



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:39 PM UTC

PDB ID : 3GVJ / pdb_00003gvj
Title : Crystal structure of an endo-neuraminidaseNF mutant
Authors : Schulz, E.C.; Dickmanns, A.; Ficner, R.
Deposited on : 2009-03-31
Resolution : 1.48 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

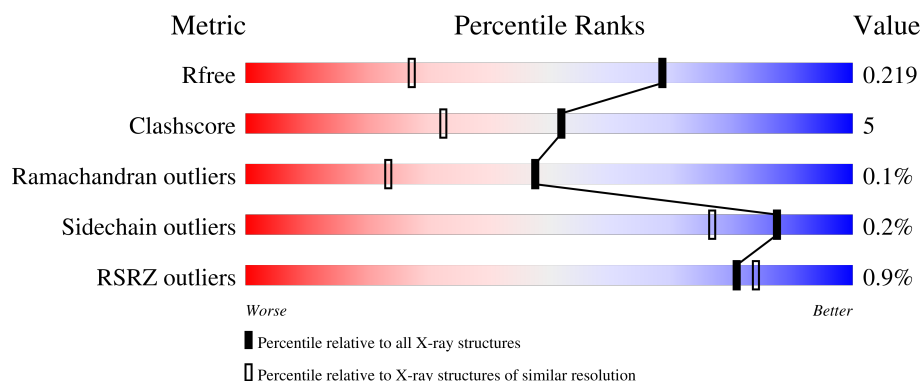
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.48 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	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	670	46% 50% .
2	B	5	80% 20%
3	C	4	50% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6457 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 Endo-N-acetylneuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	670	5425	3420	946	1040	19	0	24	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	VAL	-	expression tag	UNP Q858B1
A	242	PRO	-	expression tag	UNP Q858B1
A	243	ARG	-	expression tag	UNP Q858B1
A	244	GLY	-	expression tag	UNP Q858B1
A	245	SER	-	expression tag	UNP Q858B1
A	647	ALA	ARG	engineered mutation	UNP Q858B1

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	5	101	55	5	41	0	0	0

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			81	44	4	33			

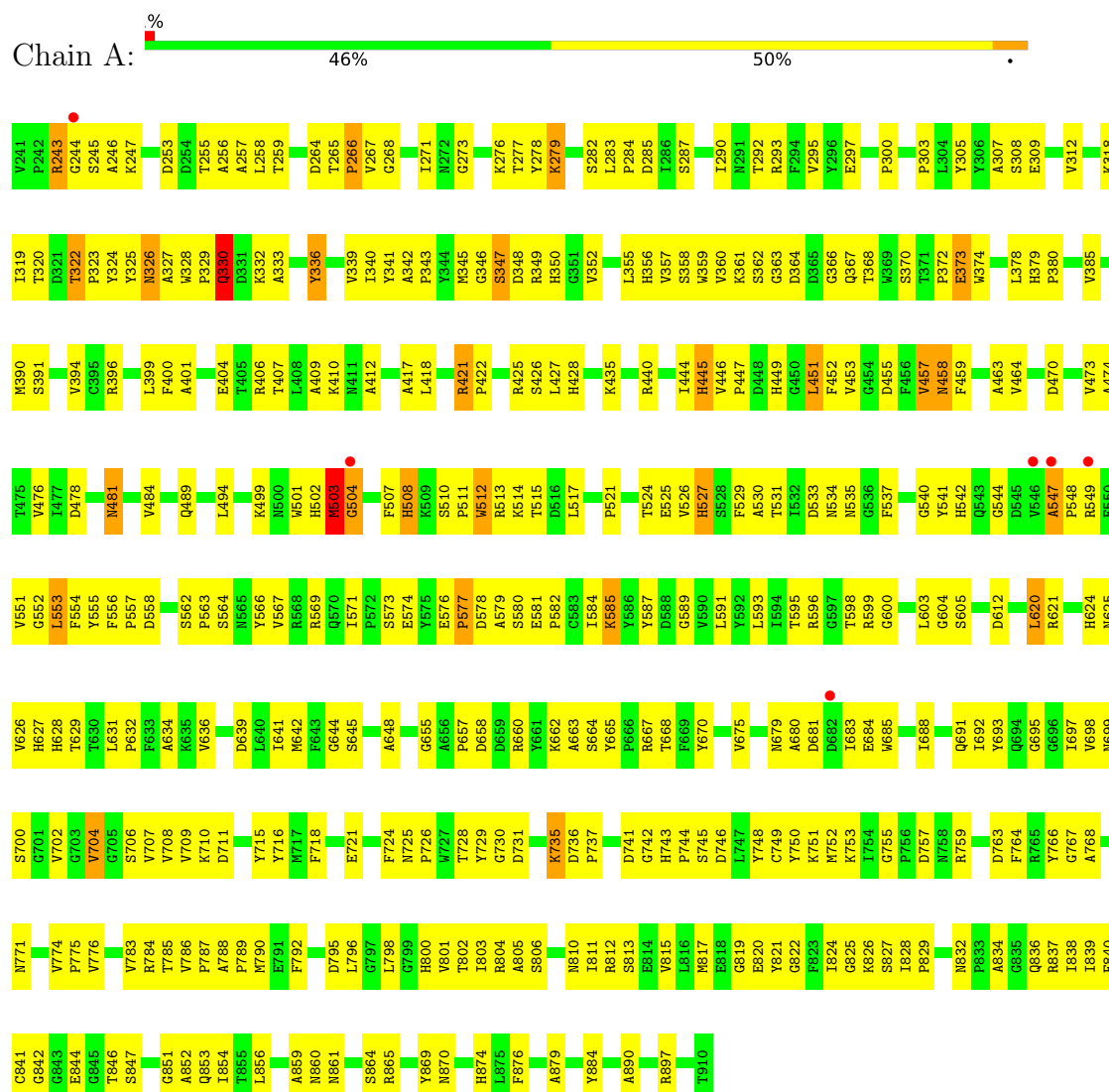
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	850	Total	O	0	0
			850	850		

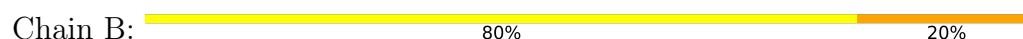
3 Residue-property plots

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: Endo-N-acetylneuraminidase



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid



SLE1
SIA2
SIA3
SIA4
SIA5

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid

Chain C:



SLE1
SIA2
SIA3
SIA4

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	119.09Å 119.09Å 175.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	12.00 – 1.48 12.00 – 1.48	Depositor EDS
% Data completeness (in resolution range)	100.0 (12.00-1.48) 99.8 (12.00-1.48)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.5.0039	Depositor
R, R_{free}	0.194 , 0.216 0.197 , 0.219	Depositor DCC
R_{free} test set	7751 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	12.3	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6457	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	2.18	336/5632 (6.0%)	1.06	8/7671 (0.1%)

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 (336) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	363	GLY	C-O	-12.18	1.15	1.24
1	A	504[A]	GLY	C-N	11.18	1.49	1.33
1	A	504[B]	GLY	C-N	11.18	1.49	1.33
1	A	533	ASP	C-O	-9.62	1.17	1.24
1	A	574[A]	GLU	N-CA	-9.53	1.34	1.46
1	A	574[B]	GLU	N-CA	-9.53	1.34	1.46
1	A	478	ASP	C-O	-9.16	1.15	1.24
1	A	551	VAL	C-O	-9.03	1.14	1.23
1	A	664	SER	C-O	-8.75	1.14	1.23
1	A	632	PRO	C-O	-8.41	1.13	1.23
1	A	451	LEU	C-O	-8.30	1.14	1.23
1	A	854	ILE	C-O	-8.18	1.15	1.24
1	A	884	TYR	C-O	-8.14	1.14	1.24
1	A	725	ASN	C-O	-8.09	1.13	1.24
1	A	394	VAL	C-O	-8.03	1.15	1.24
1	A	473	VAL	C-O	-7.94	1.15	1.24
1	A	645	SER	C-O	-7.93	1.15	1.23
1	A	255	THR	C-O	-7.91	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	783	VAL	C-O	-7.88	1.15	1.24
1	A	692	ILE	C-O	-7.86	1.15	1.24
1	A	776	VAL	C-O	-7.84	1.16	1.24
1	A	775	PRO	C-O	-7.83	1.14	1.23
1	A	815	VAL	C-O	-7.80	1.15	1.24
1	A	786	VAL	C-O	-7.76	1.15	1.24
1	A	320	THR	C-O	-7.72	1.14	1.23
1	A	702	VAL	C-O	-7.71	1.15	1.24
1	A	826	LYS	C-O	-7.68	1.15	1.24
1	A	312	VAL	C-O	-7.67	1.15	1.24
1	A	846	THR	C-O	-7.66	1.14	1.24
1	A	323	PRO	C-O	-7.61	1.14	1.24
1	A	271	ILE	C-O	-7.58	1.16	1.24
1	A	856	LEU	C-O	-7.55	1.14	1.24
1	A	282[A]	SER	C-O	-7.54	1.14	1.23
1	A	282[B]	SER	C-O	-7.54	1.14	1.23
1	A	811	ILE	C-O	-7.49	1.14	1.24
1	A	829	PRO	C-O	-7.47	1.15	1.23
1	A	817	MET	C-O	-7.46	1.15	1.24
1	A	339	VAL	C-O	-7.46	1.15	1.24
1	A	839	ILE	C-O	-7.45	1.16	1.24
1	A	457	VAL	C-O	-7.44	1.16	1.23
1	A	749	CYS	C-O	-7.44	1.15	1.23
1	A	501	TRP	C-O	-7.43	1.14	1.24
1	A	284	PRO	C-O	-7.43	1.14	1.24
1	A	869	TYR	C-O	-7.35	1.15	1.24
1	A	736	ASP	C-O	-7.35	1.14	1.24
1	A	841	CYS	C-O	-7.34	1.15	1.23
1	A	629	THR	C-O	-7.29	1.14	1.24
1	A	366	GLY	C-O	-7.26	1.14	1.24
1	A	481	ASN	C-O	-7.26	1.15	1.23
1	A	768	ALA	C-O	-7.24	1.14	1.23
1	A	340	ILE	C-O	-7.23	1.16	1.24
1	A	700	SER	C-O	-7.23	1.14	1.24
1	A	698	VAL	C-O	-7.22	1.14	1.24
1	A	502	HIS	C-O	-7.17	1.15	1.23
1	A	851	GLY	C-O	-7.17	1.14	1.23
1	A	562	SER	C-O	-7.16	1.15	1.24
1	A	569	ARG	C-O	-7.15	1.16	1.24
1	A	801	VAL	C-O	-7.14	1.16	1.24
1	A	767	GLY	C-O	-7.13	1.14	1.23
1	A	803	ILE	C-O	-7.10	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	ARG	C-O	-7.09	1.15	1.24
1	A	710	LYS	C-O	-7.08	1.16	1.24
1	A	418	LEU	C-O	-7.04	1.15	1.24
1	A	515	THR	C-O	-7.04	1.15	1.24
1	A	529	PHE	C-O	-7.00	1.15	1.23
1	A	861	ASN	C-O	-7.00	1.15	1.23
1	A	245	SER	C-O	-6.97	1.15	1.23
1	A	715	TYR	C-O	-6.96	1.16	1.24
1	A	537	PHE	C-O	-6.93	1.16	1.23
1	A	716	TYR	C-O	-6.91	1.16	1.24
1	A	571	ILE	C-O	-6.89	1.15	1.24
1	A	745	SER	C-O	-6.89	1.15	1.24
1	A	293	ARG	C-O	-6.88	1.15	1.24
1	A	596	ARG	C-O	-6.86	1.15	1.24
1	A	530	ALA	C-O	-6.86	1.16	1.24
1	A	526	VAL	C-O	-6.83	1.16	1.24
1	A	555	TYR	C-O	-6.83	1.15	1.24
1	A	668	THR	C-O	-6.79	1.15	1.24
1	A	644	GLY	C-O	-6.79	1.15	1.23
1	A	257	ALA	C-O	-6.78	1.16	1.24
1	A	752	MET	C-O	-6.78	1.15	1.24
1	A	285	ASP	C-O	-6.77	1.15	1.24
1	A	573	SER	C-O	-6.77	1.15	1.24
1	A	755	GLY	C-O	-6.77	1.14	1.24
1	A	804	ARG	C-O	-6.74	1.15	1.23
1	A	458	ASN	C-O	-6.74	1.15	1.24
1	A	463	ALA	CA-CB	-6.72	1.43	1.53
1	A	621	ARG	C-O	-6.71	1.16	1.24
1	A	838	ILE	C-O	-6.69	1.17	1.24
1	A	266	PRO	C-O	-6.68	1.15	1.23
1	A	634	ALA	C-O	-6.68	1.15	1.23
1	A	774	VAL	C-O	-6.67	1.16	1.24
1	A	598	THR	C-O	-6.67	1.15	1.24
1	A	484	VAL	C-O	-6.65	1.17	1.24
1	A	751	LYS	C-O	-6.65	1.16	1.24
1	A	327	ALA	C-O	-6.62	1.17	1.24
1	A	541	TYR	C-O	-6.61	1.15	1.23
1	A	556	PHE	C-O	-6.61	1.16	1.24
1	A	800	HIS	C-O	-6.61	1.16	1.23
1	A	510	SER	C-O	-6.60	1.15	1.24
1	A	421	ARG	C-O	-6.59	1.17	1.24
1	A	521	PRO	C-O	-6.58	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	897	ARG	C-O	-6.57	1.15	1.23
1	A	744	PRO	C-O	-6.57	1.15	1.24
1	A	361	LYS	C-O	-6.56	1.15	1.23
1	A	422	PRO	C-O	-6.56	1.16	1.23
1	A	378	LEU	C-O	-6.55	1.16	1.23
1	A	724	PHE	C-O	-6.54	1.16	1.24
1	A	759	ARG	C-O	-6.54	1.15	1.23
1	A	391	SER	C-O	-6.53	1.16	1.23
1	A	309	GLU	C-O	-6.50	1.16	1.23
1	A	407	THR	C-O	-6.49	1.16	1.23
1	A	665	TYR	C-O	-6.47	1.17	1.24
1	A	604	GLY	C-O	-6.45	1.15	1.23
1	A	828	ILE	C-O	-6.45	1.16	1.24
1	A	358	SER	C-O	-6.45	1.15	1.23
1	A	718	PHE	C-O	-6.40	1.16	1.23
1	A	557	PRO	C-O	-6.40	1.16	1.24
1	A	612	ASP	C-O	-6.40	1.15	1.23
1	A	874	HIS	C-O	-6.39	1.16	1.24
1	A	693	TYR	C-O	-6.36	1.16	1.24
1	A	750	TYR	C-O	-6.36	1.16	1.24
1	A	333	ALA	C-O	-6.33	1.15	1.23
1	A	512	TRP	C-O	-6.33	1.15	1.23
1	A	336	TYR	C-O	-6.32	1.16	1.23
1	A	264	ASP	C-O	-6.30	1.15	1.24
1	A	684	GLU	C-O	-6.29	1.16	1.23
1	A	771	ASN	C-O	-6.28	1.16	1.24
1	A	374	TRP	C-O	-6.28	1.16	1.24
1	A	657	PRO	C-O	-6.27	1.16	1.23
1	A	721	GLU	C-O	-6.26	1.14	1.24
1	A	595	THR	C-O	-6.26	1.15	1.23
1	A	531	THR	C-O	-6.25	1.16	1.23
1	A	445	HIS	C-O	-6.23	1.16	1.24
1	A	663	ALA	C-O	-6.23	1.16	1.23
1	A	864	SER	C-O	-6.22	1.16	1.24
1	A	697	ILE	C-O	-6.22	1.17	1.23
1	A	292	THR	C-O	-6.19	1.16	1.23
1	A	795	ASP	C-O	-6.19	1.16	1.23
1	A	757	ASP	C-O	-6.18	1.16	1.23
1	A	788	ALA	C-O	-6.18	1.16	1.23
1	A	305	TYR	C-O	-6.17	1.16	1.24
1	A	342	ALA	C-O	-6.17	1.17	1.24
1	A	764	PHE	C-O	-6.16	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	347	SER	C-O	-6.14	1.17	1.24
1	A	685	TRP	C-O	-6.14	1.16	1.24
1	A	699	ASN	C-O	-6.14	1.16	1.23
1	A	370	SER	C-O	-6.13	1.15	1.23
1	A	390	MET	C-O	-6.13	1.15	1.24
1	A	655	GLY	C-O	-6.10	1.15	1.24
1	A	790	MET	C-O	-6.06	1.16	1.23
1	A	890	ALA	C-O	-6.06	1.16	1.23
1	A	625	ASN	C-O	-6.04	1.15	1.23
1	A	805	ALA	C-O	-6.04	1.16	1.23
1	A	735	LYS	C-O	-6.03	1.15	1.23
1	A	507	PHE	C-O	-6.02	1.17	1.24
1	A	578	ASP	C-O	-6.01	1.16	1.23
1	A	558	ASP	C-O	-6.01	1.16	1.23
1	A	385	VAL	C-O	-6.00	1.17	1.23
1	A	360	VAL	C-O	-5.98	1.17	1.24
1	A	535	ASN	C-O	-5.98	1.16	1.24
1	A	552	GLY	C-O	-5.98	1.15	1.23
1	A	737	PRO	C-O	-5.96	1.16	1.24
1	A	379	HIS	C-O	-5.94	1.16	1.23
1	A	605	SER	C-O	-5.93	1.16	1.23
1	A	426	SER	C-O	-5.91	1.16	1.24
1	A	404	GLU	C-O	-5.90	1.16	1.23
1	A	789	PRO	C-O	-5.89	1.17	1.23
1	A	837	ARG	C-O	-5.89	1.16	1.23
1	A	362	SER	C-O	-5.88	1.17	1.24
1	A	357	VAL	C-O	-5.87	1.17	1.24
1	A	409	ALA	C-O	-5.86	1.17	1.24
1	A	318	LYS	C-O	-5.86	1.16	1.24
1	A	525	GLU	C-O	-5.85	1.16	1.23
1	A	401	ALA	C-O	-5.85	1.16	1.23
1	A	731	ASP	C-O	-5.84	1.16	1.24
1	A	836	GLN	C-O	-5.82	1.16	1.24
1	A	459	PHE	C-O	-5.82	1.16	1.24
1	A	763	ASP	C-O	-5.82	1.16	1.23
1	A	373	GLU	C-O	-5.81	1.17	1.24
1	A	641	ILE	C-O	-5.81	1.17	1.24
1	A	810	ASN	C-O	-5.80	1.15	1.23
1	A	711	ASP	C-O	-5.80	1.18	1.24
1	A	585	LYS	CG-CD	-5.79	1.35	1.52
1	A	246	ALA	C-O	-5.79	1.17	1.23
1	A	865	ARG	CZ-NH2	-5.79	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	626	VAL	C-O	-5.77	1.18	1.24
1	A	474	ALA	C-O	-5.76	1.16	1.24
1	A	825	GLY	C-O	-5.76	1.17	1.23
1	A	704	VAL	C-O	-5.76	1.17	1.24
1	A	322[A]	THR	C-O	-5.75	1.18	1.24
1	A	322[B]	THR	C-O	-5.75	1.18	1.24
1	A	470	ASP	C-O	-5.74	1.17	1.24
1	A	766	TYR	C-O	-5.74	1.17	1.24
1	A	680	ALA	C-O	-5.73	1.16	1.24
1	A	581	GLU	C-O	-5.72	1.17	1.24
1	A	341	TYR	C-O	-5.72	1.17	1.24
1	A	847	SER	C-O	-5.72	1.17	1.23
1	A	290	ILE	C-O	-5.71	1.18	1.24
1	A	428	HIS	C-O	-5.71	1.17	1.24
1	A	319	ILE	C-O	-5.71	1.18	1.24
1	A	268	GLY	C-O	-5.70	1.17	1.23
1	A	587	TYR	C-O	-5.70	1.17	1.23
1	A	648	ALA	C-O	-5.70	1.16	1.23
1	A	842	GLY	C-O	-5.70	1.16	1.23
1	A	307	ALA	C-O	-5.70	1.17	1.24
1	A	283	LEU	C-O	-5.69	1.16	1.24
1	A	412	ALA	C-O	-5.69	1.17	1.24
1	A	346	GLY	C-O	-5.68	1.16	1.23
1	A	844[A]	GLU	C-O	-5.68	1.16	1.24
1	A	844[B]	GLU	C-O	-5.68	1.16	1.24
1	A	742	GLY	C-O	-5.67	1.15	1.24
1	A	730	GLY	C-O	-5.67	1.16	1.23
1	A	464	VAL	C-O	-5.64	1.17	1.24
1	A	821	TYR	C-O	-5.62	1.16	1.23
1	A	278	TYR	C-O	-5.60	1.17	1.24
1	A	792	PHE	C-O	-5.59	1.17	1.24
1	A	593	LEU	C-O	-5.59	1.17	1.24
1	A	567	VAL	C-O	-5.58	1.18	1.24
1	A	785	THR	C-O	-5.58	1.17	1.24
1	A	253	ASP	C-O	-5.57	1.17	1.23
1	A	508	HIS	C-O	-5.57	1.17	1.24
1	A	859	ALA	C-O	-5.57	1.17	1.24
1	A	503	MET	C-O	-5.57	1.16	1.23
1	A	670	TYR	C-O	-5.57	1.16	1.23
1	A	540	GLY	C-O	-5.56	1.15	1.23
1	A	620	LEU	C-O	-5.56	1.17	1.23
1	A	455	ASP	C-O	-5.55	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	834	ALA	C-O	-5.53	1.17	1.24
1	A	279	LYS	C-O	-5.53	1.17	1.24
1	A	624	HIS	C-O	-5.53	1.15	1.23
1	A	603	LEU	C-O	-5.52	1.17	1.23
1	A	631	LEU	C-O	-5.51	1.17	1.24
1	A	824	ILE	C-O	-5.51	1.18	1.24
1	A	400	PHE	C-O	-5.50	1.17	1.24
1	A	514	LYS	C-O	-5.50	1.17	1.24
1	A	580	SER	C-O	-5.49	1.17	1.23
1	A	259	THR	C-O	-5.48	1.17	1.24
1	A	787	PRO	C-O	-5.48	1.17	1.24
1	A	579	ALA	C-O	-5.47	1.17	1.23
1	A	287	SER	C-O	-5.46	1.17	1.24
1	A	343	PRO	C-O	-5.46	1.17	1.23
1	A	812	ARG	C-O	-5.46	1.17	1.23
1	A	574[A]	GLU	C-O	-5.45	1.17	1.24
1	A	574[B]	GLU	C-O	-5.45	1.17	1.24
1	A	784	ARG	C-O	-5.45	1.17	1.23
1	A	667	ARG	C-O	-5.44	1.17	1.24
1	A	534	ASN	C-O	-5.43	1.17	1.24
1	A	527	HIS	C-O	-5.43	1.17	1.23
1	A	277	THR	C-O	-5.42	1.17	1.24
1	A	494	LEU	C-O	-5.41	1.16	1.23
1	A	599	ARG	C-O	-5.41	1.17	1.23
1	A	563	PRO	C-O	-5.39	1.17	1.24
1	A	802	THR	C-O	-5.39	1.17	1.24
1	A	380	PRO	C-O	-5.39	1.17	1.24
1	A	554	PHE	C-O	-5.37	1.17	1.24
1	A	547	ALA	CA-C	-5.36	1.47	1.53
1	A	827	SER	C-O	-5.36	1.16	1.23
1	A	295	VAL	C-O	-5.34	1.18	1.24
1	A	352	VAL	C-O	-5.33	1.17	1.24
1	A	452	PHE	C-O	-5.32	1.17	1.23
1	A	729	TYR	C-O	-5.32	1.16	1.23
1	A	330	GLN	C-O	-5.31	1.17	1.23
1	A	819	GLY	C-O	-5.31	1.15	1.23
1	A	566	TYR	C-O	-5.30	1.17	1.23
1	A	308	SER	C-O	-5.30	1.16	1.23
1	A	410	LYS	C-O	-5.29	1.17	1.24
1	A	748	TYR	C-O	-5.29	1.17	1.23
1	A	798	LEU	C-O	-5.28	1.17	1.23
1	A	435	LYS	C-O	-5.28	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	517	LEU	C-O	-5.27	1.16	1.24
1	A	396[A]	ARG	C-O	-5.27	1.17	1.23
1	A	396[B]	ARG	C-O	-5.27	1.17	1.23
1	A	322[A]	THR	CA-C	5.27	1.59	1.52
1	A	322[B]	THR	CA-C	5.27	1.59	1.52
1	A	840	PHE	C-O	-5.26	1.17	1.23
1	A	476	VAL	C-O	-5.26	1.18	1.24
1	A	524	THR	C-O	-5.25	1.16	1.23
1	A	600	GLY	C-O	-5.25	1.17	1.23
1	A	639	ASP	C-O	-5.24	1.17	1.24
1	A	852	ALA	C-O	-5.24	1.17	1.23
1	A	256	ALA	C-O	-5.24	1.18	1.24
1	A	662	LYS	C-O	-5.24	1.17	1.23
1	A	553	LEU	C-O	-5.23	1.17	1.23
1	A	589	GLY	C-O	-5.22	1.17	1.24
1	A	691	GLN	C-O	-5.22	1.16	1.23
1	A	267	VAL	C-O	-5.22	1.17	1.24
1	A	627	HIS	C-O	-5.22	1.17	1.23
1	A	741	ASP	C-O	-5.21	1.17	1.24
1	A	359	TRP	C-O	-5.20	1.17	1.23
1	A	513	ARG	C-O	-5.20	1.17	1.24
1	A	297	GLU	C-O	-5.19	1.16	1.23
1	A	820	GLU	C-O	-5.18	1.18	1.24
1	A	879	ALA	C-O	-5.17	1.17	1.23
1	A	399	LEU	C-O	-5.17	1.17	1.24
1	A	326	ASN	C-O	-5.17	1.18	1.24
1	A	746	ASP	C-O	-5.17	1.17	1.23
1	A	706	SER	C-O	-5.16	1.17	1.23
1	A	406	ARG	C-O	-5.16	1.17	1.23
1	A	822	GLY	C-O	-5.16	1.16	1.23
1	A	876	PHE	C-O	-5.16	1.17	1.24
1	A	806	SER	C-O	-5.16	1.17	1.24
1	A	303	PRO	C-O	-5.15	1.18	1.23
1	A	332	LYS	C-O	-5.14	1.17	1.24
1	A	695	GLY	C-O	-5.13	1.17	1.24
1	A	860	ASN	C-O	-5.13	1.17	1.24
1	A	577	PRO	C-O	-5.13	1.17	1.23
1	A	660	ARG	C-O	-5.12	1.16	1.23
1	A	688	ILE	C-O	-5.12	1.18	1.24
1	A	675	VAL	C-O	-5.12	1.17	1.24
1	A	348	ASP	C-O	-5.12	1.17	1.24
1	A	372	PRO	C-O	-5.11	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	447	PRO	C-O	-5.11	1.17	1.23
1	A	453	VAL	C-O	-5.09	1.19	1.24
1	A	832	ASN	C-O	-5.08	1.18	1.24
1	A	726	PRO	C-O	-5.08	1.17	1.24
1	A	258	LEU	C-O	-5.07	1.18	1.24
1	A	276	LYS	C-O	-5.07	1.17	1.23
1	A	300	PRO	C-O	-5.07	1.17	1.23
1	A	642	MET	CB-CG	-5.07	1.37	1.52
1	A	709	VAL	C-O	-5.07	1.18	1.24
1	A	367	GLN	CD-OE1	-5.06	1.14	1.23
1	A	707	VAL	C-O	-5.06	1.18	1.24
1	A	870	ASN	C-O	-5.05	1.18	1.23
1	A	511	PRO	C-O	-5.05	1.17	1.23
1	A	853	GLN	C-O	-5.04	1.17	1.23
1	A	796	LEU	C-O	-5.04	1.17	1.24
1	A	329	PRO	C-O	-5.04	1.18	1.24
1	A	683	ILE	C-O	-5.03	1.18	1.24
1	A	273	GLY	C-O	-5.03	1.17	1.23
1	A	708	VAL	C-O	-5.02	1.18	1.23
1	A	417	ALA	C-O	-5.02	1.18	1.24
1	A	564	SER	C-O	-5.01	1.17	1.24
1	A	753	LYS	C-O	-5.01	1.17	1.24
1	A	636	VAL	C-O	-5.01	1.18	1.24
1	A	813	SER	C-O	-5.01	1.17	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	MET	O-C-N	-19.62	94.89	122.94
1	A	503	MET	CA-C-N	-6.31	110.35	121.70
1	A	503	MET	C-N-CA	-6.31	110.35	121.70
1	A	728	THR	N-CA-C	-5.98	104.85	111.36
1	A	508	HIS	N-CA-C	5.32	117.99	111.82
1	A	865	ARG	NE-CZ-NH2	-5.13	114.59	119.20
1	A	574[A]	GLU	CA-C-O	-5.09	112.43	119.05
1	A	574[B]	GLU	CA-C-O	-5.09	112.43	119.05

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	330	GLN	Peptide
1	A	503	MET	Mainchain

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	5425	0	5199	54	0
2	B	101	0	82	3	0
3	C	81	0	66	2	0
4	A	850	0	0	5	0
All	All	6457	0	5347	56	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 5.

All (56) 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:347:SER:HB3	1:A:355[B]:LEU:HD23	1.38	1.04
1:A:345:MET:HB3	1:A:355[B]:LEU:HD21	1.47	0.96
1:A:449:HIS:HD2	1:A:451:LEU:H	1.17	0.88
1:A:345:MET:HB3	1:A:355[A]:LEU:HD11	1.57	0.84
1:A:503:MET:HG2	1:A:504[A]:GLY:HA3	1.60	0.83
1:A:503:MET:HG2	1:A:504[B]:GLY:HA3	1.68	0.72
1:A:373:GLU:OE2	1:A:508:HIS:HE1	1.72	0.72
1:A:449:HIS:CD2	1:A:451:LEU:H	2.05	0.72
1:A:322[A]:THR:HG22	1:A:324:TYR:H	1.59	0.68
1:A:508:HIS:HD2	4:A:984:HOH:O	1.78	0.65
1:A:347:SER:HB3	1:A:355[B]:LEU:CD2	2.22	0.65
1:A:584:ILE:O	1:A:585:LYS:HD2	1.95	0.65
1:A:499[C]:LYS:NZ	4:A:1281:HOH:O	2.30	0.64
1:A:544:GLY:HA2	1:A:549[B]:ARG:HG2	1.80	0.64
1:A:527:HIS:HD2	1:A:582:PRO:O	1.82	0.62
1:A:347:SER:HB3	1:A:355[A]:LEU:HD13	1.81	0.62
1:A:336:TYR:OH	1:A:425[B]:ARG:HD3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499[C]:LYS:CE	2:B:5:SIA:O7	2.52	0.58
1:A:425[A]:ARG:HD2	1:A:427:LEU:HD21	1.86	0.58
1:A:584:ILE:C	1:A:585:LYS:HD2	2.29	0.57
1:A:499[C]:LYS:HE2	2:B:5:SIA:O7	2.04	0.56
1:A:330:GLN:HB2	1:A:527:HIS:HE1	1.71	0.55
1:A:553:LEU:CD2	1:A:591[A]:LEU:HD21	2.36	0.54
1:A:325:TYR:OH	1:A:350:HIS:HE1	1.89	0.54
3:C:4:SIA:H92	3:C:4:SIA:O6	2.08	0.54
1:A:425[B]:ARG:HG3	1:A:425[B]:ARG:HH11	1.71	0.53
1:A:457:VAL:HA	1:A:504[B]:GLY:O	2.09	0.53
1:A:330:GLN:HB2	1:A:527:HIS:CE1	2.44	0.52
1:A:355[A]:LEU:HD12	1:A:356:HIS:N	2.25	0.51
1:A:628:HIS:HE1	1:A:658:ASP:OD1	1.94	0.50
1:A:328:TRP:HD1	1:A:330:GLN:HE21	1.57	0.50
1:A:322[A]:THR:HG21	4:A:107:HOH:O	2.11	0.49
1:A:364:ASP:OD2	1:A:368[A]:THR:OG1	2.27	0.48
1:A:542:HIS:HD2	4:A:916:HOH:O	1.95	0.48
1:A:445:HIS:HD2	1:A:481:ASN:HD21	1.62	0.47
1:A:544:GLY:HA2	1:A:549[A]:ARG:HG2	1.96	0.46
1:A:553:LEU:HD21	1:A:591[A]:LEU:HD21	1.97	0.45
1:A:425[B]:ARG:HG3	1:A:425[B]:ARG:NH1	2.32	0.45
1:A:265[C]:THR:HG23	1:A:266:PRO:N	2.32	0.45
1:A:325:TYR:OH	1:A:350:HIS:CE1	2.70	0.45
3:C:1:SLB:O6	3:C:1:SLB:H92	2.17	0.44
1:A:243:ARG:HB3	1:A:244:GLY:HA3	1.99	0.44
1:A:444:ILE:HG22	1:A:446:VAL:HG23	2.01	0.43
1:A:499[C]:LYS:HE3	2:B:5:SIA:O7	2.17	0.43
1:A:440[A]:ARG:HE	1:A:489:GLN:HE21	1.64	0.43
1:A:679[B]:ASN:ND2	1:A:681:ASP:H	2.17	0.43
1:A:445:HIS:HD2	1:A:481:ASN:ND2	2.16	0.43
1:A:279:LYS:HE2	4:A:979:HOH:O	2.18	0.43
1:A:553:LEU:HD22	1:A:591[A]:LEU:HD21	2.01	0.42
1:A:735:LYS:O	1:A:743:HIS:HE1	2.03	0.41
1:A:547:ALA:HA	1:A:548:PRO:HA	1.64	0.41
1:A:247:LYS:HD3	1:A:247:LYS:HA	1.75	0.41
1:A:576:GLU:N	1:A:577:PRO:CD	2.84	0.41
1:A:322[A]:THR:HB	1:A:326:ASN:OD1	2.20	0.40
1:A:458:ASN:O	1:A:504[A]:GLY:HA2	2.20	0.40
1:A:421:ARG:HD2	1:A:512:TRP:CD2	2.56	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	696/670 (104%)	673 (97%)	22 (3%)	1 (0%)	48	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	704	VAL

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	593/566 (105%)	592 (100%)	1 (0%)	87	77

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	620	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	GLN
1	A	338	ASN
1	A	350	HIS
1	A	415	ASN

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Mol	Chain	Res	Type
1	A	445	HIS
1	A	449	HIS
1	A	461	ASN
1	A	481	ASN
1	A	489	GLN
1	A	508	HIS
1	A	527	HIS
1	A	542	HIS
1	A	570	GLN
1	A	628	HIS
1	A	676	ASN
1	A	687	ASN
1	A	743	HIS
1	A	860	ASN
1	A	906	ASN

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](#)

9 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	SLB	B	1	2	21,21,21	1.16	2 (9%)	24,31,31	4.58	9 (37%)
2	SIA	B	2	2	20,20,21	0.57	0	21,28,31	1.29	2 (9%)
2	SIA	B	3	2	20,20,21	0.60	0	21,28,31	1.24	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SIA	B	4	2	20,20,21	0.61	0	21,28,31	1.39	4 (19%)
2	SIA	B	5	2	20,20,21	0.61	0	21,28,31	1.30	3 (14%)
3	SLB	C	1	3	21,21,21	1.13	2 (9%)	24,31,31	4.45	7 (29%)
3	SIA	C	2	3	20,20,21	0.76	1 (5%)	21,28,31	1.14	1 (4%)
3	SIA	C	3	3	20,20,21	0.63	0	21,28,31	1.15	1 (4%)
3	SIA	C	4	3	20,20,21	1.31	3 (15%)	21,28,31	2.69	6 (28%)

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	SLB	B	1	2	-	14/20/38/38	0/1/1/1
2	SIA	B	2	2	-	1/18/34/38	0/1/1/1
2	SIA	B	3	2	-	0/18/34/38	0/1/1/1
2	SIA	B	4	2	-	4/18/34/38	0/1/1/1
2	SIA	B	5	2	-	0/18/34/38	0/1/1/1
3	SLB	C	1	3	-	2/20/38/38	0/1/1/1
3	SIA	C	2	3	-	0/18/34/38	0/1/1/1
3	SIA	C	3	3	-	4/18/34/38	0/1/1/1
3	SIA	C	4	3	-	3/18/34/38	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	SLB	O2-C2	3.44	1.44	1.39
2	B	1	SLB	O2-C2	2.97	1.43	1.39
3	C	4	SIA	C9-C8	-2.67	1.45	1.52
3	C	4	SIA	C5-N5	-2.54	1.41	1.45
3	C	4	SIA	O1B-C1	-2.53	1.22	1.30
2	B	1	SLB	O10-C10	2.41	1.28	1.23
3	C	2	SIA	O1B-C1	-2.25	1.23	1.30
3	C	1	SLB	C3-C2	2.06	1.54	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	SLB	O2-C2-C3	-14.90	86.87	109.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	SLB	O2-C2-C3	-14.38	87.66	109.44
2	B	1	SLB	O2-C2-C1	-11.91	85.59	110.73
3	C	1	SLB	O2-C2-C1	-11.53	86.38	110.73
3	C	4	SIA	O9-C9-C8	-9.57	91.05	111.16
2	B	1	SLB	O2-C2-O6	-8.74	87.49	109.51
3	C	1	SLB	O2-C2-O6	-8.60	87.85	109.51
2	B	1	SLB	O6-C6-C7	4.96	114.39	106.65
2	B	1	SLB	C3-C2-C1	3.84	119.96	112.84
3	C	4	SIA	O1B-C1-C2	3.56	121.96	112.71
3	C	1	SLB	C3-C2-C1	3.50	119.34	112.84
2	B	2	SIA	C6-C5-N5	-3.45	105.41	110.91
2	B	4	SIA	C6-C5-N5	-3.43	105.43	110.91
2	B	3	SIA	C6-C5-N5	-3.42	105.45	110.91
3	C	1	SLB	O1A-C1-C2	-3.37	118.23	123.85
2	B	1	SLB	O1A-C1-C2	-3.35	118.27	123.85
3	C	4	SIA	O1A-C1-C2	-3.21	115.92	122.85
3	C	2	SIA	C6-C5-N5	-3.04	106.05	110.91
3	C	4	SIA	O6-C2-C3	-2.89	106.67	110.56
2	B	3	SIA	O6-C2-C1	2.79	112.98	107.72
2	B	1	SLB	C11-C10-N5	-2.64	111.75	116.12
2	B	5	SIA	C4-C5-N5	-2.63	105.25	110.44
2	B	5	SIA	O6-C2-C1	2.62	112.67	107.72
2	B	2	SIA	O1B-C1-C2	2.62	119.52	112.71
3	C	1	SLB	C3-C4-C5	2.60	113.74	109.72
2	B	4	SIA	C4-C5-N5	-2.54	105.43	110.44
2	B	1	SLB	C3-C4-C5	2.50	113.58	109.72
2	B	4	SIA	O6-C2-C1	2.42	112.28	107.72
3	C	1	SLB	O6-C6-C5	2.35	112.00	109.84
3	C	4	SIA	O8-C8-C7	2.35	114.74	109.25
2	B	1	SLB	C5-N5-C10	-2.34	117.62	123.11
3	C	3	SIA	O1B-C1-C2	2.34	118.80	112.71
3	C	4	SIA	C11-C10-N5	-2.32	112.27	116.12
2	B	5	SIA	O1B-C1-C2	2.29	118.67	112.71
2	B	4	SIA	O1B-C1-C2	2.24	118.54	112.71

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	SLB	O6-C6-C7-C8
2	B	1	SLB	O6-C6-C7-O7
2	B	1	SLB	C6-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
2	B	1	SLB	O7-C7-C8-C9
2	B	1	SLB	O7-C7-C8-O8
2	B	1	SLB	C7-C8-C9-O9
3	C	3	SIA	C6-C7-C8-C9
3	C	3	SIA	C6-C7-C8-O8
3	C	3	SIA	O7-C7-C8-C9
3	C	3	SIA	O7-C7-C8-O8
3	C	4	SIA	C7-C8-C9-O9
3	C	4	SIA	O8-C8-C9-O9
2	B	1	SLB	O8-C8-C9-O9
2	B	1	SLB	C6-C7-C8-C9
2	B	4	SIA	C6-C7-C8-C9
2	B	4	SIA	C6-C7-C8-O8
2	B	4	SIA	O7-C7-C8-O8
2	B	1	SLB	C6-C5-N5-C10
2	B	4	SIA	O7-C7-C8-C9
2	B	1	SLB	C4-C5-N5-C10
2	B	1	SLB	C5-C6-C7-O7
3	C	1	SLB	O1B-C1-C2-C3
2	B	1	SLB	C5-C6-C7-C8
2	B	2	SIA	C6-C7-C8-C9
3	C	4	SIA	C6-C7-C8-C9
2	B	1	SLB	O1B-C1-C2-O2
2	B	1	SLB	O1B-C1-C2-C3
3	C	1	SLB	O1A-C1-C2-C3

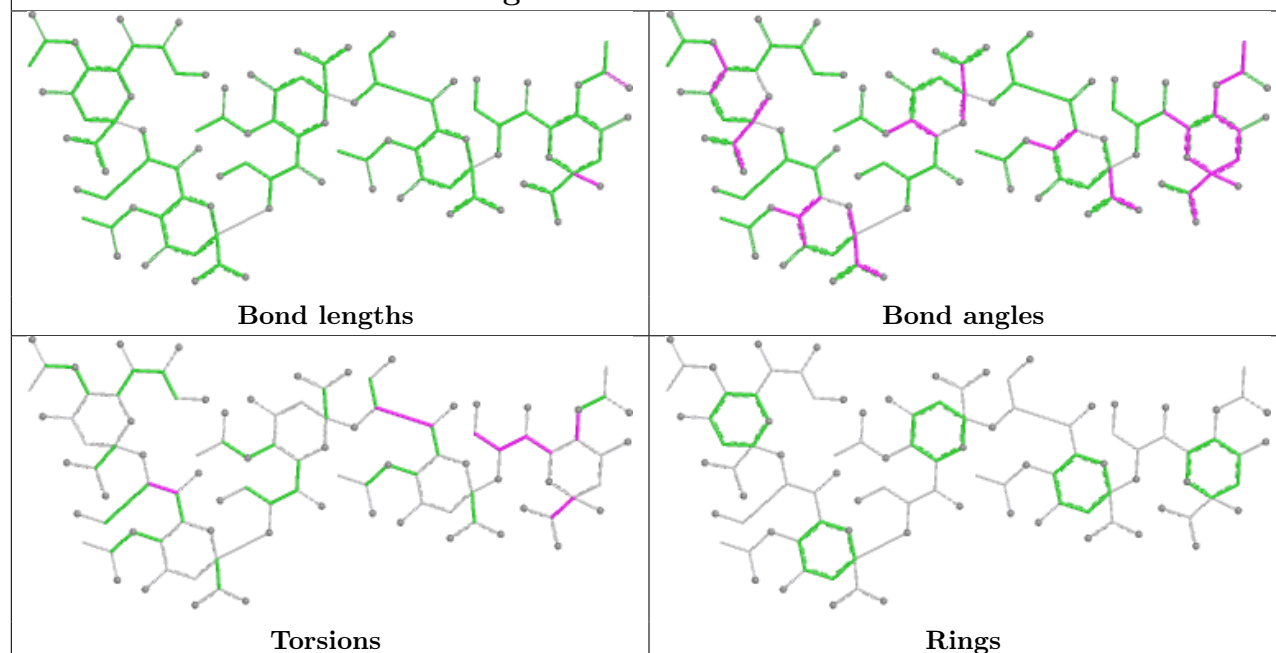
There are no ring outliers.

3 monomers are involved in 5 short contacts:

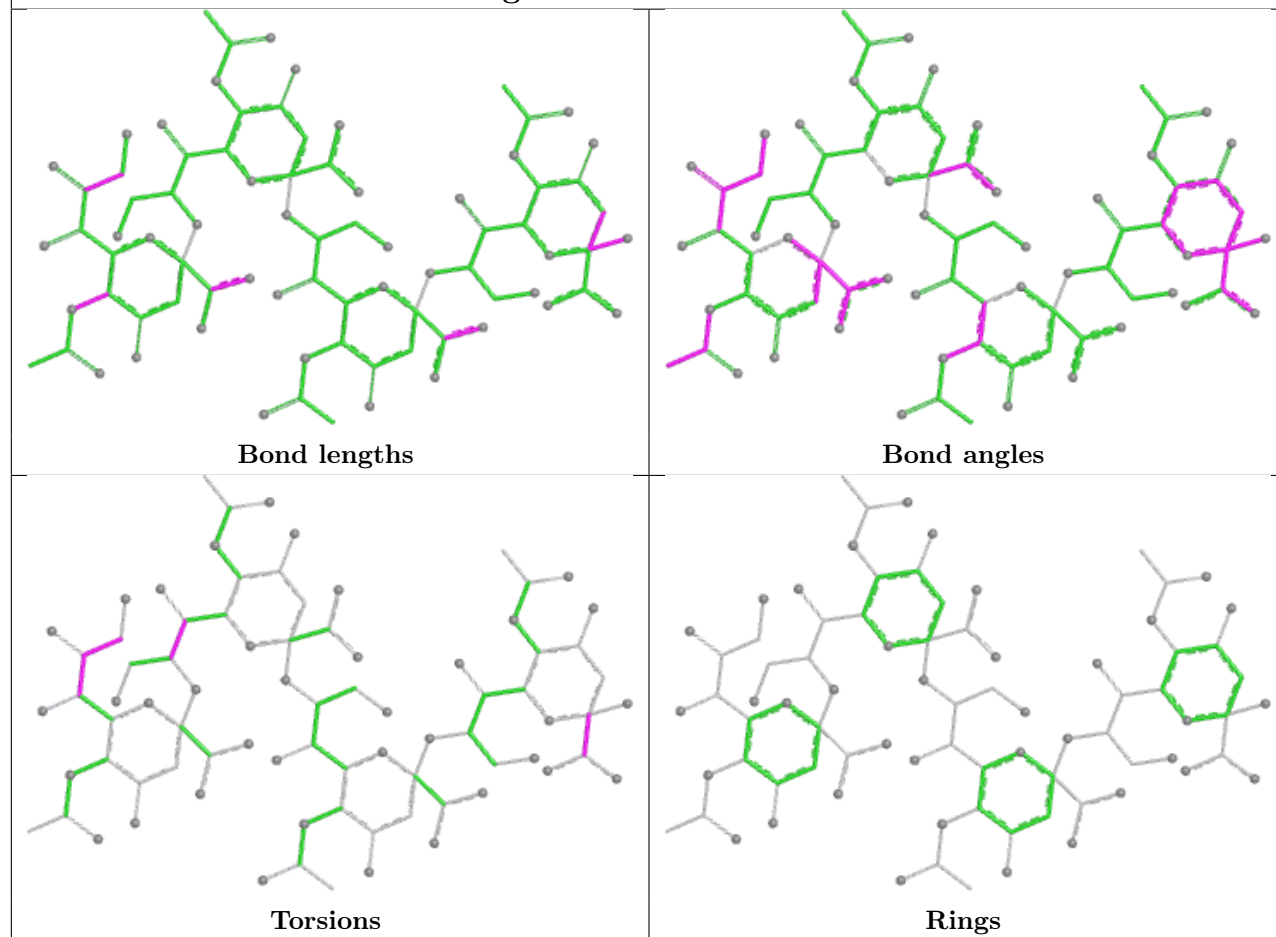
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5	SIA	3	0
3	C	4	SIA	1	0
3	C	1	SLB	1	0

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



5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	670/670 (100%)	-0.28	6 (0%) 81 84	5, 13, 21, 37	24 (3%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504[A]	GLY	4.4
1	A	244	GLY	4.1
1	A	547	ALA	2.5
1	A	546	VAL	2.5
1	A	549[A]	ARG	2.2
1	A	682	ASP	2.2

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.

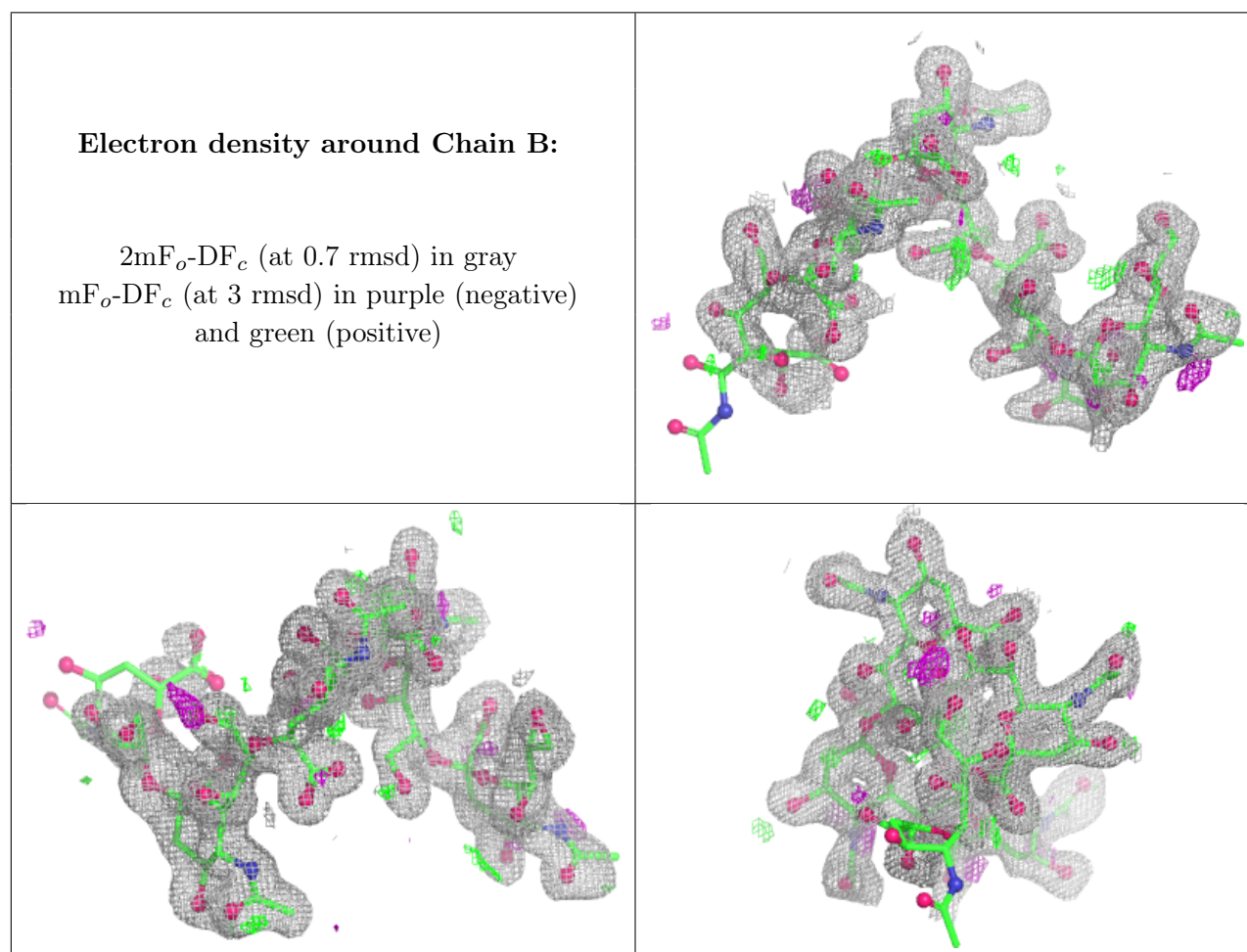
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SIA	B	4	20/21	0.80	0.12	30,32,37,38	0
2	SIA	B	5	20/21	0.84	0.11	32,36,38,39	0
2	SLB	B	1	21/21	0.88	0.22	32,36,36,36	16
3	SLB	C	1	21/21	0.88	0.10	20,26,32,35	0
2	SIA	B	2	20/21	0.91	0.09	19,22,29,30	0
2	SIA	B	3	20/21	0.92	0.08	18,20,26,27	0

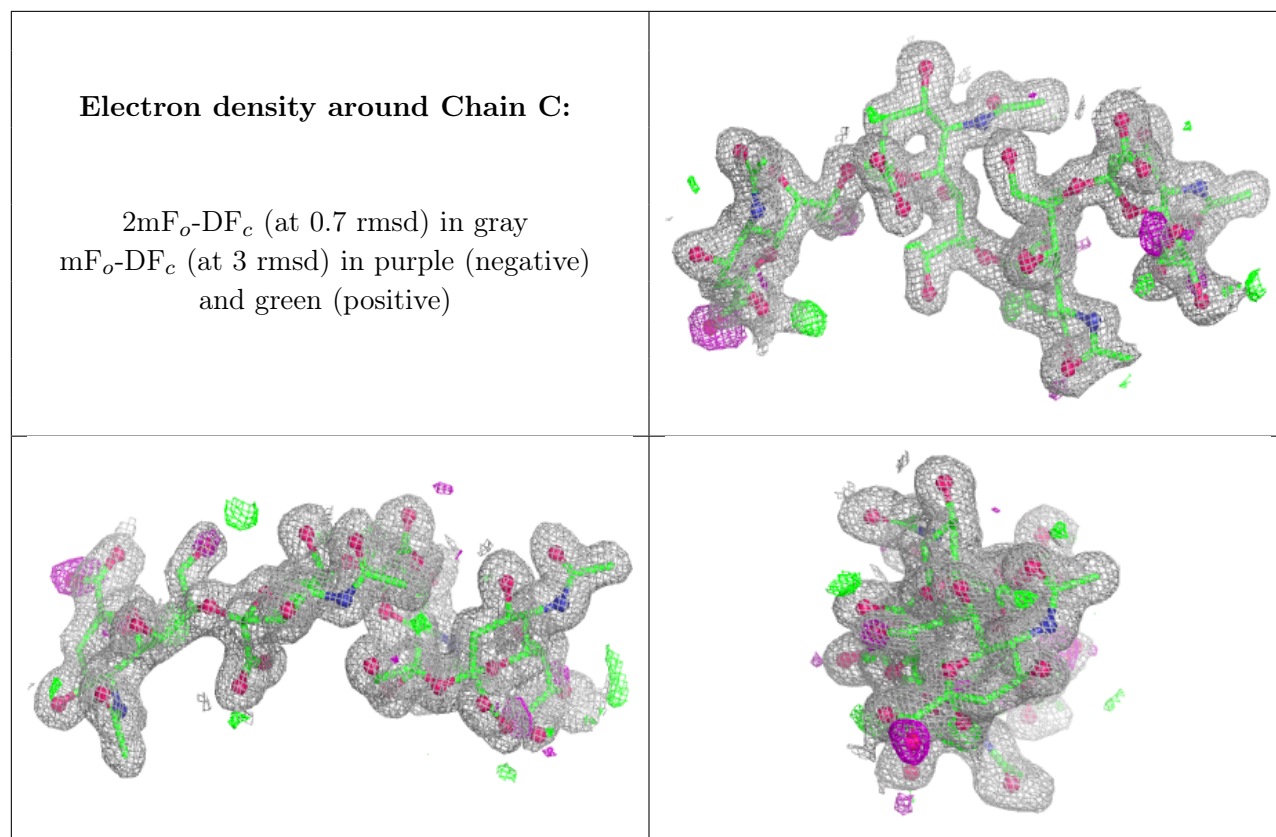
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SIA	C	3	20/21	0.92	0.08	16,24,28,29	0
3	SIA	C	4	20/21	0.92	0.09	18,21,30,34	0
3	SIA	C	2	20/21	0.95	0.07	13,18,25,28	0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.