



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:15 AM UTC

PDB ID : 4YFU / pdb_00004yfu
Title : Crystal structure of open Bacillus fragment DNA polymerase bound to DNA and dTTP
Authors : Wu, E.Y.
Deposited on : 2015-02-25
Resolution : 1.50 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

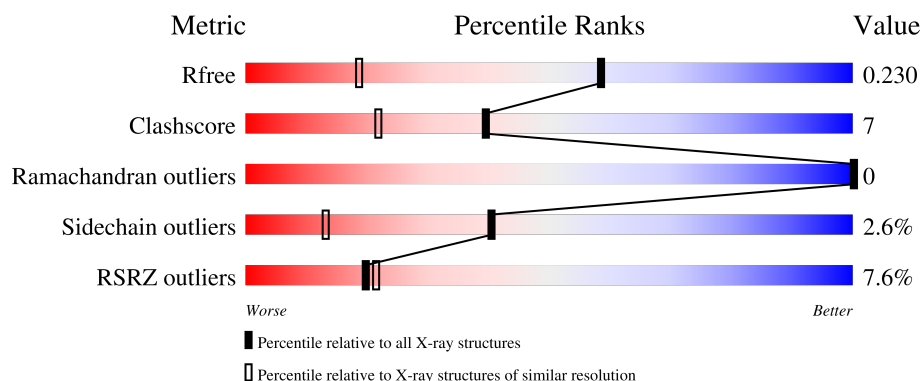
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	580	6% 79% 18% .
1	D	580	9% 77% 18% .
2	B	9	33% 44% 22%
2	E	9	11% 22% 56% 22%
3	C	14	64% 14% 21%

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Mol	Chain	Length	Quality of chain
3	F	14	 21% 79% 21%
4	G	2	 50% 50%
4	H	2	 50% 50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11744 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 DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	0	10	0
			4700	2995	812	873	20			
1	D	580	Total	C	N	O	S	0	13	0
			4719	3011	811	877	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	LYS	-	expression tag	UNP E1C9K5
A	456	GLU	ALA	conflict	UNP E1C9K5
A	505	LYS	GLU	conflict	UNP E1C9K5
A	512	GLY	ARG	conflict	UNP E1C9K5
A	550	THR	SER	conflict	UNP E1C9K5
A	598	ALA	ASP	engineered mutation	UNP E1C9K5
A	710	TYR	PHE	engineered mutation	UNP E1C9K5
A	823	HIS	ARG	conflict	UNP E1C9K5
D	297	LYS	-	expression tag	UNP E1C9K5
D	456	GLU	ALA	conflict	UNP E1C9K5
D	505	LYS	GLU	conflict	UNP E1C9K5
D	512	GLY	ARG	conflict	UNP E1C9K5
D	550	THR	SER	conflict	UNP E1C9K5
D	598	ALA	ASP	engineered mutation	UNP E1C9K5
D	710	TYR	PHE	engineered mutation	UNP E1C9K5
D	823	HIS	ARG	conflict	UNP E1C9K5

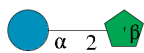
- Molecule 2 is a DNA chain called Primer DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	P	0	0	0
			180	88	32	52	8			
2	E	9	Total	C	N	O	P	0	0	0
			180	88	32	52	8			

- Molecule 3 is a DNA chain called Template DNA.

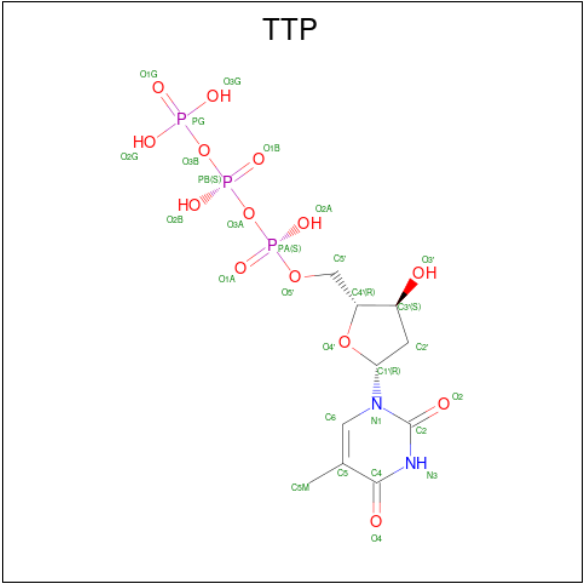
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	P	0	0	0
			226	107	43	65	11			
3	F	14	Total	C	N	O	P	0	0	0
			288	137	58	80	13			

- Molecule 4 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



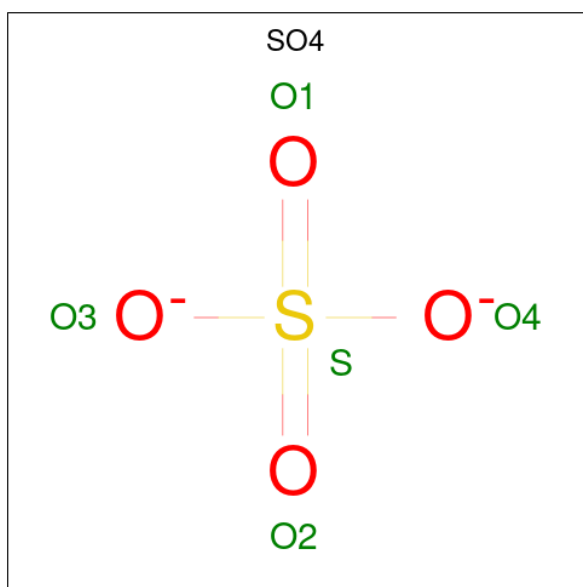
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	G	2	Total	C	O	0	0	0
			23	12	11			
4	H	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

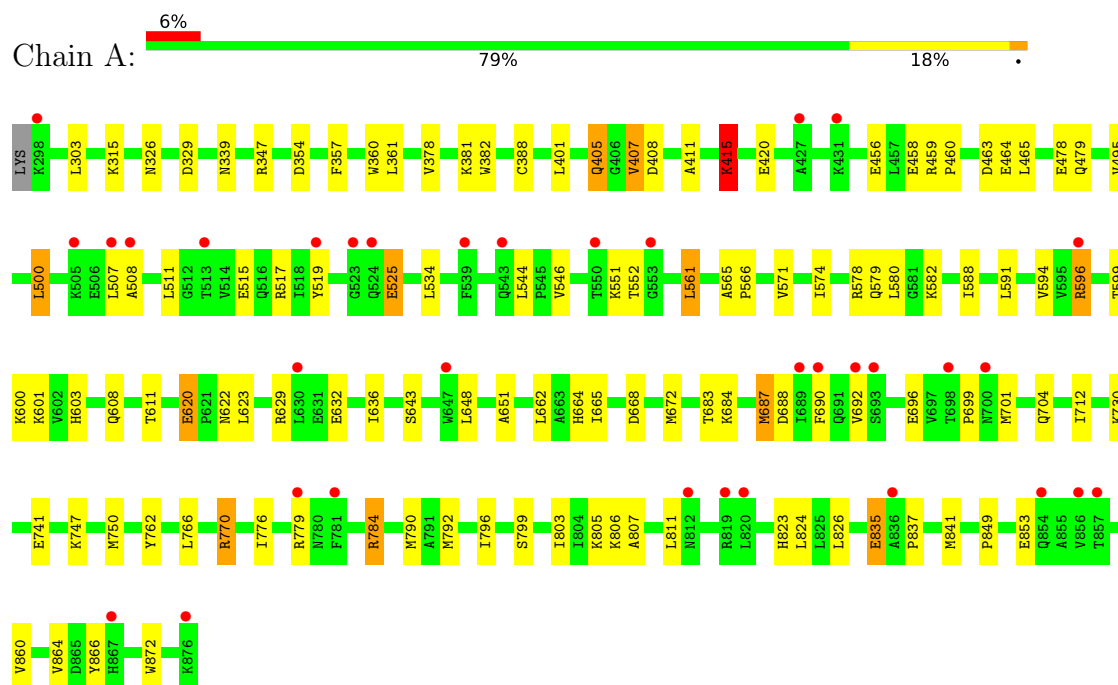
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	556	Total	O	0	0
			556	556		
7	D	622	Total	O	0	0
			622	622		
7	B	37	Total	O	0	0
			37	37		
7	C	50	Total	O	0	0
			50	50		
7	E	35	Total	O	0	0
			35	35		
7	F	71	Total	O	0	0
			71	71		

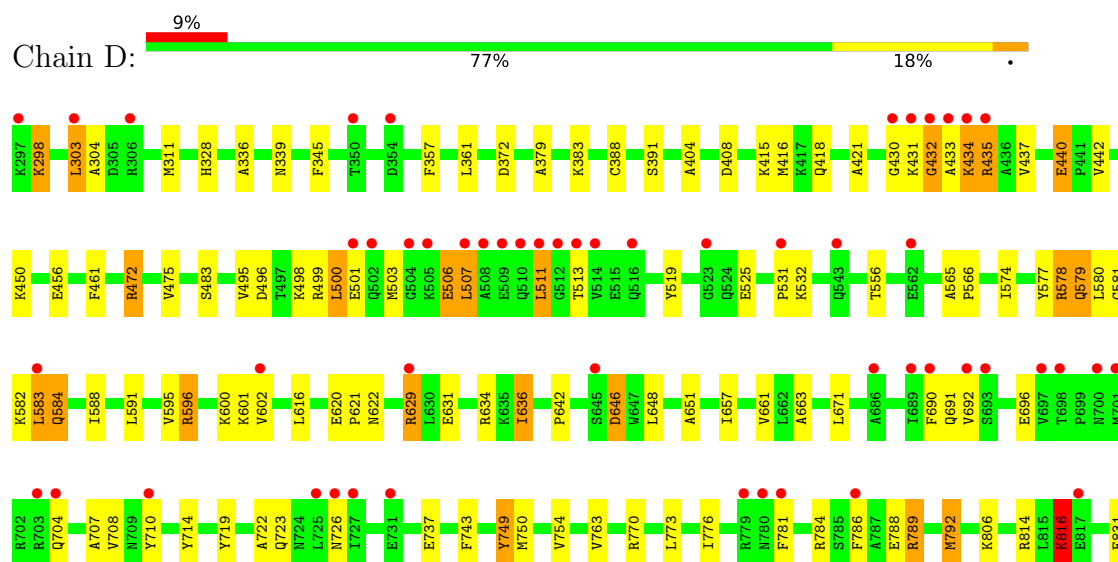
3 Residue-property plots [i](#)

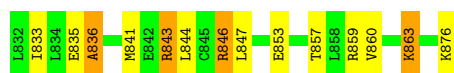
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA polymerase



• Molecule 1: DNA polymerase





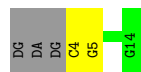
- Molecule 2: Primer DNA



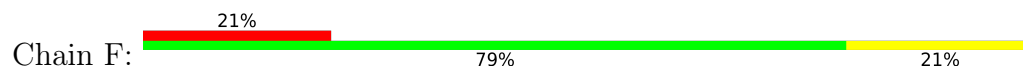
- Molecule 2: Primer DNA



- Molecule 3: Template DNA



- Molecule 3: Template DNA



- Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



- Molecule 4: beta-D-fructofuranose-(2-1)-alpha-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	93.23Å 108.10Å 151.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.68 – 1.50 44.68 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (44.68-1.50) 99.0 (44.68-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.195 , 0.230 0.195 , 0.230	Depositor DCC
R_{free} test set	11140 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11744	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: GLC, TTP, 2DT, SO4, FRU, CME

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	1.51	34/4803 (0.7%)	1.41	21/6487 (0.3%)
1	D	1.65	53/4828 (1.1%)	1.60	48/6524 (0.7%)
2	B	0.73	1/180 (0.6%)	1.42	5/276 (1.8%)
2	E	0.85	0/180	1.87	6/276 (2.2%)
3	C	0.74	1/253 (0.4%)	1.29	2/388 (0.5%)
3	F	0.82	0/324	1.15	2/499 (0.4%)
All	All	1.53	89/10568 (0.8%)	1.50	84/14450 (0.6%)

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	620	GLU	N-CA	9.71	1.53	1.46
1	D	620	GLU	N-CA	8.74	1.52	1.46
1	D	357	PHE	N-CA	8.24	1.56	1.46
1	A	622	ASN	C-O	7.55	1.32	1.24
1	A	790	MET	N-CA	7.39	1.55	1.46
1	D	498	LYS	CA-C	-7.18	1.43	1.52
1	D	379	ALA	C-O	7.09	1.32	1.24
1	A	525	GLU	CA-C	-7.05	1.43	1.52
1	D	584	GLN	N-CA	-7.03	1.38	1.46
1	D	835	GLU	CA-C	-7.00	1.44	1.52
1	A	361	LEU	N-CA	6.87	1.54	1.46
1	D	578	ARG	CD-NE	-6.83	1.36	1.46
1	D	582	LYS	N-CA	6.71	1.54	1.46
1	D	620	GLU	C-O	6.58	1.27	1.23
1	A	662	LEU	C-O	-6.58	1.16	1.24
1	D	496	ASP	N-CA	6.46	1.54	1.46
1	A	835	GLU	N-CA	6.40	1.54	1.45
1	A	824	LEU	CA-C	-6.28	1.44	1.52
1	A	401	LEU	C-O	6.23	1.31	1.24
1	D	361	LEU	N-CA	6.16	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	831	GLU	N-CA	6.15	1.53	1.45
1	A	578	ARG	CD-NE	-6.14	1.37	1.46
1	A	623	LEU	N-CA	-6.14	1.38	1.46
1	D	596	ARG	CZ-NH2	-6.13	1.25	1.33
1	D	483	SER	C-O	6.09	1.31	1.24
1	D	383	LYS	C-O	6.06	1.32	1.24
1	D	499	ARG	N-CA	-6.05	1.39	1.46
1	D	857	THR	C-O	6.04	1.31	1.24
1	D	707	ALA	C-O	-6.00	1.17	1.24
1	A	381	LYS	C-O	5.98	1.31	1.24
1	D	601	LYS	N-CA	5.94	1.52	1.45
1	D	404	ALA	CA-C	-5.89	1.44	1.52
1	D	859	ARG	CZ-NH1	5.78	1.40	1.32
1	A	458	GLU	C-O	-5.75	1.17	1.24
1	A	546	VAL	CA-C	-5.74	1.46	1.52
1	D	442	VAL	C-O	5.74	1.30	1.24
1	D	620	GLU	CA-C	-5.70	1.49	1.53
1	A	601	LYS	N-CA	5.68	1.52	1.46
1	D	642	PRO	C-O	5.66	1.30	1.23
1	D	440	GLU	CA-C	5.64	1.58	1.52
3	C	5	DG	O3'-P	-5.62	1.52	1.61
1	D	581	GLY	C-O	-5.58	1.17	1.23
1	A	479	GLN	CA-C	5.57	1.59	1.52
1	A	360	TRP	C-O	-5.53	1.17	1.24
1	D	722	ALA	N-CA	5.53	1.53	1.46
1	D	853	GLU	N-CA	5.51	1.53	1.46
1	A	805	LYS	CA-CB	5.46	1.61	1.53
1	A	357	PHE	N-CA	5.45	1.52	1.46
1	D	577	TYR	CA-C	5.45	1.59	1.52
1	D	651	ALA	N-CA	5.43	1.52	1.46
1	A	664	HIS	N-CA	5.43	1.52	1.46
1	A	608	GLN	CA-C	-5.38	1.45	1.52
1	A	860	VAL	C-O	-5.38	1.20	1.24
1	A	747	LYS	N-CA	-5.37	1.39	1.46
1	A	611	THR	N-CA	5.37	1.52	1.45
1	A	415	LYS	N-CA	5.37	1.53	1.46
1	D	507	LEU	C-O	-5.35	1.17	1.24
1	A	872	TRP	C-O	-5.35	1.17	1.24
1	A	464	GLU	N-CA	-5.34	1.39	1.46
1	D	450	LYS	N-CA	5.34	1.52	1.46
1	A	807	ALA	N-CA	5.34	1.52	1.46
1	D	749	TYR	CA-CB	5.31	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	372	ASP	N-CA	5.29	1.54	1.46
1	D	860	VAL	CA-C	5.27	1.57	1.52
1	A	339	ASN	CA-CB	5.26	1.60	1.53
1	A	811	LEU	C-O	5.24	1.30	1.24
1	D	784	ARG	C-O	5.24	1.30	1.24
1	D	616	LEU	N-CA	5.22	1.52	1.45
1	D	763	VAL	N-CA	5.21	1.52	1.46
1	A	803	ILE	N-CA	5.19	1.52	1.46
1	D	336	ALA	C-O	5.17	1.30	1.23
1	D	648	LEU	CA-C	5.15	1.59	1.52
1	D	844	LEU	N-CA	5.15	1.52	1.46
1	D	622	ASN	C-O	5.12	1.29	1.24
1	D	430	GLY	N-CA	5.08	1.50	1.44
1	D	714	TYR	N-CA	5.08	1.52	1.46
1	D	391	SER	N-CA	-5.07	1.39	1.45
1	D	737	GLU	CA-C	5.07	1.59	1.52
2	B	27	DG	O3'-P	-5.07	1.53	1.61
1	D	857	THR	N-CA	-5.06	1.40	1.46
1	D	579	GLN	N-CA	5.05	1.52	1.46
1	D	726	ASN	CA-C	-5.05	1.47	1.53
1	D	421	ALA	CA-C	5.04	1.60	1.52
1	D	566	PRO	N-CA	5.03	1.54	1.47
1	D	749	TYR	C-O	5.02	1.29	1.24
1	A	651	ALA	N-CA	5.02	1.52	1.46
1	A	378	VAL	C-O	5.01	1.30	1.24
1	D	743	PHE	N-CA	5.01	1.52	1.46
1	A	407	VAL	C-O	5.01	1.29	1.24

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	25	DA	C5'-C4'-C3'	13.37	134.96	114.90
1	D	846	ARG	CG-CD-NE	12.77	140.08	112.00
2	E	25	DA	P-O5'-C5'	12.72	139.08	120.00
1	D	843	ARG	CD-NE-CZ	10.65	139.31	124.40
3	C	5	DG	C2'-C3'-O3'	-10.59	95.62	111.50
1	D	836	ALA	O-C-N	8.63	129.56	121.71
1	D	580	LEU	N-CA-C	8.26	120.28	111.28
1	D	770	ARG	NE-CZ-NH2	8.14	126.53	119.20
3	C	5	DG	C4'-C3'-O3'	-7.83	98.26	110.00
2	E	26	DT	C2'-C3'-O3'	-7.79	99.82	111.50
1	D	831	GLU	CA-CB-CG	7.70	129.50	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	843	ARG	NE-CZ-NH2	-7.62	112.35	119.20
2	B	24	DG	C4'-C3'-O3'	-7.41	98.88	110.00
1	A	463	ASP	N-CA-C	7.00	118.91	111.28
1	D	578	ARG	NE-CZ-NH2	-7.00	112.90	119.20
2	E	22	DA	C4'-C3'-O3'	-6.97	99.55	110.00
1	D	578	ARG	CB-CG-CD	-6.89	95.46	111.30
1	A	347	ARG	CA-C-N	-6.87	112.62	119.56
1	A	347	ARG	C-N-CA	-6.87	112.62	119.56
2	B	22	DA	C4'-C3'-O3'	-6.57	100.14	110.00
1	D	475	VAL	CA-C-O	-6.56	113.17	120.25
1	A	601	LYS	CD-CE-NZ	-6.54	90.97	111.90
2	B	25	DA	O5'-P-OP1	6.54	128.60	109.00
1	A	354	ASP	CA-C-O	6.47	124.11	119.32
2	B	25	DA	O5'-P-OP2	-6.46	88.63	108.00
1	D	833	ILE	O-C-N	-6.25	116.50	123.26
1	D	601	LYS	CD-CE-NZ	-6.17	92.16	111.90
1	D	843	ARG	NE-CZ-NH1	6.17	127.67	121.50
1	D	773	LEU	O-C-N	6.14	126.88	121.17
1	D	786	PHE	N-CA-C	-6.12	104.69	111.36
1	D	583	LEU	N-CA-C	6.10	118.43	111.11
1	A	578	ARG	NE-CZ-NH2	-6.09	113.72	119.20
1	D	661	VAL	O-C-N	6.08	127.77	121.87
1	D	816	LYS	CB-CG-CD	6.04	125.19	111.30
1	A	688	ASP	N-CA-C	6.02	119.09	111.69
1	D	708	VAL	N-CA-C	-5.99	104.67	110.42
1	D	556	THR	N-CA-C	-5.97	103.31	111.56
2	E	21	DC	C2'-C3'-O3'	-5.89	102.67	111.50
1	D	749	TYR	CA-C-O	-5.77	114.76	120.82
3	F	12	DA	C4'-C3'-O3'	-5.77	101.35	110.00
1	A	478	GLU	N-CA-C	5.73	117.53	111.28
1	D	578	ARG	NE-CZ-NH1	5.70	127.20	121.50
1	D	437	VAL	CA-C-N	-5.67	114.91	120.98
1	D	437	VAL	C-N-CA	-5.67	114.91	120.98
1	D	532	LYS	N-CA-C	5.61	117.86	111.02
1	D	806	LYS	CA-C-O	-5.61	114.61	120.55
1	D	565	ALA	O-C-N	5.57	126.22	120.70
1	D	831	GLU	CB-CG-CD	-5.57	103.14	112.60
1	D	631	GLU	N-CA-C	5.54	118.03	111.33
1	A	826	LEU	CA-C-O	5.47	127.41	121.06
1	A	770	ARG	CB-CG-CD	-5.44	98.79	111.30
1	D	500	LEU	O-C-N	5.43	127.88	122.12
1	D	339	ASN	CA-C-O	-5.40	115.58	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	21	DC	C4'-C3'-O3'	5.39	118.08	110.00
1	D	843	ARG	CG-CD-NE	-5.38	100.17	112.00
2	B	25	DA	C5'-C4'-C3'	5.33	122.89	114.90
1	D	432	GLY	CA-C-N	5.29	131.22	121.70
1	D	432	GLY	C-N-CA	5.29	131.22	121.70
1	D	792	MET	N-CA-C	-5.29	105.19	111.69
1	D	661	VAL	CA-C-O	-5.25	115.48	120.95
1	D	442	VAL	N-CA-C	-5.24	105.61	110.53
1	A	360	TRP	O-C-N	5.24	127.46	122.07
1	D	657	ILE	O-C-N	5.23	126.94	121.87
1	A	508	ALA	N-CA-C	-5.22	105.67	111.36
1	D	846	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	D	328	HIS	O-C-N	5.19	129.32	122.93
1	A	806	LYS	N-CA-C	-5.18	105.63	111.28
1	D	789	ARG	N-CA-C	-5.18	105.72	111.36
1	D	646	ASP	N-CA-C	-5.17	106.28	112.59
1	D	754	VAL	N-CA-C	-5.17	105.50	110.72
1	D	574	ILE	O-C-N	5.17	127.15	121.83
1	A	465	LEU	CA-C-O	-5.16	115.06	120.63
1	A	687	MET	CG-SD-CE	5.15	112.23	100.90
1	D	501	GLU	N-CA-C	-5.15	105.75	111.36
1	A	643	SER	N-CA-C	-5.11	107.05	113.28
1	D	596	ARG	NE-CZ-NH2	-5.10	114.61	119.20
1	A	596	ARG	NE-CZ-NH2	-5.08	114.63	119.20
1	A	599	THR	O-C-N	5.07	128.15	122.27
1	D	461	PHE	O-C-N	5.07	127.92	122.15
1	A	465	LEU	O-C-N	5.04	127.46	122.12
1	D	472	ARG	CA-CB-CG	-5.03	104.03	114.10
3	F	9	DA	C4'-C3'-O3'	-5.03	102.45	110.00
1	A	565	ALA	O-C-N	5.02	127.09	121.32
1	A	411	ALA	CA-C-O	-5.01	114.44	120.10

There are no chirality outliers.

There are no planarity outliers.

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	4700	0	4794	56	0
1	D	4719	0	4817	77	0
2	B	180	0	104	3	0
2	E	180	0	104	6	0
3	C	226	0	124	1	0
3	F	288	0	158	1	0
4	G	23	0	21	1	0
4	H	23	0	21	1	0
5	A	29	0	13	2	0
6	D	5	0	0	0	0
7	A	556	0	0	16	1
7	B	37	0	0	0	0
7	C	50	0	0	1	0
7	D	622	0	0	33	1
7	E	35	0	0	1	0
7	F	71	0	0	1	0
All	All	11744	0	10156	138	1

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 7.

All (138) 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:D:749:TYR:CE2	1:D:750[A]:MET:CE	2.41	1.04
1:A:692:VAL:HG21	1:A:701:MET:HE1	1.39	1.01
1:D:418:GLN:HG2	7:D:1402:HOH:O	1.64	0.96
1:D:843:ARG:HD2	7:D:1248:HOH:O	1.66	0.95
1:D:792:MET:HB3	7:D:1460:HOH:O	1.69	0.92
1:A:690:PHE:HZ	1:A:704:GLN:NE2	1.72	0.87
1:D:781:PHE:HD2	7:D:1040:HOH:O	1.57	0.87
1:D:749:TYR:HE2	1:D:750[A]:MET:CE	1.85	0.86
1:D:749:TYR:CE2	1:D:750[A]:MET:HE2	2.10	0.85
1:A:315:LYS:HE2	7:A:1348:HOH:O	1.77	0.84
1:D:846:ARG:HD2	7:D:1064:HOH:O	1.79	0.81
1:A:690:PHE:HZ	1:A:704:GLN:HE21	1.30	0.79
1:D:507:LEU:O	7:D:1001:HOH:O	1.99	0.79
1:D:749:TYR:CD2	1:D:750[A]:MET:HE3	2.20	0.76
1:D:749:TYR:CD2	1:D:750[A]:MET:CE	2.69	0.76
1:D:578:ARG:NH2	2:E:25:DA:H5"	2.03	0.74
1:D:843:ARG:CD	7:D:1248:HOH:O	2.30	0.74
1:D:749:TYR:CE2	1:D:750[A]:MET:HE3	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:VAL:CG2	1:A:701:MET:HE1	2.15	0.73
1:A:690:PHE:CZ	1:A:704:GLN:NE2	2.56	0.72
1:D:646:ASP:OD1	1:D:646:ASP:N	2.25	0.70
1:D:591:LEU:O	1:D:595[A]:VAL:HG23	1.91	0.70
1:A:684:LYS:HA	1:A:687:MET:HE3	1.74	0.69
1:D:816:LYS:HG2	7:D:1095:HOH:O	1.94	0.67
1:A:525:GLU:HB3	7:A:1403:HOH:O	1.93	0.67
1:D:792:MET:CB	7:D:1460:HOH:O	2.33	0.67
1:A:683:THR:HG22	1:A:687:MET:HE2	1.77	0.66
1:D:584:GLN:CD	7:D:1034:HOH:O	2.41	0.63
1:D:596:ARG:CZ	7:D:1029:HOH:O	2.46	0.62
1:D:456:GLU:HG2	7:D:1116:HOH:O	1.99	0.62
1:A:594:VAL:HG13	7:A:1241:HOH:O	2.02	0.60
1:A:408:ASP:HB2	4:G:2:FRU:H11	1.84	0.59
1:A:600:LYS:NZ	7:A:1004:HOH:O	2.36	0.59
1:D:814:ARG:NH1	7:D:1006:HOH:O	2.34	0.58
1:D:503[A]:MET:HE2	7:D:1343:HOH:O	2.02	0.57
1:A:517:ARG:HD3	7:A:1405:HOH:O	2.03	0.57
1:D:749:TYR:HE2	1:D:750[A]:MET:HE1	1.69	0.57
1:A:784[B]:ARG:NH2	7:A:1001:HOH:O	2.26	0.57
1:A:456:GLU:HG2	7:A:1203:HOH:O	2.04	0.56
1:D:710:TYR:HD1	7:D:1370:HOH:O	1.89	0.56
1:D:749:TYR:HD2	1:D:750[A]:MET:HE3	1.71	0.56
1:A:750[A]:MET:SD	1:A:792[A]:MET:HB3	2.46	0.56
1:A:766[A]:LEU:HG	7:A:1323:HOH:O	2.06	0.56
1:D:692:VAL:HB	1:D:696:GLU:HG3	1.87	0.56
1:D:690:PHE:HZ	1:D:704:GLN:NE2	2.04	0.55
1:D:511:LEU:N	7:D:1001:HOH:O	2.38	0.55
1:A:766[A]:LEU:HD12	1:A:799:SER:HB3	1.88	0.55
1:D:789:ARG:NH1	7:D:1008:HOH:O	2.36	0.55
1:A:779:ARG:NH1	7:A:1005:HOH:O	2.39	0.55
1:D:788:GLU:O	1:D:792:MET:HG3	2.06	0.55
3:F:1:DG:N2	7:F:102:HOH:O	2.41	0.54
5:A:901:TTP:H2'2	7:A:1059:HOH:O	2.06	0.54
5:A:901:TTP:C2'	7:A:1059:HOH:O	2.56	0.54
1:A:692:VAL:HB	1:A:696:GLU:HB2	1.91	0.53
1:D:507:LEU:HB3	7:D:1034:HOH:O	2.09	0.53
1:D:749:TYR:CD2	1:D:750[A]:MET:HE2	2.36	0.53
1:A:415:LYS:HD3	7:A:1300:HOH:O	2.10	0.52
1:A:779:ARG:O	1:A:784[A]:ARG:NH2	2.42	0.52
1:A:551:LYS:HG3	1:A:552:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:LEU:HG	1:A:571:VAL:HG13	1.92	0.51
1:A:459:ARG:HB3	1:A:460:PRO:HD3	1.93	0.51
1:A:730:LYS:NZ	7:A:1010:HOH:O	2.43	0.51
1:A:741:GLU:HG2	7:A:1468:HOH:O	2.11	0.51
1:D:583:LEU:HB3	7:D:1517:HOH:O	2.11	0.51
1:A:629:ARG:NH2	2:B:101:2DT:OP2	2.44	0.50
1:D:503[A]:MET:CE	7:D:1343:HOH:O	2.59	0.49
2:E:26:DT:H2'	2:E:27:DG:C8	2.47	0.49
1:A:853:GLU:HG3	1:A:864:VAL:HG23	1.95	0.49
1:A:776:ILE:O	1:A:784[B]:ARG:HG3	2.14	0.48
1:D:303:LEU:HD13	1:D:345:PHE:HD2	1.78	0.48
1:A:580:LEU:HD21	1:A:632:GLU:OE1	2.13	0.48
1:D:690:PHE:CZ	1:D:704:GLN:NE2	2.81	0.48
1:D:583:LEU:HD21	7:D:1523:HOH:O	2.14	0.48
1:A:823:HIS:HE1	1:A:835:GLU:OE2	1.96	0.48
1:D:634:ARG:HH21	1:D:876:LYS:HD3	1.78	0.48
1:D:588:ILE:HD11	1:D:636:ILE:HD11	1.96	0.47
1:D:814:ARG:NH2	1:D:847[A]:LEU:HD13	2.29	0.47
1:D:846:ARG:HD2	1:D:846:ARG:HH11	1.59	0.47
1:D:431:LYS:HD2	1:D:435:ARG:HD3	1.96	0.47
1:D:588:ILE:HD11	1:D:636:ILE:CD1	2.45	0.47
1:A:511:LEU:O	1:A:515:GLU:HB2	2.14	0.47
1:D:634:ARG:NH2	1:D:876:LYS:HD3	2.29	0.47
1:A:779:ARG:C	1:A:784[A]:ARG:HH21	2.23	0.47
1:D:691:GLN:CG	7:D:1490:HOH:O	2.63	0.47
1:A:415:LYS:HD2	1:A:415:LYS:HA	1.62	0.46
1:D:495:VAL:HG11	1:D:500:LEU:HD11	1.96	0.46
1:A:329:ASP:H	1:A:382:TRP:CD1	2.33	0.46
1:D:629:ARG:NH2	2:E:28:DC:OP2	2.48	0.46
1:A:326:ASN:HD22	1:A:620:GLU:CD	2.23	0.46
1:A:534:LEU:HD11	1:A:574:ILE:HD13	1.97	0.46
2:E:25:DA:H2''	7:E:231:HOH:O	2.14	0.46
1:D:588:ILE:CD1	1:D:636:ILE:CD1	2.94	0.45
1:D:600:LYS:HD3	7:D:1156:HOH:O	2.16	0.45
1:A:668:ASP:O	1:A:672:MET:HG3	2.17	0.45
1:A:648:LEU:HD12	1:A:841:MET:HG3	1.99	0.45
1:D:408:ASP:HB2	4:H:2:FRU:H11	1.99	0.45
1:A:405:GLN:HB3	1:A:407:VAL:HG23	1.99	0.45
1:D:595[A]:VAL:HG22	1:D:602[A]:VAL:HG13	1.98	0.45
1:D:596:ARG:NH1	7:D:1029:HOH:O	2.50	0.45
1:A:770:ARG:HH12	1:D:472:ARG:NH1	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:719:TYR:O	1:D:723:GLN:HG2	2.17	0.44
1:A:849:PRO:HG3	1:A:866:TYR:CD1	2.53	0.44
1:D:416:MET:SD	7:D:1085:HOH:O	2.62	0.44
1:D:506:GLU:HG3	1:D:507:LEU:N	2.31	0.44
1:A:841:MET:HA	1:A:841:MET:HE2	1.99	0.44
1:A:582:LYS:HG2	2:B:26:DT:H2''	2.00	0.43
1:A:596:ARG:HD3	1:A:603:HIS:CD2	2.53	0.43
1:D:816:LYS:CD	7:D:1095:HOH:O	2.66	0.43
1:D:690:PHE:HZ	1:D:704:GLN:HE21	1.67	0.43
1:D:816:LYS:CG	7:D:1095:HOH:O	2.60	0.43
1:A:579:GLN:HG2	2:B:27:DG:OP1	2.18	0.43
1:D:663:ALA:HB2	1:D:671:LEU:HG	2.00	0.43
1:A:588:ILE:HD11	1:A:636:ILE:HD13	2.01	0.42
1:A:712:ILE:HD13	7:A:1011:HOH:O	2.18	0.42
1:A:823:HIS:CE1	1:A:835:GLU:OE2	2.72	0.42
1:D:298:LYS:HD2	7:D:1468:HOH:O	2.19	0.42
1:A:665:ILE:HD12	1:A:796[A]:ILE:HD13	2.00	0.42
1:D:836:ALA:HB3	1:D:841:MET:CE	2.49	0.42
1:D:435:ARG:HA	1:D:435:ARG:HD2	1.42	0.42
1:A:315:LYS:HA	1:A:315:LYS:HD2	1.68	0.42
1:D:440:GLU:HG3	7:D:1195:HOH:O	2.19	0.42
1:D:519:TYR:CD2	1:D:525:GLU:HG2	2.55	0.42
1:D:418:GLN:HA	7:D:1035:HOH:O	2.19	0.42
1:D:433:ALA:HA	1:D:434:LYS:HA	1.81	0.42
3:C:4:DC:H6	7:C:132:HOH:O	2.01	0.41
1:D:304:ALA:HB1	1:D:311:MET:HE1	2.02	0.41
1:D:531:PRO:HG3	2:E:25:DA:H5'	2.02	0.41
1:D:584:GLN:NE2	7:D:1034:HOH:O	2.52	0.41
1:D:863:LYS:HE2	7:D:1122:HOH:O	2.20	0.41
1:D:298:LYS:HE2	1:D:298:LYS:HB3	1.91	0.41
1:D:432:GLY:HA2	1:D:434:LYS:C	2.45	0.41
1:D:602[B]:VAL:HG11	1:D:621:PRO:HG3	2.02	0.41
1:A:315:LYS:CE	7:A:1348:HOH:O	2.50	0.41
1:A:495:VAL:CG1	1:A:500:LEU:HD22	2.51	0.41
1:A:762:TYR:CD1	1:A:770:ARG:HG3	2.55	0.41
1:D:691:GLN:HG3	7:D:1490:HOH:O	2.21	0.40
1:D:579:GLN:HG2	2:E:27:DG:OP1	2.21	0.40
1:A:515:GLU:HG2	1:A:519:TYR:CZ	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1004:HOH:O	7:D:1292:HOH:O[2_745]	1.99	0.21

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	586/580 (101%)	574 (98%)	12 (2%)	0	100	100
1	D	590/580 (102%)	574 (97%)	16 (3%)	0	100	100
All	All	1176/1160 (101%)	1148 (98%)	28 (2%)	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	504/495 (102%)	490 (97%)	14 (3%)	38	11
1	D	507/495 (102%)	494 (97%)	13 (3%)	40	13
All	All	1011/990 (102%)	984 (97%)	27 (3%)	40	12

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	LEU
1	A	405	GLN
1	A	415	LYS

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Mol	Chain	Res	Type
1	A	420	GLU
1	A	500	LEU
1	A	507	LEU
1	A	544	LEU
1	A	561	LEU
1	A	566	PRO
1	A	591	LEU
1	A	699	PRO
1	A	784[A]	ARG
1	A	784[B]	ARG
1	A	837	PRO
1	D	298	LYS
1	D	303	LEU
1	D	415	LYS
1	D	434	LYS
1	D	435	ARG
1	D	506	GLU
1	D	511	LEU
1	D	513	THR
1	D	629	ARG
1	D	636	ILE
1	D	776	ILE
1	D	816	LYS
1	D	863	LYS

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

Mol	Chain	Res	Type
1	A	638	GLN
1	A	691	GLN
1	A	704	GLN
1	A	726	ASN
1	A	755	GLN
1	A	823	HIS
1	A	867	HIS
1	D	468	ASN
1	D	470	GLN
1	D	612	GLN
1	D	704	GLN
1	D	768	HIS
1	D	867	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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$
1	CME	D	388	1	8,9,10	0.77	0	6,9,11	1.44	2 (33%)
2	2DT	E	101	3,2	17,20,21	1.57	5 (29%)	22,28,31	4.42	11 (50%)
2	2DT	B	101	3,2	17,20,21	1.28	1 (5%)	22,28,31	3.23	10 (45%)
1	CME	A	388	1	8,9,10	0.71	0	6,9,11	1.44	1 (16%)

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
1	CME	D	388	1	-	1/5/8/10	-
2	2DT	E	101	3,2	-	0/7/18/19	0/2/2/2
2	2DT	B	101	3,2	-	0/7/18/19	0/2/2/2
1	CME	A	388	1	-	1/5/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	101	2DT	C3'-C2'	-3.07	1.45	1.54
2	E	101	2DT	O2-C2	2.71	1.27	1.23
2	E	101	2DT	C6-C5	2.48	1.38	1.34
2	B	101	2DT	O2-C2	2.35	1.27	1.23
2	E	101	2DT	O4'-C1'	-2.04	1.37	1.42
2	E	101	2DT	C5M-C5	2.02	1.55	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	101	2DT	C4-N3-C2	-10.30	113.84	127.34
2	E	101	2DT	N3-C2-N1	9.36	127.07	114.89
2	E	101	2DT	C5-C6-N1	-7.86	114.78	123.31
2	B	101	2DT	C4-N3-C2	-7.47	117.54	127.34
2	E	101	2DT	C6-C5-C4	6.49	123.37	118.02
2	B	101	2DT	N3-C2-N1	6.46	123.31	114.89
2	B	101	2DT	C5-C4-N3	6.12	120.65	115.32
2	E	101	2DT	C5-C4-N3	5.35	119.98	115.32
2	E	101	2DT	C4'-O4'-C1'	5.22	114.74	109.81
2	B	101	2DT	O2-C2-N3	-4.61	112.98	121.49
2	E	101	2DT	O2-C2-N3	-4.59	113.03	121.49
2	E	101	2DT	C5M-C5-C6	-4.24	117.12	122.85
2	B	101	2DT	C4'-O4'-C1'	3.82	113.42	109.81
2	E	101	2DT	C3'-C2'-C1'	3.80	107.25	102.87
2	B	101	2DT	C5-C6-N1	-3.77	119.21	123.31
2	B	101	2DT	C2'-C1'-N1	2.85	117.80	112.40
2	B	101	2DT	C5M-C5-C6	-2.60	119.33	122.85
2	E	101	2DT	O2-C2-N1	-2.50	119.54	122.80
2	B	101	2DT	C5M-C5-C4	2.46	121.41	118.78
1	A	388	CME	CB-CA-C	-2.34	104.46	110.80
1	D	388	CME	CB-CA-C	-2.17	104.92	110.80
1	D	388	CME	CB-SG-SD	-2.14	98.33	103.86
2	B	101	2DT	O4-C4-C5	-2.07	122.55	124.92
2	E	101	2DT	O4-C4-N3	-2.03	116.29	120.11

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	388	CME	SD-CE-CZ-OH
1	D	388	CME	SD-CE-CZ-OH

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	101	2DT	1	0

5.5 Carbohydrates ⓘ

4 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$
4	GLC	G	1	4	11,11,12	0.77	0	15,15,17	1.48	2 (13%)
4	FRU	G	2	4	11,12,12	1.80	2 (18%)	10,18,18	1.70	2 (20%)
4	GLC	H	1	4	11,11,12	0.85	0	15,15,17	1.46	3 (20%)
4	FRU	H	2	4	11,12,12	1.31	2 (18%)	10,18,18	1.21	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLC	G	1	4	-	0/2/19/22	0/1/1/1
4	FRU	G	2	4	-	0/5/24/24	0/1/1/1
4	GLC	H	1	4	-	0/2/19/22	0/1/1/1
4	FRU	H	2	4	-	0/5/24/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2	FRU	O2-C2	4.86	1.49	1.40
4	H	2	FRU	O2-C2	2.47	1.45	1.40
4	H	2	FRU	O3-C3	2.43	1.47	1.42
4	G	2	FRU	O5-C2	2.24	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	FRU	O6-C6-C5	-4.42	96.30	111.33
4	G	1	GLC	C1-O5-C5	3.50	116.88	112.19
4	H	2	FRU	O6-C6-C5	-2.91	101.41	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	GLC	O5-C1-C2	-2.65	104.47	110.79
4	G	2	FRU	O3-C3-C4	-2.54	104.28	113.25
4	H	1	GLC	C1-O5-C5	2.38	115.38	112.19
4	G	1	GLC	O5-C5-C6	-2.09	103.60	107.66
4	H	1	GLC	O3-C3-C2	-2.05	105.87	110.05

There are no chirality outliers.

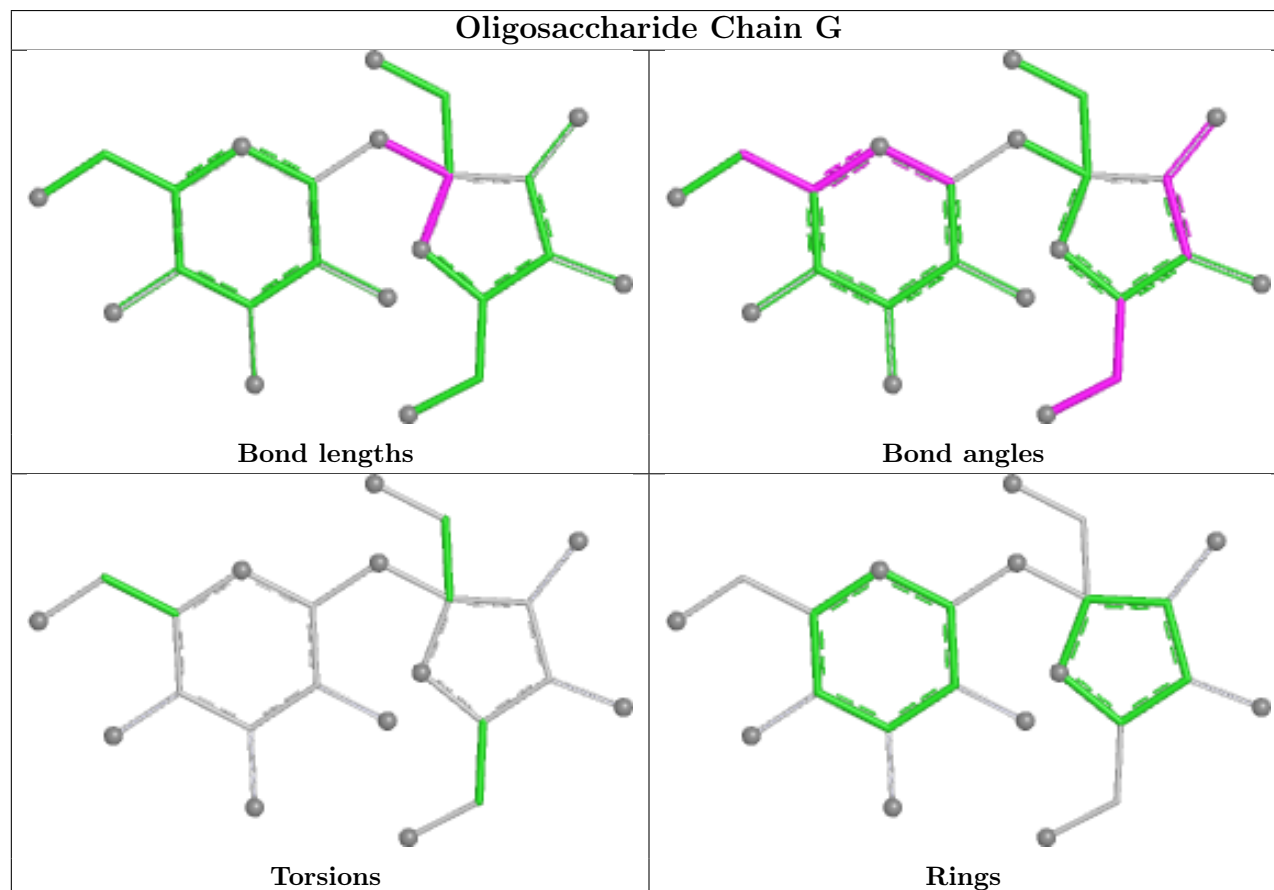
There are no torsion outliers.

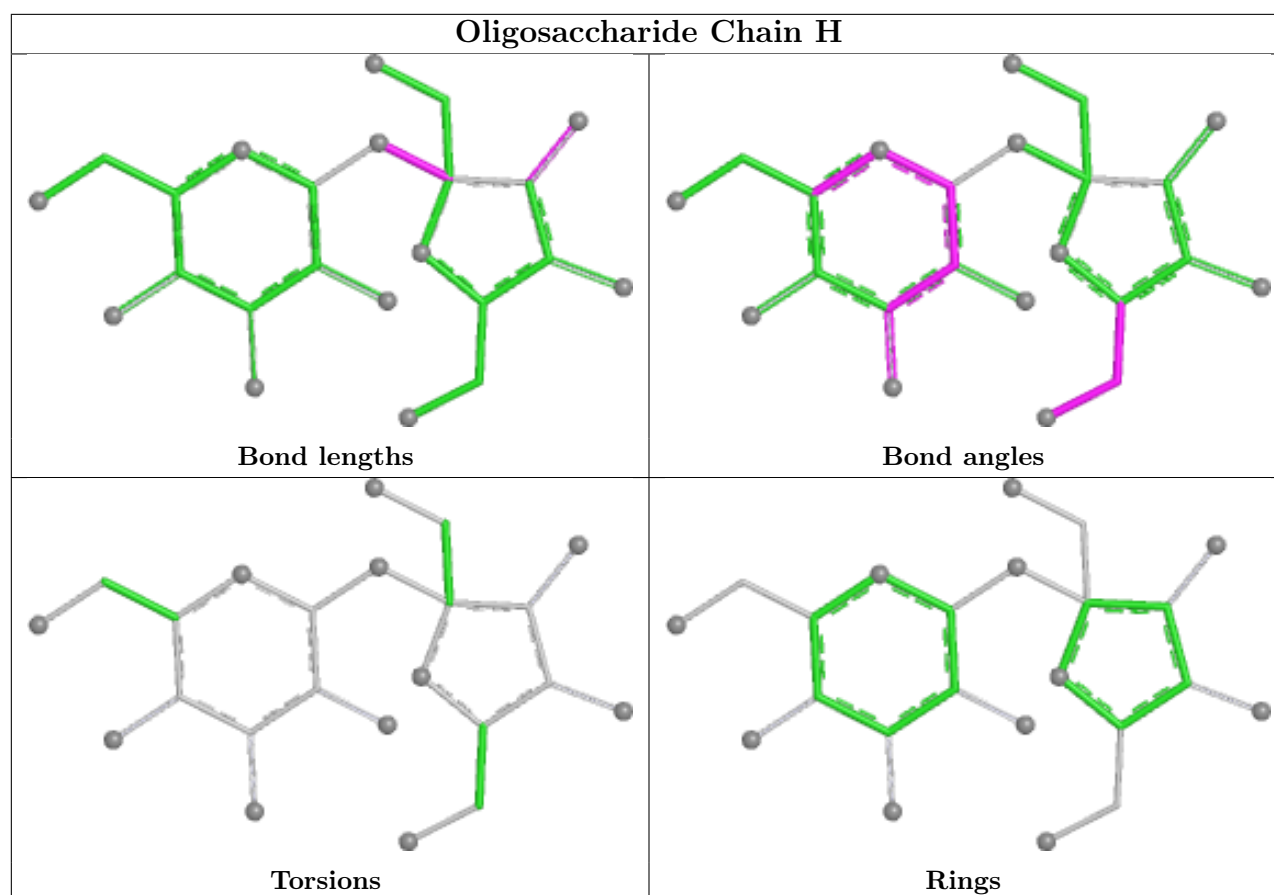
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	2	FRU	1	0
4	G	2	FRU	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.





5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	TTP	A	901	-	29,30,30	1.73	6 (20%)	43,47,47	1.86	8 (18%)
6	SO4	D	901	-	4,4,4	0.37	0	6,6,6	1.63	3 (50%)

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
5	TTP	A	901	-	-	4/22/34/34	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	TTP	PA-O3A	6.07	1.66	1.59
5	A	901	TTP	C6-C5	4.40	1.41	1.34
5	A	901	TTP	O4-C4	2.47	1.28	1.23
5	A	901	TTP	C4-N3	-2.30	1.34	1.38
5	A	901	TTP	C2-N3	-2.18	1.34	1.38
5	A	901	TTP	PB-O3A	2.06	1.61	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	TTP	C5-C6-N1	-5.03	117.85	123.31
5	A	901	TTP	C5-C4-N3	4.26	119.03	115.32
5	A	901	TTP	N3-C2-N1	4.03	120.14	114.89
5	A	901	TTP	C4-N3-C2	-3.77	122.40	127.34
5	A	901	TTP	O2B-PB-O3B	2.66	114.45	107.27
5	A	901	TTP	O3G-PG-O3B	-2.50	96.24	104.64
5	A	901	TTP	O3'-C3'-C2'	-2.48	102.26	110.88
6	D	901	SO4	O4-S-O1	2.23	121.21	109.56
6	D	901	SO4	O4-S-O2	-2.20	98.07	109.56
5	A	901	TTP	C2'-C3'-C4'	2.10	107.06	102.80
6	D	901	SO4	O3-S-O1	2.09	120.50	109.56

There are no chirality outliers.

All (4) torsion outliers are listed below:

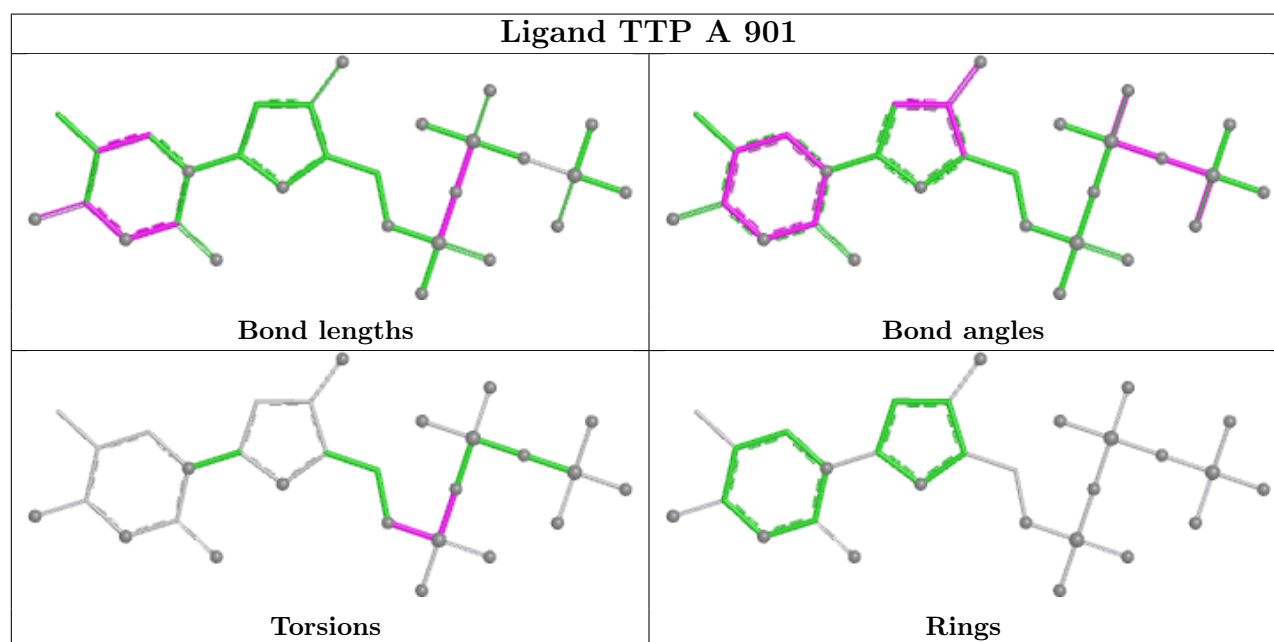
Mol	Chain	Res	Type	Atoms
5	A	901	TTP	C5'-O5'-PA-O3A
5	A	901	TTP	C5'-O5'-PA-O1A
5	A	901	TTP	PB-O3A-PA-O2A
5	A	901	TTP	PB-O3A-PA-O1A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	901	TTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	578/580 (99%)	0.61	34 (5%) 28 30	10, 27, 45, 67	11 (1%)
1	D	579/580 (99%)	0.55	53 (9%) 14 15	5, 24, 49, 89	13 (2%)
2	B	8/9 (88%)	0.17	0 100 100	22, 26, 30, 37	0
2	E	8/9 (88%)	0.17	1 (12%) 8 8	17, 24, 31, 51	0
3	C	11/14 (78%)	0.11	0 100 100	17, 22, 37, 45	0
3	F	14/14 (100%)	0.39	3 (21%) 2 2	14, 23, 41, 46	0
All	All	1198/1206 (99%)	0.57	91 (7%) 20 21	5, 25, 47, 89	24 (2%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	433	ALA	6.7
1	D	504	GLY	6.4
1	D	508	ALA	6.3
1	D	430	GLY	5.2
1	D	432	GLY	5.0
1	D	602[A]	VAL	4.4
1	D	514	VAL	4.3
1	D	693	SER	4.2
1	D	502	GLN	3.8
1	D	434	LYS	3.7
1	D	507	LEU	3.6
1	D	698	THR	3.6
1	A	689	ILE	3.6
1	D	505	LYS	3.5
1	D	692	VAL	3.5
1	D	306	ARG	3.4
1	D	431	LYS	3.4
1	D	513	THR	3.4
1	A	647	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	511	LEU	3.3
1	A	431	LYS	3.3
1	D	689	ILE	3.2
1	A	630	LEU	3.2
1	D	303	LEU	3.2
1	A	543	GLN	3.1
1	D	725	LEU	3.1
1	D	509	GLU	3.0
1	A	690	PHE	3.0
1	A	854[A]	GLN	2.9
1	A	781	PHE	2.9
1	D	435	ARG	2.9
1	A	550	THR	2.9
1	D	731	GLU	2.8
1	D	512	GLY	2.8
1	D	645	SER	2.8
1	A	836	ALA	2.8
1	D	297	LYS	2.7
3	F	1	DG	2.7
1	A	513	THR	2.7
1	D	726	ASN	2.7
1	D	690	PHE	2.7
1	A	856	VAL	2.7
1	D	510	GLN	2.7
1	D	629	ARG	2.7
1	D	710	TYR	2.6
1	D	700	ASN	2.6
1	D	703	ARG	2.6
1	D	727	ILE	2.6
1	D	354	ASP	2.6
1	A	698	THR	2.5
1	D	686	ALA	2.5
1	D	786	PHE	2.5
1	D	350	THR	2.5
1	D	780	ASN	2.5
1	D	562	GLU	2.5
1	D	817	GLU	2.5
1	D	781	PHE	2.5
1	D	779	ARG	2.5
1	D	523	GLY	2.4
2	E	21	DC	2.4
1	A	779	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	539	PHE	2.4
1	A	523	GLY	2.4
1	A	693	SER	2.4
1	D	531	PRO	2.3
1	A	553	GLY	2.3
1	A	524	GLN	2.3
1	D	701	MET	2.3
1	A	427	ALA	2.2
1	D	543	GLN	2.2
1	D	697	VAL	2.2
1	A	820	LEU	2.2
3	F	2	DA	2.2
3	F	14	DG	2.2
1	A	519	TYR	2.2
1	D	501	GLU	2.2
1	A	596	ARG	2.1
1	D	704	GLN	2.1
1	A	298	LYS	2.1
1	A	876	LYS	2.1
1	A	812[A]	ASN	2.1
1	A	508	ALA	2.1
1	A	857	THR	2.1
1	A	505	LYS	2.1
1	D	516	GLN	2.1
1	A	692	VAL	2.0
1	A	819	ARG	2.0
1	A	507	LEU	2.0
1	A	867	HIS	2.0
1	A	700	ASN	2.0
1	D	583	LEU	2.0

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

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
1	CME	A	388	10/11	0.94	0.12	19,22,55,68	0
1	CME	D	388	10/11	0.94	0.11	18,26,45,49	0
2	2DT	B	101	19/20	0.97	0.07	20,22,28,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2DT	E	101	19/20	0.98	0.05	16,18,22,22	0

6.3 Carbohydrates

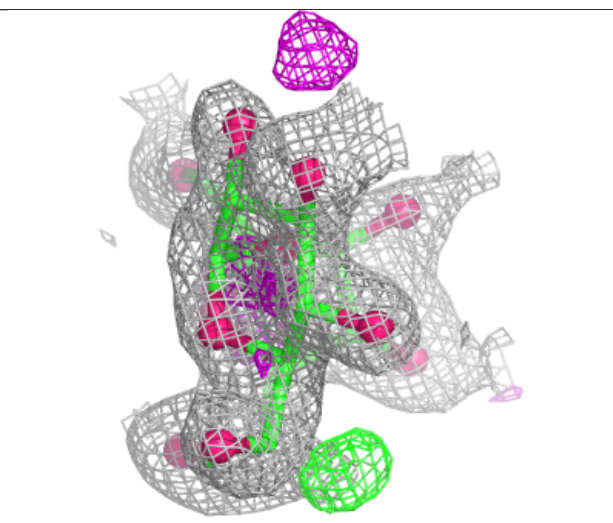
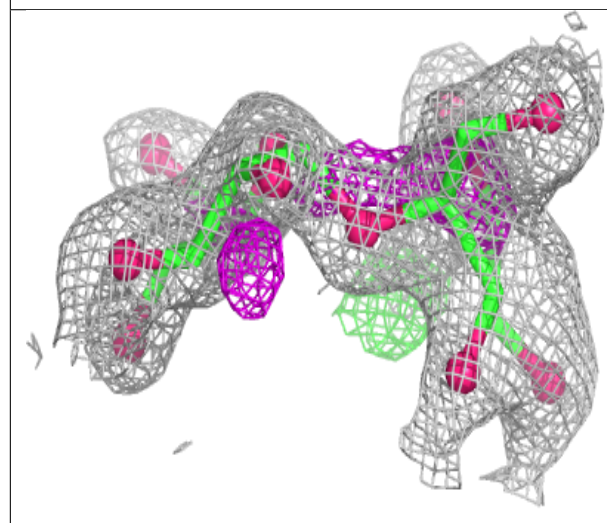
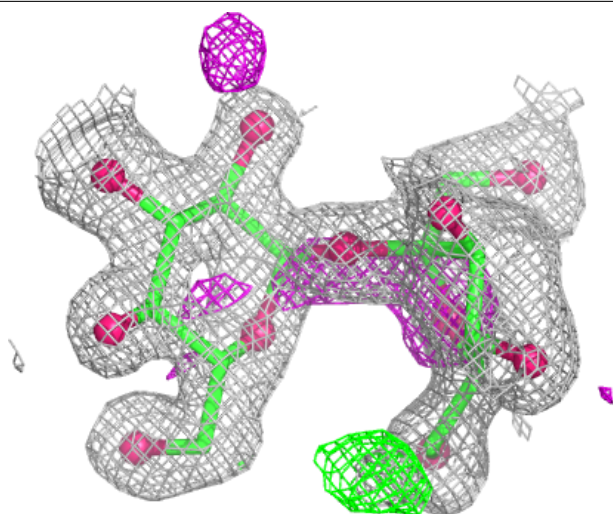
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

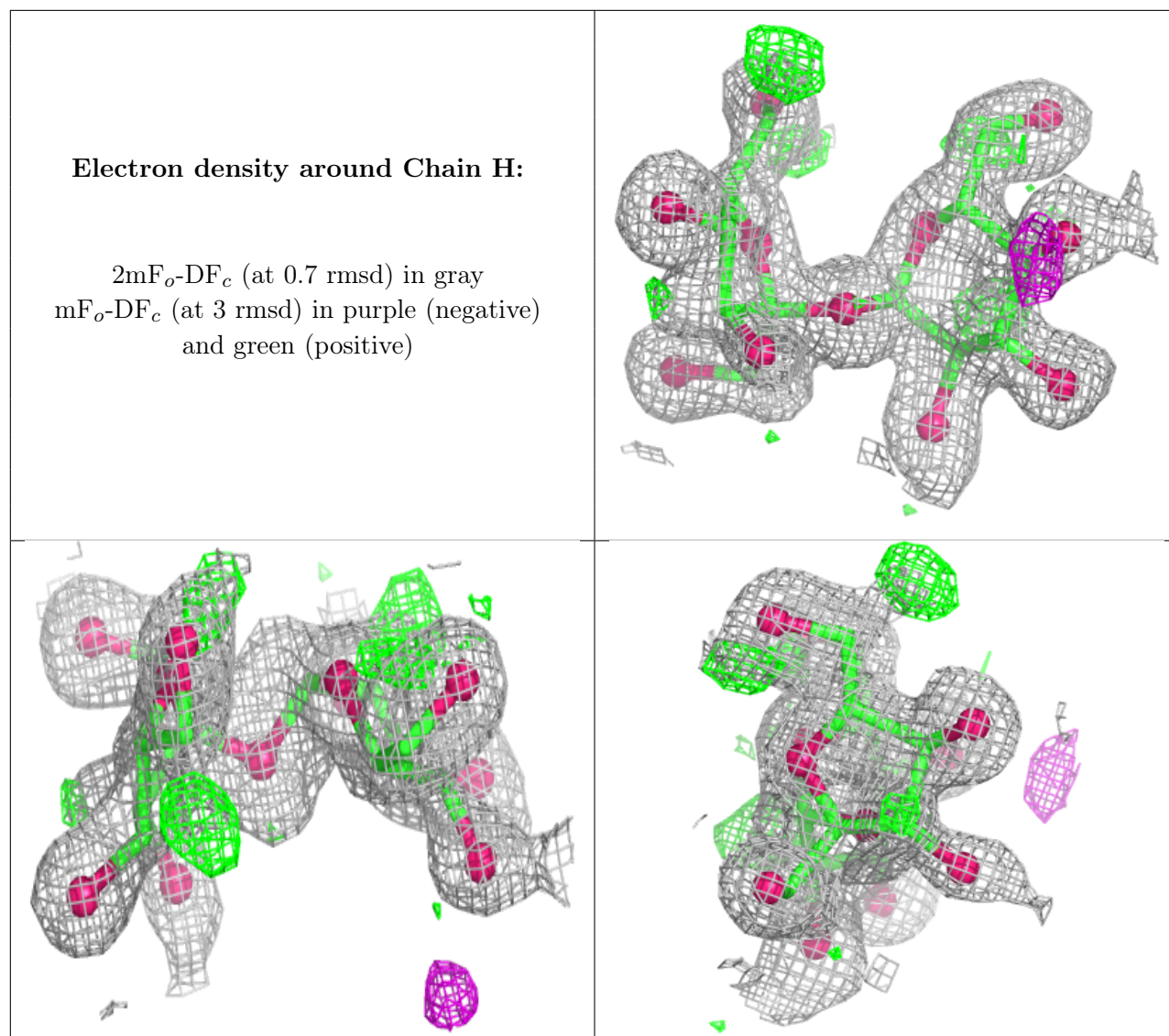
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FRU	G	2	12/12	0.82	0.14	29,34,37,43	0
4	GLC	G	1	11/12	0.85	0.12	35,37,41,45	0
4	FRU	H	2	12/12	0.85	0.13	15,19,20,20	12
4	GLC	H	1	11/12	0.86	0.11	18,20,22,24	11

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.

Electron density around Chain G:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



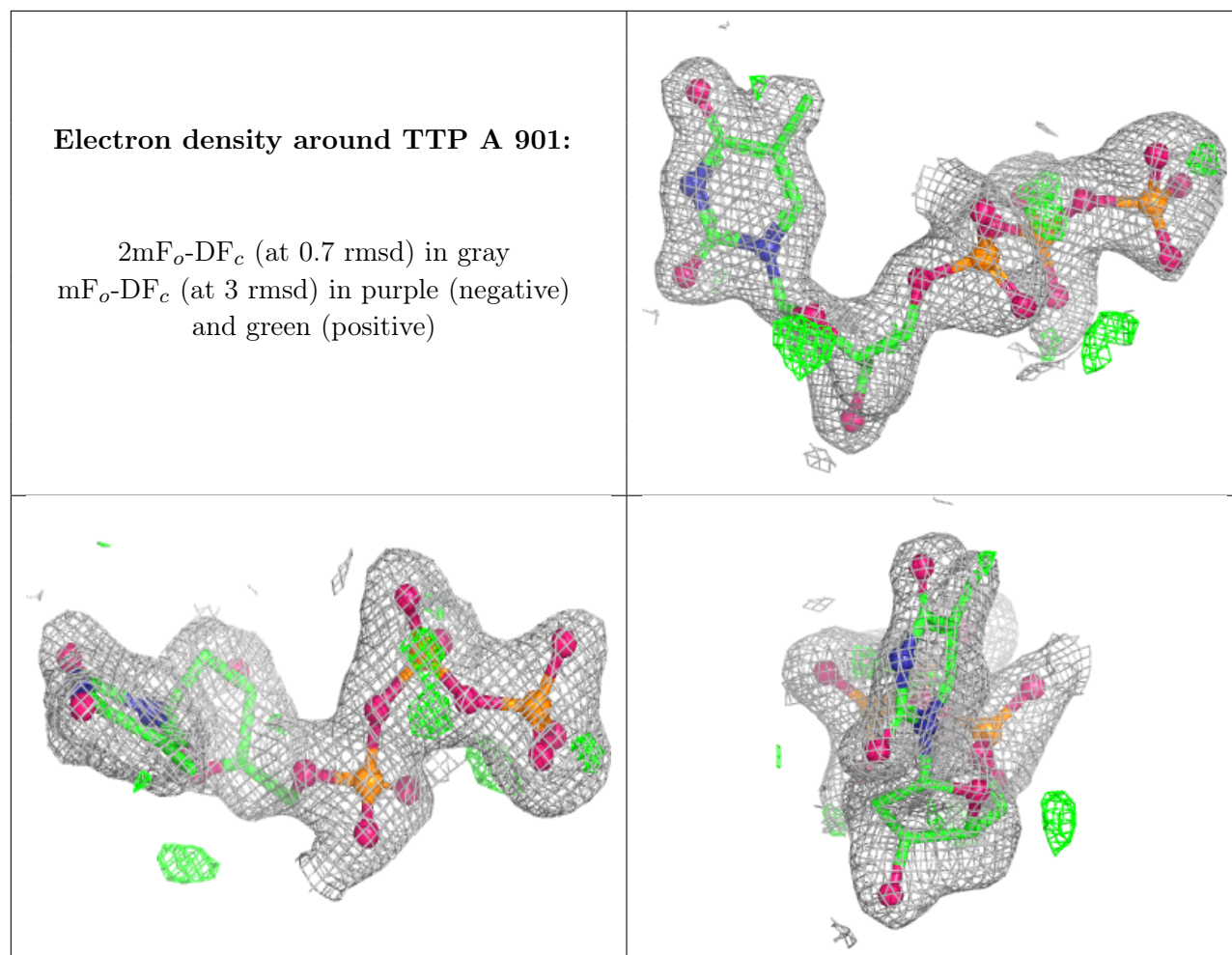


6.4 Ligands [i](#)

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(Å ²)	Q<0.9
5	TTP	A	901	29/29	0.91	0.12	28,35,43,43	29
6	SO4	D	901	5/5	0.93	0.10	36,38,50,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.