



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:08 PM UTC

PDB ID : 6KDJ / pdb_00006kdj
Title : HIV-1 reverse transcriptase with Q151M/Y115F/F116Y:DNA:lamivudine
5'-triphosphate ternary complex
Authors : Yasutake, Y.; Hattori, S.I.; Tamura, N.; Maeda, K.
Deposited on : 2019-07-02
Resolution : 2.51 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

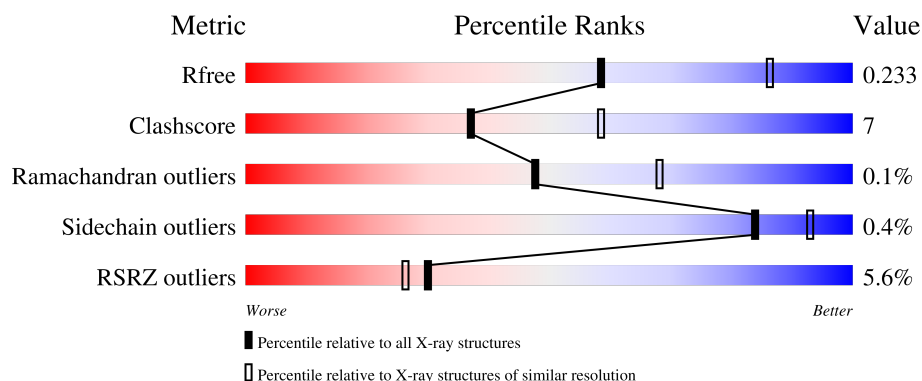
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	557	7% 82% 17% .
1	C	557	3% 84% 15% .
2	B	444	8% 75% 16% 9%
2	D	444	5% 80% 11% 9%
3	E	38	66% 24% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	38	 74%21%5%
4	G	2	 100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 17551 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	553	Total	C	N	O	S	0	0	0
			4498	2911	750	829	8			
1	C	553	Total	C	N	O	S	0	1	0
			4506	2915	751	832	8			

There are 14 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	162	SER	CYS	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	162	SER	CYS	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			
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).

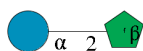
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	35	Total	C	N	O	P	0	0	0
			721	340	130	216	35			

Continued on next page...

Continued from previous page...

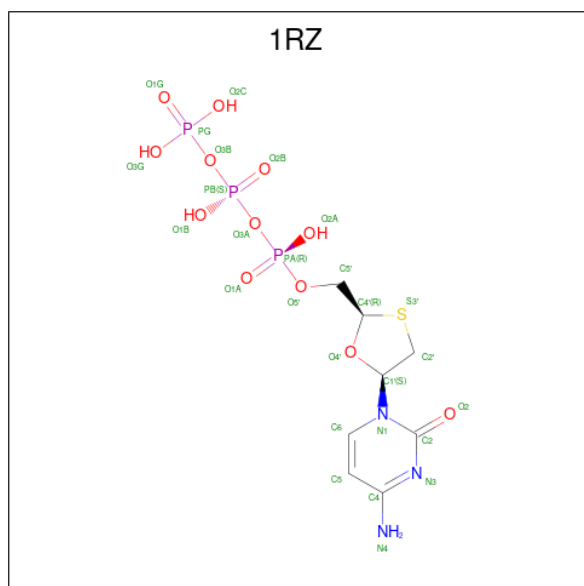
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	38	Total	C	N	O	P	0	0	0
			780	370	142	231	37			

- 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 Lamivudine Triphosphate (CCD ID: 1RZ) (formula: C₈H₁₄N₃O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			27	8	3	12	3	1		
5	C	1	Total	C	N	O	P	S	0	0
			27	8	3	12	3	1		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	71	Total O 71 71	0	0
8	B	41	Total O 41 41	0	0
8	E	29	Total O 29 29	0	0
8	C	55	Total O 55 55	0	0

Continued on next page...

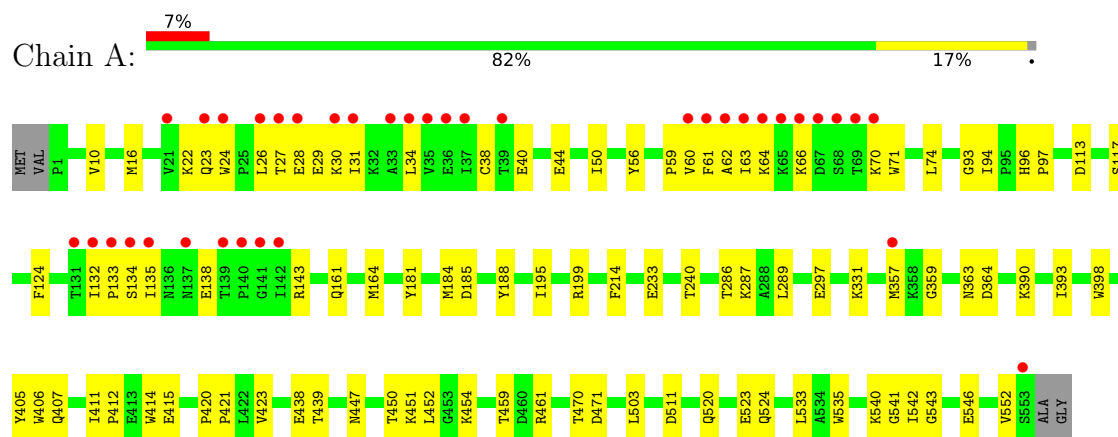
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	37	Total	O	0	0
			37	37		
8	F	16	Total	O	0	0
			16	16		

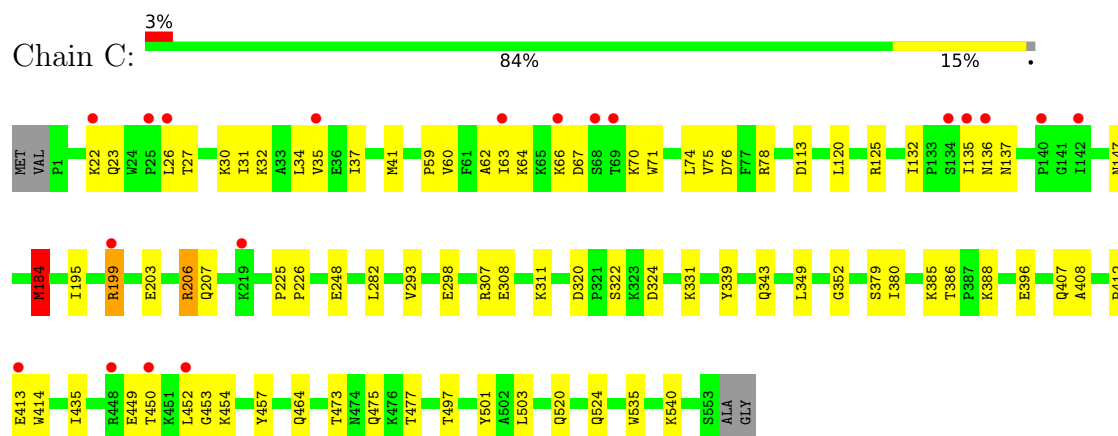
3 Residue-property plots [i](#)

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.

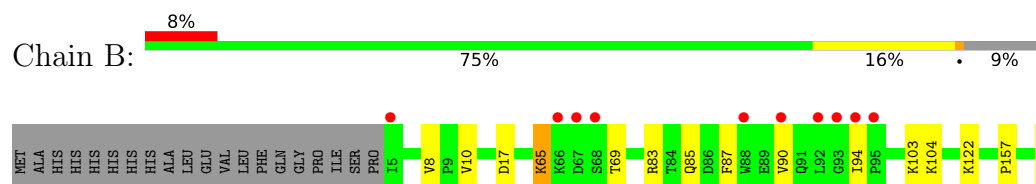
- Molecule 1: HIV-1 reverse transcriptase p66 subunit

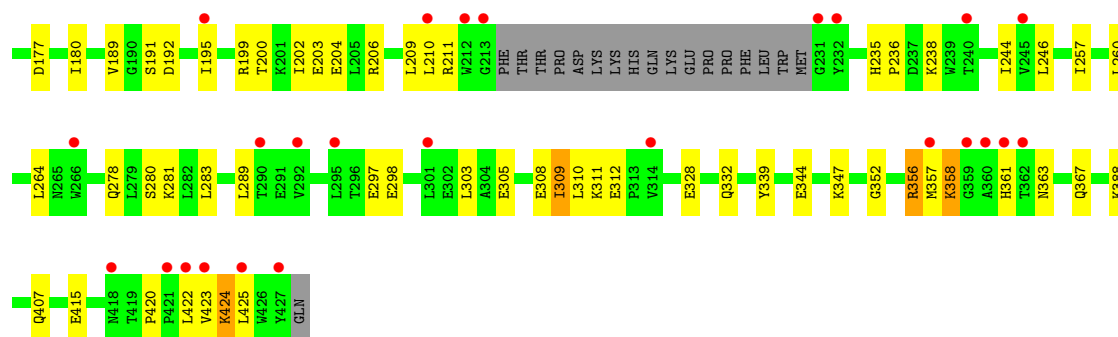


- Molecule 1: HIV-1 reverse transcriptase p66 subunit

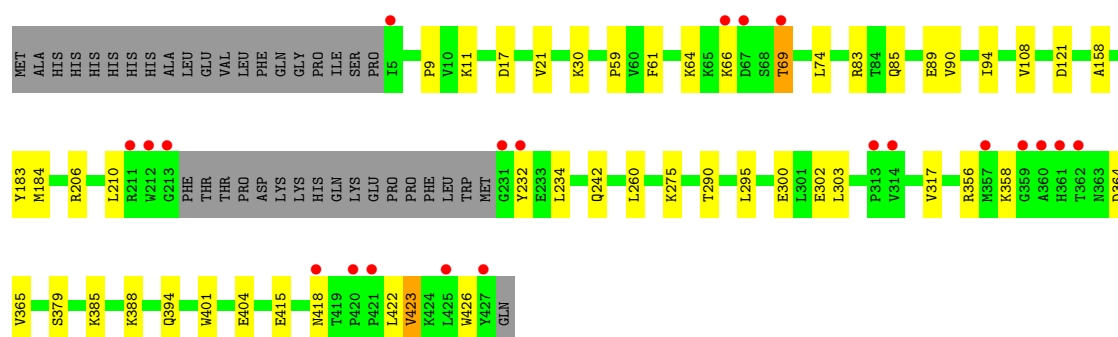
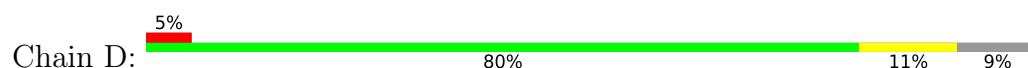


- Molecule 2: HIV-1 RT p51 subunit





• 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	285.11Å 285.11Å 96.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.79 – 2.51 48.79 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.79-2.51) 99.9 (48.79-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.182 , 0.230 0.185 , 0.233	Depositor DCC
R_{free} test set	5032 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17551	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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, 1RZ, GLC, FRU, MG

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	0.47	0/4616	0.66	4/6268 (0.1%)
1	C	0.39	0/4624	0.61	2/6279 (0.0%)
2	B	0.40	0/3441	0.66	2/4673 (0.0%)
2	D	0.41	0/3441	0.60	3/4673 (0.1%)
3	E	0.42	0/760	0.58	0/1172
3	F	0.39	0/827	0.58	0/1276
All	All	0.42	0/17709	0.63	11/24341 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	PRO	N-CA-C	9.12	125.63	113.40
2	D	426	TRP	N-CA-C	-8.48	101.94	112.88
1	C	199	ARG	CB-CG-CD	8.26	130.30	111.30
1	A	132	ILE	CA-C-N	6.06	125.46	118.85
1	A	132	ILE	C-N-CA	6.06	125.46	118.85
1	A	66	LYS	N-CA-C	-5.72	105.05	111.28
2	D	69	THR	N-CA-C	-5.61	106.33	112.72
2	B	361	HIS	CA-CB-CG	5.36	119.16	113.80
2	B	309	ILE	N-CA-C	-5.30	104.43	111.05
1	C	184	MET	CB-CA-C	-5.09	110.31	117.23
2	D	423	VAL	N-CA-C	-5.08	106.31	112.76

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	4498	0	4553	73	0
1	C	4506	0	4556	67	0
2	B	3347	0	3379	67	0
2	D	3347	0	3379	38	0
3	E	721	0	397	7	0
3	F	780	0	432	9	0
4	G	23	0	21	0	0
5	A	27	0	13	3	0
5	C	27	0	12	1	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	B	12	0	16	0	0
7	D	12	0	16	3	0
8	A	71	0	0	1	0
8	B	41	0	0	0	0
8	C	55	0	0	1	0
8	D	37	0	0	0	0
8	E	29	0	0	0	0
8	F	16	0	0	0	0
All	All	17551	0	16774	243	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 7.

All (243) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ILE:HG21	1:A:134:SER:HA	1.50	0.91
2:B:422:LEU:HD12	2:B:423:VAL:HG23	1.58	0.84
2:D:66:LYS:HD3	2:D:66:LYS:H	1.43	0.83
1:A:459:THR:HG22	1:A:461:ARG:H	1.45	0.81
2:B:311:LYS:HG2	2:B:312:GLU:OE1	1.79	0.81
2:B:424:LYS:HA	2:B:424:LYS:CE	2.10	0.81
1:C:195:ILE:O	1:C:199:ARG:HG3	1.81	0.80
2:B:332:GLN:HE22	2:B:424:LYS:HE2	1.48	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:PHE:HA	2:B:90:VAL:CG2	2.14	0.78
1:C:113:ASP:HA	5:C:601:1RZ:O1A	1.84	0.77
1:A:438:GLU:OE2	1:A:459:THR:HG21	1.86	0.76
2:B:87:PHE:HA	2:B:90:VAL:HG22	1.66	0.75
1:C:125:ARG:HD3	1:C:147:ASN:HA	1.73	0.71
2:D:394:GLN:HB2	7:D:701:GOL:H31	1.73	0.70
1:A:447:ASN:HB3	1:A:450:THR:OG1	1.92	0.68
2:B:308:GLU:HA	2:B:311:LYS:HB2	1.75	0.68
1:C:473:THR:O	1:C:477:THR:HG23	1.95	0.67
2:B:424:LYS:HA	2:B:424:LYS:HE3	1.77	0.67
1:A:540:LYS:HB2	1:A:542:ILE:HD11	1.75	0.67
1:C:298:GLU:OE2	1:C:298:GLU:N	2.22	0.65
2:B:308:GLU:HG2	2:B:311:LYS:HD2	1.79	0.65
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.78	0.65
1:C:35:VAL:HG12	1:C:132:ILE:HG21	1.77	0.65
3:F:3:DC:H2'	3:F:4:OMC:C6	2.33	0.64
1:A:331:LYS:NZ	1:A:364:ASP:OD2	2.30	0.64
2:B:422:LEU:CD1	2:B:423:VAL:HG23	2.28	0.64
1:A:27:THR:O	1:A:31:ILE:HG12	1.98	0.64
1:C:136:ASN:OD1	1:C:137:ASN:N	2.31	0.64
1:A:543:GLY:HA3	2:B:283:LEU:O	1.98	0.64
1:A:451:LYS:HG3	1:A:471:ASP:H	1.63	0.63
2:B:422:LEU:HD12	2:B:423:VAL:N	2.14	0.63
2:B:424:LYS:HE3	2:B:424:LYS:CA	2.29	0.62
1:A:56:TYR:O	1:A:143:ARG:NH2	2.32	0.62
2:D:108:VAL:HG21	2:D:232:TYR:CE2	2.35	0.62
2:D:89:GLU:HG2	2:D:90:VAL:HG23	1.80	0.62
2:B:388:LYS:NZ	2:B:415:GLU:OE1	2.32	0.62
1:A:34:LEU:O	1:A:38:CYS:N	2.33	0.61
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.80	0.61
2:B:69:THR:HG22	2:B:69:THR:O	2.00	0.61
2:D:356:ARG:NH1	2:D:358:LYS:O	2.32	0.61
2:B:85:GLN:O	2:B:85:GLN:HG3	1.99	0.61
2:B:200:THR:O	2:B:204:GLU:HG3	2.02	0.60
1:C:37:ILE:O	1:C:41:MET:HG3	2.01	0.60
2:B:260:LEU:HD21	2:B:303:LEU:HD13	1.84	0.60
2:B:166:LYS:HE2	2:B:166:LYS:HA	1.84	0.60
2:B:423:VAL:HG12	2:B:424:LYS:N	2.16	0.60
2:D:66:LYS:HE3	2:D:232:TYR:HD1	1.67	0.60
1:C:67:ASP:HB3	1:C:70:LYS:HG2	1.84	0.59
1:A:520:GLN:O	1:A:524:GLN:HG3	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:THR:O	1:C:31:ILE:HG13	2.02	0.59
1:C:34:LEU:HB3	1:C:132:ILE:HD12	1.82	0.59
1:A:22:LYS:O	1:A:59:PRO:HG3	2.02	0.59
1:A:503:LEU:HD12	1:A:533:LEU:HG	1.84	0.59
2:B:87:PHE:O	2:B:90:VAL:HG23	2.03	0.59
1:A:542:ILE:HD12	1:A:542:ILE:H	1.67	0.58
8:A:703:HOH:O	1:C:331:LYS:HE2	2.02	0.58
2:D:69:THR:HG22	2:D:69:THR:O	2.03	0.58
1:C:30:LYS:HD3	1:C:62:ALA:O	2.03	0.58
1:A:552:VAL:HG12	1:A:552:VAL:O	2.03	0.58
2:B:202:ILE:O	2:B:206:ARG:HG3	2.02	0.58
1:C:32:LYS:HA	1:C:35:VAL:HG22	1.86	0.58
1:A:161:GLN:NE2	1:A:184:MET:SD	2.77	0.58
1:A:70:LYS:HE2	1:A:71:TRP:O	2.04	0.57
1:A:28:GLU:HG2	1:A:29:GLU:N	2.18	0.57
1:C:343:GLN:HG3	1:C:349:LEU:HD11	1.84	0.57
1:A:138:GLU:O	1:A:138:GLU:HG2	2.05	0.57
1:A:447:ASN:HB3	1:A:450:THR:HG1	1.69	0.57
1:C:135:ILE:HG22	1:C:135:ILE:O	2.05	0.57
1:C:78:ARG:HE	3:F:0:DG:H5"	1.68	0.56
1:A:22:LYS:HD2	1:A:23:GLN:H	1.71	0.56
1:C:34:LEU:HD21	1:C:62:ALA:HB2	1.86	0.56
1:C:450:THR:HG23	1:C:452:LEU:H	1.71	0.56
1:A:541:GLY:HA2	1:A:546:GLU:HG3	1.88	0.56
2:B:235:HIS:HB2	2:B:238:LYS:HE2	1.88	0.56
2:B:169:GLU:O	2:B:173:LYS:HB2	2.07	0.56
1:C:76:ASP:OD1	1:C:78:ARG:HG3	2.05	0.56
1:A:74:LEU:HD22	3:E:0:DG:C4	2.41	0.55
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.87	0.55
2:B:422:LEU:HD12	2:B:423:VAL:H	1.71	0.55
1:A:439:THR:CG2	2:B:289:LEU:HD13	2.35	0.55
1:A:26:LEU:HD11	1:A:61:PHE:HA	1.87	0.55
1:A:184:MET:HE2	5:A:601:1RZ:H8	1.88	0.55
1:C:203:GLU:O	1:C:207:GLN:HG2	2.08	0.54
1:A:454:LYS:HE2	1:A:552:VAL:O	2.07	0.54
1:C:60:VAL:HG12	1:C:75:VAL:HG22	1.90	0.54
1:A:289:LEU:HD21	3:E:28:DG:H4'	1.89	0.53
2:B:423:VAL:HB	2:B:425:LEU:HD13	1.89	0.53
2:B:195:ILE:HG22	2:B:199:ARG:NH1	2.24	0.53
1:C:35:VAL:CG1	1:C:132:ILE:HG21	2.37	0.53
2:D:66:LYS:H	2:D:66:LYS:CD	2.19	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:GLN:O	1:A:523:GLU:HG2	2.08	0.53
2:B:199:ARG:O	2:B:202:ILE:HB	2.09	0.53
3:E:3:DC:H2'	3:E:4:OMC:C6	2.43	0.53
1:C:396:GLU:CD	1:C:396:GLU:H	2.17	0.53
2:B:344:GLU:HB2	2:B:347:LYS:HD3	1.90	0.53
2:B:424:LYS:CE	2:B:424:LYS:CA	2.85	0.53
1:A:117:SER:HB2	1:A:214:PHE:HE1	1.73	0.52
1:C:435:ILE:HG13	2:D:290:THR:HG21	1.90	0.52
2:B:424:LYS:HE3	2:B:424:LYS:C	2.34	0.52
1:C:78:ARG:HE	3:F:0:DG:C5'	2.23	0.52
2:D:394:GLN:CB	7:D:701:GOL:H31	2.39	0.52
1:C:408:ALA:HB1	2:D:364:ASP:HB3	1.92	0.52
3:F:1:DC:H2'	3:F:2:OMC:C6	2.45	0.52
2:B:206:ARG:O	2:B:210:LEU:HD12	2.09	0.52
2:B:278:GLN:OE1	2:B:298:GLU:HB3	2.10	0.52
1:A:184:MET:HG3	3:E:33:DG:H1'	1.92	0.52
2:D:17:ASP:O	2:D:83:ARG:HD3	2.10	0.52
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.92	0.52
1:C:136:ASN:CG	1:C:137:ASN:H	2.17	0.52
1:A:23:GLN:OE1	1:A:60:VAL:HG12	2.10	0.51
1:C:412:PRO:O	1:C:414:TRP:HD1	1.92	0.51
1:C:413:GLU:HA	8:C:748:HOH:O	2.10	0.51
2:B:356:ARG:HG2	2:B:358:LYS:H	1.76	0.51
2:D:90:VAL:HA	2:D:94:ILE:HD12	1.92	0.51
1:C:308:GLU:O	1:C:311:LYS:HG2	2.10	0.51
2:D:90:VAL:HG21	2:D:158:ALA:HA	1.91	0.51
2:B:339:TYR:CZ	2:B:352:GLY:HA3	2.46	0.51
2:B:236:PRO:C	2:B:238:LYS:H	2.18	0.51
1:A:23:GLN:OE1	1:A:59:PRO:HA	2.11	0.50
2:B:94:ILE:HD11	2:B:157:PRO:HB2	1.92	0.50
2:B:356:ARG:O	2:B:356:ARG:HD3	2.11	0.50
2:D:64:LYS:HE2	2:D:69:THR:O	2.11	0.50
1:A:406:TRP:CZ2	2:B:420:PRO:HG3	2.46	0.50
2:B:8:VAL:O	2:B:10:VAL:HG23	2.11	0.50
2:D:260:LEU:HD21	2:D:303:LEU:HD11	1.93	0.50
1:A:412:PRO:O	1:A:414:TRP:HD1	1.95	0.50
2:B:65:LYS:HA	2:B:407:GLN:OE1	2.12	0.50
2:B:195:ILE:HG22	2:B:199:ARG:HH12	1.77	0.49
1:A:297:GLU:OE2	1:C:331:LYS:NZ	2.44	0.49
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.47	0.49
2:D:365:VAL:HG11	2:D:401:TRP:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:MET:HE2	1:A:359:GLY:O	2.12	0.49
1:C:503:LEU:CD2	2:D:422:LEU:HD21	2.43	0.49
2:D:30:LYS:NZ	2:D:404:GLU:OE1	2.36	0.49
2:D:388:LYS:HE2	2:D:415:GLU:OE1	2.12	0.49
2:B:358:LYS:HE2	2:B:363:ASN:HB3	1.93	0.49
2:B:356:ARG:HB2	2:B:367:GLN:HG2	1.94	0.48
2:B:423:VAL:CG1	2:B:424:LYS:N	2.75	0.48
1:C:30:LYS:HE2	1:C:71:TRP:CZ3	2.48	0.48
3:E:23:DC:H2''	3:E:24:DG:C8	2.48	0.48
1:C:407:GLN:NE2	2:D:418:ASN:HA	2.29	0.48
1:C:66:LYS:HB2	1:C:66:LYS:HE3	1.58	0.48
1:A:22:LYS:HD2	1:A:23:GLN:N	2.29	0.48
2:B:280:SER:OG	2:B:281:LYS:HD3	2.13	0.48
1:A:117:SER:HB2	1:A:214:PHE:CE1	2.49	0.48
2:B:206:ARG:C	2:B:210:LEU:HD12	2.39	0.48
1:A:30:LYS:O	1:A:31:ILE:HD13	2.14	0.47
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.95	0.47
1:C:64:LYS:HG2	1:C:71:TRP:CZ3	2.49	0.47
2:B:209:LEU:C	2:B:211:ARG:H	2.22	0.47
1:C:184:MET:HA	1:C:184:MET:HE3	1.96	0.47
1:A:390:LYS:HG2	1:A:415:GLU:CG	2.44	0.47
1:C:339:TYR:CZ	1:C:352:GLY:HA3	2.49	0.47
3:F:2:OMC:HM22	3:F:3:DC:O4'	2.15	0.47
2:D:61:PHE:CZ	2:D:74:LEU:HD23	2.50	0.47
2:D:183:TYR:CE2	2:D:184:MET:HG3	2.49	0.47
2:B:103:LYS:HD3	2:B:191:SER:HA	1.97	0.47
2:B:244:ILE:HB	2:B:310:LEU:HD22	1.96	0.46
1:C:66:LYS:HG3	1:C:67:ASP:H	1.79	0.46
1:A:113:ASP:HA	5:A:601:1RZ:O2A	2.15	0.46
2:D:295:LEU:HD23	2:D:300:GLU:HG2	1.97	0.46
2:D:9:PRO:HA	2:D:121:ASP:OD2	2.16	0.46
2:D:275:LYS:HE3	2:D:302:GLU:HG3	1.97	0.46
1:A:50:ILE:HG13	1:A:143:ARG:HB2	1.98	0.46
1:A:94:ILE:HG12	3:E:4:OMC:H1'	1.98	0.46
1:C:66:LYS:HG3	1:C:67:ASP:N	2.30	0.46
1:C:320:ASP:OD1	1:C:322:SER:HB3	2.15	0.46
1:C:206:ARG:HE	1:C:206:ARG:HB3	1.49	0.45
1:C:248:GLU:HG3	1:C:307:ARG:NH2	2.31	0.45
2:D:206:ARG:O	2:D:210:LEU:HG	2.17	0.45
1:A:447:ASN:CG	1:A:450:THR:HG23	2.41	0.45
1:C:184:MET:HE2	1:C:184:MET:HB3	1.87	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:TYR:O	1:C:464:GLN:HA	2.16	0.45
2:D:232:TYR:HD2	2:D:234:LEU:HD21	1.80	0.45
2:B:257:ILE:HG22	2:B:283:LEU:HD11	1.97	0.45
3:E:10:DC:H2''	3:E:11:DG:C8	2.52	0.45
1:A:195:ILE:O	1:A:199:ARG:HG3	2.16	0.45
1:C:22:LYS:HD2	1:C:22:LYS:HA	1.75	0.44
1:A:23:GLN:HG3	1:A:24:TRP:N	2.32	0.44
1:A:535:TRP:CZ3	2:B:422:LEU:HD13	2.52	0.44
1:C:30:LYS:HE2	1:C:71:TRP:HZ3	1.81	0.44
2:D:232:TYR:CD2	2:D:234:LEU:HD21	2.52	0.44
2:B:199:ARG:O	2:B:203:GLU:HG2	2.18	0.44
1:C:23:GLN:OE1	1:C:59:PRO:HA	2.18	0.44
1:C:74:LEU:HD22	3:F:0:DG:C4	2.52	0.44
1:C:63:ILE:HG12	1:C:74:LEU:HD12	2.00	0.44
1:C:195:ILE:HG12	1:C:199:ARG:HH21	1.82	0.44
2:B:17:ASP:O	2:B:83:ARG:HD3	2.17	0.43
2:B:180:ILE:HG12	2:B:189:VAL:HG22	2.00	0.43
1:C:324:ASP:CG	1:C:388:LYS:HE3	2.42	0.43
1:A:93:GLY:C	1:A:94:ILE:HD13	2.43	0.43
1:A:286:THR:C	1:A:287:LYS:HG3	2.43	0.43
1:C:449:GLU:OE2	1:C:449:GLU:HA	2.18	0.43
3:F:18:DT:H4'	3:F:19:DG:C8	2.53	0.43
1:A:185:ASP:OD2	5:A:601:1RZ:H5	2.19	0.43
1:A:398:TRP:CZ2	1:A:411:ILE:HG12	2.53	0.43
2:B:423:VAL:HG12	2:B:425:LEU:N	2.33	0.43
2:D:21:VAL:HB	2:D:59:PRO:HD3	2.00	0.43
1:C:225:PRO:HA	1:C:226:PRO:C	2.44	0.43
1:C:396:GLU:CD	1:C:396:GLU:N	2.76	0.43
1:A:63:ILE:HG12	1:A:64:LYS:N	2.33	0.43
2:D:11:LYS:O	2:D:85:GLN:HG2	2.19	0.43
1:A:452:LEU:HD23	1:A:470:THR:HG22	2.00	0.42
1:C:184:MET:HG3	3:F:33:DG:H1'	2.01	0.42
1:C:120:LEU:HD23	1:C:125:ARG:HG2	2.01	0.42
1:C:540:LYS:O	1:C:540:LYS:HG3	2.18	0.42
2:B:94:ILE:CD1	2:B:157:PRO:HB2	2.49	0.42
1:A:40:GLU:O	1:A:44:GLU:HG3	2.19	0.42
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.55	0.42
2:B:103:LYS:NZ	2:B:177:ASP:O	2.51	0.42
1:C:380:ILE:HD11	1:C:386:THR:HG23	2.01	0.42
2:D:11:LYS:HB3	2:D:11:LYS:HE3	1.80	0.42
1:C:26:LEU:HB2	1:C:31:ILE:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:LEU:HB3	1:C:293:VAL:HG11	2.01	0.42
2:B:69:THR:O	2:B:69:THR:CG2	2.65	0.42
1:A:233:GLU:HB2	1:A:240:THR:OG1	2.20	0.42
2:B:297:GLU:H	2:B:297:GLU:HG3	1.55	0.42
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.20	0.42
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.54	0.42
2:D:423:VAL:O	2:D:423:VAL:HG12	2.19	0.42
1:A:393:ILE:O	1:A:414:TRP:HZ3	2.03	0.41
1:A:10:VAL:HG23	1:A:124:PHE:CD1	2.55	0.41
2:B:305:GLU:OE1	2:B:309:ILE:CD1	2.68	0.41
1:C:497:THR:O	1:C:535:TRP:HA	2.20	0.41
2:B:328:GLU:O	2:B:339:TYR:HA	2.20	0.41
2:D:242:GLN:O	2:D:242:GLN:HG3	2.19	0.41
1:A:164:MET:HE1	1:A:214:PHE:CD2	2.56	0.41
2:D:394:GLN:HG2	7:D:701:GOL:H31	2.02	0.41
2:D:422:LEU:N	2:D:422:LEU:HD22	2.36	0.41
1:A:27:THR:OG1	1:A:30:LYS:HG3	2.21	0.41
1:A:447:ASN:OD1	1:A:450:THR:HG23	2.21	0.41
2:B:104:LYS:HB3	2:B:192:ASP:HA	2.02	0.41
2:B:122:LYS:H	2:B:122:LYS:HG3	1.67	0.41
1:C:379:SER:HB3	1:C:385:LYS:O	2.21	0.41
1:C:453:GLY:C	1:C:454:LYS:HG3	2.45	0.41
1:A:450:THR:O	1:A:451:LYS:HG2	2.20	0.40
2:D:317:VAL:HG13	2:D:317:VAL:O	2.21	0.40
1:A:16:MET:HA	1:A:16:MET:HE2	2.04	0.40
1:A:70:LYS:HA	1:A:70:LYS:HD2	1.82	0.40
1:C:520:GLN:O	1:C:524:GLN:HG3	2.21	0.40
3:F:10:DC:H2"	3:F:11:DG:C8	2.57	0.40
1:A:420:PRO:HA	1:A:421:PRO:C	2.46	0.40
2:D:379:SER:HB3	2:D:385:LYS:O	2.20	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	551/557 (99%)	527 (96%)	23 (4%)	1 (0%)	43	63
1	C	552/557 (99%)	527 (96%)	25 (4%)	0	100	100
2	B	402/444 (90%)	384 (96%)	18 (4%)	0	100	100
2	D	402/444 (90%)	390 (97%)	12 (3%)	0	100	100
All	All	1907/2002 (95%)	1828 (96%)	78 (4%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	ILE

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	492/494 (100%)	492 (100%)	0	100	100
1	C	493/494 (100%)	491 (100%)	2 (0%)	84	93
2	B	365/400 (91%)	360 (99%)	5 (1%)	59	81
2	D	365/400 (91%)	365 (100%)	0	100	100
All	All	1715/1788 (96%)	1708 (100%)	7 (0%)	84	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	65	LYS
2	B	356	ARG
2	B	357	MET
2	B	358	LYS
2	B	424	LYS
1	C	184	MET
1	C	206	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	91	GLN
1	A	174	GLN
1	A	207	GLN
1	A	394	GLN
1	A	407	GLN
2	B	137	ASN
2	B	147	ASN
2	B	151	GLN
2	B	174	GLN
2	B	235	HIS
2	B	255	ASN
2	B	258	GLN
2	B	394	GLN
2	B	418	ASN
1	C	147	ASN
1	C	161	GLN
1	C	278	GLN
1	C	334	GLN
1	C	407	GLN
1	C	464	GLN
1	C	487	GLN
1	C	545	ASN
1	C	547	GLN
2	D	147	ASN
2	D	182	GLN
2	D	242	GLN
2	D	255	ASN
2	D	269	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	E	4	3	19,22,23	3.05	7 (36%)	25,31,34	0.82	1 (4%)
3	OMC	F	4	3	19,22,23	3.21	8 (42%)	25,31,34	0.81	1 (4%)
3	OMC	E	2	3	19,22,23	3.14	8 (42%)	25,31,34	0.85	1 (4%)
3	OMC	F	2	3	19,22,23	3.24	8 (42%)	25,31,34	0.99	2 (8%)

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	-	0/9/27/28	0/2/2/2
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	F	2	3	-	0/9/27/28	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	OMC	C6-C5	6.43	1.50	1.35
3	F	4	OMC	C4-N3	6.38	1.47	1.34
3	F	4	OMC	C2-N3	6.33	1.48	1.36
3	F	4	OMC	C6-C5	6.15	1.49	1.35
3	E	4	OMC	C2-N3	6.11	1.48	1.36
3	E	4	OMC	C6-C5	5.95	1.48	1.35
3	F	2	OMC	C4-N4	5.90	1.48	1.33
3	E	2	OMC	C6-C5	5.87	1.48	1.35
3	E	4	OMC	C4-N3	5.80	1.46	1.34
3	F	2	OMC	C2-N3	5.78	1.47	1.36
3	E	2	OMC	C4-N4	5.72	1.47	1.33
3	E	2	OMC	C4-N3	5.68	1.45	1.34
3	F	2	OMC	C4-N3	5.58	1.45	1.34
3	F	4	OMC	C4-N4	5.28	1.46	1.33
3	E	2	OMC	C2-N3	5.25	1.46	1.36
3	E	4	OMC	C4-N4	5.21	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	OMC	C2-N1	4.86	1.50	1.40
3	F	4	OMC	C2-N1	4.68	1.49	1.40
3	E	4	OMC	C2-N1	4.61	1.49	1.40
3	F	2	OMC	C2-N1	4.51	1.49	1.40
3	E	2	OMC	C6-N1	3.94	1.47	1.38
3	F	2	OMC	C6-N1	3.93	1.47	1.38
3	F	2	OMC	O2-C2	-3.70	1.16	1.23
3	E	2	OMC	O2-C2	-3.55	1.17	1.23
3	F	4	OMC	C6-N1	3.36	1.46	1.38
3	E	4	OMC	C6-N1	3.26	1.45	1.38
3	F	4	OMC	O2-C2	-3.23	1.17	1.23
3	E	2	OMC	C5-C4	2.88	1.49	1.42
3	F	2	OMC	C5-C4	2.83	1.49	1.42
3	E	4	OMC	O2-C2	-2.54	1.19	1.23
3	F	4	OMC	C5-C4	2.06	1.47	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4	OMC	N4-C4-N3	2.27	121.96	117.91
3	F	2	OMC	C6-C5-C4	2.24	121.21	117.53
3	F	2	OMC	C5-C6-N1	-2.23	118.22	121.84
3	E	2	OMC	C5-C6-N1	-2.04	118.52	121.84
3	F	4	OMC	N4-C4-N3	2.02	121.52	117.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	4	OMC	2	0
3	F	4	OMC	1	0
3	F	2	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	0.52	0	15,15,17	0.95	0
4	FRU	G	2	4	11,12,12	0.63	0	10,18,18	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
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.

There are no bond angle outliers.

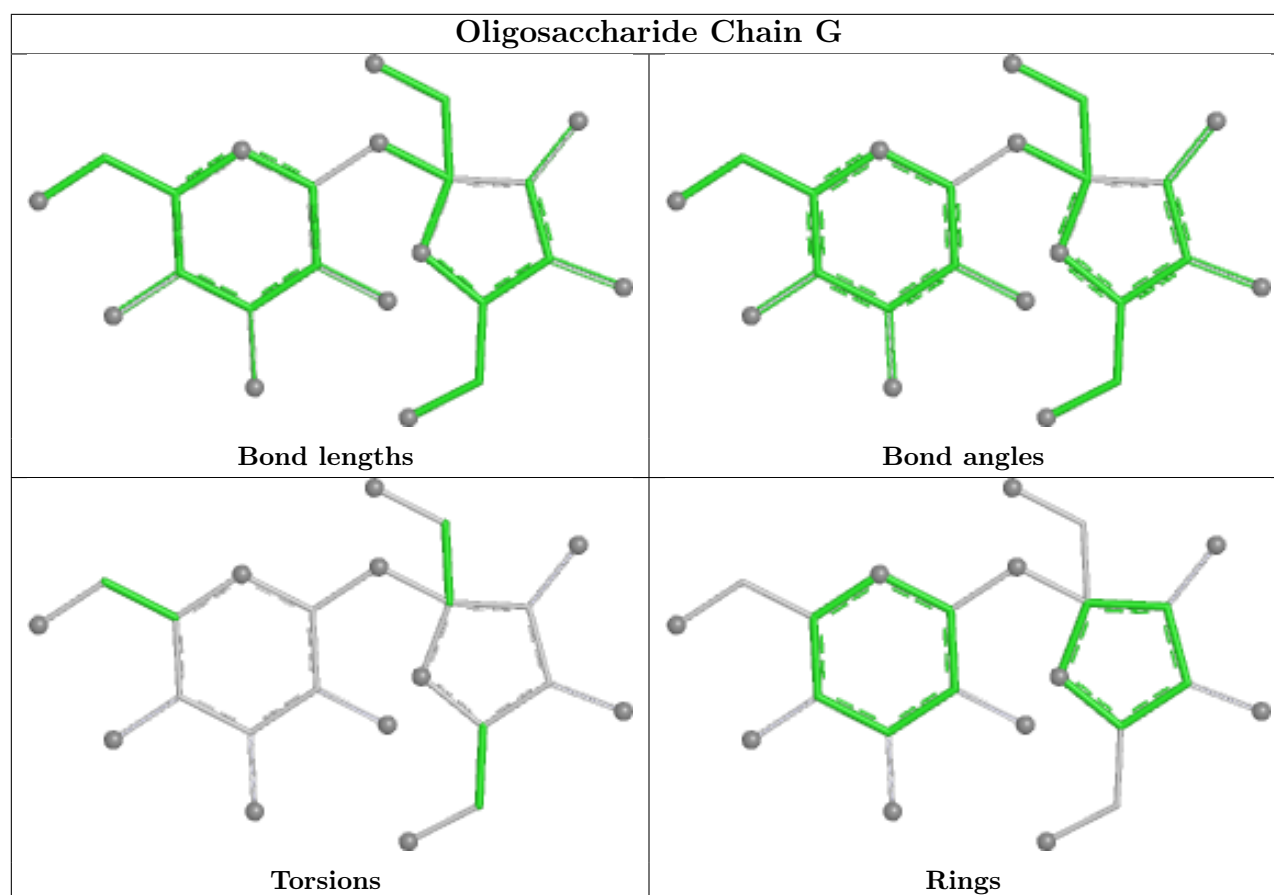
There are no chirality outliers.

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 [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
7	GOL	D	701	-	5,5,5	1.18	0	5,5,5	1.28	0
7	GOL	D	702	-	5,5,5	1.23	0	5,5,5	1.10	0
5	1RZ	C	601	6	27,28,28	1.13	1 (3%)	38,43,43	1.09	1 (2%)
5	1RZ	A	601	6	27,28,28	1.10	0	38,43,43	1.06	1 (2%)
7	GOL	B	701	-	5,5,5	1.14	0	5,5,5	1.04	0
7	GOL	B	702	-	5,5,5	0.97	0	5,5,5	1.04	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
7	GOL	D	701	-	-	0/4/4/4	-
7	GOL	D	702	-	-	0/4/4/4	-
5	1RZ	C	601	6	-	3/22/31/31	0/2/2/2
5	1RZ	A	601	6	-	3/22/31/31	0/2/2/2
7	GOL	B	701	-	-	2/4/4/4	-
7	GOL	B	702	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	601	1RZ	C2'-S3'	-2.02	1.75	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	601	1RZ	C2'-S3'-C4'	4.29	99.07	88.41
5	A	601	1RZ	C2'-S3'-C4'	4.24	98.96	88.41

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	1RZ	C5'-O5'-PA-O3A
5	A	601	1RZ	C5'-O5'-PA-O1A
7	B	701	GOL	C1-C2-C3-O3
7	B	701	GOL	O2-C2-C3-O3
5	C	601	1RZ	PA-O3A-PB-O2B
5	A	601	1RZ	C5'-O5'-PA-O2A
5	C	601	1RZ	PB-O3A-PA-O1A
5	C	601	1RZ	PB-O3A-PA-O2A

There are no ring outliers.

3 monomers are involved in 7 short contacts:

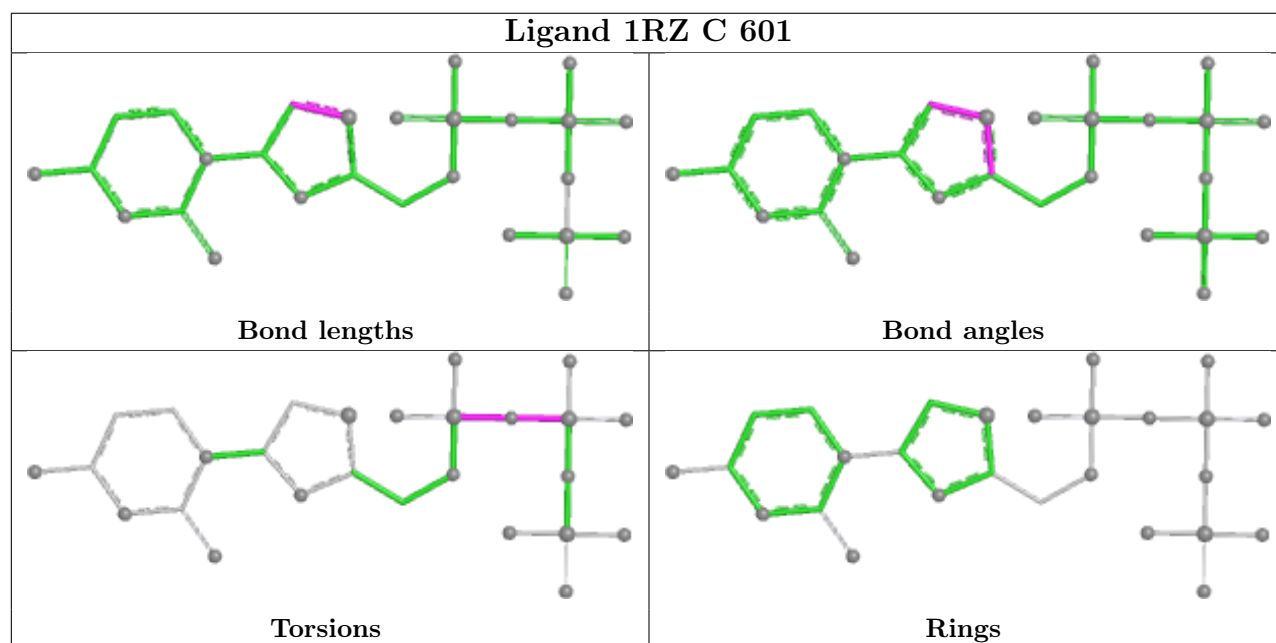
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	701	GOL	3	0

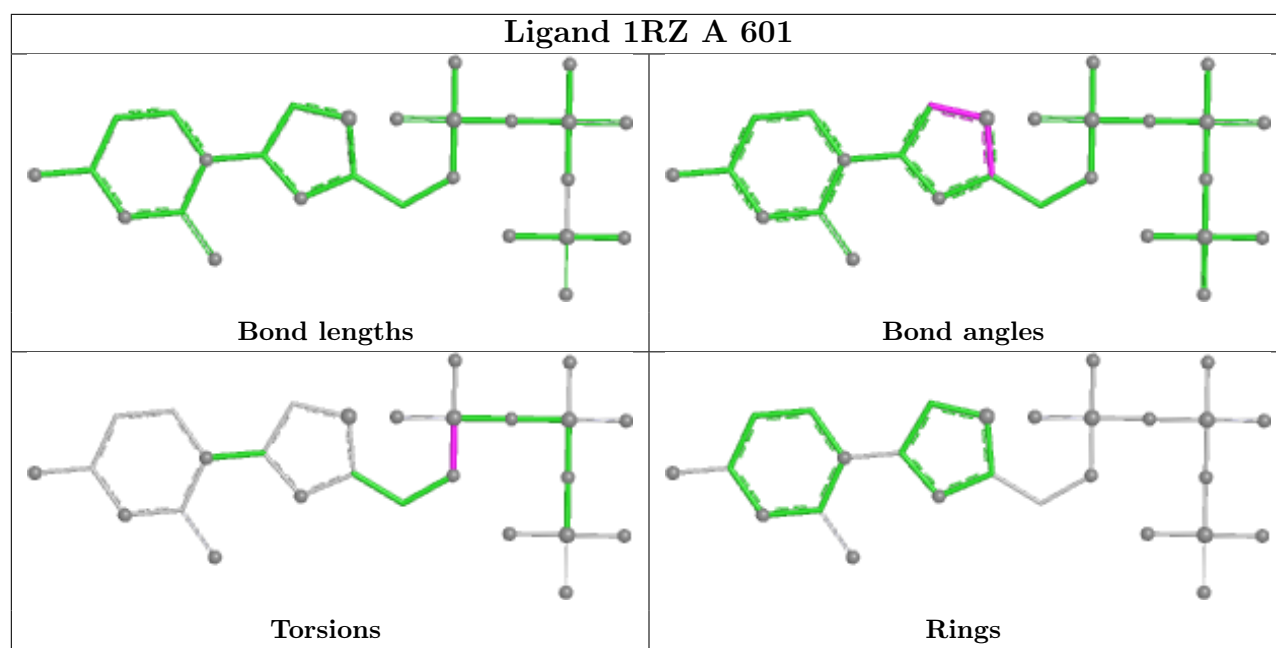
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	601	1RZ	1	0
5	A	601	1RZ	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	553/557 (99%)	0.15	37 (6%)	24	21	36, 62, 99, 131	0
1	C	553/557 (99%)	0.17	19 (3%)	48	43	37, 68, 108, 158	1 (0%)
2	B	406/444 (91%)	0.42	35 (8%)	16	14	39, 75, 120, 135	0
2	D	406/444 (91%)	0.04	21 (5%)	33	29	36, 61, 94, 112	0
3	E	33/38 (86%)	-0.60	0	100	100	38, 58, 89, 119	0
3	F	36/38 (94%)	-0.21	0	100	100	41, 72, 114, 136	0
All	All	1987/2078 (95%)	0.17	112 (5%)	30	26	36, 66, 109, 158	1 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	425	LEU	7.3
1	A	133	PRO	6.8
1	C	135	ILE	6.3
2	B	422	LEU	6.3
1	A	31	ILE	5.9
1	A	135	ILE	5.8
2	B	360	ALA	5.5
2	D	232	TYR	5.3
2	B	195	ILE	4.9
1	A	62	ALA	4.8
2	B	92	LEU	4.7
2	D	360	ALA	4.7
2	D	427	TYR	4.6
2	B	88	TRP	4.6
2	B	231	GLY	4.3
1	A	132	ILE	4.0
1	A	63	ILE	4.0
1	A	134	SER	3.9
1	A	140	PRO	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	33	ALA	3.9
1	A	34	LEU	3.9
1	A	69	THR	3.9
2	B	93	GLY	3.8
1	C	134	SER	3.8
2	B	423	VAL	3.8
1	A	64	LYS	3.7
1	C	136	ASN	3.7
1	A	28	GLU	3.6
2	D	357	MET	3.5
2	B	68	SER	3.5
2	B	427	TYR	3.4
2	B	210	LEU	3.4
2	D	212	TRP	3.3
2	B	361	HIS	3.3
1	A	27	THR	3.2
2	B	95	PRO	3.2
1	A	142	ILE	3.1
2	B	90	VAL	3.1
1	C	450	THR	3.0
1	A	141	GLY	3.0
1	A	553	SER	3.0
1	C	452	LEU	2.9
1	A	61	PHE	2.9
2	B	94	ILE	2.9
1	A	30	LYS	2.9
2	B	212	TRP	2.9
2	D	5	ILE	2.8
1	A	60	VAL	2.8
2	B	232	TYR	2.8
2	D	420	PRO	2.8
2	B	357	MET	2.8
1	A	36	GLU	2.8
1	A	131	THR	2.7
2	B	425	LEU	2.7
2	B	292	VAL	2.7
1	A	67	ASP	2.7
2	B	359	GLY	2.7
2	B	240	THR	2.7
2	B	67	ASP	2.7
2	B	301	LEU	2.7
2	D	361	HIS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	290	THR	2.6
2	D	362	THR	2.6
1	C	68	SER	2.6
1	A	39	THR	2.5
2	B	362	THR	2.5
2	B	5	ILE	2.5
2	B	66	LYS	2.5
2	D	231	GLY	2.5
2	D	359	GLY	2.5
2	D	213	GLY	2.5
1	A	66	LYS	2.5
1	A	68	SER	2.5
2	B	421	PRO	2.4
1	A	70	LYS	2.4
2	B	213	GLY	2.4
1	A	26	LEU	2.4
2	D	314	VAL	2.4
1	C	142	ILE	2.4
1	A	137	ASN	2.4
1	A	139	THR	2.3
2	D	67	ASP	2.3
1	A	65	LYS	2.3
1	C	199	ARG	2.3
1	C	66	LYS	2.3
1	C	413	GLU	2.3
2	D	66	LYS	2.3
1	C	25	PRO	2.3
1	C	63	ILE	2.2
1	A	24	TRP	2.2
2	D	418	ASN	2.2
1	A	21	VAL	2.2
1	A	357	MET	2.2
2	D	211	ARG	2.2
1	A	37	ILE	2.1
1	C	22	LYS	2.1
2	D	421	PRO	2.1
1	C	35	VAL	2.1
2	B	245	VAL	2.1
2	B	266	TRP	2.1
2	B	295	LEU	2.1
1	C	140	PRO	2.1
1	A	23	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	26	LEU	2.1
1	C	219	LYS	2.1
2	B	314	VAL	2.0
1	C	448	ARG	2.0
1	C	69	THR	2.0
2	D	313	PRO	2.0
1	A	35	VAL	2.0
2	B	418	ASN	2.0
2	D	69	THR	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.

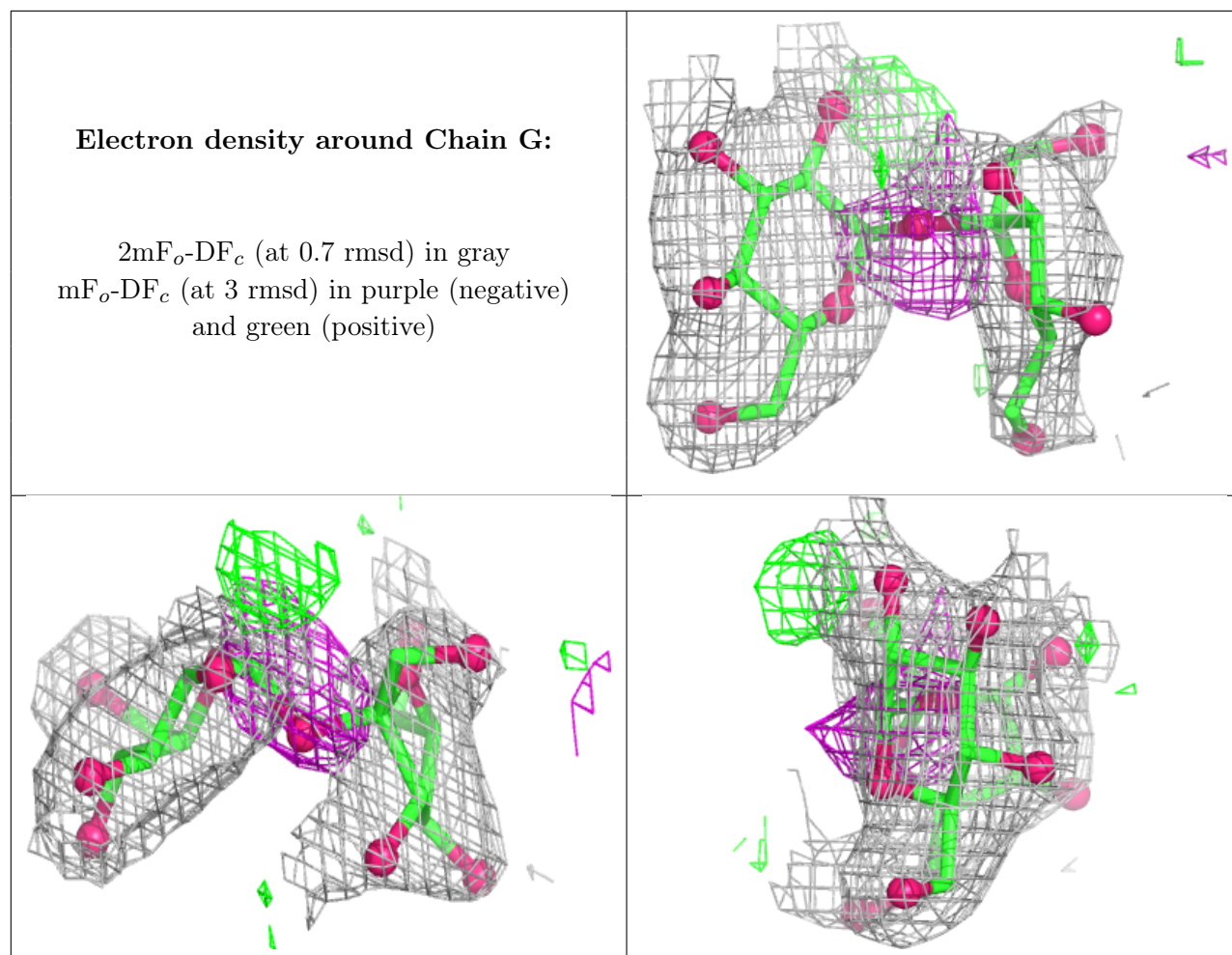
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OMC	F	4	21/22	0.95	0.09	36,48,64,88	0
3	OMC	F	2	21/22	0.96	0.08	45,58,69,79	0
3	OMC	E	2	21/22	0.97	0.07	40,48,54,57	0
3	OMC	E	4	21/22	0.98	0.06	30,44,49,52	0

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	0.79	0.17	97,107,110,110	0
4	GLC	G	1	11/12	0.91	0.11	46,70,82,90	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.

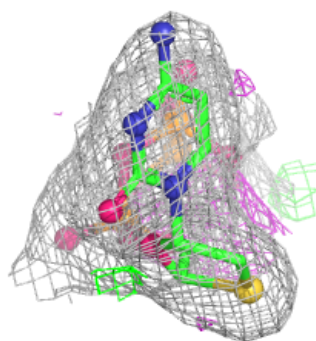
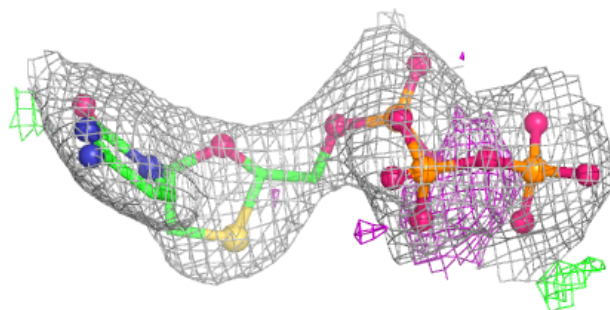
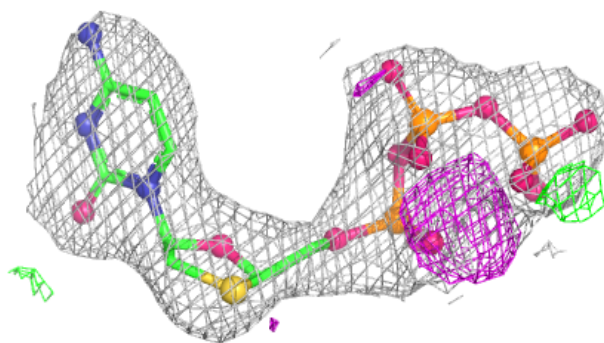
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	A	602	1/1	0.81	0.20	100,100,100,100	0
5	1RZ	C	601	27/27	0.89	0.11	63,91,120,123	0
7	GOL	B	701	6/6	0.90	0.15	58,64,67,69	0
6	MG	C	602	1/1	0.91	0.23	74,74,74,74	0
5	1RZ	A	601	27/27	0.91	0.10	73,85,106,109	0
7	GOL	D	701	6/6	0.95	0.14	46,48,51,58	0
7	GOL	D	702	6/6	0.96	0.09	48,52,54,56	0
7	GOL	B	702	6/6	0.98	0.07	45,50,56,62	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.

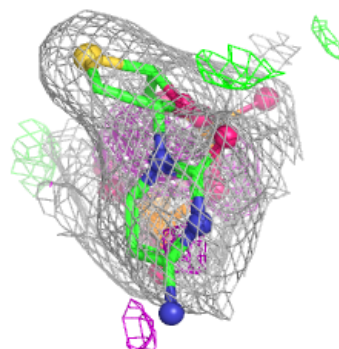
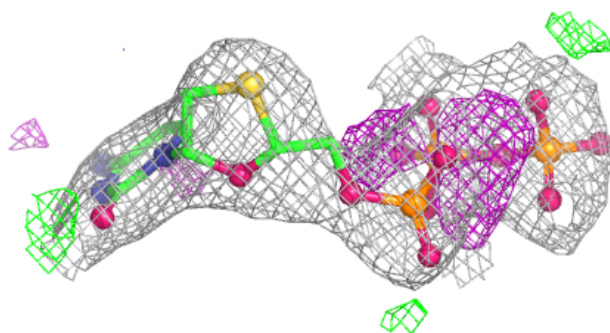
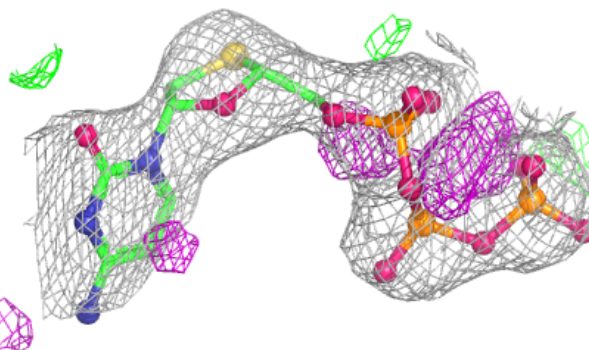
Electron density around 1RZ C 601:

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



Electron density around 1RZ A 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.