Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 12:44 AM JST

PDB ID	:	6IKA
Title	:	HIV-1 reverse transcriptase with Q151M/G112S/D113A/Y115F/F116Y/F160L/I159L:DNA:entecavir-triphosphate ternary complex
Authors	:	Yasutake, Y.; Hattori, S.I.; Tamura, N.; Maeda, K.
Deposited on	:	2018-10-15
Resolution	:	2.60 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:

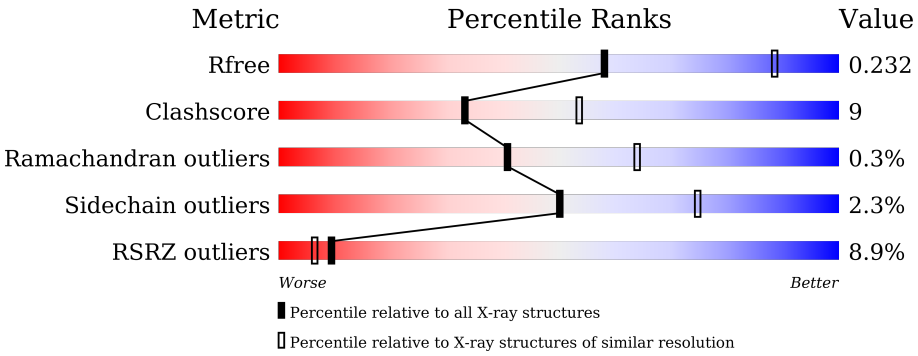
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	7% 82% 17% ••
1	C	557	12% 85% 14% ••
2	B	444	11% 69% 21% • 9%
2	D	444	4% 79% 11% • 9%
3	E	38	21% 55% 16% 8%
3	F	38	3% 55% 37% 8%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17416 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 RT p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4494	2908	750	828	8			
1	C	553	Total	C	N	O	S	0	0	0
			4494	2908	750	828	8			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP D3XFN7
A	0	VAL	-	expression tag	UNP D3XFN7
A	112	SER	GLY	engineered mutation	UNP D3XFN7
A	113	ALA	ASP	engineered mutation	UNP D3XFN7
A	115	PHE	TYR	engineered mutation	UNP D3XFN7
A	116	TYR	PHE	engineered mutation	UNP D3XFN7
A	151	MET	GLN	engineered mutation	UNP D3XFN7
A	159	LEU	ILE	engineered mutation	UNP D3XFN7
A	160	LEU	PHE	engineered mutation	UNP D3XFN7
A	162	SER	CYS	engineered mutation	UNP D3XFN7
A	280	SER	CYS	engineered mutation	UNP D3XFN7
C	-1	MET	-	expression tag	UNP D3XFN7
C	0	VAL	-	expression tag	UNP D3XFN7
C	112	SER	GLY	engineered mutation	UNP D3XFN7
C	113	ALA	ASP	engineered mutation	UNP D3XFN7
C	115	PHE	TYR	engineered mutation	UNP D3XFN7
C	116	TYR	PHE	engineered mutation	UNP D3XFN7
C	151	MET	GLN	engineered mutation	UNP D3XFN7
C	159	LEU	ILE	engineered mutation	UNP D3XFN7
C	160	LEU	PHE	engineered mutation	UNP D3XFN7
C	162	SER	CYS	engineered mutation	UNP D3XFN7
C	280	SER	CYS	engineered mutation	UNP D3XFN7

- 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			

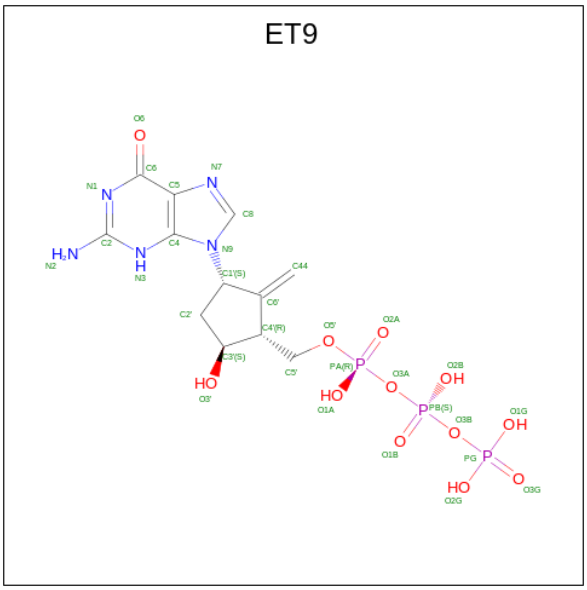
There are 36 discrepancies between the modelled and reference sequences:

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).

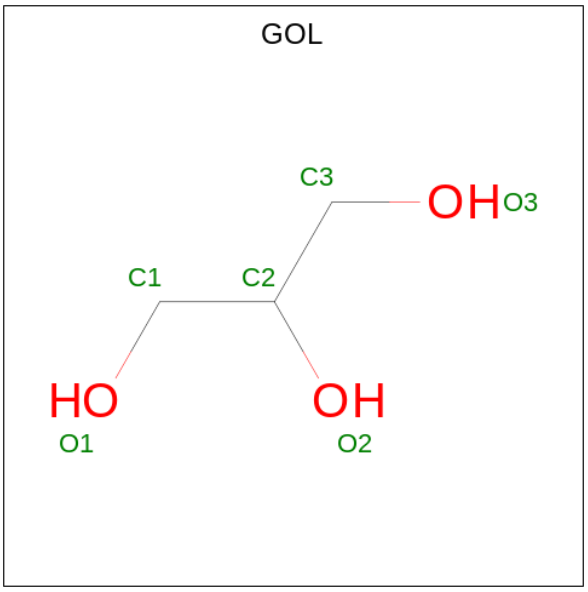
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	35	Total	C	N	O	P	0	0	0
			718	339	128	216	35			
3	F	38	Total	C	N	O	P	0	0	0
			777	369	140	231	37			

- Molecule 4 is [[(1R,3S,5S)-3-(2-azanyl-6-oxidanylidene-3H-purin-9-yl)-2-methylidene-5-oxidanyl-cyclopentyl]methoxy-oxidanyl-phosphory l] phosphono hydrogen phosphate (three-letter code: ET9) (formula: $C_{12}H_{18}N_5O_{12}P_3$).



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



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	46	Total O 46 46	0	0
7	B	29	Total O 29 29	0	0
7	E	12	Total O 12 12	0	0

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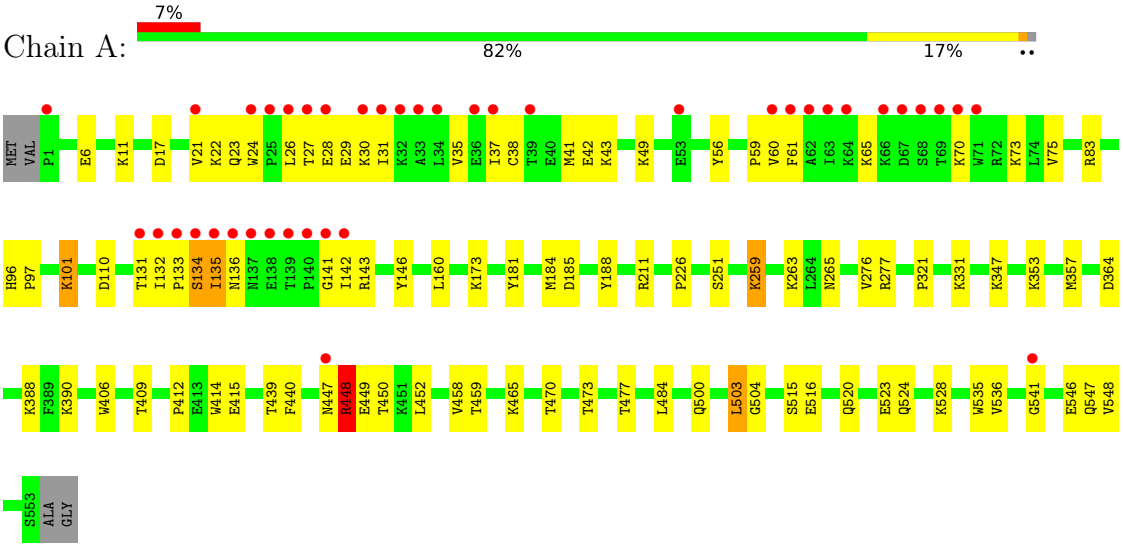
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	27	Total O 27 27	0	0
7	D	25	Total O 25 25	0	0
7	F	10	Total O 10 10	0	0

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.

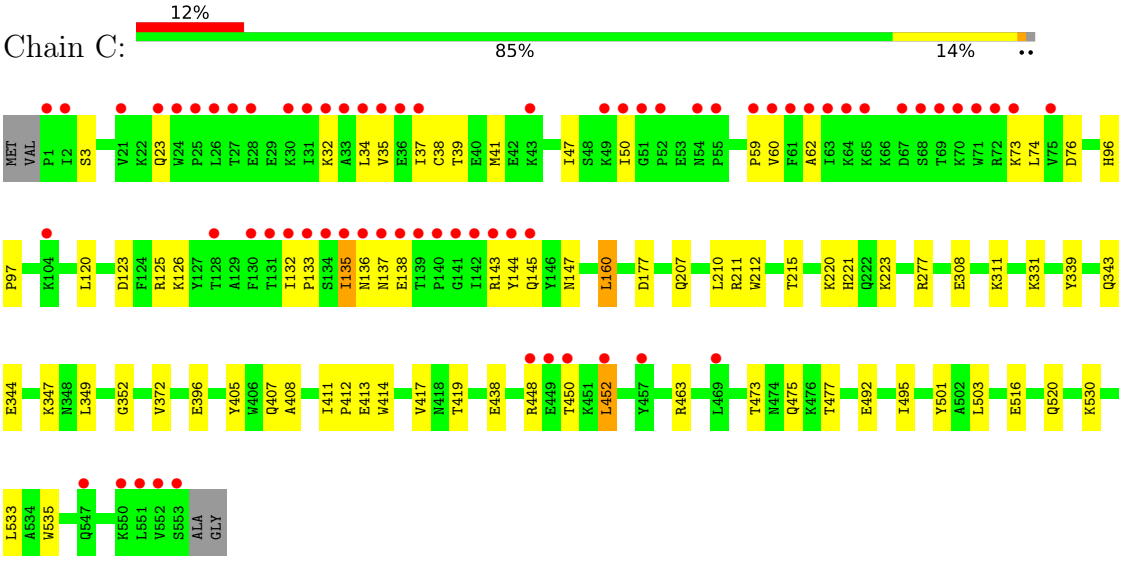
• Molecule 1: HIV-1 RT p66 subunit

Chain A:



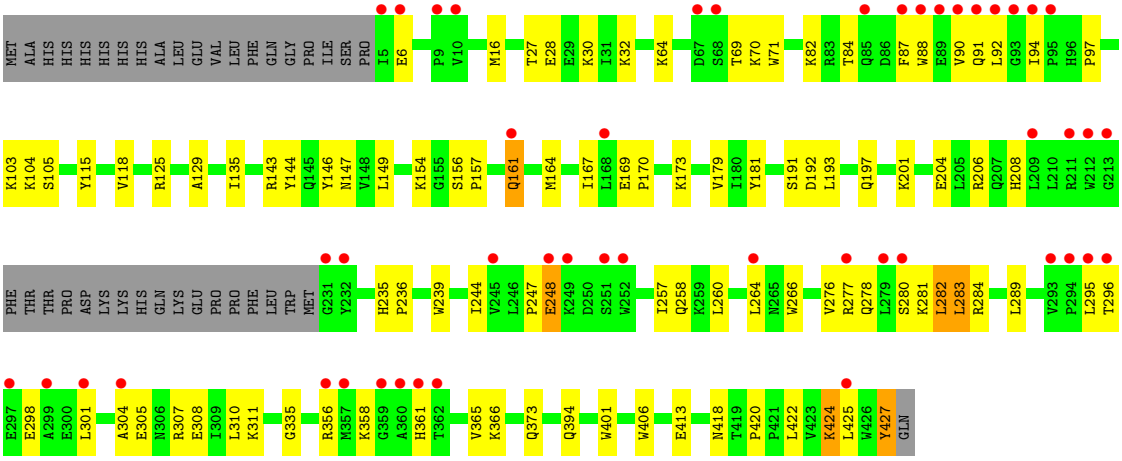
• Molecule 1: HIV-1 RT p66 subunit

Chain C:

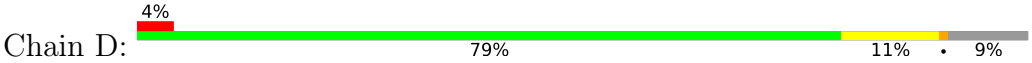


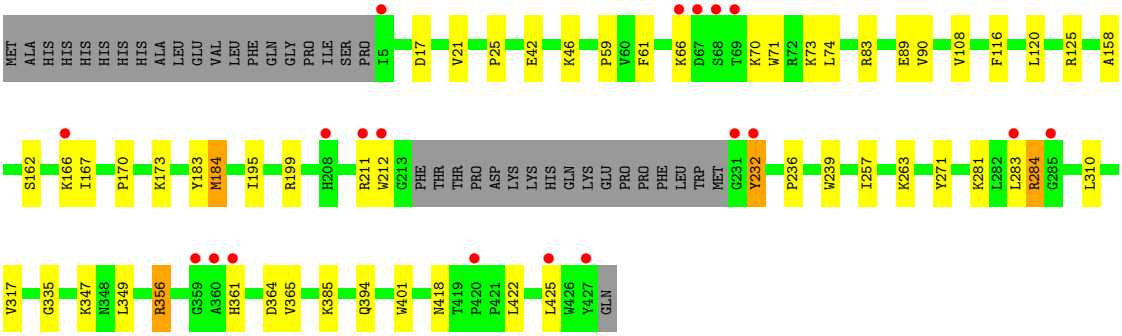
• Molecule 2: HIV-1 RT p51 subunit

Chain B:

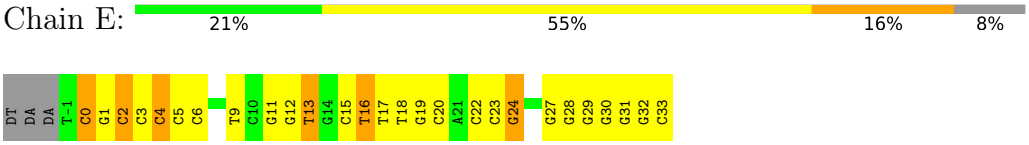


• Molecule 2: HIV-1 RT p51 subunit

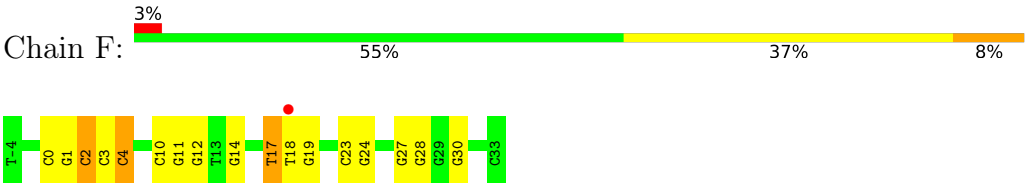




• Molecule 3: DNA/RNA (38-MER)



• Molecule 3: DNA/RNA (38-MER)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	285.40Å 285.40Å 96.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.87 – 2.60 48.87 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.87-2.60) 99.6 (48.87-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.186 , 0.232 0.186 , 0.232	Depositor DCC
R_{free} test set	4538 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17416	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.51	0/4611	0.62	0/6262
1	C	0.46	0/4611	0.59	0/6262
2	B	0.47	0/3441	0.62	0/4673
2	D	0.47	0/3441	0.57	0/4673
3	E	1.75	22/756 (2.9%)	0.81	0/1165
3	F	1.12	7/823 (0.9%)	0.85	0/1269
All	All	0.63	29/17683 (0.2%)	0.63	0/24304

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	A	0	1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	OMC	O3'-P	-8.31	1.51	1.61
3	E	19	DG	O3'-P	-8.27	1.51	1.61
3	E	5	DC	O3'-P	-8.12	1.51	1.61
3	E	30	DG	O3'-P	-7.84	1.51	1.61
3	E	29	DG	O3'-P	-7.64	1.51	1.61
3	E	17	DT	O3'-P	-7.63	1.51	1.61
3	E	6	DC	O3'-P	-7.47	1.52	1.61
3	E	31	DG	O3'-P	-7.23	1.52	1.61
3	E	18	DT	O3'-P	-6.92	1.52	1.61
3	E	22	DC	O3'-P	-6.92	1.52	1.61
3	E	13	DT	O3'-P	-6.86	1.52	1.61
3	E	24	DG	O3'-P	-6.79	1.52	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	OMC	O3'-P	-6.73	1.53	1.61
3	E	28	DG	O3'-P	-6.46	1.53	1.61
3	F	14	DG	O3'-P	-6.38	1.53	1.61
3	E	27	DG	O3'-P	-6.35	1.53	1.61
3	F	12	DG	O3'-P	-6.28	1.53	1.61
3	F	19	DG	O3'-P	-6.12	1.53	1.61
3	F	30	DG	O3'-P	-5.76	1.54	1.61
3	E	20	DC	O3'-P	-5.75	1.54	1.61
3	F	27	DG	O3'-P	-5.68	1.54	1.61
3	E	15	DC	O3'-P	-5.65	1.54	1.61
3	E	32	DG	O3'-P	-5.65	1.54	1.61
3	F	28	DG	O3'-P	-5.64	1.54	1.61
3	E	9	DT	O3'-P	-5.57	1.54	1.61
3	E	16	DT	O3'-P	-5.44	1.54	1.61
3	E	11	DG	O3'-P	-5.43	1.54	1.61
3	E	0	DC	O3'-P	-5.31	1.54	1.61
3	F	17	DT	O3'-P	-5.11	1.55	1.61

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	448	ARG	Sidechain

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	4494	0	4558	85	0
1	C	4494	0	4558	61	0
2	B	3347	0	3379	93	0
2	D	3347	0	3379	45	0
3	E	718	0	397	11	0
3	F	777	0	432	10	0
4	A	32	0	0	5	0
4	C	32	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	6	0	8	3	0
5	B	6	0	8	0	0
5	C	6	0	8	2	0
5	D	6	0	8	1	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	46	0	0	1	0
7	B	29	0	0	0	0
7	C	27	0	0	1	0
7	D	25	0	0	0	0
7	E	12	0	0	0	0
7	F	10	0	0	0	0
All	All	17416	0	16735	291	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 9.

All (291) 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:31:ILE:HG21	1:A:134:SER:HA	1.36	1.04
3:F:17:DT:H5”	3:F:17:DT:H6	1.25	1.01
1:A:131:THR:CG2	1:A:141:GLY:HA3	1.93	0.98
2:B:335:GLY:HA3	2:B:356:ARG:HD3	1.46	0.94
1:A:26:LEU:HD22	1:A:30:LYS:HD3	1.51	0.92
2:B:87:PHE:HA	2:B:90:VAL:HG22	1.53	0.91
1:C:135:ILE:HG22	1:C:136:ASN:H	1.35	0.90
1:A:131:THR:HG22	1:A:141:GLY:HA3	1.54	0.89
1:A:133:PRO:O	1:A:134:SER:O	1.93	0.86
1:A:135:ILE:HG13	1:A:136:ASN:H	1.43	0.84
2:B:201:LYS:HA	2:B:204:GLU:HG3	1.60	0.83
1:C:135:ILE:HG22	1:C:136:ASN:N	2.01	0.76
3:F:17:DT:H5”	3:F:17:DT:C6	2.15	0.76
1:A:500:GLN:HB3	2:B:422:LEU:HD21	1.68	0.75
1:A:135:ILE:HG13	1:A:136:ASN:N	2.01	0.74
1:C:450:THR:OG1	1:C:452:LEU:HD12	1.89	0.73
1:C:160:LEU:HD22	1:C:160:LEU:O	1.90	0.72
5:C:602:GOL:H11	2:D:394:GLN:HB2	1.71	0.71
1:C:50:ILE:HG13	1:C:143:ARG:HB3	1.73	0.70
3:F:3:DC:H2’	3:F:4:OMC:C6	2.26	0.70
2:B:104:LYS:HB3	2:B:191:SER:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:VAL:HG21	2:D:158:ALA:HA	1.73	0.69
2:B:296:THR:HG22	2:B:298:GLU:H	1.57	0.69
1:A:135:ILE:HG23	1:A:136:ASN:N	2.08	0.69
1:A:31:ILE:CG2	1:A:134:SER:HA	2.18	0.68
1:A:60:VAL:HG11	1:A:132:ILE:HD13	1.74	0.68
1:A:440:PHE:HA	1:A:459:THR:HG22	1.76	0.67
2:D:356:ARG:HD3	2:D:361:HIS:HB2	1.76	0.67
2:B:335:GLY:HA3	2:B:356:ARG:CD	2.23	0.67
1:A:65:LYS:HD3	1:A:70:LYS:HB2	1.76	0.67
1:A:23:GLN:HE22	1:A:60:VAL:H	1.42	0.66
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.78	0.66
1:A:134:SER:O	1:A:135:ILE:HG22	1.96	0.66
1:A:28:GLU:HG2	1:A:29:GLU:N	2.10	0.65
1:A:500:GLN:CB	2:B:422:LEU:HD21	2.27	0.65
2:D:335:GLY:HA3	2:D:356:ARG:HG2	1.79	0.65
2:B:277:ARG:HA	2:B:280:SER:HB3	1.79	0.64
2:B:90:VAL:HG23	2:B:92:LEU:HG	1.80	0.63
2:B:278:GLN:OE1	2:B:298:GLU:HB3	1.99	0.63
2:B:104:LYS:O	2:B:235:HIS:HD2	1.80	0.63
2:B:64:LYS:HD2	2:B:71:TRP:CZ2	2.34	0.63
2:B:248:GLU:HG2	2:B:307:ARG:NH2	2.14	0.63
1:A:22:LYS:HD2	1:A:23:GLN:H	1.65	0.62
1:A:450:THR:CG2	1:A:452:LEU:HD12	2.29	0.62
4:A:601:ET9:C44	3:E:33:DC:H2"	2.29	0.62
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.82	0.62
1:C:136:ASN:O	1:C:138:GLU:N	2.33	0.62
3:E:16:DT:H2'	3:E:16:DT:O2	1.99	0.61
3:F:18:DT:H2'	3:F:18:DT:O2	2.01	0.61
1:C:160:LEU:HD22	1:C:160:LEU:C	2.21	0.61
1:A:142:ILE:HD12	1:A:143:ARG:H	1.65	0.61
1:A:27:THR:OG1	1:A:30:LYS:HG3	2.00	0.61
1:C:120:LEU:HD23	1:C:125:ARG:HG2	1.82	0.61
1:C:473:THR:O	1:C:477:THR:HG23	2.01	0.61
1:A:520:GLN:O	1:A:524:GLN:HG3	2.01	0.60
1:A:448:ARG:HG3	1:A:449:GLU:N	2.15	0.60
1:C:35:VAL:O	1:C:39:THR:HG23	2.02	0.59
2:D:66:LYS:HZ2	2:D:232:TYR:HD2	1.49	0.59
1:A:541:GLY:HA2	1:A:546:GLU:HG3	1.83	0.59
2:B:356:ARG:HD2	2:B:361:HIS:CD2	2.38	0.59
2:B:356:ARG:HD2	2:B:361:HIS:CG	2.38	0.58
1:C:59:PRO:HG2	1:C:76:ASP:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TRP:CZ2	2:B:420:PRO:HG3	2.39	0.58
1:C:50:ILE:CG1	1:C:143:ARG:HB3	2.34	0.58
1:A:26:LEU:CD2	1:A:30:LYS:HD3	2.30	0.58
5:A:602:GOL:H31	2:B:394:GLN:CG	2.34	0.57
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.87	0.57
2:D:70:LYS:HD2	2:D:71:TRP:H	1.70	0.57
2:B:103:LYS:HZ1	2:B:179:VAL:HB	1.70	0.57
2:B:103:LYS:HE2	2:B:191:SER:HA	1.87	0.57
1:A:26:LEU:HD22	1:A:30:LYS:CD	2.32	0.56
2:B:266:TRP:CD1	2:B:425:LEU:HD22	2.41	0.56
1:C:339:TYR:CZ	1:C:352:GLY:HA3	2.40	0.56
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.86	0.56
2:B:358:LYS:HZ2	2:B:361:HIS:H	1.53	0.56
1:C:74:LEU:HD22	3:F:0:DC:C2	2.40	0.56
5:A:602:GOL:H31	2:B:394:GLN:HG2	1.87	0.56
2:D:46:LYS:HE2	2:D:116:PHE:HB3	1.86	0.56
1:A:135:ILE:CG1	1:A:136:ASN:H	2.11	0.56
2:B:358:LYS:HD2	2:B:366:LYS:HD3	1.88	0.56
2:B:104:LYS:CB	2:B:192:ASP:HA	2.36	0.55
1:C:344:GLU:HB2	1:C:347:LYS:HD2	1.88	0.55
2:B:247:PRO:O	2:B:307:ARG:NH2	2.38	0.55
1:A:23:GLN:OE1	1:A:60:VAL:HG12	2.07	0.55
7:A:702:HOH:O	1:C:331:LYS:HE2	2.06	0.55
2:B:64:LYS:HZ3	2:B:64:LYS:HB2	1.72	0.55
2:B:422:LEU:HD12	2:B:422:LEU:N	2.21	0.55
1:A:31:ILE:HG13	1:A:135:ILE:H	1.71	0.55
2:B:164:MET:HA	2:B:167:ILE:HG22	1.88	0.55
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.88	0.55
3:E:3:DC:H2'	3:E:4:OMC:C6	2.42	0.55
1:C:516:GLU:OE2	1:C:520:GLN:NE2	2.32	0.54
1:C:123:ASP:O	1:C:126:LYS:HE2	2.08	0.54
1:C:221:HIS:CD2	1:C:223:LYS:HD2	2.42	0.54
2:B:296:THR:HG22	2:B:298:GLU:N	2.21	0.54
2:B:244:ILE:HB	2:B:310:LEU:HG	1.89	0.54
2:B:356:ARG:NH1	2:B:361:HIS:HB3	2.22	0.54
1:C:35:VAL:HG22	1:C:132:ILE:HG21	1.89	0.54
1:A:259:LYS:HE3	1:A:263:LYS:HE2	1.90	0.54
1:A:412:PRO:O	1:A:414:TRP:HD1	1.91	0.54
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.38	0.53
2:B:424:LYS:HG3	2:B:427:TYR:HB3	1.90	0.53
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:GLN:CD	2:B:298:GLU:HB3	2.28	0.53
2:D:108:VAL:HG21	2:D:232:TYR:CE1	2.44	0.53
2:D:89:GLU:HG2	2:D:90:VAL:HG23	1.90	0.53
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.38	0.53
1:C:438:GLU:OE1	1:C:463:ARG:HD3	2.09	0.53
1:A:23:GLN:NE2	1:A:60:VAL:H	2.06	0.52
1:A:185:ASP:OD1	3:E:33:DC:O3'	2.26	0.52
2:B:64:LYS:HZ1	2:B:69:THR:HG22	1.74	0.52
1:A:131:THR:CG2	1:A:141:GLY:CA	2.79	0.52
1:A:331:LYS:NZ	1:A:364:ASP:OD2	2.41	0.52
2:B:84:THR:HB	2:B:154:LYS:HZ3	1.75	0.52
1:C:495:ILE:HB	1:C:533:LEU:HD13	1.91	0.52
1:C:34:LEU:HD21	1:C:62:ALA:HB2	1.91	0.52
1:A:56:TYR:O	1:A:143:ARG:NH2	2.42	0.52
1:A:447:ASN:HB2	1:A:450:THR:HB	1.92	0.52
4:C:601:ET9:N2	3:F:0:DC:O2	2.42	0.52
1:A:135:ILE:HG23	1:A:136:ASN:H	1.72	0.52
1:A:185:ASP:OD1	4:A:601:ET9:C5'	2.57	0.52
1:C:448:ARG:NH2	3:F:18:DT:OP2	2.43	0.51
2:B:82:LYS:HE2	2:B:413:GLU:OE1	2.10	0.51
1:C:38:CYS:HB3	1:C:144:TYR:CE2	2.44	0.51
1:A:31:ILE:O	1:A:35:VAL:HG23	2.11	0.51
1:A:37:ILE:HG22	1:A:41:MET:SD	2.51	0.51
1:A:536:VAL:HG11	2:B:258:GLN:HE21	1.74	0.51
1:C:396:GLU:CD	1:C:396:GLU:H	2.13	0.51
2:D:317:VAL:HG22	2:D:347:LYS:HB3	1.91	0.51
2:D:195:ILE:HG13	2:D:199:ARG:HE	1.75	0.51
1:A:60:VAL:HA	1:A:75:VAL:HA	1.93	0.51
1:A:276:VAL:HG22	1:A:353:LYS:HE2	1.93	0.51
1:A:520:GLN:O	1:A:523:GLU:HG2	2.09	0.51
1:C:413:GLU:HA	7:C:724:HOH:O	2.11	0.51
1:C:125:ARG:HD3	1:C:147:ASN:HA	1.92	0.51
2:B:276:VAL:O	2:B:280:SER:CB	2.59	0.51
2:D:25:PRO:HA	5:D:501:GOL:H12	1.93	0.50
3:F:1:DG:H2'	3:F:2:OMC:C6	2.46	0.50
1:A:184:MET:HG3	3:E:33:DC:H1'	1.94	0.50
1:A:73:LYS:HE2	1:A:146:TYR:OH	2.12	0.50
2:D:263:LYS:HA	2:D:425:LEU:HD22	1.94	0.50
3:E:16:DT:C6	3:E:16:DT:H5"	2.47	0.50
2:B:358:LYS:HZ2	2:B:361:HIS:N	2.10	0.49
1:C:23:GLN:HE22	1:C:60:VAL:H	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:LEU:HD13	1:A:535:TRP:HB2	1.95	0.49
5:C:602:GOL:H11	2:D:394:GLN:CB	2.41	0.49
1:A:390:LYS:HD3	1:A:415:GLU:HB3	1.94	0.49
2:B:87:PHE:CA	2:B:90:VAL:HG22	2.36	0.49
1:C:343:GLN:HG3	1:C:349:LEU:HD11	1.94	0.49
1:A:60:VAL:HB	1:A:75:VAL:HG22	1.94	0.49
1:A:465:LYS:HD3	1:A:484:LEU:HD12	1.95	0.49
1:C:503:LEU:CD2	2:D:422:LEU:HD21	2.43	0.49
2:B:88:TRP:HA	2:B:91:GLN:HA	1.94	0.49
1:A:37:ILE:O	1:A:41:MET:N	2.41	0.49
1:A:265:ASN:OD1	1:A:353:LYS:HE3	2.13	0.49
2:B:64:LYS:HZ1	2:B:69:THR:CG2	2.25	0.48
2:B:129:ALA:HA	2:B:144:TYR:O	2.13	0.48
2:B:105:SER:OG	2:B:235:HIS:NE2	2.39	0.48
3:E:23:DC:H2"	3:E:24:DG:C8	2.49	0.48
1:C:125:ARG:CD	1:C:147:ASN:HA	2.42	0.48
2:D:66:LYS:HE3	2:D:232:TYR:N	2.29	0.48
2:D:167:ILE:HD12	2:D:212:TRP:CD1	2.48	0.48
1:A:185:ASP:CG	4:A:601:ET9:C5'	2.81	0.48
1:A:21:VAL:HG23	1:A:59:PRO:HD3	1.95	0.48
1:C:220:LYS:HE3	1:C:220:LYS:HA	1.95	0.48
2:B:277:ARG:O	2:B:281:LYS:HG2	2.13	0.48
2:B:295:LEU:H	2:B:295:LEU:HD12	1.79	0.48
2:B:373:GLN:HG3	2:B:406:TRP:CZ3	2.49	0.48
2:D:183:TYR:CE2	2:D:184:MET:HG3	2.49	0.48
2:D:73:LYS:HZ3	2:D:73:LYS:HB3	1.77	0.48
2:D:271:TYR:CE1	2:D:310:LEU:HD23	2.49	0.47
2:B:105:SER:HG	2:B:235:HIS:CD2	2.31	0.47
2:D:236:PRO:HA	2:D:239:TRP:CD2	2.49	0.47
1:A:135:ILE:HG13	1:A:136:ASN:HD22	1.80	0.47
3:E:1:DG:H2'	3:E:2:OMC:C6	2.50	0.47
1:C:35:VAL:CG2	1:C:132:ILE:HG21	2.45	0.47
1:C:495:ILE:HB	1:C:533:LEU:CD1	2.43	0.47
2:D:46:LYS:HD3	2:D:116:PHE:CD1	2.49	0.47
1:A:504:GLY:HA2	2:B:420:PRO:HG2	1.95	0.47
2:B:103:LYS:NZ	2:B:179:VAL:H	2.13	0.47
1:C:223:LYS:N	1:C:223:LYS:HD3	2.30	0.47
1:C:372:VAL:HG11	1:C:411:ILE:HG23	1.97	0.47
1:C:50:ILE:HG21	1:C:145:GLN:HB3	1.97	0.46
1:C:37:ILE:O	1:C:41:MET:HG3	2.15	0.46
2:B:276:VAL:O	2:B:280:SER:N	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:LEU:HD13	1:C:215:THR:HG22	1.97	0.46
1:C:96:HIS:CG	1:C:97:PRO:HD2	2.50	0.46
1:A:23:GLN:OE1	1:A:59:PRO:HA	2.16	0.46
1:A:439:THR:CG2	2:B:289:LEU:HD13	2.43	0.46
2:B:257:ILE:CG2	2:B:283:LEU:HD21	2.45	0.46
2:D:61:PHE:CZ	2:D:74:LEU:HD23	2.51	0.46
2:D:162:SER:O	2:D:166:LYS:HG2	2.15	0.46
2:D:361:HIS:CD2	2:D:361:HIS:O	2.69	0.46
3:F:23:DC:H2"	3:F:24:DG:C8	2.51	0.46
2:B:304:ALA:O	2:B:308:GLU:HG2	2.16	0.46
1:C:408:ALA:HB1	2:D:364:ASP:HB3	1.98	0.46
2:D:17:ASP:O	2:D:83:ARG:HD3	2.16	0.46
1:A:450:THR:HG21	1:A:452:LEU:HD12	1.97	0.46
2:D:356:ARG:HD3	2:D:361:HIS:CB	2.44	0.46
2:B:125:ARG:HD3	2:B:147:ASN:HA	1.97	0.45
2:B:277:ARG:CA	2:B:280:SER:HB3	2.46	0.45
2:B:103:LYS:NZ	2:B:179:VAL:HB	2.31	0.45
2:B:118:VAL:HB	2:B:149:LEU:HG	1.98	0.45
1:A:101:LYS:HE2	1:A:321:PRO:HG3	1.99	0.45
1:A:173:LYS:HB2	1:A:173:LYS:HE3	1.71	0.45
2:D:211:ARG:O	2:D:211:ARG:HG3	2.15	0.45
1:A:6:GLU:H	1:A:6:GLU:CD	2.19	0.45
2:B:87:PHE:O	2:B:92:LEU:N	2.45	0.45
1:C:3:SER:HB2	1:C:212:TRP:O	2.17	0.45
1:A:133:PRO:O	1:A:134:SER:C	2.51	0.45
2:D:257:ILE:HG22	2:D:283:LEU:HD11	1.99	0.45
2:D:281:LYS:HG3	2:D:284:ARG:NH2	2.31	0.45
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.99	0.45
2:B:282:LEU:HD23	2:B:282:LEU:HA	1.83	0.44
2:B:308:GLU:O	2:B:311:LYS:HB3	2.17	0.44
1:A:23:GLN:HG3	1:A:24:TRP:N	2.31	0.44
2:B:169:GLU:O	2:B:173:LYS:HB2	2.18	0.44
2:B:301:LEU:O	2:B:305:GLU:HB2	2.18	0.44
2:D:365:VAL:HG11	2:D:401:TRP:HB2	2.00	0.44
1:C:38:CYS:HB3	1:C:144:TYR:HE2	1.81	0.44
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.52	0.44
2:B:94:ILE:HG22	2:B:161:GLN:OE1	2.17	0.44
1:C:220:LYS:HA	1:C:220:LYS:CE	2.47	0.44
3:F:10:DC:H2"	3:F:11:DG:C8	2.53	0.44
2:B:169:GLU:HB3	2:B:170:PRO:HD3	2.00	0.43
2:D:21:VAL:HB	2:D:59:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:VAL:HG22	1:A:548:VAL:HB	2.00	0.43
2:B:143:ARG:HG2	2:B:143:ARG:HH11	1.83	0.43
2:D:394:GLN:NE2	2:D:418:ASN:HD22	2.16	0.43
1:C:120:LEU:O	1:C:125:ARG:NH1	2.51	0.43
3:E:12:DG:C2'	3:E:13:DT:H71	2.48	0.43
2:D:422:LEU:O	2:D:425:LEU:HG	2.17	0.43
1:C:207:GLN:O	1:C:211:ARG:HG3	2.18	0.43
1:C:412:PRO:O	1:C:414:TRP:HD1	2.00	0.43
2:B:104:LYS:HB3	2:B:192:ASP:HA	2.01	0.43
1:A:504:GLY:CA	2:B:420:PRO:HG2	2.49	0.43
2:D:120:LEU:HD23	2:D:125:ARG:HG2	2.00	0.43
2:B:260:LEU:O	2:B:264:LEU:HG	2.19	0.43
2:B:32:LYS:HA	2:B:32:LYS:HD3	1.65	0.43
1:A:22:LYS:CD	1:A:23:GLN:H	2.31	0.42
4:A:601:ET9:N1	3:E:0:DC:N3	2.67	0.42
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.54	0.42
2:B:6:GLU:OE2	2:B:6:GLU:HA	2.19	0.42
2:B:105:SER:OG	2:B:235:HIS:CD2	2.72	0.42
2:D:170:PRO:HA	2:D:173:LYS:HG2	2.01	0.42
2:B:125:ARG:NH1	2:B:147:ASN:OD1	2.51	0.42
1:C:35:VAL:HG22	1:C:132:ILE:CG2	2.50	0.42
2:B:70:LYS:HG2	2:B:71:TRP:N	2.34	0.42
1:A:185:ASP:OD2	4:A:601:ET9:C5'	2.68	0.42
2:D:66:LYS:HE2	2:D:66:LYS:HB2	1.63	0.42
1:A:26:LEU:HD11	1:A:61:PHE:HA	2.00	0.42
2:B:193:LEU:HG	2:B:197:GLN:OE1	2.20	0.42
2:B:296:THR:CG2	2:B:298:GLU:HB2	2.49	0.42
1:C:160:LEU:C	1:C:160:LEU:CD2	2.86	0.42
1:A:473:THR:O	1:A:477:THR:HG23	2.20	0.42
1:A:516:GLU:CD	1:A:516:GLU:H	2.23	0.42
1:A:17:ASP:O	1:A:83:ARG:HD3	2.20	0.42
2:B:424:LYS:CE	2:B:424:LYS:HA	2.48	0.42
2:D:356:ARG:CZ	2:D:361:HIS:CG	3.03	0.42
1:A:409:THR:OG1	5:A:602:GOL:H2	2.20	0.42
1:A:450:THR:CG2	1:A:452:LEU:HB2	2.49	0.42
2:B:156:SER:N	2:B:157:PRO:HD2	2.34	0.42
1:C:50:ILE:CG2	1:C:145:GLN:HB3	2.49	0.42
2:B:97:PRO:HD3	2:B:181:TYR:CD1	2.55	0.41
1:A:28:GLU:CG	1:A:29:GLU:N	2.81	0.41
1:C:23:GLN:NE2	1:C:60:VAL:H	2.17	0.41
1:C:492:GLU:OE2	1:C:530:LYS:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:317:VAL:HG12	2:D:349:LEU:HD23	2.02	0.41
2:D:166:LYS:HD3	2:D:166:LYS:N	2.36	0.41
1:C:405:TYR:CE2	1:C:407:GLN:HB2	2.55	0.41
2:D:361:HIS:O	2:D:361:HIS:HD2	2.03	0.41
2:B:125:ARG:HD3	2:B:146:TYR:O	2.21	0.41
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.55	0.41
2:B:276:VAL:O	2:B:280:SER:HB3	2.21	0.41
2:B:365:VAL:HG11	2:B:401:TRP:HB2	2.03	0.41
1:C:417:VAL:HG22	1:C:419:THR:HG23	2.02	0.41
1:C:533:LEU:HD12	1:C:533:LEU:HA	1.84	0.41
2:B:167:ILE:O	2:B:208:HIS:NE2	2.54	0.41
3:E:2:OMC:HM23	3:E:2:OMC:H1'	1.78	0.41
2:B:358:LYS:HE3	2:B:361:HIS:HA	2.03	0.40
2:D:356:ARG:CD	2:D:361:HIS:CB	2.99	0.40
1:A:42:GLU:OE2	1:A:49:LYS:HG3	2.22	0.40
1:A:135:ILE:CG2	1:A:136:ASN:H	2.33	0.40
2:B:296:THR:HG21	2:B:298:GLU:HB2	2.04	0.40
1:C:73:LYS:HZ3	1:C:73:LYS:HG2	1.54	0.40
2:D:173:LYS:HB2	2:D:173:LYS:HE3	1.77	0.40
1:A:524:GLN:O	1:A:528:LYS:HG2	2.21	0.40
2:B:27:THR:OG1	2:B:30:LYS:HG3	2.22	0.40
1:C:41:MET:HE2	1:C:47:ILE:HD13	2.02	0.40
1:C:308:GLU:O	1:C:311:LYS:HG2	2.22	0.40
2:D:108:VAL:HG21	2:D:232:TYR:CZ	2.57	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	551/557 (99%)	526 (96%)	23 (4%)	2 (0%)	34 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	551/557 (99%)	524 (95%)	24 (4%)	3 (0%)	29 52
2	B	402/444 (90%)	378 (94%)	24 (6%)	0	100 100
2	D	402/444 (90%)	385 (96%)	17 (4%)	0	100 100
All	All	1906/2002 (95%)	1813 (95%)	88 (5%)	5 (0%)	41 64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	SER
1	C	137	ASN
1	A	135	ILE
1	C	135	ILE
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	492/494 (100%)	474 (96%)	18 (4%)	34 60
1	C	492/494 (100%)	487 (99%)	5 (1%)	76 90
2	B	365/400 (91%)	355 (97%)	10 (3%)	44 71
2	D	365/400 (91%)	359 (98%)	6 (2%)	62 82
All	All	1714/1788 (96%)	1675 (98%)	39 (2%)	50 75

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	38	CYS
1	A	43	LYS
1	A	101	LYS
1	A	110	ASP
1	A	160	LEU

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Mol	Chain	Res	Type
1	A	211	ARG
1	A	226	PRO
1	A	251	SER
1	A	259	LYS
1	A	277	ARG
1	A	347	LYS
1	A	357	MET
1	A	388	LYS
1	A	448	ARG
1	A	503	LEU
1	A	515	SER
1	A	547	GLN
2	B	16	MET
2	B	161	GLN
2	B	206	ARG
2	B	248	GLU
2	B	282	LEU
2	B	283	LEU
2	B	284	ARG
2	B	418	ASN
2	B	424	LYS
2	B	427	TYR
1	C	32	LYS
1	C	160	LEU
1	C	177	ASP
1	C	277	ARG
1	C	452	LEU
2	D	42	GLU
2	D	184	MET
2	D	232	TYR
2	D	284	ARG
2	D	356	ARG
2	D	385	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	207	GLN
1	A	221	HIS
1	A	407	GLN
1	A	428	GLN

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Mol	Chain	Res	Type
1	A	483	HIS
1	A	507	GLN
1	A	547	GLN
2	B	174	GLN
2	B	182	GLN
2	B	258	GLN
2	B	269	GLN
2	B	418	ASN
1	C	221	HIS
1	C	278	GLN
1	C	334	GLN
1	C	407	GLN
1	C	507	GLN
1	C	509	GLN
2	D	137	ASN
2	D	151	GLN
2	D	174	GLN
2	D	182	GLN
2	D	197	GLN
2	D	255	ASN
2	D	361	HIS
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	4.02	13 (68%)	26,31,34	1.19	3 (11%)

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	3.88	12 (63%)	26,31,34	1.34	3 (11%)
3	OMC	F	2	3	19,22,23	2.83	8 (42%)	26,31,34	0.96	2 (7%)
3	OMC	F	4	3	19,22,23	2.98	8 (42%)	26,31,34	0.90	1 (3%)

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	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

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	OMC	C2'-C1'	-9.34	1.29	1.53
3	E	2	OMC	C2'-C1'	-8.53	1.31	1.53
3	E	2	OMC	C3'-C4'	-7.37	1.34	1.53
3	E	4	OMC	O4'-C1'	6.72	1.57	1.42
3	E	4	OMC	C3'-C4'	-6.34	1.36	1.53
3	F	4	OMC	C2-N3	6.25	1.49	1.36
3	F	2	OMC	C6-C5	5.81	1.48	1.35
3	F	4	OMC	C6-C5	5.56	1.48	1.35
3	E	2	OMC	O4'-C1'	5.54	1.55	1.42
3	F	4	OMC	C4-N3	5.53	1.45	1.34
3	F	2	OMC	C2-N3	5.45	1.47	1.36
3	E	2	OMC	O2-C2	-5.21	1.14	1.23
3	E	4	OMC	O2-C2	-5.10	1.14	1.23
3	F	4	OMC	C4-N4	5.07	1.45	1.33
3	F	2	OMC	C4-N4	4.95	1.45	1.33
3	F	2	OMC	C4-N3	4.53	1.43	1.34
3	E	4	OMC	C6-C5	4.49	1.45	1.35
3	E	2	OMC	C6-C5	4.46	1.45	1.35
3	F	2	OMC	C2-N1	4.20	1.49	1.40
3	E	4	OMC	C2-N3	4.12	1.44	1.36
3	F	4	OMC	C2-N1	3.96	1.48	1.40
3	E	4	OMC	C3'-C2'	3.60	1.61	1.52
3	E	2	OMC	C2-N3	3.59	1.43	1.36
3	E	2	OMC	O5'-C5'	-3.53	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	OMC	O5'-C5'	-3.53	1.36	1.44
3	E	2	OMC	C4-N4	3.47	1.42	1.33
3	E	4	OMC	C4-N4	3.21	1.41	1.33
3	E	2	OMC	C3'-C2'	3.18	1.60	1.52
3	E	4	OMC	C2-N1	3.09	1.46	1.40
3	F	2	OMC	O2-C2	-3.08	1.18	1.23
3	F	4	OMC	C6-N1	3.03	1.45	1.38
3	F	2	OMC	C6-N1	3.01	1.45	1.38
3	E	2	OMC	C4-N3	2.93	1.40	1.34
3	F	4	OMC	O2-C2	-2.84	1.18	1.23
3	E	4	OMC	O4'-C4'	2.77	1.51	1.45
3	E	2	OMC	C2-N1	2.65	1.45	1.40
3	E	4	OMC	C4-N3	2.38	1.39	1.34
3	F	2	OMC	C5-C4	2.35	1.48	1.42
3	F	4	OMC	C5-C4	2.28	1.48	1.42
3	E	4	OMC	C1'-N1	-2.15	1.41	1.47
3	E	2	OMC	C6-N1	2.15	1.43	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2	OMC	O2-C2-N3	-3.38	116.84	122.33
3	E	2	OMC	C2'-C1'-N1	-2.48	109.42	114.22
3	E	4	OMC	O2-C2-N3	-2.44	118.36	122.33
3	E	4	OMC	O3'-C3'-C2'	-2.38	104.40	111.17
3	F	2	OMC	C6-C5-C4	2.20	121.05	117.50
3	F	4	OMC	N4-C4-N3	2.19	121.82	117.97
3	E	2	OMC	O2-C2-N1	2.16	123.35	118.89
3	F	2	OMC	C5-C6-N1	-2.07	118.35	121.81
3	E	4	OMC	C1'-N1-C2	2.03	122.96	118.42

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	ET9	A	601	6	25,34,34	1.93	9 (36%)	28,54,54	1.96	8 (28%)
5	GOL	B	501	-	5,5,5	1.23	0	5,5,5	0.75	0
5	GOL	A	602	-	5,5,5	1.17	0	5,5,5	1.12	0
4	ET9	C	601	6	25,34,34	1.70	4 (16%)	28,54,54	1.96	8 (28%)
5	GOL	C	602	-	5,5,5	1.14	0	5,5,5	0.73	0
5	GOL	D	501	-	5,5,5	0.85	0	5,5,5	0.95	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	ET9	A	601	6	-	7/18/38/38	0/3/3/3
5	GOL	B	501	-	-	2/4/4/4	-
5	GOL	A	602	-	-	2/4/4/4	-
4	ET9	C	601	6	-	7/18/38/38	0/3/3/3
5	GOL	C	602	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	D	501	-	-	2/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	ET9	C6-N1	-4.58	1.29	1.39
4	C	601	ET9	C6-N1	-4.11	1.30	1.39
4	A	601	ET9	C4'-C6'	-3.06	1.47	1.51
4	A	601	ET9	C2'-C1'	-3.00	1.50	1.54
4	C	601	ET9	C4'-C6'	-2.94	1.47	1.51
4	C	601	ET9	C2'-C1'	-2.73	1.51	1.54
4	A	601	ET9	C2-N3	-2.51	1.31	1.37
4	A	601	ET9	C1'-C6'	-2.39	1.46	1.51
4	A	601	ET9	PG-O2G	-2.39	1.45	1.54
4	C	601	ET9	C4'-C3'	-2.20	1.49	1.53
4	A	601	ET9	C4'-C3'	-2.12	1.49	1.53
4	A	601	ET9	C44-C6'	-2.09	1.28	1.32
4	A	601	ET9	C1'-N9	-2.04	1.46	1.49

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	601	ET9	C2'-C1'-N9	-5.21	105.92	114.73
4	C	601	ET9	C2'-C1'-N9	-4.70	106.77	114.73
4	C	601	ET9	PB-O3B-PG	-4.21	118.39	132.83
4	A	601	ET9	C4'-C6'-C1'	3.80	116.28	105.76
4	C	601	ET9	C4'-C6'-C44	-3.66	121.37	127.72
4	A	601	ET9	C4'-C6'-C44	-3.47	121.71	127.72
4	C	601	ET9	C4'-C6'-C1'	3.36	115.05	105.76
4	A	601	ET9	PB-O3B-PG	-3.28	121.56	132.83
4	C	601	ET9	PB-O3A-PA	-2.94	122.73	132.83
4	A	601	ET9	C8-N7-C5	2.89	108.49	102.99
4	A	601	ET9	C1'-C6'-C44	-2.44	121.95	125.68
4	A	601	ET9	PB-O3A-PA	-2.34	124.80	132.83
4	C	601	ET9	C8-N7-C5	2.26	107.29	102.99
4	C	601	ET9	N2-C2-N1	-2.19	115.48	119.73
4	A	601	ET9	C4-C5-C6	-2.04	116.63	121.16
4	C	601	ET9	O2G-PG-O3B	2.01	111.37	104.64

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	ET9	PB-O3B-PG-O1G
4	C	601	ET9	C3'-C4'-C5'-O5'
4	C	601	ET9	C6'-C4'-C5'-O5'
4	C	601	ET9	C5'-O5'-PA-O1A
4	C	601	ET9	C5'-O5'-PA-O2A
5	D	501	GOL	O1-C1-C2-C3
5	A	602	GOL	O1-C1-C2-C3
5	B	501	GOL	C1-C2-C3-O3
5	C	602	GOL	O1-C1-C2-C3
5	C	602	GOL	O1-C1-C2-O2
5	D	501	GOL	O1-C1-C2-O2
4	C	601	ET9	PB-O3B-PG-O3G
4	C	601	ET9	PB-O3B-PG-O2G
4	C	601	ET9	C5'-O5'-PA-O3A
4	A	601	ET9	PA-O3A-PB-O1B
5	B	501	GOL	O2-C2-C3-O3
4	A	601	ET9	PB-O3A-PA-O2A
4	A	601	ET9	PB-O3B-PG-O2G
4	A	601	ET9	C5'-O5'-PA-O3A
4	A	601	ET9	C5'-O5'-PA-O2A
4	A	601	ET9	PB-O3B-PG-O3G
5	A	602	GOL	O1-C1-C2-O2

There are no ring outliers.

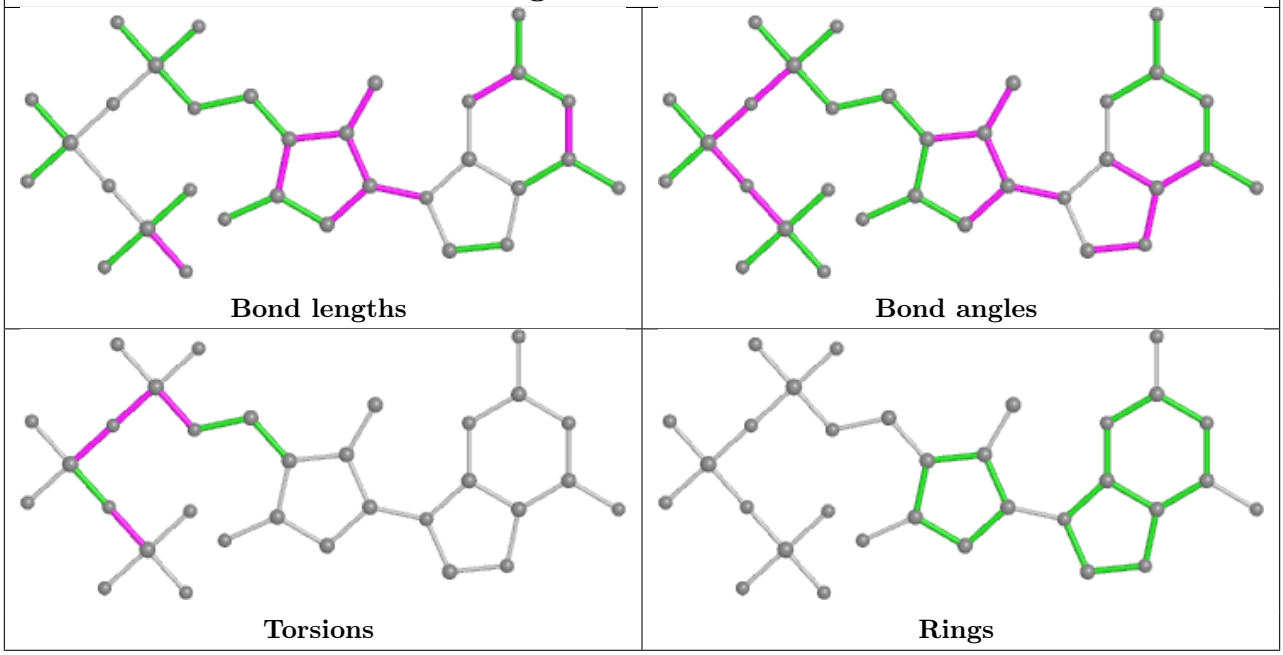
5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	ET9	5	0
5	A	602	GOL	3	0
4	C	601	ET9	1	0
5	C	602	GOL	2	0
5	D	501	GOL	1	0

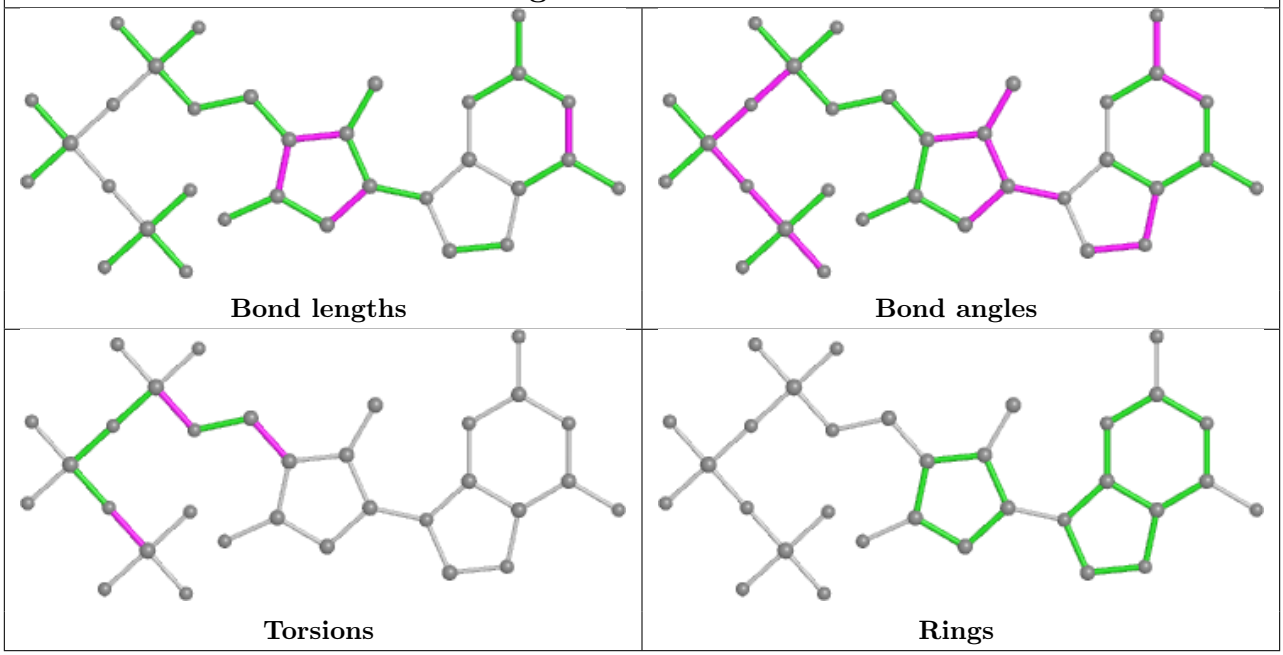
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand ET9 A 601



Ligand ET9 C 601



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, 95^{th} 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%)	0.44	41 (7%) 14 10	30, 57, 112, 189	0
1	C	553/557 (99%)	0.64	68 (12%) 4 2	30, 63, 125, 172	0
2	B	406/444 (91%)	0.71	48 (11%) 4 3	33, 71, 135, 178	0
2	D	406/444 (91%)	0.27	19 (4%) 31 25	31, 56, 100, 166	0
3	E	33/38 (86%)	-0.13	0 100 100	35, 55, 89, 129	0
3	F	36/38 (94%)	-0.02	1 (2%) 53 46	38, 65, 124, 155	0
All	All	1987/2078 (95%)	0.50	177 (8%) 9 6	30, 61, 124, 189	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	PRO	13.0
2	B	88	TRP	9.4
1	A	33	ALA	8.8
1	C	132	ILE	8.7
1	A	132	ILE	8.6
1	A	36	GLU	8.2
2	D	231	GLY	8.0
1	C	34	LEU	7.9
2	B	231	GLY	7.4
2	B	301	LEU	7.3
1	A	69	THR	7.3
1	A	28	GLU	7.2
1	C	68	SER	7.1
1	A	27	THR	7.0
1	C	69	THR	6.8
2	B	212	TRP	6.5
1	A	68	SER	6.4
1	C	50	ILE	6.4
1	C	141	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
1	C	140	PRO	6.3
1	A	136	ASN	6.3
2	B	91	GLN	6.2
1	C	63	ILE	6.1
1	C	142	ILE	6.1
1	A	62	ALA	6.1
2	B	360	ALA	5.9
1	C	26	LEU	5.8
1	C	35	VAL	5.6
1	A	67	ASP	5.6
2	B	94	ILE	5.5
2	B	93	GLY	5.5
1	A	24	TRP	5.5
1	A	138	GLU	5.5
2	B	89	GLU	5.5
2	B	295	LEU	5.5
1	C	553	SER	5.3
1	A	61	PHE	5.2
1	C	137	ASN	5.1
1	C	62	ALA	5.1
2	B	359	GLY	5.1
2	D	232	TYR	5.0
1	C	135	ILE	5.0
2	B	92	LEU	4.9
1	A	141	GLY	4.9
2	B	362	THR	4.8
2	B	361	HIS	4.8
1	C	133	PRO	4.7
2	B	213	GLY	4.6
2	D	360	ALA	4.6
2	D	359	GLY	4.6
1	C	134	SER	4.6
1	C	138	GLU	4.5
1	C	131	THR	4.5
1	C	136	ASN	4.4
2	B	232	TYR	4.3
2	D	212	TRP	4.3
2	D	5	ILE	4.3
1	A	32	LYS	4.3
2	B	357	MET	4.3
1	C	61	PHE	4.3
1	C	32	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	143	ARG	4.1
1	A	34	LEU	4.1
1	C	70	LYS	4.1
1	C	144	TYR	4.0
2	B	90	VAL	4.0
1	A	63	ILE	4.0
2	B	425	LEU	3.9
2	D	67	ASP	3.9
2	B	279	LEU	3.8
1	C	71	TRP	3.8
1	A	26	LEU	3.8
1	A	64	LYS	3.8
1	C	67	ASP	3.8
1	C	448	ARG	3.7
2	B	5	ILE	3.7
2	B	356	ARG	3.7
2	B	211	ARG	3.6
1	A	66	LYS	3.6
1	C	54	ASN	3.6
2	B	67	ASP	3.6
1	A	135	ILE	3.6
2	B	87	PHE	3.6
2	D	361	HIS	3.6
1	C	33	ALA	3.6
1	C	52	PRO	3.6
1	A	134	SER	3.5
1	C	31	ILE	3.5
1	A	31	ILE	3.5
1	C	2	ILE	3.5
2	B	6	GLU	3.5
2	B	299	ALA	3.4
2	D	427	TYR	3.4
1	C	551	LEU	3.4
1	A	30	LYS	3.4
2	D	283	LEU	3.4
1	C	55	PRO	3.3
1	A	53	GLU	3.2
1	C	452	LEU	3.2
1	C	449	GLU	3.2
1	A	137	ASN	3.2
1	C	36	GLU	3.2
2	D	425	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	37	ILE	3.2
1	C	457	TYR	3.1
2	B	209	LEU	3.1
2	B	68	SER	3.1
2	B	168	LEU	3.1
1	A	70	LYS	3.1
2	B	251	SER	3.1
1	C	469	LEU	3.0
1	A	139	THR	3.0
2	D	166	LYS	3.0
1	C	24	TRP	3.0
1	C	30	LYS	2.9
2	B	277	ARG	2.9
1	C	60	VAL	2.9
1	C	130	PHE	2.9
1	A	1	PRO	2.9
2	B	95	PRO	2.9
1	C	28	GLU	2.8
1	C	49	LYS	2.8
2	B	161	GLN	2.8
1	A	142	ILE	2.8
2	B	264	LEU	2.8
1	A	25	PRO	2.7
1	C	104	LYS	2.7
2	B	248	GLU	2.7
1	C	37	ILE	2.7
1	C	64	LYS	2.6
1	C	550	LYS	2.6
1	C	547	GLN	2.6
1	A	140	PRO	2.6
2	B	9	PRO	2.6
1	A	131	THR	2.6
1	C	65	LYS	2.5
1	C	23	GLN	2.5
1	C	51	GLY	2.5
1	C	139	THR	2.5
2	D	66	LYS	2.5
1	A	39	THR	2.5
1	A	60	VAL	2.4
2	B	245	VAL	2.4
1	A	447	ASN	2.4
2	D	208	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	25	PRO	2.4
3	F	18	DT	2.4
2	B	85	GLN	2.4
2	B	304	ALA	2.4
2	B	297	GLU	2.3
1	C	72	ARG	2.3
2	B	293	VAL	2.3
1	C	43	LYS	2.3
2	B	249	LYS	2.3
2	D	68	SER	2.3
1	C	27	THR	2.3
1	C	59	PRO	2.3
2	B	294	PRO	2.3
1	C	552	VAL	2.3
2	B	280	SER	2.2
1	A	71	TRP	2.2
2	B	296	THR	2.2
1	C	73	LYS	2.2
2	B	10	VAL	2.1
1	A	541	GLY	2.1
2	D	285	GLY	2.1
1	C	1	PRO	2.1
1	A	21	VAL	2.1
2	D	420	PRO	2.1
1	C	128	THR	2.1
1	C	450	THR	2.1
2	D	211	ARG	2.1
1	C	75	VAL	2.1
2	B	252	TRP	2.1
1	C	21	VAL	2.0
1	C	145	GLN	2.0
2	D	69	THR	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, 95^{th} 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	31,40,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OMC	F	2	21/22	0.98	0.17	39,51,58,63	0
3	OMC	E	4	21/22	0.98	0.19	25,35,46,50	0
3	OMC	F	4	21/22	0.98	0.20	32,41,46,50	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

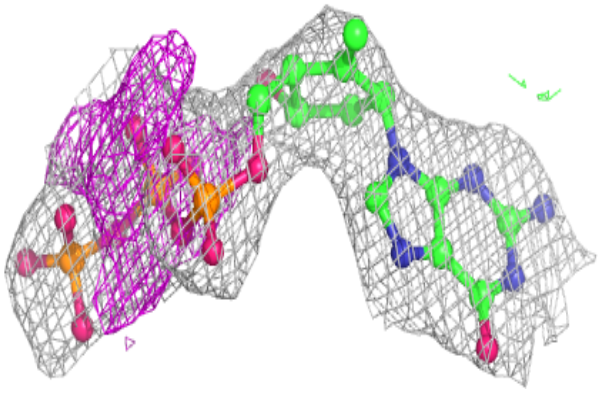
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

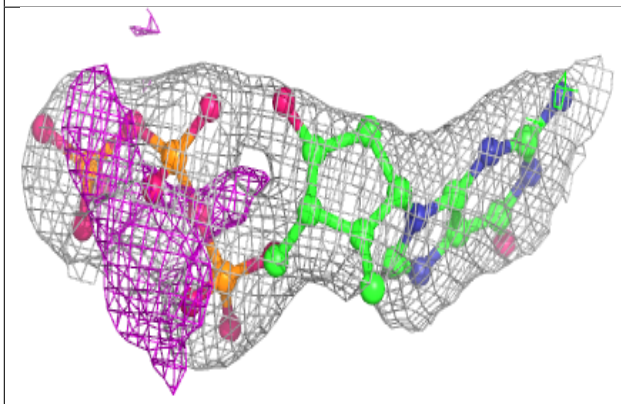
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	C	603	1/1	0.50	0.34	96,96,96,96	0
6	MG	A	603	1/1	0.65	0.20	109,109,109,109	0
5	GOL	A	602	6/6	0.84	0.24	51,61,62,63	0
4	ET9	C	601	32/32	0.87	0.20	69,91,124,126	0
4	ET9	A	601	32/32	0.88	0.20	68,89,130,138	0
5	GOL	D	501	6/6	0.94	0.25	49,54,55,65	0
5	GOL	B	501	6/6	0.95	0.26	46,52,56,65	0
5	GOL	C	602	6/6	0.96	0.20	45,47,51,52	0

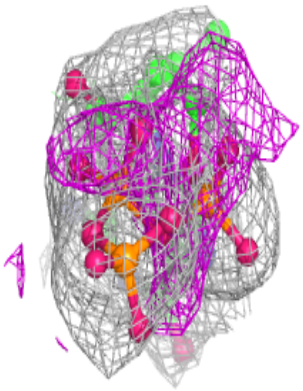
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

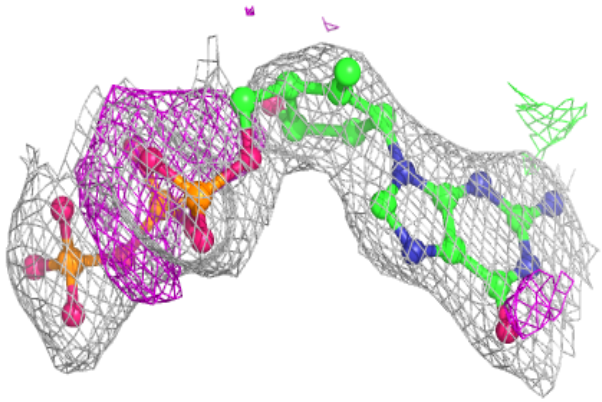


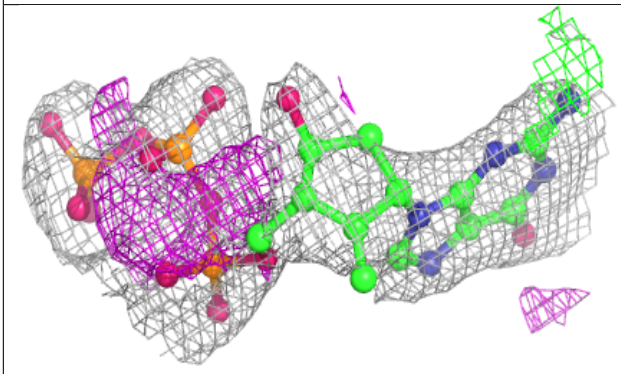


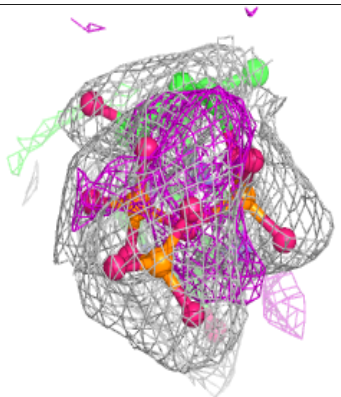


Electron density around ET9 A 601:

$2mF_o$-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.