



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:12 PM UTC

PDB ID : 1OJN / pdb_00001ojn
Title : SPECIFICITY AND MECHANISM OF STREPTOCOCCUS PNEUMONIAE HYALURONATE LYASE: COMPLEX OF THE TYR408PHE MUTANT WITH 6-SULPHATED CHONDROITIN DISACCHARIDE
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Deposited on : 2003-07-11
Resolution : 1.60 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	:	4-5-2 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

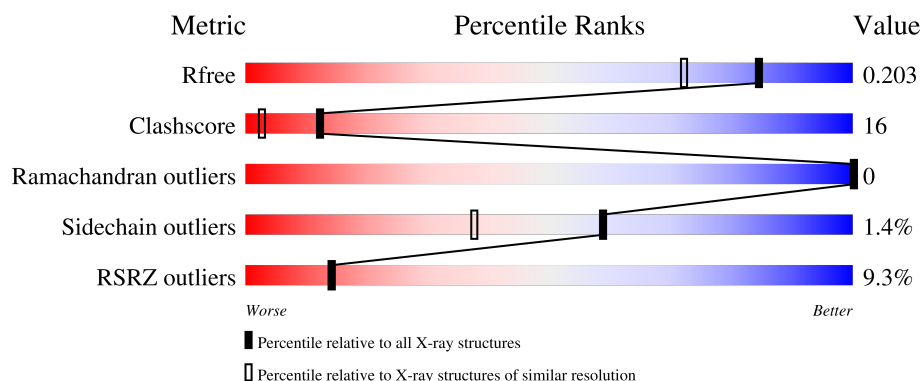
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 $\leq 5\%$. 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	731	9% 83% 13% ...
2	B	2	100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6651 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.

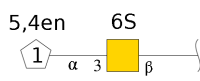
- Molecule 1 is a protein called HYALURONATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	723	5963	3750	1003	1188	22	0	19	1

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	893	HIS	-	expression tag	UNP Q54873
A	894	HIS	-	expression tag	UNP Q54873
A	895	HIS	-	expression tag	UNP Q54873
A	896	HIS	-	expression tag	UNP Q54873
A	897	HIS	-	expression tag	UNP Q54873
A	898	HIS	-	expression tag	UNP Q54873
A	173	THR	ALA	conflict	UNP Q54873
A	196	ASP	GLU	conflict	UNP Q54873
A	223	ILE	THR	conflict	UNP Q54873
A	408	PHE	TYR	conflict	UNP Q54873
A	496	ARG	CYS	conflict	UNP Q54873
A	541	THR	PRO	conflict	UNP Q54873
A	704	SER	GLY	conflict	UNP Q54873
A	736	SER	PHE	conflict	UNP Q54873
A	790	GLY	ARG	conflict	UNP Q54873

- Molecule 2 is an oligosaccharide called 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-6-O-sulfo-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	2	30	14	1	14	1	0	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

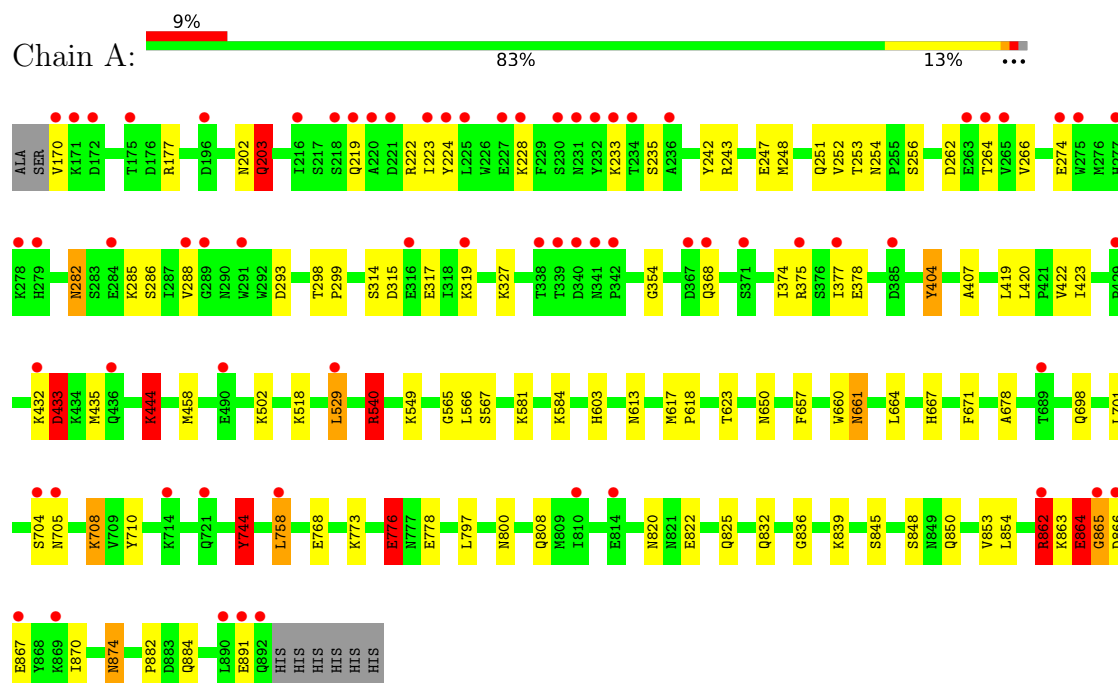
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	638	Total	O	0	0
			638	638		

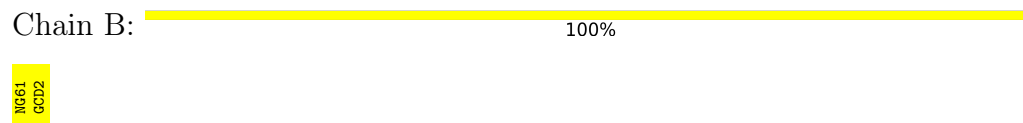
3 Residue-property plots

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: HYALURONATE LYASE



• Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-6-O-sulfo-beta-D-galactopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.91Å 104.20Å 101.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.08 – 1.60 40.08 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.08-1.60) 99.4 (40.08-1.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.45Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.194 , 0.209 0.188 , 0.203	Depositor DCC
R_{free} test set	6870 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6651	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: SO4, GCD, NG6

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	4.07	33/6084 (0.5%)	2.06	60/8209 (0.7%)

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	7

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203[A]	GLN	CD-NE2	154.66	4.58	1.33
1	A	203[B]	GLN	CD-NE2	154.66	4.58	1.33
1	A	862[A]	ARG	NE-CZ	108.19	2.52	1.33
1	A	862[B]	ARG	NE-CZ	108.19	2.52	1.33
1	A	432[A]	LYS	CD-CE	64.29	3.45	1.52
1	A	432[B]	LYS	CD-CE	64.29	3.45	1.52
1	A	433[A]	ASP	CG-OD2	58.33	2.36	1.25
1	A	433[B]	ASP	CG-OD2	58.33	2.36	1.25
1	A	203[A]	GLN	CG-CD	40.40	2.53	1.52
1	A	203[B]	GLN	CG-CD	40.40	2.53	1.52
1	A	758[A]	LEU	CG-CD2	34.15	2.65	1.52
1	A	758[B]	LEU	CG-CD2	34.15	2.65	1.52
1	A	540[A]	ARG	NE-CZ	33.58	1.70	1.33
1	A	540[B]	ARG	NE-CZ	33.58	1.70	1.33
1	A	776[A]	GLU	CD-OE2	31.35	1.84	1.25
1	A	776[B]	GLU	CD-OE2	31.35	1.84	1.25
1	A	865[A]	GLY	CA-C	26.70	1.89	1.51
1	A	865[B]	GLY	CA-C	26.70	1.89	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	744[A]	TYR	CG-CD1	-19.30	0.98	1.39
1	A	744[B]	TYR	CG-CD1	-19.30	0.98	1.39
1	A	776[A]	GLU	CD-OE1	16.68	1.57	1.25
1	A	776[B]	GLU	CD-OE1	16.68	1.57	1.25
1	A	744[A]	TYR	CG-CD2	-14.83	1.08	1.39
1	A	744[B]	TYR	CG-CD2	-14.83	1.08	1.39
1	A	744[A]	TYR	CD1-CE1	8.87	1.65	1.38
1	A	744[B]	TYR	CD1-CE1	8.87	1.65	1.38
1	A	444[A]	LYS	CG-CD	8.52	1.78	1.52
1	A	444[B]	LYS	CG-CD	8.52	1.78	1.52
1	A	744[A]	TYR	CD2-CE2	8.09	1.62	1.38
1	A	744[B]	TYR	CD2-CE2	8.09	1.62	1.38
1	A	865[A]	GLY	N-CA	-5.94	1.36	1.45
1	A	865[B]	GLY	N-CA	-5.94	1.36	1.45
1	A	891	GLU	C-N	-5.59	1.25	1.33

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203[A]	GLN	CG-CD-NE2	-62.62	22.47	116.40
1	A	203[B]	GLN	CG-CD-NE2	-62.62	22.47	116.40
1	A	203[A]	GLN	OE1-CD-NE2	-45.87	76.73	122.60
1	A	203[B]	GLN	OE1-CD-NE2	-45.87	76.73	122.60
1	A	776[A]	GLU	OE1-CD-OE2	-34.17	40.88	122.90
1	A	776[B]	GLU	OE1-CD-OE2	-34.17	40.88	122.90
1	A	862[A]	ARG	CD-NE-CZ	-31.14	80.80	124.40
1	A	862[B]	ARG	CD-NE-CZ	-31.14	80.80	124.40
1	A	862[A]	ARG	NE-CZ-NH1	-31.03	90.47	121.50
1	A	862[B]	ARG	NE-CZ-NH1	-31.03	90.47	121.50
1	A	758[A]	LEU	CD1-CG-CD2	-27.78	49.68	110.80
1	A	758[B]	LEU	CD1-CG-CD2	-27.78	49.68	110.80
1	A	203[A]	GLN	CG-CD-OE1	-24.57	71.66	120.80
1	A	203[B]	GLN	CG-CD-OE1	-24.57	71.66	120.80
1	A	203[A]	GLN	CB-CG-CD	-23.31	72.98	112.60
1	A	203[B]	GLN	CB-CG-CD	-23.31	72.98	112.60
1	A	744[A]	TYR	CB-CG-CD2	-23.23	85.96	120.80
1	A	744[B]	TYR	CB-CG-CD2	-23.23	85.96	120.80
1	A	744[A]	TYR	CB-CG-CD1	-21.83	88.05	120.80
1	A	744[B]	TYR	CB-CG-CD1	-21.83	88.05	120.80
1	A	444[A]	LYS	CG-CD-CE	20.66	158.83	111.30
1	A	444[B]	LYS	CG-CD-CE	20.66	158.83	111.30
1	A	433[A]	ASP	CB-CG-OD2	-19.79	72.89	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433[B]	ASP	CB-CG-OD2	-19.79	72.89	118.40
1	A	744[A]	TYR	CD1-CG-CD2	-15.48	94.89	118.10
1	A	744[B]	TYR	CD1-CG-CD2	-15.48	94.89	118.10
1	A	862[A]	ARG	NE-CZ-NH2	15.19	132.87	119.20
1	A	862[B]	ARG	NE-CZ-NH2	15.19	132.87	119.20
1	A	758[A]	LEU	CB-CG-CD2	-14.55	67.04	110.70
1	A	758[B]	LEU	CB-CG-CD2	-14.55	67.04	110.70
1	A	865[A]	GLY	CA-C-O	12.57	142.44	120.57
1	A	865[B]	GLY	CA-C-O	12.57	142.44	120.57
1	A	744[A]	TYR	CD1-CE1-CZ	12.48	142.06	119.60
1	A	744[B]	TYR	CD1-CE1-CZ	12.48	142.06	119.60
1	A	744[A]	TYR	CZ-CE2-CD2	11.48	140.26	119.60
1	A	744[B]	TYR	CZ-CE2-CD2	11.48	140.26	119.60
1	A	433[A]	ASP	OD1-CG-OD2	8.60	143.55	122.90
1	A	433[B]	ASP	OD1-CG-OD2	8.60	143.55	122.90
1	A	744[A]	TYR	CG-CD1-CE1	8.11	133.36	121.20
1	A	744[B]	TYR	CG-CD1-CE1	8.11	133.36	121.20
1	A	800	ASN	N-CA-C	7.12	121.36	112.24
1	A	657	PHE	N-CA-C	7.07	121.36	110.20
1	A	518	LYS	N-CA-C	6.92	120.61	112.72
1	A	854	LEU	N-CA-C	6.91	122.70	113.72
1	A	444[A]	LYS	CB-CG-CD	-6.86	95.52	111.30
1	A	444[B]	LYS	CB-CG-CD	-6.86	95.52	111.30
1	A	233	LYS	N-CA-C	-6.51	105.30	113.18
1	A	864	GLU	CA-C-N	6.51	134.17	121.41
1	A	864	GLU	C-N-CA	6.51	134.17	121.41
1	A	603	HIS	N-CA-C	6.33	118.70	111.11
1	A	870	ILE	N-CA-C	5.88	117.06	108.53
1	A	660	TRP	N-CA-C	5.66	118.99	111.75
1	A	623	THR	N-CA-C	-5.64	102.11	110.46
1	A	776[A]	GLU	CG-CD-OE2	-5.55	105.63	118.40
1	A	776[B]	GLU	CG-CD-OE2	-5.55	105.63	118.40
1	A	419	LEU	N-CA-C	5.50	117.36	111.36
1	A	865[A]	GLY	N-CA-C	-5.21	100.84	113.18
1	A	865[B]	GLY	N-CA-C	-5.21	100.84	113.18
1	A	708	LYS	N-CA-C	-5.18	100.07	108.52
1	A	836	GLY	N-CA-C	-5.08	101.15	113.18

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203[A]	GLN	Sidechain
1	A	433[A]	ASP	Sidechain
1	A	540[A]	ARG	Sidechain
1	A	744[A]	TYR	Sidechain
1	A	776[A]	GLU	Sidechain
1	A	862[A]	ARG	Sidechain
1	A	864	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5963	0	5779	184	0
2	B	30	0	14	0	0
3	A	20	0	0	1	0
4	A	638	0	0	7	0
All	All	6651	0	5793	184	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 16.

All (184) 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:549[A]:LYS:CD	1:A:549[A]:LYS:CE	1.74	1.64
1:A:444[B]:LYS:CD	1:A:444[B]:LYS:CG	1.78	1.61
1:A:758[B]:LEU:HD13	1:A:758[B]:LEU:CD2	1.26	1.56
1:A:540[A]:ARG:NE	1:A:540[A]:ARG:CZ	1.70	1.55
1:A:758[A]:LEU:HD13	1:A:758[A]:LEU:CD2	1.32	1.53
1:A:444[A]:LYS:CG	1:A:444[A]:LYS:CD	1.89	1.50
1:A:865[B]:GLY:N	1:A:865[B]:GLY:CA	1.70	1.48
1:A:865[A]:GLY:CA	1:A:865[A]:GLY:C	1.89	1.45
1:A:865[B]:GLY:CA	1:A:865[B]:GLY:C	1.93	1.42
1:A:758[B]:LEU:CD2	1:A:758[B]:LEU:CD1	2.00	1.39
1:A:744[A]:TYR:CG	1:A:744[A]:TYR:CD1	2.11	1.38
1:A:744[B]:TYR:CD2	1:A:744[B]:TYR:CG	2.10	1.38
1:A:758[A]:LEU:CD2	1:A:758[A]:LEU:CD1	2.08	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:862[A]:ARG:CZ	1:A:862[A]:ARG:HD3	1.63	1.28
1:A:203[B]:GLN:NE2	1:A:203[B]:GLN:HG2	1.51	1.22
1:A:540[B]:ARG:CZ	1:A:540[B]:ARG:NE	2.02	1.22
1:A:776[A]:GLU:OE2	1:A:776[A]:GLU:CD	1.84	1.19
1:A:203[A]:GLN:NE2	1:A:203[A]:GLN:HG2	1.57	1.17
1:A:758[A]:LEU:HD11	1:A:776[A]:GLU:HG2	1.21	1.15
1:A:744[A]:TYR:CD1	1:A:744[A]:TYR:CE1	2.37	1.13
1:A:744[B]:TYR:CD2	1:A:744[B]:TYR:CD1	2.39	1.10
1:A:758[A]:LEU:HD13	1:A:758[A]:LEU:HD21	1.23	1.09
1:A:540[A]:ARG:CZ	1:A:540[A]:ARG:CD	2.30	1.09
1:A:744[A]:TYR:CD1	1:A:744[A]:TYR:CD2	2.39	1.09
1:A:758[B]:LEU:HD13	1:A:758[B]:LEU:HD21	1.15	1.08
1:A:862[A]:ARG:CZ	1:A:862[A]:ARG:CD	2.33	1.07
1:A:758[A]:LEU:CD2	1:A:758[A]:LEU:HB2	1.86	1.06
1:A:744[B]:TYR:CD2	1:A:744[B]:TYR:CE2	2.46	1.04
1:A:444[B]:LYS:CD	1:A:444[B]:LYS:CB	2.37	1.03
1:A:758[A]:LEU:HD11	1:A:776[A]:GLU:CG	1.93	0.98
1:A:613:ASN:H	1:A:698:GLN:HE22	1.03	0.98
1:A:758[B]:LEU:CD2	1:A:758[B]:LEU:HB3	1.93	0.98
1:A:203[B]:GLN:CD	1:A:203[B]:GLN:HB3	1.91	0.96
1:A:444[B]:LYS:HB3	1:A:444[B]:LYS:HD2	1.46	0.95
1:A:758[A]:LEU:HG	1:A:776[A]:GLU:CD	1.92	0.94
1:A:864:GLU:C	1:A:865[B]:GLY:CA	2.40	0.94
1:A:744[A]:TYR:CD1	1:A:744[A]:TYR:CB	2.53	0.92
1:A:744[B]:TYR:CD2	1:A:744[B]:TYR:CB	2.52	0.92
1:A:433[A]:ASP:OD2	1:A:433[A]:ASP:HB3	1.69	0.91
1:A:758[B]:LEU:CD2	1:A:758[B]:LEU:CB	2.49	0.90
1:A:865[A]:GLY:CA	1:A:866:ASP:N	2.35	0.90
1:A:758[A]:LEU:CD2	1:A:758[A]:LEU:CB	2.50	0.88
1:A:444[B]:LYS:CB	1:A:444[B]:LYS:HD2	2.02	0.88
1:A:865[B]:GLY:CA	1:A:866:ASP:N	2.37	0.88
1:A:865[B]:GLY:N	1:A:865[B]:GLY:C	2.33	0.87
1:A:444[A]:LYS:CD	1:A:444[A]:LYS:CB	2.53	0.85
1:A:540[A]:ARG:CZ	1:A:540[A]:ARG:HD3	2.05	0.84
1:A:433[B]:ASP:OD2	1:A:433[B]:ASP:HB2	1.76	0.83
1:A:758[A]:LEU:CG	1:A:776[A]:GLU:CD	2.51	0.83
1:A:758[A]:LEU:CD1	1:A:776[A]:GLU:HG2	2.05	0.83
1:A:203[A]:GLN:CB	1:A:203[A]:GLN:CD	2.52	0.82
1:A:203[A]:GLN:CD	1:A:203[A]:GLN:CG	2.53	0.81
1:A:203[A]:GLN:NE2	1:A:203[A]:GLN:CG	2.42	0.81
1:A:744[B]:TYR:CD2	1:A:744[B]:TYR:HD1	1.97	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444[A]:LYS:HB2	1:A:444[A]:LYS:HD2	1.62	0.81
1:A:203[A]:GLN:CD	1:A:203[A]:GLN:HB2	2.05	0.81
1:A:203[B]:GLN:CD	1:A:203[B]:GLN:CB	2.53	0.80
1:A:862[B]:ARG:CZ	1:A:862[B]:ARG:HD2	2.11	0.80
1:A:540[A]:ARG:NE	1:A:540[A]:ARG:NH2	2.28	0.80
1:A:549[A]:LYS:CE	1:A:549[A]:LYS:CG	2.59	0.80
1:A:744[B]:TYR:CD2	1:A:744[B]:TYR:HB3	2.15	0.79
1:A:758[A]:LEU:CD1	1:A:776[A]:GLU:CG	2.60	0.77
1:A:444[B]:LYS:CD	1:A:444[B]:LYS:HB3	2.10	0.76
1:A:203[B]:GLN:NE2	1:A:203[B]:GLN:CG	2.42	0.74
1:A:758[B]:LEU:CD2	1:A:758[B]:LEU:CG	2.65	0.74
1:A:744[A]:TYR:CD1	1:A:744[A]:TYR:HB2	2.20	0.74
1:A:282:ASN:ND2	1:A:285:LYS:HG2	2.04	0.72
1:A:862[B]:ARG:CZ	1:A:862[B]:ARG:NE	2.52	0.72
1:A:444[B]:LYS:CG	1:A:444[B]:LYS:HD3	2.11	0.72
1:A:433[A]:ASP:OD2	1:A:433[A]:ASP:CB	2.38	0.71
1:A:203[A]:GLN:CG	1:A:203[A]:GLN:OE1	2.39	0.70
1:A:433[B]:ASP:OD2	1:A:433[B]:ASP:CB	2.40	0.70
1:A:862[B]:ARG:CZ	1:A:862[B]:ARG:CD	2.70	0.70
1:A:248:MET:O	1:A:252[A]:VAL:HG23	1.91	0.69
1:A:444[A]:LYS:CB	1:A:444[A]:LYS:HD2	2.21	0.69
1:A:433[B]:ASP:OD2	1:A:433[B]:ASP:CG	2.36	0.69
1:A:758[A]:LEU:CD2	1:A:758[A]:LEU:CG	2.71	0.68
1:A:529:LEU:C	1:A:529:LEU:HD23	2.18	0.68
1:A:540[B]:ARG:HH11	1:A:540[B]:ARG:HG2	1.59	0.68
1:A:444[A]:LYS:CG	1:A:444[A]:LYS:HD3	2.19	0.67
1:A:203[B]:GLN:CD	1:A:203[B]:GLN:CG	2.67	0.67
1:A:708:LYS:HE3	1:A:710:TYR:OH	1.95	0.67
1:A:874:ASN:C	1:A:874:ASN:HD22	2.03	0.66
1:A:744[A]:TYR:CD1	1:A:744[A]:TYR:HD2	2.06	0.66
1:A:540[B]:ARG:HG2	1:A:540[B]:ARG:NH1	2.11	0.65
1:A:865[A]:GLY:C	1:A:865[A]:GLY:N	2.53	0.65
1:A:549[A]:LYS:CD	1:A:549[A]:LYS:NZ	2.56	0.64
1:A:282:ASN:C	1:A:282:ASN:HD22	2.06	0.63
1:A:862[B]:ARG:NE	1:A:862[B]:ARG:HH11	1.97	0.63
1:A:701:LEU:HD12	1:A:778:GLU:HG2	1.81	0.62
1:A:758[B]:LEU:CD2	1:A:758[B]:LEU:HD12	2.23	0.62
1:A:458:MET:HE2	1:A:567:SER:HB2	1.81	0.61
1:A:862[B]:ARG:NE	1:A:862[B]:ARG:NH1	2.49	0.61
1:A:315:ASP:O	1:A:319[A]:LYS:HG3	2.01	0.60
1:A:776[B]:GLU:OE2	1:A:776[B]:GLU:OE1	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:GLU:H	1:A:822:GLU:CD	2.09	0.60
1:A:776[A]:GLU:OE2	1:A:776[A]:GLU:OE1	2.20	0.60
1:A:584:LYS:NZ	1:A:768:GLU:HG2	2.18	0.59
1:A:865[A]:GLY:C	1:A:867:GLU:H	2.10	0.59
1:A:444[A]:LYS:CD	1:A:444[A]:LYS:HB2	2.23	0.59
1:A:704[A]:SER:C	1:A:705:ASN:HD22	2.12	0.58
1:A:864:GLU:O	1:A:865[A]:GLY:C	2.45	0.58
1:A:243:ARG:O	1:A:247:GLU:HG3	2.04	0.58
1:A:327:LYS:HD3	1:A:327:LYS:C	2.29	0.58
1:A:758[A]:LEU:CG	1:A:776[A]:GLU:CG	2.82	0.58
1:A:581:LYS:HB3	1:A:768:GLU:HB2	1.86	0.57
1:A:223:ILE:HG13	1:A:224:TYR:CD2	2.39	0.57
1:A:420:LEU:HD13	1:A:435:MET:HE3	1.85	0.57
1:A:882:PRO:HB2	1:A:884:GLN:HE22	1.69	0.57
1:A:704[B]:SER:C	1:A:705:ASN:HD22	2.13	0.57
1:A:254:ASN:C	1:A:254:ASN:HD22	2.12	0.57
1:A:862[A]:ARG:CZ	1:A:862[A]:ARG:NE	2.67	0.57
1:A:758[A]:LEU:HB2	1:A:758[A]:LEU:HD23	1.81	0.56
1:A:808[A]:GLN:HG3	4:A:2573:HOH:O	2.05	0.55
1:A:264:THR:HG22	4:A:2082:HOH:O	2.05	0.55
1:A:458:MET:HE1	1:A:565:GLY:C	2.31	0.55
1:A:650:ASN:HD21	1:A:832:GLN:HE22	1.54	0.55
1:A:433[A]:ASP:OD2	1:A:433[A]:ASP:CG	2.51	0.54
1:A:203[B]:GLN:CG	1:A:203[B]:GLN:OE1	2.56	0.53
1:A:758[A]:LEU:HD22	1:A:778:GLU:HB2	1.90	0.53
1:A:882:PRO:HB2	1:A:884:GLN:NE2	2.23	0.53
1:A:540[A]:ARG:HD3	1:A:540[A]:ARG:NH1	2.23	0.53
1:A:758[B]:LEU:HB3	1:A:758[B]:LEU:HD23	1.83	0.53
1:A:820:ASN:HD22	1:A:825:GLN:HG2	1.73	0.53
1:A:864:GLU:O	1:A:865[A]:GLY:O	2.27	0.52
1:A:839:LYS:HD2	1:A:853:VAL:HG23	1.91	0.52
1:A:502:LYS:HB2	1:A:529:LEU:HD21	1.91	0.52
1:A:248:MET:O	1:A:252[B]:VAL:HG13	2.09	0.51
1:A:502:LYS:CB	1:A:529:LEU:HD21	2.41	0.51
1:A:354:GLY:HA3	1:A:377:ILE:HD11	1.93	0.51
1:A:298:THR:HB	1:A:299:PRO:HD3	1.93	0.50
1:A:862[A]:ARG:CD	1:A:862[A]:ARG:NH1	2.73	0.50
1:A:863:LYS:HE2	1:A:865[B]:GLY:O	2.12	0.49
1:A:584:LYS:HZ1	1:A:768:GLU:HG2	1.77	0.48
1:A:584:LYS:HE2	3:A:1200:SO4:O1	2.14	0.48
1:A:758[A]:LEU:HD11	1:A:776[A]:GLU:CD	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LEU:HD13	1:A:435:MET:CE	2.43	0.48
1:A:664:LEU:C	1:A:664:LEU:HD23	2.39	0.48
1:A:374:ILE:HD13	1:A:423:ILE:HG23	1.96	0.47
1:A:254:ASN:C	1:A:254:ASN:ND2	2.72	0.47
1:A:235:SER:HB2	1:A:293:ASP:HB2	1.97	0.47
1:A:671:PHE:HB2	1:A:678:ALA:HB3	1.97	0.47
1:A:845:SER:HB2	1:A:853:VAL:HG23	1.95	0.47
1:A:314:SER:OG	1:A:317:GLU:HG3	2.16	0.46
1:A:864:GLU:O	1:A:865[B]:GLY:CA	2.63	0.46
1:A:848:SER:O	1:A:850:GLN:HG3	2.16	0.46
1:A:864:GLU:C	1:A:865[A]:GLY:C	2.84	0.45
1:A:286:SER:O	1:A:288:VAL:HG23	2.16	0.45
1:A:242:TYR:CD2	1:A:298:THR:HG23	2.52	0.45
1:A:758[A]:LEU:CD2	1:A:758[A]:LEU:HD12	2.31	0.45
1:A:254:ASN:ND2	1:A:256:SER:H	2.15	0.44
1:A:529:LEU:C	1:A:529:LEU:CD2	2.89	0.44
1:A:661:ASN:C	1:A:661:ASN:HD22	2.26	0.44
1:A:822:GLU:CD	1:A:822:GLU:N	2.75	0.44
1:A:374:ILE:O	1:A:378:GLU:HG3	2.18	0.44
1:A:549[A]:LYS:HE3	4:A:2612:HOH:O	2.18	0.43
1:A:808[A]:GLN:HG2	4:A:2566:HOH:O	2.18	0.43
1:A:375:ARG:HD3	4:A:2182:HOH:O	2.18	0.43
1:A:404:TYR:CD1	1:A:407:ALA:HB3	2.54	0.43
1:A:758[A]:LEU:CD1	1:A:776[A]:GLU:CD	2.90	0.43
1:A:865[A]:GLY:C	1:A:867:GLU:N	2.75	0.43
1:A:170:VAL:HG23	1:A:315:ASP:OD2	2.18	0.43
1:A:422:VAL:HA	4:A:2009:HOH:O	2.18	0.43
1:A:540[B]:ARG:CZ	1:A:540[B]:ARG:HG2	2.49	0.42
1:A:650:ASN:ND2	1:A:862[A]:ARG:NH2	2.68	0.42
1:A:882:PRO:CB	1:A:884:GLN:HE22	2.31	0.42
1:A:354:GLY:CA	1:A:377:ILE:HD11	2.49	0.42
1:A:581:LYS:HD3	1:A:768:GLU:HG3	2.02	0.42
1:A:252[B]:VAL:HG23	1:A:253:THR:HG23	2.01	0.42
1:A:228[B]:LYS:O	1:A:228[B]:LYS:HG2	2.19	0.42
1:A:282:ASN:HD21	1:A:285:LYS:HG2	1.81	0.41
1:A:222:ARG:H	1:A:222:ARG:HG2	1.61	0.41
1:A:744[A]:TYR:CZ	1:A:797:LEU:HD13	2.55	0.41
1:A:617:MET:HA	1:A:618[B]:PRO:HD3	1.95	0.41
1:A:667:HIS:HD2	4:A:2583:HOH:O	2.03	0.41
1:A:274:GLU:HA	1:A:274:GLU:OE1	2.21	0.40
1:A:865[A]:GLY:O	1:A:867:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASN:ND2	1:A:251:GLN:HE22	2.18	0.40
1:A:671:PHE:N	1:A:671:PHE:CD1	2.89	0.40
1:A:458:MET:HE1	1:A:566:LEU:N	2.37	0.40
1:A:177:ARG:HA	1:A:177:ARG:NE	2.36	0.40
1:A:262:ASP:O	1:A:266:VAL:HG23	2.20	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	740/731 (101%)	715 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	659/649 (102%)	649 (98%)	10 (2%)	57	35

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	GLN

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Mol	Chain	Res	Type
1	A	282	ASN
1	A	368	GLN
1	A	404	TYR
1	A	444[A]	LYS
1	A	444[B]	LYS
1	A	529	LEU
1	A	661	ASN
1	A	773	LYS
1	A	874	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	202	ASN
1	A	231	ASN
1	A	237	ASN
1	A	254	ASN
1	A	261	GLN
1	A	277	HIS
1	A	282	ASN
1	A	349	ASN
1	A	368	GLN
1	A	386	GLN
1	A	392	GLN
1	A	418	GLN
1	A	580	ASN
1	A	650	ASN
1	A	661	ASN
1	A	667	HIS
1	A	683	ASN
1	A	698	GLN
1	A	729	GLN
1	A	759	GLN
1	A	788	GLN
1	A	820	ASN
1	A	825	GLN
1	A	874	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 ⓘ

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	NG6	B	1	2	19,19,19	2.43	8 (42%)	27,28,28	1.80	3 (11%)
2	GCD	B	2	2	10,11,12	5.05	5 (50%)	12,15,17	3.16	7 (58%)

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	NG6	B	1	2	-	1/10/30/30	0/1/1/1
2	GCD	B	2	2	-	0/4/17/20	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	GCD	O5-C5	12.99	1.55	1.37
2	B	2	GCD	O5-C1	6.85	1.56	1.45
2	B	1	NG6	C2-N2	5.36	1.54	1.45
2	B	2	GCD	C3-C4	4.16	1.55	1.50
2	B	1	NG6	O5-C1	3.97	1.52	1.42
2	B	1	NG6	O5-C5	3.77	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NG6	O6-S	-3.39	1.47	1.56
2	B	1	NG6	C7-N2	3.34	1.45	1.34
2	B	1	NG6	C4-C3	3.05	1.60	1.52
2	B	2	GCD	O6A-C6	2.80	1.29	1.22
2	B	2	GCD	C4-C5	2.64	1.37	1.33
2	B	1	NG6	O6-C6	2.39	1.55	1.46
2	B	1	NG6	C1-C2	2.37	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	GCD	O5-C5-C4	-7.35	118.19	124.94
2	B	1	NG6	O6-C6-C5	7.23	120.46	107.57
2	B	2	GCD	O3-C3-C4	4.56	119.58	109.27
2	B	2	GCD	O3-C3-C2	-4.05	102.22	109.44
2	B	2	GCD	O6B-C6-O6A	2.79	130.54	123.90
2	B	2	GCD	O5-C5-C6	2.75	116.91	111.85
2	B	1	NG6	O4-C4-C5	2.54	115.58	109.32
2	B	2	GCD	C3-C4-C5	-2.27	117.61	121.45
2	B	1	NG6	O4-C4-C3	-2.27	105.03	110.38
2	B	2	GCD	C1-C2-C3	-2.20	106.44	109.64

There are no chirality outliers.

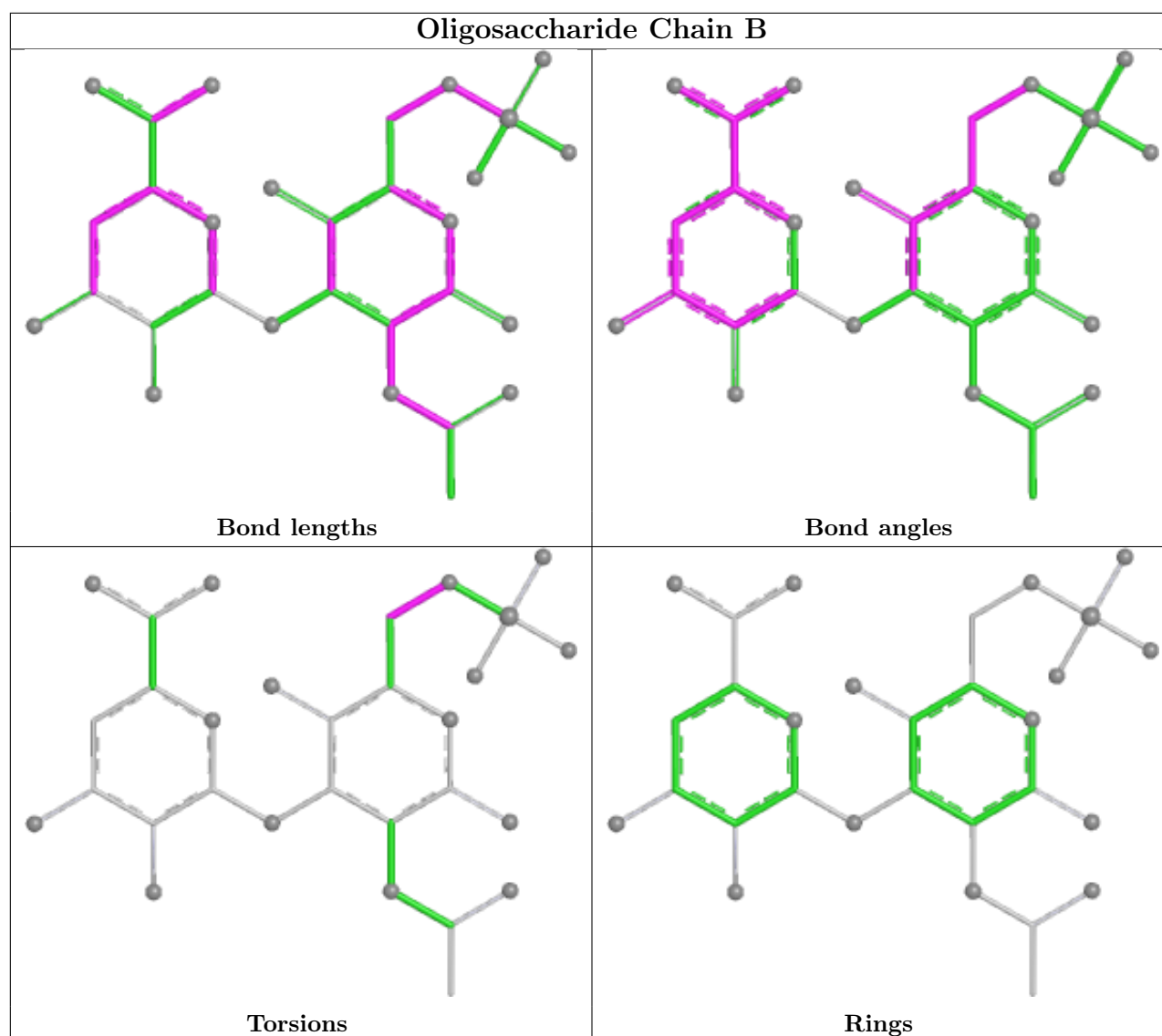
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NG6	C5-C6-O6-S

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](#)

4 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	$\# Z > 2$
3	SO4	A	1201	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	A	1203	-	4,4,4	0.24	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	1200	-	4,4,4	0.21	0	6,6,6	0.07	0
3	SO4	A	1202	-	4,4,4	0.24	0	6,6,6	0.09	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1200	SO4	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

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	723/731 (98%)	0.37	67 (9%) 14 14	7, 21, 39, 56	19 (2%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	ASP	6.0
1	A	340	ASP	6.0
1	A	220	ALA	5.7
1	A	228[A]	LYS	5.3
1	A	865[A]	GLY	5.2
1	A	170	VAL	4.3
1	A	319[A]	LYS	4.3
1	A	219	GLN	3.9
1	A	234	THR	3.5
1	A	171	LYS	3.4
1	A	432[A]	LYS	3.4
1	A	264	THR	3.4
1	A	279	HIS	3.3
1	A	385	ASP	3.3
1	A	230	SER	3.2
1	A	891	GLU	3.1
1	A	232	TYR	3.1
1	A	368	GLN	3.1
1	A	218	SER	3.1
1	A	224	TYR	3.0
1	A	869[A]	LYS	3.0
1	A	375	ARG	3.0
1	A	278	LYS	3.0
1	A	275	TRP	2.9
1	A	866	ASP	2.9
1	A	289	GLY	2.9
1	A	341	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	316	GLU	2.8
1	A	436	GLN	2.7
1	A	704[A]	SER	2.7
1	A	862[A]	ARG	2.6
1	A	274	GLU	2.6
1	A	890	LEU	2.6
1	A	367	ASP	2.6
1	A	721	GLN	2.6
1	A	758[A]	LEU	2.5
1	A	705	ASN	2.5
1	A	867	GLU	2.5
1	A	377	ILE	2.5
1	A	227	GLU	2.4
1	A	196	ASP	2.4
1	A	231	ASN	2.4
1	A	892	GLN	2.4
1	A	689	THR	2.4
1	A	291	TRP	2.4
1	A	216	ILE	2.4
1	A	223	ILE	2.4
1	A	284	GLU	2.3
1	A	225	LEU	2.3
1	A	288	VAL	2.2
1	A	342	PRO	2.2
1	A	175	THR	2.2
1	A	338	THR	2.2
1	A	236	ALA	2.2
1	A	714	LYS	2.2
1	A	810	ILE	2.2
1	A	429	PRO	2.2
1	A	277	HIS	2.2
1	A	529	LEU	2.1
1	A	490	GLU	2.1
1	A	263[A]	GLU	2.1
1	A	233	LYS	2.1
1	A	265	VAL	2.1
1	A	814	GLU	2.1
1	A	371	SER	2.1
1	A	172	ASP	2.0
1	A	339	THR	2.0

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

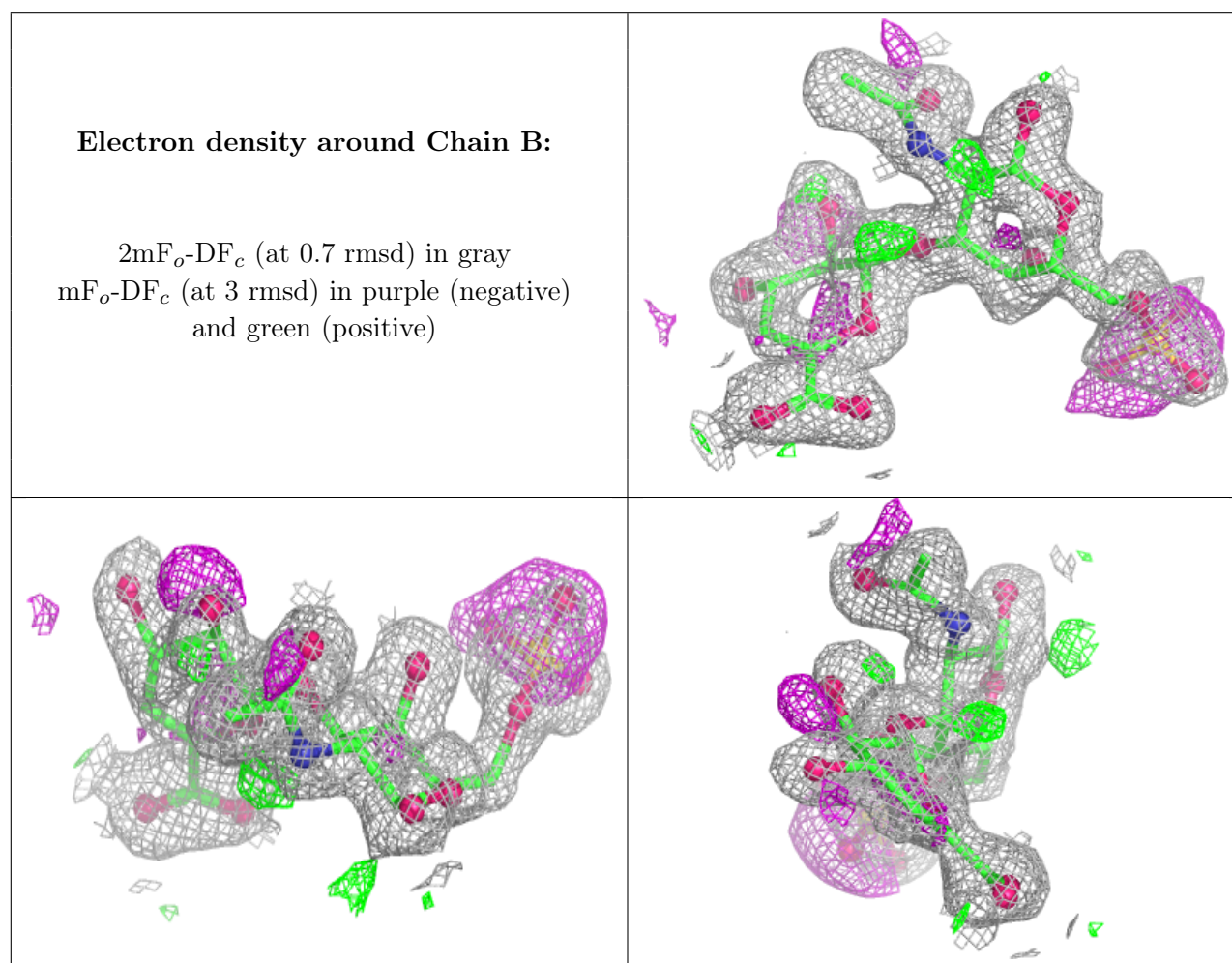
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	GCD	B	2	11/12	0.81	0.13	25,32,37,38	0
2	NG6	B	1	19/19	0.84	0.13	23,31,49,52	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	SO4	A	1203	5/5	0.78	0.14	62,63,63,65	0
3	SO4	A	1200	5/5	0.81	0.14	39,47,53,53	0
3	SO4	A	1202	5/5	0.87	0.13	53,54,55,56	0
3	SO4	A	1201	5/5	0.89	0.10	29,35,42,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.