



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:14 pm BST

PDB ID : 6KDM
Title : HIV-1 reverse transcriptase with Q151M/Y115F/F116Y:DNA:entecavir
5'-triphosphate ternary complex
Authors : Yasutake, Y.; Hattori, S.I.; Tamura, N.; Maeda, K.
Deposited on : 2019-07-02
Resolution : 2.32 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 : 2.11
buster-report : 1.1.7 (2018)
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) : 2.11

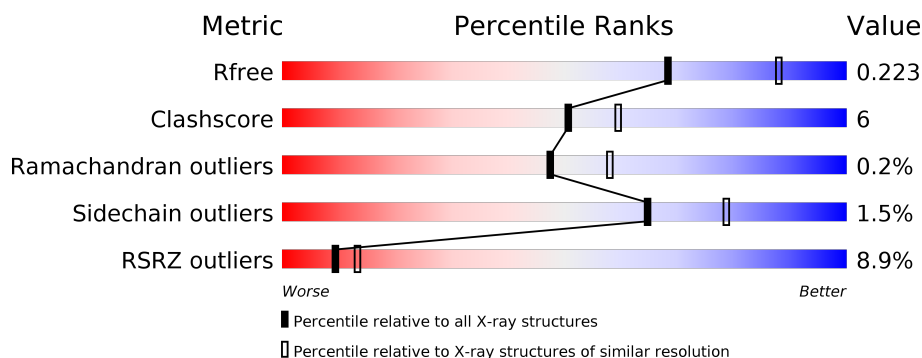
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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>6%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>
1	C	557	<div> <div>10%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>..</div> </div> </div>
2	B	444	<div> <div>14%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>9%</div> </div> </div>
2	D	444	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>9%</div> </div> </div>
3	E	38	<div> <div></div> <div> <div></div> <div>68%</div> <div>24%</div> <div>8%</div> </div> </div>
3	F	38	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>26%</div> </div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 17780 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	1	0
			4503	2914	750	831	8			
1	C	553	Total	C	N	O	S	0	1	0
			4503	2915	750	829	9			

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	1	0
			3352	2182	557	606	7			

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).

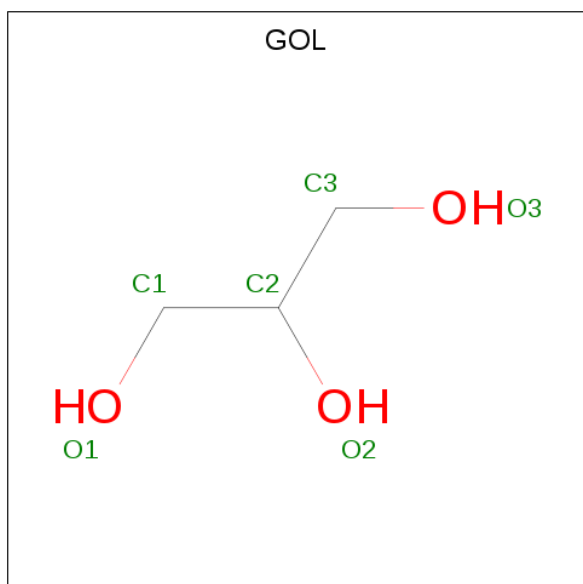
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	35	Total	C	N	O	P	0	0	0
			718	339	128	216	35			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	38	Total	C	N	O	P	0	0	0
			777	369	140	231	37			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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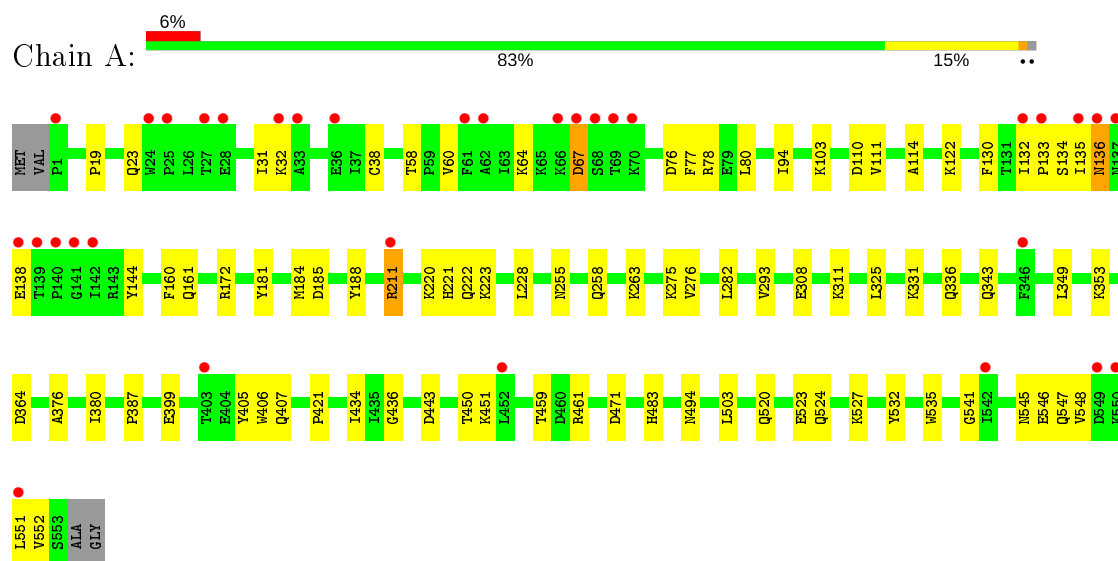
- Molecule 7 is water.

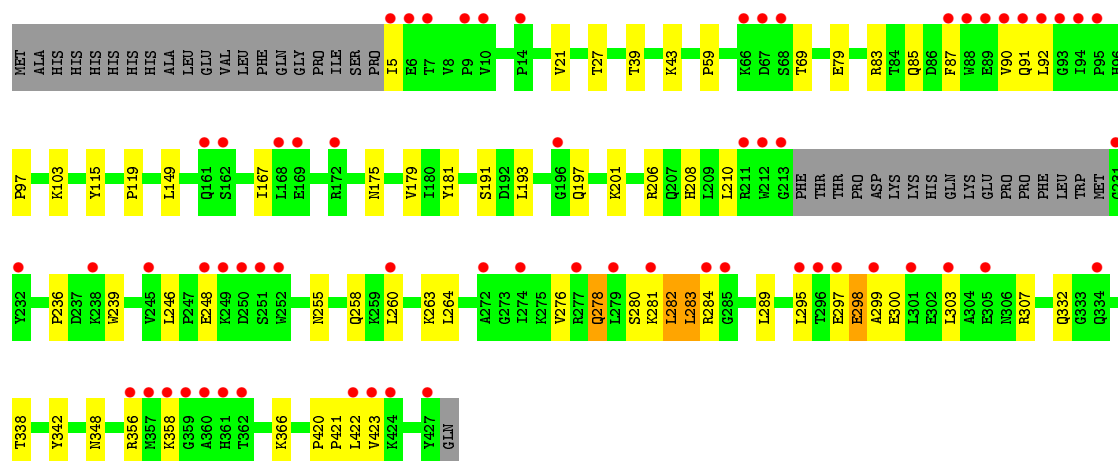


3 Residue-property plots [i](#)

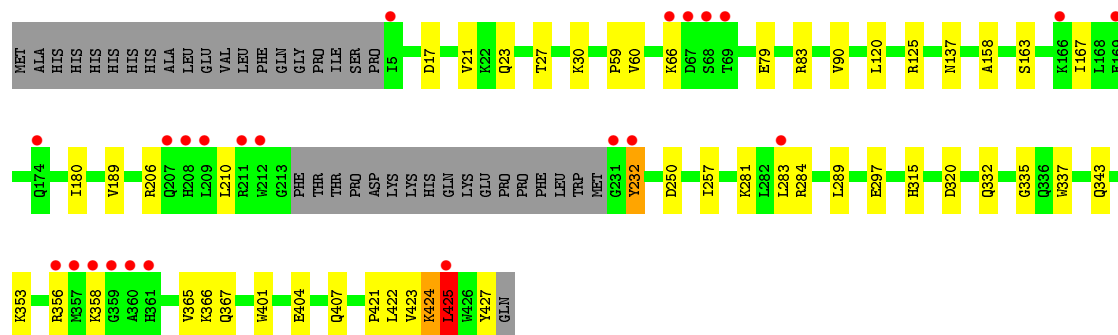
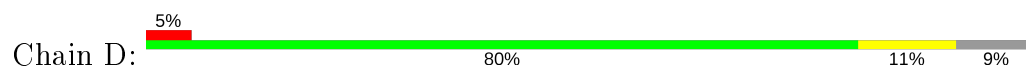
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

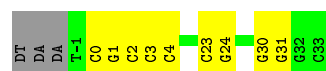




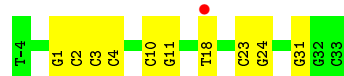
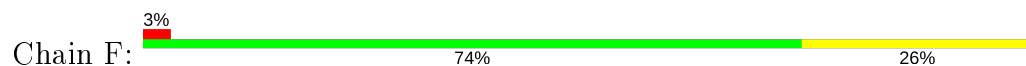
- Molecule 2: HIV-1 RT p51 subunit



- Molecule 3: DNA/RNA (38-MER)



- Molecule 3: DNA/RNA (38-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	284.45Å 284.45Å 95.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.67 – 2.32 48.67 – 2.32	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.67-2.32) 100.0 (48.67-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.32Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.190 , 0.223 0.190 , 0.223	Depositor DCC
R_{free} test set	6352 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17780	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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, MG, ET9

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	0.31	0/4624	0.49	1/6279 (0.0%)
1	C	0.30	0/4624	0.46	0/6278
2	B	0.31	0/3441	0.47	0/4673
2	D	0.39	0/3449	0.49	0/4683
3	E	0.52	0/756	0.95	1/1165 (0.1%)
3	F	0.50	0/823	0.93	0/1269
All	All	0.35	0/17717	0.54	2/24347 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
2	D	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ASP	N-CA-C	-6.45	93.60	111.00
3	E	31	DG	O4'-C4'-C3'	-5.64	102.24	104.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	357[A]	MET	Mainchain
1	C	357[B]	MET	Mainchain
2	D	425	LEU	Mainchain

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	4503	0	4557	62	0
1	C	4503	0	4562	40	0
2	B	3347	0	3379	43	0
2	D	3352	0	3388	42	0
3	E	718	0	397	8	0
3	F	777	0	432	8	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	D	18	0	24	2	0
4	E	6	0	8	3	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	32	0	0	2	0
6	C	32	0	0	0	0
7	A	133	0	0	4	0
7	B	53	0	0	0	0
7	C	116	0	0	1	0
7	D	93	0	0	0	0
7	E	42	0	0	0	0
7	F	41	0	0	0	0
All	All	17780	0	16763	193	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 6.

All (193) 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:450:THR:HG22	1:A:451:LYS:H	1.19	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:THR:HG22	1:A:451:LYS:N	1.77	0.98
2:D:425:LEU:H	2:D:425:LEU:CD1	1.78	0.95
2:D:320:ASP:H	2:D:343:GLN:HE22	1.10	0.92
1:A:222:GLN:HE22	1:A:228:LEU:H	1.19	0.90
2:D:23:GLN:HE22	2:D:60:VAL:H	1.21	0.87
2:B:298:GLU:N	2:B:298:GLU:OE2	2.07	0.86
1:A:450:THR:CG2	1:A:451:LYS:H	1.91	0.83
1:A:211:ARG:CG	1:A:211:ARG:HH11	1.91	0.83
2:D:425:LEU:HD13	2:D:425:LEU:N	1.92	0.81
1:A:31:ILE:HD13	1:A:135:ILE:H	1.45	0.80
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.46	0.79
2:D:425:LEU:N	2:D:425:LEU:CD1	2.42	0.78
1:A:211:ARG:HG2	1:A:211:ARG:NH1	1.97	0.78
2:D:425:LEU:H	2:D:425:LEU:HD12	1.47	0.78
1:A:434:ILE:H	1:A:494:ASN:HD21	1.32	0.78
2:B:297:GLU:HG2	2:B:298:GLU:OE2	1.84	0.78
2:B:69:THR:O	2:B:69:THR:HG22	1.83	0.77
2:D:425:LEU:O	2:D:425:LEU:HD22	1.85	0.76
2:D:423:VAL:HG12	2:D:423:VAL:O	1.87	0.75
2:B:255:ASN:HA	2:B:258:GLN:HE21	1.54	0.72
1:A:135:ILE:O	1:A:135:ILE:HG22	1.89	0.71
1:A:451:LYS:HB2	1:A:471:ASP:HA	1.73	0.71
1:C:521:ILE:HA	1:C:524:GLN:HE21	1.58	0.69
1:A:421:PRO:HG2	1:C:301:LEU:HD13	1.76	0.68
2:D:337:TRP:HE1	2:D:367:GLN:HE21	1.38	0.67
1:A:172:ARG:NH1	7:A:704:HOH:O	2.28	0.66
2:B:278:GLN:CD	2:B:298:GLU:HB2	2.17	0.65
2:B:278:GLN:NE2	2:B:298:GLU:HB2	2.12	0.64
2:B:281:LYS:C	2:B:283:LEU:N	2.48	0.63
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.39	0.63
2:B:258:GLN:HE22	2:B:289:LEU:HD22	1.62	0.63
1:A:122:LYS:HG3	7:A:753:HOH:O	1.98	0.62
1:A:331:LYS:NZ	1:A:364:ASP:OD2	2.29	0.62
2:B:281:LYS:C	2:B:283:LEU:H	2.02	0.61
2:D:90:VAL:HG21	2:D:158:ALA:HA	1.82	0.61
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.83	0.60
1:A:110[A]:ASP:HB2	1:A:220:LYS:HB3	1.83	0.60
3:E:30:DG:N2	4:E:101:GOL:O3	2.31	0.60
2:D:425:LEU:C	2:D:425:LEU:HD22	2.23	0.59
2:D:425:LEU:CD2	2:D:425:LEU:O	2.49	0.58
1:A:263:LYS:NZ	7:A:707:HOH:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:VAL:HG22	1:A:353:LYS:HE3	1.86	0.58
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.86	0.58
2:B:281:LYS:O	2:B:283:LEU:N	2.37	0.57
1:A:450:THR:CG2	1:A:451:LYS:N	2.49	0.57
2:B:342:TYR:HB3	2:B:348:ASN:HD22	1.69	0.57
1:A:135:ILE:HG22	1:A:138:GLU:HG3	1.87	0.56
1:A:494:ASN:HD22	1:A:532:TYR:HB3	1.70	0.56
2:D:320:ASP:H	2:D:343:GLN:NE2	1.91	0.56
2:B:248:GLU:HG3	2:B:307:ARG:HH22	1.72	0.55
2:D:423:VAL:CG1	2:D:423:VAL:O	2.54	0.55
2:D:425:LEU:HD13	2:D:425:LEU:H	1.55	0.55
1:C:448:ARG:NH1	3:F:18:DT:O2	2.39	0.55
2:B:303:LEU:O	2:B:307:ARG:HG3	2.06	0.55
2:B:276:VAL:O	2:B:280:SER:HB3	2.06	0.55
1:A:31:ILE:CD1	1:A:135:ILE:H	2.19	0.54
3:E:3:DC:H2'	3:E:4:OMC:C6	2.43	0.54
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.43	0.54
1:A:443:ASP:OD2	1:A:552:VAL:HG21	2.08	0.54
3:F:3:DC:H2'	3:F:4:OMC:C6	2.43	0.54
2:B:246:LEU:HD13	2:B:260:LEU:HD11	1.90	0.53
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.90	0.53
2:B:167:ILE:O	2:B:208:HIS:HE1	1.92	0.53
1:C:331:LYS:NZ	1:C:364:ASP:OD1	2.37	0.53
2:D:335:GLY:HA3	2:D:356:ARG:HE	1.74	0.53
1:C:381:VAL:HG13	4:D:501:GOL:H11	1.91	0.53
3:E:30:DG:H21	4:E:101:GOL:HO3	1.54	0.53
7:A:765:HOH:O	4:E:101:GOL:H11	2.08	0.53
1:A:406:TRP:CZ2	2:B:420:PRO:HG3	2.44	0.53
1:C:342:TYR:HA	1:C:349:LEU:HD23	1.90	0.53
2:D:335:GLY:HA2	2:D:367:GLN:HE22	1.74	0.52
1:C:343:GLN:HG3	1:C:349:LEU:HD21	1.91	0.52
1:A:133:PRO:HB2	1:A:136:ASN:ND2	2.25	0.52
1:A:275:LYS:HB3	1:A:336:GLN:HE22	1.74	0.51
2:B:69:THR:CG2	2:B:69:THR:O	2.56	0.51
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.76	0.51
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.92	0.51
1:A:161:GLN:NE2	1:A:184:MET:SD	2.80	0.51
3:F:1:DG:H2'	3:F:2:OMC:C6	2.46	0.51
2:B:103:LYS:HE2	2:B:179:VAL:HG12	1.92	0.50
2:B:103:LYS:HE3	2:B:191:SER:HA	1.93	0.50
1:A:380:ILE:HD12	2:B:27:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:ARG:O	1:C:451:LYS:NZ	2.44	0.50
1:A:541:GLY:HA2	1:A:546:GLU:HB2	1.93	0.50
1:C:137:ASN:O	1:C:137:ASN:ND2	2.44	0.50
1:A:421:PRO:HG2	1:C:301:LEU:CD1	2.41	0.50
1:C:448:ARG:NH2	3:F:18:DT:H5'	2.27	0.49
1:C:162:SER:O	1:C:166:LYS:HG2	2.12	0.49
2:D:281:LYS:HG2	2:D:284:ARG:HH21	1.78	0.49
1:A:421:PRO:CG	1:C:301:LEU:HD13	2.42	0.49
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.95	0.49
1:C:34:LEU:HD21	1:C:62:ALA:HB2	1.94	0.49
1:C:22:LYS:HA	1:C:22:LYS:HD2	1.69	0.49
1:C:30:LYS:O	1:C:34:LEU:HG	2.13	0.48
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.96	0.48
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.48	0.48
2:B:276:VAL:O	2:B:280:SER:CB	2.61	0.48
2:D:232:TYR:CD1	2:D:232:TYR:C	2.85	0.48
3:E:1:DG:H2'	3:E:2:OMC:C6	2.49	0.48
2:B:193:LEU:HG	2:B:197:GLN:HG3	1.95	0.47
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.96	0.47
2:D:137:ASN:HD21	4:D:501:GOL:H12	1.80	0.47
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.96	0.47
2:B:358:LYS:HD2	2:B:366:LYS:HE2	1.97	0.47
1:A:221:HIS:CE1	1:A:223:LYS:HE3	2.50	0.47
2:D:163:SER:O	2:D:167:ILE:HG12	2.15	0.46
1:A:31:ILE:HG21	1:A:134:SER:HA	1.97	0.46
1:A:545:ASN:HA	1:A:548:VAL:HG12	1.97	0.46
2:D:421:PRO:CB	2:D:424:LYS:HE3	2.45	0.46
2:B:5:ILE:HG21	2:B:119:PRO:HD2	1.98	0.46
2:B:278:GLN:HG2	2:B:298:GLU:C	2.36	0.46
1:C:377:THR:OG1	7:C:701:HOH:O	2.20	0.46
1:C:412:PRO:O	1:C:414:TRP:HD1	1.97	0.46
1:C:444:GLY:HA2	1:C:552:VAL:HG11	1.97	0.46
2:B:278:GLN:HG2	2:B:299:ALA:HA	1.98	0.46
3:F:10:DC:H2''	3:F:11:DG:C8	2.51	0.46
1:C:405:TYR:CE2	1:C:407:GLN:HB2	2.51	0.45
1:A:282:LEU:HB3	1:A:293:VAL:HG11	1.99	0.45
2:D:79:GLU:HG3	2:D:83:ARG:HE	1.82	0.45
1:A:135:ILE:CG2	1:A:138:GLU:HG3	2.46	0.45
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.99	0.45
2:B:281:LYS:O	2:B:282:LEU:C	2.51	0.45
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:LYS:HE3	1:C:23:GLN:H	1.81	0.45
1:A:436:GLY:O	1:A:461:ARG:NH2	2.50	0.45
6:A:603:ET9:N2	3:E:0:DC:O2	2.50	0.45
2:D:353:LYS:HE3	2:D:353:LYS:HB2	1.75	0.45
1:C:136:ASN:O	1:C:138:GLU:N	2.44	0.44
2:D:337:TRP:HE1	2:D:367:GLN:NE2	2.11	0.44
1:C:227:PHE:HB2	1:C:234:LEU:HB2	1.98	0.44
2:B:332:GLN:HG3	2:B:338:THR:HG23	2.00	0.44
2:B:97:PRO:HD3	2:B:181:TYR:CD1	2.52	0.44
1:C:469:LEU:HD12	1:C:477:THR:HG22	1.98	0.44
2:D:206:ARG:O	2:D:210:LEU:HG	2.18	0.44
2:D:365:VAL:HG11	2:D:401:TRP:HB2	2.00	0.44
1:C:380:ILE:HD12	2:D:27:THR:HG22	2.00	0.44
1:C:465:LYS:HD3	1:C:484:LEU:HD11	2.00	0.44
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.52	0.43
1:C:494:ASN:HB3	2:D:289:LEU:HD12	2.00	0.43
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.52	0.43
1:A:308:GLU:O	1:A:311:LYS:HG2	2.18	0.43
1:A:275:LYS:HB3	1:A:336:GLN:NE2	2.33	0.43
1:A:483:HIS:ND1	1:A:524:GLN:OE1	2.52	0.43
1:A:94:ILE:HG12	3:E:4:OMC:H1'	2.01	0.43
2:B:39:THR:HG22	2:B:43:LYS:HE2	2.00	0.43
1:C:266:TRP:CE2	3:F:31:DG:H4'	2.53	0.43
6:A:603:ET9:N1	3:E:0:DC:N3	2.66	0.43
2:D:332:GLN:OE1	2:D:424:LYS:HD3	2.18	0.43
2:D:17:ASP:O	2:D:83:ARG:HD3	2.18	0.43
1:A:111:VAL:HB	1:A:185:ASP:HB2	2.01	0.43
1:A:523:GLU:O	1:A:527:LYS:HG2	2.19	0.43
1:C:325:LEU:HB3	1:C:387:PRO:HB3	2.01	0.43
2:D:66:LYS:HE3	2:D:407:GLN:OE1	2.19	0.43
2:D:297:GLU:H	2:D:297:GLU:HG2	1.63	0.42
2:D:358:LYS:HB2	2:D:358:LYS:HE3	1.72	0.42
1:A:135:ILE:CG2	1:A:135:ILE:O	2.61	0.42
1:A:520:GLN:O	1:A:523:GLU:HG2	2.20	0.42
1:C:96:HIS:CG	1:C:97:PRO:HD2	2.54	0.42
3:E:23:DC:H2''	3:E:24:DG:C8	2.54	0.42
1:A:376:ALA:O	1:A:380:ILE:HG12	2.20	0.42
1:C:438:GLU:OE1	1:C:463:ARG:HD3	2.19	0.42
2:D:257:ILE:HB	2:D:283:LEU:HD21	2.01	0.42
3:F:4:OMC:HM23	3:F:4:OMC:H1'	1.83	0.42
1:A:103:LYS:HA	1:A:103:LYS:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:422:LEU:HA	2:D:422:LEU:HD23	1.91	0.42
2:B:90:VAL:C	2:B:91:GLN:HG2	2.39	0.42
2:B:87:PHE:HB3	2:B:92:LEU:HB2	2.02	0.42
1:C:339:TYR:CZ	1:C:352:GLY:HA3	2.55	0.42
1:C:181:TYR:HB2	1:C:188:TYR:HB3	2.02	0.42
1:A:255:ASN:HA	1:A:258:GLN:HE21	1.85	0.41
2:B:263:LYS:HB2	2:B:423:VAL:HG11	2.01	0.41
1:C:503:LEU:HG	1:C:507:GLN:HG3	2.01	0.41
1:C:199:ARG:HH11	1:C:223:LYS:HD3	1.85	0.41
2:B:85:GLN:HE22	2:B:90:VAL:HG21	1.85	0.41
2:D:30:LYS:NZ	2:D:404:GLU:OE1	2.44	0.41
2:B:206:ARG:O	2:B:210:LEU:HG	2.21	0.41
2:D:180:ILE:HG12	2:D:189:VAL:HG13	2.03	0.41
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.56	0.41
1:A:325:LEU:HB3	1:A:387:PRO:HB3	2.02	0.41
1:A:32:LYS:HD2	1:A:32:LYS:HA	1.94	0.41
1:A:23:GLN:OE1	1:A:60:VAL:HG12	2.20	0.41
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.19	0.40
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.96	0.40
1:C:130:PHE:CZ	1:C:144:TYR:HB2	2.56	0.40
1:A:76:ASP:OD2	1:A:78:ARG:NH2	2.53	0.40
1:C:257:ILE:HB	1:C:283:LEU:HD21	2.03	0.40
2:D:120:LEU:HD23	2:D:125:ARG:HG2	2.03	0.40
2:D:356:ARG:HG3	2:D:356:ARG:H	1.61	0.40
3:F:23:DC:H2"	3:F:24:DG:C8	2.56	0.40
1:C:379:SER:CB	1:C:387:PRO:HD3	2.51	0.40
1:C:451:LYS:HB3	1:C:471:ASP:HA	2.04	0.40
2:D:358:LYS:HD3	2:D:366:LYS:NZ	2.35	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	552/557 (99%)	536 (97%)	15 (3%)	1 (0%)	47	58
1	C	552/557 (99%)	535 (97%)	15 (3%)	2 (0%)	34	41
2	B	402/444 (90%)	383 (95%)	18 (4%)	1 (0%)	47	58
2	D	403/444 (91%)	388 (96%)	15 (4%)	0	100	100
All	All	1909/2002 (95%)	1842 (96%)	63 (3%)	4 (0%)	47	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	C	137	ASN
2	B	282	LEU
1	C	133	PRO

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	493/494 (100%)	486 (99%)	7 (1%)	67	80
1	C	493/494 (100%)	489 (99%)	4 (1%)	81	90
2	B	365/400 (91%)	357 (98%)	8 (2%)	52	68
2	D	366/400 (92%)	360 (98%)	6 (2%)	62	77
All	All	1717/1788 (96%)	1692 (98%)	25 (2%)	65	79

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LYS
1	A	67	ASP
1	A	211	ARG
1	A	399	GLU
1	A	459	THR
1	A	547	GLN
1	A	551	LEU

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Mol	Chain	Res	Type
2	B	278	GLN
2	B	283	LEU
2	B	284	ARG
2	B	295	LEU
2	B	298	GLU
2	B	300	GLU
2	B	356	ARG
2	B	422	LEU
1	C	177	ASP
1	C	199	ARG
1	C	277	ARG
1	C	301	LEU
2	D	232	TYR
2	D	250	ASP
2	D	315	HIS
2	D	424	LYS
2	D	425	LEU
2	D	427	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	207	GLN
1	A	222	GLN
1	A	258	GLN
1	A	336	GLN
1	A	464	GLN
1	A	480	GLN
1	A	494	ASN
2	B	151	GLN
2	B	161	GLN
2	B	175	ASN
2	B	208	HIS
2	B	258	GLN
2	B	348	ASN
1	C	258	GLN
1	C	330	GLN
1	C	340	GLN
1	C	524	GLN
1	C	547	GLN
2	D	23	GLN

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Mol	Chain	Res	Type
2	D	182	GLN
2	D	343	GLN
2	D	367	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	OMC	F	2	3	15,22,23	3.27	5 (33%)	17,31,34	1.36	1 (5%)
3	OMC	E	2	3	15,22,23	3.22	5 (33%)	17,31,34	1.27	2 (11%)
3	OMC	E	4	3	15,22,23	3.23	5 (33%)	17,31,34	1.38	2 (11%)
3	OMC	F	4	3	15,22,23	3.28	5 (33%)	17,31,34	1.42	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	F	2	3	-	0/7/27/28	0/2/2/2
3	OMC	E	2	3	-	0/7/27/28	0/2/2/2
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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	OMC	C6-N1	7.89	1.45	1.35
3	E	2	OMC	C6-N1	7.77	1.45	1.35
3	E	4	OMC	C6-N1	7.55	1.45	1.35
3	F	4	OMC	C6-N1	7.50	1.45	1.35
3	F	4	OMC	C4-N3	5.90	1.45	1.35
3	F	4	OMC	C2-N3	5.59	1.49	1.38
3	E	4	OMC	C4-N3	5.53	1.44	1.35
3	E	4	OMC	C2-N3	5.48	1.49	1.38
3	F	2	OMC	C4-N3	5.44	1.44	1.35
3	E	2	OMC	C4-N3	5.37	1.44	1.35
3	F	2	OMC	C2-N3	5.24	1.48	1.38
3	E	2	OMC	C2-N3	5.15	1.48	1.38
3	F	2	OMC	C6-C5	4.90	1.48	1.38
3	E	4	OMC	C6-C5	4.84	1.48	1.38
3	E	2	OMC	C6-C5	4.84	1.48	1.38
3	F	4	OMC	C6-C5	4.82	1.48	1.38
3	F	2	OMC	C5-C4	3.35	1.49	1.41
3	E	2	OMC	C5-C4	3.32	1.49	1.41
3	F	4	OMC	C5-C4	3.24	1.49	1.41
3	E	4	OMC	C5-C4	3.24	1.49	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	OMC	C2-N3-C4	4.51	120.91	116.34
3	F	4	OMC	C2-N3-C4	4.39	120.80	116.34
3	E	4	OMC	C2-N3-C4	4.03	120.43	116.34
3	E	2	OMC	C2-N3-C4	3.96	120.35	116.34
3	E	4	OMC	N4-C4-N3	2.77	120.87	116.49
3	F	4	OMC	N4-C4-N3	2.72	120.78	116.49
3	E	2	OMC	N4-C4-N3	2.10	119.81	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	F	2	OMC	1	0
3	E	2	OMC	1	0
3	E	4	OMC	2	0
3	F	4	OMC	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 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
4	GOL	A	601	-	5,5,5	0.36	0	5,5,5	0.25	0
4	GOL	D	503	-	5,5,5	0.52	0	5,5,5	0.30	0
6	ET9	C	602	5	26,34,34	1.80	5 (19%)	28,54,54	2.14	8 (28%)
4	GOL	B	501	-	5,5,5	0.37	0	5,5,5	0.29	0
4	GOL	D	501	-	5,5,5	0.36	0	5,5,5	0.28	0
4	GOL	D	502	-	5,5,5	0.37	0	5,5,5	0.25	0
6	ET9	A	603	5	26,34,34	1.61	3 (11%)	28,54,54	2.21	11 (39%)
4	GOL	E	101	-	5,5,5	0.29	0	5,5,5	0.31	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	GOL	A	601	-	-	0/4/4/4	-
4	GOL	D	503	-	-	2/4/4/4	-
6	ET9	C	602	5	-	4/18/38/38	0/3/3/3
4	GOL	B	501	-	-	1/4/4/4	-
4	GOL	D	501	-	-	0/4/4/4	-
4	GOL	D	502	-	-	2/4/4/4	-
6	ET9	A	603	5	-	4/18/38/38	0/3/3/3
4	GOL	E	101	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	ET9	C2'-C1'	-6.19	1.46	1.54
6	C	602	ET9	C2'-C1'	-5.97	1.47	1.54
6	C	602	ET9	C4'-C6'	-3.69	1.46	1.51
6	C	602	ET9	C6-C5	3.38	1.47	1.41
6	A	603	ET9	C6-C5	3.09	1.46	1.41
6	C	602	ET9	C5-C4	2.39	1.47	1.40
6	C	602	ET9	C1'-C6'	-2.31	1.47	1.51
6	A	603	ET9	C5-C4	2.11	1.46	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	602	ET9	C6-C5-C4	-5.26	115.77	120.80
6	A	603	ET9	C6-C5-C4	-4.60	116.41	120.80
6	C	602	ET9	C6-N1-C2	4.57	123.19	115.93
6	A	603	ET9	C5-C6-N1	-4.25	117.62	123.43
6	C	602	ET9	C5-C6-N1	-4.00	117.96	123.43
6	C	602	ET9	N3-C2-N1	-3.89	122.03	127.22
6	A	603	ET9	N2-C2-N1	3.69	122.99	117.25
6	A	603	ET9	C6-N1-C2	3.64	121.72	115.93
6	A	603	ET9	O1G-PG-O3B	3.42	116.11	104.64
6	C	602	ET9	C2-N3-C4	3.15	118.95	115.36
6	A	603	ET9	C2-N3-C4	2.99	118.77	115.36
6	A	603	ET9	N2-C2-N3	-2.96	112.96	117.79
6	C	602	ET9	O2G-PG-O3B	2.95	114.52	104.64
6	C	602	ET9	C5'-C4'-C3'	-2.78	106.73	115.61
6	A	603	ET9	C5'-C4'-C3'	-2.66	107.10	115.61
6	A	603	ET9	PB-O3B-PG	-2.61	123.87	132.83
6	A	603	ET9	O3B-PG-O3G	-2.59	96.84	111.19
6	A	603	ET9	N3-C2-N1	-2.40	124.02	127.22
6	C	602	ET9	C2'-C1'-N9	-2.01	111.33	114.73

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	602	ET9	PB-O3B-PG-O2G
4	D	503	GOL	O1-C1-C2-C3
4	E	101	GOL	O1-C1-C2-O2
4	E	101	GOL	O1-C1-C2-C3
6	A	603	ET9	PB-O3B-PG-O1G
6	A	603	ET9	PB-O3B-PG-O2G

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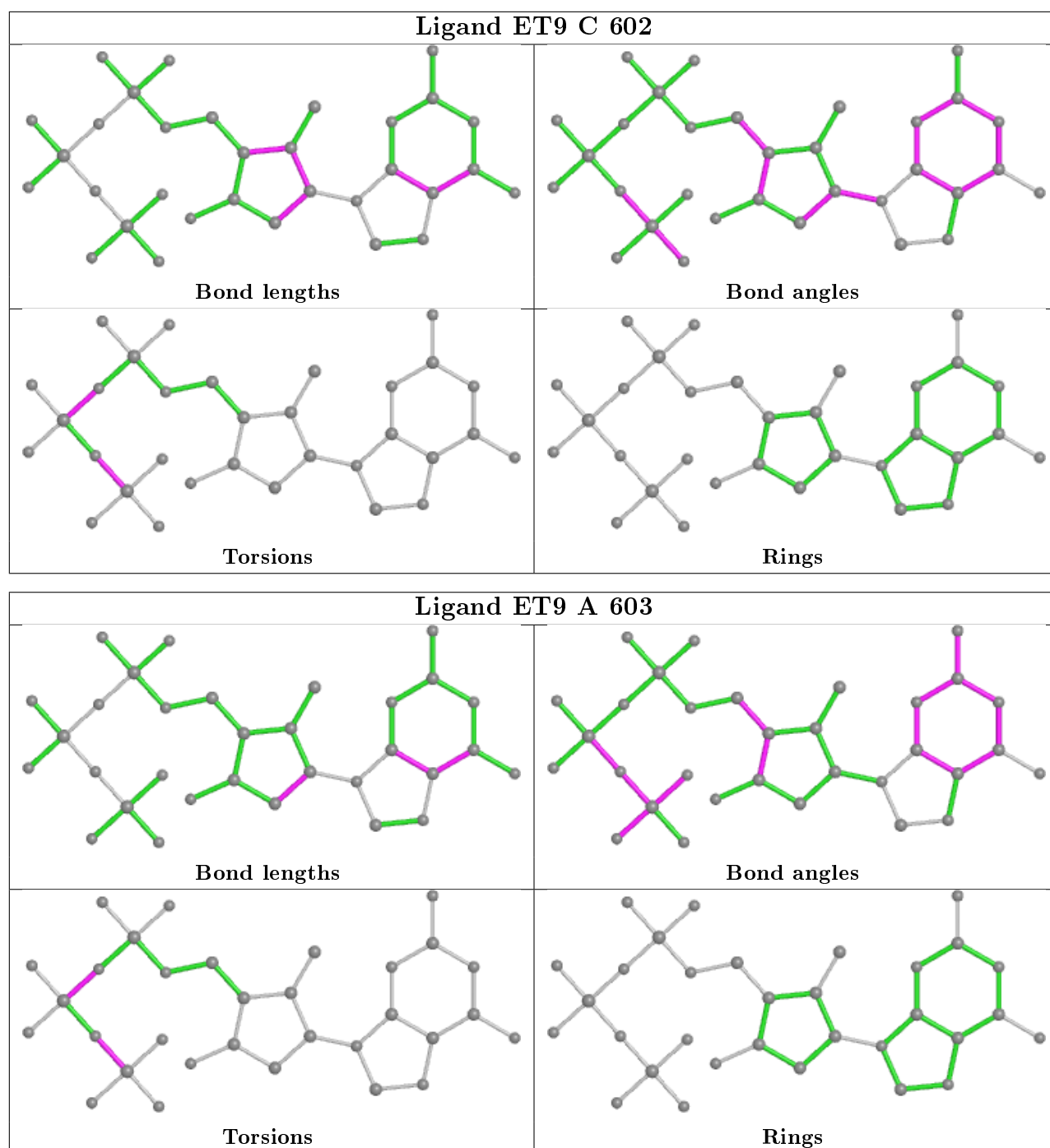
Mol	Chain	Res	Type	Atoms
4	D	503	GOL	O1-C1-C2-O2
4	D	502	GOL	O1-C1-C2-O2
6	C	602	ET9	PA-O3A-PB-O2B
6	C	602	ET9	PB-O3B-PG-O3G
4	B	501	GOL	O1-C1-C2-C3
6	A	603	ET9	PB-O3B-PG-O3G
6	C	602	ET9	PA-O3A-PB-O1B
6	A	603	ET9	PA-O3A-PB-O2B
4	D	502	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	501	GOL	2	0
6	A	603	ET9	2	0
4	E	101	GOL	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%)	0.49	33 (5%) 21 28	26, 52, 94, 143	0
1	C	553/557 (99%)	0.57	56 (10%) 7 10	29, 53, 96, 149	0
2	B	406/444 (91%)	1.00	63 (15%) 2 3	31, 65, 129, 161	0
2	D	406/444 (91%)	0.43	23 (5%) 23 30	28, 50, 91, 156	0
3	E	33/38 (86%)	-0.12	0 100 100	29, 48, 81, 125	0
3	F	36/38 (94%)	-0.03	1 (2%) 53 60	35, 59, 101, 140	0
All	All	1987/2078 (95%)	0.58	176 (8%) 9 13	26, 54, 110, 161	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	301	LEU	14.7
2	B	90	VAL	11.1
2	D	360	ALA	10.8
2	D	67	ASP	10.8
2	B	88	TRP	9.9
2	B	5	ILE	9.5
2	D	359	GLY	9.2
2	B	93	GLY	8.6
2	B	92	LEU	8.1
2	B	357	MET	7.2
1	C	140	PRO	7.2
1	A	28	GLU	6.8
1	A	137	ASN	6.7
1	C	68	SER	6.6
2	D	212	TRP	6.6
2	B	361	HIS	6.5
2	B	360	ALA	6.5
2	B	359	GLY	6.4
1	A	140	PRO	6.3

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Mol	Chain	Res	Type	RSRZ
2	B	91	GLN	6.3
1	A	139	THR	6.2
2	D	361	HIS	6.1
1	A	69	THR	6.0
1	C	69	THR	5.9
2	B	295	LEU	5.9
2	B	94	ILE	5.7
2	B	89	GLU	5.7
1	C	141	GLY	5.7
1	A	133	PRO	5.4
2	B	212	TRP	5.4
1	C	142	ILE	5.4
2	B	168	LEU	5.3
1	C	132	ILE	5.2
1	C	133	PRO	5.1
2	B	279	LEU	4.9
1	C	67	ASP	4.9
1	C	139	THR	4.8
2	B	95	PRO	4.8
1	A	66	LYS	4.8
2	D	5	ILE	4.7
2	B	297	GLU	4.7
1	C	50	ILE	4.6
2	D	232	TYR	4.5
2	B	213	GLY	4.5
1	C	52	PRO	4.4
1	A	135	ILE	4.4
1	A	142	ILE	4.4
2	B	303	LEU	4.3
2	B	422	LEU	4.3
1	A	136	ASN	4.3
1	A	27	THR	4.2
2	B	252	TRP	4.2
2	B	245	VAL	4.2
1	C	28	GLU	4.2
2	D	68	SER	4.2
2	D	174	GLN	4.1
1	C	135	ILE	4.1
1	C	136	ASN	4.1
2	B	66	LYS	4.1
2	B	251	SER	4.1
1	A	138	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	68	SER	4.0
1	C	35	VAL	4.0
1	C	26	LEU	3.9
1	C	449	GLU	3.9
1	C	469	LEU	3.9
1	C	137	ASN	3.8
2	D	425	LEU	3.8
1	C	452	LEU	3.8
1	C	34	LEU	3.7
2	B	248	GLU	3.7
2	B	68	SER	3.7
1	C	37	ILE	3.7
2	B	305	GLU	3.7
1	A	132	ILE	3.7
1	C	131	THR	3.7
2	B	231	GLY	3.6
1	A	67	ASP	3.6
1	C	553	SER	3.6
2	B	67	ASP	3.6
1	C	39	THR	3.5
1	A	32	LYS	3.5
1	C	357[A]	MET	3.5
1	C	448	ARG	3.5
2	B	249	LYS	3.4
2	D	66	LYS	3.4
1	C	51	GLY	3.4
1	C	70	LYS	3.4
1	C	550	LYS	3.4
2	B	362	THR	3.3
1	A	33	ALA	3.3
2	B	423	VAL	3.3
2	D	211	ARG	3.3
2	B	277	ARG	3.3
2	B	232	TYR	3.2
1	C	138	GLU	3.2
2	B	238	LYS	3.2
3	F	18	DT	3.2
1	A	141	GLY	3.2
1	A	550	LYS	3.1
1	C	58	THR	3.1
1	A	24	TRP	3.1
1	C	219	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	71	TRP	3.0
1	C	54	ASN	3.0
1	A	25	PRO	3.0
2	B	250	ASP	3.0
2	B	274	ILE	2.9
1	C	33	ALA	2.9
2	D	356	ARG	2.9
2	B	285	GLY	2.9
1	A	549	ASP	2.9
2	B	7	THR	2.8
2	B	162	SER	2.8
1	A	36	GLU	2.8
1	C	49	LYS	2.8
1	C	32	LYS	2.7
2	B	6	GLU	2.7
2	B	296	THR	2.7
2	B	358	LYS	2.6
2	B	424	LYS	2.6
2	B	211	ARG	2.6
2	B	427	TYR	2.6
2	B	14	PRO	2.6
2	B	260	LEU	2.6
1	C	552	VAL	2.6
1	C	64	LYS	2.5
1	C	143	ARG	2.5
1	A	1	PRO	2.5
1	A	62	ALA	2.5
2	B	272	ALA	2.5
1	A	403	THR	2.5
2	B	9	PRO	2.4
2	B	10	VAL	2.4
2	B	299	ALA	2.4
2	D	357	MET	2.4
2	B	172	ARG	2.4
2	B	169	GLU	2.4
2	B	281	LYS	2.4
1	C	457	TYR	2.4
2	D	207	GLN	2.4
1	A	346	PHE	2.4
1	C	547	GLN	2.4
1	C	36	GLU	2.3
2	B	284	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	356	ARG	2.3
1	A	551	LEU	2.3
1	A	61	PHE	2.3
2	B	87	PHE	2.3
1	C	17	ASP	2.3
2	B	161	GLN	2.2
1	A	70	LYS	2.2
1	C	134	SER	2.2
1	A	542	ILE	2.2
1	C	450	THR	2.1
1	C	144	TYR	2.1
2	D	69	THR	2.1
2	B	196	GLY	2.1
1	C	104	LYS	2.1
1	C	14	PRO	2.1
1	C	41	MET	2.1
1	C	40	GLU	2.1
1	C	55	PRO	2.1
1	A	452	LEU	2.1
2	D	283	LEU	2.1
2	D	208	HIS	2.1
2	B	334	GLN	2.1
1	C	470	THR	2.1
2	D	166	LYS	2.1
1	A	211	ARG	2.0
2	D	231	GLY	2.0
2	D	169	GLU	2.0
2	D	209	LEU	2.0
1	C	59	PRO	2.0
1	C	454	LYS	2.0
2	D	358	LYS	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	E	2	21/22	0.96	0.19	29,34,40,42	0
3	OMC	F	2	21/22	0.97	0.15	39,45,50,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	OMC	F	4	21/22	0.97	0.20	30,35,40,48	0
3	OMC	E	4	21/22	0.98	0.19	25,29,35,40	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

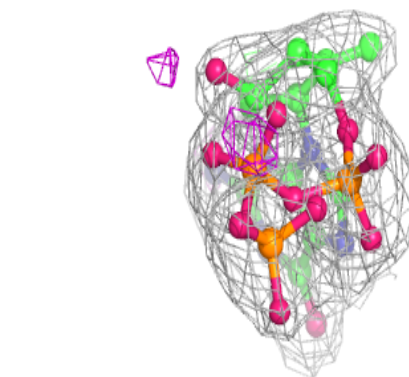
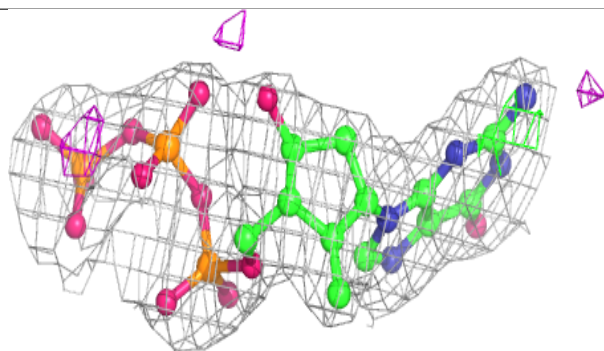
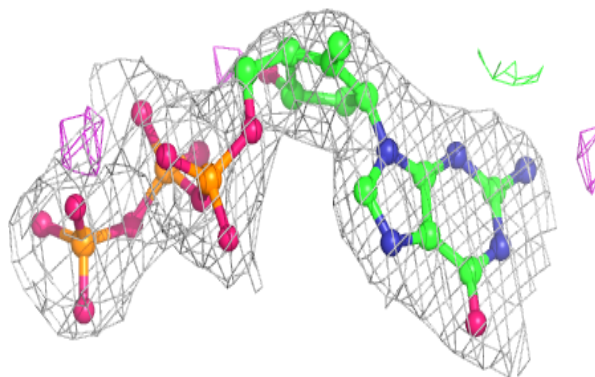
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	A	602	1/1	0.72	0.10	55,55,55,55	0
4	GOL	A	601	6/6	0.79	0.26	49,58,60,61	0
5	MG	C	601	1/1	0.83	0.15	65,65,65,65	0
4	GOL	E	101	6/6	0.89	0.30	63,70,71,72	0
4	GOL	D	502	6/6	0.89	0.20	41,46,47,48	0
4	GOL	D	503	6/6	0.89	0.20	55,59,61,61	0
6	ET9	C	602	32/32	0.92	0.14	51,60,79,83	0
4	GOL	B	501	6/6	0.92	0.26	41,47,49,50	0
6	ET9	A	603	32/32	0.94	0.14	48,57,68,68	0
4	GOL	D	501	6/6	0.95	0.24	46,49,49,51	0

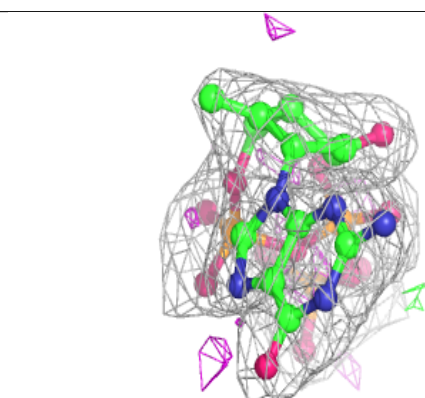
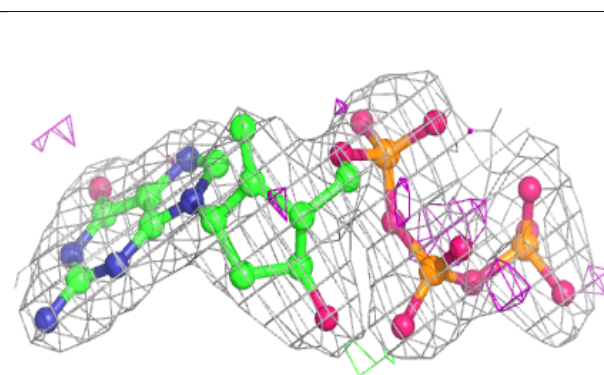
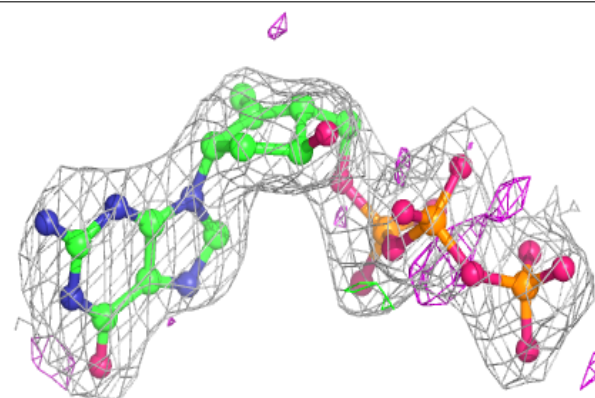
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ET9 C 602:

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

**Electron density around ET9 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.