	117.14	108.34
1	A	229	HIS	CB-CA-C	5.26	116.78	108.88
1	A	255	ASN	CA-C-N	5.22	126.36	119.84
1	A	255	ASN	C-N-CA	5.22	126.36	119.84
1	A	82	SER	N-CA-C	5.16	116.15	109.65
1	A	298	PHE	N-CA-C	5.13	121.74	110.80
1	A	107	VAL	N-CA-C	5.11	114.55	106.32
1	A	50	ASN	CA-CB-CG	-5.10	107.50	112.60
1	A	72	ARG	CA-C-N	-5.07	113.50	119.84
1	A	72	ARG	C-N-CA	-5.07	113.50	119.84
1	A	267	ARG	N-CA-C	-5.03	105.80	111.28
1	A	302	ASN	N-CA-C	5.02	117.76	109.72
1	A	136	LEU	N-CA-C	-5.02	102.27	110.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ALA	Peptide
1	A	313	ARG	Peptide
1	A	321	LEU	Peptide
1	A	361	HIS	Peptide

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	2631	0	2556	380	0
2	B	28	0	25	0	0
3	A	1	0	0	0	0
4	A	52	0	0	10	0
All	All	2712	0	2581	380	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 73.

All (380) 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:171:LEU:O	1:A:175:LEU:HD21	1.37	1.19
1:A:344:THR:O	1:A:348:LEU:HD13	1.42	1.17
1:A:267:ARG:HH11	1:A:267:ARG:HB2	1.08	1.14
1:A:171:LEU:HD11	1:A:352:ILE:HD12	1.33	1.09
1:A:346:ASP:O	1:A:349:ASN:N	1.83	1.09
1:A:175:LEU:H	1:A:175:LEU:HD23	1.16	1.06
1:A:228:PRO:HA	1:A:237:ASN:HA	1.33	1.05
1:A:134:ARG:O	1:A:192:LEU:HA	1.57	1.04
1:A:279:LEU:CD1	1:A:285:LEU:HD13	1.88	1.03
1:A:142:TYR:CE2	1:A:200:ASP:HB2	1.97	0.99
1:A:279:LEU:CD1	1:A:285:LEU:CD1	2.41	0.98
1:A:204:ALA:HB2	1:A:212:ASP:O	1.64	0.97
1:A:280:TYR:HB2	1:A:285:LEU:HD22	1.46	0.96
1:A:78:ARG:NH1	1:A:156:VAL:O	1.98	0.96
1:A:247:LEU:HD22	1:A:308:HIS:HB3	1.48	0.96
1:A:227:SER:HB2	1:A:238:GLN:HE21	1.31	0.95
1:A:277:LYS:C	1:A:279:LEU:H	1.76	0.94
1:A:281:GLU:HB2	4:A:379:HOH:O	1.67	0.93
1:A:53:SER:HA	1:A:56:GLN:HE21	1.33	0.92
1:A:342:ALA:O	1:A:343:SER:C	2.13	0.90
1:A:175:LEU:H	1:A:175:LEU:CD2	1.85	0.89
1:A:171:LEU:C	1:A:175:LEU:HD21	1.98	0.88
1:A:337:GLU:HA	1:A:340:LEU:HD12	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ARG:HB2	1:A:267:ARG:NH1	1.89	0.88
1:A:227:SER:HB2	1:A:238:GLN:NE2	1.89	0.87
1:A:285:LEU:HD23	1:A:288:HIS:HD2	1.40	0.87
1:A:260:ASN:HB2	1:A:269:PHE:CD1	2.11	0.86
1:A:247:LEU:CD2	1:A:308:HIS:HB3	2.05	0.85
1:A:346:ASP:O	1:A:347:ASN:C	2.19	0.85
1:A:134:ARG:HB3	1:A:243:ASP:OD1	1.76	0.85
1:A:344:THR:C	1:A:348:LEU:HD13	2.02	0.84
1:A:279:LEU:HD12	1:A:285:LEU:CD1	2.06	0.84
1:A:72:ARG:HA	1:A:75:LEU:HD12	1.59	0.83
1:A:37:TRP:O	1:A:39:GLN:N	2.12	0.82
1:A:204:ALA:CB	1:A:212:ASP:O	2.26	0.82
1:A:279:LEU:HD13	1:A:285:LEU:HD13	1.61	0.82
1:A:218:ARG:HH11	1:A:218:ARG:HB2	1.44	0.81
1:A:139:ALA:O	1:A:247:LEU:HD12	1.81	0.81
1:A:102:GLU:HB3	1:A:128:LEU:CD2	2.11	0.80
1:A:112:SER:HB3	1:A:121:PHE:CE2	2.17	0.80
1:A:62:SER:OG	1:A:65:GLU:HB3	1.81	0.80
1:A:148:PRO:HB2	1:A:150:TRP:HE1	1.47	0.80
1:A:347:ASN:HB2	1:A:348:LEU:HD12	1.63	0.80
1:A:133:LYS:H	1:A:191:ASP:HB3	1.46	0.79
1:A:92:ILE:O	1:A:95:ARG:N	2.16	0.78
1:A:99:LEU:HB2	4:A:34:HOH:O	1.83	0.78
1:A:158:ALA:O	1:A:163:VAL:HG23	1.83	0.78
1:A:279:LEU:HD12	1:A:285:LEU:HD11	1.66	0.78
1:A:178:LYS:H	1:A:178:LYS:HZ2	1.32	0.78
1:A:214:LEU:HB3	1:A:217:SER:OG	1.83	0.77
1:A:229:HIS:HA	1:A:230:PRO:C	2.10	0.77
1:A:167:MET:HE3	1:A:349:ASN:OD1	1.84	0.77
1:A:114:THR:HG21	1:A:119:ARG:HG2	1.65	0.77
1:A:263:PRO:HB3	1:A:300:TYR:OH	1.86	0.76
1:A:123:ASN:OD1	1:A:199:PHE:HA	1.87	0.75
1:A:348:LEU:HA	1:A:351:ILE:HD12	1.69	0.75
1:A:148:PRO:HB2	1:A:150:TRP:NE1	2.02	0.75
1:A:276:GLU:OE1	4:A:377:HOH:O	2.05	0.75
1:A:176:ASP:O	1:A:179:LEU:HB2	1.87	0.74
1:A:311:PHE:O	1:A:313:ARG:N	2.20	0.74
1:A:63:ILE:HG12	1:A:63:ILE:O	1.87	0.74
1:A:37:TRP:CG	1:A:38:THR:H	2.05	0.74
1:A:114:THR:HG21	1:A:119:ARG:CG	2.18	0.73
1:A:184:ASP:H	1:A:185:VAL:HA	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:TRP:O	1:A:271:ARG:N	2.15	0.72
1:A:360:LEU:O	1:A:362:LEU:N	2.16	0.72
1:A:353:GLN:O	1:A:357:LEU:HD12	1.90	0.72
1:A:112:SER:O	1:A:118:TYR:HD1	1.73	0.72
1:A:175:LEU:HD23	1:A:175:LEU:N	1.96	0.72
1:A:259:PRO:O	1:A:269:PHE:HE1	1.71	0.72
1:A:88:ALA:O	1:A:89:ARG:C	2.33	0.72
1:A:214:LEU:HD22	1:A:307:ASP:HA	1.70	0.72
1:A:349:ASN:O	1:A:353:GLN:HG3	1.90	0.71
1:A:66:MET:HE1	1:A:345:ILE:HG21	1.71	0.71
1:A:171:LEU:CD1	1:A:352:ILE:HD12	2.18	0.70
1:A:303:ILE:HG23	1:A:303:ILE:O	1.90	0.70
1:A:103:TRP:HZ3	1:A:194:LEU:O	1.74	0.70
1:A:137:VAL:HG23	1:A:195:ARG:HB3	1.74	0.69
1:A:214:LEU:O	1:A:215:TYR:C	2.35	0.69
1:A:227:SER:CB	1:A:238:GLN:HE21	2.05	0.69
1:A:322:ILE:O	1:A:323:ALA:C	2.34	0.69
1:A:270:ASN:HA	1:A:273:GLN:CG	2.23	0.69
1:A:248:LEU:N	1:A:248:LEU:HD12	2.09	0.68
1:A:322:ILE:O	1:A:322:ILE:HG23	1.93	0.68
1:A:72:ARG:HA	1:A:75:LEU:CD1	2.24	0.68
1:A:88:ALA:O	1:A:91:HIS:N	2.27	0.68
1:A:164:PRO:O	1:A:167:MET:HG2	1.94	0.67
1:A:126:SER:HB3	1:A:196:LEU:HB2	1.76	0.67
1:A:63:ILE:HD12	1:A:346:ASP:H	1.60	0.67
1:A:167:MET:HB3	1:A:349:ASN:OD1	1.94	0.67
1:A:228:PRO:CA	1:A:237:ASN:HA	2.18	0.66
1:A:137:VAL:HG12	1:A:244:LEU:O	1.96	0.66
1:A:357:LEU:O	1:A:358:GLU:C	2.38	0.66
1:A:134:ARG:CB	1:A:243:ASP:OD1	2.44	0.66
1:A:159:THR:O	1:A:161:SER:OG	2.10	0.66
1:A:277:LYS:C	1:A:279:LEU:N	2.47	0.66
1:A:102:GLU:HB3	1:A:128:LEU:HD23	1.76	0.66
1:A:259:PRO:O	1:A:269:PHE:CE1	2.48	0.66
1:A:346:ASP:O	1:A:348:LEU:N	2.28	0.65
1:A:96:ILE:HG22	1:A:97:GLN:N	2.10	0.65
1:A:142:TYR:HE2	1:A:200:ASP:HB2	1.56	0.65
1:A:280:TYR:HB2	1:A:285:LEU:CD2	2.22	0.65
1:A:277:LYS:NZ	1:A:281:GLU:OE2	2.29	0.65
1:A:270:ASN:HA	1:A:273:GLN:HG2	1.77	0.65
1:A:53:SER:O	1:A:56:GLN:HG2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LYS:O	1:A:279:LEU:N	2.28	0.64
1:A:343:SER:O	1:A:344:THR:C	2.40	0.64
1:A:37:TRP:CG	1:A:38:THR:N	2.64	0.63
1:A:275:ILE:O	1:A:279:LEU:HB2	1.97	0.63
1:A:58:ALA:HB3	1:A:284:LEU:HD22	1.79	0.63
1:A:114:THR:C	1:A:116:TYR:H	2.06	0.63
1:A:348:LEU:H	1:A:348:LEU:CD1	2.11	0.63
1:A:84:GLY:C	1:A:86:TYR:H	2.07	0.62
1:A:354:VAL:O	1:A:355:PHE:C	2.42	0.62
1:A:137:VAL:HA	1:A:195:ARG:O	1.99	0.62
1:A:263:PRO:HD3	1:A:300:TYR:CE2	2.35	0.62
1:A:356:VAL:O	1:A:360:LEU:HG	2.00	0.62
1:A:96:ILE:HG23	1:A:103:TRP:CD1	2.34	0.62
1:A:336:ASN:HD21	1:A:338:GLU:HB3	1.65	0.62
1:A:57:VAL:O	1:A:57:VAL:HG12	1.99	0.62
1:A:280:TYR:HB3	1:A:290:LEU:HD21	1.81	0.61
1:A:112:SER:O	1:A:118:TYR:CD1	2.53	0.61
1:A:353:GLN:O	1:A:357:LEU:CD1	2.47	0.61
1:A:342:ALA:O	1:A:343:SER:O	2.16	0.61
1:A:155:PHE:HE1	1:A:335:ASP:HB3	1.65	0.61
1:A:262:PHE:N	1:A:262:PHE:CD2	2.67	0.61
1:A:267:ARG:O	1:A:270:ASN:HB2	2.01	0.61
1:A:347:ASN:HB2	1:A:348:LEU:CD1	2.29	0.60
1:A:350:LYS:O	1:A:352:ILE:N	2.33	0.60
1:A:348:LEU:N	1:A:348:LEU:CD1	2.65	0.60
1:A:216:GLY:O	1:A:217:SER:C	2.45	0.60
1:A:86:TYR:CE2	1:A:90:GLN:HG3	2.37	0.59
1:A:343:SER:O	1:A:346:ASP:HB3	2.02	0.59
1:A:280:TYR:CB	1:A:285:LEU:HD22	2.28	0.59
1:A:57:VAL:O	1:A:57:VAL:CG1	2.51	0.59
1:A:58:ALA:CB	1:A:284:LEU:HD22	2.33	0.59
1:A:267:ARG:HH11	1:A:267:ARG:CB	2.00	0.59
1:A:295:PHE:HB2	4:A:377:HOH:O	2.03	0.59
1:A:337:GLU:O	1:A:340:LEU:N	2.36	0.59
1:A:164:PRO:O	1:A:165:CYS:C	2.45	0.59
1:A:86:TYR:CE1	1:A:89:ARG:NH2	2.72	0.58
1:A:278:GLU:C	4:A:379:HOH:O	2.46	0.58
1:A:336:ASN:ND2	1:A:338:GLU:HB3	2.19	0.58
1:A:279:LEU:HD12	1:A:285:LEU:HD13	1.74	0.58
1:A:102:GLU:HG2	1:A:183:LYS:HD2	1.85	0.58
1:A:102:GLU:H	1:A:128:LEU:HD21	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HG	1:A:353:GLN:HG2	1.84	0.58
1:A:279:LEU:CD1	1:A:285:LEU:HD11	2.22	0.58
1:A:79:TYR:CD1	1:A:79:TYR:N	2.71	0.57
1:A:358:GLU:O	1:A:359:TYR:C	2.47	0.57
1:A:199:PHE:CE1	1:A:220:LEU:HD23	2.40	0.57
1:A:357:LEU:O	1:A:360:LEU:N	2.38	0.57
1:A:354:VAL:HG12	1:A:355:PHE:N	2.20	0.57
1:A:260:ASN:HB2	1:A:269:PHE:CE1	2.38	0.57
1:A:346:ASP:OD1	1:A:347:ASN:N	2.38	0.57
1:A:284:LEU:O	1:A:285:LEU:HD12	2.05	0.57
1:A:92:ILE:O	1:A:93:MET:C	2.47	0.56
1:A:163:VAL:HB	1:A:251:ILE:O	2.05	0.56
1:A:173:ARG:O	1:A:174:ALA:C	2.48	0.56
1:A:70:ASP:OD2	1:A:95:ARG:NH2	2.38	0.56
1:A:220:LEU:HB3	1:A:311:PHE:HZ	1.69	0.56
1:A:279:LEU:N	4:A:379:HOH:O	2.39	0.56
1:A:283:GLY:C	1:A:285:LEU:H	2.12	0.56
1:A:79:TYR:HD1	1:A:79:TYR:H	1.53	0.56
1:A:66:MET:HE1	1:A:345:ILE:CG2	2.36	0.56
1:A:146:TYR:OH	1:A:148:PRO:HA	2.05	0.56
1:A:70:ASP:OD1	1:A:169:LEU:HB3	2.06	0.56
1:A:178:LYS:HZ3	1:A:178:LYS:HB2	1.70	0.56
1:A:91:HIS:C	1:A:91:HIS:CD2	2.84	0.56
1:A:69:ASN:N	1:A:69:ASN:HD22	2.03	0.56
1:A:311:PHE:C	1:A:313:ARG:N	2.63	0.56
1:A:92:ILE:HG22	1:A:93:MET:N	2.21	0.55
1:A:161:SER:HB3	1:A:164:PRO:HG2	1.88	0.55
1:A:346:ASP:C	1:A:348:LEU:N	2.63	0.55
1:A:351:ILE:O	1:A:354:VAL:HB	2.06	0.55
1:A:84:GLY:O	1:A:86:TYR:N	2.40	0.55
1:A:214:LEU:O	1:A:216:GLY:N	2.40	0.55
1:A:258:PHE:CD2	1:A:294:TYR:HB2	2.42	0.55
1:A:109:THR:HA	1:A:121:PHE:O	2.07	0.54
1:A:346:ASP:OD1	1:A:346:ASP:C	2.48	0.54
1:A:57:VAL:HG22	1:A:60:GLY:HA3	1.89	0.54
1:A:287:ASP:OD1	1:A:343:SER:OG	2.24	0.54
1:A:82:SER:O	1:A:83:PRO:C	2.50	0.54
1:A:349:ASN:C	1:A:353:GLN:HE21	2.15	0.54
1:A:47:ALA:HB2	1:A:361:HIS:HD2	1.72	0.54
1:A:243:ASP:HB3	1:A:359:TYR:OH	2.08	0.54
1:A:279:LEU:HD11	1:A:285:LEU:CD1	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LEU:HD12	1:A:348:LEU:N	2.23	0.53
1:A:106:GLU:HG2	1:A:125:ILE:HD13	1.89	0.53
1:A:135:HIS:HD2	1:A:194:LEU:N	2.06	0.53
1:A:234:ARG:NH2	4:A:16:HOH:O	2.40	0.53
1:A:114:THR:HG21	1:A:119:ARG:CB	2.37	0.53
1:A:285:LEU:HD23	1:A:288:HIS:CD2	2.31	0.53
1:A:82:SER:O	1:A:84:GLY:N	2.42	0.53
1:A:102:GLU:HB3	1:A:128:LEU:HD22	1.90	0.53
1:A:183:LYS:HA	1:A:185:VAL:HG22	1.91	0.53
1:A:273:GLN:HE22	1:A:297:ASN:HB2	1.74	0.53
1:A:92:ILE:O	1:A:95:ARG:HB2	2.09	0.53
1:A:345:ILE:O	1:A:349:ASN:N	2.42	0.53
1:A:158:ALA:HB1	1:A:340:LEU:HD11	1.91	0.52
1:A:142:TYR:HB3	1:A:198:PHE:HB3	1.91	0.52
1:A:150:TRP:CD1	1:A:150:TRP:N	2.77	0.52
1:A:110:PHE:CD1	1:A:219:HIS:CD2	2.98	0.52
1:A:57:VAL:HA	1:A:60:GLY:H	1.75	0.52
1:A:337:GLU:O	1:A:338:GLU:C	2.52	0.52
1:A:51:SER:HA	1:A:54:LEU:HB2	1.92	0.52
1:A:163:VAL:HG21	1:A:251:ILE:O	2.10	0.51
1:A:86:TYR:CD2	1:A:90:GLN:HG3	2.45	0.51
1:A:115:PRO:HD2	1:A:205:PHE:HD1	1.74	0.51
1:A:247:LEU:C	1:A:248:LEU:HD12	2.35	0.51
1:A:44:HIS:O	1:A:267:ARG:NH2	2.43	0.51
1:A:163:VAL:HB	1:A:164:PRO:HD3	1.91	0.51
1:A:167:MET:O	1:A:171:LEU:N	2.29	0.51
1:A:212:ASP:O	1:A:213:SER:HB3	2.11	0.51
1:A:248:LEU:N	1:A:248:LEU:CD1	2.73	0.51
1:A:51:SER:O	1:A:52:SER:C	2.53	0.51
1:A:163:VAL:CB	1:A:251:ILE:O	2.58	0.51
1:A:198:PHE:N	1:A:198:PHE:CD2	2.78	0.51
1:A:255:ASN:N	1:A:256:PRO:HD3	2.25	0.51
1:A:346:ASP:HA	1:A:349:ASN:HB2	1.92	0.50
1:A:63:ILE:CD1	1:A:345:ILE:HB	2.41	0.50
1:A:134:ARG:HG2	1:A:243:ASP:OD1	2.11	0.50
1:A:184:ASP:N	1:A:185:VAL:HA	2.21	0.50
1:A:311:PHE:C	1:A:313:ARG:H	2.18	0.50
1:A:134:ARG:HG3	1:A:241:GLY:HA2	1.94	0.50
1:A:258:PHE:CD2	1:A:258:PHE:N	2.80	0.50
1:A:288:HIS:CE1	1:A:289:SER:O	2.65	0.50
1:A:344:THR:O	1:A:345:ILE:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ARG:C	1:A:74:LEU:H	2.20	0.50
1:A:79:TYR:HA	1:A:143:ASP:HB2	1.93	0.50
1:A:270:ASN:HA	1:A:273:GLN:HG3	1.93	0.50
1:A:348:LEU:HD13	1:A:348:LEU:H	1.76	0.50
1:A:362:LEU:N	1:A:362:LEU:HD23	2.27	0.50
1:A:68:GLN:NE2	1:A:72:ARG:HD2	2.27	0.49
1:A:262:PHE:HZ	1:A:320:HIS:H	1.60	0.49
1:A:136:LEU:HD21	1:A:356:VAL:HG22	1.94	0.49
1:A:280:TYR:CD2	1:A:290:LEU:HG	2.47	0.49
1:A:311:PHE:O	1:A:312:LEU:C	2.55	0.49
1:A:354:VAL:HA	1:A:357:LEU:HD12	1.94	0.49
1:A:37:TRP:CZ2	1:A:38:THR:HG22	2.48	0.49
1:A:167:MET:O	1:A:170:GLU:N	2.45	0.49
1:A:112:SER:O	1:A:118:TYR:HA	2.12	0.49
1:A:204:ALA:CB	1:A:208:TRP:HA	2.42	0.49
1:A:82:SER:C	1:A:84:GLY:N	2.70	0.49
1:A:70:ASP:O	1:A:74:LEU:HD12	2.13	0.49
1:A:114:THR:HG21	1:A:119:ARG:HB2	1.95	0.48
1:A:181:SER:HA	4:A:5:HOH:O	2.13	0.48
1:A:350:LYS:O	1:A:353:GLN:N	2.44	0.48
1:A:82:SER:O	1:A:85:SER:N	2.46	0.48
1:A:136:LEU:O	1:A:194:LEU:HA	2.14	0.48
1:A:159:THR:HA	1:A:251:ILE:O	2.14	0.48
1:A:213:SER:O	1:A:214:LEU:HB2	2.14	0.48
1:A:260:ASN:ND2	1:A:266:THR:OG1	2.46	0.48
1:A:53:SER:HA	1:A:56:GLN:NE2	2.15	0.48
1:A:191:ASP:O	1:A:192:LEU:HB2	2.14	0.48
1:A:102:GLU:HA	1:A:102:GLU:OE2	2.14	0.48
1:A:105:VAL:HG23	1:A:105:VAL:O	2.12	0.48
1:A:356:VAL:O	1:A:357:LEU:O	2.32	0.48
1:A:265:THR:O	1:A:268:TRP:HB2	2.14	0.47
1:A:280:TYR:HD2	1:A:290:LEU:HG	1.79	0.47
1:A:327:PRO:C	1:A:329:VAL:H	2.20	0.47
1:A:352:ILE:C	1:A:354:VAL:N	2.72	0.47
1:A:227:SER:O	1:A:237:ASN:HB2	2.15	0.47
1:A:175:LEU:HG	1:A:175:LEU:O	2.14	0.47
1:A:137:VAL:HG23	1:A:195:ARG:O	2.14	0.47
1:A:313:ARG:NE	4:A:29:HOH:O	2.31	0.47
1:A:350:LYS:O	1:A:351:ILE:C	2.58	0.47
1:A:96:ILE:CG2	1:A:103:TRP:CD1	2.97	0.47
1:A:77:GLU:O	1:A:84:GLY:HA3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:HIS:CG	1:A:202:GLU:HB2	2.50	0.47
1:A:167:MET:C	1:A:169:LEU:N	2.70	0.47
1:A:69:ASN:N	1:A:69:ASN:ND2	2.63	0.47
1:A:227:SER:O	1:A:238:GLN:HG3	2.15	0.46
1:A:354:VAL:O	1:A:357:LEU:HB2	2.15	0.46
1:A:134:ARG:CG	1:A:243:ASP:OD1	2.63	0.46
1:A:84:GLY:C	1:A:86:TYR:N	2.74	0.46
1:A:171:LEU:O	1:A:171:LEU:HD23	2.16	0.46
1:A:256:PRO:O	1:A:257:THR:HG23	2.16	0.46
1:A:329:VAL:O	1:A:329:VAL:HG23	2.15	0.46
1:A:171:LEU:HD11	1:A:352:ILE:CD1	2.25	0.46
1:A:149:ARG:CZ	1:A:154:VAL:HG11	2.46	0.46
1:A:354:VAL:CG1	1:A:358:GLU:HG3	2.46	0.46
1:A:108:ASP:OD1	1:A:219:HIS:HE1	1.99	0.46
1:A:231:PRO:HA	1:A:232:GLY:HA2	1.71	0.46
1:A:261:PHE:CZ	1:A:304:ILE:HD12	2.51	0.46
1:A:72:ARG:HH21	1:A:337:GLU:CD	2.24	0.46
1:A:343:SER:O	1:A:344:THR:O	2.33	0.45
1:A:272:LEU:O	1:A:276:GLU:HB2	2.15	0.45
1:A:147:PHE:HD1	1:A:147:PHE:HA	1.67	0.45
1:A:355:PHE:O	1:A:356:VAL:C	2.59	0.45
1:A:178:LYS:HB2	1:A:178:LYS:NZ	2.31	0.45
1:A:66:MET:O	1:A:67:TRP:C	2.59	0.45
1:A:257:THR:HG22	1:A:294:TYR:HA	1.99	0.45
1:A:37:TRP:CD2	1:A:38:THR:N	2.84	0.45
1:A:103:TRP:CZ3	1:A:194:LEU:O	2.64	0.44
1:A:112:SER:HB3	1:A:121:PHE:CZ	2.50	0.44
1:A:112:SER:CB	1:A:121:PHE:CE2	2.96	0.44
1:A:258:PHE:HD2	1:A:294:TYR:HB2	1.80	0.44
1:A:82:SER:HA	1:A:83:PRO:HD2	1.84	0.44
1:A:175:LEU:CD2	1:A:175:LEU:N	2.61	0.44
1:A:247:LEU:HD23	1:A:308:HIS:HB3	1.92	0.44
1:A:76:ILE:CD1	1:A:87:SER:OG	2.66	0.44
1:A:237:ASN:N	1:A:240:ASP:OD2	2.50	0.44
1:A:178:LYS:H	1:A:178:LYS:NZ	2.10	0.44
1:A:78:ARG:HG2	1:A:144:SER:HB3	1.99	0.44
1:A:262:PHE:HZ	1:A:320:HIS:N	2.15	0.44
1:A:308:HIS:HB2	1:A:318:VAL:HG11	1.99	0.44
1:A:37:TRP:CE2	1:A:38:THR:HG22	2.53	0.44
1:A:114:THR:HB	1:A:205:PHE:CE1	2.53	0.44
1:A:93:MET:C	1:A:97:GLN:OE1	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLU:H	1:A:131:GLU:HG3	1.29	0.43
1:A:37:TRP:C	1:A:39:GLN:H	2.22	0.43
1:A:227:SER:CB	1:A:238:GLN:NE2	2.70	0.43
1:A:279:LEU:HD13	1:A:279:LEU:C	2.43	0.43
1:A:55:GLN:O	1:A:57:VAL:N	2.52	0.43
1:A:135:HIS:HD2	1:A:193:SER:C	2.25	0.43
1:A:202:GLU:HB3	1:A:203:GLU:HG2	1.99	0.43
1:A:272:LEU:O	1:A:273:GLN:C	2.61	0.43
1:A:97:GLN:C	1:A:99:LEU:N	2.75	0.43
1:A:163:VAL:CG2	1:A:251:ILE:O	2.66	0.43
1:A:277:LYS:HG3	1:A:278:GLU:H	1.82	0.43
1:A:141:HIS:CD2	1:A:143:ASP:O	2.72	0.43
1:A:354:VAL:HG12	1:A:358:GLU:HG3	2.01	0.43
1:A:90:GLN:HE21	1:A:93:MET:HE2	1.84	0.43
1:A:110:PHE:CG	1:A:219:HIS:CD2	3.07	0.43
1:A:120:SER:C	1:A:121:PHE:CD2	2.97	0.43
1:A:218:ARG:HB2	1:A:218:ARG:NH1	2.23	0.43
1:A:228:PRO:HA	1:A:237:ASN:CA	2.25	0.43
1:A:283:GLY:C	1:A:285:LEU:N	2.77	0.43
1:A:47:ALA:HB2	1:A:361:HIS:CD2	2.53	0.43
1:A:262:PHE:HA	1:A:263:PRO:HD2	1.69	0.43
1:A:80:PRO:C	1:A:82:SER:H	2.27	0.42
1:A:141:HIS:ND1	1:A:202:GLU:HG3	2.34	0.42
1:A:160:ASP:HA	1:A:161:SER:OG	2.19	0.42
1:A:88:ALA:O	1:A:90:GLN:N	2.52	0.42
1:A:352:ILE:H	1:A:352:ILE:HG13	1.45	0.42
1:A:114:THR:C	1:A:116:TYR:N	2.72	0.42
1:A:72:ARG:O	1:A:74:LEU:N	2.53	0.42
1:A:90:GLN:O	1:A:91:HIS:C	2.62	0.42
1:A:134:ARG:HA	1:A:241:GLY:O	2.19	0.42
1:A:354:VAL:HG13	1:A:358:GLU:CG	2.49	0.42
1:A:357:LEU:O	1:A:359:TYR:N	2.52	0.42
1:A:275:ILE:HG21	1:A:351:ILE:HA	2.00	0.42
1:A:110:PHE:CG	1:A:219:HIS:NE2	2.88	0.42
1:A:293:LYS:H	1:A:293:LYS:HG3	1.56	0.42
1:A:344:THR:HA	1:A:348:LEU:CD1	2.50	0.42
1:A:94:GLN:OE1	1:A:95:ARG:N	2.52	0.42
1:A:116:TYR:HB3	1:A:119:ARG:HH22	1.84	0.42
1:A:350:LYS:HB2	1:A:351:ILE:H	1.40	0.42
1:A:63:ILE:HD12	1:A:345:ILE:HB	2.01	0.41
1:A:95:ARG:HD2	1:A:95:ARG:HA	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:PHE:CE2	1:A:319:LEU:HA	2.55	0.41
1:A:71:LEU:HD13	1:A:166:ALA:HB2	2.01	0.41
1:A:46:PRO:HB2	1:A:358:GLU:HB3	2.02	0.41
1:A:263:PRO:HD3	1:A:300:TYR:CZ	2.55	0.41
1:A:355:PHE:C	1:A:355:PHE:CD2	2.98	0.41
1:A:209:SER:HA	1:A:210:PRO:HD2	1.87	0.41
1:A:63:ILE:HD11	1:A:345:ILE:HB	2.02	0.41
1:A:229:HIS:ND1	1:A:238:GLN:HG2	2.35	0.41
1:A:244:LEU:HD12	1:A:317:PRO:O	2.20	0.41
1:A:284:LEU:C	1:A:285:LEU:HD12	2.46	0.41
1:A:286:LYS:O	1:A:287:ASP:C	2.64	0.41
1:A:341:HIS:O	1:A:342:ALA:C	2.64	0.41
1:A:96:ILE:CG2	1:A:97:GLN:N	2.72	0.41
1:A:213:SER:O	1:A:218:ARG:NH2	2.53	0.41
1:A:171:LEU:C	1:A:175:LEU:CD2	2.83	0.41
1:A:242:MET:HE3	1:A:242:MET:HB3	1.67	0.41
1:A:164:PRO:O	1:A:166:ALA:N	2.54	0.41
1:A:103:TRP:HE3	1:A:127:THR:C	2.28	0.40
1:A:114:THR:O	1:A:116:TYR:N	2.54	0.40
1:A:330:TRP:O	1:A:331:HIS:HB2	2.22	0.40
1:A:36:ALA:N	4:A:363:HOH:O	2.53	0.40
1:A:60:GLY:O	1:A:174:ALA:HB1	2.21	0.40
1:A:79:TYR:CZ	1:A:82:SER:HB2	2.57	0.40
1:A:135:HIS:CD2	1:A:193:SER:C	3.00	0.40
1:A:355:PHE:O	1:A:358:GLU:HB2	2.21	0.40
1:A:37:TRP:HZ3	1:A:241:GLY:HA2	1.86	0.40
1:A:49:LEU:N	1:A:49:LEU:HD23	2.37	0.40
1:A:199:PHE:HE1	1:A:220:LEU:HD23	1.84	0.40
1:A:345:ILE:H	1:A:345:ILE:HG12	1.53	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	319/327 (98%)	185 (58%)	81 (25%)	53 (17%)	0 0

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	85	SER
1	A	92	ILE
1	A	93	MET
1	A	96	ILE
1	A	168	MET
1	A	182	LEU
1	A	215	TYR
1	A	259	PRO
1	A	278	GLU
1	A	312	LEU
1	A	322	ILE
1	A	338	GLU
1	A	341	HIS
1	A	342	ALA
1	A	343	SER
1	A	344	THR
1	A	345	ILE
1	A	346	ASP
1	A	350	LYS
1	A	351	ILE
1	A	357	LEU
1	A	358	GLU
1	A	359	TYR
1	A	361	HIS
1	A	83	PRO
1	A	164	PRO
1	A	192	LEU
1	A	219	HIS
1	A	89	ARG
1	A	97	GLN
1	A	101	ALA
1	A	115	PRO
1	A	217	SER
1	A	264	LYS
1	A	356	VAL
1	A	37	TRP
1	A	88	ALA

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Mol	Chain	Res	Type
1	A	193	SER
1	A	284	LEU
1	A	323	ALA
1	A	337	GLU
1	A	347	ASN
1	A	157	GLY
1	A	173	ARG
1	A	205	PHE
1	A	213	SER
1	A	221	ALA
1	A	210	PRO
1	A	252	GLY
1	A	328	GLU
1	A	216	GLY
1	A	156	VAL

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	288/291 (99%)	206 (72%)	82 (28%)	0 1

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	42	ASN
1	A	45	GLN
1	A	48	HIS
1	A	49	LEU
1	A	55	GLN
1	A	65	GLU
1	A	68	GLN
1	A	69	ASN
1	A	74	LEU
1	A	77	GLU

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Mol	Chain	Res	Type
1	A	85	SER
1	A	87	SER
1	A	89	ARG
1	A	93	MET
1	A	94	GLN
1	A	97	GLN
1	A	100	GLN
1	A	102	GLU
1	A	106	GLU
1	A	108	ASP
1	A	111	LEU
1	A	124	ILE
1	A	131	GLU
1	A	133	LYS
1	A	147	PHE
1	A	150	TRP
1	A	153	ARG
1	A	154	VAL
1	A	156	VAL
1	A	161	SER
1	A	167	MET
1	A	170	GLU
1	A	171	LEU
1	A	175	LEU
1	A	178	LYS
1	A	182	LEU
1	A	183	LYS
1	A	192	LEU
1	A	202	GLU
1	A	203	GLU
1	A	211	GLN
1	A	218	ARG
1	A	236	THR
1	A	239	LEU
1	A	242	MET
1	A	243	ASP
1	A	246	VAL
1	A	248	LEU
1	A	251	ILE
1	A	257	THR
1	A	260	ASN
1	A	262	PHE

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Mol	Chain	Res	Type
1	A	267	ARG
1	A	275	ILE
1	A	276	GLU
1	A	277	LYS
1	A	279	LEU
1	A	286	LYS
1	A	287	ASP
1	A	291	GLU
1	A	293	LYS
1	A	294	TYR
1	A	304	ILE
1	A	308	HIS
1	A	309	ILE
1	A	314	LYS
1	A	321	LEU
1	A	328	GLU
1	A	329	VAL
1	A	334	ASP
1	A	336	ASN
1	A	339	ASN
1	A	344	THR
1	A	345	ILE
1	A	348	LEU
1	A	350	LYS
1	A	352	ILE
1	A	354	VAL
1	A	355	PHE
1	A	360	LEU
1	A	362	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	48	HIS
1	A	56	GLN
1	A	68	GLN
1	A	69	ASN
1	A	90	GLN
1	A	91	HIS
1	A	135	HIS
1	A	211	GLN

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Mol	Chain	Res	Type
1	A	219	HIS
1	A	238	GLN
1	A	260	ASN
1	A	288	HIS
1	A	297	ASN
1	A	331	HIS
1	A	336	ASN
1	A	353	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

2 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	2,1	14,14,15	0.70	0	17,19,21	1.76	5 (29%)
2	NAG	B	2	2	14,14,15	0.96	1 (7%)	17,19,21	3.28	9 (52%)

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	2,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	2	2	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	C1-C2	2.03	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C2-N2-C7	9.72	135.93	122.90
2	B	2	NAG	C1-C2-N2	4.29	117.19	110.43
2	B	2	NAG	C1-O5-C5	4.28	117.92	112.19
2	B	1	NAG	C1-O5-C5	3.73	117.19	112.19
2	B	2	NAG	O5-C5-C6	3.39	114.26	107.66
2	B	2	NAG	O5-C1-C2	-3.05	106.57	111.29
2	B	1	NAG	C1-C2-N2	-2.84	105.95	110.43
2	B	2	NAG	O7-C7-N2	2.83	126.98	121.98
2	B	2	NAG	C8-C7-N2	-2.42	112.11	116.12
2	B	1	NAG	C8-C7-N2	2.40	120.10	116.12
2	B	1	NAG	O5-C1-C2	-2.22	107.86	111.29
2	B	1	NAG	O5-C5-C6	-2.15	103.47	107.66
2	B	2	NAG	C3-C4-C5	2.15	114.13	110.23
2	B	2	NAG	O6-C6-C5	-2.03	104.41	111.33

There are no chirality outliers.

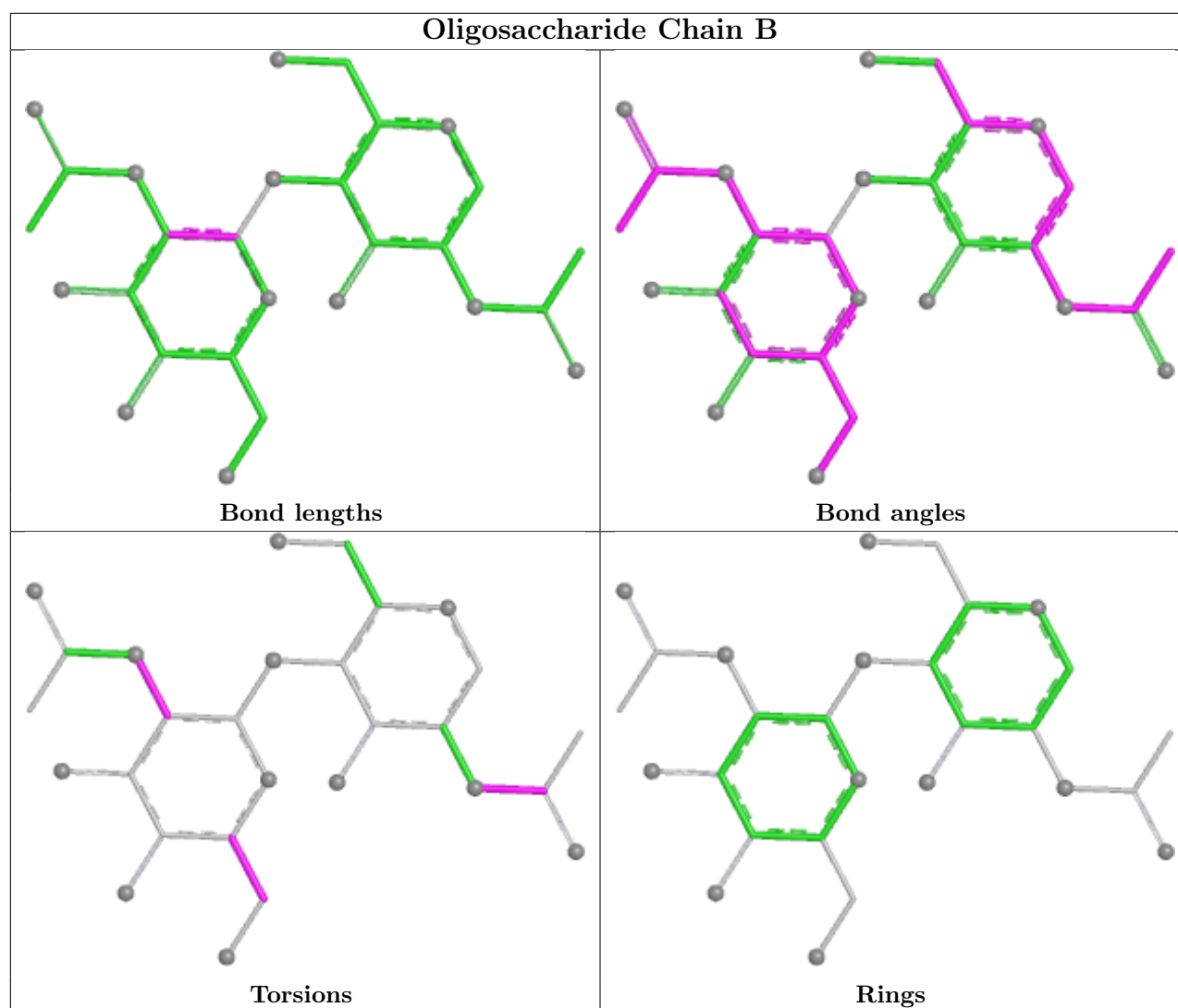
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C1-C2-N2-C7
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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, 95th 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 ²)	Q<0.9
1	A	323/327 (98%)	-0.08	1 (0%) 90 87	21, 47, 69, 84	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	GLY	2.0

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

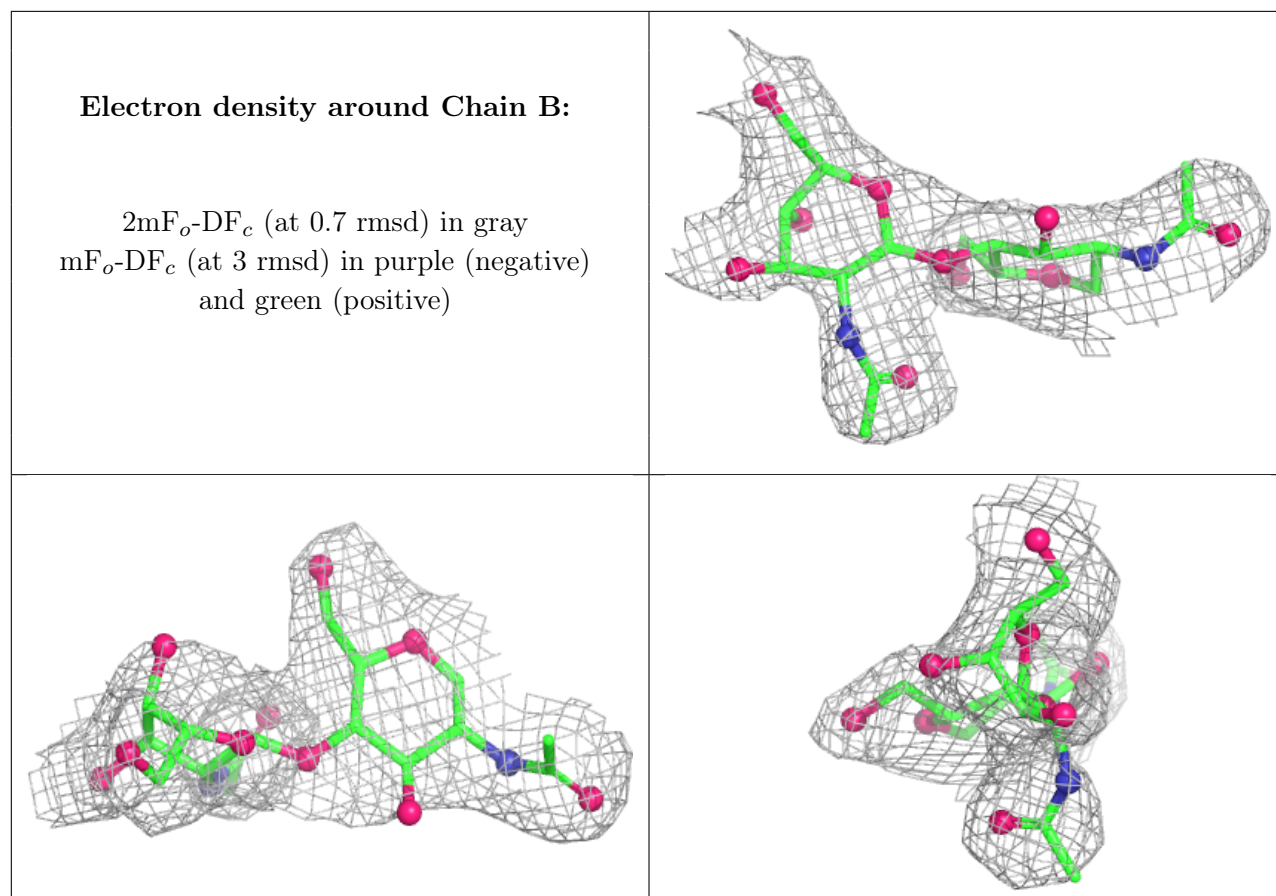
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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. The B-factors column lists the minimum, median, 95th 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	2	14/15	0.81	0.10	57,62,64,67	0
2	NAG	B	1	14/15	0.83	0.10	61,62,64,65	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95th 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	601	1/1	1.00	0.01	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.