



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:40 PM UTC

PDB ID : 6KDO / pdb_00006kdo
Title : HIV-1 reverse transcriptase with Q151M/Y115F/F116Y/M184V/F160M:DN
A:lamivudine 5'-triphosphate ternary complex
Authors : Yasutake, Y.; Hattori, S.I.; Tamura, N.; Maeda, K.
Deposited on : 2019-07-02
Resolution : 2.57 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

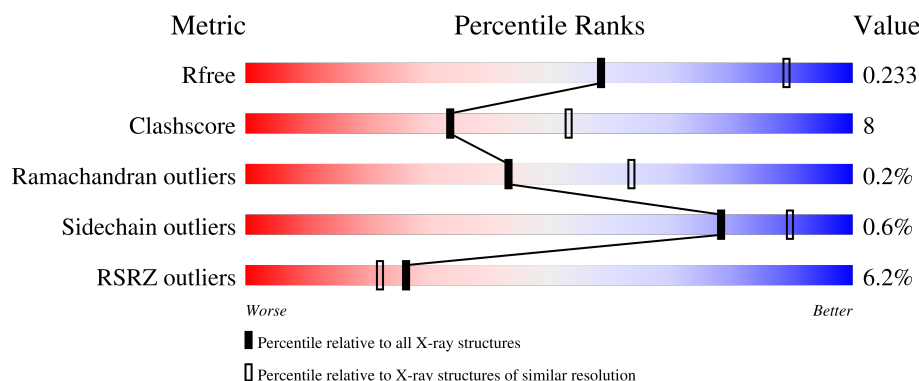
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	557	6% 83% 16% .
1	C	557	4% 83% 15% ..
2	B	444	10% 75% 16% 9%
2	D	444	6% 77% 14% 9%
3	E	38	61% 29% . 8%

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Mol	Chain	Length	Quality of chain
3	F	38	 76% 18% 5%
4	G	2	 50% 50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17434 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 HIV-1 reverse transcriptase p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4487	2902	749	828	8			
1	C	552	Total	C	N	O	S	0	0	0
			4487	2902	749	828	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP D3XFN5
A	0	VAL	-	expression tag	UNP D3XFN5
A	115	PHE	TYR	engineered mutation	UNP D3XFN5
A	116	TYR	PHE	engineered mutation	UNP D3XFN5
A	151	MET	GLN	engineered mutation	UNP D3XFN5
A	160	MET	PHE	engineered mutation	UNP D3XFN5
A	162	SER	CYS	engineered mutation	UNP D3XFN5
A	184	VAL	MET	engineered mutation	UNP D3XFN5
A	280	SER	CYS	engineered mutation	UNP D3XFN5
C	-1	MET	-	expression tag	UNP D3XFN5
C	0	VAL	-	expression tag	UNP D3XFN5
C	115	PHE	TYR	engineered mutation	UNP D3XFN5
C	116	TYR	PHE	engineered mutation	UNP D3XFN5
C	151	MET	GLN	engineered mutation	UNP D3XFN5
C	160	MET	PHE	engineered mutation	UNP D3XFN5
C	162	SER	CYS	engineered mutation	UNP D3XFN5
C	184	VAL	MET	engineered mutation	UNP D3XFN5
C	280	SER	CYS	engineered mutation	UNP D3XFN5

- Molecule 2 is a protein called HIV-1 RT p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	406	Total	C	N	O	S	0	0	0
			3347	2178	557	606	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	406	Total	C	N	O	S	0	0	0
			3347	2178	557	606	6			

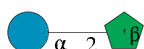
There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	expression tag	UNP P12497
B	-14	ALA	-	expression tag	UNP P12497
B	-13	HIS	-	expression tag	UNP P12497
B	-12	HIS	-	expression tag	UNP P12497
B	-11	HIS	-	expression tag	UNP P12497
B	-10	HIS	-	expression tag	UNP P12497
B	-9	HIS	-	expression tag	UNP P12497
B	-8	HIS	-	expression tag	UNP P12497
B	-7	ALA	-	expression tag	UNP P12497
B	-6	LEU	-	expression tag	UNP P12497
B	-5	GLU	-	expression tag	UNP P12497
B	-4	VAL	-	expression tag	UNP P12497
B	-3	LEU	-	expression tag	UNP P12497
B	-2	PHE	-	expression tag	UNP P12497
B	-1	GLN	-	expression tag	UNP P12497
B	0	GLY	-	expression tag	UNP P12497
B	162	SER	CYS	engineered mutation	UNP P12497
B	280	SER	CYS	engineered mutation	UNP P12497
D	-15	MET	-	expression tag	UNP P12497
D	-14	ALA	-	expression tag	UNP P12497
D	-13	HIS	-	expression tag	UNP P12497
D	-12	HIS	-	expression tag	UNP P12497
D	-11	HIS	-	expression tag	UNP P12497
D	-10	HIS	-	expression tag	UNP P12497
D	-9	HIS	-	expression tag	UNP P12497
D	-8	HIS	-	expression tag	UNP P12497
D	-7	ALA	-	expression tag	UNP P12497
D	-6	LEU	-	expression tag	UNP P12497
D	-5	GLU	-	expression tag	UNP P12497
D	-4	VAL	-	expression tag	UNP P12497
D	-3	LEU	-	expression tag	UNP P12497
D	-2	PHE	-	expression tag	UNP P12497
D	-1	GLN	-	expression tag	UNP P12497
D	0	GLY	-	expression tag	UNP P12497
D	162	SER	CYS	engineered mutation	UNP P12497
D	280	SER	CYS	engineered mutation	UNP P12497

- Molecule 3 is a DNA chain called DNA/RNA (38-MER).

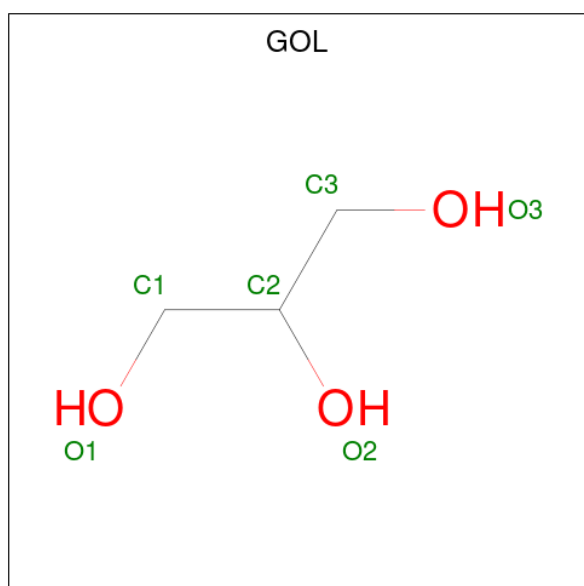
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	35	Total	C	N	O	P	0	0	0
			721	340	130	216	35			
3	F	38	Total	C	N	O	P	0	0	0
			780	370	142	231	37			

- 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			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



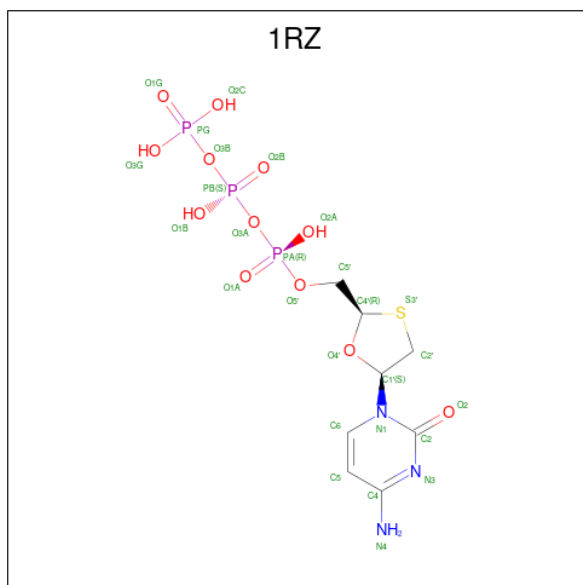
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is Lamivudine Triphosphate (CCD ID: 1RZ) (formula: $C_8H_{14}N_3O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	S	0	0
			13	7	3	2	1		
6	C	1	Total	C	N	O	S	0	0
			13	7	3	2	1		

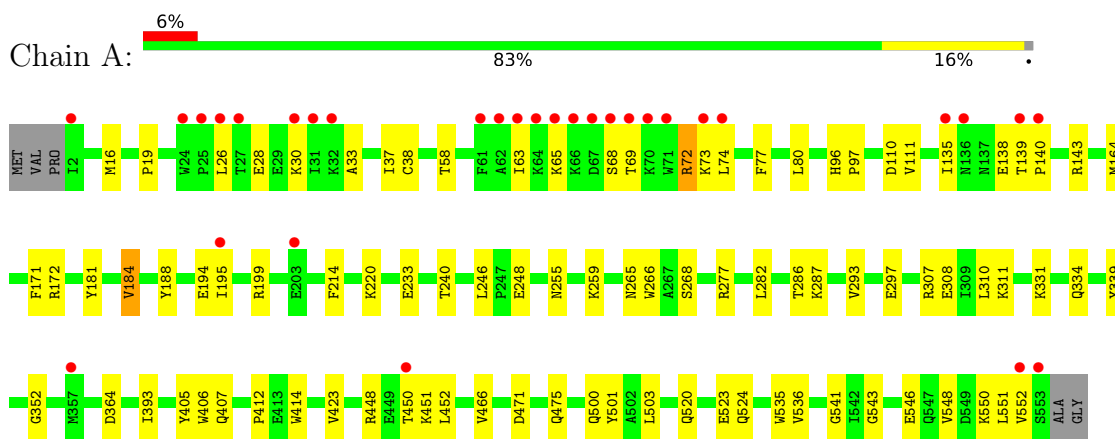
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	56	Total	O	0	0
			56	56		
7	B	23	Total	O	0	0
			23	23		
7	E	23	Total	O	0	0
			23	23		
7	C	44	Total	O	0	0
			44	44		
7	D	31	Total	O	0	0
			31	31		
7	F	15	Total	O	0	0
			15	15		

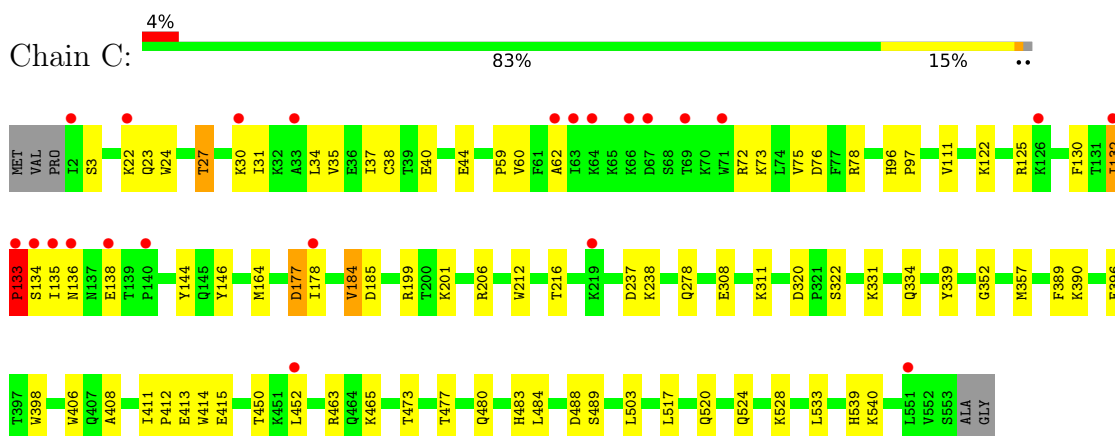
3 Residue-property plots [i](#)

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.

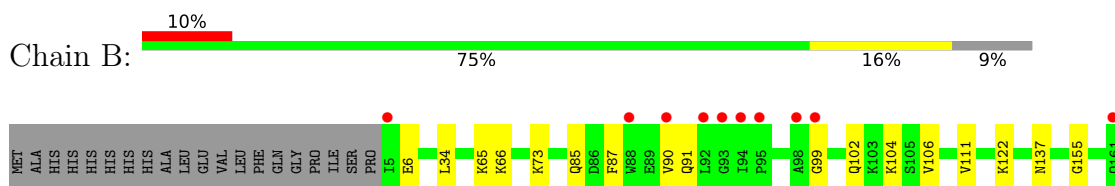
- Molecule 1: HIV-1 reverse transcriptase p66 subunit

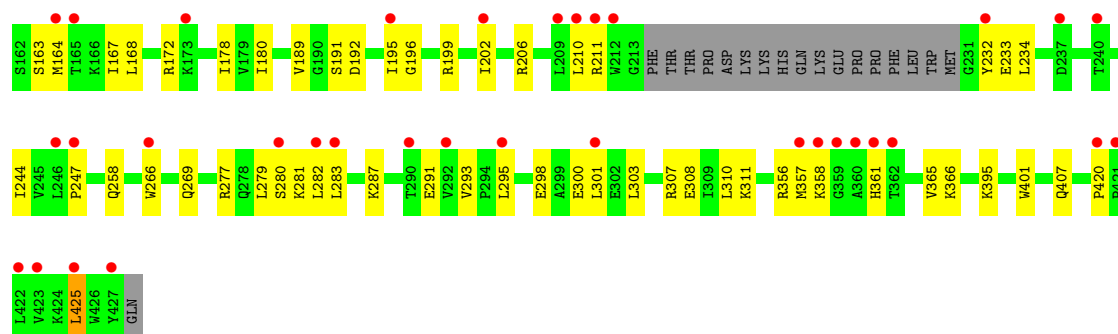


- Molecule 1: HIV-1 reverse transcriptase p66 subunit

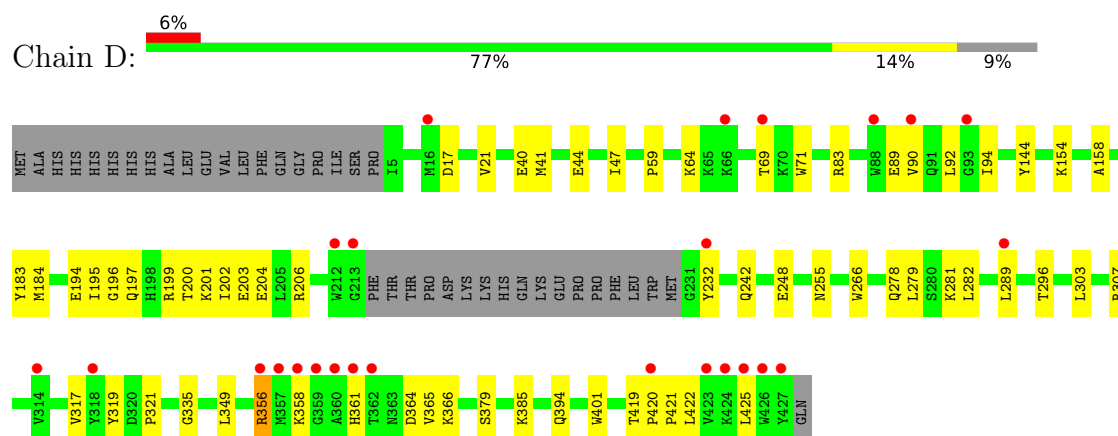


- Molecule 2: HIV-1 RT p51 subunit





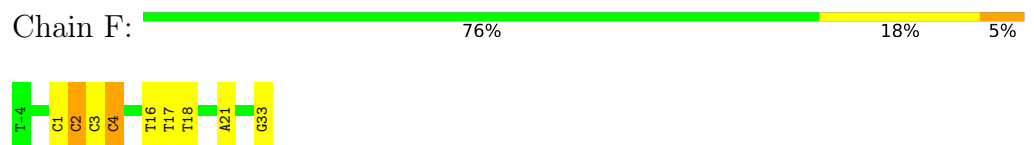
• Molecule 2: HIV-1 RT p51 subunit



• Molecule 3: DNA/RNA (38-MER)



• Molecule 3: DNA/RNA (38-MER)



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



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	284.24Å 284.24Å 95.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.67 – 2.57 48.67 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.67-2.57) 99.8 (48.67-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.192 , 0.230 0.196 , 0.233	Depositor DCC
R_{free} test set	4639 reflections (4.27%)	wwPDB-VP
Wilson B-factor (Å ²)	60.5	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17434	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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: GOL, OMC, GLC, 1RZ, FRU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	0/4603	0.55	0/6251
1	C	0.32	0/4603	0.59	4/6251 (0.1%)
2	B	0.29	0/3441	0.65	1/4673 (0.0%)
2	D	0.25	0/3441	0.48	0/4673
3	E	0.21	0/760	0.44	0/1172
3	F	0.33	0/827	0.56	1/1276 (0.1%)
All	All	0.30	0/17675	0.56	6/24296 (0.0%)

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
2	D	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	PRO	CA-N-CD	-9.79	98.30	112.00
1	C	27	THR	CA-C-N	-7.09	109.99	122.26
1	C	27	THR	C-N-CA	-7.09	109.99	122.26
3	F	17	DT	C2'-C3'-O3'	-6.55	101.67	111.50
2	B	211	ARG	CB-CG-CD	-6.18	97.09	111.30
1	C	199	ARG	CB-CG-CD	5.53	124.02	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	356	ARG	Sidechain

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	4487	0	4543	75	0
1	C	4487	0	4543	64	0
2	B	3347	0	3379	70	0
2	D	3347	0	3379	46	0
3	E	721	0	397	10	0
3	F	780	0	432	7	0
4	G	23	0	21	0	0
5	A	6	0	8	0	0
5	B	6	0	8	1	0
5	C	6	0	8	1	0
5	D	6	0	8	0	0
6	C	13	0	7	3	0
6	E	13	0	7	3	0
7	A	56	0	0	0	0
7	B	23	0	0	0	0
7	C	44	0	0	1	0
7	D	31	0	0	0	0
7	E	23	0	0	0	0
7	F	15	0	0	0	0
All	All	17434	0	16740	262	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 8.

All (262) 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)
2:B:425:LEU:O	2:B:425:LEU:CD1	2.13	0.96
2:B:425:LEU:O	2:B:425:LEU:HD12	1.64	0.95
1:A:450:THR:HG22	1:A:452:LEU:HG	1.56	0.87
2:B:425:LEU:HD12	2:B:425:LEU:C	2.03	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:LEU:CD1	2:B:425:LEU:C	2.51	0.83
2:B:111:VAL:HG11	2:B:164:MET:HE1	1.63	0.80
1:A:72:ARG:HB2	1:A:72:ARG:NH2	1.96	0.80
2:D:356:ARG:HD2	2:D:361:HIS:HB2	1.63	0.80
2:D:47:ILE:HD12	2:D:144:TYR:CD2	2.18	0.79
2:B:266:TRP:CD1	2:B:425:LEU:HD23	2.18	0.79
1:C:31:ILE:HD13	1:C:133:PRO:O	1.83	0.78
2:B:199:ARG:HA	2:B:202:ILE:HD12	1.69	0.74
2:B:266:TRP:CD1	2:B:425:LEU:CD2	2.72	0.72
2:B:172:ARG:HH21	2:B:180:ILE:HB	1.55	0.72
2:B:425:LEU:O	2:B:425:LEU:HD13	1.88	0.72
2:D:335:GLY:HA3	2:D:356:ARG:HD3	1.70	0.72
1:A:536:VAL:HG11	2:B:258:GLN:HE21	1.54	0.72
2:D:356:ARG:HD2	2:D:361:HIS:CB	2.20	0.71
1:A:503:LEU:HD13	1:A:535:TRP:HB2	1.75	0.69
1:C:27:THR:OG1	1:C:30:LYS:HB2	1.93	0.69
1:C:177:ASP:OD1	1:C:177:ASP:N	2.26	0.69
2:B:244:ILE:HD13	2:B:425:LEU:HD11	1.74	0.68
1:A:72:ARG:HB2	1:A:72:ARG:HH21	1.59	0.68
2:D:282:LEU:HD21	2:D:296:THR:HG23	1.74	0.68
1:A:541:GLY:HA2	1:A:546:GLU:HG3	1.76	0.68
1:C:133:PRO:O	1:C:133:PRO:HD2	1.94	0.67
1:A:33:ALA:O	1:A:37:ILE:HG13	1.95	0.67
1:C:34:LEU:HD21	1:C:62:ALA:HB2	1.76	0.67
2:B:90:VAL:O	2:B:91:GLN:HB2	1.94	0.66
1:A:331:LYS:NZ	1:A:364:ASP:OD2	2.28	0.66
1:A:65:LYS:HE2	1:A:72:ARG:HH12	1.60	0.65
1:A:143:ARG:HG2	1:A:143:ARG:HH21	1.62	0.65
1:C:473:THR:O	1:C:477:THR:HG23	1.96	0.65
2:D:203:GLU:HA	2:D:206:ARG:HG3	1.81	0.63
2:B:180:ILE:HG12	2:B:189:VAL:HG22	1.81	0.63
1:A:543:GLY:HA2	2:B:283:LEU:O	1.99	0.62
1:C:390:LYS:HD3	1:C:415:GLU:OE2	2.00	0.62
1:A:548:VAL:O	1:A:552:VAL:HG23	1.99	0.62
1:A:69:THR:O	1:A:69:THR:HG22	1.99	0.62
2:B:303:LEU:O	2:B:307:ARG:HB2	1.99	0.62
3:E:0:DG:H22	6:E:601:1RZ:C2	2.13	0.61
1:C:23:GLN:OE1	1:C:59:PRO:HA	2.01	0.61
1:C:178:ILE:HD11	1:C:201:LYS:HG3	1.82	0.61
1:C:27:THR:O	1:C:31:ILE:HG13	2.01	0.61
3:F:3:DC:H2'	3:F:4:OMC:C6	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:THR:HG22	1:A:450:THR:O	2.01	0.60
2:B:85:GLN:O	2:B:85:GLN:HG3	2.02	0.60
1:A:63:ILE:HD12	1:A:74:LEU:HD12	1.83	0.59
1:A:65:LYS:CE	1:A:72:ARG:HH12	2.14	0.59
6:C:601:1RZ:H7	3:F:33:DG:H2'	1.84	0.59
1:A:520:GLN:O	1:A:523:GLU:HG3	2.02	0.58
3:E:3:DC:H2'	3:E:4:OMC:C6	2.38	0.58
1:A:500:GLN:CD	1:A:500:GLN:H	2.12	0.58
2:B:168:LEU:O	2:B:172:ARG:HG2	2.03	0.58
6:C:601:1RZ:C2'	3:F:33:DG:H2'	2.34	0.58
1:A:111:VAL:HG11	1:A:214:PHE:CD1	2.39	0.58
2:D:195:ILE:HG12	2:D:199:ARG:HH21	1.69	0.58
1:C:122:LYS:HA	1:C:125:ARG:HD2	1.84	0.57
1:A:520:GLN:O	1:A:524:GLN:HG3	2.04	0.57
2:D:196:GLY:O	2:D:200:THR:HG23	2.04	0.57
2:B:244:ILE:HB	2:B:310:LEU:CD1	2.34	0.57
1:C:480:GLN:HG3	1:C:517:LEU:HD11	1.87	0.57
1:C:35:VAL:HG22	1:C:132:ILE:HG21	1.85	0.57
2:B:244:ILE:O	2:B:310:LEU:HD12	2.05	0.57
2:B:206:ARG:O	2:B:210:LEU:HG	2.05	0.56
1:C:135:ILE:HG22	1:C:136:ASN:N	2.19	0.56
1:C:489:SER:OG	1:C:528:LYS:NZ	2.22	0.56
3:E:0:DG:N2	6:E:601:1RZ:O2	2.35	0.56
2:B:137:ASN:HD21	5:B:501:GOL:H11	1.70	0.56
2:B:106:VAL:HG13	2:B:234:LEU:HD12	1.88	0.55
2:D:422:LEU:O	2:D:425:LEU:HD23	2.07	0.55
1:A:194:GLU:OE2	1:A:195:ILE:HG13	2.06	0.55
2:D:356:ARG:CD	2:D:361:HIS:HB2	2.35	0.55
2:D:365:VAL:HG11	2:D:401:TRP:HB2	1.88	0.55
1:C:72:ARG:HG3	1:C:72:ARG:HH11	1.72	0.54
1:A:26:LEU:HD22	1:A:30:LYS:HD3	1.89	0.54
1:A:28:GLU:HB3	1:A:135:ILE:HG21	1.89	0.54
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.88	0.54
2:B:277:ARG:HA	2:B:277:ARG:NE	2.22	0.54
1:C:465:LYS:HD3	1:C:484:LEU:HD11	1.89	0.54
2:B:244:ILE:CD1	2:B:425:LEU:HD11	2.37	0.54
1:A:68:SER:O	1:A:69:THR:HB	2.08	0.53
1:C:206:ARG:NE	1:C:216:THR:OG1	2.31	0.53
2:D:194:GLU:HG3	2:D:197:GLN:HE21	1.72	0.53
2:B:87:PHE:CE1	2:B:155:GLY:HA2	2.44	0.53
2:D:40:GLU:OE1	2:D:40:GLU:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:419:THR:HG22	2:D:420:PRO:O	2.07	0.53
1:A:308:GLU:O	1:A:311:LYS:HG2	2.09	0.53
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.90	0.53
1:C:60:VAL:HG12	1:C:75:VAL:HG22	1.90	0.53
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.91	0.52
2:B:356:ARG:NH1	2:B:361:HIS:HB2	2.25	0.52
1:A:233:GLU:HB2	1:A:240:THR:HB	1.91	0.52
1:C:23:GLN:HE22	1:C:60:VAL:H	1.56	0.52
3:F:18:DT:OP2	3:F:18:DT:H3'	2.10	0.52
1:A:450:THR:O	1:A:450:THR:CG2	2.57	0.52
1:A:255:ASN:O	1:A:259:LYS:HG3	2.10	0.51
1:A:111:VAL:HG21	1:A:164:MET:HE1	1.91	0.51
2:B:122:LYS:H	2:B:122:LYS:HD3	1.74	0.51
2:B:308:GLU:O	2:B:311:LYS:HB2	2.10	0.51
1:A:297:GLU:OE2	1:C:331:LYS:NZ	2.41	0.51
2:D:278:GLN:OE1	2:D:281:LYS:HD3	2.11	0.51
2:B:279:LEU:HA	2:B:282:LEU:CD1	2.41	0.51
1:A:308:GLU:HA	1:A:311:LYS:HD3	1.92	0.50
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.46	0.50
1:C:135:ILE:CG2	1:C:136:ASN:N	2.73	0.50
1:C:396:GLU:CD	1:C:396:GLU:H	2.19	0.50
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.93	0.50
1:A:65:LYS:HD2	1:A:72:ARG:HH22	1.77	0.50
2:D:90:VAL:HA	2:D:94:ILE:HD12	1.93	0.50
1:C:503:LEU:HD12	1:C:533:LEU:HG	1.92	0.50
1:C:37:ILE:CD1	1:C:73:LYS:HB2	2.41	0.50
2:B:356:ARG:HD2	2:B:357:MET:N	2.26	0.50
1:C:23:GLN:NE2	1:C:60:VAL:H	2.08	0.50
1:C:308:GLU:O	1:C:311:LYS:HG2	2.12	0.50
2:D:200:THR:O	2:D:204:GLU:HG3	2.12	0.50
2:D:183:TYR:CE2	2:D:184:MET:HG3	2.47	0.50
1:A:248:GLU:HG2	1:A:307:ARG:HH22	1.77	0.49
1:A:248:GLU:HG2	1:A:307:ARG:NH2	2.27	0.49
1:A:450:THR:HG22	1:A:452:LEU:CG	2.37	0.49
1:A:38:CYS:SG	1:A:73:LYS:HE2	2.53	0.49
1:A:135:ILE:HG13	1:A:135:ILE:O	2.11	0.49
1:A:450:THR:O	1:A:451:LYS:HB2	2.11	0.49
1:A:65:LYS:HG3	1:A:72:ARG:NH1	2.28	0.49
2:B:195:ILE:HG13	2:B:196:GLY:N	2.28	0.49
1:C:520:GLN:O	1:C:524:GLN:HG3	2.12	0.49
1:A:466:VAL:CG2	1:A:551:LEU:HG	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.48	0.48
2:D:89:GLU:HG2	2:D:90:VAL:HG23	1.95	0.48
2:D:317:VAL:HG12	2:D:349:LEU:HD23	1.95	0.48
1:A:412:PRO:O	1:A:414:TRP:HD1	1.97	0.48
1:A:500:GLN:H	1:A:500:GLN:NE2	2.10	0.48
2:B:163:SER:O	2:B:167:ILE:HG13	2.14	0.48
1:C:539:HIS:O	1:C:540:LYS:HD3	2.13	0.48
3:F:1:DC:H2'	3:F:2:OMC:C6	2.49	0.48
2:B:247:PRO:O	2:B:307:ARG:NH2	2.47	0.47
1:C:73:LYS:HD3	1:C:146:TYR:OH	2.14	0.47
1:C:133:PRO:O	1:C:133:PRO:CD	2.62	0.47
1:C:483:HIS:ND1	1:C:524:GLN:OE1	2.47	0.47
1:A:195:ILE:O	1:A:199:ARG:HG3	2.13	0.47
1:C:37:ILE:HG13	1:C:38:CYS:N	2.29	0.47
2:B:106:VAL:CG1	2:B:234:LEU:HB2	2.45	0.47
2:D:90:VAL:HG21	2:D:158:ALA:HA	1.95	0.47
2:D:202:ILE:O	2:D:206:ARG:HG3	2.15	0.47
2:D:255:ASN:HB2	2:D:289:LEU:HB3	1.97	0.47
2:B:282:LEU:HD12	2:B:282:LEU:H	1.79	0.47
1:C:111:VAL:HG21	1:C:164:MET:HE1	1.96	0.47
1:C:413:GLU:HA	7:C:737:HOH:O	2.14	0.47
2:B:99:GLY:HA2	2:B:102:GLN:OE1	2.15	0.47
2:B:232:TYR:HD2	2:B:233:GLU:H	1.63	0.47
1:C:72:ARG:HG3	1:C:72:ARG:NH1	2.29	0.47
2:D:379:SER:HB3	2:D:385:LYS:O	2.15	0.47
2:B:90:VAL:O	2:B:91:GLN:CB	2.63	0.46
2:B:199:ARG:O	2:B:202:ILE:HB	2.15	0.46
1:C:38:CYS:SG	1:C:73:LYS:NZ	2.88	0.46
6:C:601:1RZ:H7	6:C:601:1RZ:H13	1.49	0.46
2:B:282:LEU:HB3	2:B:293:VAL:HG11	1.97	0.46
1:C:30:LYS:O	1:C:34:LEU:HG	2.15	0.46
5:C:602:GOL:H12	2:D:394:GLN:HG2	1.96	0.46
2:D:266:TRP:CE3	2:D:425:LEU:HD11	2.51	0.46
2:B:287:LYS:NZ	2:B:291:GLU:OE2	2.49	0.46
3:E:10:DC:H2''	3:E:11:DG:C8	2.51	0.46
1:C:27:THR:O	1:C:30:LYS:HB3	2.15	0.46
2:D:358:LYS:HD2	2:D:366:LYS:HZ2	1.80	0.46
1:C:3:SER:HB2	1:C:212:TRP:O	2.15	0.45
2:B:66:LYS:HE2	2:B:66:LYS:HB2	1.78	0.45
1:A:110:ASP:HB2	1:A:220:LYS:HB3	1.98	0.45
1:A:265:ASN:O	1:A:268:SER:OG	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:THR:C	1:A:287:LYS:HG3	2.42	0.45
1:A:406:TRP:CZ2	2:B:420:PRO:HG3	2.51	0.45
1:A:536:VAL:CG1	2:B:258:GLN:HE21	2.27	0.45
2:B:6:GLU:OE2	2:B:6:GLU:HA	2.16	0.45
2:B:34:LEU:HD22	2:B:73:LYS:HD2	1.99	0.45
2:B:356:ARG:HD2	2:B:357:MET:CA	2.47	0.45
1:A:135:ILE:O	1:A:138:GLU:HG3	2.16	0.45
1:A:139:THR:HB	1:A:140:PRO:CD	2.47	0.45
2:B:90:VAL:O	2:B:90:VAL:HG12	2.17	0.45
1:C:450:THR:HG22	1:C:452:LEU:H	1.81	0.45
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.52	0.45
1:A:393:ILE:O	1:A:414:TRP:HZ3	1.99	0.45
1:A:448:ARG:HG3	3:E:18:DT:H2''	1.99	0.45
1:A:139:THR:HB	1:A:140:PRO:HD2	2.00	0.44
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.99	0.44
1:A:450:THR:CG2	1:A:452:LEU:HG	2.37	0.44
1:C:412:PRO:O	1:C:413:GLU:C	2.61	0.44
2:D:356:ARG:HD2	2:D:361:HIS:HB3	1.98	0.44
1:A:69:THR:O	1:A:69:THR:CG2	2.63	0.44
1:C:463:ARG:NH2	1:C:488:ASP:O	2.51	0.44
2:B:266:TRP:O	2:B:269:GLN:HG3	2.17	0.44
1:C:40:GLU:O	1:C:44:GLU:HG3	2.18	0.44
1:C:237:ASP:OD1	1:C:238:LYS:HE3	2.17	0.44
1:C:389:PHE:O	1:C:414:TRP:HA	2.18	0.44
2:D:40:GLU:OE2	2:D:44:GLU:OE1	2.36	0.44
1:C:184:VAL:HG21	3:F:33:DG:H1'	2.00	0.44
3:E:23:DC:H2''	3:E:24:DG:C8	2.52	0.44
2:D:69:THR:HG22	2:D:69:THR:O	2.18	0.44
2:D:197:GLN:O	2:D:201:LYS:HG2	2.17	0.44
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.99	0.44
2:D:64:LYS:HE3	2:D:71:TRP:CE2	2.52	0.44
2:B:303:LEU:HD21	2:B:307:ARG:HH12	1.81	0.43
1:C:480:GLN:HE21	1:C:517:LEU:HD13	1.83	0.43
2:B:104:LYS:CB	2:B:192:ASP:HA	2.47	0.43
2:B:280:SER:OG	2:B:281:LYS:HD3	2.17	0.43
3:F:16:DT:O4	3:F:21:DA:O4'	2.36	0.43
2:B:199:ARG:HA	2:B:202:ILE:CD1	2.46	0.43
1:A:65:LYS:HG3	1:A:72:ARG:CZ	2.49	0.43
1:C:406:TRP:CE3	2:D:421:PRO:HD3	2.53	0.43
2:D:195:ILE:HG13	2:D:199:ARG:HE	1.83	0.43
1:A:282:LEU:HB3	1:A:293:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:VAL:HG21	1:A:551:LEU:HG	1.99	0.43
1:C:76:ASP:OD1	1:C:78:ARG:NH2	2.52	0.43
1:C:408:ALA:HB1	2:D:364:ASP:HB3	2.00	0.43
6:E:601:1RZ:H13	6:E:601:1RZ:H7	1.76	0.43
1:C:135:ILE:CG2	1:C:136:ASN:H	2.32	0.43
2:D:92:LEU:CD2	2:D:321:PRO:HB2	2.48	0.43
2:B:244:ILE:HG23	2:B:425:LEU:O	2.19	0.43
2:B:365:VAL:HG11	2:B:401:TRP:HB2	2.00	0.43
1:C:135:ILE:HB	1:C:138:GLU:HB3	2.00	0.43
2:D:183:TYR:CD2	2:D:184:MET:HG3	2.54	0.43
1:A:277:ARG:CZ	1:A:334:GLN:HB3	2.48	0.43
2:D:422:LEU:HD13	2:D:422:LEU:HA	1.84	0.43
1:A:450:THR:HG21	1:A:452:LEU:HD12	2.01	0.42
2:B:295:LEU:HD13	2:B:300:GLU:HG2	2.01	0.42
2:B:395:LYS:HE3	3:E:24:DG:OP1	2.19	0.42
2:B:106:VAL:HG13	2:B:234:LEU:HB2	2.02	0.42
1:C:278:GLN:NE2	1:C:334:GLN:OE1	2.51	0.42
2:B:358:LYS:CD	2:B:366:LYS:HD3	2.49	0.42
1:A:451:LYS:HB3	1:A:471:ASP:HA	2.01	0.42
2:B:266:TRP:HD1	2:B:425:LEU:CD2	2.27	0.42
1:C:96:HIS:CG	1:C:97:PRO:HD2	2.54	0.42
2:D:248:GLU:HG2	2:D:307:ARG:NH2	2.34	0.42
1:C:35:VAL:CG2	1:C:132:ILE:HG21	2.49	0.42
2:D:242:GLN:O	2:D:242:GLN:HG3	2.19	0.42
2:D:279:LEU:HD11	2:D:303:LEU:HD13	2.02	0.42
1:A:550:LYS:HD3	1:A:550:LYS:HA	1.92	0.42
2:B:361:HIS:O	2:B:361:HIS:CG	2.73	0.42
1:C:339:TYR:CZ	1:C:352:GLY:HA3	2.54	0.42
2:D:41:MET:HB3	2:D:47:ILE:HG12	2.01	0.42
2:B:178:ILE:HD13	2:B:191:SER:OG	2.20	0.42
2:B:244:ILE:CG2	2:B:425:LEU:CD1	2.98	0.42
1:A:28:GLU:HB3	1:A:135:ILE:CG2	2.49	0.42
2:B:277:ARG:HA	2:B:277:ARG:HE	1.82	0.42
1:C:23:GLN:HG3	1:C:24:TRP:N	2.35	0.42
2:D:202:ILE:HD13	2:D:202:ILE:HA	1.91	0.42
1:A:184:VAL:HG21	3:E:33:DG:H1'	2.01	0.41
2:B:258:GLN:HG3	2:B:283:LEU:CD1	2.51	0.41
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.55	0.41
1:C:22:LYS:HD3	1:C:22:LYS:HA	1.70	0.41
1:C:184:VAL:HG12	1:C:185:ASP:N	2.35	0.41
2:B:65:LYS:HA	2:B:407:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ASP:OD2	1:C:322:SER:HB3	2.21	0.41
2:D:319:TYR:OH	2:D:385:LYS:HE2	2.19	0.41
2:B:90:VAL:O	2:B:90:VAL:CG1	2.69	0.41
1:A:171:PHE:CD1	1:A:171:PHE:C	2.99	0.41
1:C:130:PHE:CZ	1:C:144:TYR:HB2	2.55	0.41
1:C:135:ILE:HD12	1:C:138:GLU:HG2	2.03	0.41
3:E:18:DT:H5''	3:E:19:DG:O4'	2.21	0.41
1:A:266:TRP:CE2	3:E:31:DG:H4'	2.56	0.41
2:B:298:GLU:HA	2:B:301:LEU:HD12	2.03	0.40
1:C:398:TRP:CZ3	1:C:411:ILE:CD1	3.04	0.40
2:D:17:ASP:O	2:D:83:ARG:HD3	2.21	0.40
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/557 (99%)	532 (97%)	17 (3%)	1 (0%)	43	63
1	C	550/557 (99%)	530 (96%)	18 (3%)	2 (0%)	30	49
2	B	402/444 (90%)	390 (97%)	12 (3%)	0	100	100
2	D	402/444 (90%)	391 (97%)	11 (3%)	0	100	100
All	All	1904/2002 (95%)	1843 (97%)	58 (3%)	3 (0%)	43	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	133	PRO
1	A	184	VAL
1	C	184	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	491/494 (99%)	488 (99%)	3 (1%)	78	89
1	C	491/494 (99%)	487 (99%)	4 (1%)	73	87
2	B	365/400 (91%)	364 (100%)	1 (0%)	86	94
2	D	365/400 (91%)	363 (100%)	2 (0%)	81	91
All	All	1712/1788 (96%)	1702 (99%)	10 (1%)	78	89

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

Mol	Chain	Res	Type
1	A	16	MET
1	A	72	ARG
1	A	172	ARG
2	B	425	LEU
1	C	132	ILE
1	C	134	SER
1	C	177	ASP
1	C	357	MET
2	D	154	LYS
2	D	232	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	265	ASN
1	A	330	GLN
1	A	340	GLN
1	A	475	GLN
1	A	480	GLN
1	A	483	HIS
1	A	500	GLN
2	B	85	GLN

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Mol	Chain	Res	Type
2	B	137	ASN
2	B	147	ASN
2	B	151	GLN
2	B	207	GLN
2	B	208	HIS
2	B	235	HIS
2	B	258	GLN
2	B	394	GLN
2	B	407	GLN
2	B	418	ASN
1	C	278	GLN
1	C	334	GLN
1	C	394	GLN
1	C	407	GLN
1	C	464	GLN
1	C	480	GLN
1	C	487	GLN
1	C	507	GLN
1	C	545	ASN
1	C	547	GLN
2	D	102	GLN
2	D	147	ASN
2	D	182	GLN
2	D	197	GLN
2	D	394	GLN

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
3	OMC	F	4	3	19,22,23	3.38	8 (42%)	25,31,34	0.70	0
3	OMC	E	2	3	19,22,23	3.36	8 (42%)	25,31,34	0.73	0
3	OMC	E	4	3	19,22,23	3.33	8 (42%)	25,31,34	0.71	0
3	OMC	F	2	3	19,22,23	3.35	8 (42%)	25,31,34	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	F	4	3	-	0/9/27/28	0/2/2/2
3	OMC	E	2	3	-	0/9/27/28	0/2/2/2
3	OMC	E	4	3	-	0/9/27/28	0/2/2/2
3	OMC	F	2	3	-	0/9/27/28	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	OMC	C2-N3	6.63	1.49	1.36
3	F	2	OMC	C6-C5	6.55	1.50	1.35
3	E	4	OMC	C2-N3	6.51	1.49	1.36
3	E	2	OMC	C6-C5	6.48	1.50	1.35
3	E	2	OMC	C2-N3	6.43	1.49	1.36
3	F	4	OMC	C6-C5	6.38	1.49	1.35
3	F	4	OMC	C4-N3	6.31	1.47	1.34
3	F	2	OMC	C2-N3	6.31	1.48	1.36
3	E	4	OMC	C6-C5	6.30	1.49	1.35
3	E	4	OMC	C4-N3	6.27	1.46	1.34
3	E	2	OMC	C4-N3	6.19	1.46	1.34
3	F	2	OMC	C4-N3	6.18	1.46	1.34
3	E	2	OMC	C4-N4	5.82	1.48	1.33
3	F	2	OMC	C4-N4	5.80	1.48	1.33
3	F	4	OMC	C4-N4	5.79	1.47	1.33
3	E	4	OMC	C4-N4	5.71	1.47	1.33
3	F	4	OMC	C2-N1	5.15	1.50	1.40
3	E	4	OMC	C2-N1	5.10	1.50	1.40
3	E	2	OMC	C2-N1	5.06	1.50	1.40
3	F	2	OMC	C2-N1	4.96	1.50	1.40
3	F	2	OMC	C6-N1	4.06	1.47	1.38
3	E	2	OMC	C6-N1	4.05	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	OMC	C6-N1	3.96	1.47	1.38
3	E	4	OMC	C6-N1	3.83	1.47	1.38
3	E	2	OMC	O2-C2	-2.98	1.18	1.23
3	F	2	OMC	O2-C2	-2.98	1.18	1.23
3	F	4	OMC	O2-C2	-2.96	1.18	1.23
3	E	4	OMC	O2-C2	-2.89	1.18	1.23
3	F	2	OMC	C5-C4	2.80	1.49	1.42
3	E	2	OMC	C5-C4	2.78	1.49	1.42
3	F	4	OMC	C5-C4	2.64	1.49	1.42
3	E	4	OMC	C5-C4	2.61	1.49	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4	OMC	1	0
3	E	4	OMC	1	0
3	F	2	OMC	1	0

5.5 Carbohydrates [i](#)

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GLC	G	1	4	11,11,12	0.51	0	15,15,17	1.00	1 (6%)
4	FRU	G	2	4	11,12,12	0.57	0	10,18,18	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	GLC	C1-O5-C5	3.16	116.42	112.19

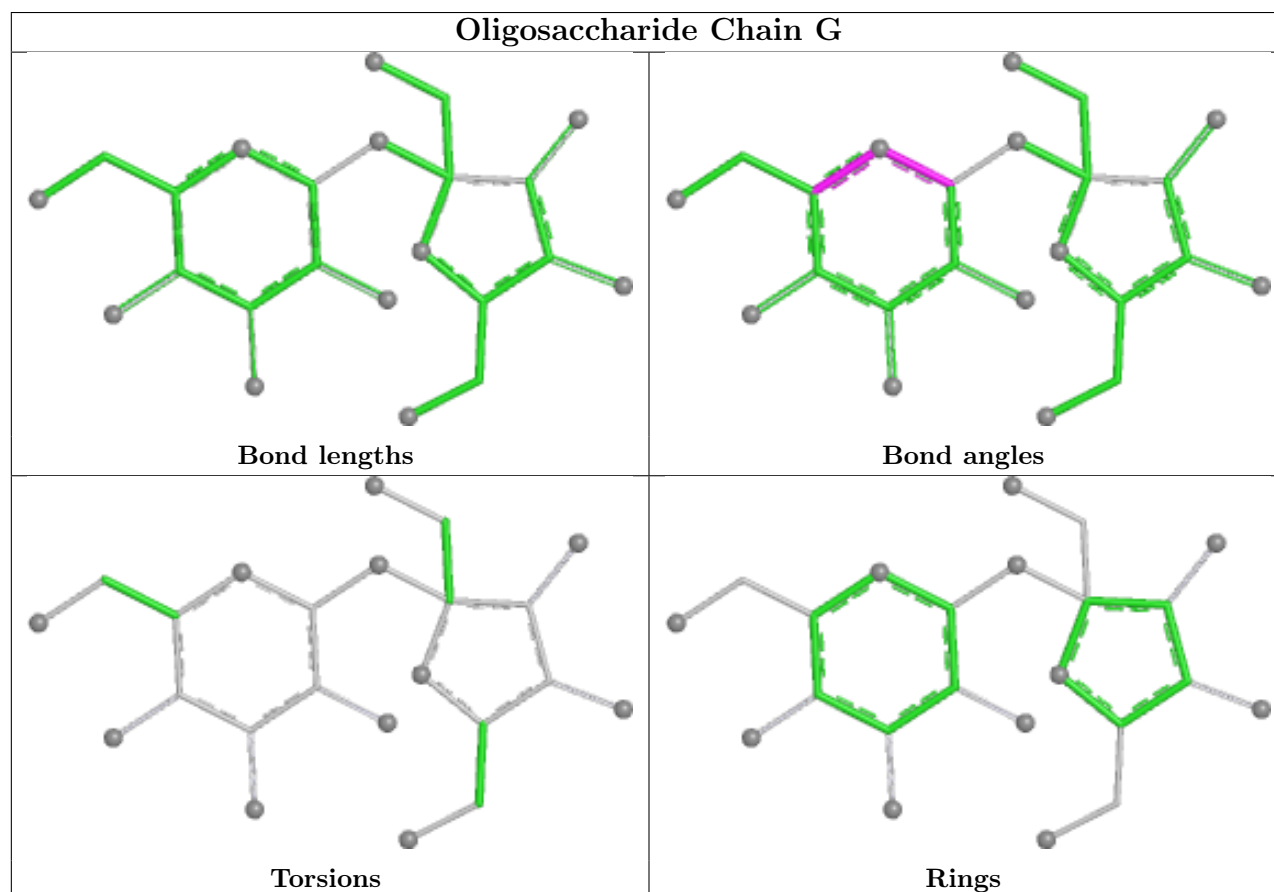
There are no chirality outliers.

There are no torsion outliers.

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

6 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	GOL	A	701	-	5,5,5	0.93	0	5,5,5	1.07	0
5	GOL	D	501	-	5,5,5	0.94	0	5,5,5	1.07	0
6	1RZ	E	601	-	13,14,28	1.14	0	18,19,43	1.37	2 (11%)
6	1RZ	C	601	-	13,14,28	1.15	0	18,19,43	1.43	2 (11%)
5	GOL	B	501	-	5,5,5	0.95	0	5,5,5	1.08	0
5	GOL	C	602	-	5,5,5	0.94	0	5,5,5	1.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	701	-	-	0/4/4/4	-
5	GOL	D	501	-	-	0/4/4/4	-
6	1RZ	E	601	-	-	3/4/11/31	0/2/2/2
6	1RZ	C	601	-	-	4/4/11/31	0/2/2/2
5	GOL	B	501	-	-	2/4/4/4	-
5	GOL	C	602	-	-	4/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	601	1RZ	C4'-O4'-C1'	3.45	115.67	106.16
6	E	601	1RZ	C4'-O4'-C1'	3.20	115.00	106.16
6	C	601	1RZ	C2'-S3'-C4'	3.12	99.19	91.46
6	E	601	1RZ	C2'-S3'-C4'	3.08	99.10	91.46

There are no chirality outliers.

All (13) torsion outliers are listed below:

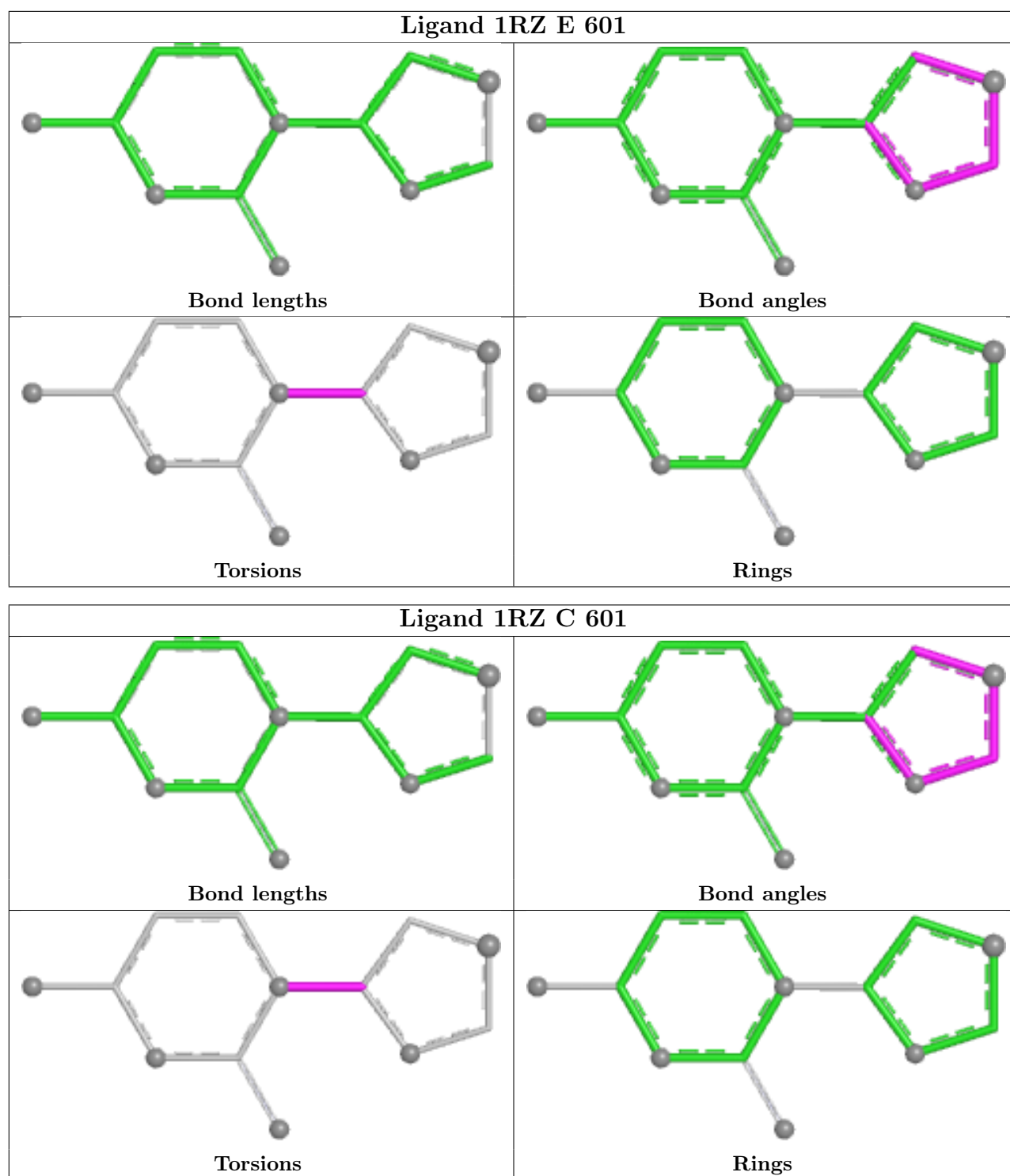
Mol	Chain	Res	Type	Atoms
5	B	501	GOL	C1-C2-C3-O3
5	C	602	GOL	O1-C1-C2-C3
5	C	602	GOL	C1-C2-C3-O3
5	B	501	GOL	O2-C2-C3-O3
5	C	602	GOL	O2-C2-C3-O3
5	C	602	GOL	O1-C1-C2-O2
6	C	601	1RZ	O4'-C1'-N1-C6
6	C	601	1RZ	C2'-C1'-N1-C6
6	C	601	1RZ	C2'-C1'-N1-C2
6	C	601	1RZ	O4'-C1'-N1-C2
6	E	601	1RZ	O4'-C1'-N1-C6
6	E	601	1RZ	O4'-C1'-N1-C2
6	E	601	1RZ	C2'-C1'-N1-C6

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	601	1RZ	3	0
6	C	601	1RZ	3	0
5	B	501	GOL	1	0
5	C	602	GOL	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 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 ⓘ

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

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	552/557 (99%)	0.22	31 (5%)	30	25	40, 67, 105, 146	0
1	C	552/557 (99%)	0.35	23 (4%)	40	36	41, 74, 117, 162	0
2	B	406/444 (91%)	0.59	44 (10%)	11	9	43, 82, 125, 137	0
2	D	406/444 (91%)	0.23	25 (6%)	26	22	39, 68, 105, 118	0
3	E	33/38 (86%)	-0.44	0	100	100	41, 66, 93, 127	0
3	F	36/38 (94%)	-0.08	0	100	100	46, 78, 130, 154	0
All	All	1985/2078 (95%)	0.32	123 (6%)	26	22	39, 71, 117, 162	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	422	LEU	6.0
2	B	360	ALA	5.8
2	D	232	TYR	5.4
2	B	88	TRP	5.4
1	C	133	PRO	5.0
1	A	24	TRP	5.0
1	A	69	THR	5.0
2	D	425	LEU	4.9
2	B	423	VAL	4.7
1	C	135	ILE	4.7
2	B	92	LEU	4.7
2	D	360	ALA	4.6
1	A	63	ILE	4.5
2	D	427	TYR	4.5
2	B	90	VAL	4.5
1	A	62	ALA	4.4
2	B	212	TRP	4.1
2	B	94	ILE	4.0
2	B	195	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	361	HIS	4.0
2	D	212	TRP	3.8
2	B	209	LEU	3.8
1	A	68	SER	3.7
1	A	25	PRO	3.7
2	B	425	LEU	3.7
1	A	552	VAL	3.6
2	B	93	GLY	3.6
1	C	71	TRP	3.5
1	A	70	LYS	3.5
1	A	135	ILE	3.4
2	B	98	ALA	3.4
1	A	61	PHE	3.3
2	D	66	LYS	3.3
1	C	452	LEU	3.3
1	A	71	TRP	3.3
1	A	26	LEU	3.2
2	D	424	LYS	3.1
2	B	427	TYR	3.1
1	A	357	MET	3.1
2	B	95	PRO	3.1
2	D	357	MET	3.1
2	D	361	HIS	3.1
2	B	232	TYR	3.0
1	A	64	LYS	3.0
1	A	65	LYS	3.0
1	A	66	LYS	2.9
1	C	63	ILE	2.9
2	D	93	GLY	2.9
2	B	362	THR	2.9
1	A	73	LYS	2.8
1	C	136	ASN	2.8
2	B	295	LEU	2.8
2	B	99	GLY	2.7
2	B	290	THR	2.7
1	C	126	LYS	2.7
1	C	62	ALA	2.7
2	D	213	GLY	2.6
2	D	362	THR	2.6
1	A	32	LYS	2.6
1	A	27	THR	2.6
2	B	237	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	357	MET	2.5
2	D	359	GLY	2.5
2	D	420	PRO	2.5
1	C	64	LYS	2.5
1	C	69	THR	2.5
2	B	247	PRO	2.5
2	B	358	LYS	2.5
2	B	421	PRO	2.5
1	A	67	ASP	2.5
2	B	246	LEU	2.5
2	B	5	ILE	2.4
1	C	33	ALA	2.4
2	B	359	GLY	2.4
1	A	74	LEU	2.4
2	B	282	LEU	2.4
2	D	356	ARG	2.4
2	B	173	LYS	2.4
1	A	31	ILE	2.3
1	C	2	ILE	2.3
1	C	67	ASP	2.3
1	A	30	LYS	2.3
1	A	140	PRO	2.3
2	D	88	TRP	2.3
1	C	178	ILE	2.3
2	D	289	LEU	2.3
2	D	358	LYS	2.3
1	A	136	ASN	2.3
1	C	22	LYS	2.3
2	B	165	THR	2.3
1	C	134	SER	2.3
2	B	266	TRP	2.3
2	D	426	TRP	2.3
2	B	420	PRO	2.3
2	B	283	LEU	2.2
1	A	203	GLU	2.2
1	C	219	LYS	2.2
2	D	318	TYR	2.2
2	B	301	LEU	2.2
2	B	164	MET	2.2
1	A	139	THR	2.2
2	D	69	THR	2.2
2	B	211	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	66	LYS	2.1
2	D	90	VAL	2.1
2	B	210	LEU	2.1
2	B	202	ILE	2.1
1	C	138	GLU	2.1
1	A	2	ILE	2.1
1	C	132	ILE	2.1
1	C	30	LYS	2.1
1	A	553	SER	2.1
1	C	140	PRO	2.1
2	B	161	GLN	2.1
1	A	450	THR	2.1
2	D	314	VAL	2.0
2	D	423	VAL	2.0
1	C	551	LEU	2.0
2	B	240	THR	2.0
2	D	16	MET	2.0
2	B	292	VAL	2.0
1	A	195	ILE	2.0
2	B	280	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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.

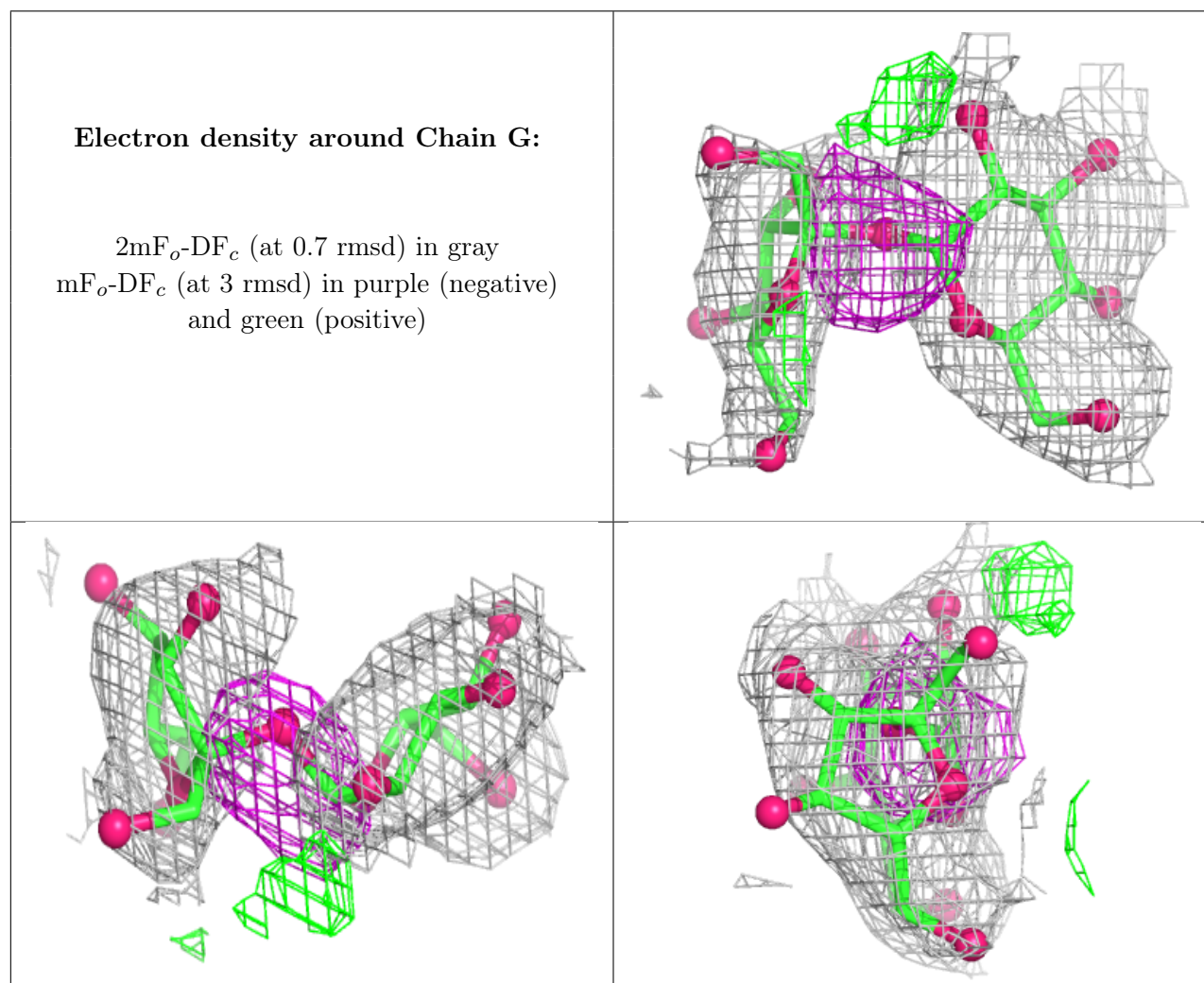
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OMC	F	2	21/22	0.95	0.10	59,67,75,83	0
3	OMC	E	2	21/22	0.96	0.09	45,53,59,68	0
3	OMC	F	4	21/22	0.96	0.10	44,60,70,76	0
3	OMC	E	4	21/22	0.97	0.07	33,49,55,64	0

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
4	FRU	G	2	12/12	0.79	0.16	88,103,105,110	0
4	GLC	G	1	11/12	0.93	0.10	52,77,82,88	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 ⓘ

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
6	1RZ	C	601	13/27	0.84	0.19	99,106,125,125	0
6	1RZ	E	601	13/27	0.85	0.19	108,111,113,113	0

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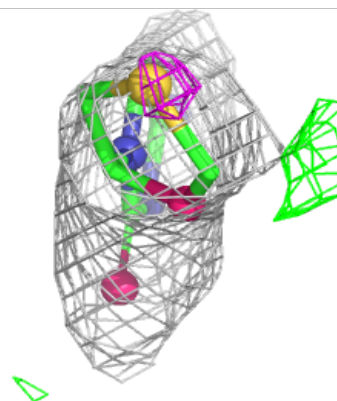
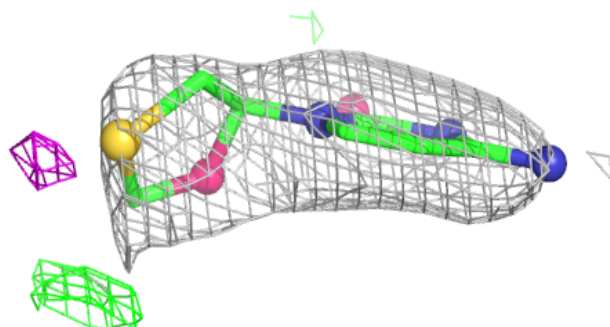
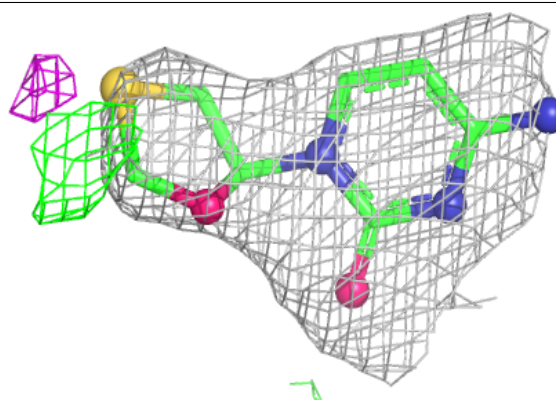
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	701	6/6	0.90	0.19	62,69,72,79	0
5	GOL	C	602	6/6	0.93	0.17	55,57,61,63	0
5	GOL	B	501	6/6	0.95	0.10	53,60,65,70	0
5	GOL	D	501	6/6	0.97	0.08	49,59,63,66	0

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.

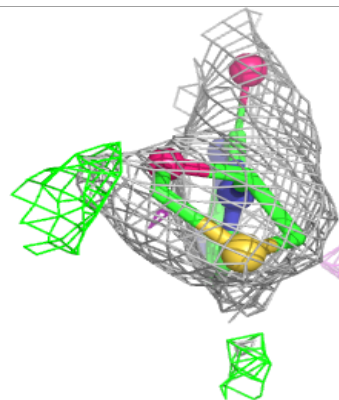
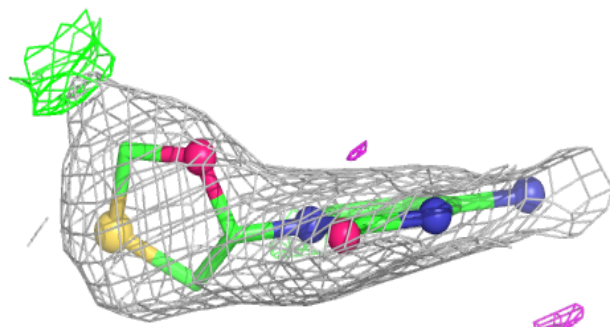
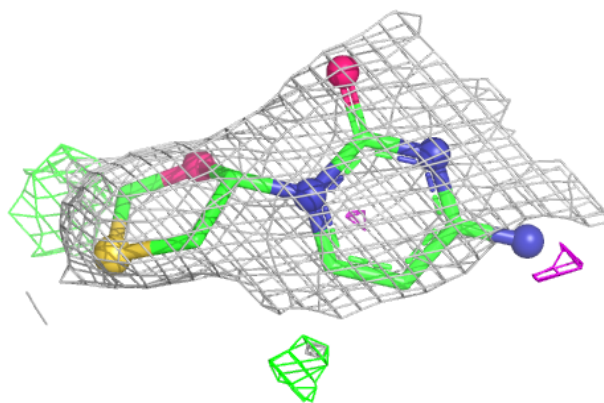
Electron density around 1RZ C 601:

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



Electron density around 1RZ E 601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.