



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:08 AM UTC

PDB ID : 6KDM / pdb_00006kdm
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 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)
Xtrriage (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

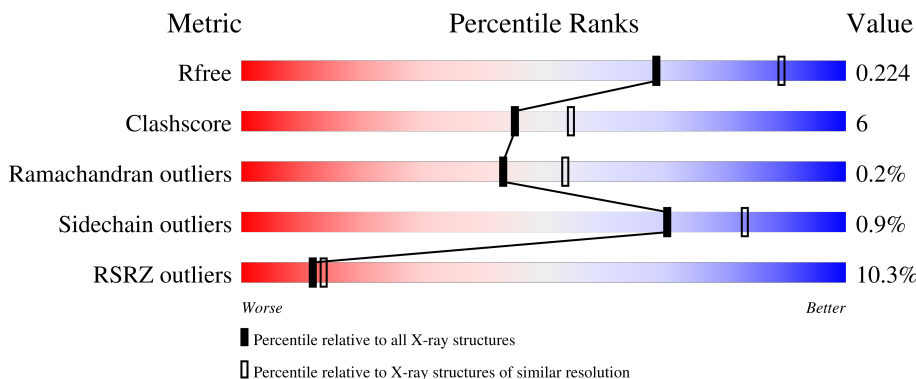
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (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 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	 11% 82% 17%
1	C	557	 5% 89% 10%
2	B	444	 18% 77% 14% 9%
2	D	444	 8% 79% 11% 9%
3	E	38	 71% 16% 5% 8%

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Mol	Chain	Length	Quality of chain
3	F	38	 74% 21% 5%

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
			Total	C	N	O	S			
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
			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	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
			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 (CCD ID: GOL) (formula: C₃H₈O₃).

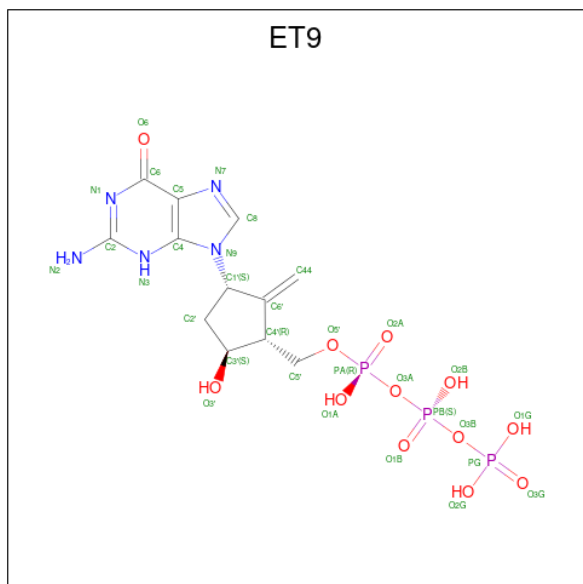


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	E	1	6	3	3	0	0
4	D	1	6	3	3	0	0
4	D	1	6	3	3	0	0
4	D	1	6	3	3	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: 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 [[(1R,3S,5S)-3-(2-azanyl-6-oxidanylidene-3H-purin-9-yl)-2-methylidene-5-oxidanyl-cyclopentyl]methoxy-oxidanyl-phosphoryl l] phosphono hydrogen phosphate (CCD ID: ET9) (formula: C₁₂H₁₈N₅O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



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

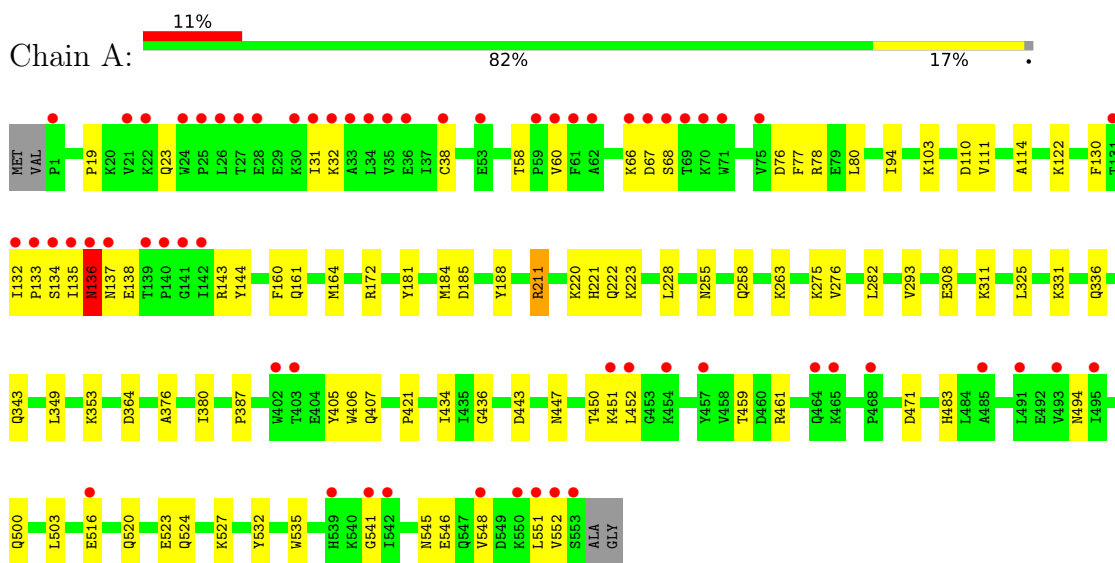
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	133	Total	O	0	0
				133		
7	B	53	Total	O	0	0
				53		
7	E	42	Total	O	0	0
				42		
7	C	116	Total	O	0	0
				116		
7	D	93	Total	O	0	0
				93		
7	F	41	Total	O	0	0
				41		

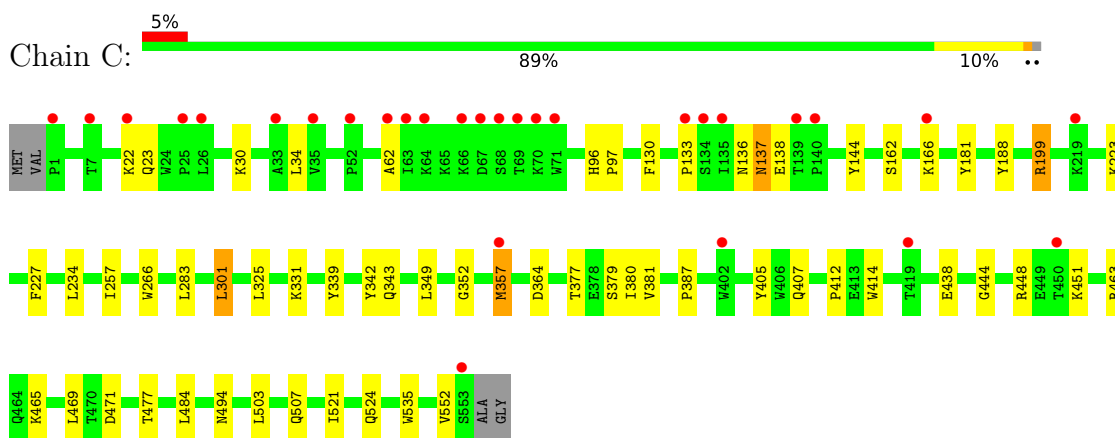
3 Residue-property plots i

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.

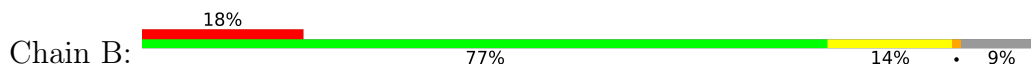
- Molecule 1: HIV-1 reverse transcriptase p66 subunit

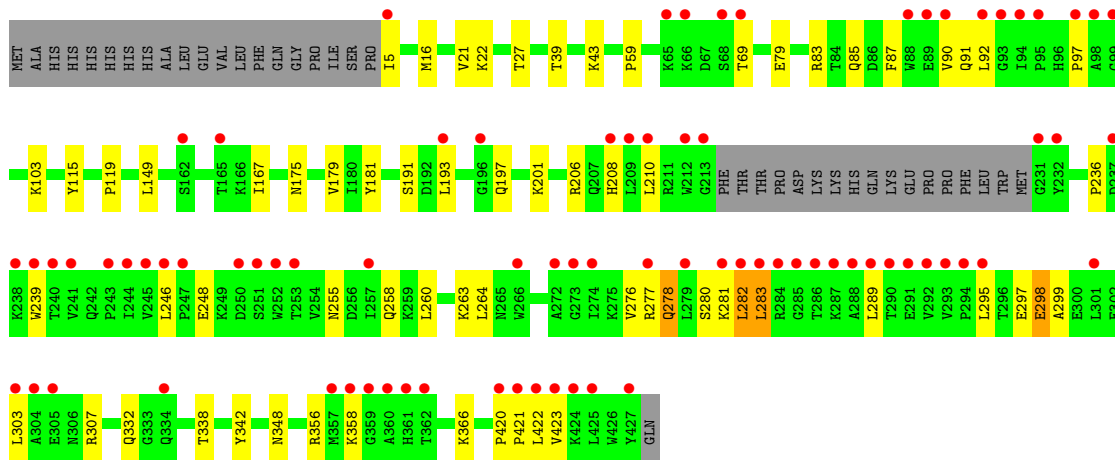


- Molecule 1: HIV-1 reverse transcriptase p66 subunit

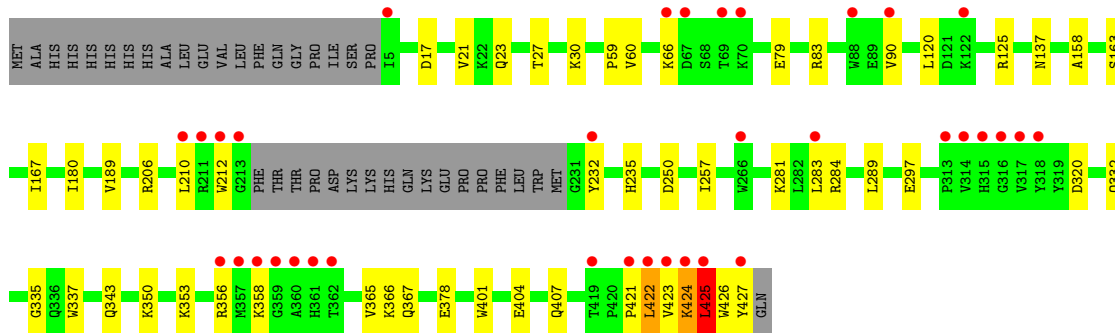
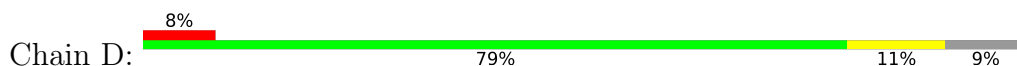


- Molecule 2: HIV-1 RT p51 subunit





• 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	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) 99.9 (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)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.190 , 0.223 0.192 , 0.224	Depositor DCC
R_{free} test set	6352 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtrriage
Anisotropy	0.113	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.010 for h,-h-k,-l	Xtrriage
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

Xtrriage'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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ET9, GOL, OMC, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	1/4624 (0.0%)	0.49	7/6279 (0.1%)
1	C	0.27	2/4624 (0.0%)	0.40	2/6278 (0.0%)
2	B	0.31	0/3441	0.42	2/4673 (0.0%)
2	D	0.39	2/3449 (0.1%)	0.43	2/4683 (0.0%)
3	E	0.20	0/756	0.40	0/1165
3	F	0.19	0/823	0.39	0/1269
All	All	0.31	5/17717 (0.0%)	0.43	13/24347 (0.1%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	357[A]	MET	N-CA	6.13	1.54	1.46
1	C	357[B]	MET	N-CA	6.13	1.54	1.46
2	D	235	HIS	C-O	-5.55	1.17	1.24
1	A	447	ASN	C-O	-5.48	1.17	1.24
2	D	235	HIS	CA-C	-5.19	1.46	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ASP	N-CA-C	-10.88	93.60	109.59
1	A	68	SER	N-CA-C	7.45	119.40	111.28
1	A	452	LEU	N-CA-C	6.91	121.31	110.32
1	C	357[A]	MET	N-CA-C	6.63	119.65	107.99
1	C	357[B]	MET	N-CA-C	6.63	119.65	107.99
2	D	422	LEU	CA-C-N	6.54	130.94	121.52
2	D	422	LEU	C-N-CA	6.54	130.94	121.52
1	A	137	ASN	N-CA-C	6.40	118.34	111.36
2	B	277	ARG	N-CA-C	6.01	117.63	111.14
1	A	143	ARG	N-CA-C	5.92	119.91	109.96
1	A	66	LYS	N-CA-C	-5.54	105.24	111.28
2	B	22	LYS	N-CA-C	5.14	117.89	110.28
1	A	136	ASN	N-CA-C	5.05	121.55	110.80

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 [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	4503	0	4557	65	0
1	C	4503	0	4562	40	0
2	B	3347	0	3379	45	0
2	D	3352	0	3388	45	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	201	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 (201) 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
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:450:THR:HG22	1:A:451:LYS:N	1.77	0.91
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:N	2:D:425:LEU:HD13	1.92	0.81
1:A:31:ILE:HD13	1:A:135:ILE:H	1.45	0.80
1:A:211:ARG:HH11	1:A:211:ARG:HG2	1.46	0.79
2:D:425:LEU:CD1	2:D:425:LEU:N	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:HG22	2:B:69:THR:O	1.83	0.77
2:D:425:LEU:HD22	2:D:425:LEU:O	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:HG22	1:A:135:ILE:O	1.89	0.71
1:A:451:LYS:HB2	1:A:471:ASP:HA	1.73	0.71
2:B:278:GLN:CD	2:B:298:GLU:HB2	2.17	0.69
1:C:521:ILE:HA	1:C:524:GLN:HE21	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:281:LYS:C	2:B:283:LEU:N	2.48	0.67
1:A:172:ARG:NH1	7:A:704:HOH:O	2.28	0.66
2:B:281:LYS:C	2:B:283:LEU:H	2.02	0.65
2:B:278:GLN:NE2	2:B:298:GLU:HB2	2.12	0.64
2:D:425:LEU:HD22	2:D:425:LEU:C	2.23	0.64
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:331:LYS:NZ	1:A:364:ASP:OD2	2.29	0.62
1:A:122:LYS:HG3	7:A:753:HOH:O	1.98	0.62
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:O	2:D:425:LEU:CD2	2.49	0.58
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:O	2:D:423:VAL:CG1	2.54	0.55
1:C:448:ARG:NH1	3:F:18:DT:O2	2.39	0.55
2:D:425:LEU:H	2:D:425:LEU:HD13	1.55	0.55
2:B:303:LEU:O	2:B:307:ARG:HG3	2.06	0.55
1:A:111:VAL:HG21	1:A:164:MET:HE1	1.88	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
3:E:30:DG:H21	4:E:101:GOL:HO3	1.54	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
2:B:16:MET:HE3	2:B:83:ARG:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:O	2:B:69:THR:CG2	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:278:GLN:HG2	2:B:298:GLU:C	2.36	0.51
2:B:103:LYS:HE2	2:B:179:VAL:HG12	1.92	0.50
1:A:380:ILE:HD12	2:B:27:THR:HG22	1.93	0.50
2:B:103:LYS:HE3	2:B:191:SER:HA	1.93	0.50
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
2:D:232:TYR:C	2:D:232:TYR:CD1	2.85	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
2:B:281:LYS:O	2:B:282:LEU:C	2.51	0.50
2:D:426:TRP:CD1	2:D:426:TRP:H	2.30	0.49
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
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:21:VAL:HB	2:D:59:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:137:ASN:HD21	4:D:501:GOL:H12	1.80	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:B:90:VAL:C	2:B:91:GLN:HG2	2.39	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
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:263:LYS:NZ	7:A:707:HOH:O	2.35	0.45
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.99	0.45
1:A:516:GLU:H	1:A:516:GLU:CD	2.24	0.45
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.52	0.45
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
2:D:350:LYS:NZ	2:D:378:GLU:OE2	2.45	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:275:LYS:HB3	1:A:336:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLU:O	1:A:311:LYS:HG2	2.18	0.43
1:A:94:ILE:HG12	3:E:4:OMC:H1'	2.01	0.43
1:A:483:HIS:ND1	1:A:524:GLN:OE1	2.52	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:17:ASP:O	2:D:83:ARG:HD3	2.18	0.43
2:D:332:GLN:OE1	2:D:424:LYS: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:O	1:A:135:ILE:CG2	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
2:D:422:LEU:HD23	2:D:422:LEU:HA	1.91	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:500:GLN:H	1:A:500:GLN:CD	2.29	0.41
1:A:23:GLN:OE1	1:A:60:VAL:HG12	2.20	0.41
1:A:32:LYS:HA	1:A:32:LYS:HD2	1.94	0.41
2:B:298:GLU:H	2:B:298:GLU:CD	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:332:GLN:CD	2:D:427:TYR:HB2	2.46	0.40
2:D:356:ARG:H	2:D:356:ARG:HG3	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%)	43	53
1	C	552/557 (99%)	535 (97%)	15 (3%)	2 (0%)	30	37
2	B	402/444 (90%)	383 (95%)	18 (4%)	1 (0%)	43	53
2	D	403/444 (91%)	388 (96%)	15 (4%)	0	100	100
All	All	1909/2002 (95%)	1842 (96%)	63 (3%)	4 (0%)	43	53

All (4) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	C	133	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%)	490 (99%)	3 (1%)	78	88
1	C	493/494 (100%)	491 (100%)	2 (0%)	84	91
2	B	365/400 (91%)	359 (98%)	6 (2%)	55	72
2	D	366/400 (92%)	362 (99%)	4 (1%)	65	80
All	All	1717/1788 (96%)	1702 (99%)	15 (1%)	70	83

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	ARG
1	A	459	THR
1	A	551	LEU
2	B	278	GLN
2	B	283	LEU
2	B	295	LEU
2	B	298	GLU
2	B	356	ARG
2	B	422	LEU
1	C	199	ARG
1	C	301	LEU
2	D	212	TRP
2	D	250	ASP
2	D	424	LYS
2	D	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	207	GLN
1	A	221	HIS
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	137	ASN
2	B	147	ASN
2	B	151	GLN
2	B	161	GLN
2	B	175	ASN
2	B	208	HIS
2	B	258	GLN
2	B	269	GLN
2	B	278	GLN
2	B	348	ASN
1	C	197	GLN
1	C	258	GLN
1	C	330	GLN
1	C	340	GLN
1	C	407	GLN
1	C	524	GLN
1	C	539	HIS
1	C	547	GLN
2	D	23	GLN
2	D	175	ASN
2	D	182	GLN
2	D	255	ASN
2	D	343	GLN
2	D	367	GLN
2	D	394	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	E	4	3	19,22,23	2.85	8 (42%)	25,31,34	0.79	0
3	OMC	F	2	3	19,22,23	2.83	8 (42%)	25,31,34	0.75	0
3	OMC	F	4	3	19,22,23	2.87	8 (42%)	25,31,34	0.66	0
3	OMC	E	2	3	19,22,23	2.81	8 (42%)	25,31,34	0.81	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	E	4	3	-	0/9/27/28	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	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	F	4	OMC	C2-N3	6.50	1.49	1.36
3	E	4	OMC	C2-N3	6.39	1.49	1.36
3	F	2	OMC	C2-N3	6.15	1.48	1.36
3	E	2	OMC	C2-N3	6.06	1.48	1.36
3	F	2	OMC	C6-C5	5.96	1.48	1.35
3	E	4	OMC	C6-C5	5.90	1.48	1.35
3	E	2	OMC	C6-C5	5.90	1.48	1.35
3	F	4	OMC	C6-C5	5.88	1.48	1.35
3	F	4	OMC	C4-N3	5.33	1.45	1.34
3	E	4	OMC	C4-N3	5.03	1.44	1.34
3	F	2	OMC	C4-N3	4.96	1.44	1.34
3	E	4	OMC	C2-N1	4.92	1.50	1.40
3	E	2	OMC	C2-N1	4.91	1.50	1.40
3	E	2	OMC	C4-N3	4.90	1.44	1.34
3	F	2	OMC	C2-N1	4.78	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	OMC	C2-N1	4.73	1.50	1.40
3	F	2	OMC	C6-N1	3.14	1.45	1.38
3	E	2	OMC	C6-N1	3.08	1.45	1.38
3	E	4	OMC	C6-N1	2.96	1.45	1.38
3	F	4	OMC	C6-N1	2.94	1.45	1.38
3	F	4	OMC	C4-N4	2.94	1.41	1.33
3	F	2	OMC	C4-N4	2.93	1.41	1.33
3	E	4	OMC	C4-N4	2.91	1.40	1.33
3	E	2	OMC	C4-N4	2.87	1.40	1.33
3	F	2	OMC	C5-C4	2.73	1.49	1.42
3	E	2	OMC	C5-C4	2.70	1.49	1.42
3	F	4	OMC	C5-C4	2.62	1.49	1.42
3	E	4	OMC	C5-C4	2.62	1.49	1.42
3	E	2	OMC	O2-C2	-2.22	1.19	1.23
3	E	4	OMC	O2-C2	-2.16	1.19	1.23
3	F	2	OMC	O2-C2	-2.11	1.19	1.23
3	F	4	OMC	O2-C2	-2.03	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	E	4	OMC	2	0
3	F	2	OMC	1	0
3	F	4	OMC	2	0
3	E	2	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
4	GOL	E	101	-	5,5,5	0.29	0	5,5,5	0.32	0
4	GOL	D	501	-	5,5,5	0.36	0	5,5,5	0.31	0
6	ET9	A	603	5	33,34,34	2.29	7 (21%)	37,54,54	1.93	9 (24%)
4	GOL	D	503	-	5,5,5	0.54	0	5,5,5	0.31	0
4	GOL	D	502	-	5,5,5	0.38	0	5,5,5	0.27	0
6	ET9	C	602	5	33,34,34	2.39	10 (30%)	37,54,54	1.88	10 (27%)
4	GOL	A	601	-	5,5,5	0.37	0	5,5,5	0.27	0
4	GOL	B	501	-	5,5,5	0.37	0	5,5,5	0.33	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	E	101	-	-	2/4/4/4	-
4	GOL	D	501	-	-	0/4/4/4	-
6	ET9	A	603	5	-	4/22/38/38	0/3/3/3
4	GOL	D	503	-	-	2/4/4/4	-
4	GOL	D	502	-	-	1/4/4/4	-
6	ET9	C	602	5	-	4/22/38/38	0/3/3/3
4	GOL	A	601	-	-	0/4/4/4	-
4	GOL	B	501	-	-	1/4/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	602	ET9	C4-N9	-6.99	1.30	1.37
6	A	603	ET9	C4-N9	-6.72	1.30	1.37
6	C	602	ET9	C5-C4	5.47	1.47	1.38
6	A	603	ET9	C5-C4	5.01	1.46	1.38
6	A	603	ET9	PB-O3A	4.91	1.64	1.59
6	A	603	ET9	C1'-N9	-4.87	1.39	1.47
6	C	602	ET9	C1'-N9	-4.20	1.40	1.47
6	C	602	ET9	C4'-C6'	-3.92	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	ET9	C2'-C1'	-3.90	1.46	1.53
6	C	602	ET9	C2'-C1'	-3.74	1.47	1.53
6	C	602	ET9	PB-O3B	3.55	1.63	1.59
6	C	602	ET9	PA-O3A	3.46	1.63	1.59
6	C	602	ET9	PB-O3A	2.99	1.62	1.59
6	A	603	ET9	C5-N7	-2.71	1.33	1.39
6	C	602	ET9	C1'-C6'	-2.64	1.47	1.51
6	C	602	ET9	C5-N7	-2.09	1.34	1.39
6	A	603	ET9	C1'-C6'	-2.04	1.48	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	ET9	C2'-C3'-C4'	-5.74	95.89	103.62
6	C	602	ET9	C8-N9-C4	5.18	111.04	106.67
6	A	603	ET9	C8-N9-C4	4.14	110.16	106.67
6	C	602	ET9	O1A-PA-O3A	4.04	118.19	107.27
6	C	602	ET9	C5-C4-N9	-3.58	104.59	106.25
6	A	603	ET9	O1G-PG-O3B	3.42	116.11	104.64
6	A	603	ET9	O1A-PA-O3A	3.28	116.15	107.27
6	C	602	ET9	O3A-PA-O2A	-3.01	101.66	110.70
6	C	602	ET9	C5'-C4'-C3'	-2.98	106.73	115.60
6	C	602	ET9	O2G-PG-O3B	2.95	114.52	104.64
6	A	603	ET9	C5'-C4'-C3'	-2.85	107.10	115.60
6	C	602	ET9	C1'-N9-C8	-2.75	122.82	126.98
6	A	603	ET9	C5-C4-N9	-2.75	104.97	106.25
6	A	603	ET9	O3B-PG-O3G	-2.70	96.84	111.04
6	C	602	ET9	O2B-PB-O3B	2.65	114.43	107.27
6	A	603	ET9	O6-C6-N1	2.52	124.51	120.27
6	C	602	ET9	C2'-C1'-N9	-2.33	111.33	115.32
6	A	603	ET9	C1'-N9-C8	-2.11	123.79	126.98
6	C	602	ET9	N9-C8-N7	-2.08	109.55	113.40

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	101	GOL	O1-C1-C2-O2
4	E	101	GOL	O1-C1-C2-C3
4	D	503	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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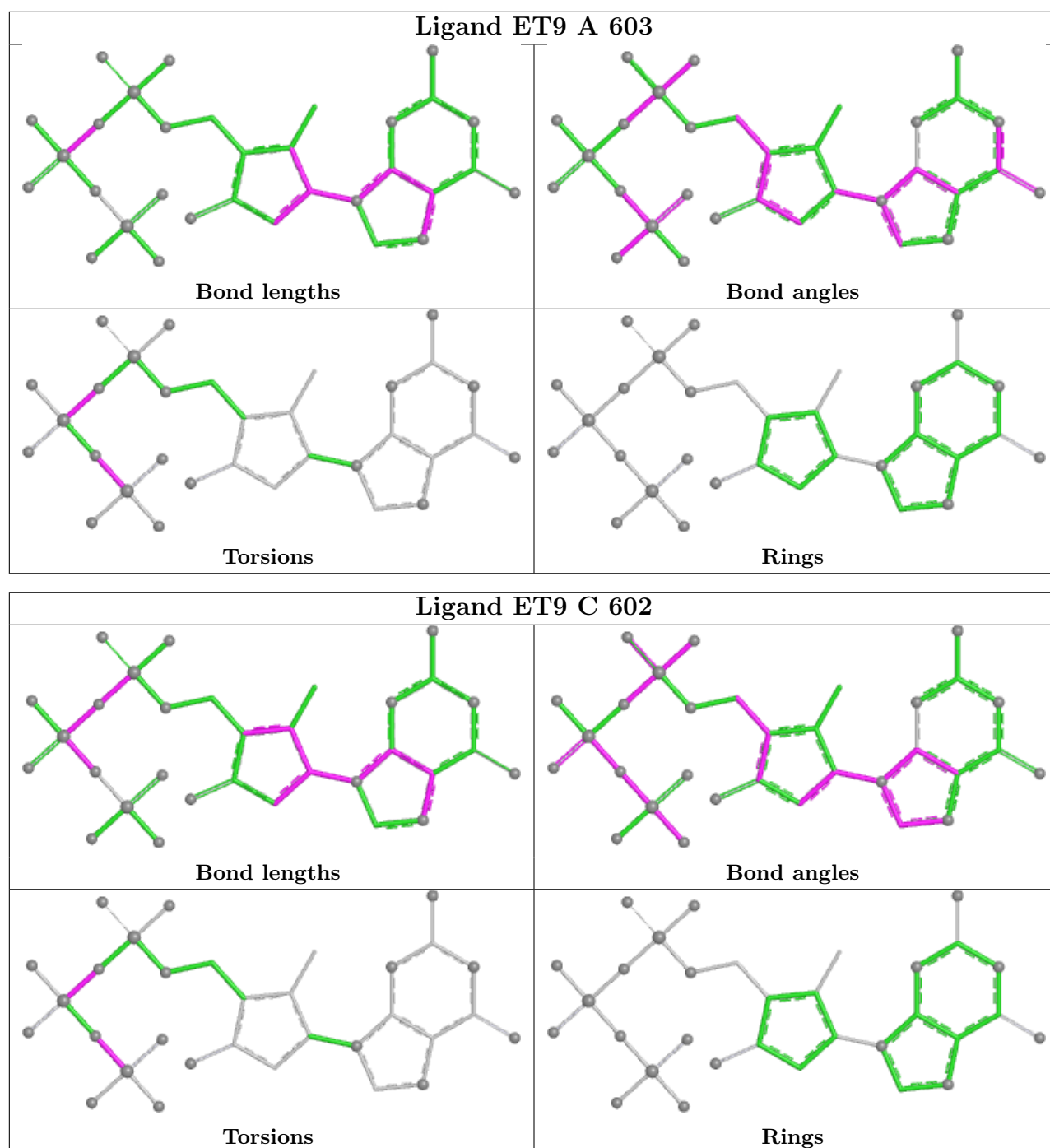
Mol	Chain	Res	Type	Atoms
6	C	602	ET9	PB-O3B-PG-O2G
4	D	503	GOL	O1-C1-C2-O2
4	D	502	GOL	O1-C1-C2-O2
6	C	602	ET9	PA-O3A-PB-O2B
6	C	602	ET9	PB-O3B-PG-O3G
4	B	501	GOL	O1-C1-C2-C3
6	A	603	ET9	PB-O3B-PG-O3G
6	A	603	ET9	PA-O3A-PB-O2B
6	C	602	ET9	PA-O3A-PB-O1B

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	101	GOL	3	0
4	D	501	GOL	2	0
6	A	603	ET9	2	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 i

6.1 Protein, DNA and RNA chains i

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%)	0.53	61 (11%) 10 12	26, 52, 94, 143	1 (0%)
1	C	553/557 (99%)	0.31	29 (5%) 33 35	27, 53, 96, 149	1 (0%)
2	B	406/444 (91%)	0.87	80 (19%) 3 3	31, 65, 129, 161	0
2	D	406/444 (91%)	0.34	35 (8%) 16 18	25, 50, 91, 156	1 (0%)
3	E	33/38 (86%)	-0.43	0 100 100	29, 48, 81, 125	0
3	F	36/38 (94%)	-0.16	0 100 100	35, 59, 101, 140	0
All	All	1987/2078 (95%)	0.47	205 (10%) 12 13	25, 54, 110, 161	3 (0%)

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	ILE	6.6
2	D	360	ALA	6.5
2	B	88	TRP	6.5
2	B	360	ALA	6.4
1	C	135	ILE	6.2
2	D	232	TYR	6.2
2	B	422	LEU	6.0
2	D	422	LEU	5.9
2	B	92	LEU	5.7
2	B	95	PRO	5.6
2	B	423	VAL	5.6
2	D	423	VAL	5.6
2	B	90	VAL	5.5
2	D	212	TRP	5.4
2	B	213	GLY	5.3
2	D	425	LEU	5.2
2	B	94	ILE	5.1
2	B	301	LEU	5.0
2	D	427	TYR	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	140	PRO	4.8
2	D	213	GLY	4.7
2	B	5	ILE	4.7
1	A	139	THR	4.6
1	A	132	ILE	4.6
2	B	245	VAL	4.5
1	A	62	ALA	4.5
2	B	232	TYR	4.4
2	B	93	GLY	4.3
1	A	141	GLY	4.3
2	B	210	LEU	4.3
2	D	5	ILE	4.2
1	A	133	PRO	4.1
1	A	136	ASN	4.0
1	C	133	PRO	4.0
2	D	359	GLY	4.0
2	D	361	HIS	3.8
1	A	67	ASP	3.8
1	C	69	THR	3.8
2	B	420	PRO	3.7
1	A	451	LYS	3.7
1	A	33	ALA	3.7
1	A	31	ILE	3.6
1	A	32	LYS	3.6
2	B	212	TRP	3.5
2	D	66	LYS	3.5
2	B	231	GLY	3.5
1	A	69	THR	3.5
1	A	28	GLU	3.5
2	B	247	PRO	3.4
1	A	142	ILE	3.4
2	B	243	PRO	3.4
2	B	266	TRP	3.4
2	B	294	PRO	3.4
1	A	60	VAL	3.4
1	C	67	ASP	3.4
2	B	290	THR	3.3
2	B	361	HIS	3.3
2	B	285	GLY	3.3
1	A	68	SER	3.3
2	B	209	LEU	3.2
2	B	295	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	424	LYS	3.2
1	C	219	LYS	3.2
1	A	551	LEU	3.2
2	D	210	LEU	3.2
2	B	66	LYS	3.2
1	A	66	LYS	3.2
2	B	357	MET	3.2
1	A	75	VAL	3.1
2	D	67	ASP	3.1
1	A	35	VAL	3.0
1	A	21	VAL	3.0
2	B	362	THR	3.0
2	D	419	THR	3.0
2	B	424	LYS	3.0
2	D	358	LYS	3.0
2	D	69	THR	3.0
2	B	252	TRP	3.0
1	C	66	LYS	2.9
1	A	134	SER	2.9
1	A	30	LYS	2.9
2	B	69	THR	2.9
1	C	68	SER	2.9
2	B	286	THR	2.9
1	A	541	GLY	2.9
2	B	98	ALA	2.9
1	C	35	VAL	2.9
2	B	241	VAL	2.9
2	D	314	VAL	2.9
1	C	450	THR	2.9
2	B	287	LYS	2.8
2	B	358	LYS	2.8
1	A	553	SER	2.8
2	D	313	PRO	2.8
2	B	292	VAL	2.8
1	A	402	TRP	2.8
2	D	357	MET	2.8
2	B	251	SER	2.8
2	B	421	PRO	2.8
1	A	457	TYR	2.8
1	C	26	LEU	2.8
2	B	303	LEU	2.8
2	B	427	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	239	TRP	2.7
2	B	425	LEU	2.7
1	C	1	PRO	2.7
1	A	24	TRP	2.7
1	A	38	CYS	2.7
2	D	356	ARG	2.7
1	C	140	PRO	2.7
1	A	71	TRP	2.7
1	A	26	LEU	2.7
1	A	485	ALA	2.7
2	B	334	GLN	2.7
2	B	237	ASP	2.7
2	B	281	LYS	2.7
2	B	283	LEU	2.7
1	A	464	GLN	2.6
1	A	550	LYS	2.6
1	A	542	ILE	2.6
2	D	318	TYR	2.6
1	A	1	PRO	2.6
1	C	134	SER	2.6
2	B	273	GLY	2.6
2	B	274	ILE	2.6
1	C	62	ALA	2.6
2	B	293	VAL	2.5
2	D	315	HIS	2.5
2	B	305	GLU	2.5
2	D	70	LYS	2.5
1	A	403	THR	2.5
1	A	552	VAL	2.5
2	B	89	GLU	2.5
1	A	70	LYS	2.5
1	A	59	PRO	2.5
1	C	402	TRP	2.5
1	C	71	TRP	2.4
1	A	36	GLU	2.4
1	C	357[A]	MET	2.4
1	A	468	PRO	2.4
1	A	27	THR	2.4
2	B	208	HIS	2.4
2	B	97	PRO	2.3
1	A	465	LYS	2.3
2	B	288	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	7	THR	2.3
1	A	131	THR	2.3
1	C	139	THR	2.3
2	B	291	GLU	2.3
1	A	22	LYS	2.3
2	B	99	GLY	2.3
2	D	88	TRP	2.3
2	B	284	ARG	2.3
1	A	34	LEU	2.3
2	B	238	LYS	2.3
2	D	421	PRO	2.3
2	B	359	GLY	2.3
1	C	63	ILE	2.3
2	D	122	LYS	2.3
2	D	90	VAL	2.3
2	D	283	LEU	2.2
2	D	211	ARG	2.2
1	A	53	GLU	2.2
1	C	166	LYS	2.2
2	B	65	LYS	2.2
1	A	539	HIS	2.2
1	A	454	LYS	2.2
1	C	22	LYS	2.2
1	C	419	THR	2.2
2	B	240	THR	2.2
2	B	253	THR	2.2
2	B	162	SER	2.2
1	C	52	PRO	2.2
1	C	33	ALA	2.2
1	C	553	SER	2.2
2	B	165	THR	2.2
2	B	282	LEU	2.2
2	B	289	LEU	2.2
2	D	317	VAL	2.2
1	A	25	PRO	2.2
1	C	64	LYS	2.2
2	B	196	GLY	2.2
2	B	272	ALA	2.2
2	D	362	THR	2.2
1	A	137	ASN	2.1
1	A	61	PHE	2.1
1	A	452	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	495	ILE	2.1
1	C	70	LYS	2.1
2	B	279	LEU	2.1
2	D	266	TRP	2.1
2	D	316	GLY	2.1
2	B	277	ARG	2.1
2	B	304	ALA	2.1
2	B	250	ASP	2.1
1	A	548	VAL	2.1
2	B	68	SER	2.1
1	A	516	GLU	2.1
1	A	491	LEU	2.1
1	A	493	VAL	2.1
2	B	246	LEU	2.0
2	B	244	ILE	2.0
2	B	257	ILE	2.0
2	B	193	LEU	2.0
1	C	25	PRO	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	0.08	39,45,50,56	0
3	OMC	F	4	21/22	0.97	0.07	30,35,40,48	0
3	OMC	E	4	21/22	0.98	0.05	25,29,35,40	0
3	OMC	E	2	21/22	0.98	0.06	29,34,40,42	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

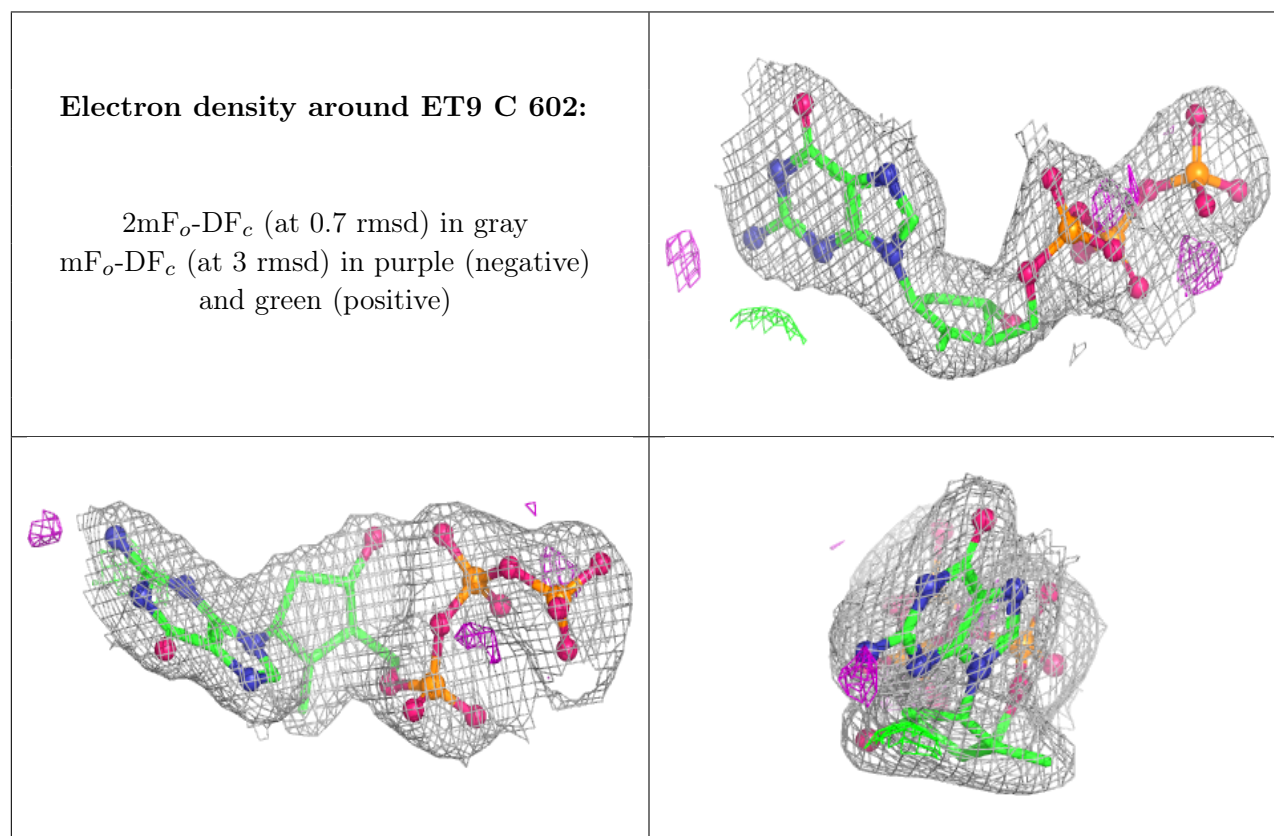
6.4 Ligands [i](#)

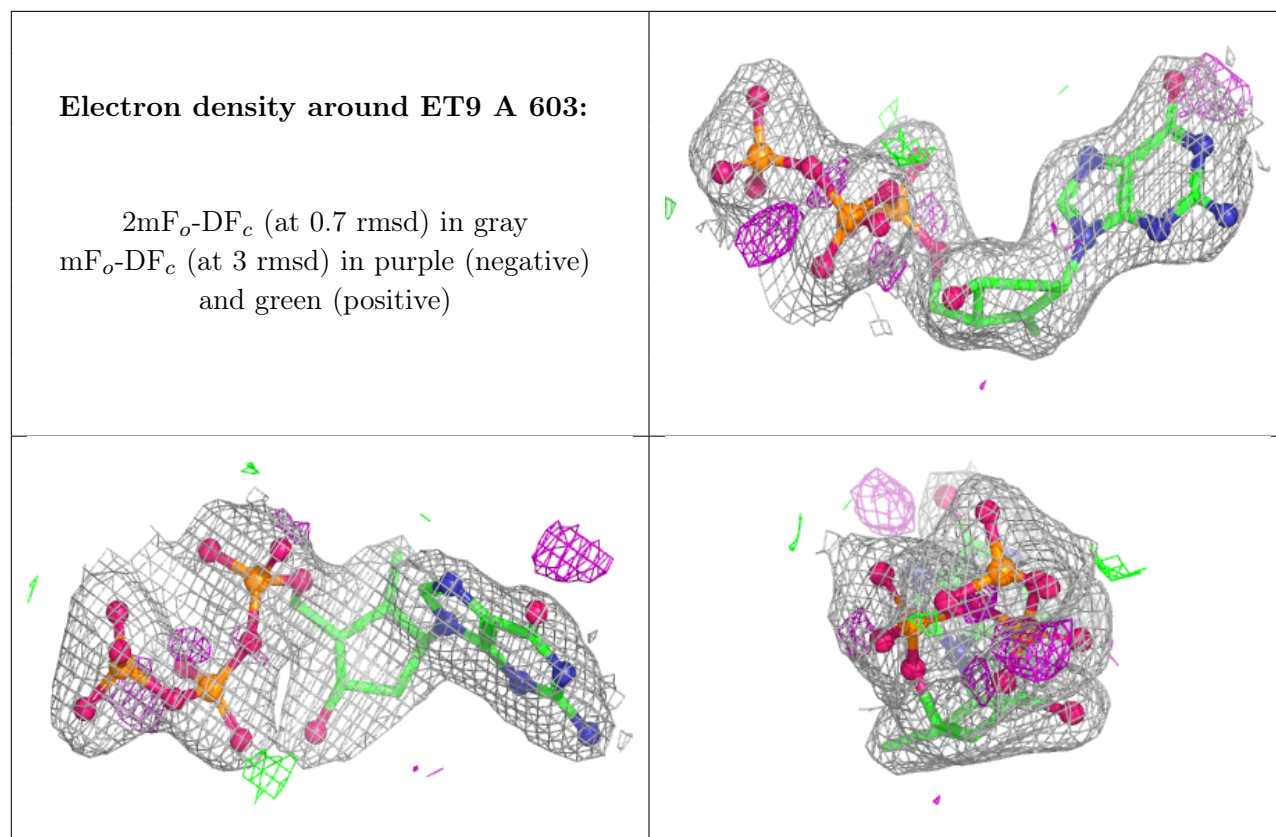
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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
4	GOL	A	601	6/6	0.87	0.17	49,58,60,61	0
4	GOL	E	101	6/6	0.92	0.15	63,70,71,72	0
4	GOL	D	501	6/6	0.93	0.13	46,49,49,51	0
4	GOL	D	502	6/6	0.93	0.14	41,46,47,48	0
4	GOL	D	503	6/6	0.93	0.17	55,59,61,61	0
6	ET9	C	602	32/32	0.94	0.08	51,60,79,83	0
6	ET9	A	603	32/32	0.95	0.08	48,57,68,68	0
4	GOL	B	501	6/6	0.95	0.11	41,47,49,50	0
5	MG	C	601	1/1	0.96	0.10	65,65,65,65	0
5	MG	A	602	1/1	0.98	0.08	55,55,55,55	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.