



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:56 AM UTC

PDB ID : 5XN0 / pdb_00005xn0
Title : HIV-1 reverse transcriptase Q151M:DNA binary complex
Authors : Yasutake, Y.; Tamura, N.; Hayashi, H.; Maeda, K.
Deposited on : 2017-05-17
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

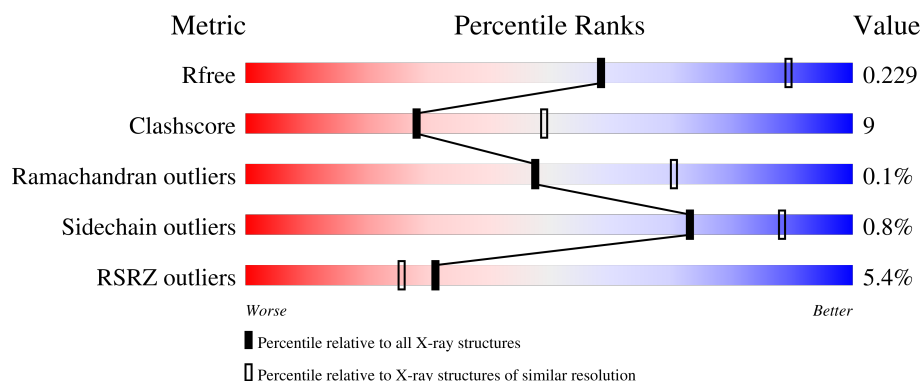
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	557	% 85% 14% .
1	C	557	7% 73% 24% ..
2	B	444	8% 74% 16% • 8%
2	D	444	7% 74% 16% • 8%
3	E	38	% 74% 13% 5% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	38	 66% 26% 8%
4	G	2	 50% 50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17318 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 Pol protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4483	2900	748	827	8			
1	C	551	Total	C	N	O	S	0	0	0
			4483	2900	748	827	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP D3XFN7
A	0	VAL	-	expression tag	UNP D3XFN7
A	151	MET	GLN	engineered mutation	UNP D3XFN7
A	162	SER	CYS	engineered mutation	UNP D3XFN7
A	280	SER	CYS	engineered mutation	UNP D3XFN7
C	-1	MET	-	expression tag	UNP D3XFN7
C	0	VAL	-	expression tag	UNP D3XFN7
C	151	MET	GLN	engineered mutation	UNP D3XFN7
C	162	SER	CYS	engineered mutation	UNP D3XFN7
C	280	SER	CYS	engineered mutation	UNP D3XFN7

- Molecule 2 is a protein called Pol protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	407	Total	C	N	O	S	0	0	0
			3354	2183	558	607	6			
2	D	407	Total	C	N	O	S	0	0	0
			3354	2183	558	607	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	expression tag	UNP D3XFN7
B	-14	ALA	-	expression tag	UNP D3XFN7

Continued on next page...

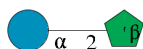
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP D3XFN7
B	-12	HIS	-	expression tag	UNP D3XFN7
B	-11	HIS	-	expression tag	UNP D3XFN7
B	-10	HIS	-	expression tag	UNP D3XFN7
B	-9	HIS	-	expression tag	UNP D3XFN7
B	-8	HIS	-	expression tag	UNP D3XFN7
B	-7	ALA	-	expression tag	UNP D3XFN7
B	-6	LEU	-	expression tag	UNP D3XFN7
B	-5	GLU	-	expression tag	UNP D3XFN7
B	-4	VAL	-	expression tag	UNP D3XFN7
B	-3	LEU	-	expression tag	UNP D3XFN7
B	-2	PHE	-	expression tag	UNP D3XFN7
B	-1	GLN	-	expression tag	UNP D3XFN7
B	0	GLY	-	expression tag	UNP D3XFN7
B	162	SER	CYS	engineered mutation	UNP D3XFN7
B	280	SER	CYS	engineered mutation	UNP D3XFN7
D	-15	MET	-	expression tag	UNP D3XFN7
D	-14	ALA	-	expression tag	UNP D3XFN7
D	-13	HIS	-	expression tag	UNP D3XFN7
D	-12	HIS	-	expression tag	UNP D3XFN7
D	-11	HIS	-	expression tag	UNP D3XFN7
D	-10	HIS	-	expression tag	UNP D3XFN7
D	-9	HIS	-	expression tag	UNP D3XFN7
D	-8	HIS	-	expression tag	UNP D3XFN7
D	-7	ALA	-	expression tag	UNP D3XFN7
D	-6	LEU	-	expression tag	UNP D3XFN7
D	-5	GLU	-	expression tag	UNP D3XFN7
D	-4	VAL	-	expression tag	UNP D3XFN7
D	-3	LEU	-	expression tag	UNP D3XFN7
D	-2	PHE	-	expression tag	UNP D3XFN7
D	-1	GLN	-	expression tag	UNP D3XFN7
D	0	GLY	-	expression tag	UNP D3XFN7
D	162	SER	CYS	engineered mutation	UNP D3XFN7
D	280	SER	CYS	engineered mutation	UNP D3XFN7

- Molecule 3 is DNA/RNA hybrid called 38-MER DNA aptamer.

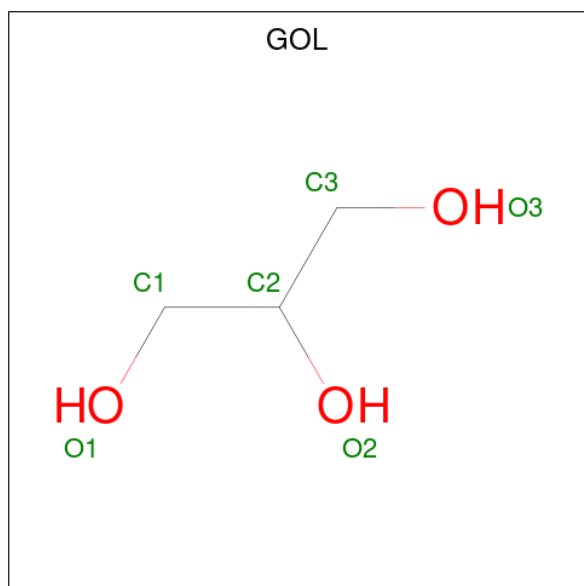
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	35	Total	C	N	O	P	0	0	0
			718	339	128	216	35			
3	F	38	Total	C	N	O	P	0	0	0
			777	369	140	231	37			

- 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	E	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

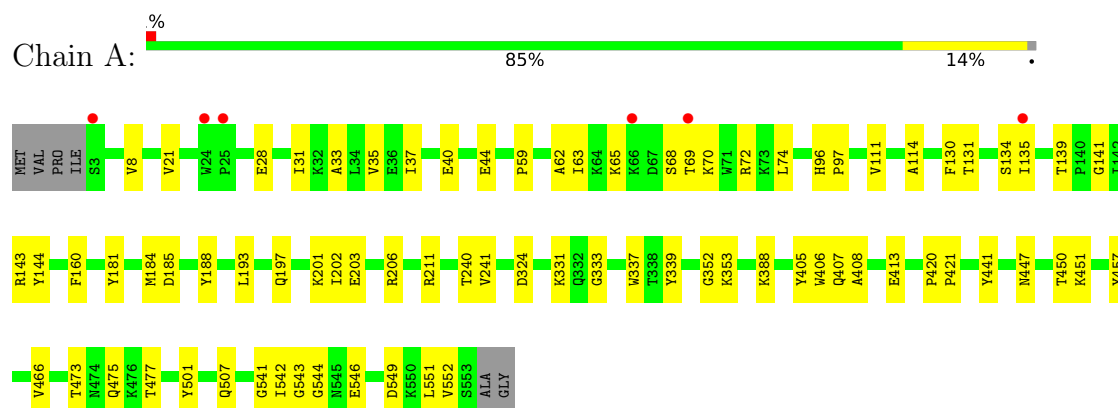
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	33	Total 33	O 33	0	0
6	B	13	Total 13	O 13	0	0
6	E	18	Total 18	O 18	0	0
6	C	19	Total 19	O 19	0	0
6	D	7	Total 7	O 7	0	0
6	F	6	Total 6	O 6	0	0

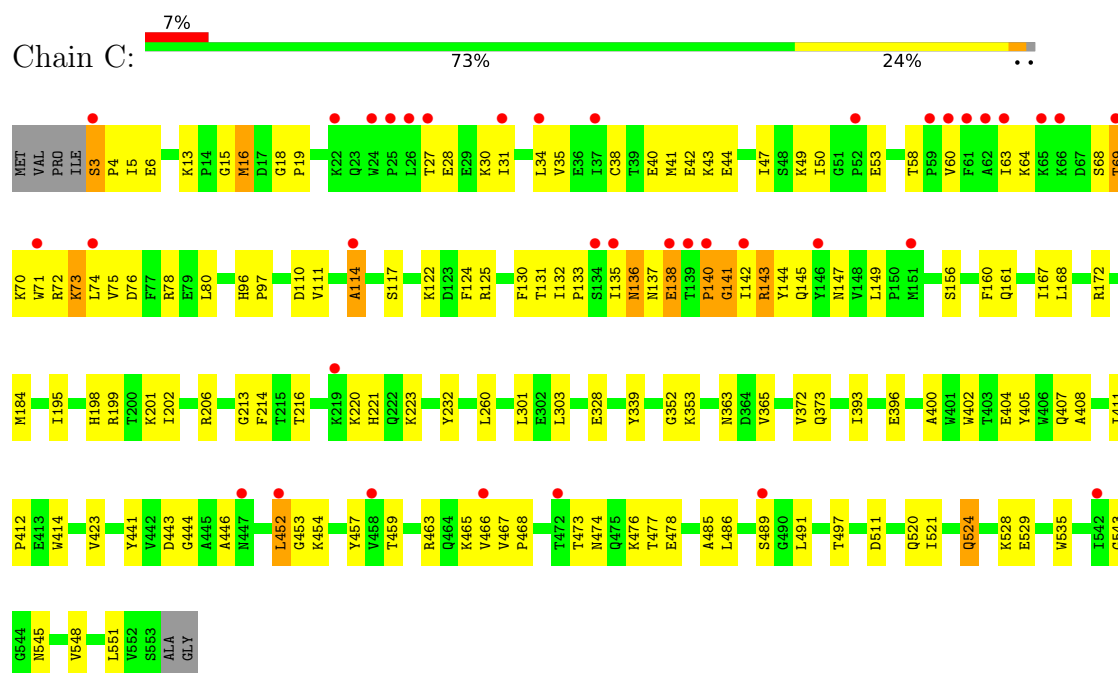
3 Residue-property plots

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.

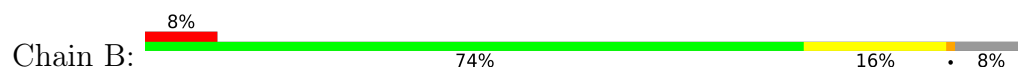
• Molecule 1: Pol protein

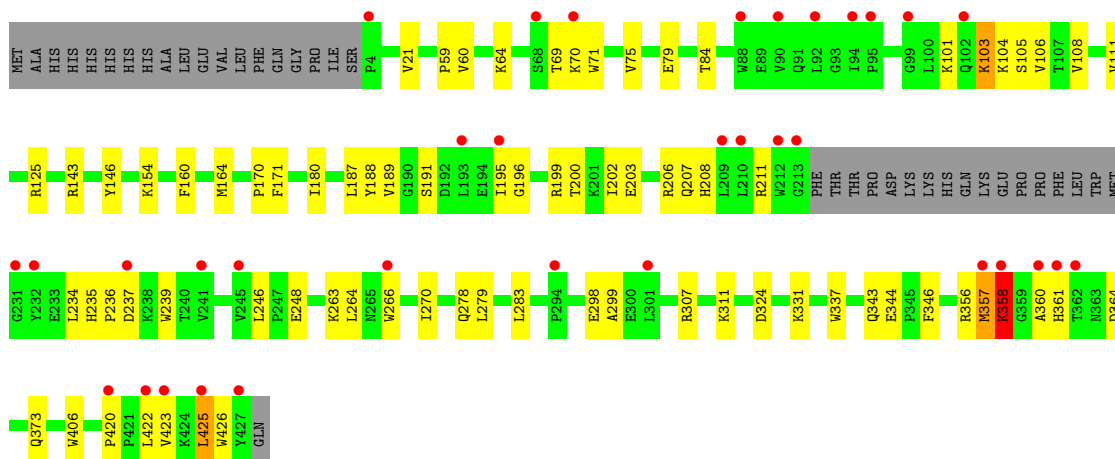


• Molecule 1: Pol protein

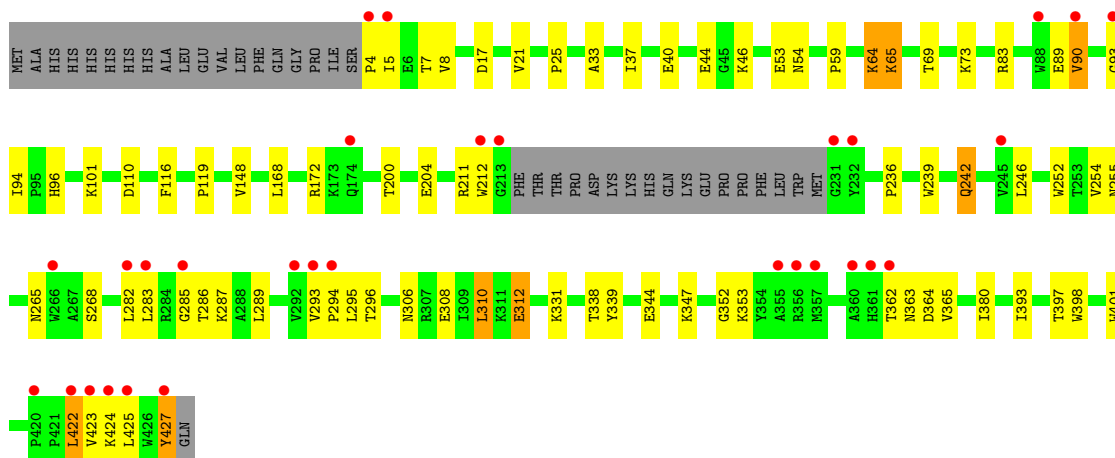
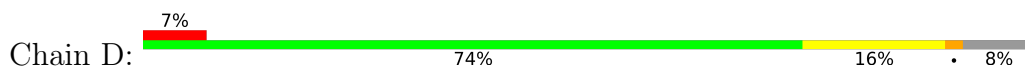


• Molecule 2: Pol protein





• Molecule 2: Pol protein



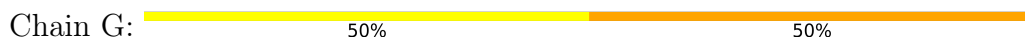
• Molecule 3: 38-MER DNA aptamer



• Molecule 3: 38-MER DNA aptamer



• 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	284.09Å 284.09Å 95.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.60 – 2.60 48.60 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.60-2.60) 99.9 (48.60-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.185 , 0.226 0.187 , 0.229	Depositor DCC
R_{free} test set	4479 reflections (3.96%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17318	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: GLC, FRU, OMC, GOL

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	0.52	0/4600	0.66	5/6246 (0.1%)
1	C	0.52	1/4600 (0.0%)	0.74	12/6246 (0.2%)
2	B	0.47	0/3449	0.67	7/4684 (0.1%)
2	D	0.51	0/3449	0.71	11/4684 (0.2%)
3	E	0.43	0/756	0.59	0/1165
3	F	0.36	0/823	0.61	1/1269 (0.1%)
All	All	0.50	1/17677 (0.0%)	0.69	36/24294 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3	SER	C-N	6.43	1.38	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	141	GLY	N-CA-C	11.01	131.71	115.64
2	D	362	THR	N-CA-C	9.84	123.24	111.33
1	C	138	GLU	N-CA-C	-7.81	102.77	111.28
3	F	-1	DT	C2'-C3'-O3'	-7.58	100.14	111.50
1	C	136	ASN	N-CA-C	7.03	121.09	111.39
2	D	363	ASN	N-CA-C	7.00	120.18	108.20
1	C	111	VAL	N-CA-C	-6.57	101.07	109.80
2	B	311	LYS	N-CA-C	6.45	118.31	111.28
1	A	542	ILE	N-CA-C	6.25	116.82	107.51
2	B	103	LYS	N-CA-C	6.04	119.08	109.24
2	D	242	GLN	CA-C-N	-5.86	114.72	120.52
2	D	242	GLN	C-N-CA	-5.86	114.72	120.52
2	D	90	VAL	N-CA-C	5.73	115.92	110.53
2	D	312	GLU	CA-C-N	-5.66	114.76	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	312	GLU	C-N-CA	-5.66	114.76	120.31
1	A	542	ILE	CB-CA-C	-5.64	103.41	111.31
2	D	8	VAL	CA-C-N	-5.64	114.16	120.14
2	D	8	VAL	C-N-CA	-5.64	114.16	120.14
1	A	131	THR	N-CA-C	5.63	118.28	108.76
2	D	422	LEU	N-CA-C	-5.63	105.29	111.82
1	C	58	THR	CA-C-N	-5.59	114.20	119.85
1	C	58	THR	C-N-CA	-5.59	114.20	119.85
1	A	8	VAL	CA-C-N	-5.53	114.23	119.76
1	A	8	VAL	C-N-CA	-5.53	114.23	119.76
2	B	358	LYS	N-CA-C	5.42	117.18	111.28
1	C	3	SER	CA-C-N	-5.40	114.79	120.94
1	C	3	SER	C-N-CA	-5.40	114.79	120.94
1	C	140	PRO	CA-N-CD	-5.36	104.50	112.00
2	D	64	LYS	N-CA-C	-5.30	99.88	108.52
1	C	114	ALA	N-CA-C	5.27	116.70	111.07
2	B	425	LEU	N-CA-C	5.23	116.98	111.28
2	B	344	GLU	CA-C-N	-5.15	114.45	119.76
2	B	344	GLU	C-N-CA	-5.15	114.45	119.76
1	C	69	THR	N-CA-C	-5.09	105.17	111.90
2	B	426	TRP	N-CA-C	5.02	119.41	113.28
1	C	143	ARG	N-CA-C	5.02	117.30	109.52

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	4483	0	4532	51	0
1	C	4483	0	4532	133	0
2	B	3354	0	3387	56	0
2	D	3354	0	3387	59	0
3	E	718	0	397	5	0
3	F	777	0	432	10	0
4	G	23	0	21	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	1	0
5	E	6	0	8	0	0
6	A	33	0	0	1	0
6	B	13	0	0	0	0
6	C	19	0	0	0	0
6	D	7	0	0	0	0
6	E	18	0	0	0	0
6	F	6	0	0	0	0
All	All	17318	0	16728	303	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 9.

All (303) 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:C:132:ILE:HG23	1:C:133:PRO:HD2	1.36	1.07
1:C:31:ILE:HG12	1:C:133:PRO:HG2	1.07	1.05
1:C:132:ILE:CG2	1:C:133:PRO:HD2	2.01	0.90
1:C:31:ILE:CG1	1:C:133:PRO:HG2	2.01	0.88
1:C:114:ALA:HB1	1:C:160:PHE:CE1	2.14	0.82
2:B:358:LYS:HG3	2:B:360:ALA:H	1.47	0.79
2:B:195:ILE:O	2:B:199:ARG:HG3	1.82	0.78
1:A:68:SER:O	1:A:69:THR:HB	1.84	0.77
1:A:143:ARG:HG2	1:A:143:ARG:HH21	1.50	0.76
1:C:43:LYS:HD3	1:C:43:LYS:C	2.13	0.74
1:C:31:ILE:HG12	1:C:133:PRO:CG	2.02	0.73
2:B:207:GLN:O	2:B:211:ARG:HG2	1.89	0.73
2:B:195:ILE:HG13	2:B:196:GLY:N	2.05	0.72
1:C:5:ILE:HD11	1:C:167:ILE:HD11	1.72	0.72
1:C:452:LEU:C	1:C:452:LEU:HD13	2.16	0.71
1:A:33:ALA:O	1:A:37:ILE:HG13	1.92	0.70
1:C:132:ILE:CG2	1:C:133:PRO:CD	2.70	0.69
1:C:132:ILE:HG23	1:C:133:PRO:CD	2.18	0.69
1:A:139:THR:HG22	1:A:141:GLY:H	1.58	0.68
2:B:356:ARG:HD3	2:B:358:LYS:HG2	1.75	0.68
2:B:263:LYS:HG3	2:B:425:LEU:HD23	1.75	0.68
2:D:353:LYS:NZ	2:D:427:TYR:CD1	2.61	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLU:HB3	1:A:135:ILE:HG12	1.75	0.67
1:A:68:SER:OG	1:A:70:LYS:HB2	1.95	0.67
2:B:356:ARG:C	2:B:356:ARG:HD2	2.20	0.67
1:C:463:ARG:HH11	1:C:463:ARG:HB2	1.60	0.67
2:D:89:GLU:HG2	2:D:90:VAL:N	2.08	0.67
1:C:136:ASN:O	1:C:137:ASN:HB2	1.94	0.66
2:D:252:TRP:CD1	2:D:295:LEU:HD23	2.31	0.66
1:C:521:ILE:HA	1:C:524:GLN:HG3	1.77	0.66
1:C:27:THR:CG2	1:C:30:LYS:HD2	2.26	0.65
1:C:457:TYR:CE2	1:C:465:LYS:HB3	2.31	0.65
1:C:42:GLU:OE2	1:C:49:LYS:HE3	1.96	0.65
2:B:195:ILE:HG13	2:B:196:GLY:H	1.62	0.65
2:D:353:LYS:NZ	2:D:427:TYR:CE1	2.63	0.64
1:C:27:THR:HG22	1:C:30:LYS:HD2	1.80	0.64
2:B:324:ASP:O	2:B:343:GLN:HG2	1.98	0.64
1:C:135:ILE:O	1:C:138:GLU:HB2	1.98	0.64
1:C:49:LYS:HG2	1:C:144:TYR:CE1	2.33	0.63
1:C:396:GLU:CD	1:C:396:GLU:H	2.06	0.63
1:C:38:CYS:HB3	1:C:144:TYR:CE2	2.33	0.63
1:C:195:ILE:O	1:C:199:ARG:HG3	1.99	0.63
1:C:76:ASP:OD1	1:C:78:ARG:NH1	2.32	0.62
2:B:108:VAL:HG22	2:B:188:TYR:CE2	2.33	0.62
2:D:422:LEU:O	2:D:425:LEU:HG	1.99	0.62
2:D:89:GLU:O	2:D:93:GLY:HA3	2.00	0.62
1:C:466:VAL:HG12	1:C:467:VAL:N	2.14	0.61
1:C:467:VAL:HG13	1:C:468:PRO:HD2	1.82	0.61
2:D:353:LYS:HZ2	2:D:427:TYR:HE1	1.42	0.61
1:C:3:SER:OG	1:C:213:GLY:HA3	2.00	0.61
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.35	0.61
1:C:452:LEU:HD13	1:C:453:GLY:N	2.16	0.60
3:F:3:DC:H2'	3:F:4:OMC:C6	2.36	0.60
2:B:248:GLU:HB3	2:B:307:ARG:NH2	2.17	0.59
1:A:65:LYS:HE2	1:A:72:ARG:HD2	1.84	0.59
1:C:131:THR:HG23	1:C:142:ILE:O	2.03	0.59
1:A:40:GLU:O	1:A:44:GLU:HG3	2.03	0.59
2:B:199:ARG:O	2:B:202:ILE:HB	2.01	0.59
2:D:25:PRO:HA	5:D:501:GOL:H31	1.85	0.59
1:C:5:ILE:HG22	1:C:6:GLU:O	2.02	0.58
2:B:200:THR:HA	2:B:203:GLU:HG3	1.86	0.58
1:C:3:SER:HB3	1:C:4:PRO:CD	2.34	0.57
2:D:255:ASN:HB2	2:D:289:LEU:HB3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:LYS:HB2	2:B:423:VAL:HG11	1.86	0.57
1:C:68:SER:O	1:C:69:THR:C	2.47	0.57
1:C:122:LYS:HA	1:C:125:ARG:HG3	1.86	0.57
2:D:393:ILE:HD13	2:D:398:TRP:HB2	1.87	0.57
1:C:372:VAL:HG11	1:C:411:ILE:HG23	1.86	0.57
1:C:28:GLU:HA	1:C:31:ILE:HD12	1.87	0.56
1:C:63:ILE:CG2	1:C:64:LYS:N	2.68	0.56
2:B:208:HIS:HD1	2:B:208:HIS:C	2.13	0.56
2:B:180:ILE:HG12	2:B:189:VAL:HG22	1.88	0.56
2:D:40:GLU:O	2:D:44:GLU:HG3	2.04	0.56
1:C:63:ILE:HG22	1:C:64:LYS:N	2.20	0.56
1:C:149:LEU:HB3	1:C:156:SER:HB2	1.88	0.56
1:C:486:LEU:O	1:C:528:LYS:NZ	2.36	0.56
1:C:64:LYS:HA	1:C:70:LYS:O	2.06	0.55
2:B:202:ILE:O	2:B:206:ARG:HG3	2.06	0.55
1:C:117:SER:HB2	1:C:214:PHE:CE1	2.41	0.55
1:A:143:ARG:HG2	1:A:143:ARG:NH2	2.19	0.55
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.41	0.55
3:F:17:DT:H5''	3:F:17:DT:H6	1.72	0.55
1:A:68:SER:O	1:A:69:THR:CB	2.51	0.55
1:C:400:ALA:O	1:C:404:GLU:HG3	2.07	0.55
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.89	0.55
1:C:467:VAL:HG12	1:C:468:PRO:N	2.22	0.54
1:C:117:SER:HB2	1:C:214:PHE:HE1	1.73	0.54
1:C:457:TYR:CZ	1:C:465:LYS:HB3	2.43	0.54
1:A:541:GLY:HA2	1:A:546:GLU:HG3	1.90	0.54
1:C:452:LEU:C	1:C:452:LEU:CD1	2.80	0.53
2:D:53:GLU:HG2	2:D:54:ASN:N	2.23	0.53
1:C:68:SER:HB2	1:C:70:LYS:HB2	1.91	0.53
1:C:114:ALA:HB1	1:C:160:PHE:CZ	2.43	0.53
3:E:3:DC:H2'	3:E:4:OMC:C6	2.43	0.53
1:C:41:MET:HB2	1:C:47:ILE:HD11	1.90	0.53
3:F:1:DG:H2'	3:F:2:OMC:C6	2.43	0.53
2:B:356:ARG:HD2	2:B:357:MET:N	2.23	0.53
2:B:170:PRO:HG2	2:B:171:PHE:H	1.73	0.53
2:D:17:ASP:O	2:D:83:ARG:HD3	2.09	0.53
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.90	0.52
1:A:211:ARG:HD2	1:A:211:ARG:O	2.09	0.52
1:C:543:GLY:HA2	2:D:285:GLY:O	2.09	0.52
2:D:282:LEU:HD21	2:D:296:THR:HG23	1.91	0.52
1:A:543:GLY:HA2	2:B:283:LEU:O	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:551:LEU:HD12	1:C:551:LEU:H	1.73	0.52
2:D:353:LYS:NZ	2:D:427:TYR:HD1	2.05	0.52
1:C:466:VAL:CG1	1:C:467:VAL:N	2.73	0.51
1:A:457:TYR:CD1	1:A:457:TYR:C	2.88	0.51
1:C:31:ILE:O	1:C:35:VAL:HG23	2.10	0.51
2:D:212:TRP:N	2:D:212:TRP:CD1	2.77	0.51
1:C:5:ILE:HG22	1:C:6:GLU:N	2.25	0.51
1:C:198:HIS:O	1:C:202:ILE:HG12	2.11	0.50
2:D:116:PHE:HA	2:D:148:VAL:HG21	1.94	0.50
2:D:242:GLN:HG2	2:D:353:LYS:HE2	1.94	0.50
2:D:211:ARG:HB2	2:D:212:TRP:HD1	1.75	0.50
2:B:103:LYS:O	2:B:104:LYS:C	2.54	0.50
2:B:143:ARG:HG2	2:B:143:ARG:HH11	1.76	0.49
2:B:356:ARG:C	2:B:356:ARG:CD	2.85	0.49
1:A:450:THR:O	1:A:451:LYS:HB2	2.12	0.49
2:B:105:SER:HA	2:B:234:LEU:O	2.11	0.49
1:C:5:ILE:CG2	1:C:6:GLU:N	2.75	0.49
1:A:413:GLU:HA	6:A:720:HOH:O	2.11	0.49
1:C:96:HIS:CG	1:C:97:PRO:HD2	2.47	0.49
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.47	0.49
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.48	0.49
2:D:46:LYS:HE2	2:D:116:PHE:HB3	1.94	0.49
2:B:361:HIS:O	2:B:361:HIS:CG	2.66	0.48
1:A:441:TYR:CG	1:A:544:GLY:HA3	2.49	0.48
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.48	0.48
1:C:467:VAL:CG1	1:C:468:PRO:HD2	2.43	0.48
2:D:33:ALA:O	2:D:37:ILE:HG13	2.12	0.48
2:D:365:VAL:HG11	2:D:401:TRP:HB2	1.95	0.48
1:C:63:ILE:O	1:C:72:ARG:N	2.44	0.48
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.95	0.48
1:C:110:ASP:HB2	1:C:220:LYS:HB3	1.96	0.48
1:C:221:HIS:CE1	1:C:223:LYS:HG2	2.49	0.48
1:C:13:LYS:O	1:C:16:MET:HG3	2.14	0.47
1:C:260:LEU:HD21	1:C:303:LEU:HD13	1.94	0.47
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.49	0.47
1:C:405:TYR:CE2	1:C:407:GLN:HB2	2.49	0.47
1:C:131:THR:HG22	1:C:132:ILE:O	2.14	0.47
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.13	0.47
2:D:4:PRO:C	2:D:5:ILE:HG13	2.38	0.47
2:B:208:HIS:C	2:B:208:HIS:ND1	2.73	0.47
2:B:266:TRP:C	2:B:266:TRP:CD1	2.92	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:GLN:HG2	2:B:299:ALA:N	2.30	0.47
1:C:161:GLN:HG3	1:C:184:MET:HE3	1.97	0.47
2:D:96:HIS:HE1	2:D:380:ILE:O	1.97	0.47
1:A:420:PRO:HA	1:A:421:PRO:C	2.40	0.47
1:C:34:LEU:HD12	1:C:34:LEU:HA	1.74	0.47
1:A:201:LYS:HA	1:A:201:LYS:HD3	1.58	0.46
1:A:193:LEU:HD13	1:A:197:GLN:HG3	1.96	0.46
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.97	0.46
3:F:27:DG:H2'	3:F:28:DG:C8	2.50	0.46
2:D:65:LYS:NZ	2:D:110:ASP:OD1	2.47	0.46
1:C:328:GLU:O	1:C:339:TYR:HA	2.16	0.46
1:C:441:TYR:O	1:C:457:TYR:HA	2.15	0.46
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.51	0.46
1:C:141:GLY:O	1:C:143:ARG:HG3	2.15	0.46
1:C:520:GLN:O	1:C:524:GLN:HG3	2.15	0.46
2:B:70:LYS:HG3	2:B:71:TRP:N	2.31	0.46
1:C:206:ARG:HE	1:C:216:THR:HG1	1.64	0.46
1:C:40:GLU:O	1:C:44:GLU:HG3	2.15	0.46
1:C:41:MET:HB3	1:C:47:ILE:HG12	1.98	0.46
2:D:254:VAL:HG21	2:D:287:LYS:HD2	1.98	0.46
2:B:111:VAL:HG12	2:B:111:VAL:O	2.16	0.46
1:C:63:ILE:O	1:C:71:TRP:HA	2.15	0.46
1:A:203:GLU:HG3	1:A:206:ARG:HD3	1.98	0.46
1:A:111:VAL:HG22	1:A:185:ASP:HB2	1.99	0.45
1:A:473:THR:O	1:A:477:THR:HG23	2.17	0.45
2:B:279:LEU:HD23	2:B:299:ALA:HB1	1.98	0.45
1:C:454:LYS:HA	1:C:467:VAL:O	2.16	0.45
2:D:254:VAL:HG21	2:D:287:LYS:CD	2.46	0.45
2:B:237:ASP:OD1	2:B:237:ASP:N	2.50	0.45
1:C:443:ASP:OD1	1:C:444:GLY:N	2.50	0.45
2:D:90:VAL:HG23	2:D:94:ILE:HD12	1.98	0.45
1:A:406:TRP:CZ2	2:B:420:PRO:HG3	2.51	0.45
1:C:520:GLN:O	1:C:524:GLN:CG	2.65	0.45
1:C:339:TYR:CZ	1:C:352:GLY:HA3	2.52	0.45
1:C:373:GLN:NE2	2:D:397:THR:HA	2.31	0.45
2:D:254:VAL:HG13	2:D:283:LEU:CD2	2.47	0.45
1:C:485:ALA:O	1:C:489:SER:OG	2.31	0.45
2:D:236:PRO:HA	2:D:239:TRP:CD2	2.51	0.45
1:C:402:TRP:HE1	2:D:364:ASP:CG	2.24	0.45
2:D:308:GLU:O	2:D:312:GLU:HG3	2.17	0.45
1:A:184:MET:HG3	3:E:33:DC:H1'	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:LYS:NZ	3:F:7:DC:OP1	2.43	0.45
1:C:473:THR:OG1	1:C:476:LYS:HG3	2.17	0.45
1:C:73:LYS:CE	1:C:75:VAL:HG23	2.48	0.44
1:C:491:LEU:HB3	1:C:529:GLU:HB2	1.99	0.44
1:C:31:ILE:HD13	1:C:133:PRO:O	2.18	0.44
2:D:211:ARG:CB	2:D:212:TRP:HD1	2.30	0.44
2:D:331:LYS:NZ	2:D:364:ASP:OD2	2.45	0.44
2:D:353:LYS:NZ	2:D:427:TYR:HE1	2.09	0.44
1:A:31:ILE:O	1:A:35:VAL:HG23	2.17	0.44
2:B:106:VAL:HA	2:B:189:VAL:O	2.17	0.44
1:C:38:CYS:O	1:C:47:ILE:HD11	2.16	0.44
1:C:132:ILE:HG22	1:C:133:PRO:N	2.31	0.44
2:D:7:THR:HG22	2:D:119:PRO:HG2	1.99	0.44
1:A:466:VAL:CG2	1:A:551:LEU:HG	2.47	0.44
2:D:423:VAL:HG12	2:D:423:VAL:O	2.16	0.44
2:B:111:VAL:HG21	2:B:187:LEU:HB2	2.00	0.44
1:A:406:TRP:HZ3	1:A:507:GLN:HB3	1.83	0.44
1:C:160:PHE:CD2	1:C:184:MET:HE2	2.52	0.44
1:A:331:LYS:HB2	1:A:337:TRP:CZ3	2.53	0.44
1:C:64:LYS:HD2	1:C:69:THR:O	2.18	0.44
1:C:446:ALA:HA	1:C:452:LEU:O	2.16	0.44
1:C:124:PHE:CD2	1:C:124:PHE:O	2.70	0.44
1:C:473:THR:O	1:C:477:THR:HG23	2.17	0.44
2:D:286:THR:HG22	2:D:287:LYS:N	2.33	0.44
1:A:134:SER:OG	1:A:139:THR:HB	2.18	0.44
2:B:79:GLU:OE1	4:G:1:GLC:O3	2.30	0.43
2:B:270:ILE:HG23	2:B:346:PHE:O	2.18	0.43
1:C:125:ARG:NH1	1:C:147:ASN:HB3	2.33	0.43
1:C:465:LYS:O	1:C:466:VAL:HG23	2.17	0.43
2:D:293:VAL:CG1	2:D:294:PRO:HD2	2.47	0.43
2:B:64:LYS:HD2	2:B:69:THR:HG22	2.01	0.43
1:C:489:SER:HB2	1:C:528:LYS:NZ	2.34	0.43
1:C:466:VAL:C	1:C:467:VAL:HG23	2.43	0.43
1:C:545:ASN:HA	1:C:548:VAL:HG12	2.01	0.43
2:D:306:ASN:O	2:D:310:LEU:HD22	2.17	0.43
1:C:363:ASN:HA	1:C:511:ASP:OD1	2.17	0.43
2:B:104:LYS:HB3	2:B:191:SER:O	2.18	0.43
2:B:248:GLU:HB3	2:B:307:ARG:HH22	1.80	0.43
1:C:42:GLU:OE2	1:C:49:LYS:HG3	2.18	0.43
1:C:53:GLU:CD	1:C:53:GLU:H	2.26	0.43
2:D:254:VAL:HG13	2:D:283:LEU:HD22	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:VAL:HB	1:A:59:PRO:HD3	2.01	0.43
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.54	0.43
1:C:68:SER:C	1:C:70:LYS:N	2.75	0.42
2:D:339:TYR:CZ	2:D:352:GLY:HA3	2.54	0.42
1:C:50:ILE:HG21	1:C:145:GLN:HB3	2.01	0.42
2:D:168:LEU:O	2:D:172:ARG:HG3	2.19	0.42
1:A:62:ALA:C	1:A:63:ILE:HD12	2.44	0.42
1:C:467:VAL:CG1	1:C:468:PRO:N	2.82	0.42
1:A:333:GLY:HA3	1:C:301:LEU:HD11	2.01	0.42
2:B:160:PHE:CE2	2:B:164:MET:HE2	2.55	0.42
1:C:457:TYR:HE1	1:C:463:ARG:HG2	1.85	0.42
2:B:125:ARG:HB3	2:B:146:TYR:O	2.20	0.42
3:E:4:OMC:HM23	3:E:4:OMC:H1'	1.80	0.42
1:C:15:GLY:C	1:C:16:MET:HG2	2.44	0.42
1:C:184:MET:HG2	3:F:33:DC:H2''	2.02	0.42
2:D:40:GLU:OE2	2:D:44:GLU:OE1	2.38	0.42
2:D:73:LYS:HZ3	2:D:73:LYS:HB3	1.84	0.42
2:D:101:LYS:O	2:D:236:PRO:HB2	2.20	0.42
2:B:180:ILE:HA	2:B:188:TYR:O	2.20	0.42
1:C:412:PRO:O	1:C:414:TRP:HD1	2.03	0.42
3:F:10:DC:H2''	3:F:11:DG:C8	2.54	0.42
2:D:338:THR:HG22	2:D:353:LYS:HG3	2.02	0.42
1:C:60:VAL:HG21	1:C:130:PHE:HD2	1.85	0.41
1:C:97:PRO:HD3	1:C:232:TYR:CE2	2.55	0.41
1:C:396:GLU:CD	1:C:396:GLU:N	2.76	0.41
2:D:265:ASN:O	2:D:268:SER:OG	2.37	0.41
3:F:17:DT:H5''	3:F:17:DT:C6	2.53	0.41
1:C:393:ILE:HB	1:C:423:VAL:HB	2.01	0.41
1:C:408:ALA:HB1	2:D:364:ASP:HB3	2.01	0.41
3:F:4:OMC:HM23	3:F:4:OMC:H1'	1.93	0.41
1:A:65:LYS:HD3	1:A:65:LYS:HA	1.93	0.41
1:C:19:PRO:HG3	1:C:80:LEU:HB2	2.02	0.41
1:C:60:VAL:CG2	1:C:130:PHE:HB2	2.49	0.41
1:C:365:VAL:HG12	1:C:423:VAL:HG12	2.02	0.41
1:C:459:THR:OG1	1:C:463:ARG:N	2.53	0.41
1:C:474:ASN:O	1:C:478:GLU:HG2	2.21	0.41
2:B:84:THR:HB	2:B:154:LYS:HE2	2.03	0.41
3:E:13:DT:H2''	3:E:14:DG:C8	2.55	0.41
1:C:13:LYS:C	1:C:16:MET:HG3	2.46	0.41
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.56	0.41
2:D:344:GLU:CD	2:D:347:LYS:HD2	2.44	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:LYS:HD3	1:C:43:LYS:O	2.20	0.41
1:C:132:ILE:CG2	1:C:133:PRO:N	2.83	0.41
1:C:132:ILE:HB	1:C:142:ILE:HB	2.02	0.41
2:D:200:THR:O	2:D:204:GLU:HG3	2.21	0.41
1:A:69:THR:O	1:A:69:THR:HG22	2.21	0.41
1:C:74:LEU:HD23	1:C:74:LEU:HA	1.77	0.41
2:D:344:GLU:CG	2:D:347:LYS:HD2	2.50	0.41
1:A:406:TRP:CZ3	1:A:507:GLN:HB3	2.56	0.41
1:C:463:ARG:HB2	1:C:463:ARG:NH1	2.31	0.41
1:C:463:ARG:NH1	1:C:463:ARG:CB	2.84	0.41
3:F:-2:DA:C8	3:F:-1:DT:H71	2.55	0.41
1:A:549:ASP:O	1:A:552:VAL:HG22	2.21	0.41
1:C:168:LEU:O	1:C:172:ARG:HG3	2.21	0.41
1:C:489:SER:HB2	1:C:528:LYS:HZ2	1.84	0.41
1:C:497:THR:O	1:C:535:TRP:HA	2.21	0.41
2:D:246:LEU:HD11	2:D:310:LEU:CD2	2.51	0.41
1:A:240:THR:HG22	1:A:241:VAL:O	2.20	0.40
2:B:278:GLN:HG2	2:B:298:GLU:C	2.46	0.40
3:E:1:DG:H2'	3:E:2:OMC:C6	2.56	0.40
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.56	0.40
2:B:60:VAL:HG23	2:B:75:VAL:HG22	2.03	0.40
2:B:105:SER:OG	2:B:235:HIS:CE1	2.75	0.40
1:C:130:PHE:CZ	1:C:144:TYR:HB2	2.57	0.40
1:C:201:LYS:HA	1:C:201:LYS:HD3	1.73	0.40
1:A:202:ILE:O	1:A:206:ARG:HG3	2.21	0.40
1:A:211:ARG:HD2	1:A:211:ARG:C	2.46	0.40
2:B:373:GLN:HG3	2:B:406:TRP:CZ3	2.56	0.40
1:C:60:VAL:HG21	1:C:130:PHE:CD2	2.56	0.40
2:D:211:ARG:HB2	2:D:212:TRP:CD1	2.56	0.40
2:D:293:VAL:HG13	2:D:294:PRO:HD2	2.03	0.40
2:B:160:PHE:HE2	2:B:164:MET:HE2	1.87	0.40
2:B:266:TRP:CD1	2:B:425:LEU:HD13	2.56	0.40
1:A:324:ASP:OD2	1:A:388:LYS:NZ	2.49	0.40
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.03	0.40
2:D:64:LYS:HE3	2:D:69:THR:O	2.21	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	549/557 (99%)	537 (98%)	12 (2%)	0	100	100
1	C	549/557 (99%)	528 (96%)	19 (4%)	2 (0%)	30	51
2	B	403/444 (91%)	391 (97%)	12 (3%)	0	100	100
2	D	403/444 (91%)	393 (98%)	10 (2%)	0	100	100
All	All	1904/2002 (95%)	1849 (97%)	53 (3%)	2 (0%)	48	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	140	PRO
1	C	18	GLY

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	490/494 (99%)	488 (100%)	2 (0%)	84	93
1	C	490/494 (99%)	486 (99%)	4 (1%)	73	88
2	B	366/400 (92%)	362 (99%)	4 (1%)	65	84
2	D	366/400 (92%)	362 (99%)	4 (1%)	65	84
All	All	1712/1788 (96%)	1698 (99%)	14 (1%)	73	88

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LEU
1	A	353	LYS
2	B	101	LYS
2	B	357	MET
2	B	358	LYS
2	B	422	LEU
1	C	16	MET
1	C	73	LYS
1	C	452	LEU
1	C	524	GLN
2	D	65	LYS
2	D	310	LEU
2	D	424	LYS
2	D	427	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	ASN
1	A	278	GLN
1	A	330	GLN
1	A	340	GLN
1	A	507	GLN
2	B	147	ASN
2	B	161	GLN
2	B	265	ASN
2	B	336	GLN
1	C	136	ASN
1	C	278	GLN
1	C	340	GLN
1	C	447	ASN
1	C	464	GLN
1	C	545	ASN
2	D	137	ASN
2	D	151	GLN
2	D	197	GLN
2	D	207	GLN
2	D	242	GLN
2	D	336	GLN
2	D	407	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	2	3	19,22,23	2.79	8 (42%)	25,31,34	0.83	0
3	OMC	E	4	3	19,22,23	2.58	8 (42%)	25,31,34	0.73	0
3	OMC	E	2	3	19,22,23	2.63	8 (42%)	25,31,34	0.89	1 (4%)
3	OMC	F	4	3	19,22,23	2.84	8 (42%)	25,31,34	0.62	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	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	E	2	3	-	0/9/27/28	0/2/2/2
3	OMC	F	4	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	6.32	1.48	1.36
3	F	2	OMC	C2-N3	5.94	1.48	1.36
3	F	2	OMC	C6-C5	5.92	1.48	1.35
3	E	2	OMC	C6-C5	5.92	1.48	1.35
3	F	4	OMC	C6-C5	5.88	1.48	1.35
3	E	4	OMC	C2-N3	5.58	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	OMC	C6-C5	5.46	1.47	1.35
3	F	4	OMC	C4-N3	5.20	1.44	1.34
3	F	2	OMC	C4-N3	5.10	1.44	1.34
3	E	2	OMC	C2-N3	4.98	1.46	1.36
3	E	4	OMC	C4-N3	4.46	1.43	1.34
3	E	2	OMC	C2-N1	4.43	1.49	1.40
3	E	2	OMC	C4-N3	4.42	1.43	1.34
3	E	4	OMC	C2-N1	4.27	1.49	1.40
3	F	4	OMC	C2-N1	4.24	1.49	1.40
3	F	2	OMC	C2-N1	4.20	1.48	1.40
3	F	4	OMC	C4-N4	3.17	1.41	1.33
3	F	2	OMC	C6-N1	3.10	1.45	1.38
3	E	2	OMC	C6-N1	3.04	1.45	1.38
3	E	4	OMC	C6-N1	2.98	1.45	1.38
3	F	4	OMC	C6-N1	2.95	1.45	1.38
3	F	2	OMC	C4-N4	2.94	1.41	1.33
3	E	2	OMC	O2-C2	-2.87	1.18	1.23
3	F	2	OMC	C5-C4	2.76	1.49	1.42
3	E	4	OMC	C4-N4	2.75	1.40	1.33
3	E	2	OMC	C5-C4	2.67	1.49	1.42
3	F	2	OMC	O2-C2	-2.62	1.18	1.23
3	F	4	OMC	C5-C4	2.61	1.49	1.42
3	F	4	OMC	O2-C2	-2.51	1.19	1.23
3	E	2	OMC	C4-N4	2.49	1.39	1.33
3	E	4	OMC	O2-C2	-2.21	1.19	1.23
3	E	4	OMC	C5-C4	2.15	1.47	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	OMC	O2-C2-N3	-2.18	118.89	122.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

Continued on next page...

Continued from previous page...

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

5.5 Carbohydrates

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GLC	G	1	4	11,11,12	0.56	0	15,15,17	1.62	1 (6%)
4	FRU	G	2	4	11,12,12	0.60	0	10,18,18	0.83	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	-	1/2/19/22	0/1/1/1
4	FRU	G	2	4	-	3/5/24/24	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	GLC	C1-O5-C5	5.86	120.04	112.19
4	G	2	FRU	O2-C2-O5	2.10	113.36	109.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	2	FRU	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

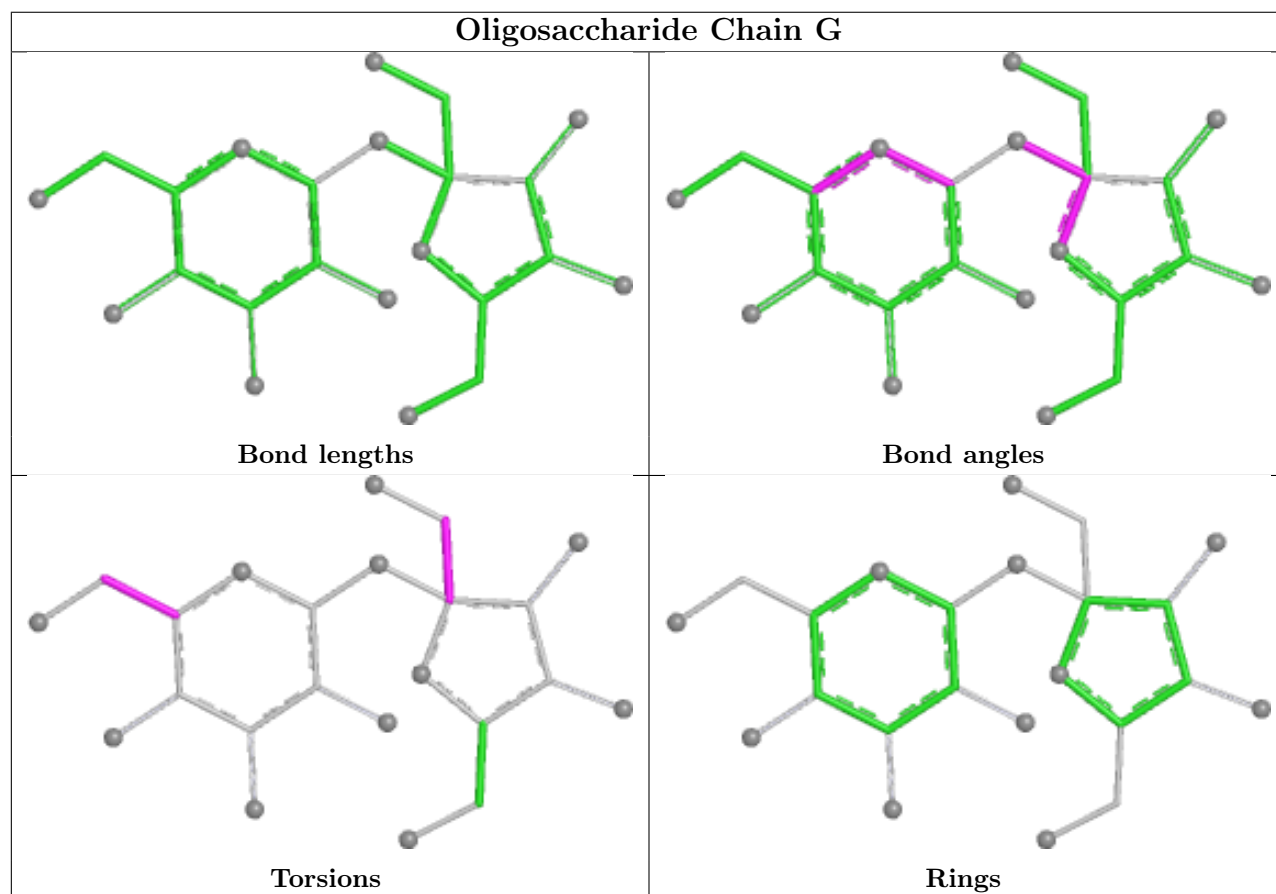
Mol	Chain	Res	Type	Atoms
4	G	2	FRU	O1-C1-C2-O2
4	G	2	FRU	O1-C1-C2-O5
4	G	1	GLC	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	GLC	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](#)

5 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	C	601	-	5,5,5	0.20	0	5,5,5	0.77	0
5	GOL	D	501	-	5,5,5	0.31	0	5,5,5	0.44	0
5	GOL	B	501	-	5,5,5	0.48	0	5,5,5	0.48	0
5	GOL	E	101	-	5,5,5	0.05	0	5,5,5	0.54	0
5	GOL	A	601	-	5,5,5	0.51	0	5,5,5	0.70	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	C	601	-	-	2/4/4/4	-
5	GOL	D	501	-	-	2/4/4/4	-
5	GOL	B	501	-	-	0/4/4/4	-
5	GOL	E	101	-	-	2/4/4/4	-
5	GOL	A	601	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	601	GOL	O1-C1-C2-C3
5	D	501	GOL	C1-C2-C3-O3
5	A	601	GOL	C1-C2-C3-O3
5	E	101	GOL	C1-C2-C3-O3
5	C	601	GOL	O1-C1-C2-O2
5	D	501	GOL	O2-C2-C3-O3
5	E	101	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	501	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	551/557 (98%)	-0.20	6 (1%) 78 74	31, 55, 90, 172	0
1	C	551/557 (98%)	0.32	37 (6%) 24 19	36, 71, 138, 195	0
2	B	407/444 (91%)	0.33	34 (8%) 17 13	36, 73, 127, 199	0
2	D	407/444 (91%)	0.32	30 (7%) 20 16	42, 71, 116, 174	0
3	E	33/38 (86%)	-0.68	0 100 100	35, 50, 104, 127	0
3	F	36/38 (94%)	-0.18	0 100 100	43, 69, 145, 175	0
All	All	1985/2078 (95%)	0.15	107 (5%) 31 26	31, 65, 125, 199	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	90	VAL	5.5
2	B	422	LEU	5.5
1	C	74	LEU	5.4
2	D	232	TYR	5.0
1	A	24	TRP	4.7
2	D	360	ALA	4.7
1	C	27	THR	4.7
1	C	26	LEU	4.5
1	C	61	PHE	4.4
1	C	24	TRP	4.4
2	B	209	LEU	4.3
2	B	423	VAL	4.3
2	B	360	ALA	4.3
2	B	212	TRP	4.2
2	D	425	LEU	4.2
1	C	71	TRP	4.1
2	B	425	LEU	4.1
2	B	88	TRP	4.0
1	C	60	VAL	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	142	ILE	3.9
2	D	5	ILE	3.9
1	C	135	ILE	3.9
2	B	195	ILE	3.6
2	D	362	THR	3.6
1	C	452	LEU	3.5
2	D	4	PRO	3.5
2	D	90	VAL	3.5
2	D	423	VAL	3.4
2	D	427	TYR	3.4
2	D	282	LEU	3.4
2	D	212	TRP	3.3
2	D	293	VAL	3.3
2	D	424	LYS	3.3
2	B	92	LEU	3.3
2	B	231	GLY	3.3
1	A	135	ILE	3.2
1	C	140	PRO	3.2
1	A	69	THR	3.2
1	C	34	LEU	3.1
1	C	63	ILE	2.9
2	D	213	GLY	2.9
1	C	62	ALA	2.9
2	B	357	MET	2.8
2	D	361	HIS	2.8
2	B	361	HIS	2.8
1	C	59	PRO	2.8
2	D	294	PRO	2.8
2	B	95	PRO	2.7
2	B	420	PRO	2.7
1	C	69	THR	2.7
2	D	422	LEU	2.7
2	D	231	GLY	2.6
2	B	94	ILE	2.6
2	B	210	LEU	2.6
1	C	25	PRO	2.6
2	B	232	TYR	2.6
1	C	31	ILE	2.6
2	B	301	LEU	2.6
2	B	68	SER	2.6
1	A	3	SER	2.5
1	C	472	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	362	THR	2.5
1	C	65	LYS	2.5
2	B	102	GLN	2.5
1	C	3	SER	2.5
1	C	134	SER	2.5
1	C	542	ILE	2.4
2	B	193	LEU	2.4
2	D	292	VAL	2.4
2	B	4	PRO	2.4
1	C	146	TYR	2.4
2	B	241	VAL	2.3
2	D	93	GLY	2.3
2	B	358	LYS	2.3
2	B	213	GLY	2.3
1	C	466	VAL	2.3
2	B	427	TYR	2.3
1	C	52	PRO	2.3
1	C	37	ILE	2.3
1	C	22	LYS	2.3
2	B	245	VAL	2.3
1	A	25	PRO	2.3
2	D	356	ARG	2.3
2	B	266	TRP	2.2
2	D	420	PRO	2.2
2	B	70	LYS	2.2
2	D	283	LEU	2.2
2	B	237	ASP	2.2
1	C	458	VAL	2.1
1	C	114	ALA	2.1
2	B	99	GLY	2.1
1	C	138	GLU	2.1
1	C	66	LYS	2.1
2	D	266	TRP	2.1
2	D	174	GLN	2.1
2	D	355	ALA	2.1
2	D	245	VAL	2.1
2	D	357	MET	2.1
1	A	66	LYS	2.1
1	C	447	ASN	2.0
2	D	285	GLY	2.0
1	C	219	LYS	2.0
1	C	139	THR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	88	TRP	2.0
1	C	151	MET	2.0
2	B	294	PRO	2.0
1	C	489	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.

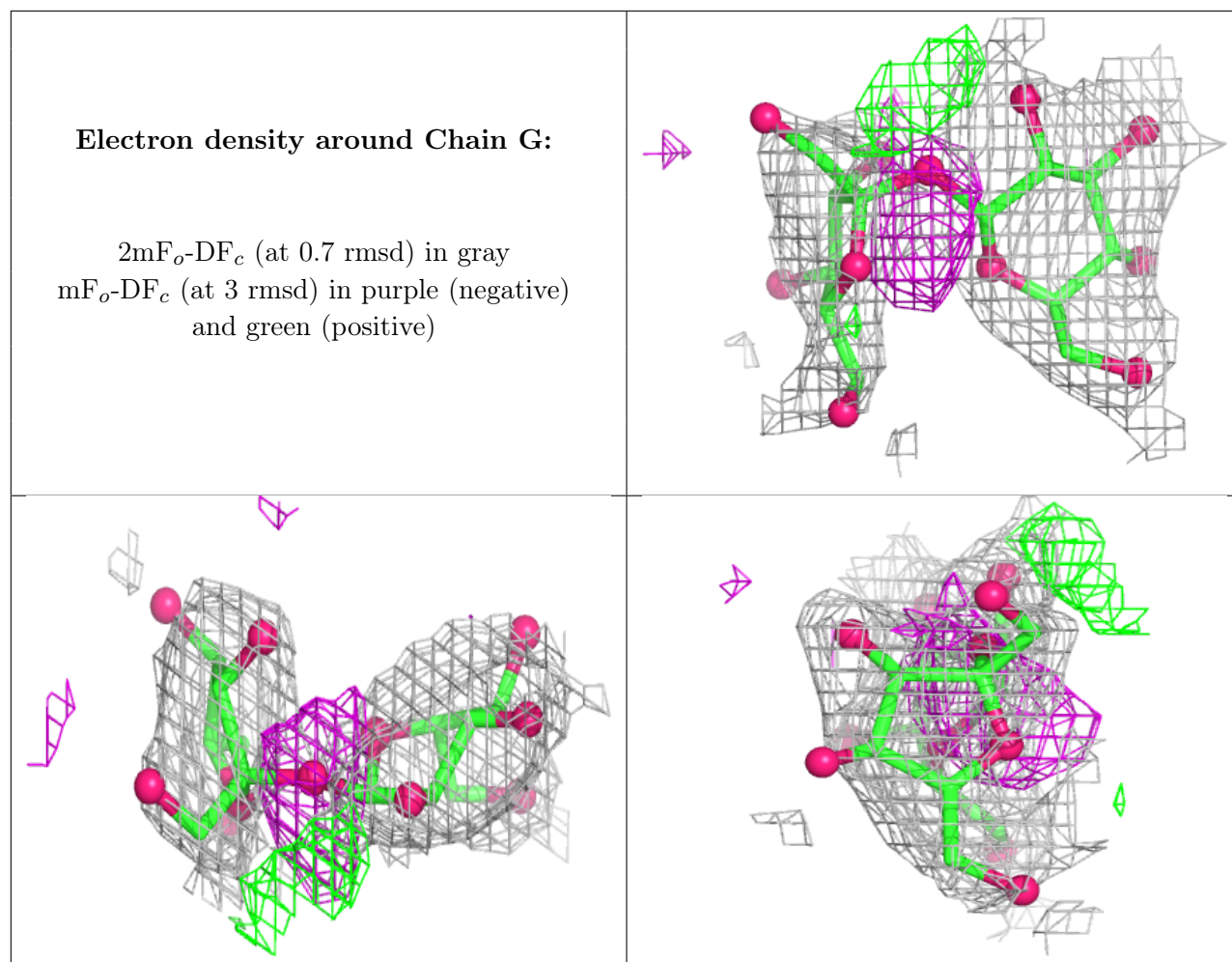
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OMC	F	2	21/22	0.95	0.09	59,63,72,77	0
3	OMC	E	2	21/22	0.97	0.08	38,44,52,70	0
3	OMC	F	4	21/22	0.97	0.07	37,46,53,55	0
3	OMC	E	4	21/22	0.98	0.06	30,37,43,44	0

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(Å ²)	Q<0.9
4	FRU	G	2	12/12	0.80	0.23	105,121,128,130	0
4	GLC	G	1	11/12	0.90	0.14	65,77,92,100	0

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	601	6/6	0.85	0.20	60,71,73,79	0
5	GOL	C	601	6/6	0.91	0.23	82,91,106,113	0
5	GOL	D	501	6/6	0.93	0.12	51,61,63,65	0
5	GOL	E	101	6/6	0.94	0.17	72,85,89,96	0
5	GOL	B	501	6/6	0.96	0.10	48,55,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.