



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:39 AM UTC

PDB ID : 5HRO / pdb_00005hro
Title : STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE In COMPLEX
WITH A DNA aptamer and an Alpha-carboxy nucleoside phosphonate in-
hibitor (alpha-CNP)
Authors : Das, K.; Arnold, E.
Deposited on : 2016-01-23
Resolution : 2.75 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

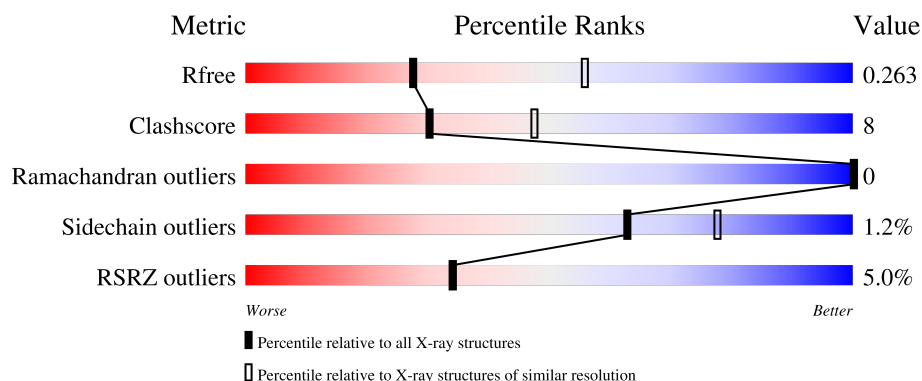
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

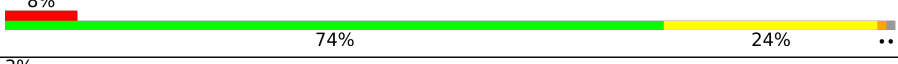
The reported resolution of this entry is 2.75 Å.

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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	555	
1	C	555	
2	B	444	
2	D	444	

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Mol	Chain	Length	Quality of chain
3	E	38	53% 37% • 8%
3	F	38	5% 61% 26% 5% 8%
4	G	2	50% 50%
4	H	2	100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17349 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	551	Total	C	N	O	S	0	0	0
			4488	2905	747	829	7			
1	C	551	Total	C	N	O	S	0	0	0
			4488	2905	747	829	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			
2	D	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP P03366
B	-14	ALA	-	expression tag	UNP P03366
B	-13	HIS	-	expression tag	UNP P03366
B	-12	HIS	-	expression tag	UNP P03366
B	-11	HIS	-	expression tag	UNP P03366
B	-10	HIS	-	expression tag	UNP P03366
B	-9	HIS	-	expression tag	UNP P03366
B	-8	HIS	-	expression tag	UNP P03366
B	-7	ALA	-	expression tag	UNP P03366
B	-6	LEU	-	expression tag	UNP P03366

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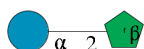
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLU	-	expression tag	UNP P03366
B	-4	VAL	-	expression tag	UNP P03366
B	-3	LEU	-	expression tag	UNP P03366
B	-2	PHE	-	expression tag	UNP P03366
B	-1	GLN	-	expression tag	UNP P03366
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366
D	-15	MET	-	initiating methionine	UNP P03366
D	-14	ALA	-	expression tag	UNP P03366
D	-13	HIS	-	expression tag	UNP P03366
D	-12	HIS	-	expression tag	UNP P03366
D	-11	HIS	-	expression tag	UNP P03366
D	-10	HIS	-	expression tag	UNP P03366
D	-9	HIS	-	expression tag	UNP P03366
D	-8	HIS	-	expression tag	UNP P03366
D	-7	ALA	-	expression tag	UNP P03366
D	-6	LEU	-	expression tag	UNP P03366
D	-5	GLU	-	expression tag	UNP P03366
D	-4	VAL	-	expression tag	UNP P03366
D	-3	LEU	-	expression tag	UNP P03366
D	-2	PHE	-	expression tag	UNP P03366
D	-1	GLN	-	expression tag	UNP P03366
D	0	GLY	-	expression tag	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	35	Total	C	N	O	P	0	0	0
			720	340	130	215	35			
3	F	35	Total	C	N	O	P	0	0	0
			720	340	130	215	35			

- 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			

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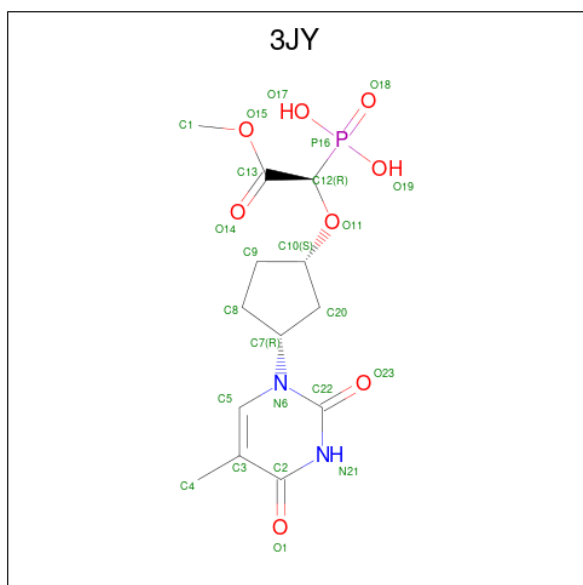
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	H	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

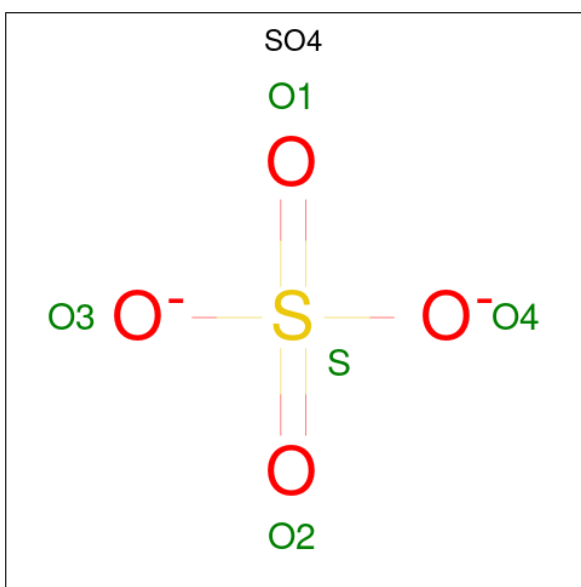
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Mg	0	0
			3	3		
5	C	3	Total	Mg	0	0
			3	3		

- Molecule 6 is [(1R)-2-methoxy-1-{[(1S,3R)-3-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)cyclopentyl]oxy}-2-oxoethyl]phosphonic acid (CCD ID: 3JY) (formula: C₁₃H₁₉N₂O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			23	12	2	8	1		
6	F	1	Total	C	N	O	P	0	0
			23	12	2	8	1		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		

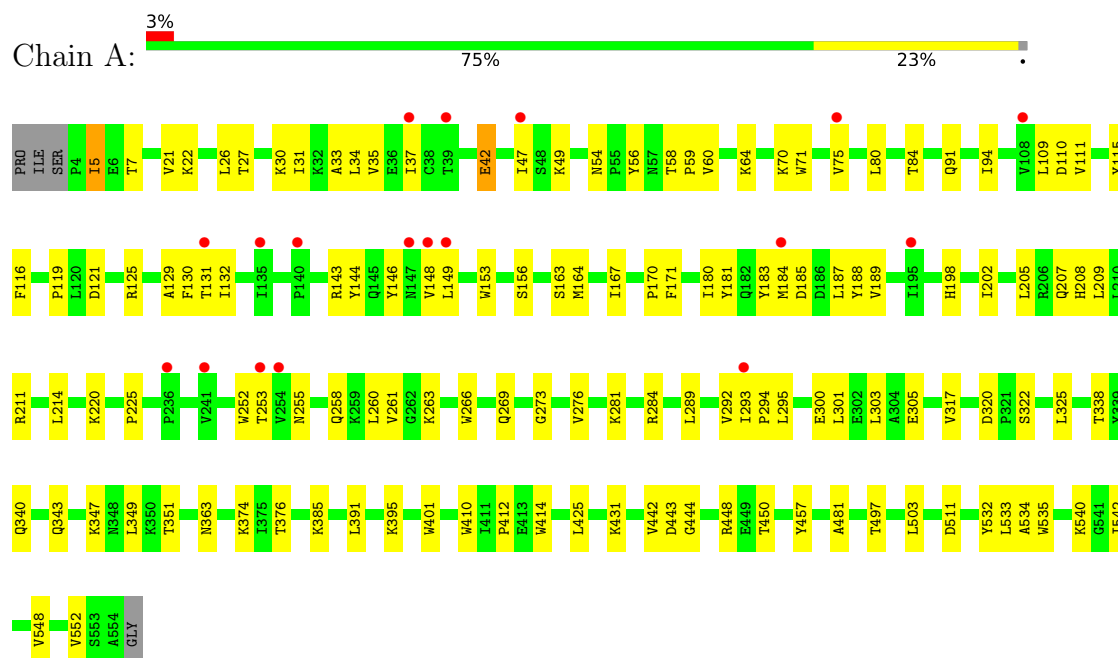
- Molecule 8 is water.

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

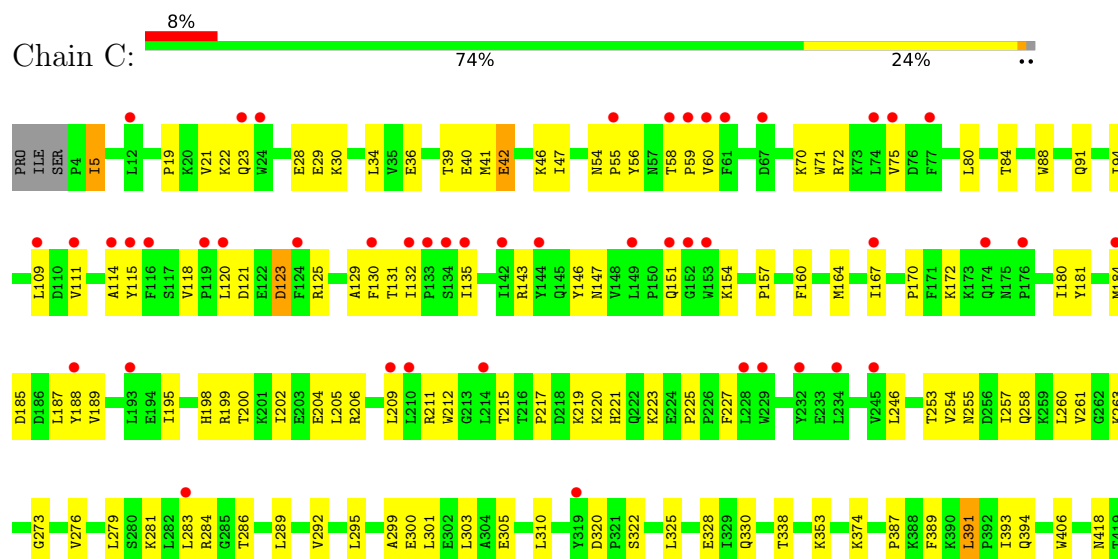
3 Residue-property plots [i](#)

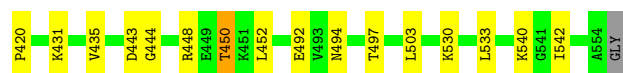
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

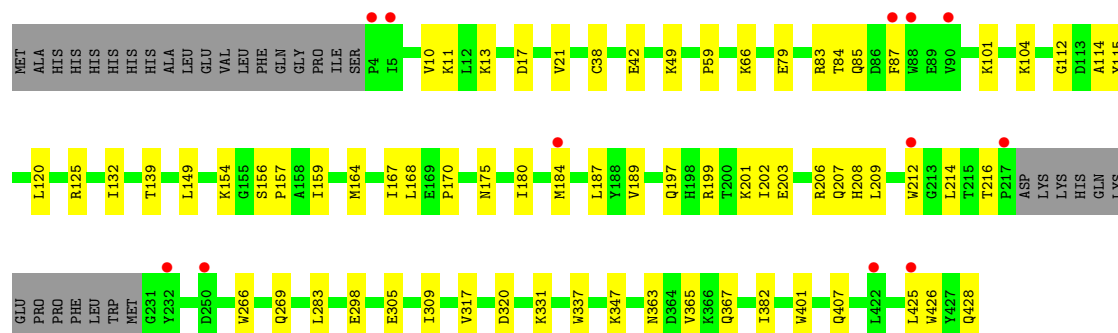
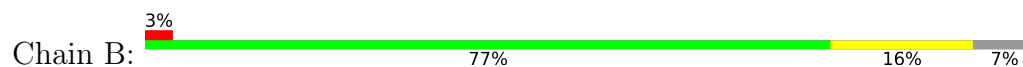


• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT

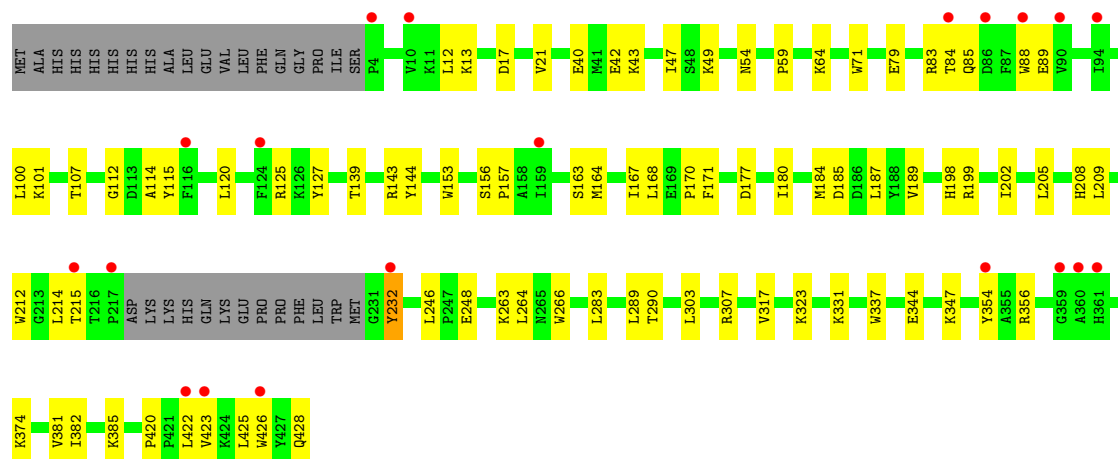
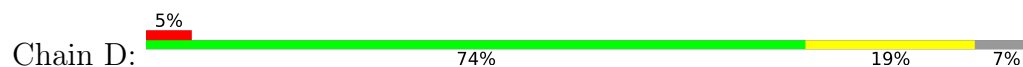




• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT



• Molecule 3: DNA (38-MER)



• Molecule 3: DNA (38-MER)

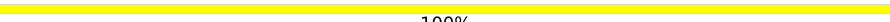


- Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain G:  50% 50%



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

Chain H:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.25Å 128.96Å 131.05Å 90.00° 101.47° 90.00°	Depositor
Resolution (Å)	38.52 – 2.75 38.52 – 2.75	Depositor EDS
% Data completeness (in resolution range)	95.8 (38.52-2.75) 95.7 (38.52-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.72Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.235 , 0.265 0.237 , 0.263	Depositor DCC
R_{free} test set	2960 reflections (3.77%)	wwPDB-VP
Wilson B-factor (Å ²)	73.1	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17349	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FRU, MG, 3JY, OMC, SO4, GLC

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	0.20	0/4605	0.42	1/6255 (0.0%)
1	C	0.20	0/4605	0.42	2/6255 (0.0%)
2	B	0.17	0/3497	0.39	0/4751
2	D	0.17	0/3497	0.41	0/4751
3	E	0.27	0/759	0.53	2/1170 (0.2%)
3	F	0.31	0/759	0.54	1/1170 (0.1%)
All	All	0.20	0/17722	0.43	6/24352 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	55	PRO	N-CA-C	6.40	125.65	112.47
3	E	19	DC	C5'-C4'-O4'	5.89	118.23	109.40
3	F	19	DC	C5'-C4'-O4'	5.74	118.02	109.40
1	C	225	PRO	O-C-N	5.56	123.76	121.15
1	A	225	PRO	O-C-N	5.26	123.62	121.15
3	E	23	DG	C5'-C4'-O4'	5.21	117.21	109.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4488	0	4545	88	0
1	C	4488	0	4545	95	0
2	B	3400	0	3431	46	0
2	D	3400	0	3430	57	0
3	E	720	0	396	14	0
3	F	720	0	396	12	0
4	G	23	0	21	1	0
4	H	23	0	21	0	0
5	A	3	0	0	0	0
5	C	3	0	0	0	0
6	A	23	0	14	0	0
6	F	23	0	14	4	0
7	A	5	0	0	0	0
7	B	20	0	0	0	0
7	C	5	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	3	0	0	0	0
All	All	17349	0	16813	287	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 (287) 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:255:ASN:HB2	1:A:289:LEU:HD21	1.27	1.09
1:A:255:ASN:HB2	1:A:289:LEU:CD2	1.98	0.92
1:C:221:HIS:HE1	1:C:223:LYS:HG3	1.39	0.88
1:A:255:ASN:CB	1:A:289:LEU:HD21	2.11	0.80
1:C:255:ASN:HB2	1:C:289:LEU:CD2	2.10	0.80
2:D:248:GLU:OE1	2:D:307:ARG:NH2	2.15	0.80
1:C:56:TYR:HB2	1:C:129:ALA:HB3	1.65	0.78
1:C:221:HIS:CE1	1:C:223:LYS:HG3	2.20	0.76
1:A:110:ASP:HB3	1:A:220:LYS:HB3	1.70	0.73
1:C:255:ASN:HB2	1:C:289:LEU:HD21	1.71	0.71
6:F:101:3JY:H11	6:F:101:3JY:H6	1.73	0.70
1:C:261:VAL:HG13	1:C:276:VAL:HG11	1.72	0.70
1:C:172:LYS:HE2	1:C:180:ILE:HB	1.75	0.69
1:A:56:TYR:HB2	1:A:129:ALA:HB3	1.74	0.69
2:D:115:TYR:CD2	2:D:156:SER:HB3	2.28	0.69
1:C:72:ARG:NH1	6:F:101:3JY:O19	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:VAL:HB	1:C:185:ASP:HB2	1.75	0.67
1:A:207:GLN:O	1:A:211:ARG:N	2.26	0.67
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.76	0.66
2:D:180:ILE:HG12	2:D:189:VAL:HG22	1.78	0.66
1:A:183:TYR:OH	3:E:36:DG:N3	2.29	0.63
1:A:255:ASN:HD22	1:A:289:LEU:HD11	1.62	0.63
1:C:60:VAL:HG22	1:C:75:VAL:HG13	1.79	0.63
1:C:41:MET:HB3	1:C:46:LYS:HB2	1.81	0.62
1:C:19:PRO:HB2	1:C:58:THR:HG23	1.79	0.62
1:A:94:ILE:HD11	3:E:35:DG:H21	1.65	0.62
3:E:27:DC:H2''	3:E:28:DG:C8	2.35	0.61
1:C:5:ILE:HG22	1:C:212:TRP:HD1	1.64	0.61
2:B:13:LYS:HD2	2:B:85:GLN:HB3	1.83	0.61
2:B:206:ARG:NH2	2:B:216:THR:O	2.33	0.61
1:A:64:LYS:HA	1:A:71:TRP:HA	1.83	0.61
1:A:21:VAL:HG23	1:A:59:PRO:HD3	1.82	0.60
1:A:448:ARG:HH21	3:E:22:DT:H5''	1.65	0.60
2:D:199:ARG:HA	2:D:202:ILE:HD12	1.84	0.60
1:C:184:MET:HG2	3:F:37:DG:H2''	1.83	0.59
1:A:164:MET:HE2	1:A:187:LEU:HD11	1.85	0.59
2:B:180:ILE:HG12	2:B:189:VAL:HG22	1.84	0.59
1:A:253:THR:HA	1:A:292:VAL:HA	1.85	0.59
1:C:118:VAL:HG21	1:C:160:PHE:HD1	1.68	0.59
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.84	0.59
2:D:266:TRP:NE1	2:D:425:LEU:HD22	2.17	0.59
2:D:170:PRO:HB2	2:D:208:HIS:CE1	2.37	0.58
1:C:257:ILE:HB	1:C:283:LEU:HD21	1.85	0.58
2:B:157:PRO:HG3	2:B:184:MET:HA	1.85	0.58
2:B:115:TYR:CD2	2:B:156:SER:HB3	2.38	0.58
1:C:258:GLN:CD	3:F:32:DG:H2''	2.28	0.58
1:A:70:LYS:HG2	1:A:71:TRP:H	1.69	0.58
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.86	0.57
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.87	0.57
1:C:180:ILE:HG23	1:C:189:VAL:HG22	1.87	0.57
1:C:125:ARG:HE	1:C:147:ASN:HA	1.68	0.57
2:B:170:PRO:HB2	2:B:208:HIS:CE1	2.40	0.57
1:C:202:ILE:O	1:C:206:ARG:HG3	2.06	0.56
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.87	0.56
2:D:114:ALA:HB2	2:D:214:LEU:HD22	1.88	0.56
2:B:199:ARG:HA	2:B:202:ILE:HD12	1.87	0.56
1:C:23:GLN:NE2	1:C:131:THR:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:LYS:HE2	1:C:220:LYS:HE2	1.88	0.56
1:C:5:ILE:HG22	1:C:212:TRP:CD1	2.40	0.55
1:C:23:GLN:HG3	1:C:131:THR:HG23	1.89	0.55
1:C:181:TYR:HB2	1:C:188:TYR:HB3	1.87	0.55
2:D:198:HIS:CD2	2:D:202:ILE:HD11	2.42	0.55
1:C:279:LEU:HD23	1:C:299:ALA:HB1	1.88	0.55
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.89	0.54
1:A:34:LEU:HD21	1:A:132:ILE:HD12	1.88	0.54
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.88	0.54
3:E:12:DT:H2'	3:E:13:DT:H71	1.89	0.54
1:C:123:ASP:N	1:C:123:ASP:OD1	2.40	0.54
1:A:395:LYS:NZ	1:A:414:TRP:O	2.40	0.54
2:B:363:ASN:O	2:B:367:GLN:HG3	2.08	0.54
2:B:17:ASP:O	2:B:83:ARG:NH1	2.40	0.54
1:C:253:THR:HA	1:C:292:VAL:HA	1.90	0.54
1:A:252:TRP:O	1:A:292:VAL:HG23	2.09	0.53
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.91	0.53
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.43	0.53
1:C:72:ARG:NH2	6:F:101:3JY:O19	2.42	0.53
1:C:255:ASN:HB2	1:C:289:LEU:HD23	1.89	0.53
1:A:281:LYS:O	1:A:284:ARG:HG2	2.07	0.53
2:B:164:MET:HE3	2:B:168:LEU:HD21	1.91	0.53
1:C:281:LYS:O	1:C:284:ARG:HG2	2.09	0.53
2:B:87:PHE:HZ	2:B:159:ILE:HG13	1.73	0.53
1:C:60:VAL:HG21	1:C:130:PHE:CD2	2.44	0.53
1:A:180:ILE:HG23	1:A:189:VAL:HG22	1.89	0.53
1:C:255:ASN:CB	1:C:289:LEU:HD21	2.38	0.53
2:D:54:ASN:HB3	2:D:143:ARG:HH21	1.74	0.52
1:C:202:ILE:HG22	1:C:206:ARG:HD2	1.90	0.52
2:B:167:ILE:HG23	2:B:212:TRP:CD1	2.44	0.52
2:D:64:LYS:HE3	2:D:71:TRP:CE2	2.45	0.52
1:A:273:GLY:HA2	1:A:338:THR:HG21	1.91	0.52
1:A:94:ILE:HD11	3:E:35:DG:N2	2.25	0.52
1:C:448:ARG:HH21	3:F:22:DT:H5''	1.73	0.52
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.90	0.52
2:B:203:GLU:O	2:B:207:GLN:HG2	2.10	0.52
1:C:94:ILE:HD12	3:F:8:OMC:HM23	1.91	0.51
2:D:263:LYS:HA	2:D:423:VAL:HG21	1.92	0.51
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.93	0.51
1:A:27:THR:O	1:A:31:ILE:HG13	2.10	0.51
2:D:266:TRP:CD1	2:D:266:TRP:C	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.93	0.51
2:D:115:TYR:HD2	2:D:156:SER:HB3	1.75	0.51
2:D:266:TRP:CD1	2:D:425:LEU:HD13	2.46	0.51
2:D:13:LYS:HD2	2:D:85:GLN:HB3	1.93	0.51
1:A:47:ILE:HG13	1:A:144:TYR:HB3	1.94	0.50
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.93	0.50
1:A:503:LEU:HD11	1:A:533:LEU:HB3	1.92	0.50
2:B:197:GLN:O	2:B:201:LYS:HG2	2.12	0.50
3:E:7:DC:H2'	3:E:8:OMC:C6	2.47	0.50
2:D:84:THR:HG21	2:D:153:TRP:HZ2	1.77	0.50
2:D:425:LEU:HD23	2:D:426:TRP:CE2	2.47	0.50
3:E:7:DC:H2'	3:E:8:OMC:H6	1.77	0.49
1:C:492:GLU:HG2	1:C:530:LYS:HB2	1.94	0.49
2:B:167:ILE:HG12	2:B:212:TRP:CD2	2.47	0.49
2:B:209:LEU:HD13	2:B:214:LEU:HD23	1.94	0.49
2:D:209:LEU:HD13	2:D:214:LEU:HD23	1.94	0.49
1:A:293:ILE:HG13	1:A:294:PRO:HD2	1.95	0.49
1:C:260:LEU:HD21	1:C:303:LEU:HD13	1.94	0.49
1:A:47:ILE:HD12	1:A:146:TYR:HA	1.95	0.49
2:B:320:ASP:OD2	1:C:418:ASN:ND2	2.39	0.49
2:D:42:GLU:OE2	2:D:49:LYS:HG3	2.12	0.49
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.94	0.48
1:C:28:GLU:HB2	1:C:135:ILE:HD12	1.95	0.48
2:D:120:LEU:HD23	2:D:125:ARG:HG2	1.94	0.48
1:A:443:ASP:OD1	1:A:444:GLY:N	2.46	0.48
2:D:177:ASP:OD1	2:D:177:ASP:N	2.37	0.48
2:D:356:ARG:HG3	2:D:356:ARG:O	2.13	0.48
1:A:548:VAL:O	1:A:552:VAL:HG22	2.14	0.48
3:F:17:DT:H4'	3:F:18:DG:OP1	2.14	0.48
1:C:542:ILE:HG23	2:D:283:LEU:HD13	1.94	0.48
1:C:205:LEU:O	1:C:209:LEU:HG	2.14	0.48
2:D:167:ILE:HG23	2:D:212:TRP:CD1	2.49	0.48
1:A:110:ASP:HB3	1:A:220:LYS:CB	2.43	0.47
1:C:70:LYS:HG2	1:C:71:TRP:H	1.79	0.47
1:A:301:LEU:O	1:A:305:GLU:HG2	2.14	0.47
1:A:5:ILE:HD11	1:A:163:SER:HB3	1.96	0.47
2:B:317:VAL:HG12	2:B:347:LYS:HB3	1.95	0.47
1:C:255:ASN:ND2	1:C:289:LEU:HD21	2.29	0.47
2:D:17:ASP:O	2:D:83:ARG:HD3	2.14	0.47
1:A:30:LYS:HG2	1:A:71:TRP:CZ3	2.50	0.47
1:C:254:VAL:HG13	1:C:283:LEU:HD22	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:LEU:HB3	1:C:393:ILE:HG22	1.97	0.47
2:D:428:GLN:HE21	2:D:428:GLN:HA	1.80	0.47
1:A:317:VAL:HG11	1:A:347:LYS:HB3	1.97	0.47
1:C:389:PHE:HB3	1:C:391:LEU:HD13	1.97	0.47
1:C:494:ASN:HB3	2:D:289:LEU:HD12	1.96	0.47
1:C:540:LYS:HA	1:C:540:LYS:HD3	1.68	0.47
2:D:100:LEU:HG	2:D:381:VAL:HG13	1.96	0.47
2:D:163:SER:O	2:D:167:ILE:HG13	2.15	0.47
1:A:167:ILE:O	1:A:170:PRO:HD2	2.14	0.47
1:C:263:LYS:HD2	3:F:34:DG:H4'	1.97	0.47
1:A:266:TRP:O	1:A:269:GLN:HG2	2.15	0.47
1:C:114:ALA:HB1	1:C:160:PHE:CE1	2.50	0.47
6:F:101:3JY:H6	6:F:101:3JY:H3	1.58	0.47
1:C:120:LEU:HD12	1:C:121:ASP:H	1.80	0.46
2:D:79:GLU:HG3	2:D:83:ARG:HE	1.80	0.46
2:D:112:GLY:HA2	2:D:115:TYR:CD1	2.51	0.46
3:F:17:DT:H2''	3:F:18:DG:C8	2.50	0.46
1:A:31:ILE:O	1:A:35:VAL:HG23	2.14	0.46
1:A:263:LYS:HD2	3:E:34:DG:H4'	1.97	0.46
2:B:115:TYR:O	2:B:149:LEU:HB2	2.16	0.46
1:A:121:ASP:O	1:A:125:ARG:HG3	2.15	0.46
2:B:66:LYS:NZ	2:B:407:GLN:OE1	2.39	0.46
1:C:29:GLU:HG3	1:C:30:LYS:N	2.31	0.46
1:C:125:ARG:NE	1:C:147:ASN:HA	2.30	0.46
1:C:131:THR:HB	1:C:143:ARG:HG2	1.98	0.46
1:C:167:ILE:O	1:C:170:PRO:HD2	2.16	0.46
1:C:200:THR:O	1:C:204:GLU:HG3	2.16	0.46
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.51	0.46
1:C:198:HIS:O	1:C:202:ILE:HG12	2.16	0.46
2:B:428:GLN:HE21	2:B:428:GLN:HA	1.80	0.45
1:C:34:LEU:HD21	1:C:132:ILE:HD12	1.98	0.45
2:D:12:LEU:HD11	2:D:127:TYR:CE1	2.50	0.45
1:A:7:THR:OG1	1:A:121:ASP:HA	2.16	0.45
1:A:60:VAL:HG22	1:A:75:VAL:HG13	1.98	0.45
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.56	0.45
1:C:273:GLY:HA2	1:C:338:THR:HG21	1.97	0.45
1:A:54:ASN:O	1:A:143:ARG:NH2	2.49	0.45
2:B:154:LYS:HG2	2:B:184:MET:SD	2.57	0.45
1:A:5:ILE:HD12	1:A:167:ILE:HD11	1.99	0.45
1:C:255:ASN:CG	1:C:289:LEU:HD21	2.42	0.45
2:D:323:LYS:NZ	2:D:344:GLU:OE2	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:GLN:HG3	1:A:351:THR:HG22	1.98	0.45
1:C:211:ARG:HB2	1:C:212:TRP:CE3	2.52	0.45
1:C:227:PHE:CD2	1:C:227:PHE:N	2.84	0.45
2:D:171:PHE:CD2	2:D:205:LEU:HD13	2.51	0.45
1:C:80:LEU:O	1:C:84:THR:OG1	2.33	0.45
1:A:116:PHE:O	1:A:148:VAL:HG11	2.17	0.45
1:A:295:LEU:HB3	1:A:300:GLU:HG2	1.99	0.45
2:D:40:GLU:HA	2:D:43:LYS:HG2	1.98	0.45
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.52	0.44
1:C:246:LEU:HD11	1:C:310:LEU:HD22	1.99	0.44
1:C:320:ASP:OD1	1:C:322:SER:OG	2.29	0.44
1:A:153:TRP:HB3	1:A:156:SER:OG	2.17	0.44
2:D:88:TRP:CE3	2:D:89:GLU:HG3	2.52	0.44
1:C:54:ASN:O	1:C:143:ARG:NH2	2.50	0.44
2:B:112:GLY:HA2	2:B:115:TYR:CD1	2.53	0.44
1:C:338:THR:HG22	1:C:353:LYS:HB3	2.00	0.44
2:D:303:LEU:HG	2:D:307:ARG:NH1	2.33	0.44
2:D:331:LYS:HB2	2:D:337:TRP:CZ3	2.53	0.44
1:A:171:PHE:CD2	1:A:205:LEU:HD13	2.53	0.44
1:C:36:GLU:O	1:C:40:GLU:HG3	2.18	0.44
1:C:258:GLN:NE2	3:F:32:DG:H2''	2.33	0.44
1:A:60:VAL:HG21	1:A:130:PHE:CD2	2.53	0.44
2:B:425:LEU:HD23	2:B:426:TRP:CE2	2.52	0.43
1:C:21:VAL:HG23	1:C:59:PRO:HD3	2.00	0.43
2:D:317:VAL:HG12	2:D:347:LYS:HB3	1.98	0.43
1:A:325:LEU:HD12	1:A:385:LYS:HG3	2.00	0.43
2:B:66:LYS:HG2	2:B:407:GLN:CD	2.43	0.43
2:B:101:LYS:HD3	2:B:382:ILE:HG23	2.01	0.43
2:D:323:LYS:O	2:D:385:LYS:NZ	2.50	0.43
1:A:320:ASP:OD1	1:A:322:SER:OG	2.25	0.43
1:C:418:ASN:O	1:C:420:PRO:HD3	2.18	0.43
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.53	0.43
1:C:435:VAL:HG22	2:D:290:THR:HG21	2.00	0.43
2:D:47:ILE:HD12	2:D:144:TYR:CD2	2.53	0.43
1:A:70:LYS:HG2	1:A:71:TRP:N	2.32	0.43
1:C:91:GLN:O	3:F:7:DC:H4'	2.19	0.43
1:C:157:PRO:HG2	3:F:6:OMC:H1'	2.00	0.43
1:A:208:HIS:O	1:A:211:ARG:HB2	2.19	0.43
2:D:354:TYR:HD2	2:D:374:LYS:HD3	1.83	0.43
1:C:115:TYR:CD2	1:C:151:GLN:HG2	2.53	0.43
1:C:443:ASP:OD1	1:C:444:GLY:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:GLU:O	2:B:309:ILE:HG13	2.19	0.42
1:C:295:LEU:HB3	1:C:300:GLU:HG2	2.00	0.42
2:D:101:LYS:HD3	2:D:382:ILE:HG23	2.01	0.42
2:D:164:MET:HE3	2:D:168:LEU:HD21	2.00	0.42
1:A:198:HIS:O	1:A:202:ILE:HG12	2.19	0.42
1:C:88:TRP:CD1	2:D:143:ARG:NH1	2.88	0.42
2:D:107:THR:HA	2:D:232:TYR:O	2.20	0.42
1:A:442:VAL:HG12	1:A:457:TYR:HB3	2.01	0.42
1:C:450:THR:HG22	1:C:452:LEU:HG	2.00	0.42
2:D:112:GLY:HA2	2:D:115:TYR:CE1	2.55	0.42
2:D:422:LEU:HG	2:D:423:VAL:HG12	2.00	0.42
3:F:8:OMC:HM23	3:F:8:OMC:H1'	1.83	0.42
1:A:115:TYR:HB3	1:A:149:LEU:O	2.18	0.42
2:D:185:ASP:OD1	2:D:185:ASP:N	2.50	0.42
1:C:39:THR:O	1:C:42:GLU:HG3	2.20	0.42
1:C:215:THR:C	1:C:217:PRO:HD3	2.45	0.42
1:C:254:VAL:HG21	1:C:286:THR:HG21	2.02	0.42
1:A:457:TYR:HA	1:A:548:VAL:HG21	2.02	0.42
2:B:298:GLU:H	2:B:298:GLU:CD	2.28	0.42
2:B:120:LEU:HD23	2:B:125:ARG:HG2	2.02	0.42
1:C:84:THR:HB	1:C:154:LYS:HE2	2.02	0.42
1:A:91:GLN:O	3:E:7:DC:H4'	2.19	0.42
1:A:410:TRP:CH2	1:A:412:PRO:HA	2.55	0.42
2:B:115:TYR:HE2	2:B:157:PRO:HA	1.85	0.42
1:A:258:GLN:HB3	3:E:33:DG:H4'	2.02	0.42
1:A:22:LYS:HD3	1:A:22:LYS:HA	1.79	0.41
1:A:33:ALA:O	1:A:37:ILE:HG12	2.21	0.41
1:A:266:TRP:CE2	3:E:35:DG:H4'	2.55	0.41
1:C:164:MET:HE2	1:C:187:LEU:HD11	2.01	0.41
1:A:5:ILE:CG2	1:A:119:PRO:HD2	2.50	0.41
2:B:164:MET:HE2	2:B:187:LEU:HD13	2.02	0.41
1:A:184:MET:HE3	3:E:37:DG:N3	2.35	0.41
2:B:10:VAL:C	2:B:11:LYS:HD2	2.45	0.41
2:B:42:GLU:OE2	2:B:49:LYS:HG3	2.20	0.41
2:B:104:LYS:HB3	2:B:104:LYS:HE2	1.77	0.41
3:F:27:DC:H2''	3:F:28:DG:C8	2.54	0.41
1:A:26:LEU:HD21	1:A:34:LEU:HD13	2.01	0.41
1:A:412:PRO:HD3	2:B:401:TRP:CZ2	2.55	0.41
1:C:22:LYS:HD3	1:C:22:LYS:HA	1.88	0.41
1:A:21:VAL:HG23	1:A:58:THR:HA	2.02	0.41
2:B:79:GLU:OE1	4:G:1:GLC:O3	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ILE:HD12	1:C:146:TYR:HA	2.02	0.41
2:D:157:PRO:HG3	2:D:184:MET:HA	2.03	0.41
1:A:94:ILE:CD1	3:E:35:DG:H21	2.33	0.41
2:D:164:MET:HE2	2:D:187:LEU:HD13	2.03	0.41
1:A:5:ILE:CD1	1:A:163:SER:HB3	2.51	0.41
1:A:343:GLN:HG3	1:A:349:LEU:HD11	2.01	0.41
1:A:401:TRP:HB2	1:A:425:LEU:HD11	2.02	0.41
2:B:84:THR:HG22	2:B:87:PHE:HB3	2.03	0.41
1:C:325:LEU:HB3	1:C:387:PRO:HB3	2.03	0.41
1:C:195:ILE:O	1:C:199:ARG:HG3	2.20	0.41
2:D:422:LEU:HG	2:D:423:VAL:N	2.36	0.41
2:B:266:TRP:O	2:B:269:GLN:HG3	2.21	0.40
1:C:28:GLU:CB	1:C:135:ILE:HD12	2.51	0.40
1:C:406:TRP:CZ2	2:D:420:PRO:HG3	2.57	0.40
2:D:214:LEU:HD12	2:D:215:THR:H	1.87	0.40
1:A:80:LEU:O	1:A:84:THR:OG1	2.32	0.40
1:A:131:THR:HB	1:A:143:ARG:HG2	2.03	0.40
2:B:175:ASN:OD1	2:B:201:LYS:HE2	2.22	0.40
1:C:301:LEU:O	1:C:305:GLU:HG2	2.20	0.40
1:C:503:LEU:HD11	1:C:533:LEU:HB3	2.02	0.40
1:A:42:GLU:OE1	1:A:49:LYS:HE3	2.22	0.40
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.22	0.40
1:A:540:LYS:HA	1:A:540:LYS:HD3	1.88	0.40
1:C:215:THR:O	1:C:217:PRO:HD3	2.22	0.40
1:C:328:GLU:HG2	1:C:330:GLN:NE2	2.36	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	549/555 (99%)	536 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	549/555 (99%)	533 (97%)	16 (3%)	0	100	100
2	B	408/444 (92%)	396 (97%)	12 (3%)	0	100	100
2	D	408/444 (92%)	396 (97%)	12 (3%)	0	100	100
All	All	1914/1998 (96%)	1861 (97%)	53 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	492/495 (99%)	484 (98%)	8 (2%)	55	73
1	C	492/495 (99%)	482 (98%)	10 (2%)	48	69
2	B	374/403 (93%)	373 (100%)	1 (0%)	86	93
2	D	374/403 (93%)	372 (100%)	2 (0%)	81	89
All	All	1732/1796 (96%)	1711 (99%)	21 (1%)	63	78

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	42	GLU
1	A	109	LEU
1	A	374	LYS
1	A	391	LEU
1	A	431	LYS
1	A	450	THR
1	A	497	THR
2	B	139	THR
1	C	5	ILE
1	C	42	GLU
1	C	109	LEU
1	C	123	ASP

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Mol	Chain	Res	Type
1	C	374	LYS
1	C	391	LEU
1	C	394	GLN
1	C	431	LYS
1	C	450	THR
1	C	497	THR
2	D	139	THR
2	D	232	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
1	A	207	GLN
1	A	235	HIS
1	A	407	GLN
1	A	474	ASN
1	A	487	GLN
1	A	509	GLN
1	A	524	GLN
1	A	545	ASN
2	B	315	HIS
2	B	361	HIS
2	B	428	GLN
1	C	136	ASN
1	C	145	GLN
1	C	175	ASN
1	C	221	HIS
1	C	255	ASN
1	C	394	GLN
1	C	474	ASN
1	C	487	GLN
1	C	507	GLN
1	C	524	GLN
2	D	96	HIS
2	D	151	GLN
2	D	197	GLN
2	D	208	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	OMC	F	6	3	19,22,23	0.93	1 (5%)	25,31,34	0.79	0
3	OMC	F	8	3	19,22,23	0.93	1 (5%)	25,31,34	0.81	0
3	OMC	E	6	3	19,22,23	0.93	1 (5%)	25,31,34	0.75	0
3	OMC	E	8	3	19,22,23	0.94	1 (5%)	25,31,34	0.87	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	6	3	-	0/9/27/28	0/2/2/2
3	OMC	F	8	3	-	1/9/27/28	0/2/2/2
3	OMC	E	6	3	-	1/9/27/28	0/2/2/2
3	OMC	E	8	3	-	0/9/27/28	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	8	OMC	C4-N4	3.84	1.43	1.33
3	E	6	OMC	C4-N4	3.81	1.43	1.33
3	F	6	OMC	C4-N4	3.81	1.43	1.33
3	F	8	OMC	C4-N4	3.78	1.43	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	6	OMC	C1'-C2'-O2'-CM2
3	F	8	OMC	C1'-C2'-O2'-CM2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	6	OMC	1	0
3	F	8	OMC	2	0
3	E	8	OMC	2	0

5.5 Carbohydrates [i](#)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GLC	G	1	4	11,11,12	0.60	0	15,15,17	0.78	1 (6%)
4	FRU	G	2	4	11,12,12	0.62	0	10,18,18	0.90	0
4	GLC	H	1	4	11,11,12	0.54	0	15,15,17	1.01	2 (13%)
4	FRU	H	2	4	11,12,12	0.68	0	10,18,18	1.16	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLC	G	1	4	-	0/2/19/22	0/1/1/1
4	FRU	G	2	4	-	3/5/24/24	0/1/1/1
4	GLC	H	1	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FRU	H	2	4	-	3/5/24/24	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	GLC	C1-O5-C5	2.28	115.24	112.19
4	H	1	GLC	C1-O5-C5	2.25	115.20	112.19
4	H	2	FRU	C6-C5-C4	-2.22	109.85	115.10
4	H	1	GLC	C1-C2-C3	2.14	112.75	109.64

There are no chirality outliers.

All (6) 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	H	2	FRU	O1-C1-C2-O2
4	H	2	FRU	O1-C1-C2-O5
4	H	2	FRU	O1-C1-C2-C3

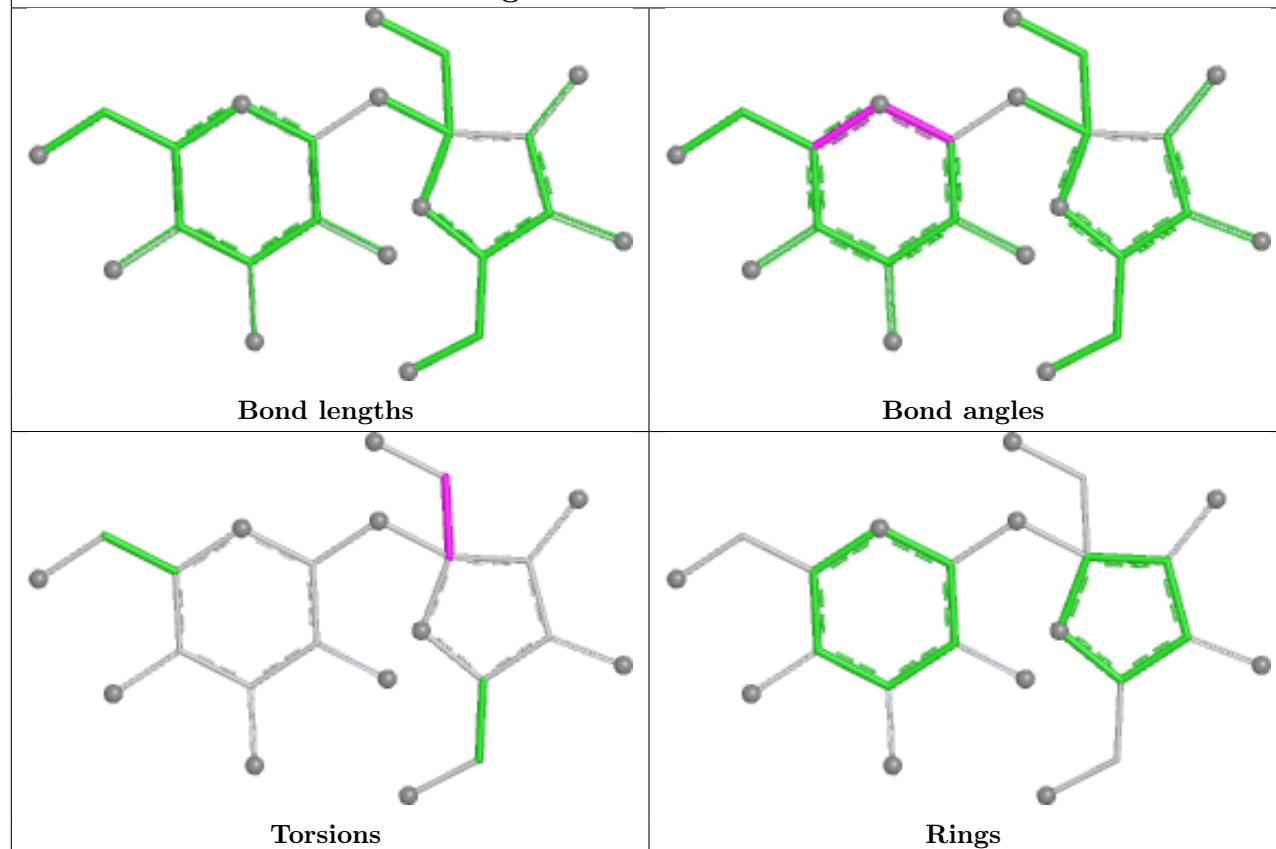
There are no ring outliers.

1 monomer is involved in 1 short contact:

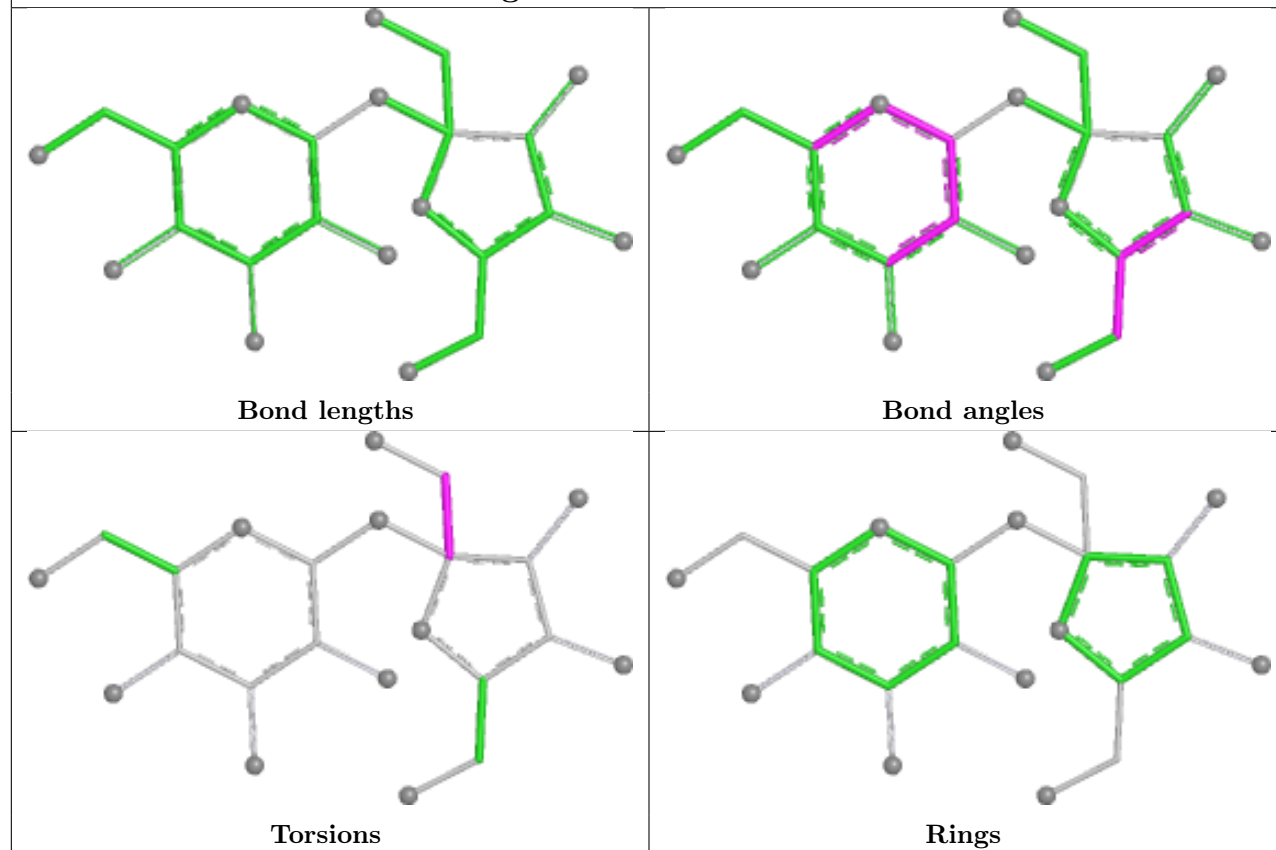
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	GLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain G



Oligosaccharide Chain H



5.6 Ligand geometry

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	SO4	C	604	-	4,4,4	0.23	0	6,6,6	0.17	0
7	SO4	B	502	-	4,4,4	0.23	0	6,6,6	0.13	0
7	SO4	B	501	-	4,4,4	0.27	0	6,6,6	0.37	0
6	3JY	F	101	5	21,24,25	2.89	11 (52%)	29,36,37	2.42	16 (55%)
7	SO4	A	605	-	4,4,4	0.24	0	6,6,6	0.10	0
7	SO4	B	504	-	4,4,4	0.26	0	6,6,6	0.17	0
6	3JY	A	603	5	21,24,25	2.83	10 (47%)	29,36,37	2.54	14 (48%)
7	SO4	B	503	-	4,4,4	0.25	0	6,6,6	0.20	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
6	3JY	F	101	5	-	7/13/27/29	0/2/2/2
6	3JY	A	603	5	-	8/13/27/29	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	101	3JY	O11-C10	-7.83	1.34	1.44
6	A	603	3JY	O11-C10	-7.80	1.34	1.44
6	F	101	3JY	O1-C2	5.72	1.34	1.23
6	A	603	3JY	O1-C2	5.69	1.34	1.23
6	A	603	3JY	C2-C3	-3.54	1.39	1.44
6	F	101	3JY	C2-C3	-3.46	1.39	1.44
6	F	101	3JY	C22-N6	-3.15	1.33	1.38
6	A	603	3JY	O15-C13	-3.06	1.20	1.30
6	A	603	3JY	C22-N6	-3.04	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	101	3JY	O15-C13	-3.02	1.21	1.30
6	F	101	3JY	C5-C3	2.97	1.39	1.34
6	A	603	3JY	C5-C3	2.95	1.39	1.34
6	A	603	3JY	O23-C22	-2.70	1.18	1.23
6	F	101	3JY	O23-C22	-2.64	1.18	1.23
6	A	603	3JY	C22-N21	-2.58	1.33	1.38
6	F	101	3JY	P16-O18	2.49	1.53	1.49
6	F	101	3JY	C22-N21	-2.47	1.33	1.38
6	F	101	3JY	C20-C7	-2.23	1.50	1.53
6	A	603	3JY	C20-C7	-2.21	1.50	1.53
6	A	603	3JY	C2-N21	-2.20	1.34	1.38
6	F	101	3JY	C2-N21	-2.16	1.34	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	3JY	C12-O11-C10	5.69	135.79	115.47
6	A	603	3JY	C3-C2-N21	4.88	119.57	115.32
6	F	101	3JY	C3-C2-N21	4.87	119.55	115.32
6	A	603	3JY	C2-N21-C22	-4.46	121.49	127.34
6	F	101	3JY	C2-N21-C22	-4.39	121.58	127.34
6	F	101	3JY	P16-C12-C13	-4.28	100.94	110.75
6	A	603	3JY	N21-C22-N6	4.21	120.37	114.89
6	F	101	3JY	N21-C22-N6	4.14	120.28	114.89
6	A	603	3JY	O1-C2-C3	-3.97	120.37	124.92
6	F	101	3JY	O1-C2-C3	-3.94	120.41	124.92
6	A	603	3JY	P16-C12-C13	-3.33	103.10	110.75
6	F	101	3JY	O11-C12-C13	3.02	116.86	109.18
6	A	603	3JY	C3-C5-N6	-2.99	120.06	123.31
6	F	101	3JY	C12-O11-C10	2.85	125.66	115.47
6	F	101	3JY	C3-C5-N6	-2.80	120.27	123.31
6	A	603	3JY	O18-P16-C12	-2.78	108.20	113.40
6	A	603	3JY	C7-N6-C22	2.66	120.43	117.13
6	F	101	3JY	C10-C20-C7	2.62	108.66	102.36
6	A	603	3JY	C20-C7-C8	2.57	106.53	102.68
6	A	603	3JY	C10-C20-C7	2.55	108.49	102.36
6	A	603	3JY	C8-C9-C10	2.30	107.02	102.75
6	F	101	3JY	O23-C22-N6	-2.28	119.83	122.80
6	F	101	3JY	C20-C7-C8	2.27	106.08	102.68
6	F	101	3JY	C8-C9-C10	2.21	106.86	102.75
6	F	101	3JY	C7-N6-C22	2.21	119.87	117.13
6	F	101	3JY	C4-C3-C2	2.15	121.08	118.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	101	3JY	O18-P16-C12	-2.14	109.40	113.40
6	A	603	3JY	O23-C22-N6	-2.10	120.07	122.80
6	A	603	3JY	C4-C3-C2	2.03	120.95	118.78
6	F	101	3JY	O14-C13-C12	-2.01	119.44	122.98

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	603	3JY	C20-C10-O11-C12
6	A	603	3JY	O11-C12-C13-O14
6	A	603	3JY	C13-C12-P16-O18
6	A	603	3JY	C13-C12-P16-O19
6	A	603	3JY	C13-C12-P16-O17
6	A	603	3JY	O11-C12-P16-O18
6	F	101	3JY	C20-C10-O11-C12
6	F	101	3JY	C13-C12-P16-O18
6	F	101	3JY	C13-C12-P16-O19
6	F	101	3JY	C13-C12-P16-O17
6	F	101	3JY	O11-C12-P16-O18
6	A	603	3JY	O11-C12-C13-O15
6	F	101	3JY	O11-C12-C13-O15
6	A	603	3JY	C9-C10-O11-C12
6	F	101	3JY	O11-C12-C13-O14

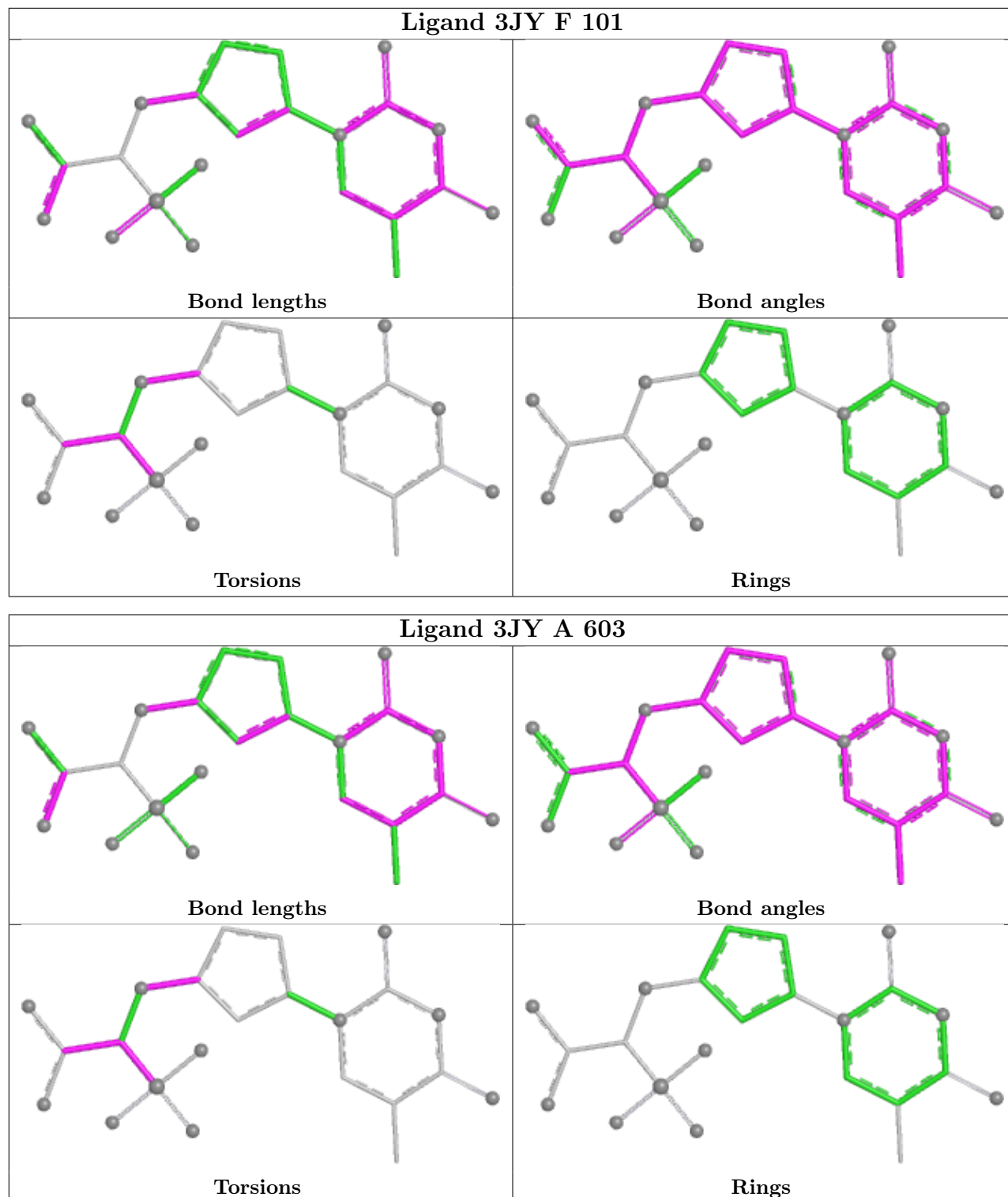
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	101	3JY	4	0

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

equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	551/555 (99%)	0.43	18 (3%) 49 47	41, 96, 151, 190	0
1	C	551/555 (99%)	0.62	47 (8%) 16 17	43, 113, 162, 182	0
2	B	412/444 (92%)	0.24	12 (2%) 53 52	41, 81, 127, 142	0
2	D	412/444 (92%)	0.44	20 (4%) 35 34	44, 92, 136, 160	0
3	E	33/38 (86%)	0.18	0 100 100	70, 97, 113, 152	0
3	F	33/38 (86%)	0.58	2 (6%) 27 27	82, 112, 131, 169	0
All	All	1992/2074 (96%)	0.44	99 (4%) 34 34	41, 93, 152, 190	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	THR	5.6
1	C	60	VAL	4.7
2	D	360	ALA	4.6
2	D	423	VAL	4.5
2	D	359	GLY	4.3
1	A	148	VAL	4.3
1	A	37	ILE	4.1
2	B	90	VAL	3.8
2	D	90	VAL	3.7
1	C	130	PHE	3.7
1	C	75	VAL	3.7
1	C	115	TYR	3.6
1	C	153	TRP	3.5
2	D	86	ASP	3.5
2	B	88	TRP	3.5
2	B	250	ASP	3.4
1	C	283	LEU	3.4
2	D	116	PHE	3.4
1	C	135	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	61	PHE	3.3
2	D	422	LEU	3.3
1	C	132	ILE	3.2
1	C	74	LEU	3.2
1	C	55	PRO	3.2
1	A	254	VAL	3.1
2	B	87	PHE	3.1
1	C	152	GLY	3.1
1	C	210	LEU	3.0
1	C	77	PHE	3.0
1	C	124	PHE	3.0
1	C	188	TYR	3.0
1	C	142	ILE	3.0
1	C	58	THR	3.0
1	C	24	TRP	2.9
2	D	354	TYR	2.9
1	C	111	VAL	2.9
2	B	232	TYR	2.9
1	A	75	VAL	2.9
1	C	116	PHE	2.9
1	C	109	LEU	2.8
1	C	151	GLN	2.8
1	C	193	LEU	2.8
2	D	361	HIS	2.8
1	C	23	GLN	2.8
2	D	10	VAL	2.8
2	D	88	TRP	2.7
2	D	232	TYR	2.7
2	B	212	TRP	2.7
2	B	4	PRO	2.7
1	C	319	TYR	2.6
1	C	120	LEU	2.6
1	A	135	ILE	2.6
2	B	5	ILE	2.6
1	C	234	LEU	2.5
1	C	133	PRO	2.5
1	C	174	GLN	2.5
1	C	134	SER	2.5
1	C	229	TRP	2.5
2	D	159	ILE	2.5
1	C	149	LEU	2.5
2	B	217	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	140	PRO	2.4
1	A	293	ILE	2.4
1	C	12	LEU	2.4
3	F	20	DT	2.4
2	B	422	LEU	2.4
2	D	426	TRP	2.4
2	D	215	THR	2.4
1	C	59	PRO	2.4
1	C	176	PRO	2.3
1	C	167	ILE	2.3
1	A	108	VAL	2.3
2	D	124	PHE	2.3
1	C	114	ALA	2.3
2	D	94	ILE	2.3
2	D	84	THR	2.2
1	C	214	LEU	2.2
1	C	245	VAL	2.2
1	C	144	TYR	2.2
1	C	232	TYR	2.2
1	C	119	PRO	2.2
1	C	67	ASP	2.2
1	A	47	ILE	2.2
1	A	236	PRO	2.1
1	C	184	MET	2.1
2	D	217	PRO	2.1
1	A	149	LEU	2.1
1	C	228	LEU	2.1
1	A	184	MET	2.0
2	D	4	PRO	2.0
1	C	209	LEU	2.0
1	A	195	ILE	2.0
3	F	21	DT	2.0
1	A	39	THR	2.0
1	A	253	THR	2.0
2	B	184	MET	2.0
2	B	425	LEU	2.0
1	A	147	ASN	2.0
1	A	241	VAL	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($\text{\AA}^2$)	Q<0.9
3	OMC	F	6	21/22	0.85	0.13	85,98,111,120	0
3	OMC	F	8	21/22	0.88	0.12	95,103,106,118	0
3	OMC	E	8	21/22	0.93	0.10	67,73,76,90	0
3	OMC	E	6	21/22	0.94	0.09	82,91,95,98	0

6.3 Carbohydrates [i](#)

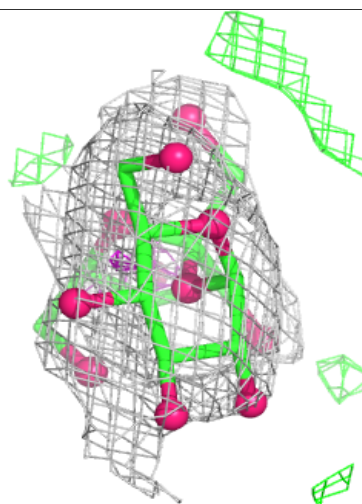
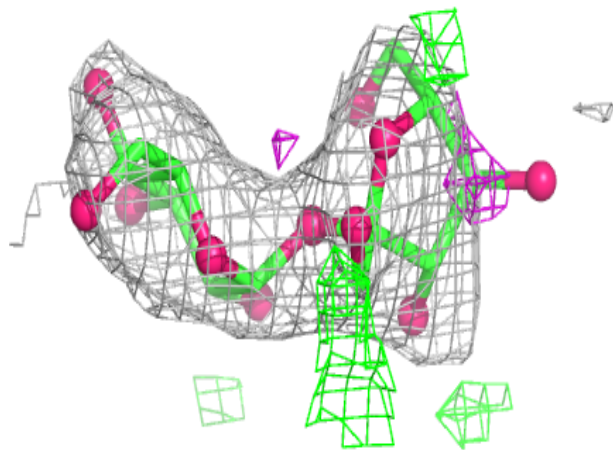
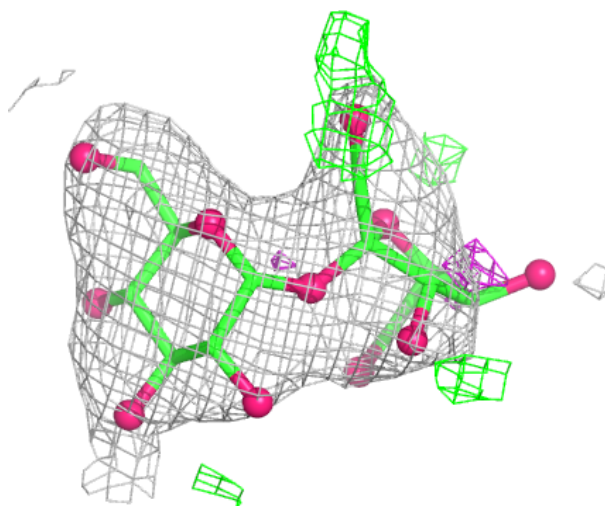
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

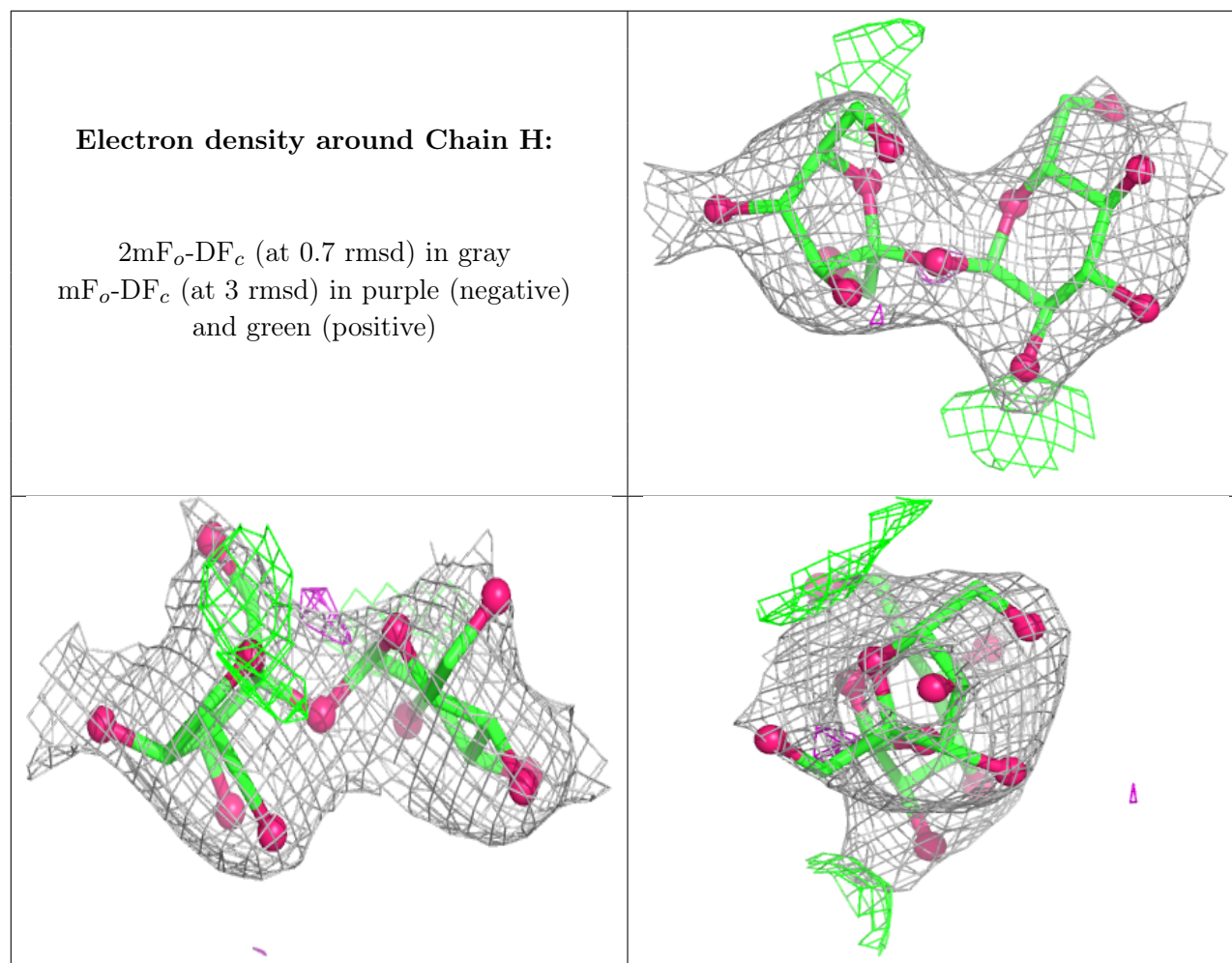
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FRU	G	2	12/12	0.66	0.18	82,97,108,109	0
4	FRU	H	2	12/12	0.75	0.12	93,101,102,104	0
4	GLC	H	1	11/12	0.86	0.11	82,92,96,101	0
4	GLC	G	1	11/12	0.93	0.10	67,77,86,87	0

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.

Electron density around Chain G:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	SO4	B	503	5/5	0.74	0.24	87,98,102,121	0
6	3JY	F	101	23/24	0.79	0.15	98,119,137,145	0
7	SO4	B	502	5/5	0.80	0.18	94,100,109,113	0
7	SO4	B	501	5/5	0.81	0.20	78,79,85,101	0
7	SO4	B	504	5/5	0.83	0.22	78,78,84,111	0
7	SO4	A	605	5/5	0.86	0.10	98,102,110,116	0
5	MG	A	604	1/1	0.89	0.13	70,70,70,70	0
5	MG	C	603	1/1	0.89	0.06	172,172,172,172	0
6	3JY	A	603	23/24	0.89	0.11	103,107,123,129	0
7	SO4	C	604	5/5	0.89	0.27	84,92,112,112	0

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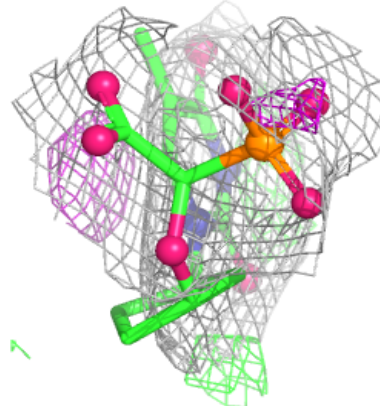
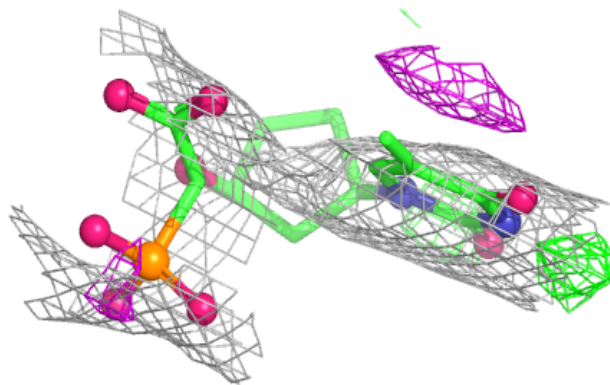
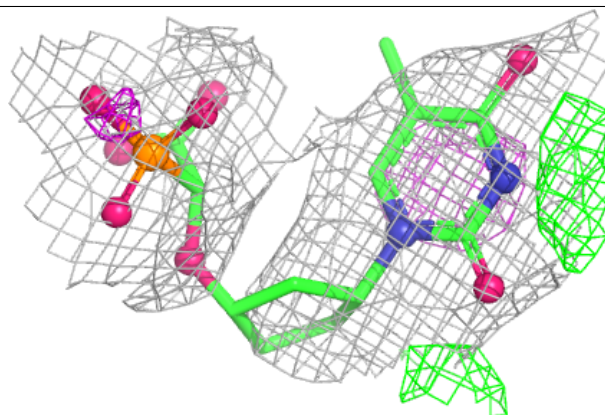
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	C	601	1/1	0.91	0.09	122,122,122,122	0
5	MG	C	602	1/1	0.92	0.08	70,70,70,70	0
5	MG	A	601	1/1	0.93	0.09	114,114,114,114	0
5	MG	A	602	1/1	0.93	0.05	114,114,114,114	0

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.

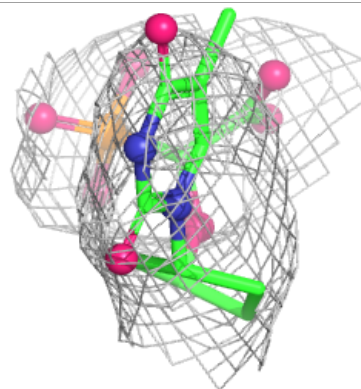
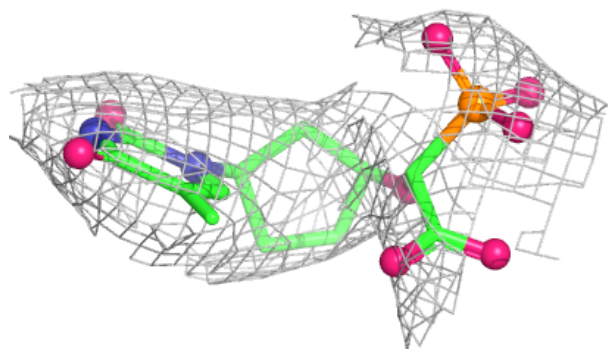
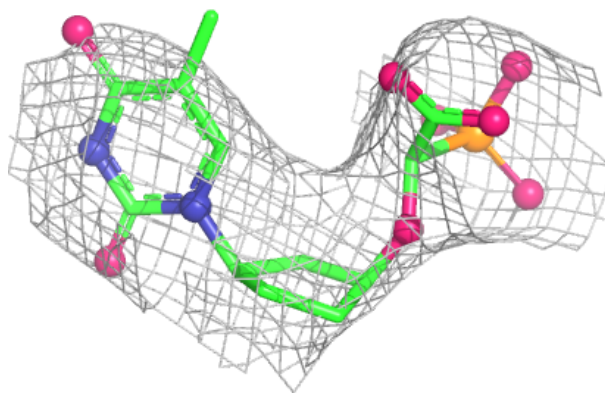
Electron density around 3JY F 101:

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



Electron density around 3JY A 603:

$2mF_o-DF_c$ (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.