



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 10, 2024 – 10:11 AM JST

PDB ID : 8X1Z
Title : HIV-1 reverse transcriptase mutant Q151M/Y115F/F116Y:DNA:E-CFCP-T
P ternary complex
Authors : Yasutake, Y.; Hattori, S.I.; Mitsuya, H.
Deposited on : 2023-11-09
Resolution : 2.62 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

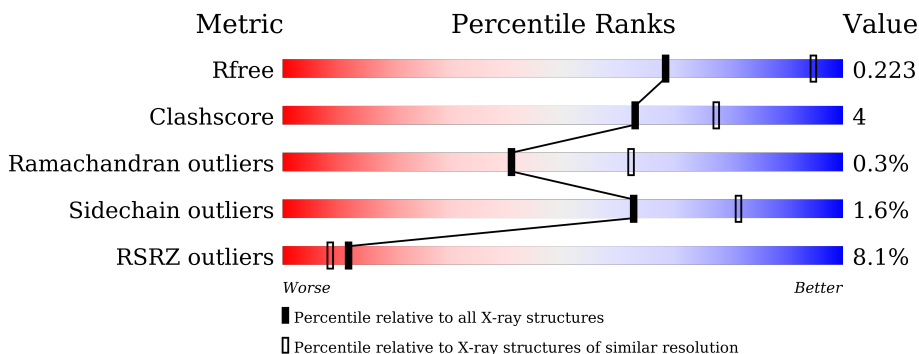
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	
1	C	557	
2	B	444	
2	D	444	
3	E	38	
3	F	38	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 17553 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
			Total	C	N	O	S			
1	A	553	Total	C	N	O	S	0	1	0
			4506	2916	753	829	8			
1	C	553	Total	C	N	O	S	0	1	0
			4503	2914	750	831	8			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP D3XFN5
A	0	VAL	-	expression tag	UNP D3XFN5
A	115	PHE	TYR	engineered mutation	UNP D3XFN5
A	116	TYR	PHE	engineered mutation	UNP D3XFN5
A	151	MET	GLN	engineered mutation	UNP D3XFN5
A	162	SER	CYS	engineered mutation	UNP D3XFN5
A	280	SER	CYS	engineered mutation	UNP D3XFN5
C	-1	MET	-	expression tag	UNP D3XFN5
C	0	VAL	-	expression tag	UNP D3XFN5
C	115	PHE	TYR	engineered mutation	UNP D3XFN5
C	116	TYR	PHE	engineered mutation	UNP D3XFN5
C	151	MET	GLN	engineered mutation	UNP D3XFN5
C	162	SER	CYS	engineered mutation	UNP D3XFN5
C	280	SER	CYS	engineered mutation	UNP D3XFN5

- Molecule 2 is a protein called HIV-1 RT p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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).

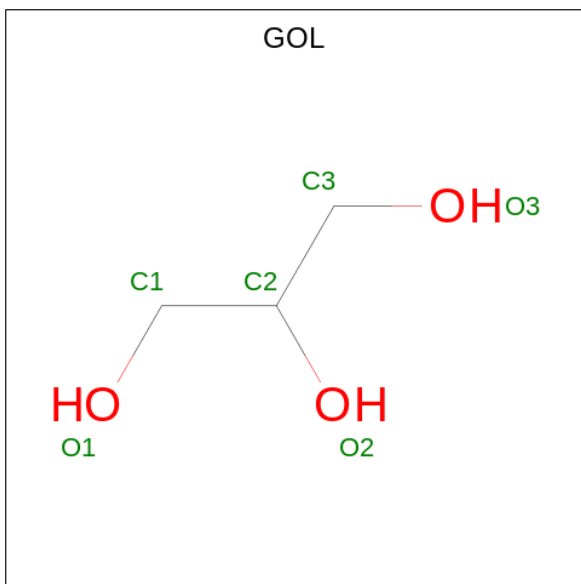
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	35	718	339	128	216	35	0	0	0

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



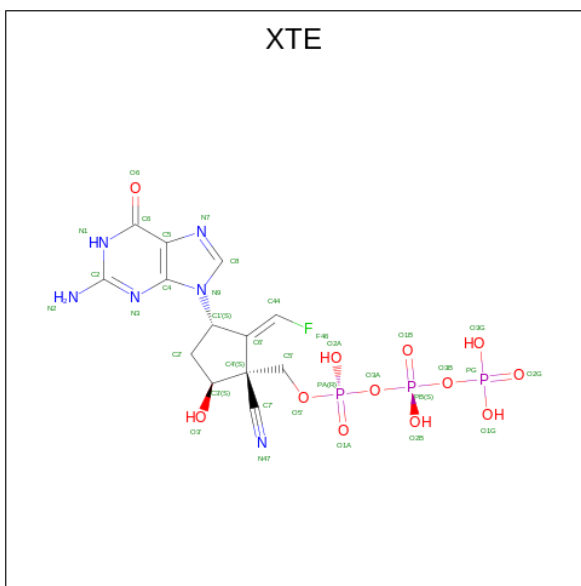
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	D	1	6	3	3	0	0
4	D	1	6	3	3	0	0
4	F	1	6	3	3	0	0

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

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

- Molecule 6 is E-CFCP-triphosphate (three-letter code: XTE) (formula: C₁₃H₁₆FN₆O₁₂P₃)

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			P
6	A	1	35	13	1	6	12	3	0	0
6	C	1	35	13	1	6	12	3	0	0

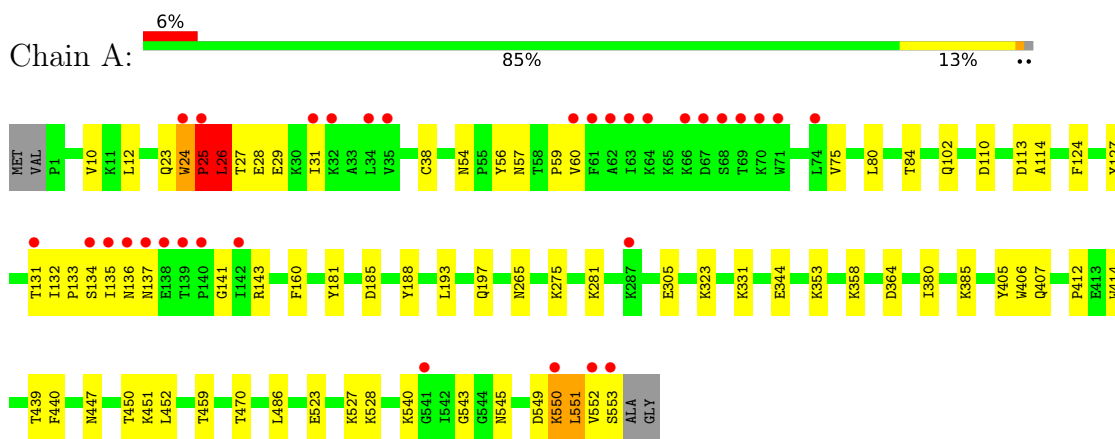
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	73	Total	O	0	0
			73	73		
7	B	26	Total	O	0	0
			26	26		
7	E	36	Total	O	0	0
			36	36		
7	C	48	Total	O	0	0
			48	48		
7	D	50	Total	O	0	0
			50	50		
7	F	20	Total	O	0	0
			20	20		

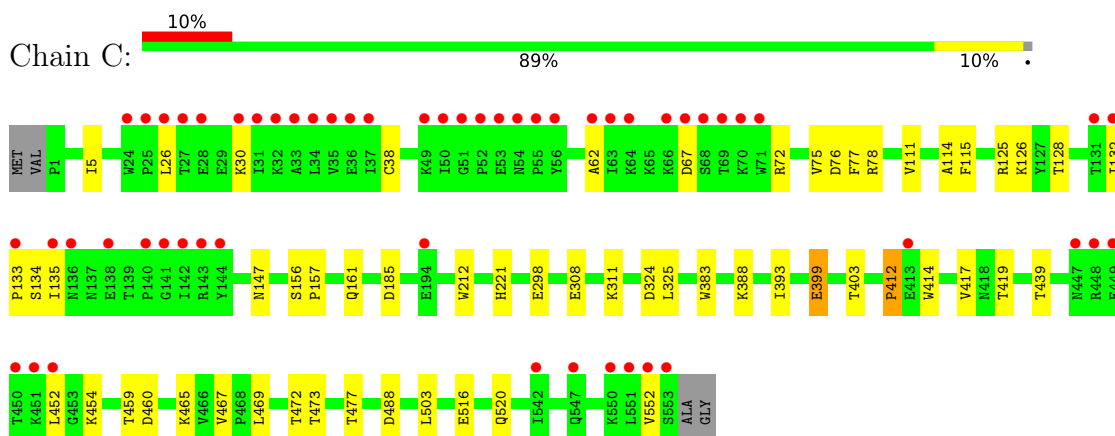
3 Residue-property plots [i](#)

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

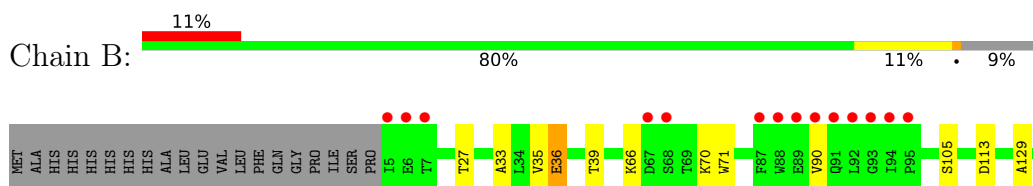
- Molecule 1: HIV-1 reverse transcriptase p66 subunit

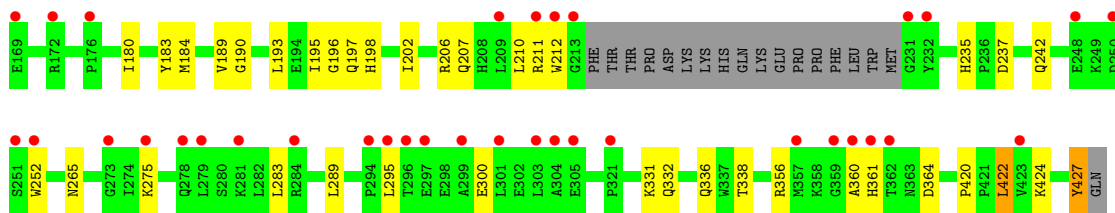


- Molecule 1: HIV-1 reverse transcriptase p66 subunit

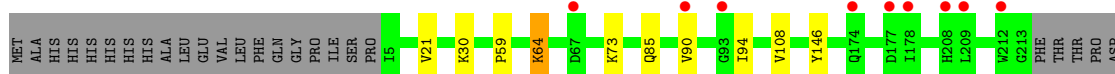
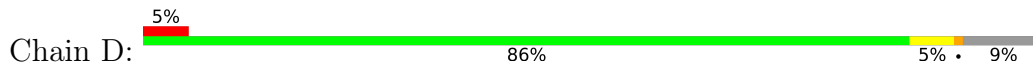


- Molecule 2: HIV-1 RT p51 subunit





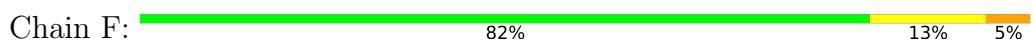
● Molecule 2: HIV-1 RT p51 subunit



● Molecule 3: DNA/RNA (38-MER)



● Molecule 3: DNA/RNA (38-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	283.14Å 283.14Å 95.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.47 – 2.62 44.47 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.47-2.62) 99.9 (44.47-2.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.61Å)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.179 , 0.223 0.179 , 0.223	Depositor DCC
R_{free} test set	4364 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtrriage
Anisotropy	0.091	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.013 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17553	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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: XTE, MG, OMC, GOL

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	0.42	0/4627	0.55	1/6282 (0.0%)
1	C	0.35	0/4624	0.48	0/6279
2	B	0.33	0/3441	0.49	0/4673
2	D	0.31	0/3441	0.48	0/4673
3	E	0.87	5/756 (0.7%)	0.89	0/1165
3	F	0.58	0/823	0.93	1/1269 (0.1%)
All	All	0.41	5/17712 (0.0%)	0.56	2/24341 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	32	DG	O3'-P	-7.49	1.52	1.61
3	E	0	DC	O3'-P	-7.24	1.52	1.61
3	E	-1	DT	O3'-P	-5.57	1.54	1.61
3	E	32	DG	P-OP2	-5.07	1.40	1.49
3	E	31	DG	O3'-P	-5.01	1.55	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	PRO	CA-N-CD	-6.83	101.94	111.50
3	F	18	DT	O4'-C1'-N1	5.21	111.65	108.00

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	4506	0	4566	52	0
1	C	4503	0	4557	39	0
2	B	3347	0	3379	34	0
2	D	3347	0	3379	15	0
3	E	718	0	397	7	0
3	F	777	0	432	5	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	D	12	0	16	0	0
4	F	6	0	8	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	35	0	0	5	0
6	C	35	0	0	5	0
7	A	73	0	0	0	0
7	B	26	0	0	1	0
7	C	48	0	0	0	0
7	D	50	0	0	0	0
7	E	36	0	0	0	0
7	F	20	0	0	0	0
All	All	17553	0	16750	146	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 4.

All (146) 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:135:ILE:HG22	1:A:135:ILE:O	1.49	1.09
1:A:27:THR:HG22	1:A:28:GLU:N	1.84	0.91
2:B:193:LEU:HD13	2:B:197:GLN:HG3	1.55	0.86
1:A:135:ILE:O	1:A:135:ILE:CG2	2.23	0.83
2:D:356:ARG:HD2	2:D:361:HIS:HB3	1.63	0.81
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.62	0.80
2:B:195:ILE:HG13	2:B:196:GLY:N	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:CG2	1:A:28:GLU:N	2.48	0.77
1:C:26:LEU:HD21	1:C:30:LYS:HB3	1.65	0.76
2:D:356:ARG:HD2	2:D:361:HIS:CB	2.18	0.73
2:B:207:GLN:O	2:B:211:ARG:HG2	1.92	0.69
6:A:603:XTE:F46	3:E:33:DC:H2''	1.84	0.68
1:A:27:THR:HG22	1:A:28:GLU:H	1.60	0.67
1:A:27:THR:HG22	1:A:29:GLU:H	1.58	0.67
2:B:193:LEU:HD13	2:B:197:GLN:CG	2.24	0.66
1:C:38:CYS:SG	1:C:132:ILE:HD11	2.35	0.66
1:A:331:LYS:NZ	1:A:364:ASP:OD2	2.29	0.65
6:A:603:XTE:N2	3:E:0:DC:O2	2.29	0.65
2:D:64:LYS:O	2:D:407:GLN:NE2	2.30	0.64
1:A:136:ASN:O	1:A:137:ASN:HB2	1.97	0.64
1:A:27:THR:CG2	1:A:28:GLU:H	2.10	0.63
2:B:206:ARG:HG2	2:B:210:LEU:HD12	1.82	0.62
2:B:252:TRP:CD1	2:B:295:LEU:HD11	2.35	0.61
1:C:452:LEU:HD12	1:C:469:LEU:O	2.00	0.60
1:C:115:PHE:CE1	1:C:156:SER:HB3	2.37	0.60
2:B:198:HIS:CE1	2:B:202:ILE:HD11	2.38	0.59
1:A:23:GLN:OE1	1:A:59:PRO:HA	2.02	0.59
1:A:114:ALA:HB3	6:A:603:XTE:N47	2.18	0.59
2:B:252:TRP:CD1	2:B:295:LEU:HD21	2.39	0.58
1:C:38:CYS:SG	1:C:132:ILE:CD1	2.92	0.58
1:C:516:GLU:OE2	1:C:520:GLN:NE2	2.38	0.57
1:A:27:THR:HG22	1:A:29:GLU:N	2.19	0.56
1:A:57:ASN:OD1	1:A:131:THR:HG23	2.06	0.56
1:C:115:PHE:CD2	6:C:602:XTE:N47	2.73	0.56
2:D:30:LYS:NZ	2:D:404:GLU:OE1	2.39	0.55
2:B:195:ILE:CG1	2:B:196:GLY:N	2.69	0.54
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.88	0.54
1:C:125:ARG:O	1:C:128:THR:OG1	2.25	0.54
1:C:67:ASP:OD2	1:C:67:ASP:N	2.41	0.54
3:F:3:DC:H2'	3:F:4:OMC:C6	2.44	0.53
1:C:26:LEU:CD2	1:C:30:LYS:HB3	2.38	0.53
1:A:56:TYR:O	1:A:143:ARG:NH2	2.41	0.53
3:E:3:DC:H2'	3:E:4:OMC:C6	2.45	0.52
1:A:545:ASN:O	1:A:549:ASP:HB2	2.10	0.52
1:C:125:ARG:HD3	1:C:147:ASN:HA	1.91	0.51
1:A:551:LEU:HD12	1:A:551:LEU:O	2.09	0.51
2:B:331:LYS:NZ	2:B:364:ASP:OD2	2.42	0.51
2:B:105:SER:OG	2:B:235:HIS:NE2	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:SER:OG	1:A:141:GLY:HA2	2.11	0.51
1:A:447:ASN:HB3	1:A:450:THR:HB	1.94	0.50
1:C:134:SER:OG	1:C:135:ILE:N	2.37	0.50
1:A:440:PHE:HA	1:A:459:THR:HG22	1.94	0.50
2:B:105:SER:HG	2:B:235:HIS:HE2	1.53	0.50
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.42	0.50
1:A:323:LYS:NZ	1:A:344:GLU:OE2	2.41	0.50
1:C:465:LYS:NZ	1:C:488:ASP:OD2	2.29	0.50
1:A:54:ASN:O	1:A:143:ARG:NH1	2.43	0.49
1:C:30:LYS:HE3	1:C:62:ALA:O	2.11	0.49
1:C:399:GLU:O	1:C:403:THR:HG23	2.12	0.49
1:A:24:TRP:CB	1:A:25:PRO:HD2	2.36	0.49
1:A:450:THR:O	1:A:451:LYS:HB2	2.12	0.49
1:A:543:GLY:HA3	2:B:283:LEU:O	2.15	0.47
1:A:80:LEU:O	1:A:84:THR:OG1	2.29	0.47
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.96	0.47
1:C:76:ASP:OD1	1:C:78:ARG:NH2	2.39	0.47
1:C:111:VAL:HB	1:C:185:ASP:HB2	1.96	0.47
1:A:540:LYS:HE3	2:B:265:ASN:OD1	2.14	0.47
2:B:206:ARG:HG2	2:B:210:LEU:CD1	2.45	0.46
1:C:157:PRO:O	1:C:161:GLN:HG3	2.15	0.46
2:B:180:ILE:HG12	2:B:189:VAL:HG22	1.98	0.46
2:B:360:ALA:O	2:B:361:HIS:ND1	2.47	0.46
2:B:422:LEU:N	2:B:422:LEU:HD13	2.31	0.46
3:F:1:DG:H2'	3:F:2:OMC:C6	2.51	0.46
2:B:336:GLN:HG3	2:B:427:TYR:OH	2.17	0.45
2:D:257:ILE:HG22	2:D:283:LEU:HD11	1.98	0.45
1:C:503:LEU:HD23	2:D:422:LEU:HD21	1.98	0.45
2:D:73:LYS:NZ	2:D:146:TYR:OH	2.50	0.45
2:D:90:VAL:HG12	2:D:94:ILE:HD11	1.99	0.45
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.56	0.44
1:A:552:VAL:O	1:A:553:SER:C	2.56	0.44
1:C:417:VAL:HG22	1:C:419:THR:HG23	1.99	0.44
1:A:57:ASN:OD1	1:A:131:THR:N	2.51	0.44
2:D:252:TRP:HB3	2:D:257:ILE:CD1	2.47	0.44
1:A:60:VAL:HG22	1:A:75:VAL:HG22	1.99	0.44
2:B:35:VAL:O	2:B:39:THR:HG23	2.18	0.44
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.99	0.44
2:B:33:ALA:O	2:B:36:GLU:HG3	2.18	0.44
1:A:523:GLU:O	1:A:527:LYS:HG2	2.18	0.43
1:A:31:ILE:HD11	1:A:133:PRO:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.53	0.43
1:C:75:VAL:HB	1:C:77:PHE:CD2	2.53	0.43
1:C:114:ALA:HB3	6:C:602:XTE:N47	2.32	0.43
1:C:115:PHE:CE2	6:C:602:XTE:N47	2.86	0.43
1:A:380:ILE:HD12	2:B:27:THR:HG22	2.00	0.43
1:A:550:LYS:O	1:A:553:SER:OG	2.35	0.43
1:A:26:LEU:H	1:A:26:LEU:HG	1.25	0.43
1:A:265:ASN:OD1	1:A:353:LYS:HE3	2.19	0.43
1:C:298:GLU:OE1	1:C:298:GLU:N	2.39	0.43
2:B:167:ILE:HG12	2:B:212:TRP:CE3	2.54	0.43
2:B:422:LEU:HD22	2:B:422:LEU:H	1.84	0.43
1:C:472:THR:CG2	1:C:473:THR:N	2.81	0.43
1:C:472:THR:CG2	1:C:477:THR:HG23	2.49	0.43
6:C:602:XTE:F46	3:F:33:DC:H2''	2.09	0.43
1:A:486:LEU:O	1:A:528:LYS:NZ	2.39	0.42
2:D:317:VAL:O	2:D:318:TYR:CD1	2.72	0.42
6:A:603:XTE:F46	3:E:33:DC:C2'	2.56	0.42
1:C:62:ALA:HA	1:C:72:ARG:O	2.19	0.42
1:C:393:ILE:HG23	1:C:414:TRP:CH2	2.55	0.42
1:C:454:LYS:HA	1:C:467:VAL:O	2.19	0.42
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.55	0.42
1:A:412:PRO:O	1:A:414:TRP:HD1	2.02	0.42
3:E:23:DC:H2''	3:E:24:DG:C8	2.54	0.42
2:B:242:GLN:HG3	2:B:242:GLN:O	2.20	0.42
3:E:1:DG:H2'	3:E:2:OMC:C6	2.53	0.42
1:C:325:LEU:HD11	1:C:383:TRP:CE3	2.55	0.42
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.55	0.42
1:C:308:GLU:O	1:C:311:LYS:HG2	2.19	0.42
1:C:324:ASP:OD2	1:C:388:LYS:NZ	2.43	0.42
1:C:412:PRO:O	1:C:414:TRP:HD1	2.02	0.41
2:D:252:TRP:HB3	2:D:257:ILE:HD11	2.01	0.41
1:A:185:ASP:OD2	6:A:603:XTE:O2A	2.38	0.41
3:E:4:OMC:HM23	3:E:4:OMC:H1'	1.93	0.41
2:B:129:ALA:HA	2:B:144:TYR:O	2.20	0.41
2:B:332:GLN:HG3	2:B:338:THR:HG23	2.02	0.41
1:C:454:LYS:HE2	1:C:552:VAL:O	2.19	0.41
2:D:317:VAL:O	2:D:317:VAL:HG13	2.19	0.41
1:A:193:LEU:HD13	1:A:197:GLN:HG3	2.00	0.41
2:B:360:ALA:O	2:B:361:HIS:CG	2.73	0.41
1:C:439:THR:O	1:C:459:THR:HA	2.21	0.41
2:B:105:SER:O	2:B:190:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:552:VAL:O	1:C:552:VAL:HG12	2.20	0.41
2:D:275:LYS:CG	2:D:302:GLU:HG3	2.51	0.41
1:A:406:TRP:CZ2	2:B:420:PRO:HG3	2.55	0.41
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.56	0.41
1:A:275:LYS:NZ	1:A:305:GLU:OE1	2.37	0.41
1:C:5:ILE:HG23	1:C:212:TRP:CE3	2.55	0.41
1:C:393:ILE:O	1:C:414:TRP:CZ3	2.74	0.41
1:A:10:VAL:HG23	1:A:124:PHE:CD1	2.56	0.41
2:B:90:VAL:O	2:B:90:VAL:HG12	2.22	0.40
2:B:70:LYS:HG3	2:B:71:TRP:N	2.37	0.40
1:C:439:THR:N	1:C:460:ASP:OD2	2.34	0.40
3:F:4:OMC:HM23	3:F:4:OMC:H1'	1.96	0.40
6:C:602:XTE:N2	3:F:0:DC:O2	2.54	0.40
1:A:358:LYS:HE2	7:B:618:HOH:O	2.21	0.40
2:D:108:VAL:HG21	2:D:232:TYR:CE1	2.57	0.40
1:A:551:LEU:HD12	1:A:551:LEU:C	2.41	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%)	530 (96%)	20 (4%)	2 (0%)	34	55
1	C	552/557 (99%)	531 (96%)	19 (3%)	2 (0%)	34	55
2	B	402/444 (90%)	381 (95%)	21 (5%)	0	100	100
2	D	402/444 (90%)	386 (96%)	15 (4%)	1 (0%)	47	69
All	All	1908/2002 (95%)	1828 (96%)	75 (4%)	5 (0%)	41	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	PRO
1	C	133	PRO
1	A	26	LEU
2	D	282	LEU
1	C	412	PRO

5.3.2 Protein sidechains [i](#)

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%)	483 (98%)	10 (2%)	55	77
1	C	493/494 (100%)	490 (99%)	3 (1%)	86	94
2	B	365/400 (91%)	355 (97%)	10 (3%)	44	69
2	D	365/400 (91%)	360 (99%)	5 (1%)	67	84
All	All	1716/1788 (96%)	1688 (98%)	28 (2%)	62	81

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

Mol	Chain	Res	Type
1	A	24	TRP
1	A	25	PRO
1	A	26	LEU
1	A	102	GLN
1	A	110	ASP
1	A	113	ASP
1	A	281	LYS
1	A	385	LYS
1	A	550	LYS
1	A	551	LEU
2	B	36	GLU
2	B	66	LYS
2	B	113	ASP
2	B	237	ASP
2	B	275	LYS
2	B	300	GLU
2	B	356	ARG

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Mol	Chain	Res	Type
2	B	422	LEU
2	B	424	LYS
2	B	427	TYR
1	C	126	LYS
1	C	221	HIS
1	C	399	GLU
2	D	64	LYS
2	D	85	GLN
2	D	275	LYS
2	D	356	ARG
2	D	361	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	161	GLN
2	B	367	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	4	3	19,22,23	2.74	8 (42%)	26,31,34	0.57	0
3	OMC	E	2	3	19,22,23	2.73	8 (42%)	26,31,34	0.64	0
3	OMC	E	4	3	19,22,23	2.67	8 (42%)	26,31,34	0.64	0
3	OMC	F	2	3	19,22,23	2.68	8 (42%)	26,31,34	0.77	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	4	3	-	0/9/27/28	0/2/2/2
3	OMC	E	2	3	-	0/9/27/28	0/2/2/2
3	OMC	E	4	3	-	0/9/27/28	0/2/2/2
3	OMC	F	2	3	-	0/9/27/28	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	OMC	C6-C5	6.02	1.49	1.35
3	F	4	OMC	C2-N3	5.99	1.48	1.36
3	F	2	OMC	C6-C5	5.95	1.48	1.35
3	E	4	OMC	C2-N3	5.85	1.48	1.36
3	E	4	OMC	C6-C5	5.84	1.48	1.35
3	E	2	OMC	C2-N3	5.74	1.48	1.36
3	F	4	OMC	C6-C5	5.74	1.48	1.35
3	F	2	OMC	C2-N3	5.57	1.47	1.36
3	F	4	OMC	C4-N3	5.13	1.44	1.34
3	E	2	OMC	C4-N3	4.78	1.44	1.34
3	E	4	OMC	C4-N3	4.70	1.44	1.34
3	F	2	OMC	C4-N3	4.48	1.43	1.34
3	F	2	OMC	C2-N1	4.33	1.49	1.40
3	E	2	OMC	C2-N1	4.23	1.49	1.40
3	F	4	OMC	C2-N1	4.21	1.49	1.40
3	E	4	OMC	C2-N1	4.14	1.49	1.40
3	E	2	OMC	C6-N1	3.08	1.45	1.38
3	E	2	OMC	C4-N4	3.00	1.41	1.33
3	F	2	OMC	C6-N1	3.00	1.45	1.38
3	F	4	OMC	C4-N4	2.89	1.40	1.33
3	F	4	OMC	C6-N1	2.88	1.45	1.38
3	F	2	OMC	C4-N4	2.82	1.40	1.33
3	E	4	OMC	C4-N4	2.79	1.40	1.33
3	E	4	OMC	C6-N1	2.77	1.44	1.38
3	F	2	OMC	C5-C4	2.70	1.49	1.42
3	E	2	OMC	C5-C4	2.60	1.48	1.42
3	F	4	OMC	C5-C4	2.54	1.48	1.42
3	E	4	OMC	C5-C4	2.36	1.48	1.42
3	F	2	OMC	O2-C2	-2.34	1.19	1.23
3	E	4	OMC	O2-C2	-2.31	1.19	1.23
3	E	2	OMC	O2-C2	-2.26	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	OMC	O2-C2	-2.23	1.19	1.23

There are no bond angle outliers.

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	4	OMC	2	0
3	E	2	OMC	1	0
3	E	4	OMC	2	0
3	F	2	OMC	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	F	101	-	5,5,5	0.47	0	5,5,5	0.33	0
4	GOL	D	502	-	5,5,5	0.51	0	5,5,5	0.24	0
4	GOL	B	501	-	5,5,5	0.42	0	5,5,5	0.27	0
6	XTE	C	602	5	26,37,37	1.56	5 (19%)	27,59,59	1.69	4 (14%)
4	GOL	A	601	-	5,5,5	0.62	0	5,5,5	0.57	0
6	XTE	A	603	5	26,37,37	1.86	5 (19%)	27,59,59	1.83	6 (22%)
4	GOL	D	501	-	5,5,5	0.39	0	5,5,5	0.11	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	F	101	-	-	2/4/4/4	-
4	GOL	D	502	-	-	2/4/4/4	-
4	GOL	B	501	-	-	2/4/4/4	-
6	XTE	C	602	5	-	6/18/48/48	0/3/3/3
4	GOL	A	601	-	-	4/4/4/4	-
6	XTE	A	603	5	-	4/18/48/48	0/3/3/3
4	GOL	D	501	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	XTE	C6-N1	-5.30	1.30	1.37
6	C	602	XTE	C6-N1	-3.74	1.32	1.37
6	C	602	XTE	C1'-C6'	-3.42	1.44	1.51
6	A	603	XTE	C1'-C6'	-3.29	1.45	1.51
6	A	603	XTE	C1'-N9	-2.87	1.45	1.49
6	C	602	XTE	C2'-C1'	-2.74	1.51	1.54
6	A	603	XTE	C2-N1	-2.59	1.31	1.37
6	C	602	XTE	C4-N3	-2.16	1.32	1.37
6	A	603	XTE	C2'-C1'	-2.14	1.52	1.54
6	C	602	XTE	C1'-N9	-2.11	1.46	1.49

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	XTE	C2'-C1'-N9	-4.96	106.33	114.73
6	C	602	XTE	PB-O3B-PG	-4.82	116.28	132.83
6	A	603	XTE	C3'-C2'-C1'	4.25	109.43	103.98
6	A	603	XTE	PB-O3B-PG	-3.48	120.88	132.83
6	C	602	XTE	PB-O3A-PA	-3.26	121.64	132.83
6	C	602	XTE	C3'-C2'-C1'	3.08	107.93	103.98
6	A	603	XTE	C8-N7-C5	2.64	108.02	102.99
6	A	603	XTE	O3G-PG-O3B	2.17	111.91	104.64
6	A	603	XTE	C5-C6-N1	2.10	117.67	113.95
6	C	602	XTE	C2'-C1'-N9	-2.09	111.20	114.73

There are no chirality outliers.

All (22) torsion outliers are listed below:

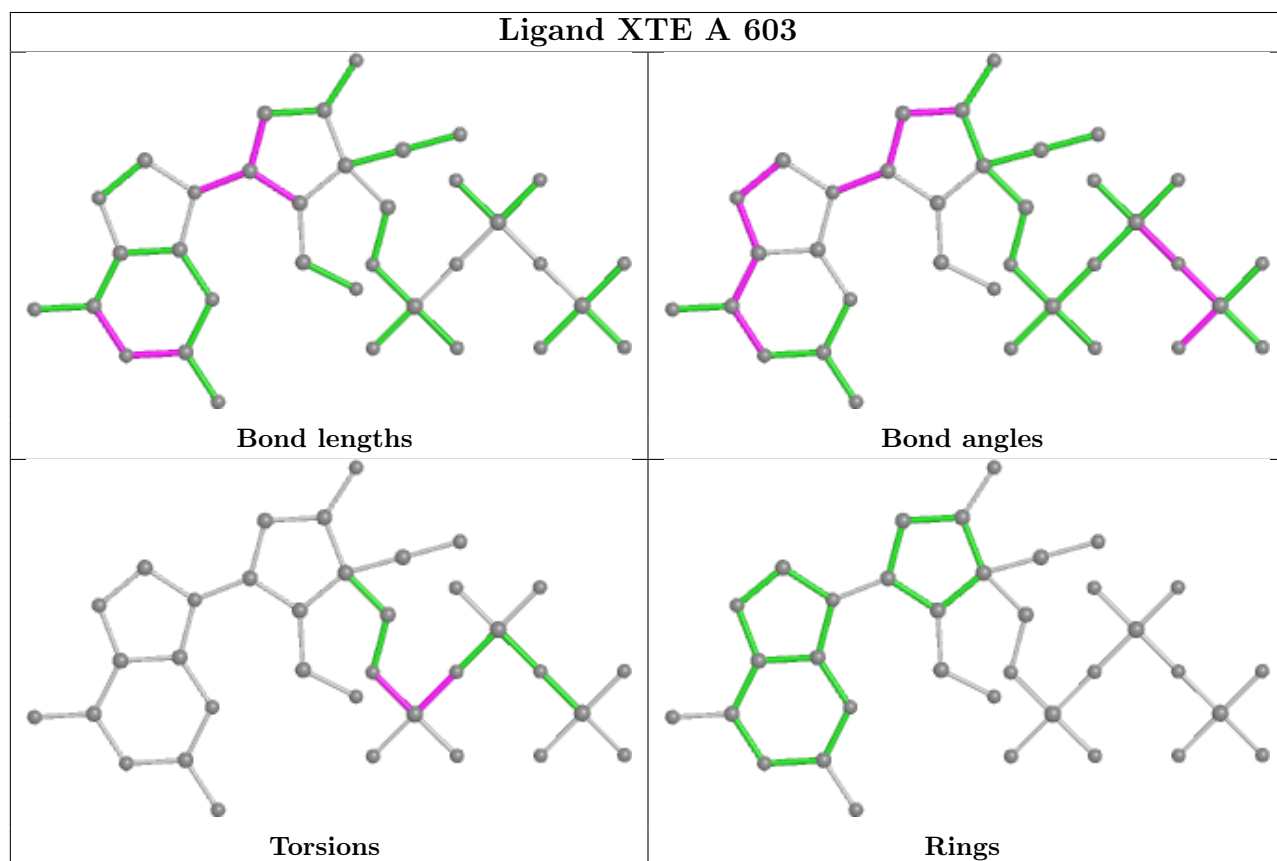
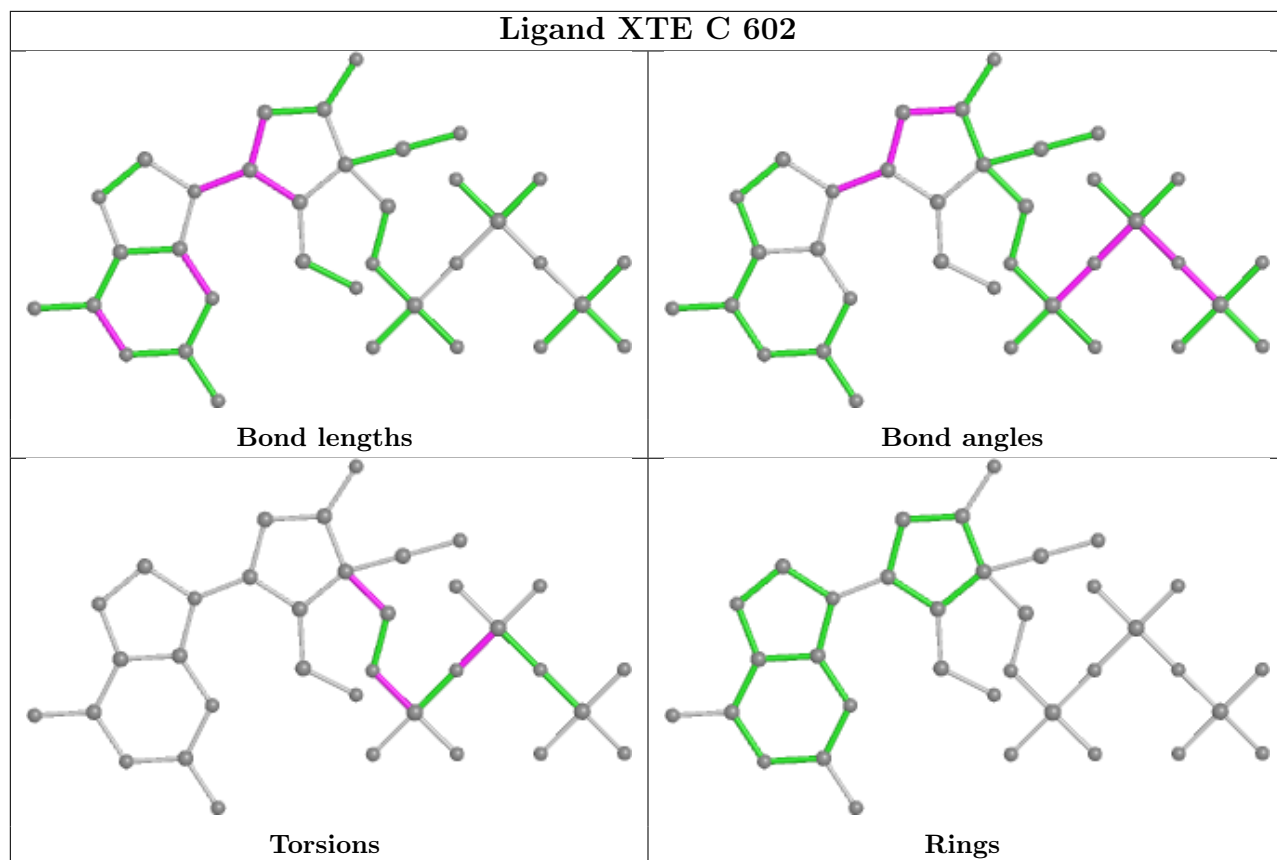
Mol	Chain	Res	Type	Atoms
4	A	601	GOL	O1-C1-C2-C3
4	A	601	GOL	C1-C2-C3-O3
4	D	501	GOL	C1-C2-C3-O3
4	D	501	GOL	O2-C2-C3-O3
4	D	502	GOL	O1-C1-C2-C3
4	F	101	GOL	O1-C1-C2-C3
6	A	603	XTE	PB-O3A-PA-O5'
6	A	603	XTE	C5'-O5'-PA-O2A
6	C	602	XTE	C5'-O5'-PA-O1A
6	C	602	XTE	C5'-O5'-PA-O2A
4	F	101	GOL	O1-C1-C2-O2
4	B	501	GOL	O1-C1-C2-C3
4	A	601	GOL	O2-C2-C3-O3
4	A	601	GOL	O1-C1-C2-O2
4	B	501	GOL	O1-C1-C2-O2
4	D	502	GOL	O1-C1-C2-O2
6	A	603	XTE	C5'-O5'-PA-O3A
6	C	602	XTE	C5'-O5'-PA-O3A
6	A	603	XTE	C5'-O5'-PA-O1A
6	C	602	XTE	C6'-C4'-C5'-O5'
6	C	602	XTE	PA-O3A-PB-O2B
6	C	602	XTE	PA-O3A-PB-O1B

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	602	XTE	5	0
6	A	603	XTE	5	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%)	0.30	32 (5%) 23 18	41, 63, 118, 197	0
1	C	553/557 (99%)	0.46	55 (9%) 7 5	40, 72, 133, 195	0
2	B	406/444 (91%)	0.74	50 (12%) 4 2	42, 77, 136, 206	0
2	D	406/444 (91%)	0.25	24 (5%) 22 17	43, 69, 116, 172	0
3	E	33/38 (86%)	-0.17	0 100 100	42, 60, 102, 135	0
3	F	36/38 (94%)	-0.03	0 100 100	44, 71, 136, 173	0
All	All	1987/2078 (95%)	0.41	161 (8%) 12 8	40, 70, 129, 206	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	360	ALA	10.0
2	D	360	ALA	8.0
1	A	68	SER	7.6
2	B	92	LEU	7.4
1	C	34	LEU	7.3
1	C	136	ASN	7.1
2	B	231	GLY	6.9
1	A	69	THR	6.9
1	C	132	ILE	6.8
2	B	301	LEU	6.6
1	A	136	ASN	6.5
1	C	69	THR	6.1
1	A	140	PRO	6.0
2	B	361	HIS	6.0
2	B	357	MET	5.8
1	A	63	ILE	5.8
1	A	137	ASN	5.6
2	B	88	TRP	5.5
2	D	232	TYR	5.4

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Mol	Chain	Res	Type	RSRZ
2	B	95	PRO	5.3
1	A	139	THR	5.2
1	C	452	LEU	5.2
1	C	28	GLU	5.2
1	C	68	SER	5.2
2	B	67	ASP	5.1
2	B	93	GLY	5.0
2	B	89	GLU	5.0
1	A	67	ASP	4.8
2	B	91	GLN	4.8
2	B	359	GLY	4.7
2	D	231	GLY	4.6
2	D	359	GLY	4.6
2	B	295	LEU	4.6
2	B	213	GLY	4.5
2	B	297	GLU	4.5
1	A	24	TRP	4.4
2	B	296	THR	4.4
2	B	423	VAL	4.3
1	C	141	GLY	4.3
1	A	25	PRO	4.3
1	A	62	ALA	4.2
1	C	142	ILE	4.2
1	C	63	ILE	4.2
1	C	140	PRO	4.1
1	C	449	GLU	4.0
1	C	26	LEU	4.0
1	C	135	ILE	4.0
2	B	278	GLN	3.9
1	C	50	ILE	3.9
2	D	93	GLY	3.9
2	B	94	ILE	3.8
1	C	37	ILE	3.8
1	A	64	LYS	3.8
1	A	61	PHE	3.8
1	C	52	PRO	3.7
1	C	447	ASN	3.6
2	D	283	LEU	3.6
2	B	305	GLU	3.6
1	C	448	ARG	3.6
1	C	67	ASP	3.6
1	C	553	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	144	TYR	3.6
2	B	168	LEU	3.5
1	A	70	LYS	3.5
2	B	87	PHE	3.5
1	A	135	ILE	3.4
2	D	67	ASP	3.4
1	C	71	TRP	3.4
2	B	248	GLU	3.4
2	D	357	MET	3.4
2	D	295	LEU	3.4
1	A	66	LYS	3.3
1	C	66	LYS	3.3
1	A	553	SER	3.3
1	C	32	LYS	3.3
1	C	35	VAL	3.3
1	C	30	LYS	3.3
2	D	284	ARG	3.2
1	C	54	ASN	3.2
2	D	361	HIS	3.2
2	B	232	TYR	3.2
1	A	134	SER	3.2
2	B	279	LEU	3.2
2	D	281	LYS	3.1
2	D	212	TRP	3.1
2	B	212	TRP	3.1
1	C	552	VAL	3.1
2	B	251	SER	3.1
1	C	27	THR	3.0
1	C	70	LYS	3.0
2	B	281	LYS	3.0
1	A	35	VAL	3.0
2	B	252	TRP	3.0
1	A	34	LEU	3.0
1	C	31	ILE	3.0
1	C	138	GLU	3.0
1	C	24	TRP	3.0
2	B	90	VAL	3.0
1	C	62	ALA	3.0
1	C	25	PRO	2.9
1	C	53	GLU	2.9
2	D	282	LEU	2.9
1	C	551	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	550	LYS	2.9
1	A	71	TRP	2.9
1	C	547	GLN	2.9
1	C	133	PRO	2.9
2	B	211	ARG	2.8
1	A	550	LYS	2.8
1	C	49	LYS	2.8
1	C	450	THR	2.8
2	D	177	ASP	2.8
2	B	362	THR	2.7
2	B	299	ALA	2.6
1	A	552	VAL	2.6
2	B	172	ARG	2.6
2	D	90	VAL	2.6
2	B	303	LEU	2.6
2	B	7	THR	2.5
2	B	68	SER	2.5
2	B	273	GLY	2.5
1	A	32	LYS	2.5
1	A	142	ILE	2.4
2	B	275	LYS	2.4
1	A	74	LEU	2.4
2	D	178	ILE	2.4
1	A	131	THR	2.4
2	B	284	ARG	2.4
1	C	64	LYS	2.4
2	B	294	PRO	2.4
2	B	209	LEU	2.4
1	A	60	VAL	2.4
1	C	36	GLU	2.4
1	C	33	ALA	2.3
1	A	287	LYS	2.3
1	C	194	GLU	2.3
2	B	6	GLU	2.3
1	C	143	ARG	2.2
1	C	413	GLU	2.2
1	A	31	ILE	2.2
2	B	176	PRO	2.2
1	A	541	GLY	2.2
2	D	427	TYR	2.2
2	B	250	ASP	2.2
1	C	51	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	56	TYR	2.1
1	C	55	PRO	2.1
2	D	300	GLU	2.1
1	C	451	LYS	2.1
2	D	297	GLU	2.1
1	C	131	THR	2.1
1	C	542	ILE	2.1
2	B	169	GLU	2.1
2	D	294	PRO	2.1
1	A	138	GLU	2.1
2	D	208	HIS	2.1
2	B	304	ALA	2.1
2	D	174	GLN	2.0
2	B	321	PRO	2.0
2	D	209	LEU	2.0
2	B	5	ILE	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	0.98	0.19	40,46,51,58	0
3	OMC	F	2	21/22	0.98	0.18	52,57,64,72	0
3	OMC	F	4	21/22	0.98	0.21	42,49,53,55	0
3	OMC	E	4	21/22	0.99	0.19	33,41,48,54	0

6.3 Carbohydrates [i](#)

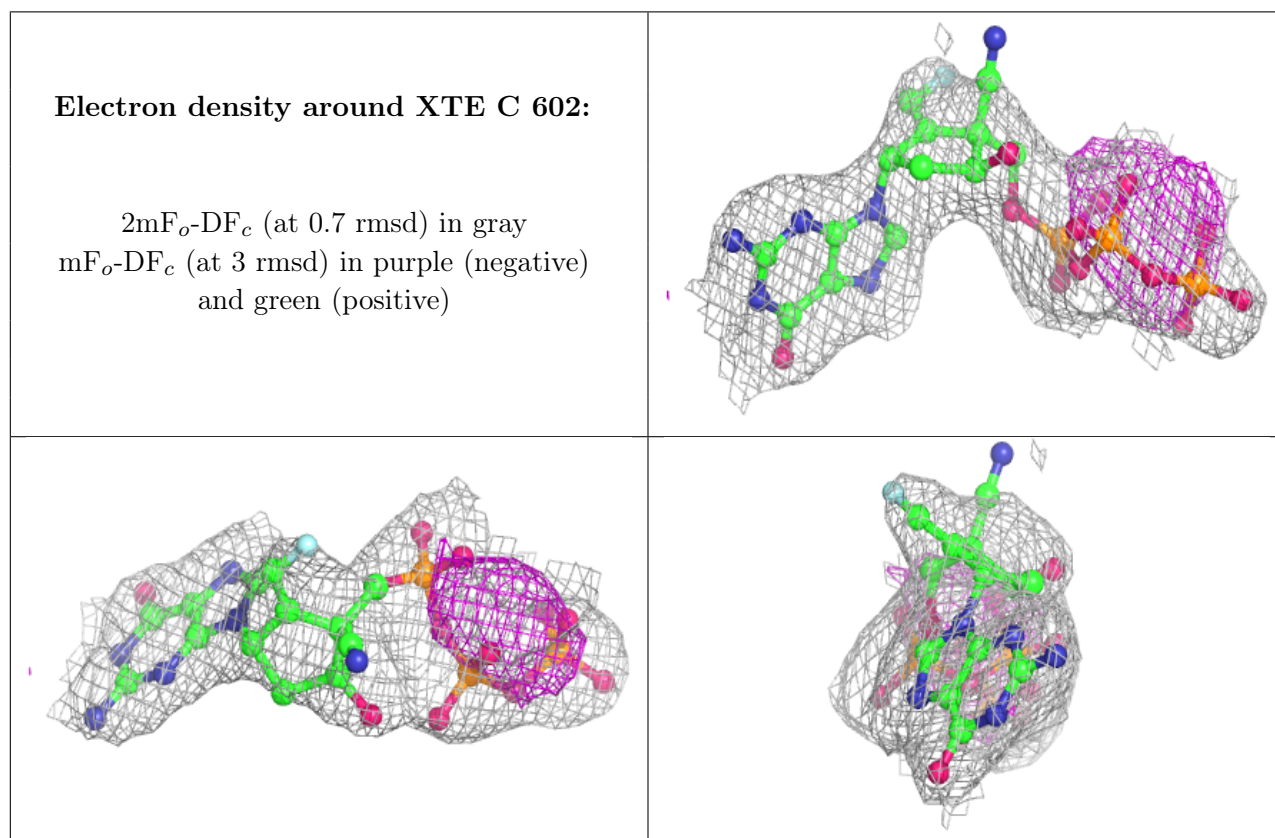
There are no monosaccharides in this entry.

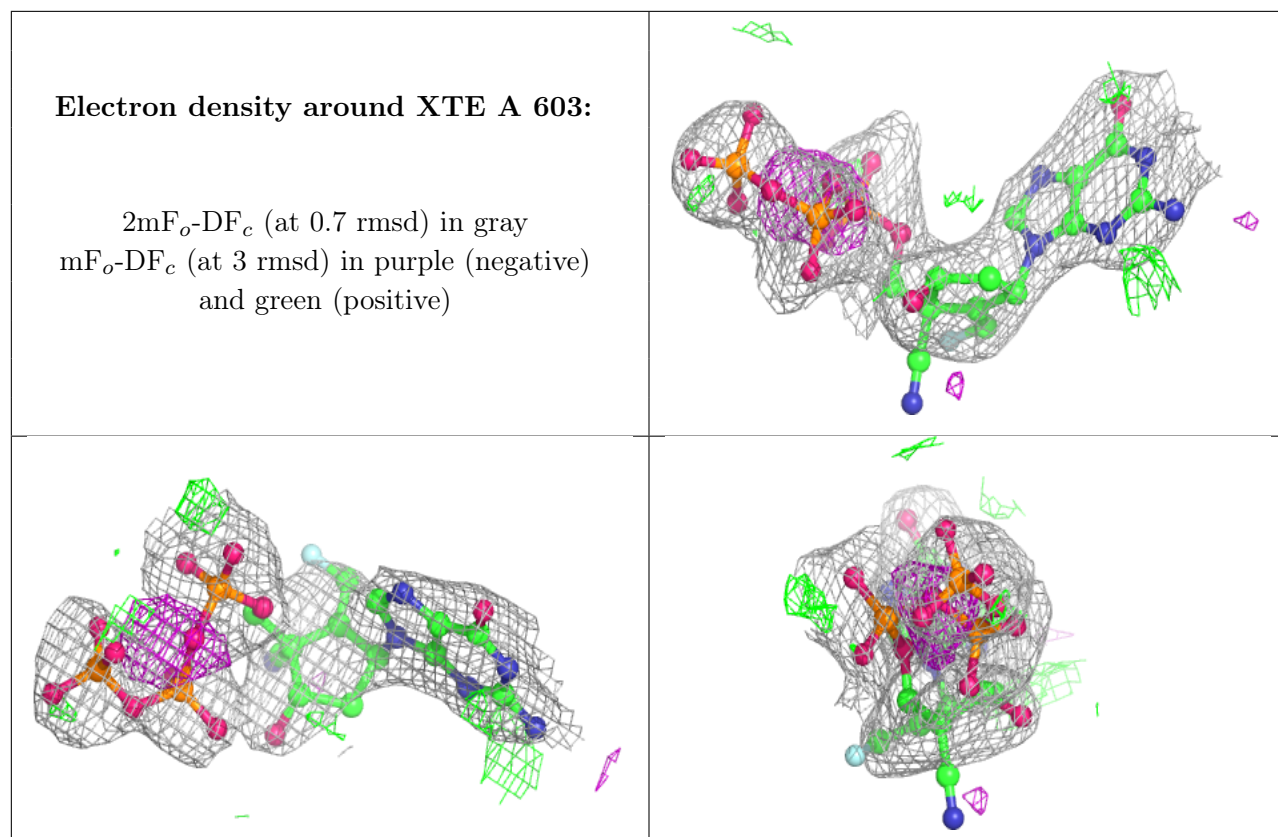
6.4 Ligands [i](#)

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	C	601	1/1	0.49	0.27	90,90,90,90	0
6	XTE	C	602	35/35	0.80	0.23	82,106,129,132	0
6	XTE	A	603	35/35	0.82	0.27	75,92,123,128	35
4	GOL	A	601	6/6	0.88	0.33	79,81,83,84	0
4	GOL	F	101	6/6	0.88	0.33	74,75,79,84	0
5	MG	A	602	1/1	0.88	0.29	83,83,83,83	1
4	GOL	D	502	6/6	0.92	0.27	66,73,76,78	0
4	GOL	B	501	6/6	0.92	0.28	50,53,60,65	0
4	GOL	D	501	6/6	0.96	0.24	57,65,66,68	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.