



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 05:00 AM BST

PDB ID : 5XN0
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

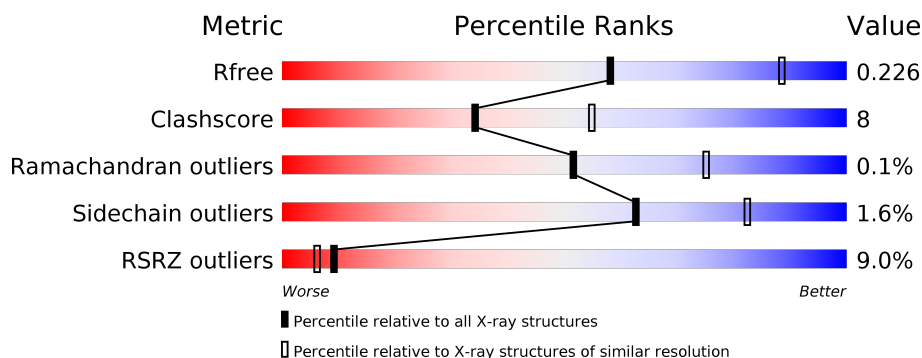
1 Overall quality at a glance

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on 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	<div> <div>2%</div> <div>85%</div> <div>14%</div> <div>•</div> </div>
1	C	557	<div> <div>14%</div> <div>73%</div> <div>24%</div> <div>••</div> </div>
2	B	444	<div> <div>11%</div> <div>75%</div> <div>16%</div> <div>• 8%</div> </div>
2	D	444	<div> <div>8%</div> <div>75%</div> <div>17%</div> <div>8%</div> </div>
3	E	38	<div> <div>3%</div> <div>68%</div> <div>18%</div> <div>5% 8%</div> </div>
3	F	38	<div> <div>8%</div> <div>66%</div> <div>29%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
4	G	2	

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

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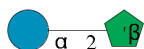
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP D3XFN7
B	-12	HIS	-	expression tag	UNP D3XFN7
B	-11	HIS	-	expression tag	UNP D3XFN7
B	-10	HIS	-	expression tag	UNP D3XFN7
B	-9	HIS	-	expression tag	UNP D3XFN7
B	-8	HIS	-	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.

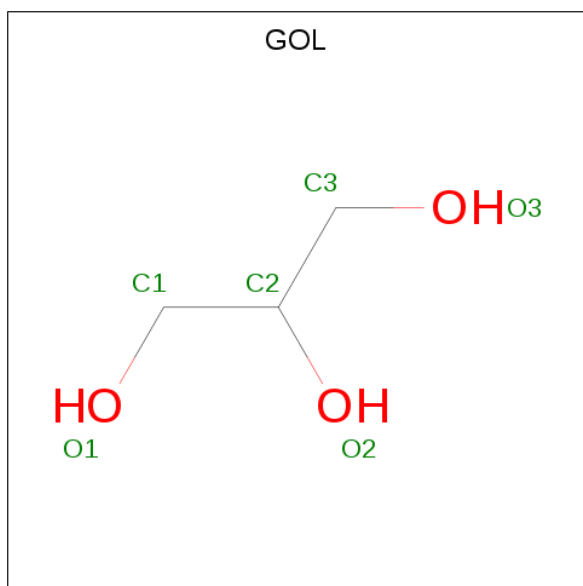
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	35	Total	C	N	O	P	0	0	0
			718	339	128	216	35			
3	F	38	Total	C	N	O	P	0	0	0
			777	369	140	231	37			

- 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 (three-letter code: 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		

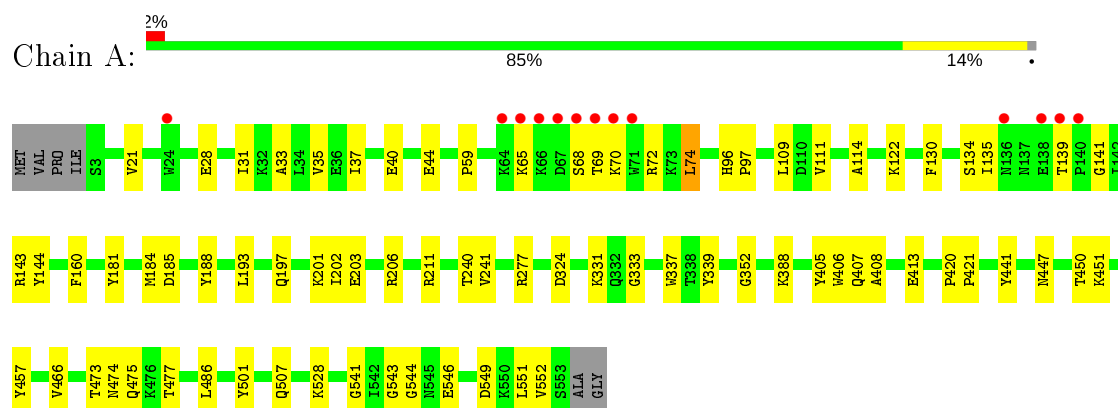
- Molecule 6 is water.

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

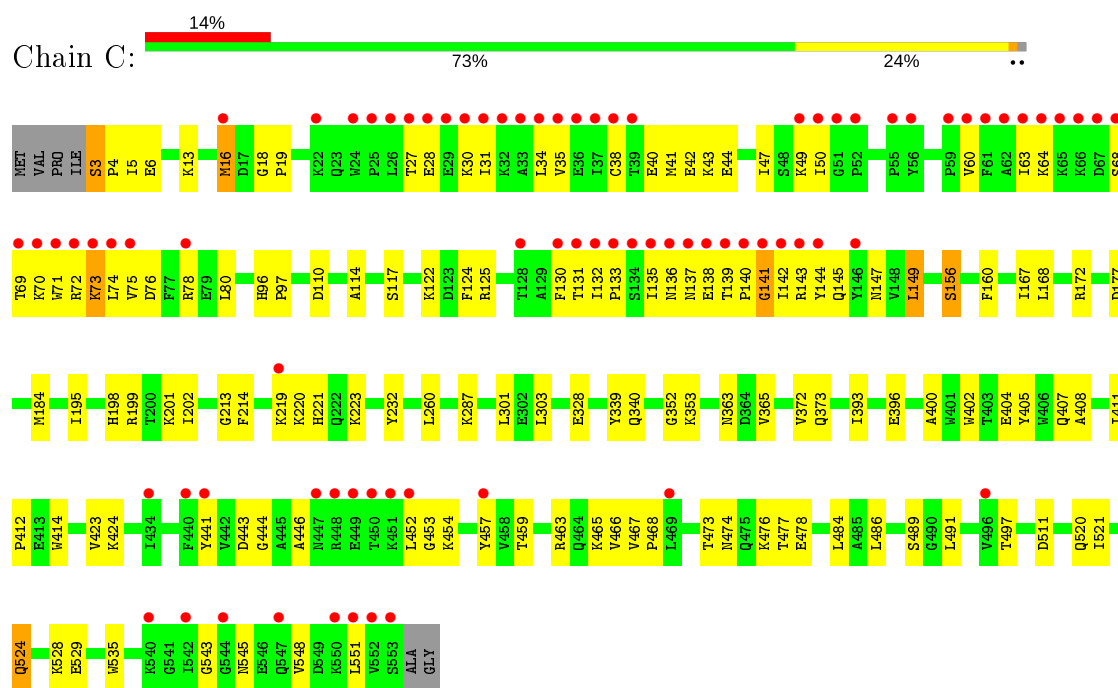
3 Residue-property plots [i](#)

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: Pol protein

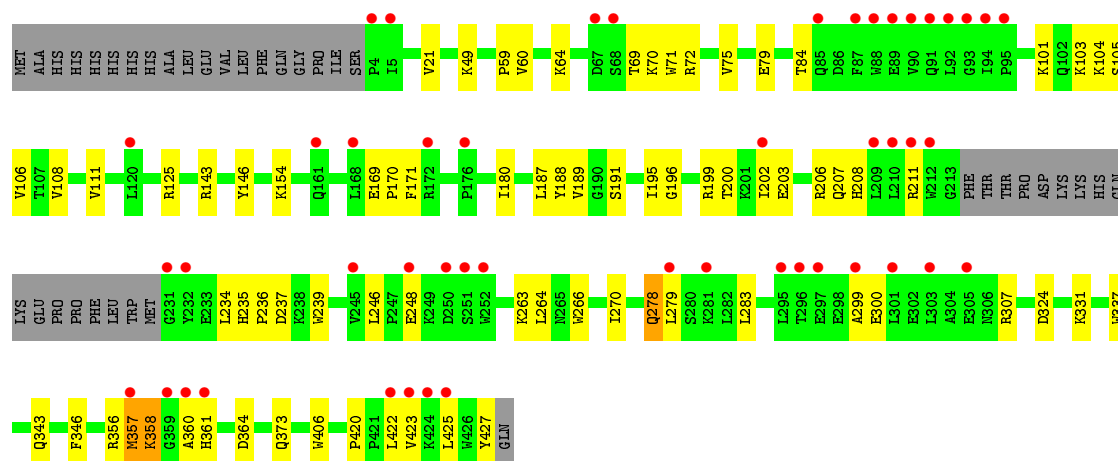


• Molecule 1: Pol protein

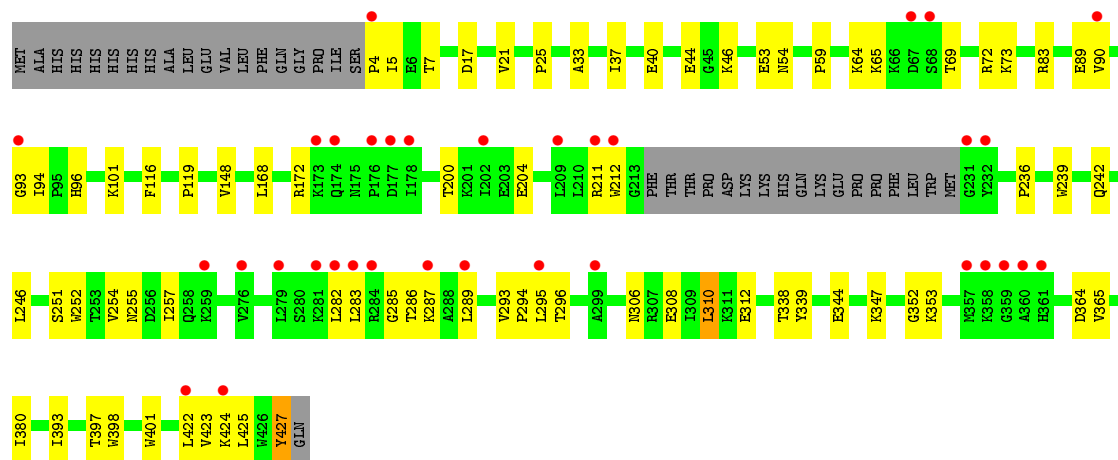
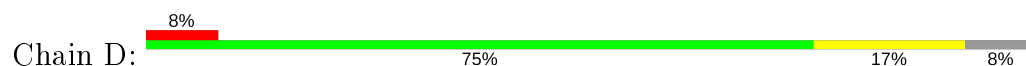


• Molecule 2: Pol protein

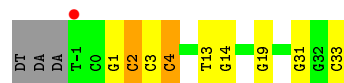




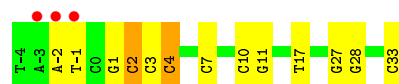
• Molecule 2: Pol protein



• 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	284.09 Å 284.09 Å 95.61 Å 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) 100.0 (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 2.61 Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.185 , 0.226 0.185 , 0.226	Depositor DCC
R_{free} test set	4479 reflections (5.04%)	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)	0.34 , 54.5	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: OMC, GOL, GLC, 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	0.49	0/4600	0.60	2/6246 (0.0%)
1	C	0.46	0/4600	0.62	4/6246 (0.1%)
2	B	0.44	0/3449	0.60	2/4684 (0.0%)
2	D	0.46	0/3449	0.62	1/4684 (0.0%)
3	E	0.93	0/756	1.03	3/1165 (0.3%)
3	F	0.76	0/823	0.95	0/1269
All	All	0.51	0/17677	0.66	12/24294 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	19	DG	O5'-P-OP2	-8.69	97.88	105.70
1	C	141	GLY	N-CA-C	7.45	131.71	113.10
1	A	74	LEU	CA-CB-CG	7.29	132.06	115.30
1	A	109	LEU	CA-CB-CG	5.75	128.51	115.30
2	D	257	ILE	CG1-CB-CG2	-5.73	98.80	111.40
3	E	31	DG	C4'-C3'-C2'	-5.30	98.33	103.10
2	B	169	GLU	C-N-CD	5.22	139.36	128.40
1	C	139	THR	C-N-CD	5.17	139.26	128.40
2	B	422	LEU	CA-CB-CG	5.12	127.08	115.30
1	C	3	SER	C-N-CD	5.09	139.09	128.40
1	C	149	LEU	C-N-CD	5.09	139.09	128.40
3	E	31	DG	O4'-C4'-C3'	-5.04	102.48	104.50

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	50	0
1	C	4483	0	4532	123	0
2	B	3354	0	3387	53	0
2	D	3354	0	3387	55	0
3	E	718	0	397	5	0
3	F	777	0	432	10	0
4	G	23	0	21	1	0
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	285	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 (285) 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:HH21	1:A:143:ARG:HG2	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:43:LYS:C	1:C:43:LYS:HD3	2.13	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
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
1:C:463:ARG:HB2	1:C:463:ARG:HH11	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
1:C:452:LEU:C	1:C:452:LEU:HD13	2.16	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: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:B:356:ARG:HD2	2:B:356:ARG:C	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:396:GLU:H	1:C:396:GLU:CD	2.06	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
2:B:263:LYS:HB2	2:B:423:VAL:HG11	1.86	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: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: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:63:ILE:HG22	1:C:64:LYS:N	2.20	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
2:D:53:GLU:HG2	2:D:54:ASN:N	2.23	0.54
1:C:114:ALA:HB1	1:C:160:PHE:CZ	2.43	0.53
1:C:68:SER:HB2	1:C:70:LYS:HB2	1.91	0.53
1:C:41:MET:HB2	1:C:47:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:3:DC:H2'	3:E:4:OMC:C6	2.43	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:O	1:A:211:ARG:HD2	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
1:C:551:LEU:H	1:C:551:LEU:HD12	1.73	0.52
1:C:68:SER:O	1:C:69:THR:C	2.47	0.52
2:D:353:LYS:NZ	2:D:427:TYR:HD1	2.05	0.52
2:B:208:HIS:C	2:B:208:HIS:HD1	2.13	0.52
1:C:466:VAL:CG1	1:C:467:VAL:N	2.73	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
1:A:450:THR:O	1:A:451:LYS:HB2	2.12	0.50
2:B:143:ARG:HG2	2:B:143:ARG:HH11	1.76	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
1:C:452:LEU:C	1:C:452:LEU:CD1	2.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:278:GLN:HG2	2:B:299:ALA:N	2.30	0.47
2:D:96:HIS:HE1	2:D:380:ILE:O	1.97	0.47
1:A:457:TYR:C	1:A:457:TYR:CD1	2.88	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
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: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:103:LYS:O	2:B:104:LYS:C	2.54	0.45
2:B:237:ASP:N	2:B:237:ASP:OD1	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
2:B:356:ARG:CD	2:B:356:ARG:C	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:254:VAL:HG13	2:D:283:LEU:CD2	2.47	0.45
2:D:236:PRO:HA	2:D:239:TRP:CD2	2.51	0.45
2:D:308:GLU:O	2:D:312:GLU:HG3	2.17	0.45
1:C:473:THR:OG1	1:C:476:LYS:HG3	2.17	0.45
1:A:184:MET:HG3	3:E:33:DC:H1'	1.99	0.45
1:C:353:LYS:NZ	3:F:7:DC:OP1	2.43	0.45
1:C:491:LEU:HB3	1:C:529:GLU:HB2	1.99	0.44
1:C:73:LYS:CE	1:C:75:VAL:HG23	2.48	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: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:132:ILE:HG22	1:C:133:PRO:N	2.31	0.44
1:C:38:CYS:O	1:C:47:ILE:HD11	2.16	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:A:331:LYS:HB2	1:A:337:TRP:CZ3	2.53	0.44
1:C:446:ALA:HA	1:C:452:LEU:O	2.16	0.44
1:C:64:LYS:HD2	1:C:69:THR:O	2.18	0.44
1:C:124:PHE:O	1:C:124:PHE:CD2	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:270:ILE:HG23	2:B:346:PHE:O	2.18	0.43
2:B:79:GLU:OE1	4:G:1:GLC:O3	2.30	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: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:D:4:PRO:C	2:D:5:ILE:HG13	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:LYS:HB3	2:D:73:LYS:HZ2	1.84	0.43
2:D:254:VAL:HG13	2:D:283:LEU:HD22	2.01	0.43
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.54	0.43
1:A:21:VAL:HB	1:A:59:PRO:HD3	2.01	0.43
2:D:339:TYR:CZ	2:D:352:GLY:HA3	2.54	0.42
1:A:486:LEU:O	1:A:528:LYS:NZ	2.38	0.42
1:C:50:ILE:HG21	1:C:145:GLN:HB3	2.01	0.42
2:B:208:HIS:ND1	2:B:208:HIS:C	2.73	0.42
2:D:168:LEU:O	2:D:172:ARG:HG3	2.19	0.42
2:B:266:TRP:C	2:B:266:TRP:CD1	2.92	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
1:C:457:TYR:HE1	1:C:463:ARG:HG2	1.85	0.42
1:A:420:PRO:HA	1:A:421:PRO:C	2.40	0.42
2:B:125:ARG:HB3	2:B:146:TYR:O	2.20	0.42
1:C:184:MET:HG2	3:F:33:DC:H2"	2.02	0.42
2:D:101:LYS:O	2:D:236:PRO:HB2	2.20	0.42
2:D:40:GLU:OE2	2:D:44:GLU:OE1	2.38	0.42
3:E:4:OMC:H1'	3:E:4:OMC:HM23	1.80	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
3:F:17:DT:H5"	3:F:17:DT:C6	2.53	0.41
1:C:408:ALA:HB1	2:D:364:ASP:HB3	2.01	0.41
1:C:393:ILE:HB	1:C:423:VAL:HB	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:60:VAL:CG2	1:C:130:PHE:HB2	2.49	0.41
1:C:19:PRO:HG3	1:C:80:LEU:HB2	2.02	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
1:C:132:ILE:CG2	1:C:133:PRO:N	2.83	0.41
3:E:13:DT:H2"	3:E:14:DG:C8	2.55	0.41
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.56	0.41
1:C:132:ILE:HB	1:C:142:ILE:HB	2.02	0.41
1:C:43:LYS:HD3	1:C:43:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:THR:O	2:D:204:GLU:HG3	2.21	0.41
1:A:69:THR:HG22	1:A:69:THR:O	2.21	0.41
1:C:74:LEU:HA	1:C:74:LEU:HD23	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:NH1	1:C:463:ARG:HB2	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
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:105:SER:OG	2:B:235:HIS:CE1	2.75	0.40
2:B:60:VAL:HG23	2:B:75:VAL:HG22	2.03	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
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: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
1:C:402:TRP:HE1	2:D:364:ASP:CG	2.24	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%)	34	57
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%)	51	75

All (2) Ramachandran outliers are listed below:

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

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	490/494 (99%)	486 (99%)	4 (1%)	81	92
1	C	490/494 (99%)	480 (98%)	10 (2%)	55	78
2	B	366/400 (92%)	358 (98%)	8 (2%)	52	76
2	D	366/400 (92%)	360 (98%)	6 (2%)	62	82
All	All	1712/1788 (96%)	1684 (98%)	28 (2%)	62	82

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LEU
1	A	122	LYS
1	A	277	ARG
1	A	474	ASN
2	B	49	LYS
2	B	72	ARG

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Mol	Chain	Res	Type
2	B	101	LYS
2	B	278	GLN
2	B	300	GLU
2	B	357	MET
2	B	358	LYS
2	B	427	TYR
1	C	16	MET
1	C	73	LYS
1	C	156	SER
1	C	177	ASP
1	C	219	LYS
1	C	287	LYS
1	C	340	GLN
1	C	424	LYS
1	C	484	LEU
1	C	524	GLN
2	D	65	LYS
2	D	72	ARG
2	D	251	SER
2	D	310	LEU
2	D	424	LYS
2	D	427	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	ASN
2	B	137	ASN
2	B	161	GLN
1	C	340	GLN
1	C	373	GLN
1	C	447	ASN
2	D	242	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	E	4	3	15,22,23	2.99	5 (33%)	17,31,34	1.45	2 (11%)
3	OMC	F	4	3	15,22,23	3.27	6 (40%)	17,31,34	1.29	2 (11%)
3	OMC	F	2	3	15,22,23	3.26	5 (33%)	17,31,34	1.27	1 (5%)
3	OMC	E	2	3	15,22,23	3.03	5 (33%)	17,31,34	1.05	1 (5%)

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	E	4	3	-	0/7/27/28	0/2/2/2
3	OMC	F	4	3	-	0/7/27/28	0/2/2/2
3	OMC	F	2	3	-	0/7/27/28	0/2/2/2
3	OMC	E	2	3	-	0/7/27/28	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	OMC	C6-N1	7.82	1.45	1.35
3	E	2	OMC	C6-N1	7.69	1.45	1.35
3	E	4	OMC	C6-N1	7.59	1.45	1.35
3	F	4	OMC	C6-N1	7.53	1.45	1.35
3	F	4	OMC	C4-N3	5.74	1.44	1.35
3	F	2	OMC	C4-N3	5.61	1.44	1.35
3	F	4	OMC	C2-N3	5.41	1.48	1.38
3	F	2	OMC	C2-N3	5.03	1.48	1.38
3	F	2	OMC	C6-C5	4.86	1.48	1.38
3	E	2	OMC	C6-C5	4.86	1.48	1.38
3	E	4	OMC	C4-N3	4.84	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	OMC	C6-C5	4.81	1.48	1.38
3	E	2	OMC	C4-N3	4.80	1.43	1.35
3	E	4	OMC	C2-N3	4.66	1.47	1.38
3	E	4	OMC	C6-C5	4.38	1.47	1.38
3	E	2	OMC	C2-N3	4.07	1.46	1.38
3	F	2	OMC	C5-C4	3.38	1.49	1.41
3	E	2	OMC	C5-C4	3.29	1.49	1.41
3	F	4	OMC	C5-C4	3.23	1.49	1.41
3	E	4	OMC	C5-C4	2.78	1.47	1.41
3	F	4	OMC	C4-N4	2.18	1.41	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4	OMC	C2-N3-C4	4.78	121.18	116.34
3	F	4	OMC	C2-N3-C4	4.03	120.42	116.34
3	F	2	OMC	C2-N3-C4	3.94	120.34	116.34
3	E	2	OMC	C2-N3-C4	3.14	119.52	116.34
3	F	4	OMC	N4-C4-N3	2.48	120.41	116.49
3	E	4	OMC	N4-C4-N3	2.29	120.11	116.49

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	E	4	OMC	2	0
3	F	4	OMC	2	0
3	F	2	OMC	1	0
3	E	2	OMC	1	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	0.58	0	15,15,17	1.65	1 (6%)
4	FRU	G	2	4	11,12,12	0.60	0	10,18,18	0.82	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	-	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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	G	1	GLC	C1-O5-C5	5.79	120.04	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

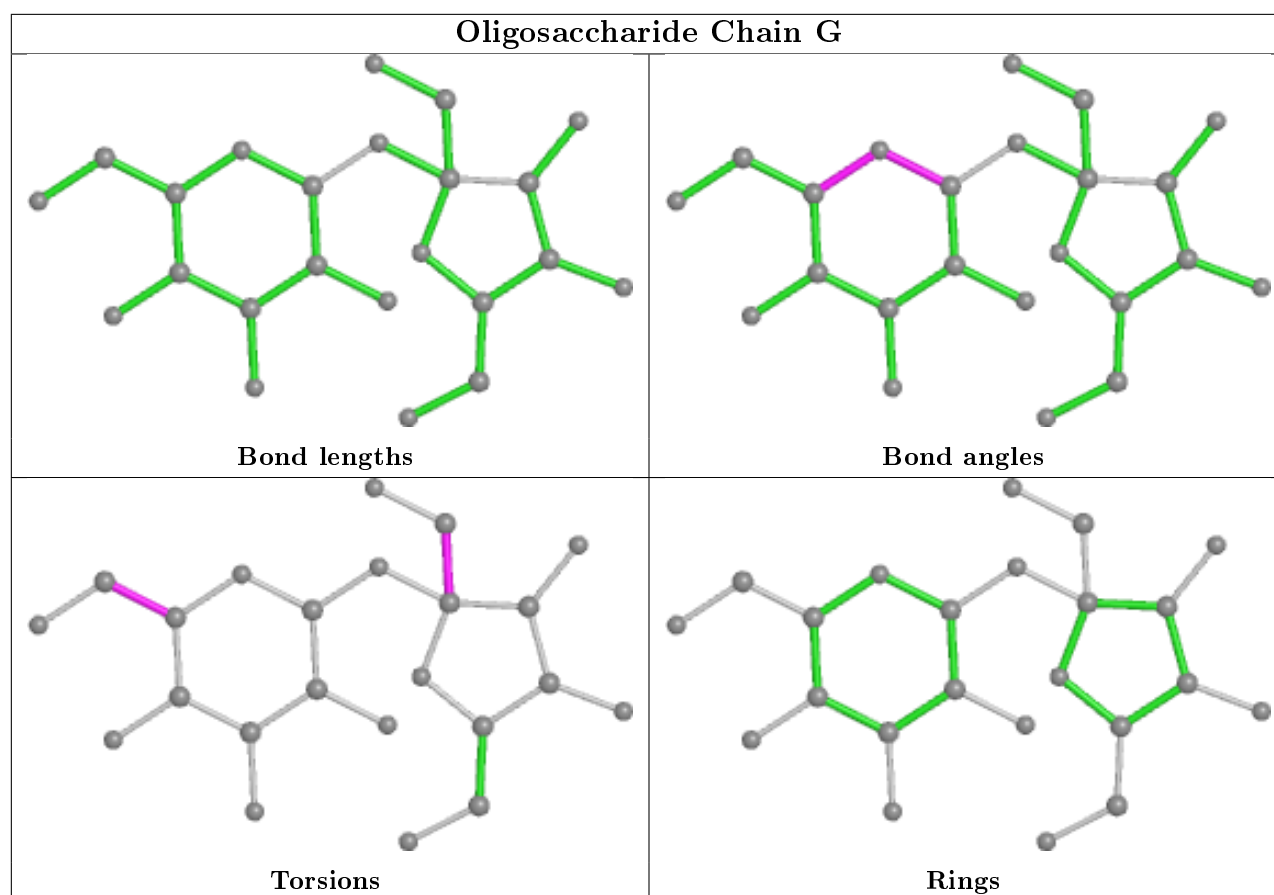
Mol	Chain	Res	Type	Atoms
4	G	2	FRU	O1-C1-C2-C3
4	G	2	FRU	O1-C1-C2-O2
4	G	2	FRU	O1-C1-C2-O5
4	G	1	GLC	O5-C5-C6-O6

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	D	501	-	5,5,5	0.30	0	5,5,5	0.42	0
5	GOL	A	601	-	5,5,5	0.48	0	5,5,5	0.68	0
5	GOL	C	601	-	5,5,5	0.20	0	5,5,5	0.72	0
5	GOL	B	501	-	5,5,5	0.47	0	5,5,5	0.45	0
5	GOL	E	101	-	5,5,5	0.05	0	5,5,5	0.50	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	D	501	-	-	2/4/4/4	-
5	GOL	A	601	-	-	1/4/4/4	-
5	GOL	C	601	-	-	2/4/4/4	-
5	GOL	B	501	-	-	0/4/4/4	-
5	GOL	E	101	-	-	2/4/4/4	-

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	D	501	GOL	C1-C2-C3-O3
5	C	601	GOL	O1-C1-C2-C3
5	A	601	GOL	C1-C2-C3-O3
5	E	101	GOL	C1-C2-C3-O3
5	D	501	GOL	O2-C2-C3-O3
5	C	601	GOL	O1-C1-C2-O2
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%)	0.17	13 (2%) 59 53	31, 55, 90, 172	0
1	C	551/557 (98%)	0.74	80 (14%) 2 1	36, 71, 138, 195	0
2	B	407/444 (91%)	0.70	48 (11%) 4 3	36, 73, 127, 199	0
2	D	407/444 (91%)	0.47	34 (8%) 11 7	42, 71, 116, 174	0
3	E	33/38 (86%)	0.03	1 (3%) 50 43	35, 50, 104, 127	0
3	F	36/38 (94%)	0.14	3 (8%) 11 8	43, 69, 145, 175	0
All	All	1985/2078 (95%)	0.49	179 (9%) 9 6	31, 65, 125, 199	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	360	ALA	11.2
2	B	88	TRP	9.9
1	C	61	PHE	9.5
2	B	4	PRO	8.8
1	C	34	LEU	8.3
2	B	92	LEU	8.2
1	C	136	ASN	8.1
1	C	68	SER	7.6
2	D	4	PRO	7.1
2	B	91	GLN	7.1
2	B	212	TRP	6.9
2	D	67	ASP	6.7
1	C	60	VAL	6.6
1	C	26	LEU	6.5
1	C	71	TRP	6.5
1	C	27	THR	6.4
1	C	67	ASP	6.3
1	C	142	ILE	6.1
2	B	357	MET	6.0

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Mol	Chain	Res	Type	RSRZ
2	B	361	HIS	5.8
1	C	62	ALA	5.8
1	C	32	LYS	5.7
1	C	63	ILE	5.7
1	C	452	LEU	5.6
1	A	67	ASP	5.6
2	B	359	GLY	5.6
1	A	66	LYS	5.6
2	B	231	GLY	5.5
1	C	542	ILE	5.5
1	C	144	TYR	5.4
2	B	209	LEU	5.4
2	D	283	LEU	5.4
2	B	423	VAL	5.3
1	C	50	ILE	5.3
1	C	135	ILE	5.2
1	C	74	LEU	5.2
1	C	31	ILE	5.2
1	C	24	TRP	5.2
1	C	134	SER	5.1
1	C	69	THR	5.1
1	A	65	LYS	5.0
1	A	69	THR	5.0
1	C	141	GLY	5.0
2	B	90	VAL	5.0
2	B	301	LEU	4.9
1	C	66	LYS	4.9
1	C	35	VAL	4.8
2	D	358	LYS	4.8
1	C	72	ARG	4.8
1	C	28	GLU	4.7
1	C	140	PRO	4.7
2	B	252	TRP	4.6
1	C	133	PRO	4.6
2	B	67	ASP	4.5
1	C	132	ILE	4.5
1	C	36	GLU	4.5
2	B	5	ILE	4.4
2	D	360	ALA	4.4
1	A	24	TRP	4.3
1	A	136	ASN	4.3
2	D	212	TRP	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	231	GLY	4.2
1	A	68	SER	4.2
2	D	232	TYR	4.2
2	B	95	PRO	4.1
1	A	138	GLU	4.1
1	A	140	PRO	4.1
1	C	73	LYS	4.0
1	C	39	THR	4.0
1	C	51	GLY	3.9
1	C	448	ARG	3.9
1	C	59	PRO	3.8
2	B	94	ILE	3.8
2	B	93	GLY	3.8
2	D	284	ARG	3.8
2	D	361	HIS	3.7
1	C	70	LYS	3.7
2	D	276	VAL	3.7
1	C	75	VAL	3.6
2	B	87	PHE	3.5
1	C	65	LYS	3.5
1	C	131	THR	3.5
1	C	29	GLU	3.4
1	C	38	CYS	3.4
1	C	457	TYR	3.4
2	D	279	LEU	3.4
2	D	282	LEU	3.3
2	B	232	TYR	3.2
2	B	248	GLU	3.2
1	A	139	THR	3.2
1	C	130	PHE	3.2
1	C	25	PRO	3.1
1	C	139	THR	3.1
2	B	89	GLU	3.1
2	D	211	ARG	3.1
1	C	37	ILE	3.0
2	D	295	LEU	3.0
2	D	299	ALA	3.0
2	B	211	ARG	3.0
2	B	245	VAL	3.0
2	B	279	LEU	2.9
1	C	33	ALA	2.9
2	B	168	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	250	ASP	2.9
2	D	357	MET	2.9
2	D	90	VAL	2.8
1	A	70	LYS	2.8
2	D	177	ASP	2.8
2	D	424	LYS	2.8
2	B	251	SER	2.8
1	A	64	LYS	2.7
1	C	550	LYS	2.7
2	B	305	GLU	2.7
1	C	49	LYS	2.7
3	F	-3	DA	2.7
1	C	52	PRO	2.7
2	B	68	SER	2.7
3	F	-2	DA	2.7
1	C	551	LEU	2.6
1	C	128	THR	2.6
3	F	-1	DT	2.6
2	D	259	LYS	2.6
1	C	55	PRO	2.6
1	C	146	TYR	2.6
2	D	178	ILE	2.5
2	D	281	LYS	2.5
2	D	68	SER	2.5
1	C	143	ARG	2.5
2	B	172	ARG	2.5
1	C	451	LYS	2.5
1	C	22	LYS	2.4
1	C	552	VAL	2.4
1	C	544	GLY	2.4
2	B	422	LEU	2.4
2	B	120	LEU	2.4
1	C	441	TYR	2.4
1	C	434	ILE	2.4
1	C	449	GLU	2.4
2	D	174	GLN	2.4
1	C	440	PHE	2.4
1	C	219	LYS	2.4
1	C	137	ASN	2.4
2	B	425	LEU	2.4
1	C	16	MET	2.3
1	C	496	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	176	PRO	2.3
1	C	540	LYS	2.3
2	B	424	LYS	2.3
2	B	303	LEU	2.3
2	D	209	LEU	2.3
2	D	93	GLY	2.2
2	B	210	LEU	2.2
1	C	56	TYR	2.2
2	D	359	GLY	2.2
1	C	450	THR	2.2
1	C	447	ASN	2.2
1	A	71	TRP	2.2
2	D	176	PRO	2.2
2	D	422	LEU	2.2
1	C	78	ARG	2.1
1	C	469	LEU	2.1
2	B	299	ALA	2.1
1	C	547	GLN	2.1
2	B	297	GLU	2.1
2	D	289	LEU	2.1
2	B	161	GLN	2.1
2	B	296	THR	2.1
1	C	138	GLU	2.1
2	B	202	ILE	2.1
2	B	85	GLN	2.1
1	C	30	LYS	2.1
1	C	64	LYS	2.0
2	B	281	LYS	2.0
2	D	173	LYS	2.0
2	D	202	ILE	2.0
2	D	287	LYS	2.0
2	B	295	LEU	2.0
3	E	-1	DT	2.0
1	C	553	SER	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.

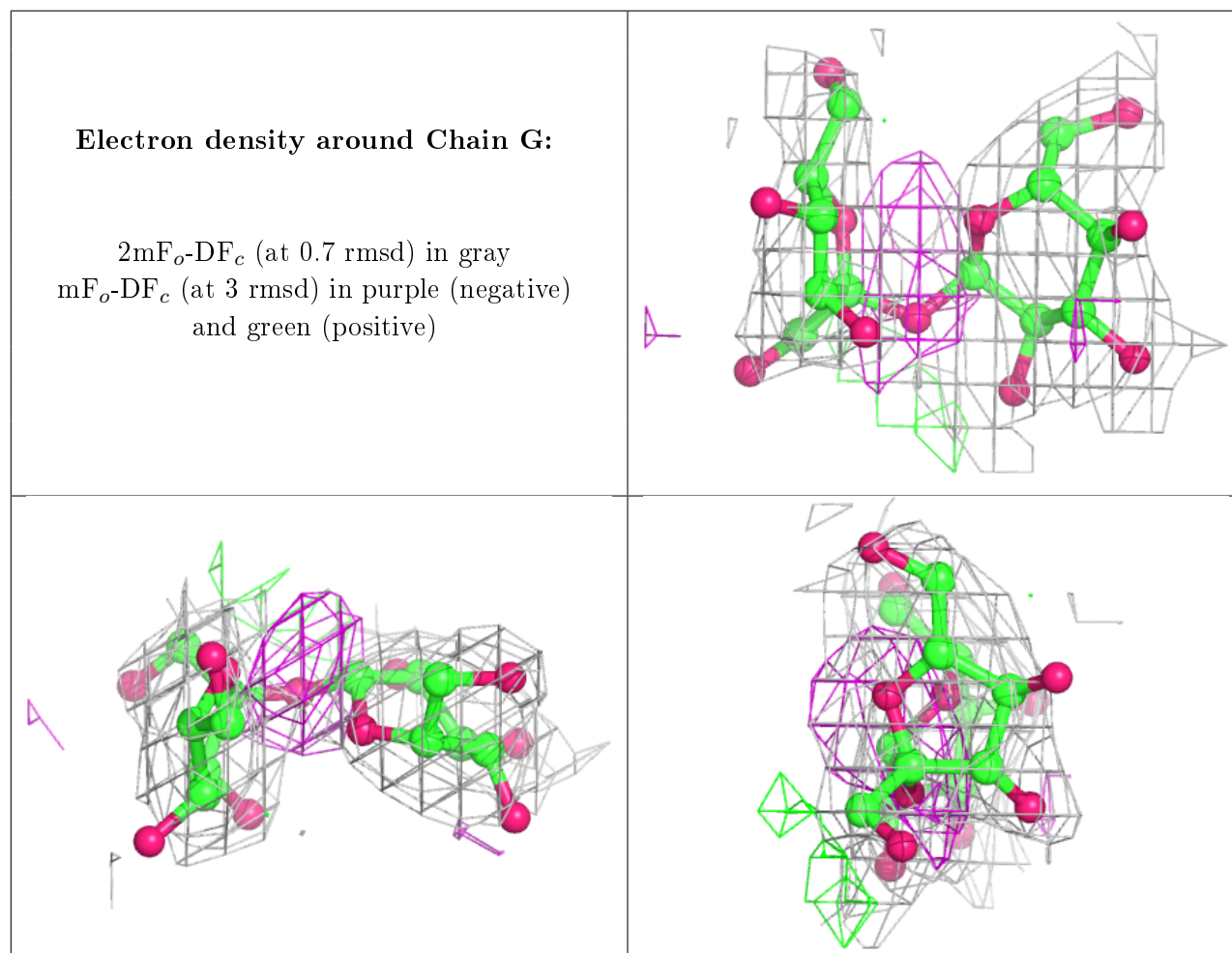
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	OMC	F	2	21/22	0.97	0.16	59,63,72,77	0
3	OMC	F	4	21/22	0.98	0.19	37,46,53,55	0
3	OMC	E	4	21/22	0.98	0.19	30,37,43,44	0
3	OMC	E	2	21/22	0.98	0.19	38,44,52,70	0

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(\AA^2)	Q<0.9
4	FRU	G	2	12/12	0.64	0.31	105,121,128,130	0
4	GLC	G	1	11/12	0.85	0.26	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

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	GOL	A	601	6/6	0.79	0.27	60,71,73,79	0
5	GOL	C	601	6/6	0.85	0.37	82,91,106,113	0
5	GOL	E	101	6/6	0.88	0.33	72,85,89,96	0
5	GOL	D	501	6/6	0.89	0.25	51,61,63,65	0
5	GOL	B	501	6/6	0.96	0.22	48,55,59,59	0

6.5 Other polymers

There are no such residues in this entry.