



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:36 PM UTC

PDB ID : 8X21 / pdb_00008x21
Title : HIV-1 reverse transcriptase mutant Q151M/Y115F/F116Y/L74V:DNA:ETV
-TP ternary complex
Authors : Yasutake, Y.; Hattori, S.I.; Mitsuya, H.
Deposited on : 2023-11-09
Resolution : 2.33 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

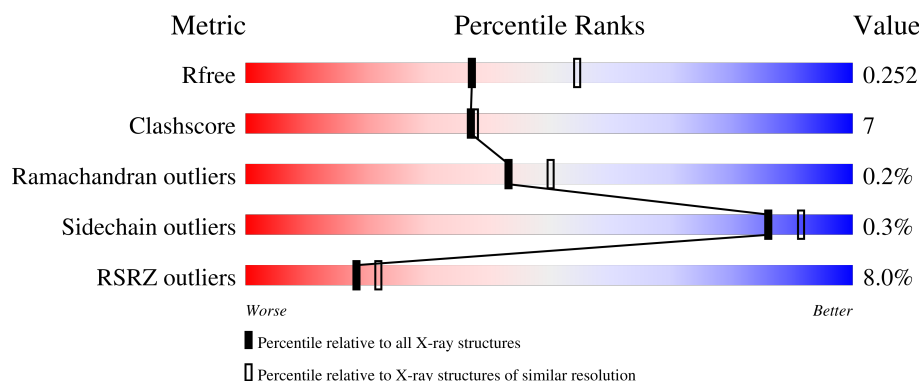
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	8% 83% 15% ..
1	C	557	8% 83% 16% ..
2	B	444	10% 75% 16% 9%
2	D	444	6% 79% 13% 9%
3	E	38	68% 18% 5% 8%

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Mol	Chain	Length	Quality of chain
3	F	38	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (74%), yellow (21%), and orange (5%). The percentages are labeled below the bar.

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17751 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pol protein (Fragment).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4497	2910	750	829	8			
1	C	553	Total	C	N	O	S	0	1	0
			4505	2915	751	830	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP D3XFN5
A	0	VAL	-	expression tag	UNP D3XFN5
A	74	VAL	LEU	engineered mutation	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	-	initiating methionine	UNP D3XFN5
C	0	VAL	-	expression tag	UNP D3XFN5
C	74	VAL	LEU	engineered mutation	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).

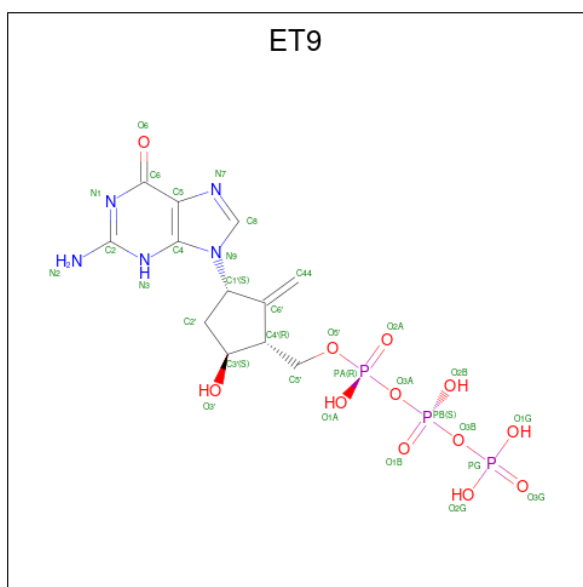
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	35	Total	C	N	O	P	0	0	0
			718	339	128	216	35			

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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 [[(1R,3S,5S)-3-(2-azanyl-6-oxidanylidene-3H-purin-9-yl)-2-methylidene-5-oxidanyl-cyclopentyl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (CCD ID: ET9) (formula: $C_{12}H_{18}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	12	5	12	3		
4	C	1	Total	C	N	O	P	0	0
			32	12	5	12	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: 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		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

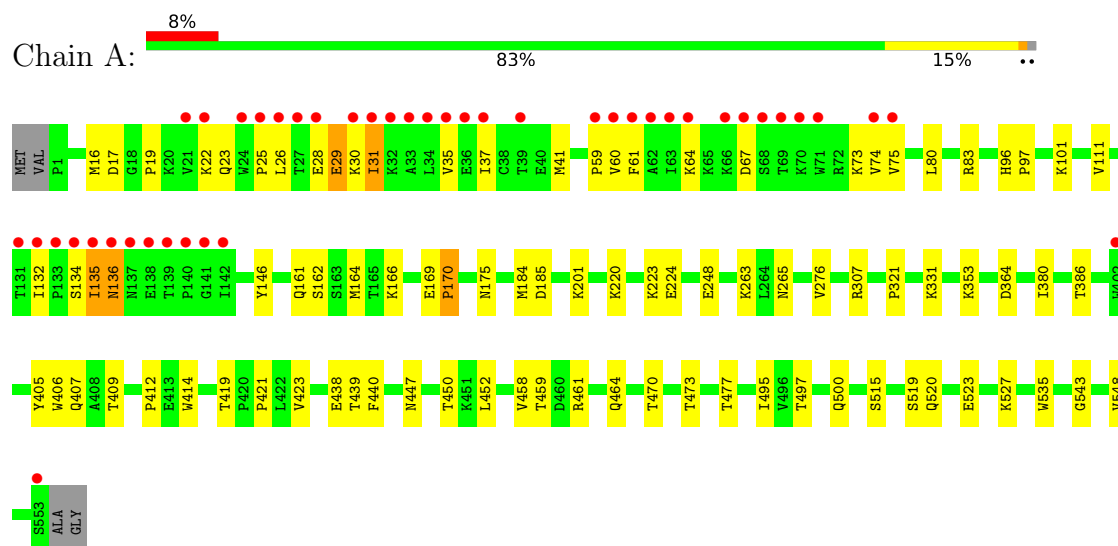
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	122	Total	O	0	0
			122	122		
7	B	58	Total	O	0	0
			58	58		
7	E	43	Total	O	0	0
			43	43		
7	C	111	Total	O	0	0
			111	111		
7	D	92	Total	O	0	0
			92	92		
7	F	32	Total	O	0	0
			32	32		

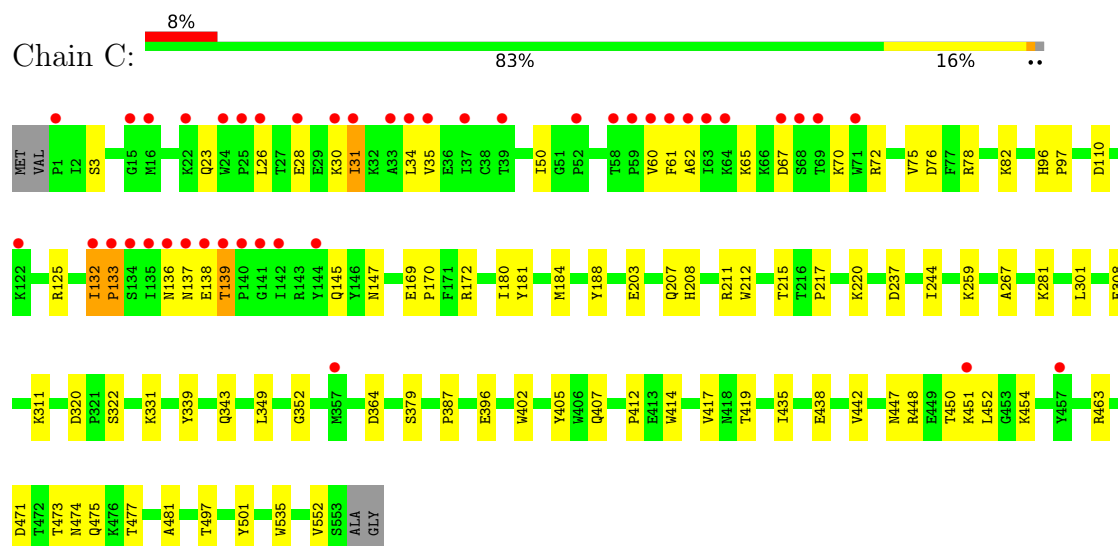
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

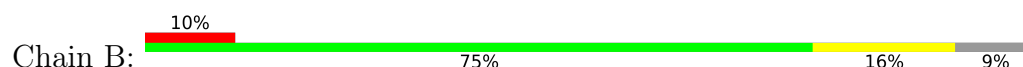
- Molecule 1: Pol protein (Fragment)



- Molecule 1: Pol protein (Fragment)



- Molecule 2: HIV-1 RT p51 subunit



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 95.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.67 – 2.33 48.67 – 2.33	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.67-2.33) 100.0 (48.67-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.175 , 0.218 (Not available) , 0.252	Depositor DCC
R_{free} test set	6262 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17751	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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: GOL, MG, OMC, 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	0.62	2/4615 (0.0%)	0.75	5/6267 (0.1%)
1	C	0.55	2/4623 (0.0%)	0.74	5/6277 (0.1%)
2	B	0.51	0/3441	0.73	3/4673 (0.1%)
2	D	0.51	0/3441	0.63	2/4673 (0.0%)
3	E	0.61	0/756	0.69	0/1165
3	F	0.51	0/823	0.62	0/1269
All	All	0.56	4/17699 (0.0%)	0.71	15/24324 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	PRO	N-CA	16.34	1.68	1.47
1	C	139	THR	C-N	13.01	1.50	1.33
1	C	132	ILE	N-CA	5.41	1.50	1.46
1	A	170	PRO	C-O	-5.24	1.17	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	139	THR	CA-C-N	15.44	135.66	119.76
1	C	139	THR	C-N-CA	15.44	135.66	119.76
1	C	133	PRO	N-CA-C	14.44	132.74	113.40
1	A	169	GLU	CA-C-N	12.67	135.68	119.84
1	A	169	GLU	C-N-CA	12.67	135.68	119.84
2	B	36	GLU	CA-CB-CG	-8.83	96.45	114.10
2	D	426	TRP	N-CA-C	-7.81	102.25	112.41
1	A	170	PRO	N-CA-C	-7.23	97.58	112.47
2	D	422	LEU	N-CA-C	-7.17	105.06	113.88
1	A	170	PRO	CA-N-CD	-6.48	102.93	112.00
1	A	169	GLU	O-C-N	-5.69	115.41	120.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	ILE	CA-C-N	5.67	125.03	118.85
1	C	132	ILE	C-N-CA	5.67	125.03	118.85
2	B	363	ASN	N-CA-C	5.40	118.25	107.62
2	B	362	THR	N-CA-C	5.32	117.15	111.36

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	4497	0	4551	77	0
1	C	4505	0	4559	64	0
2	B	3347	0	3379	61	0
2	D	3347	0	3379	37	0
3	E	718	0	397	8	0
3	F	777	0	432	7	0
4	A	32	0	0	0	0
4	C	32	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	6	0	8	3	0
6	B	6	0	7	0	0
6	D	18	0	24	1	0
6	E	6	0	7	0	0
7	A	122	0	0	3	0
7	B	58	0	0	0	0
7	C	111	0	0	0	0
7	D	92	0	0	1	0
7	E	43	0	0	0	0
7	F	32	0	0	0	0
All	All	17751	0	16743	240	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 (240) 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:170:PRO:N	1:A:170:PRO:CA	1.68	1.35
1:C:26:LEU:HD11	1:C:31:ILE:HD12	1.12	1.11
2:B:248:GLU:HG2	2:B:307:ARG:NH2	1.75	1.00
1:A:439:THR:CG2	2:B:289:LEU:HD13	1.94	0.97
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.47	0.93
1:C:26:LEU:HD11	1:C:31:ILE:CD1	2.00	0.91
1:A:31:ILE:HG21	1:A:134:SER:HA	1.53	0.88
1:C:67:ASP:OD1	1:C:70:LYS:HD2	1.73	0.88
1:C:26:LEU:CD1	1:C:31:ILE:HD12	2.01	0.86
2:B:248:GLU:HG2	2:B:307:ARG:HH22	1.35	0.85
1:A:439:THR:HG21	2:B:289:LEU:CD1	2.06	0.84
1:A:459:THR:HG22	1:A:461:ARG:H	1.39	0.84
1:C:31:ILE:HD11	1:C:133:PRO:HG2	1.59	0.84
1:C:60:VAL:HG12	1:C:75:VAL:HG22	1.60	0.83
2:B:87:PHE:HB3	2:B:92:LEU:HB2	1.61	0.82
6:A:603:GOL:H11	7:A:752:HOH:O	1.81	0.79
1:A:170:PRO:N	1:A:170:PRO:C	2.42	0.78
1:A:31:ILE:HD13	1:A:135:ILE:H	1.49	0.78
1:A:26:LEU:HD22	1:A:30:LYS:HE2	1.66	0.77
2:B:311:LYS:HG2	2:B:312:GLU:HG2	1.66	0.76
1:A:37:ILE:HG22	1:A:41:MET:HE2	1.67	0.75
1:A:135:ILE:HG22	1:A:135:ILE:O	1.86	0.74
1:A:35:VAL:HG23	1:A:132:ILE:HD11	1.74	0.70
1:C:136:ASN:O	1:C:138:GLU:N	2.25	0.69
1:A:459:THR:CG2	1:A:461:ARG:H	2.06	0.69
2:B:388:LYS:NZ	2:B:415:GLU:OE1	2.26	0.69
2:B:85:GLN:O	2:B:85:GLN:HG3	1.92	0.68
1:A:459:THR:HG22	1:A:461:ARG:N	2.07	0.67
2:D:90:VAL:HG21	2:D:158:ALA:HA	1.77	0.67
2:B:298:GLU:CD	2:B:298:GLU:H	2.01	0.67
1:A:439:THR:HG23	2:B:289:LEU:HD13	1.75	0.67
1:C:438:GLU:OE1	1:C:463:ARG:HD3	1.94	0.67
1:A:331:LYS:NZ	1:A:364:ASP:OD2	2.24	0.66
1:A:447:ASN:HB3	1:A:450:THR:HB	1.78	0.66
2:B:35:VAL:O	2:B:39:THR:HG23	1.94	0.66
1:A:26:LEU:HD22	1:A:30:LYS:CE	2.26	0.66
1:A:438:GLU:OE2	1:A:459:THR:HG21	1.95	0.66
1:A:31:ILE:CG2	1:A:134:SER:HA	2.24	0.65
1:A:161:GLN:NE2	1:A:184:MET:SD	2.69	0.64
1:C:343:GLN:HG3	1:C:349:LEU:HD11	1.79	0.64
2:B:358:LYS:HZ1	2:B:367:GLN:HG3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:O	1:A:135:ILE:CG2	2.47	0.63
1:C:203:GLU:O	1:C:207:GLN:HG2	1.98	0.63
1:A:74:VAL:HG11	3:E:0:DC:C2	2.34	0.62
1:A:439:THR:CG2	2:B:289:LEU:CD1	2.73	0.61
2:B:278:GLN:HE21	2:B:298:GLU:CB	2.13	0.61
3:F:3:DC:H2'	3:F:4:OMC:C6	2.36	0.61
2:D:232:TYR:CE1	2:D:234:LEU:HD21	2.37	0.60
1:A:223:LYS:HG3	1:A:224:GLU:HG2	1.84	0.59
1:C:208:HIS:HA	1:C:211:ARG:CZ	2.31	0.59
2:D:164:MET:HE2	2:D:168:LEU:HG	1.83	0.59
2:D:108:VAL:HG21	2:D:232:TYR:CZ	2.38	0.59
2:B:207:GLN:HA	2:B:210:LEU:HD12	1.85	0.58
1:C:31:ILE:CD1	1:C:133:PRO:HG2	2.32	0.58
3:F:1:DG:H2'	3:F:2:OMC:C6	2.39	0.58
2:B:85:GLN:HE22	2:B:90:VAL:HG21	1.67	0.58
1:A:184:MET:HG3	3:E:33:DC:H1'	1.86	0.57
1:C:396:GLU:CD	1:C:396:GLU:H	2.12	0.57
3:E:23:DC:H2''	3:E:24:DG:C8	2.39	0.57
1:C:339:TYR:CZ	1:C:352:GLY:HA3	2.40	0.57
2:D:122:LYS:HG2	2:D:125:ARG:CZ	2.34	0.57
1:A:111:VAL:HG21	1:A:164:MET:HE1	1.86	0.57
2:D:170:PRO:O	2:D:174:GLN:HG3	2.04	0.57
1:A:35:VAL:HG23	1:A:132:ILE:CD1	2.35	0.57
1:C:50:ILE:HD11	1:C:145:GLN:HB3	1.86	0.56
2:B:64:LYS:NZ	2:B:69:THR:HG22	2.19	0.56
1:A:28:GLU:HG2	1:A:29:GLU:N	2.20	0.56
1:C:331:LYS:NZ	1:C:364:ASP:OD1	2.32	0.56
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.41	0.56
2:B:278:GLN:HE21	2:B:298:GLU:HB2	1.71	0.55
1:A:543:GLY:HA3	2:B:283:LEU:O	2.06	0.55
1:A:458:VAL:HG22	1:A:548:VAL:HB	1.88	0.55
1:C:3:SER:HB2	1:C:212:TRP:O	2.07	0.55
2:B:424:LYS:HA	2:B:424:LYS:CE	2.37	0.55
1:C:435:ILE:HG13	2:D:290:THR:HG21	1.88	0.55
1:A:23:GLN:HA	1:A:59:PRO:HB3	1.89	0.54
1:C:417:VAL:HG22	1:C:419:THR:HG23	1.90	0.54
1:A:22:LYS:HD2	1:A:23:GLN:H	1.72	0.54
2:B:90:VAL:HG12	2:B:90:VAL:O	2.08	0.54
1:C:110:ASP:HB3	1:C:220:LYS:HD3	1.89	0.54
1:C:34:LEU:HD21	1:C:62:ALA:HB2	1.91	0.53
2:D:356:ARG:NH1	2:D:361:HIS:HB2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:GLN:OE1	2:B:424:LYS:HD2	2.08	0.53
1:A:248:GLU:HG2	1:A:307:ARG:HH22	1.75	0.52
2:D:68:SER:OG	2:D:70:LYS:N	2.26	0.52
1:C:447:ASN:HB3	1:C:450:THR:HG22	1.92	0.52
1:C:30:LYS:HE3	1:C:62:ALA:H	1.74	0.52
1:A:31:ILE:CD1	1:A:135:ILE:H	2.21	0.52
1:A:17:ASP:O	1:A:83:ARG:HD3	2.09	0.51
1:A:440:PHE:HB2	1:A:495:ILE:CD1	2.40	0.51
6:D:503:GOL:H32	7:D:610:HOH:O	2.10	0.51
2:B:85:GLN:NE2	2:B:90:VAL:HG21	2.26	0.51
1:C:451:LYS:HD3	1:C:471:ASP:HA	1.93	0.51
2:D:350:LYS:NZ	2:D:378:GLU:OE2	2.39	0.51
3:E:1:DG:H2'	3:E:2:OMC:C6	2.45	0.51
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.92	0.50
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.94	0.50
2:B:143:ARG:HG2	2:B:143:ARG:HH11	1.75	0.50
2:B:87:PHE:HD2	2:B:92:LEU:HD12	1.77	0.50
2:B:423:VAL:HB	2:B:425:LEU:CD2	2.42	0.50
1:A:500:GLN:CD	1:A:500:GLN:H	2.19	0.50
2:B:94:ILE:HG12	2:B:161:GLN:NE2	2.26	0.50
2:D:358:LYS:HG2	2:D:359:GLY:N	2.27	0.50
1:A:73:LYS:HE2	1:A:146:TYR:OH	2.12	0.50
1:A:26:LEU:HD11	1:A:61:PHE:HA	1.93	0.50
1:C:30:LYS:NZ	1:C:61:PHE:HB2	2.27	0.49
1:C:450:THR:HG23	1:C:452:LEU:H	1.77	0.49
1:A:162:SER:O	1:A:166:LYS:HG3	2.12	0.49
1:C:78:ARG:HE	3:F:0:DC:H5''	1.78	0.49
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.94	0.49
1:C:379:SER:OG	1:C:387:PRO:HD3	2.13	0.49
2:D:365:VAL:HG11	2:D:401:TRP:HB2	1.95	0.49
1:C:65:LYS:HD3	1:C:72:ARG:CZ	2.43	0.48
1:A:25:PRO:HA	1:A:136:ASN:OD1	2.13	0.48
2:D:46:LYS:HE3	2:D:116:PHE:CD2	2.48	0.48
1:C:320:ASP:OD2	1:C:322:SER:HB3	2.13	0.48
3:F:10:DC:H2''	3:F:11:DG:C8	2.49	0.48
2:B:73:LYS:HE2	2:B:75:VAL:HG23	1.95	0.48
2:D:244:ILE:HB	2:D:310:LEU:HD13	1.94	0.48
1:C:237:ASP:OD1	1:C:237:ASP:N	2.45	0.48
2:D:201:LYS:HA	2:D:204:GLU:HG3	1.95	0.48
1:A:380:ILE:HD11	1:A:386:THR:HG23	1.96	0.48
2:D:236:PRO:HA	2:D:239:TRP:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:MET:HE2	2:D:168:LEU:CG	2.44	0.47
1:A:23:GLN:OE1	1:A:60:VAL:HG12	2.14	0.47
1:C:181:TYR:HB2	1:C:188:TYR:HB3	1.97	0.47
2:B:180:ILE:HG12	2:B:189:VAL:HG22	1.97	0.47
1:C:23:GLN:OE1	1:C:60:VAL:HG22	2.14	0.47
2:D:297:GLU:HG2	2:D:298:GLU:OE1	2.14	0.47
3:F:23:DC:H2"	3:F:24:DG:C8	2.50	0.47
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.95	0.47
2:B:237:ASP:OD1	2:B:237:ASP:O	2.32	0.47
1:A:23:GLN:OE1	1:A:59:PRO:HA	2.15	0.47
1:A:263:LYS:NZ	7:A:706:HOH:O	2.47	0.47
2:D:108:VAL:O	2:D:231:GLY:HA3	2.15	0.47
6:A:603:GOL:C1	7:A:752:HOH:O	2.52	0.46
1:C:448:ARG:NH2	1:C:474:ASN:HD21	2.14	0.46
2:B:280:SER:HB2	2:B:281:LYS:HE2	1.97	0.46
2:B:363:ASN:HB3	2:B:366:LYS:HB3	1.96	0.46
2:D:68:SER:OG	2:D:70:LYS:HB3	2.16	0.46
1:A:276:VAL:HG22	1:A:353:LYS:HE2	1.98	0.46
1:C:35:VAL:HG22	1:C:132:ILE:HG21	1.97	0.46
1:C:412:PRO:O	1:C:414:TRP:HD1	1.98	0.46
1:C:244:ILE:HD13	1:C:267:ALA:HB2	1.97	0.46
1:C:402:TRP:HE1	2:D:364:ASP:CG	2.23	0.46
1:A:452:LEU:HD23	1:A:470:THR:HA	1.97	0.46
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.97	0.46
1:C:473:THR:O	1:C:477:THR:HG23	2.15	0.46
1:C:78:ARG:O	1:C:82:LYS:HG3	2.16	0.46
1:A:31:ILE:HG12	1:A:134:SER:H	1.81	0.45
1:A:67:ASP:OD2	1:A:220:LYS:HE2	2.16	0.45
1:A:248:GLU:HG2	1:A:307:ARG:NH2	2.31	0.45
1:A:458:VAL:HG12	1:A:464:GLN:HG2	1.99	0.45
2:B:357:MET:CA	2:B:357:MET:HE2	2.46	0.45
2:B:266:TRP:CE3	2:B:425:LEU:HG	2.51	0.45
2:D:6:GLU:HG2	2:D:7:THR:N	2.31	0.45
1:C:76:ASP:OD1	1:C:78:ARG:HG3	2.16	0.45
2:D:281:LYS:HG2	2:D:284:ARG:HH21	1.83	0.44
1:C:96:HIS:CG	1:C:97:PRO:HD2	2.52	0.44
2:D:361:HIS:CD2	2:D:361:HIS:H	2.35	0.44
2:B:424:LYS:HA	2:B:424:LYS:HE2	1.99	0.44
2:D:17:ASP:O	2:D:83:ARG:HD3	2.18	0.44
2:D:232:TYR:CD1	2:D:234:LEU:HD21	2.51	0.44
1:A:175:ASN:HD21	1:A:201:LYS:NZ	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:423:VAL:HB	2:B:425:LEU:HD22	2.00	0.44
1:A:523:GLU:O	1:A:527:LYS:HG3	2.18	0.44
1:C:442:VAL:HB	1:C:481:ALA:HB1	1.99	0.44
1:C:139:THR:O	1:C:139:THR:OG1	2.27	0.44
2:B:129:ALA:HA	2:B:144:TYR:O	2.18	0.43
2:B:161:GLN:O	2:B:165:THR:HG23	2.18	0.43
2:B:175:ASN:CG	2:B:201:LYS:HE3	2.43	0.43
2:D:120:LEU:HD23	2:D:125:ARG:HG2	1.99	0.43
1:A:497:THR:O	1:A:535:TRP:HA	2.18	0.43
2:B:64:LYS:CE	2:B:69:THR:HG22	2.48	0.43
1:A:419:THR:O	1:A:419:THR:OG1	2.33	0.43
2:B:276:VAL:O	2:B:280:SER:OG	2.35	0.43
1:A:64:LYS:HB3	1:A:64:LYS:HE2	1.71	0.43
2:B:200:THR:O	2:B:204:GLU:HG3	2.17	0.43
1:C:26:LEU:CD1	1:C:31:ILE:CD1	2.80	0.43
2:B:354:TYR:OH	2:B:356:ARG:HD2	2.17	0.43
2:B:357:MET:SD	2:B:361:HIS:CE1	3.11	0.43
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.53	0.43
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.54	0.43
1:A:101:LYS:HE2	1:A:321:PRO:HG3	2.00	0.43
1:A:412:PRO:O	1:A:414:TRP:HD1	2.01	0.43
2:B:151:GLN:HE21	2:B:151:GLN:HB2	1.61	0.43
1:C:450:THR:C	1:C:451:LYS:HG3	2.42	0.43
1:A:265:ASN:OD1	1:A:353:LYS:HE3	2.19	0.42
1:C:450:THR:O	1:C:452:LEU:HD12	2.19	0.42
2:D:336:GLN:HG3	2:D:427:TYR:OH	2.19	0.42
2:D:379:SER:HB3	2:D:385:LYS:O	2.18	0.42
1:A:406:TRP:CZ2	2:B:420:PRO:HG3	2.54	0.42
1:A:500:GLN:CD	1:A:500:GLN:N	2.78	0.42
2:B:280:SER:HB2	2:B:281:LYS:NZ	2.33	0.42
2:B:263:LYS:HB2	2:B:423:VAL:HG11	2.01	0.42
2:D:208:HIS:CE1	2:D:212:TRP:HE1	2.36	0.42
1:A:515:SER:O	1:A:519:SER:OG	2.35	0.42
2:B:105:SER:O	2:B:190:GLY:HA2	2.18	0.42
2:D:336:GLN:OE1	2:D:353:LYS:HE3	2.19	0.42
1:A:409:THR:OG1	6:A:603:GOL:H31	2.20	0.42
3:E:3:DC:H2'	3:E:4:OMC:C6	2.54	0.42
1:C:28:GLU:N	1:C:28:GLU:OE1	2.52	0.42
1:A:61:PHE:HZ	3:E:0:DC:C6	2.36	0.42
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.00	0.42
2:B:109:LEU:HD22	2:B:206:ARG:HE	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ARG:HE	1:C:147:ASN:HA	1.83	0.42
2:D:335:GLY:HA3	2:D:356:ARG:HG2	2.01	0.42
3:F:4:OMC:HM23	3:F:4:OMC:H1'	1.82	0.42
1:C:172:ARG:NH2	1:C:180:ILE:HB	2.34	0.42
2:B:73:LYS:HE2	2:B:75:VAL:CG2	2.50	0.42
2:D:298:GLU:H	2:D:298:GLU:CD	2.28	0.42
1:C:308:GLU:O	1:C:311:LYS:HG2	2.20	0.42
1:A:60:VAL:HB	1:A:75:VAL:HG22	2.02	0.42
1:A:74:VAL:HG11	3:E:0:DC:N1	2.35	0.42
2:B:246:LEU:HD12	2:B:307:ARG:HG2	2.02	0.42
1:C:207:GLN:O	1:C:211:ARG:HG3	2.20	0.42
1:C:497:THR:O	1:C:535:TRP:HA	2.20	0.41
1:A:473:THR:O	1:A:477:THR:HG23	2.20	0.41
1:A:520:GLN:O	1:A:523:GLU:HG3	2.19	0.41
1:C:405:TYR:CE2	1:C:407:GLN:HB2	2.54	0.41
1:C:30:LYS:HB3	1:C:30:LYS:HE2	1.78	0.41
2:B:97:PRO:HD3	2:B:181:TYR:CD1	2.55	0.41
1:C:110:ASP:HB3	1:C:220:LYS:HB3	2.02	0.41
1:C:454:LYS:HG3	1:C:552:VAL:HG13	2.02	0.41
1:A:353:LYS:NZ	3:E:7:DC:OP1	2.53	0.41
2:B:173:LYS:HA	2:B:173:LYS:HD3	1.79	0.41
2:B:104:LYS:O	2:B:235:HIS:ND1	2.36	0.41
1:C:169:GLU:N	1:C:170:PRO:HD2	2.36	0.41
1:A:421:PRO:HG2	1:C:301:LEU:HD23	2.02	0.41
2:B:39:THR:O	2:B:43:LYS:HG3	2.21	0.41
1:C:259:LYS:HG2	3:F:29:DG:O3'	2.21	0.41
1:C:31:ILE:HD11	1:C:133:PRO:CG	2.41	0.41
2:B:164:MET:O	2:B:168:LEU:HG	2.21	0.40
2:D:21:VAL:HB	2:D:59:PRO:HD3	2.02	0.40
1:A:16:MET:HE2	1:A:16:MET:HA	2.04	0.40
1:C:281:LYS:HB3	1:C:281:LYS:HE3	1.92	0.40
2:D:424:LYS:HG2	2:D:424:LYS:O	2.21	0.40
1:C:215:THR:HG23	1:C:217:PRO:HD3	2.04	0.40
2:D:232:TYR:HE1	2:D:234:LEU:HD21	1.81	0.40
2:D:328:GLU:O	2:D:339:TYR:HA	2.21	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%)	533 (97%)	16 (3%)	2 (0%)	30	32
1	C	552/557 (99%)	528 (96%)	23 (4%)	1 (0%)	43	50
2	B	402/444 (90%)	386 (96%)	16 (4%)	0	100	100
2	D	402/444 (90%)	387 (96%)	15 (4%)	0	100	100
All	All	1907/2002 (95%)	1834 (96%)	70 (4%)	3 (0%)	43	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	137	ASN
1	A	135	ILE
1	A	136	ASN

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%)	490 (100%)	2 (0%)	84	89
1	C	493/494 (100%)	491 (100%)	2 (0%)	84	89
2	B	365/400 (91%)	364 (100%)	1 (0%)	86	91
2	D	365/400 (91%)	365 (100%)	0	100	100
All	All	1715/1788 (96%)	1710 (100%)	5 (0%)	86	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	31	ILE
2	B	358	LYS
1	C	31	ILE
1	C	184	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	174	GLN
1	A	175	ASN
1	A	221	HIS
1	A	235	HIS
1	A	278	GLN
1	A	332	GLN
1	A	394	GLN
1	A	464	GLN
1	A	547	GLN
2	B	137	ASN
2	B	151	GLN
2	B	161	GLN
2	B	182	GLN
2	B	255	ASN
2	B	269	GLN
2	B	278	GLN
1	C	91	GLN
1	C	147	ASN
1	C	161	GLN
1	C	174	GLN
1	C	221	HIS
1	C	330	GLN
1	C	334	GLN
1	C	340	GLN
1	C	373	GLN
1	C	407	GLN
1	C	500	GLN
1	C	539	HIS
2	D	147	ASN
2	D	151	GLN
2	D	182	GLN
2	D	258	GLN
2	D	269	GLN

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Mol	Chain	Res	Type
2	D	394	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	2	3	19,22,23	2.48	8 (42%)	25,31,34	0.81	0
3	OMC	F	2	3	19,22,23	2.75	8 (42%)	25,31,34	1.09	1 (4%)
3	OMC	F	4	3	19,22,23	2.50	7 (36%)	25,31,34	0.62	0
3	OMC	E	4	3	19,22,23	2.59	8 (42%)	25,31,34	0.94	1 (4%)

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	2	3	-	1/9/27/28	0/2/2/2
3	OMC	F	2	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	4	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	6.30	1.49	1.35
3	F	4	OMC	C6-C5	5.86	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	OMC	C2-N3	5.56	1.47	1.36
3	F	2	OMC	C2-N3	5.13	1.46	1.36
3	E	4	OMC	C6-C5	5.11	1.46	1.35
3	F	4	OMC	C2-N3	4.89	1.46	1.36
3	E	2	OMC	C6-C5	4.81	1.46	1.35
3	F	2	OMC	C2-N1	4.79	1.50	1.40
3	E	2	OMC	C4-N3	4.62	1.43	1.34
3	E	4	OMC	C2-N1	4.44	1.49	1.40
3	F	2	OMC	C4-N3	4.32	1.43	1.34
3	E	2	OMC	C2-N1	4.31	1.49	1.40
3	E	2	OMC	C2-N3	4.07	1.44	1.36
3	F	4	OMC	C2-N1	4.02	1.48	1.40
3	F	4	OMC	C4-N3	3.79	1.42	1.34
3	E	4	OMC	C4-N3	3.61	1.41	1.34
3	F	4	OMC	C6-N1	3.47	1.46	1.38
3	E	4	OMC	C4-N4	3.39	1.42	1.33
3	E	4	OMC	C6-N1	3.33	1.46	1.38
3	E	2	OMC	C5-C4	3.24	1.50	1.42
3	F	2	OMC	C6-N1	3.20	1.45	1.38
3	F	2	OMC	C4-N4	3.17	1.41	1.33
3	E	2	OMC	C6-N1	3.09	1.45	1.38
3	F	2	OMC	O2-C2	-2.89	1.18	1.23
3	E	2	OMC	C4-N4	2.84	1.40	1.33
3	E	2	OMC	O2-C2	-2.73	1.18	1.23
3	F	2	OMC	C5-C4	2.55	1.48	1.42
3	E	4	OMC	C5-C4	2.52	1.48	1.42
3	F	4	OMC	O2-C2	-2.52	1.19	1.23
3	E	4	OMC	O2-C2	-2.32	1.19	1.23
3	F	4	OMC	C5-C4	2.31	1.48	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	OMC	O2-C2-N3	-2.75	118.00	122.33
3	E	4	OMC	C6-C5-C4	2.37	121.41	117.53

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	OMC	C1'-C2'-O2'-CM2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
6	GOL	D	501	-	5,5,5	0.98	0	5,5,5	1.01	0
4	ET9	C	601	5	33,34,34	1.61	4 (12%)	37,54,54	1.79	7 (18%)
6	GOL	D	502	-	5,5,5	1.53	1 (20%)	5,5,5	1.40	1 (20%)
6	GOL	B	501	-	5,5,5	1.79	2 (40%)	5,5,5	0.77	0
6	GOL	D	503	-	5,5,5	1.45	1 (20%)	5,5,5	1.00	0
6	GOL	E	101	-	5,5,5	1.00	0	5,5,5	1.31	1 (20%)
4	ET9	A	601	5	33,34,34	1.78	7 (21%)	37,54,54	1.91	10 (27%)
6	GOL	A	603	-	5,5,5	0.14	0	5,5,5	0.71	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	GOL	D	501	-	-	0/4/4/4	-
4	ET9	C	601	5	-	5/22/38/38	0/3/3/3
6	GOL	D	502	-	-	2/4/4/4	-
6	GOL	B	501	-	-	2/4/4/4	-
6	GOL	D	503	-	-	3/4/4/4	-
6	GOL	E	101	-	-	4/4/4/4	-
4	ET9	A	601	5	-	8/22/38/38	0/3/3/3
6	GOL	A	603	-	-	2/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	ET9	C4-N9	-6.00	1.31	1.37
4	C	601	ET9	C4-N9	-5.20	1.31	1.37
4	C	601	ET9	C5-C4	4.62	1.45	1.38
4	A	601	ET9	C5-C4	4.35	1.45	1.38
4	A	601	ET9	C4'-C6'	-2.70	1.48	1.51
6	B	501	GOL	O2-C2	-2.61	1.35	1.43
4	A	601	ET9	C6-N1	-2.58	1.33	1.38
4	C	601	ET9	C6-N1	-2.46	1.33	1.38
6	D	502	GOL	C1-C2	2.46	1.61	1.51
4	C	601	ET9	C5-N7	-2.36	1.34	1.39
6	B	501	GOL	C1-C2	2.32	1.60	1.51
4	A	601	ET9	C5-N7	-2.30	1.34	1.39
4	A	601	ET9	C1'-C6'	-2.04	1.48	1.51
4	A	601	ET9	C4-N3	-2.02	1.33	1.37
6	D	503	GOL	O2-C2	-2.01	1.37	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	ET9	C2'-C1'-N9	-6.01	105.05	115.32
4	A	601	ET9	C2'-C1'-N9	-5.78	105.44	115.32
4	A	601	ET9	C4'-C6'-C1'	4.83	115.32	106.12
4	C	601	ET9	C4'-C6'-C1'	4.35	114.41	106.12
4	A	601	ET9	C4'-C6'-C44	-3.86	121.30	127.68
4	C	601	ET9	C4'-C6'-C44	-3.51	121.89	127.68
4	A	601	ET9	C2'-C3'-C4'	3.17	107.89	103.62
4	C	601	ET9	C2'-C3'-C4'	2.85	107.46	103.62
6	D	502	GOL	C3-C2-C1	-2.58	102.33	111.80
4	A	601	ET9	C1'-N9-C8	2.53	130.79	126.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	101	GOL	C3-C2-C1	-2.51	102.57	111.80
4	A	601	ET9	C8-N9-C4	2.41	108.70	106.67
4	C	601	ET9	C8-N9-C4	2.41	108.70	106.67
4	A	601	ET9	C4-C5-N7	-2.36	106.20	109.26
4	C	601	ET9	C4-C5-N7	-2.27	106.31	109.26
4	A	601	ET9	C6-C5-N7	2.26	137.47	130.12
4	A	601	ET9	O2B-PB-O3A	2.15	113.08	107.27
4	C	601	ET9	C6-C5-N7	2.13	137.06	130.12
4	A	601	ET9	C5-C4-N9	2.08	107.21	106.25

There are no chirality outliers.

All (26) torsion outliers are listed below:

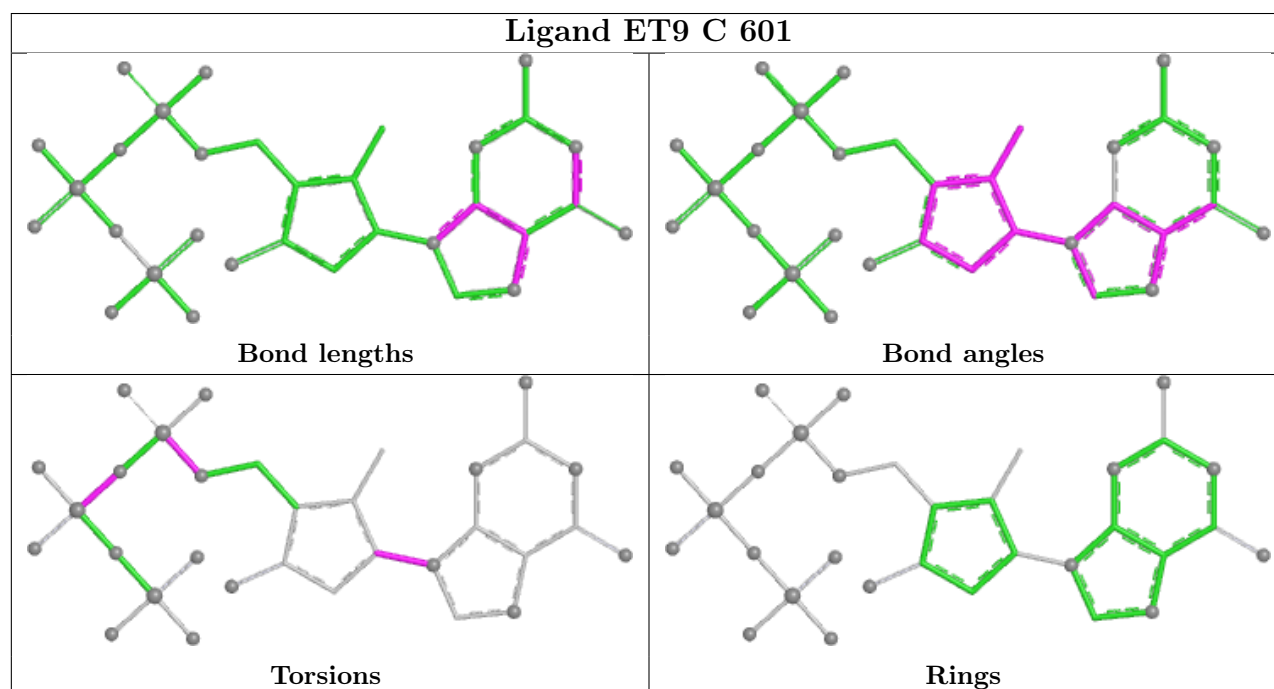
Mol	Chain	Res	Type	Atoms
4	A	601	ET9	C3'-C4'-C5'-O5'
4	A	601	ET9	C6'-C4'-C5'-O5'
4	A	601	ET9	C5'-O5'-PA-O1A
4	A	601	ET9	C5'-O5'-PA-O2A
4	A	601	ET9	C5'-O5'-PA-O3A
6	A	603	GOL	C1-C2-C3-O3
6	D	503	GOL	O1-C1-C2-C3
6	B	501	GOL	O1-C1-C2-C3
6	E	101	GOL	O1-C1-C2-C3
6	E	101	GOL	C1-C2-C3-O3
6	E	101	GOL	O1-C1-C2-O2
6	A	603	GOL	O2-C2-C3-O3
6	D	503	GOL	O1-C1-C2-O2
6	D	502	GOL	O1-C1-C2-O2
6	D	503	GOL	O2-C2-C3-O3
6	E	101	GOL	O2-C2-C3-O3
6	D	502	GOL	O1-C1-C2-C3
4	C	601	ET9	C5'-O5'-PA-O2A
4	C	601	ET9	C5'-O5'-PA-O3A
4	A	601	ET9	PA-O3A-PB-O2B
4	C	601	ET9	PA-O3A-PB-O2B
6	B	501	GOL	O1-C1-C2-O2
4	A	601	ET9	C6'-C1'-N9-C8
4	C	601	ET9	C6'-C1'-N9-C8
4	A	601	ET9	C2'-C1'-N9-C4
4	C	601	ET9	PA-O3A-PB-O1B

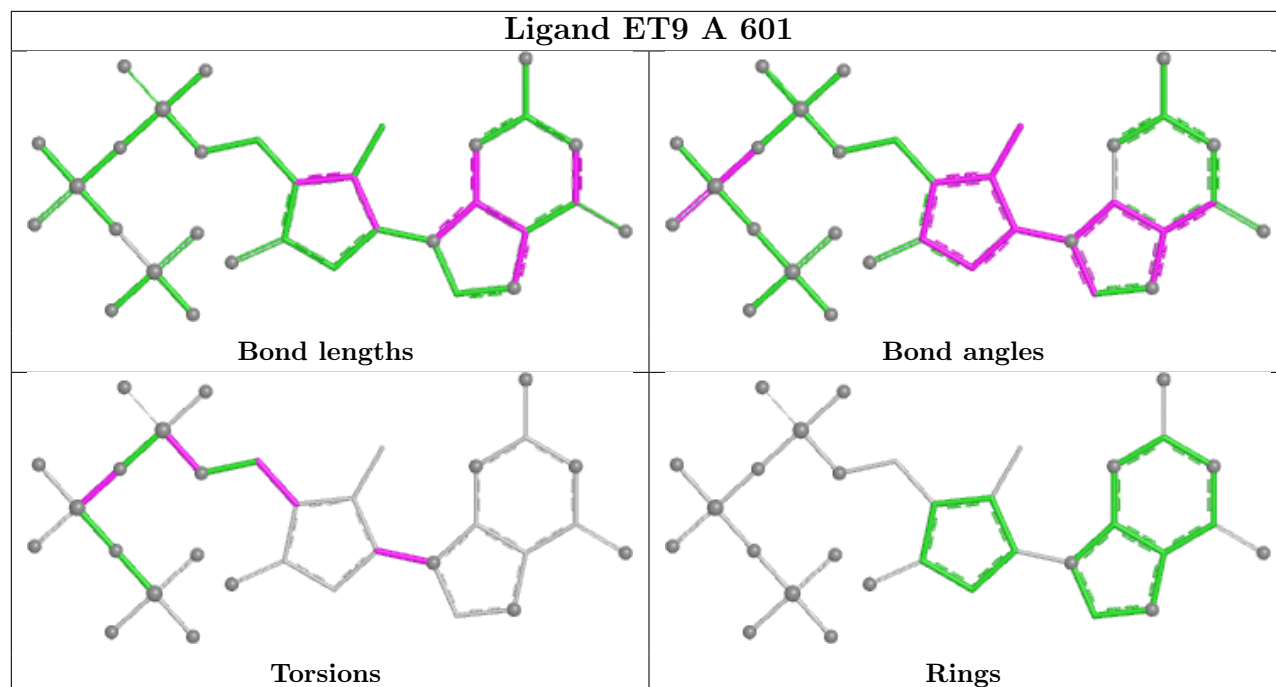
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	503	GOL	1	0
6	A	603	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%)	0.24	44 (7%)	18	22	32, 55, 101, 170	0
1	C	553/557 (99%)	0.30	43 (7%)	19	23	26, 60, 127, 181	1 (0%)
2	B	406/444 (91%)	0.51	44 (10%)	11	12	35, 68, 128, 174	0
2	D	406/444 (91%)	0.15	27 (6%)	24	28	34, 55, 99, 163	0
3	E	33/38 (86%)	-0.60	0	100	100	35, 52, 85, 140	0
3	F	36/38 (94%)	-0.32	0	100	100	38, 65, 113, 168	0
All	All	1987/2078 (95%)	0.27	158 (7%)	18	22	26, 59, 118, 181	1 (0%)

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	425	LEU	8.4
1	C	135	ILE	7.5
1	A	132	ILE	7.0
1	A	135	ILE	6.7
1	A	133	PRO	6.4
1	C	62	ALA	6.1
1	A	62	ALA	6.1
1	A	134	SER	6.1
1	A	141	GLY	5.7
2	B	92	LEU	5.4
1	A	140	PRO	5.4
1	A	33	ALA	5.1
2	D	422	LEU	5.0
2	D	232	TYR	5.0
1	C	35	VAL	4.9
2	B	301	LEU	4.9
1	A	31	ILE	4.8
2	B	360	ALA	4.8
2	D	360	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
2	B	212	TRP	4.6
2	B	90	VAL	4.6
2	B	422	LEU	4.6
1	C	134	SER	4.5
2	B	362	THR	4.5
1	C	37	ILE	4.4
1	A	69	THR	4.4
2	B	88	TRP	4.4
2	D	212	TRP	4.4
1	A	21	VAL	4.3
2	B	213	GLY	4.3
1	A	34	LEU	4.2
1	A	60	VAL	4.2
2	D	427	TYR	4.2
1	A	24	TRP	4.2
2	B	425	LEU	4.2
1	A	61	PHE	4.1
1	A	74	VAL	4.1
2	D	423	VAL	3.9
2	B	105	SER	3.8
2	D	213	GLY	3.8
2	B	5	ILE	3.7
1	C	71	TRP	3.7
1	A	139	THR	3.7
1	C	33	ALA	3.7
2	D	361	HIS	3.7
1	C	22	LYS	3.7
1	C	26	LEU	3.7
1	A	26	LEU	3.6
1	C	357[A]	MET	3.6
1	A	131	THR	3.6
1	C	31	ILE	3.6
1	A	68	SER	3.6
2	B	423	VAL	3.6
1	C	140	PRO	3.6
1	A	28	GLU	3.5
2	B	421	PRO	3.5
2	B	94	ILE	3.5
2	D	5	ILE	3.5
2	B	95	PRO	3.4
2	B	245	VAL	3.4
2	B	420	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	138	GLU	3.4
1	A	71	TRP	3.4
1	A	27	THR	3.3
2	B	210	LEU	3.3
2	B	232	TYR	3.3
1	A	136	ASN	3.3
1	A	35	VAL	3.3
1	C	30	LYS	3.2
2	B	427	TYR	3.2
1	C	133	PRO	3.1
1	A	30	LYS	3.1
1	C	52	PRO	3.1
2	D	358	LYS	3.1
2	D	424	LYS	3.0
1	C	142	ILE	3.0
1	A	63	ILE	3.0
2	B	237	ASP	3.0
1	C	25	PRO	3.0
1	A	70	LYS	2.9
1	A	75	VAL	2.9
2	B	93	GLY	2.9
2	D	421	PRO	2.9
1	C	60	VAL	2.9
1	C	63	ILE	2.9
1	C	61	PHE	2.8
1	A	39	THR	2.8
2	B	359	GLY	2.8
2	B	231	GLY	2.7
1	C	34	LEU	2.7
1	A	66	LYS	2.7
2	B	313	PRO	2.7
2	B	357	MET	2.7
1	C	136	ASN	2.6
2	D	359	GLY	2.6
1	C	64	LYS	2.6
1	C	59	PRO	2.6
1	C	132	ILE	2.6
1	A	32	LYS	2.6
2	D	419	THR	2.5
2	B	361	HIS	2.5
2	B	293	VAL	2.5
1	C	69	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	278	GLN	2.5
1	C	68	SER	2.5
2	B	280	SER	2.5
1	A	59	PRO	2.5
1	A	37	ILE	2.4
2	B	247	PRO	2.4
2	B	162	SER	2.4
2	B	241	VAL	2.4
1	C	24	TRP	2.4
1	A	67	ASP	2.4
1	C	67	ASP	2.4
1	C	141	GLY	2.4
1	A	22	LYS	2.4
2	B	356	ARG	2.4
2	D	88	TRP	2.4
1	C	144	TYR	2.3
2	B	281	LYS	2.3
2	D	313	PRO	2.3
1	C	58	THR	2.3
2	D	90	VAL	2.3
2	D	315	HIS	2.3
2	D	420	PRO	2.3
1	C	39	THR	2.3
1	A	36	GLU	2.3
1	A	142	ILE	2.3
1	A	137	ASN	2.2
2	B	238	LYS	2.2
1	A	553	SER	2.2
1	C	457	TYR	2.2
2	D	210	LEU	2.2
2	B	308	GLU	2.2
2	B	266	TRP	2.2
2	B	209	LEU	2.2
1	C	1	PRO	2.2
2	D	231	GLY	2.2
1	C	16	MET	2.1
1	C	122	LYS	2.1
2	B	66	LYS	2.1
1	A	64	LYS	2.1
1	A	402	TRP	2.1
2	D	362	THR	2.1
2	D	66	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	28	GLU	2.1
1	C	15	GLY	2.1
2	B	273	GLY	2.1
2	B	68	SER	2.1
2	B	240	THR	2.1
1	C	137	ASN	2.1
1	A	25	PRO	2.1
1	C	451	LYS	2.0
1	C	139	THR	2.0
2	D	69	THR	2.0
1	A	138	GLU	2.0
2	D	67	ASP	2.0
2	D	356	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OMC	F	2	21/22	0.97	0.07	48,53,58,61	0
3	OMC	E	2	21/22	0.98	0.06	33,39,42,48	0
3	OMC	E	4	21/22	0.98	0.05	28,35,42,46	0
3	OMC	F	4	21/22	0.98	0.05	32,40,45,50	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(Å ²)	Q<0.9
6	GOL	A	603	6/6	0.85	0.19	52,65,69,70	0

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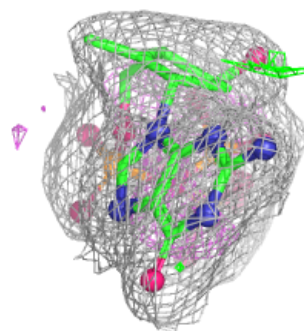
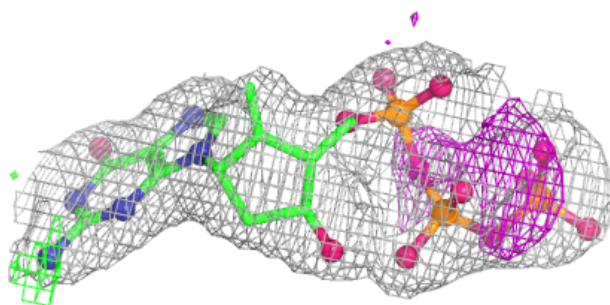
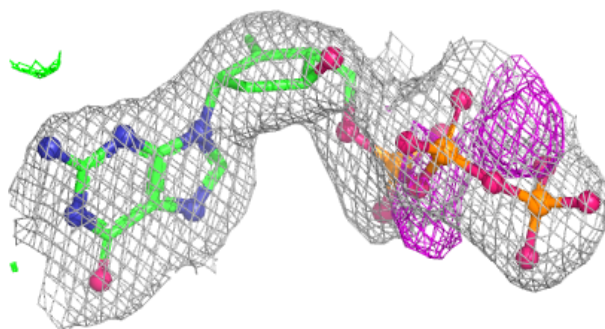
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ET9	C	601	32/32	0.92	0.10	66,73,93,96	0
4	ET9	A	601	32/32	0.92	0.10	47,63,87,94	0
5	MG	C	602	1/1	0.94	0.15	65,65,65,65	0
6	GOL	E	101	6/6	0.95	0.12	59,67,68,70	0
6	GOL	D	503	6/6	0.95	0.12	50,59,61,64	0
6	GOL	D	502	6/6	0.96	0.12	49,52,54,55	0
6	GOL	B	501	6/6	0.97	0.07	44,46,51,53	0
5	MG	A	602	1/1	0.97	0.07	61,61,61,61	0
6	GOL	D	501	6/6	0.98	0.06	39,43,47,48	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.

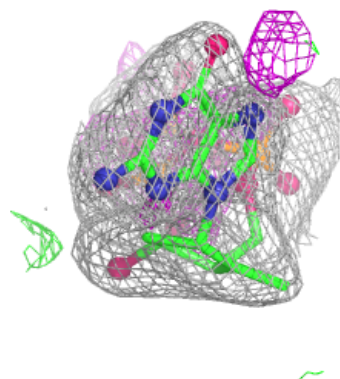
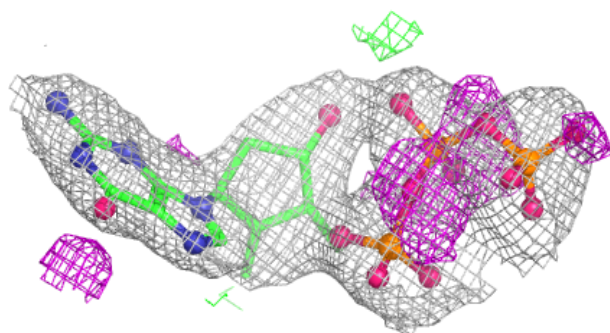
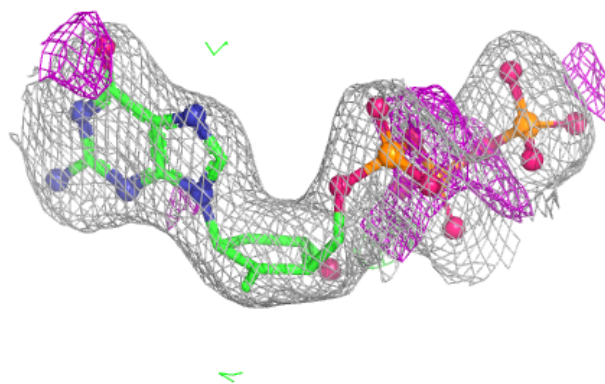
Electron density around ET9 C 601:

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 ET9 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.