



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:11 PM UTC

PDB ID : 7SR6 / pdb_00007sr6
Title : Human Endogenous Retrovirus (HERV-K) reverse transcriptase ternary complex with dsDNA template Primer and dNTP
Authors : Baldwin, E.T.; Nichols, C.
Deposited on : 2021-11-08
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

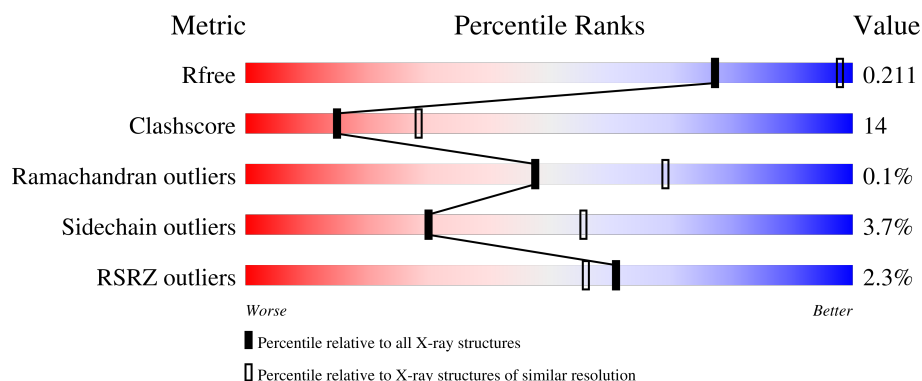
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (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	618	% 66% 24% 8%
1	B	618	3% 49% 20% 30%
1	F	618	% 64% 25% 8%
1	G	618	3% 50% 19% 30%
2	D	24	46% 46%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	24	
3	E	21	
3	I	21	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	DIO	G	601	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18265 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 Polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	566	Total	C	N	O	S	17	3	0
			4507	2912	760	820	15			
1	B	432	Total	C	N	O	S	11	2	0
			3423	2225	579	606	13			
1	F	566	Total	C	N	O	S	3	4	0
			4510	2913	762	819	16			
1	G	432	Total	C	N	O	S	13	4	0
			3428	2230	572	613	13			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP V9H0F6
A	-20	ALA	-	expression tag	UNP V9H0F6
A	-19	HIS	-	expression tag	UNP V9H0F6
A	-18	HIS	-	expression tag	UNP V9H0F6
A	-17	HIS	-	expression tag	UNP V9H0F6
A	-16	HIS	-	expression tag	UNP V9H0F6
A	-15	HIS	-	expression tag	UNP V9H0F6
A	-14	HIS	-	expression tag	UNP V9H0F6
A	-13	ASP	-	expression tag	UNP V9H0F6
A	-12	TYR	-	expression tag	UNP V9H0F6
A	-11	ASP	-	expression tag	UNP V9H0F6
A	-10	ILE	-	expression tag	UNP V9H0F6
A	-9	PRO	-	expression tag	UNP V9H0F6
A	-8	THR	-	expression tag	UNP V9H0F6
A	-7	THR	-	expression tag	UNP V9H0F6
A	-6	GLU	-	expression tag	UNP V9H0F6
A	-5	ASN	-	expression tag	UNP V9H0F6
A	-4	LEU	-	expression tag	UNP V9H0F6
A	-3	TYR	-	expression tag	UNP V9H0F6
A	-2	PHE	-	expression tag	UNP V9H0F6
A	-1	GLN	-	expression tag	UNP V9H0F6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP V9H0F6
B	-21	MET	-	initiating methionine	UNP V9H0F6
B	-20	ALA	-	expression tag	UNP V9H0F6
B	-19	HIS	-	expression tag	UNP V9H0F6
B	-18	HIS	-	expression tag	UNP V9H0F6
B	-17	HIS	-	expression tag	UNP V9H0F6
B	-16	HIS	-	expression tag	UNP V9H0F6
B	-15	HIS	-	expression tag	UNP V9H0F6
B	-14	HIS	-	expression tag	UNP V9H0F6
B	-13	ASP	-	expression tag	UNP V9H0F6
B	-12	TYR	-	expression tag	UNP V9H0F6
B	-11	ASP	-	expression tag	UNP V9H0F6
B	-10	ILE	-	expression tag	UNP V9H0F6
B	-9	PRO	-	expression tag	UNP V9H0F6
B	-8	THR	-	expression tag	UNP V9H0F6
B	-7	THR	-	expression tag	UNP V9H0F6
B	-6	GLU	-	expression tag	UNP V9H0F6
B	-5	ASN	-	expression tag	UNP V9H0F6
B	-4	LEU	-	expression tag	UNP V9H0F6
B	-3	TYR	-	expression tag	UNP V9H0F6
B	-2	PHE	-	expression tag	UNP V9H0F6
B	-1	GLN	-	expression tag	UNP V9H0F6
B	0	GLY	-	expression tag	UNP V9H0F6
F	-21	MET	-	initiating methionine	UNP V9H0F6
F	-20	ALA	-	expression tag	UNP V9H0F6
F	-19	HIS	-	expression tag	UNP V9H0F6
F	-18	HIS	-	expression tag	UNP V9H0F6
F	-17	HIS	-	expression tag	UNP V9H0F6
F	-16	HIS	-	expression tag	UNP V9H0F6
F	-15	HIS	-	expression tag	UNP V9H0F6
F	-14	HIS	-	expression tag	UNP V9H0F6
F	-13	ASP	-	expression tag	UNP V9H0F6
F	-12	TYR	-	expression tag	UNP V9H0F6
F	-11	ASP	-	expression tag	UNP V9H0F6
F	-10	ILE	-	expression tag	UNP V9H0F6
F	-9	PRO	-	expression tag	UNP V9H0F6
F	-8	THR	-	expression tag	UNP V9H0F6
F	-7	THR	-	expression tag	UNP V9H0F6
F	-6	GLU	-	expression tag	UNP V9H0F6
F	-5	ASN	-	expression tag	UNP V9H0F6
F	-4	LEU	-	expression tag	UNP V9H0F6
F	-3	TYR	-	expression tag	UNP V9H0F6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	PHE	-	expression tag	UNP V9H0F6
F	-1	GLN	-	expression tag	UNP V9H0F6
F	0	GLY	-	expression tag	UNP V9H0F6
G	-21	MET	-	initiating methionine	UNP V9H0F6
G	-20	ALA	-	expression tag	UNP V9H0F6
G	-19	HIS	-	expression tag	UNP V9H0F6
G	-18	HIS	-	expression tag	UNP V9H0F6
G	-17	HIS	-	expression tag	UNP V9H0F6
G	-16	HIS	-	expression tag	UNP V9H0F6
G	-15	HIS	-	expression tag	UNP V9H0F6
G	-14	HIS	-	expression tag	UNP V9H0F6
G	-13	ASP	-	expression tag	UNP V9H0F6
G	-12	TYR	-	expression tag	UNP V9H0F6
G	-11	ASP	-	expression tag	UNP V9H0F6
G	-10	ILE	-	expression tag	UNP V9H0F6
G	-9	PRO	-	expression tag	UNP V9H0F6
G	-8	THR	-	expression tag	UNP V9H0F6
G	-7	THR	-	expression tag	UNP V9H0F6
G	-6	GLU	-	expression tag	UNP V9H0F6
G	-5	ASN	-	expression tag	UNP V9H0F6
G	-4	LEU	-	expression tag	UNP V9H0F6
G	-3	TYR	-	expression tag	UNP V9H0F6
G	-2	PHE	-	expression tag	UNP V9H0F6
G	-1	GLN	-	expression tag	UNP V9H0F6
G	0	GLY	-	expression tag	UNP V9H0F6

- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*GP*GP*AP*CP*CP*TP*GP*AP*AP*AP*GP*CP*GP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	23	Total	C	N	O	P	0	0	0
			485	227	106	129	23			
2	H	23	Total	C	N	O	P	0	0	0
			482	226	104	129	23			

- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*TP*TP*CP*CP*CP*TP*TP*TP*CP*GP*CP*TP*TP*TP*CP*AP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	20	Total	C	N	O	P	0	0	0
			400	194	58	128	20			

Continued on next page...

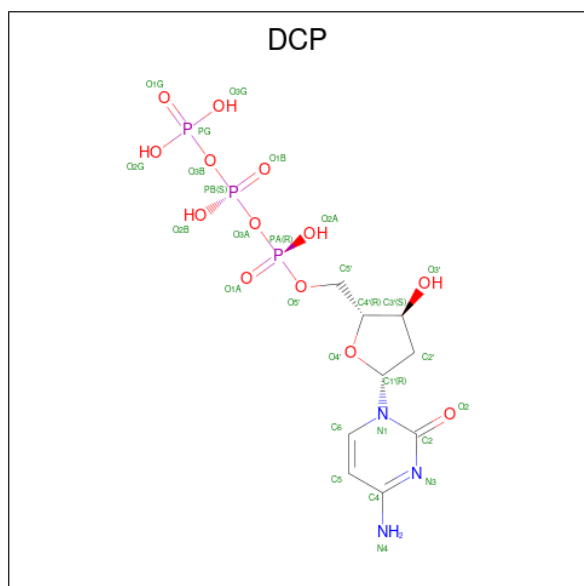
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	20	Total	C	N	O	P	0	0	0
			403	194	61	128	20			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

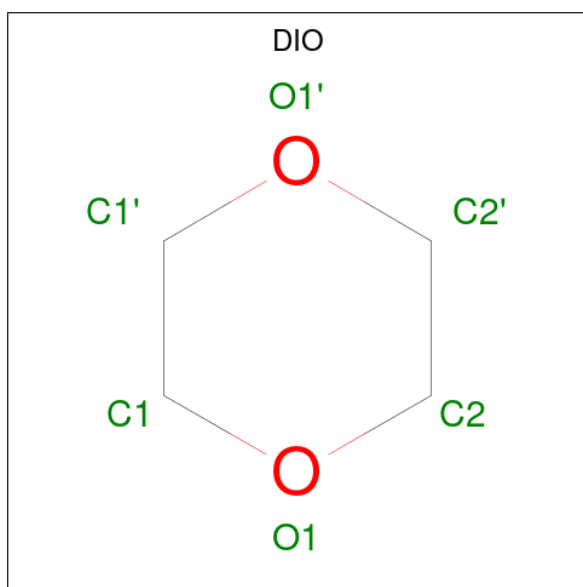
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	D	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (CCD ID: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

- Molecule 6 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: C₄H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	B	1	Total	C	O	0	0
			6	4	2		
6	B	1	Total	C	O	0	0
			6	4	2		
6	B	1	Total	C	O	0	0
			6	4	2		
6	B	1	Total	C	O	0	0
			6	4	2		
6	B	1	Total	C	O	0	0
			6	4	2		
6	B	1	Total	C	O	0	0
			6	4	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	4	2		
6	B	1	Total	C	O	0	0
			6	4	2		
6	F	1	Total	C	O	0	0
			6	4	2		
6	F	1	Total	C	O	0	0
			6	4	2		
6	F	1	Total	C	O	0	0
			6	4	2		
6	F	1	Total	C	O	0	0
			6	4	2		
6	F	1	Total	C	O	0	0
			6	4	2		
6	F	1	Total	C	O	0	0
			6	4	2		
6	F	1	Total	C	O	0	0
			6	4	2		
6	F	1	Total	C	O	0	0
			6	4	2		
6	F	1	Total	C	O	0	0
			6	4	2		
6	F	1	Total	C	O	0	0
			6	4	2		
6	G	1	Total	C	O	0	0
			6	4	2		
6	G	1	Total	C	O	0	0
			6	4	2		
6	G	1	Total	C	O	0	0
			6	4	2		
6	G	1	Total	C	O	0	0
			6	4	2		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

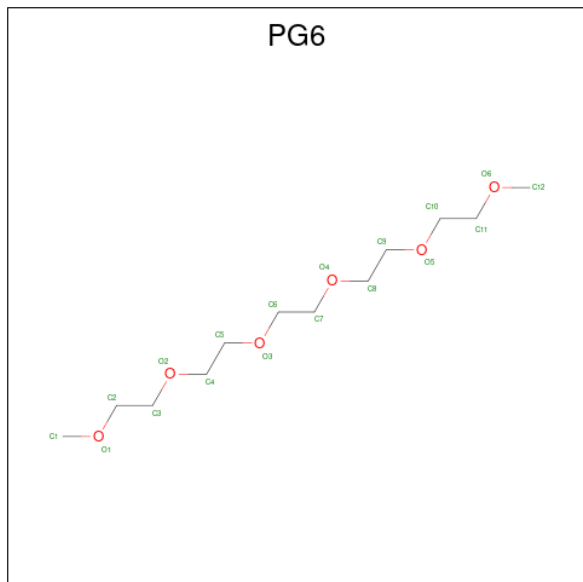


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		
7	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is POTASSIUM ION (CCD ID: K) (formula: K).

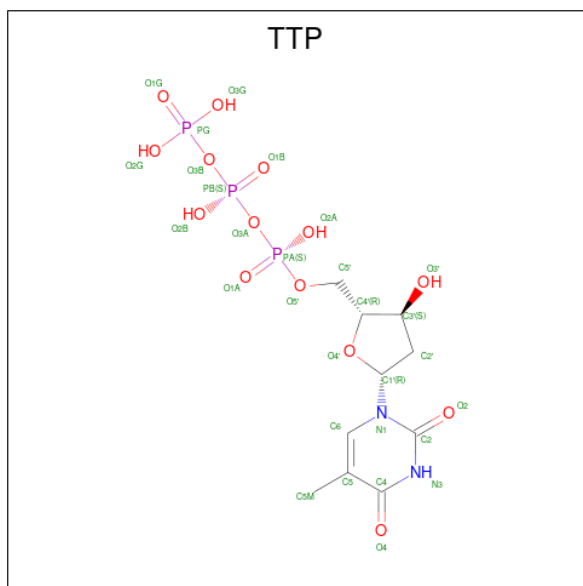
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total	K	0	0
			3	3		
8	B	2	Total	K	0	0
			2	2		
8	D	2	Total	K	0	0
			2	2		
8	F	2	Total	K	0	0
			2	2		
8	G	2	Total	K	0	0
			2	2		

- Molecule 9 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHANE (CCD ID: PG6) (formula: $C_{12}H_{26}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			18	12	6		
9	G	1	Total	C	O	0	0
			18	12	6		

- Molecule 10 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	F	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	F	1	Total	Cl	0	0
			1	1		
11	G	1	Total	Cl	0	0
			1	1		

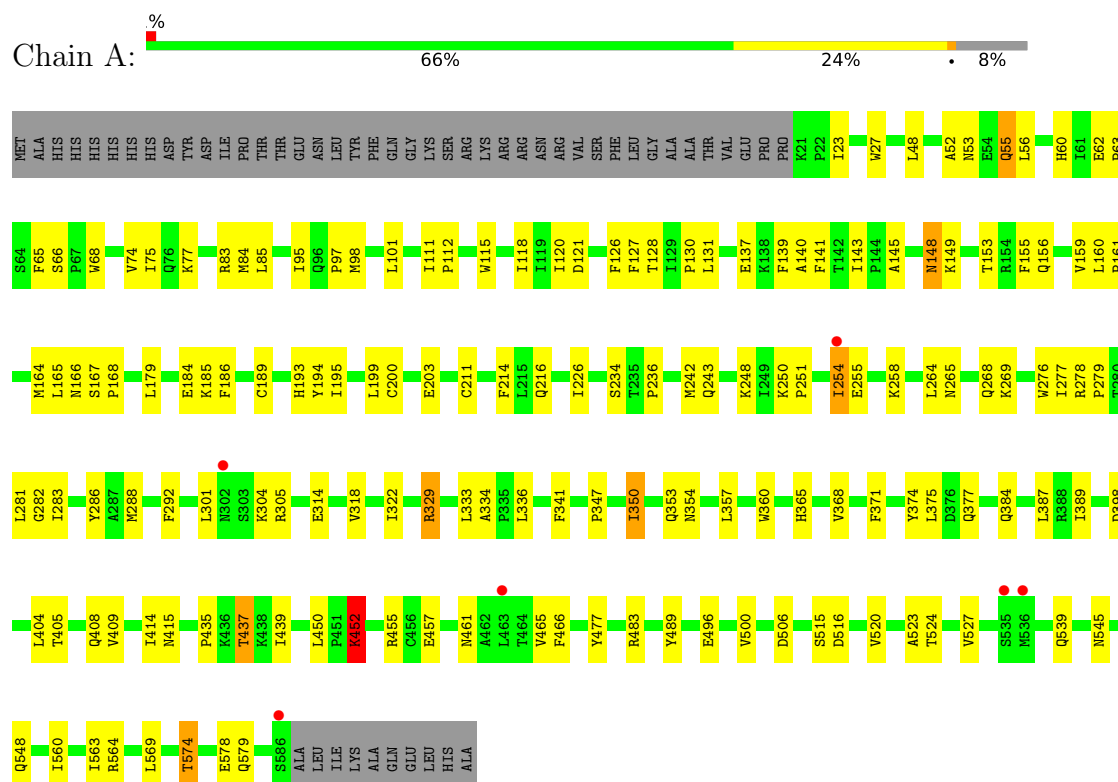
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	90	Total	O	0	0
			90	90		
12	B	54	Total	O	0	0
			54	54		
12	D	4	Total	O	0	0
			4	4		
12	E	1	Total	O	0	0
			1	1		
12	F	75	Total	O	0	0
			75	75		
12	G	58	Total	O	0	0
			58	58		
12	H	2	Total	O	0	0
			2	2		

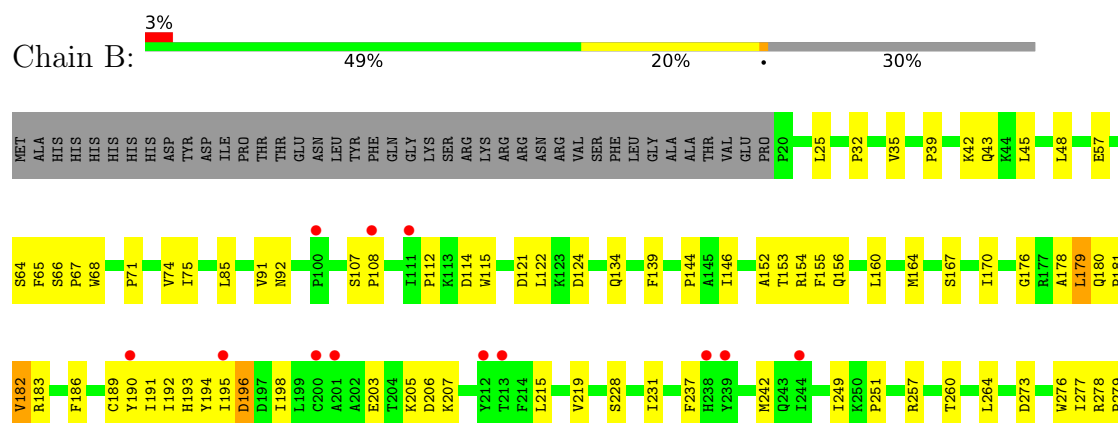
3 Residue-property plots

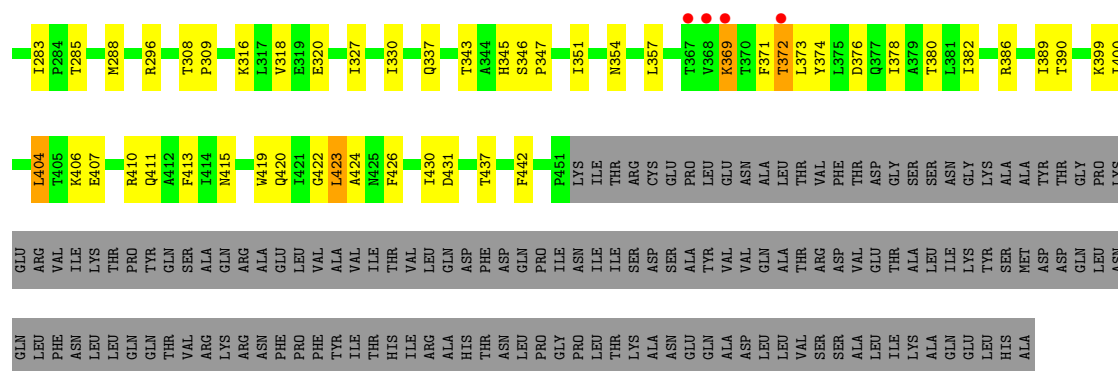
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

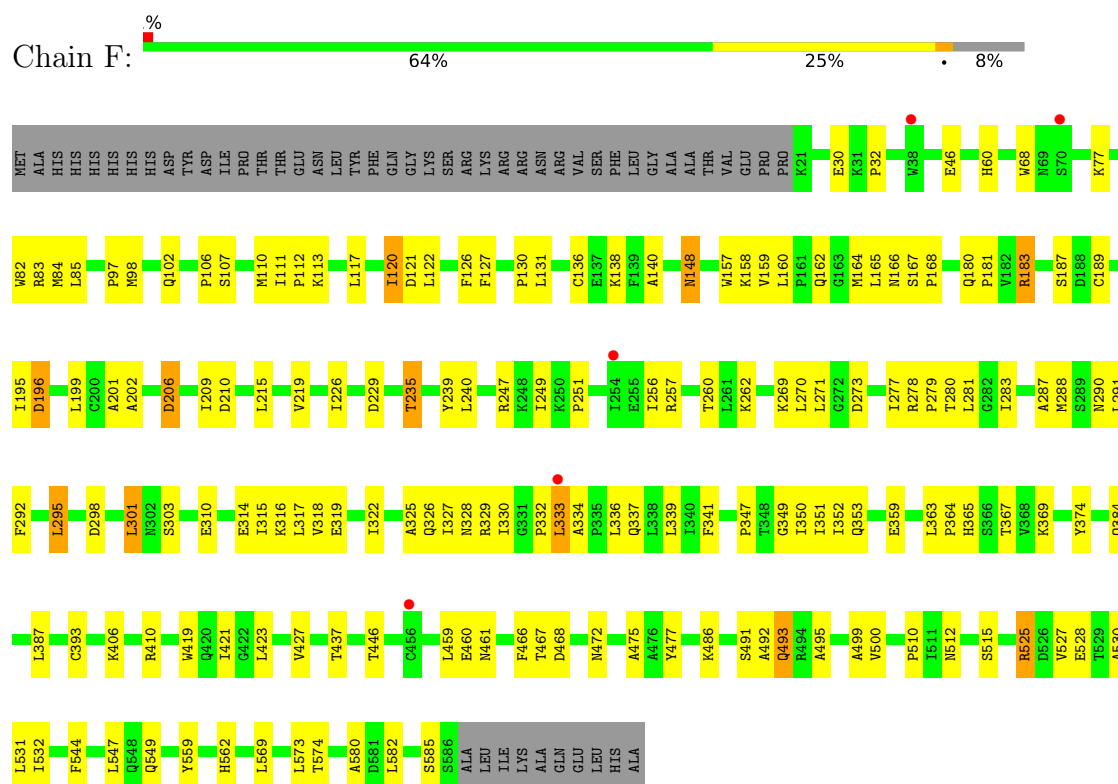


• Molecule 1: Polymerase

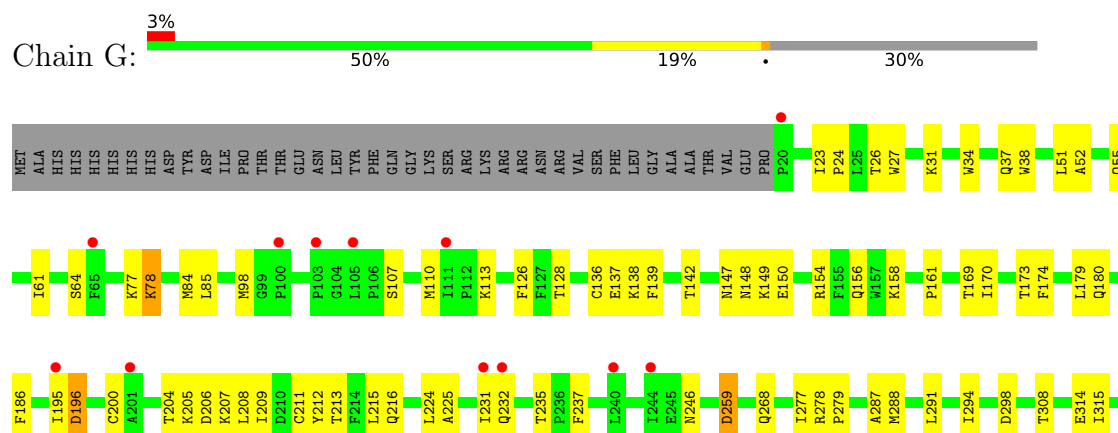


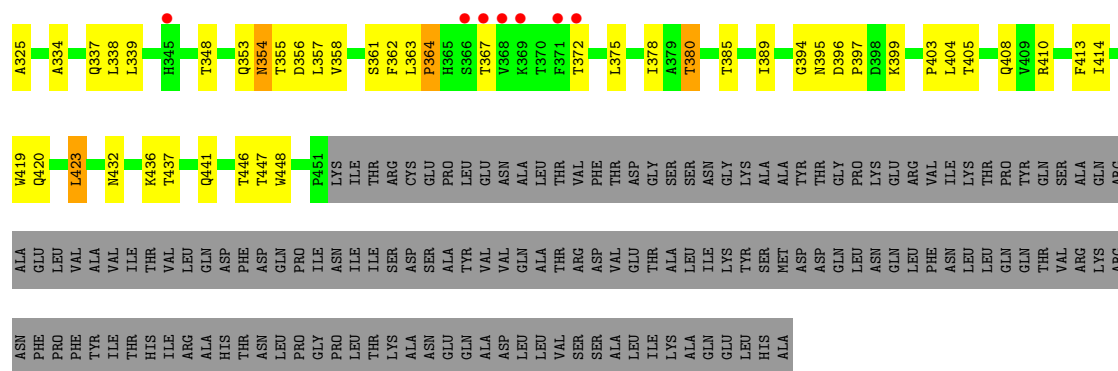


- Molecule 1: Polymerase



- Molecule 1: Polymerase





- Molecule 2: DNA (5'-D(P*GP*GP*GP*AP*CP*CP*TP*GP*AP*AP*AP*GP*CP*GP*AP*A P*AP*GP*GP*GP*AP*AP*A)-3')

Chain D: 46% 46%



- Molecule 2: DNA (5'-D(P*GP*GP*GP*AP*CP*CP*TP*GP*AP*AP*AP*GP*CP*GP*AP*A P*AP*GP*GP*GP*AP*AP*A)-3')

Chain H: 4% 29% 67%



- Molecule 3: DNA (5'-D(P*TP*TP*TP*CP*CP*CP*TP*TP*TP*CP*GP*CP*TP*TP*TP*C P*AP*GP*GP*T)-3')

Chain E: 38% 52% 5% 5%



- Molecule 3: DNA (5'-D(P*TP*TP*TP*CP*CP*CP*TP*TP*TP*CP*GP*CP*TP*TP*TP*C P*AP*GP*GP*T)-3')

Chain I: 33% 57% 5% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	177.70Å 177.70Å 117.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	88.85 – 2.62 88.85 – 2.62	Depositor EDS
% Data completeness (in resolution range)	91.8 (88.85-2.62) 92.6 (88.85-2.62)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.168 , 0.218 0.172 , 0.211	Depositor DCC
R_{free} test set	5690 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.207 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.499 for H, K, L 0.501 for -h,-k,l	Depositor
Outliers	0 of 115355 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18265	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TTP, K, DCP, MG, PG6, DIO, CL, EDO

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	1.03	3/4618 (0.1%)	1.40	6/6297 (0.1%)
1	B	1.04	0/3517	1.40	6/4795 (0.1%)
1	F	1.01	0/4621	1.40	6/6302 (0.1%)
1	G	1.06	1/3522 (0.0%)	1.43	7/4808 (0.1%)
2	D	0.67	0/549	1.12	2/847 (0.2%)
2	H	0.67	0/545	1.05	1/840 (0.1%)
3	E	0.70	0/443	1.25	4/680 (0.6%)
3	I	0.70	0/447	1.25	2/687 (0.3%)
All	All	1.00	4/18262 (0.0%)	1.38	34/25256 (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	A	0	1
1	B	0	2
1	F	0	2
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	31	LYS	CE-NZ	-8.81	1.23	1.49
1	A	333	LEU	CB-CG	-5.82	1.41	1.53
1	A	55	GLN	C-O	5.56	1.30	1.24
1	A	283	ILE	N-CA	5.18	1.50	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	ASP	CA-CB-CG	8.39	121.00	112.60
2	D	4	DG	P-O3'-C3'	-7.15	109.47	120.20
3	E	20	DA	P-O3'-C3'	-6.94	109.79	120.20
1	F	183	ARG	CA-C-N	6.27	131.03	120.88
1	F	183	ARG	C-N-CA	6.27	131.03	120.88
1	B	371	PHE	CB-CA-C	-6.15	100.95	111.41
3	E	10	DT	P-O3'-C3'	-6.12	111.01	120.20
3	I	15	DC	P-O3'-C3'	-6.01	111.18	120.20
1	A	574	THR	CA-CB-OG1	-5.85	100.83	109.60
1	F	210	ASP	CA-C-N	5.83	128.02	120.44
1	F	210	ASP	C-N-CA	5.83	128.02	120.44
1	B	190	TYR	CB-CA-C	5.82	120.11	110.74
3	E	21	DG	P-O3'-C3'	-5.76	111.56	120.20
1	B	380	THR	CA-CB-OG1	-5.63	101.15	109.60
2	H	6	DC	P-O3'-C3'	-5.56	111.86	120.20
1	G	55	GLN	N-CA-C	-5.52	105.67	112.90
1	G	354	ASN	CB-CA-C	-5.51	110.24	116.63
1	G	403	PRO	CA-C-O	-5.43	117.20	121.38
1	F	196	ASP	N-CA-C	-5.43	107.91	114.75
1	B	182	VAL	CA-C-O	-5.37	115.69	121.27
1	A	452	LYS	N-CA-C	-5.33	107.44	114.04
1	A	130	PRO	CA-C-N	5.32	130.22	121.39
1	A	130	PRO	C-N-CA	5.32	130.22	121.39
3	E	19	DC	P-O3'-C3'	-5.24	112.34	120.20
3	I	11	DT	C4'-C3'-O3'	-5.23	102.16	110.00
1	A	329	ARG	CA-C-O	-5.22	116.02	121.55
1	A	63	PRO	CA-C-O	-5.20	115.49	121.36
1	G	364	PRO	CA-C-O	-5.17	115.84	121.27
1	B	179	LEU	N-CA-C	-5.14	107.18	113.50
2	D	6	DC	C2'-C3'-O3'	5.14	119.21	111.50
1	F	525	ARG	N-CA-C	-5.12	106.98	113.18
1	G	446	THR	CA-CB-OG1	-5.07	101.99	109.60
1	G	436	LYS	CA-C-N	5.04	127.93	120.82
1	G	436	LYS	C-N-CA	5.04	127.93	120.82

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	354	ASN	Mainchain
1	B	194	TYR	Mainchain
1	B	423	LEU	Mainchain
1	F	235	THR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	F	530	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4507	0	4584	114	0
1	B	3423	0	3454	94	0
1	F	4510	0	4583	137	0
1	G	3428	0	3458	96	0
2	D	485	0	255	10	0
2	H	482	0	255	21	0
3	E	400	0	229	12	0
3	I	403	0	230	20	0
4	A	2	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
5	A	28	0	12	1	0
6	A	30	0	40	1	0
6	B	66	0	88	10	0
6	F	78	0	104	10	0
6	G	30	0	40	12	0
7	A	4	0	6	0	0
7	B	4	0	6	0	0
7	F	16	0	24	0	0
7	G	4	0	6	0	0
8	A	3	0	0	0	0
8	B	2	0	0	0	0
8	D	2	0	0	0	0
8	F	2	0	0	0	0
8	G	2	0	0	0	0
9	B	18	0	26	2	0
9	G	18	0	26	2	0
10	F	29	0	13	4	0
11	F	1	0	0	0	0
11	G	1	0	0	0	0
12	A	90	0	0	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	B	54	0	0	5	0
12	D	4	0	0	0	0
12	E	1	0	0	0	0
12	F	75	0	0	7	0
12	G	58	0	0	5	0
12	H	2	0	0	0	0
All	All	18265	0	17439	481	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 14.

All (481) 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:F:247:ARG:HB3	12:F:753:HOH:O	1.44	1.15
1:F:206:ASP:HB3	12:F:769:HOH:O	1.65	0.96
1:G:98:MET:H	1:G:169[A]:THR:HG21	1.39	0.88
2:H:23:DA:H2''	2:H:24:DA:OP2	1.77	0.84
1:B:372:THR:HG23	12:B:735:HOH:O	1.82	0.80
2:H:21:DG:H2''	2:H:22:DA:OP2	1.79	0.80
1:A:77:LYS:NZ	5:A:602:DCP:O3G	2.15	0.79
1:A:281:LEU:HD13	1:A:322:ILE:HA	1.65	0.79
1:B:66:SER:O	1:B:154:ARG:NH2	2.15	0.78
1:A:452:LYS:O	1:A:455:ARG:NH2	2.15	0.78
1:A:127:PHE:O	1:A:159:VAL:HG11	1.87	0.75
2:D:21:DG:H2''	2:D:22:DA:OP2	1.87	0.74
2:H:19:DG:H2''	2:H:20:DG:OP2	1.87	0.74
1:B:186:PHE:HB3	1:B:189:CYS:SG	2.26	0.74
1:A:414:ILE:HG22	1:A:415:ASN:OD1	1.89	0.73
1:A:161:PRO:HG2	1:A:164:MET:HB2	1.71	0.73
1:F:341:PHE:HE2	1:F:350:ILE:HD13	1.55	0.71
1:F:131:LEU:CD1	1:F:159:VAL:C	2.64	0.71
1:F:333:LEU:HD12	1:F:334:ALA:H	1.55	0.70
1:F:271:LEU:HD21	1:F:291:LEU:HB3	1.74	0.69
1:G:404:LEU:CD2	6:G:601:DIO:H11	2.22	0.69
1:F:256:ILE:CG2	1:F:270:LEU:CD1	2.71	0.68
1:B:180:GLN:O	1:B:183[B]:ARG:HG3	1.93	0.68
1:G:136:CYS:HG	1:G:158:LYS:HA	1.59	0.68
1:B:257:ARG:HH12	1:B:345[B]:HIS:CE1	2.11	0.68
1:F:319:GLU:HA	1:F:322:ILE:HD12	1.76	0.68
1:B:413:PHE:O	1:B:420:GLN:NE2	2.25	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:PHE:HB2	1:G:225:ALA:HB3	1.75	0.67
1:F:136:CYS:SG	1:F:158:LYS:HA	2.35	0.66
1:F:189:CYS:SG	1:F:202:ALA:HB2	2.35	0.66
1:A:111:ILE:O	1:A:329:ARG:HD2	1.96	0.66
1:F:98:MET:HB2	1:F:166:ASN:OD1	1.94	0.66
3:I:3:DG:H2''	3:I:4:DT:H5'	1.77	0.66
2:H:21:DG:H1'	2:H:22:DA:H5'	1.78	0.66
1:G:136:CYS:SG	1:G:158:LYS:HA	2.36	0.65
1:B:354:ASN:HB3	6:B:607:DIO:H12	1.78	0.65
1:F:281:LEU:HD13	1:F:322:ILE:HA	1.79	0.65
1:A:278:ARG:HB2	1:A:279:PRO:HD3	1.78	0.65
1:A:48:LEU:HD22	1:A:143:ILE:HG23	1.78	0.65
1:A:483:ARG:NH1	1:A:506:ASP:OD2	2.30	0.64
1:F:121:ASP:OD1	1:F:122:LEU:N	2.31	0.64
2:H:22:DA:C2	3:I:7:DC:C2	2.85	0.64
1:A:250:LYS:NZ	1:A:322:ILE:O	2.26	0.64
1:F:167:SER:N	1:F:168:PRO:CD	2.60	0.64
1:G:325:ALA:HB1	6:G:606:DIO:H1'2	1.79	0.64
1:F:419:TRP:CE2	1:F:423:LEU:CD1	2.81	0.63
1:B:257:ARG:NH1	1:B:345[B]:HIS:ND1	2.40	0.63
1:B:399:LYS:NZ	12:B:702:HOH:O	2.31	0.63
1:B:337:GLN:OE1	9:B:605:PG6:H71	1.98	0.62
1:F:83:ARG:NH1	1:F:162:GLN:OE1	2.29	0.62
1:B:273:ASP:O	1:B:277:ILE:HG22	1.99	0.62
1:G:355:THR:O	6:G:606:DIO:H2'2	1.99	0.62
1:A:127:PHE:HA	1:A:159:VAL:CG2	2.30	0.62
1:G:139:PHE:CD1	1:G:161:PRO:HG2	2.34	0.62
1:F:131:LEU:HD13	1:F:159:VAL:C	2.24	0.62
1:A:377:GLN:HG3	12:A:761:HOH:O	2.00	0.62
1:A:153:THR:HG23	1:A:155:PHE:HE1	1.64	0.62
1:A:277:ILE:C	1:A:277:ILE:HD12	2.25	0.62
2:D:3:DG:H4'	2:D:4:DG:OP1	1.98	0.62
2:H:3:DG:C8	2:H:3:DG:P	2.93	0.62
1:F:256:ILE:HG22	1:F:270:LEU:CD1	2.30	0.61
1:B:277:ILE:HG21	1:B:442:PHE:CD1	2.35	0.61
1:F:387:LEU:HD13	1:G:414:ILE:HG21	1.81	0.61
1:A:62:GLU:OE1	1:A:156:GLN:NE2	2.34	0.61
1:A:545:ASN:OD1	12:A:701:HOH:O	2.16	0.61
1:G:77:LYS:HG3	1:G:78:LYS:H	1.65	0.61
3:I:3:DG:H2'	3:I:4:DT:C6	2.36	0.61
1:F:317:LEU:HB3	6:F:613:DIO:C2'	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ALA:HA	1:A:84:MET:HE1	1.83	0.60
1:A:496:GLU:OE1	1:A:515:SER:OG	2.14	0.60
1:B:182:VAL:HG21	1:B:215:LEU:HB2	1.83	0.60
1:A:167:SER:N	1:A:168:PRO:CD	2.64	0.60
1:B:179:LEU:O	1:B:183[B]:ARG:HG2	2.01	0.60
1:B:337:GLN:NE2	9:B:605:PG6:H81	2.16	0.60
2:D:18:DA:H2''	2:D:19:DG:C8	2.37	0.60
1:F:68:TRP:O	1:F:140:ALA:HB3	2.02	0.59
1:A:126:PHE:CE2	1:A:167:SER:HB3	2.38	0.59
1:G:404:LEU:CD2	6:G:601:DIO:C1	2.81	0.59
1:B:112:PRO:HB2	1:B:115:TRP:CD1	2.38	0.59
1:G:64:SER:CB	1:G:156:GLN:HG3	2.32	0.59
1:F:32:PRO:HA	1:F:68:TRP:CH2	2.38	0.58
1:A:186:PHE:HB3	1:A:189:CYS:SG	2.43	0.58
1:B:277:ILE:HG21	1:B:442:PHE:CE1	2.38	0.58
1:B:75:ILE:CD1	1:B:85:LEU:HD12	2.33	0.58
1:A:165:LEU:HG	1:A:166:ASN:OD1	2.04	0.58
6:B:604:DIO:H1'1	12:F:716:HOH:O	2.03	0.58
1:G:64:SER:HB2	1:G:156:GLN:HG3	1.86	0.58
1:A:97:PRO:O	1:B:67:PRO:HG3	2.04	0.58
1:F:333:LEU:HD12	1:F:334:ALA:N	2.17	0.58
1:G:364:PRO:HG2	1:G:367:THR:OG1	2.04	0.58
1:F:367:THR:CG2	1:F:531:LEU:HD23	2.34	0.58
1:F:460:GLU:HA	12:G:709:HOH:O	2.03	0.58
1:A:145:ALA:HA	12:A:775:HOH:O	2.04	0.58
1:F:257:ARG:NH2	1:F:269:LYS:HD3	2.19	0.58
1:G:399:LYS:HE2	9:G:602:PG6:O5	2.03	0.58
1:A:574:THR:HG22	1:A:578:GLU:OE1	2.03	0.57
1:F:327:ILE:C	1:F:328:ASN:ND2	2.63	0.57
1:B:176:GLY:HA3	12:B:731:HOH:O	2.04	0.57
1:G:128:THR:HG22	1:G:128:THR:O	2.03	0.57
1:G:224:LEU:C	1:G:224:LEU:HD23	2.30	0.57
1:G:338:LEU:HD12	1:G:339:LEU:N	2.20	0.57
2:H:20:DG:H2''	2:H:21:DG:OP2	2.03	0.57
6:B:604:DIO:H11	12:B:742:HOH:O	2.04	0.57
1:G:357:LEU:HD23	1:G:358:VAL:N	2.19	0.57
1:A:115:TRP:CZ2	1:A:203[B]:GLU:HG3	2.39	0.57
1:F:180:GLN:HB3	1:F:181:PRO:HD3	1.87	0.57
1:G:404:LEU:HD22	6:G:601:DIO:H11	1.86	0.57
1:F:341:PHE:CE2	1:F:350:ILE:HD13	2.38	0.56
1:B:178:ALA:HB1	1:B:219:VAL:HG12	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:TYR:HE1	1:A:539:GLN:HG3	1.71	0.56
1:F:256:ILE:CG2	1:F:270:LEU:HD12	2.35	0.56
1:A:265:ASN:O	1:A:269:LYS:HG3	2.06	0.56
1:B:92:ASN:OD1	1:B:164:MET:HE1	2.06	0.56
1:B:183[B]:ARG:NH1	1:B:191:ILE:O	2.36	0.56
1:G:389:ILE:CD1	1:G:397:PRO:HG3	2.36	0.56
1:A:574:THR:CG2	1:A:578:GLU:OE1	2.54	0.55
1:F:106:PRO:HB3	1:G:147:ASN:O	2.06	0.55
2:H:3:DG:P	2:H:3:DG:O4'	2.65	0.55
1:F:111:ILE:O	1:F:329:ARG:HB3	2.07	0.55
1:F:251:PRO:HG2	1:F:277:ILE:HG22	1.89	0.55
1:A:350:ILE:HG21	1:A:357:LEU:HD23	1.89	0.55
1:B:195:ILE:O	1:B:195:ILE:HG22	2.07	0.55
1:F:60:HIS:HD2	6:F:616:DIO:H2'1	1.71	0.55
1:F:527:VAL:HG11	1:F:547:LEU:HD23	1.89	0.55
1:A:126:PHE:O	1:A:160:LEU:HB2	2.06	0.55
1:A:127:PHE:HA	1:A:159:VAL:HG21	1.89	0.54
1:F:288:MET:HB2	1:F:292:PHE:CE2	2.42	0.54
3:I:6:DT:C2	3:I:7:DC:C6	2.95	0.54
1:F:351:ILE:HD12	1:F:359:GLU:HB3	1.88	0.54
1:A:83:ARG:HA	12:A:726:HOH:O	2.06	0.54
1:A:405:THR:N	1:A:408:GLN:OE1	2.27	0.54
1:F:314:GLU:O	1:F:318:VAL:HG23	2.08	0.54
1:G:357:LEU:HD23	1:G:357:LEU:C	2.32	0.54
1:B:179:LEU:O	1:B:183[B]:ARG:CG	2.56	0.54
1:F:549[A]:GLN:HA	1:F:549[A]:GLN:NE2	2.23	0.54
1:F:113:LYS:HA	1:F:329:ARG:HD2	1.90	0.54
1:G:137:GLU:HA	1:G:156:GLN:NE2	2.22	0.54
3:I:6:DT:C2	3:I:7:DC:C5	2.96	0.54
1:G:389:ILE:HD12	1:G:397:PRO:HG3	1.90	0.54
1:B:42:LYS:HG3	1:B:146:ILE:HD11	1.89	0.54
1:A:148:ASN:ND2	1:A:148:ASN:H	2.05	0.54
1:A:350:ILE:CG2	1:A:357:LEU:HD23	2.38	0.54
3:E:4:DT:H2'	3:E:5:DT:C6	2.43	0.54
1:F:582:LEU:O	1:F:585:SER:OG	2.24	0.54
1:F:183:ARG:HB3	12:F:733:HOH:O	2.07	0.53
1:F:270:LEU:HA	1:F:273:ASP:OD2	2.09	0.53
1:A:264:LEU:O	1:A:268:GLN:HG3	2.07	0.53
1:F:459:LEU:HD13	1:F:510:PRO:HB3	1.90	0.53
1:G:212:TYR:O	1:G:215:LEU:HB3	2.08	0.53
2:H:23:DA:C2'	2:H:24:DA:OP2	2.54	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLN:HG3	12:A:778:HOH:O	2.07	0.53
1:G:399:LYS:HZ3	9:G:602:PG6:H122	1.72	0.53
1:B:354:ASN:OD1	6:B:607:DIO:H21	2.09	0.53
1:F:32:PRO:HA	1:F:68:TRP:CZ2	2.43	0.53
3:I:4:DT:H4'	3:I:5:DT:OP1	2.09	0.53
1:A:398:ASP:HB2	12:A:740:HOH:O	2.07	0.53
1:A:569:LEU:O	1:A:574:THR:HG21	2.09	0.52
1:B:278:ARG:HB3	1:B:279:PRO:HD3	1.91	0.52
3:E:4:DT:H6	3:E:4:DT:P	2.32	0.52
1:G:170:ILE:O	1:G:173:THR:HG22	2.10	0.52
1:G:410:ARG:O	1:G:414:ILE:HG13	2.10	0.52
1:F:112:PRO:HB3	1:F:332:PRO:HD3	1.91	0.52
1:G:195:ILE:O	1:G:195:ILE:HG22	2.08	0.52
2:D:15:DG:C2	3:E:14:DG:N2	2.78	0.52
1:F:467:THR:HG21	1:F:500:VAL:HG22	1.91	0.52
1:G:64:SER:OG	1:G:156:GLN:HG3	2.10	0.52
1:G:27:TRP:CZ2	1:G:138:LYS:HG3	2.44	0.52
1:B:277:ILE:O	1:B:277:ILE:HG13	2.10	0.52
1:B:386:ARG:NH1	1:B:422:GLY:O	2.42	0.52
1:F:102:GLN:HG2	12:G:719:HOH:O	2.10	0.52
1:F:341:PHE:CE2	1:F:350:ILE:CD1	2.93	0.52
1:G:37:GLN:HG3	1:G:38:TRP:N	2.24	0.52
1:A:195:ILE:HD13	3:E:23:DT:O2	2.10	0.52
1:F:196:ASP:OD2	10:F:605:TTP:C5'	2.57	0.52
1:G:334:ALA:O	1:G:353:GLN:NE2	2.40	0.51
1:A:350:ILE:N	1:A:350:ILE:HD12	2.24	0.51
1:A:141:PHE:CE1	1:A:155:PHE:HB2	2.45	0.51
1:G:180:GLN:NE2	1:G:180:GLN:HA	2.25	0.51
1:F:106:PRO:HG3	1:G:148:ASN:O	2.10	0.51
2:H:19:DG:C2'	2:H:20:DG:OP2	2.58	0.51
1:F:468:ASP:HB2	1:F:580:ALA:HB1	1.92	0.51
2:D:23:DA:C2	3:E:6:DT:O2	2.64	0.51
1:G:363:LEU:HD21	1:G:380:THR:HG22	1.91	0.51
1:A:288:MET:HE2	1:A:292:PHE:CE1	2.46	0.51
1:A:371:PHE:CE2	1:A:523:ALA:HA	2.46	0.51
1:B:91:VAL:HG11	1:B:139:PHE:CE1	2.46	0.51
1:G:23:ILE:HG23	1:G:24:PRO:HD2	1.93	0.51
1:G:213:THR:HA	1:G:216:GLN:HG2	1.91	0.51
1:B:115:TRP:CE2	1:B:203:GLU:HB3	2.45	0.51
1:F:466:PHE:O	1:F:477:TYR:HA	2.11	0.51
1:F:569:LEU:HB2	1:F:574:THR:HG21	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:ILE:O	1:G:196:ASP:CG	2.54	0.51
1:A:66:SER:HB2	1:A:137:GLU:HG2	1.94	0.50
1:B:228:SER:HA	1:B:231:ILE:HD12	1.93	0.50
1:F:97:PRO:HB3	12:F:759:HOH:O	2.11	0.50
1:A:276:TRP:CE2	3:E:21:DG:H4'	2.46	0.50
1:F:269:LYS:O	1:F:273:ASP:OD2	2.28	0.50
1:F:493:GLN:OE1	3:I:9:DC:H5'	2.11	0.50
1:B:48:LEU:HD13	1:B:74:VAL:HG13	1.93	0.50
1:G:419:TRP:CE2	1:G:423:LEU:HD13	2.46	0.50
3:I:10:DT:C6	3:I:11:DT:H72	2.46	0.50
1:A:55:GLN:OE1	1:A:60:HIS:ND1	2.37	0.50
1:F:110:MET:HE2	1:F:393:CYS:HA	1.94	0.50
1:B:153:THR:HG22	1:B:155:PHE:CE2	2.47	0.50
1:F:281:LEU:HD22	1:F:325:ALA:HB3	1.94	0.50
1:F:84:MET:HE3	1:F:157:TRP:CH2	2.47	0.50
1:F:127:PHE:HA	1:F:159:VAL:CG2	2.41	0.50
6:F:604:DIO:H22	6:G:601:DIO:H21	1.94	0.50
1:F:472:ASN:OD1	1:F:472:ASN:C	2.55	0.50
1:G:180:GLN:HA	1:G:180:GLN:HE21	1.75	0.50
1:G:113:LYS:CG	1:G:237:PHE:HB2	2.42	0.50
1:B:374:TYR:CD2	6:B:603:DIO:H1'2	2.47	0.49
1:A:334:ALA:HB3	1:A:353:GLN:NE2	2.28	0.49
1:B:424:ALA:HB3	6:B:606:DIO:H22	1.94	0.49
1:G:174:PHE:CD1	1:G:174:PHE:C	2.89	0.49
2:H:24:DA:C4	2:H:25:DC:C5	3.00	0.49
3:I:3:DG:C2	3:I:4:DT:C2	2.99	0.49
2:D:22:DA:H2	3:E:7:DC:O2	1.96	0.49
2:D:23:DA:H2	3:E:6:DT:O2	1.95	0.49
1:G:372:THR:HB	12:G:703:HOH:O	2.11	0.49
1:A:194:TYR:CE2	1:A:195:ILE:HD12	2.46	0.49
1:F:102:GLN:CG	12:G:719:HOH:O	2.61	0.49
1:F:106:PRO:HG3	1:G:148:ASN:C	2.37	0.49
3:I:5:DT:H2'	3:I:6:DT:H71	1.94	0.49
1:F:127:PHE:O	1:F:159:VAL:HG11	2.13	0.49
3:I:6:DT:O2	3:I:7:DC:C6	2.66	0.49
1:A:193:HIS:C	1:A:193:HIS:CD2	2.90	0.49
1:A:276:TRP:CD2	3:E:21:DG:H4'	2.48	0.49
1:A:384:GLN:HB2	12:A:766:HOH:O	2.12	0.49
1:F:189:CYS:SG	1:F:202:ALA:CB	3.00	0.49
1:G:51:LEU:HD13	1:G:84:MET:HB2	1.95	0.49
1:B:45:LEU:HD21	1:B:144:PRO:HG2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:PRO:HG2	1:B:115:TRP:CE2	2.48	0.49
1:F:292:PHE:CD1	2:H:12:DA:H4'	2.48	0.49
1:A:234:SER:HA	12:A:734:HOH:O	2.12	0.49
1:B:205:LYS:HZ1	1:B:206:ASP:CG	2.21	0.49
1:F:60:HIS:CD2	6:F:616:DIO:H2'1	2.48	0.49
1:F:127:PHE:HA	1:F:159:VAL:HG21	1.93	0.49
1:F:512:ASN:OD1	1:F:559:TYR:HB3	2.13	0.49
1:G:204:THR:HB	1:G:206[B]:ASP:OD1	2.13	0.49
1:A:371:PHE:HE2	1:A:523:ALA:HA	1.78	0.48
1:A:53:ASN:O	1:A:56:LEU:HB3	2.12	0.48
1:A:301:LEU:HD23	1:A:301:LEU:N	2.27	0.48
1:A:408:GLN:HG2	1:A:450:LEU:HD13	1.95	0.48
1:F:367:THR:HG21	1:F:531:LEU:HD23	1.94	0.48
1:G:107:SER:HB3	1:G:110:MET:HE3	1.95	0.48
1:G:348:THR:HG23	1:G:362:PHE:CE1	2.48	0.48
1:A:375:LEU:HD13	1:A:450:LEU:HD21	1.95	0.48
1:A:120:ILE:HG23	1:A:226:ILE:HG23	1.95	0.48
1:F:215:LEU:O	1:F:219:VAL:HG13	2.13	0.48
1:F:290:ASN:OD1	1:F:310:GLU:HB2	2.13	0.48
1:A:409:VAL:HG21	6:A:603:DIO:H21	1.94	0.48
6:F:604:DIO:H22	6:G:601:DIO:H2'2	1.95	0.48
1:A:48:LEU:CD2	1:A:143:ILE:HG23	2.42	0.48
1:F:298:ASP:OD2	1:F:303:SER:OG	2.26	0.48
1:A:120:ILE:HD12	1:A:120:ILE:N	2.29	0.48
1:F:287:ALA:O	1:F:314:GLU:CD	2.57	0.48
1:F:330:ILE:HB	1:F:353:GLN:OE1	2.13	0.48
1:F:337:GLN:HB2	1:F:352:ILE:CG2	2.43	0.48
1:G:137:GLU:HA	1:G:156:GLN:HE21	1.77	0.48
1:B:115:TRP:NE1	1:B:203:GLU:HB3	2.29	0.47
1:B:296:ARG:HD3	6:B:604:DIO:H21	1.96	0.47
1:F:301:LEU:HD23	1:F:301:LEU:N	2.28	0.47
1:F:326:GLN:NE2	1:F:328:ASN:OD1	2.47	0.47
1:B:192:ILE:HG13	1:B:193:HIS:N	2.29	0.47
1:F:532:ILE:HD13	1:F:544:PHE:HB3	1.95	0.47
1:G:77:LYS:CG	1:G:78:LYS:H	2.26	0.47
3:I:5:DT:H2''	3:I:6:DT:C6	2.48	0.47
1:F:271:LEU:HD12	1:F:295:LEU:HD13	1.96	0.47
1:F:492:ALA:O	1:F:495:ALA:HB3	2.13	0.47
1:F:68:TRP:CE2	1:F:138:LYS:HG2	2.49	0.47
1:F:421:ILE:HG13	1:G:375:LEU:HD22	1.96	0.47
2:H:21:DG:OP2	2:H:21:DG:H2'	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:PHE:CD1	1:B:237:PHE:C	2.92	0.47
1:F:446:THR:HA	6:F:617:DIO:H2'2	1.96	0.47
2:H:3:DG:C8	2:H:4:DG:C2	3.03	0.47
1:B:343:THR:HA	6:B:608:DIO:H1'2	1.97	0.47
1:B:400:ILE:HD12	1:B:426:PHE:CE2	2.49	0.47
1:B:373:LEU:O	1:B:376:ASP:HB2	2.15	0.47
1:B:407:GLU:OE2	1:B:410:ARG:NH2	2.47	0.47
2:D:15:DG:H2''	2:D:16:DA:OP2	2.15	0.47
1:F:336:LEU:HD12	1:F:393:CYS:SG	2.55	0.47
1:B:48:LEU:HD13	1:B:74:VAL:CG1	2.45	0.47
1:B:411:GLN:OE1	1:B:415:ASN:ND2	2.48	0.47
1:F:271:LEU:CD1	1:F:295:LEU:HD13	2.45	0.47
1:G:52:ALA:O	1:G:61:ILE:HD11	2.14	0.47
1:B:192:ILE:HG13	1:B:193:HIS:H	1.79	0.47
1:B:431:ASP:OD1	1:B:431:ASP:C	2.56	0.47
1:G:98:MET:H	1:G:169[A]:THR:CG2	2.20	0.46
1:G:208:LEU:O	1:G:211:CYS:HB3	2.16	0.46
1:B:75:ILE:CD1	1:B:85:LEU:CD1	2.93	0.46
1:B:423:LEU:HD22	1:B:430:ILE:HD11	1.97	0.46
1:G:179:LEU:HD12	1:G:179:LEU:C	2.39	0.46
1:A:185:LYS:HD2	1:A:214:PHE:CZ	2.50	0.46
1:F:98:MET:CB	1:F:166:ASN:OD1	2.62	0.46
1:A:516:ASP:OD1	1:A:516:ASP:C	2.59	0.46
1:A:466:PHE:O	1:A:477:TYR:HA	2.16	0.46
1:B:264:LEU:HD12	1:B:264:LEU:O	2.16	0.46
1:F:32:PRO:HA	1:F:68:TRP:CZ3	2.50	0.46
1:F:347:PRO:HB3	1:F:374:TYR:CE1	2.50	0.46
1:G:259:ASP:C	1:G:259:ASP:OD1	2.59	0.46
1:B:32:PRO:HA	1:B:68:TRP:CZ2	2.50	0.46
1:F:367:THR:HG23	1:F:531:LEU:HD23	1.97	0.46
1:A:439:ILE:HD13	12:A:718:HOH:O	2.16	0.46
1:A:496:GLU:HB3	1:A:520:VAL:HG21	1.96	0.46
1:B:180:GLN:HA	1:B:183[B]:ARG:HD3	1.98	0.46
1:F:256:ILE:HG22	1:F:270:LEU:HD13	1.97	0.46
1:A:350:ILE:HG21	1:A:357:LEU:CD2	2.46	0.46
1:A:465:VAL:HG12	1:A:477:TYR:HB2	1.98	0.46
1:B:122:LEU:HD21	1:B:198:ILE:CG1	2.46	0.46
1:F:196:ASP:OD2	10:F:605:TTP:H5'2	2.16	0.46
1:G:196:ASP:OD1	1:G:196:ASP:O	2.33	0.46
1:G:363:LEU:CD2	1:G:380:THR:HG22	2.46	0.46
1:A:314:GLU:O	1:A:318:VAL:HG23	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:DG:C2'	2:D:22:DA:OP2	2.63	0.45
1:F:333:LEU:H	1:F:333:LEU:HG	1.59	0.45
1:A:516:ASP:HA	1:A:563:ILE:O	2.16	0.45
1:B:406:LYS:HG3	12:B:744:HOH:O	2.14	0.45
1:A:131:LEU:HD21	1:A:139:PHE:CD2	2.52	0.45
1:F:515:SER:O	1:F:562:HIS:HA	2.16	0.45
2:H:22:DA:H2''	2:H:23:DA:C8	2.51	0.45
1:F:130:PRO:HB3	6:F:616:DIO:H11	1.98	0.45
1:F:315:ILE:O	1:F:316:LYS:C	2.60	0.45
1:F:328:ASN:HB3	12:F:753:HOH:O	2.16	0.45
1:F:527:VAL:O	1:F:528:GLU:C	2.59	0.45
1:G:291:LEU:O	1:G:294:ILE:HG12	2.16	0.45
1:B:25:LEU:HD21	6:B:611:DIO:H1'2	1.99	0.45
1:A:405:THR:OG1	1:A:408:GLN:OE1	2.31	0.45
1:B:180:GLN:HA	1:B:183[B]:ARG:CD	2.47	0.45
1:B:228:SER:HA	1:B:231:ILE:CD1	2.47	0.45
1:G:325:ALA:HB1	6:G:606:DIO:C1'	2.46	0.45
1:A:564:ARG:NH1	1:B:276:TRP:CD1	2.85	0.45
1:F:278:ARG:NH2	1:F:283:ILE:O	2.46	0.45
1:F:196:ASP:OD2	10:F:605:TTP:H5'1	2.17	0.45
1:F:206:ASP:OD1	1:F:206:ASP:N	2.48	0.45
1:F:341:PHE:HE2	1:F:350:ILE:CD1	2.25	0.45
1:A:128:THR:HG21	12:A:732:HOH:O	2.16	0.45
1:A:579:GLN:OE1	1:A:579:GLN:HA	2.17	0.45
1:F:365:HIS:ND1	2:H:13:DG:OP1	2.34	0.45
1:G:413:PHE:O	1:G:420:GLN:NE2	2.42	0.45
1:G:437:THR:O	1:G:441:GLN:HG3	2.17	0.45
1:F:278:ARG:HB2	1:F:279:PRO:HD3	1.98	0.45
1:A:277:ILE:HD13	1:A:281:LEU:HD12	2.00	0.44
1:G:432:ASN:OD1	1:G:432:ASN:C	2.60	0.44
1:A:292:PHE:CE2	1:A:365:HIS:HB2	2.52	0.44
1:F:148:ASN:OD1	1:F:148:ASN:N	2.50	0.44
1:G:142:THR:OG1	1:G:154:ARG:HD2	2.17	0.44
1:B:121:ASP:HB3	1:B:124:ASP:OD2	2.17	0.44
1:G:85:LEU:N	1:G:85:LEU:HD22	2.32	0.44
1:G:354:ASN:HB3	1:G:355:THR:H	1.61	0.44
1:A:98:MET:HA	1:B:65:PHE:O	2.18	0.44
1:F:256:ILE:HG23	1:F:270:LEU:HD12	1.99	0.44
6:F:604:DIO:H22	6:G:601:DIO:C2'	2.47	0.44
1:F:239:TYR:CD2	1:F:240:LEU:HG	2.53	0.44
1:F:475:ALA:HB1	1:F:499:ALA:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:26:THR:HG21	1:G:98:MET:HE2	1.98	0.44
1:G:447:THR:C	1:G:448:TRP:CD1	2.96	0.44
3:I:7:DC:H2'	3:I:8:DC:O4'	2.18	0.44
1:A:404:LEU:HD22	1:A:450:LEU:HD11	1.98	0.44
1:F:106:PRO:CB	1:G:147:ASN:O	2.65	0.44
1:G:278:ARG:HB3	1:G:279:PRO:HD3	1.99	0.44
1:B:327:ILE:HG12	1:B:357:LEU:O	2.17	0.44
1:F:117:LEU:HB3	1:F:201:ALA:HB2	1.99	0.44
1:B:369:LYS:HD2	1:B:369:LYS:HA	1.72	0.44
1:F:183:ARG:O	1:F:187:SER:HA	2.18	0.44
1:F:363:LEU:HB3	1:F:364:PRO:HD2	2.00	0.44
1:A:336:LEU:HD12	1:A:389:ILE:HG23	2.00	0.43
1:G:186:PHE:CE2	1:G:211:CYS:HA	2.53	0.43
1:F:102:GLN:NE2	1:G:148:ASN:O	2.50	0.43
1:F:271:LEU:HD12	1:F:295:LEU:CD1	2.48	0.43
1:F:573:LEU:HD12	1:G:268:GLN:HG2	2.00	0.43
3:I:6:DT:H2''	3:I:7:DC:O5'	2.18	0.43
1:F:527:VAL:HG23	1:F:528:GLU:N	2.33	0.43
1:G:356:ASP:OD2	6:G:604:DIO:H1'1	2.18	0.43
1:G:405:THR:OG1	1:G:408:GLN:HG3	2.18	0.43
1:B:182:VAL:HG21	1:B:215:LEU:HD12	2.01	0.43
1:G:34:TRP:CD1	1:G:34:TRP:C	2.97	0.43
1:G:308:THR:HG21	12:G:732:HOH:O	2.17	0.43
1:A:118:ILE:HG23	1:A:120:ILE:HD11	1.99	0.43
1:A:278:ARG:CB	1:A:279:PRO:HD3	2.45	0.43
1:A:527:VAL:HG22	1:A:548:GLN:HG3	2.00	0.43
1:B:153:THR:CG2	1:B:155:PHE:CE2	3.02	0.43
3:E:7:DC:H2''	3:E:8:DC:C5	2.53	0.43
1:F:121:ASP:OD1	1:F:121:ASP:C	2.60	0.43
2:H:8:DT:H2'	2:H:9:DG:C8	2.54	0.43
1:G:385:THR:O	1:G:389:ILE:HG13	2.19	0.43
1:A:112:PRO:O	1:A:115:TRP:HB2	2.19	0.43
1:B:160:LEU:HD11	1:B:164:MET:CB	2.48	0.43
1:A:153:THR:HG23	1:A:155:PHE:CE1	2.50	0.43
1:A:282:GLY:HA3	1:A:360:TRP:CE2	2.54	0.43
1:B:35:VAL:HG12	1:B:71:PRO:HG3	2.01	0.43
1:B:283:ILE:HD13	1:B:288:MET:HE3	2.00	0.43
3:I:4:DT:H2''	3:I:5:DT:H72	2.00	0.43
1:A:304:LYS:O	1:A:305:ARG:HD3	2.19	0.43
1:B:373:LEU:HA	1:B:373:LEU:HD12	1.79	0.43
1:A:23:ILE:CG2	1:A:98:MET:HE1	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:HE3	1:A:250:LYS:HG3	2.02	0.42
1:B:42:LYS:O	1:B:43:GLN:C	2.62	0.42
1:B:330:ILE:O	1:B:330:ILE:HG13	2.19	0.42
1:F:317:LEU:HB3	6:F:613:DIO:H2'2	1.99	0.42
1:F:460:GLU:O	1:F:461:ASN:C	2.62	0.42
1:G:205:LYS:O	1:G:209:ILE:HG13	2.19	0.42
1:A:27:TRP:CZ3	1:A:95:ILE:HG12	2.54	0.42
1:B:115:TRP:CG	1:B:203:GLU:HA	2.54	0.42
1:A:500:VAL:HG21	1:A:520:VAL:CG1	2.49	0.42
1:B:316:LYS:HE3	1:B:320:GLU:CD	2.44	0.42
1:F:249:ILE:HD11	1:F:329:ARG:HG2	2.01	0.42
1:A:341:PHE:CE1	1:A:350:ILE:HD13	2.54	0.42
1:G:98:MET:N	1:G:169[A]:THR:HG21	2.21	0.42
1:G:288:MET:HE3	1:G:291:LEU:HD23	2.02	0.42
3:I:8:DC:C4	3:I:9:DC:C4	3.08	0.42
1:B:308:THR:HB	1:B:309:PRO:HD2	2.01	0.42
1:F:196:ASP:OD1	3:I:22:DG:O3'	2.37	0.42
1:G:78:LYS:HA	1:G:78:LYS:NZ	2.34	0.42
1:A:101:LEU:HD22	1:B:152:ALA:O	2.19	0.42
1:F:328:ASN:ND2	1:F:328:ASN:N	2.68	0.42
1:G:196:ASP:OD1	1:G:196:ASP:C	2.62	0.42
3:I:5:DT:H2'	3:I:6:DT:C7	2.49	0.42
1:A:74:VAL:HA	1:A:83:ARG:O	2.19	0.42
1:B:351:ILE:HD13	1:B:389:ILE:HG12	2.02	0.42
1:B:378:ILE:O	1:B:382:ILE:HD12	2.20	0.42
1:F:347:PRO:HD2	1:F:363:LEU:HD12	2.02	0.42
2:H:22:DA:H2	3:I:7:DC:C2	2.34	0.42
1:A:286:TYR:CD1	1:A:286:TYR:C	2.98	0.42
1:A:368:VAL:CG1	3:E:13:DC:OP2	2.68	0.42
1:B:48:LEU:HD12	1:B:48:LEU:HA	1.84	0.42
1:B:167:SER:HB3	1:B:170:ILE:HD12	2.02	0.42
1:F:30:GLU:O	1:F:32:PRO:HD3	2.20	0.42
1:A:65:PHE:HA	12:A:745:HOH:O	2.20	0.42
1:F:107:SER:HA	6:F:611:DIO:H11	2.02	0.42
1:F:339:LEU:O	1:F:349:GLY:HA2	2.20	0.42
1:A:405:THR:HG1	1:A:408:GLN:CD	2.27	0.41
1:F:32:PRO:HA	1:F:68:TRP:CE2	2.55	0.41
1:G:357:LEU:C	1:G:357:LEU:CD2	2.92	0.41
1:A:167:SER:N	1:A:168:PRO:HD2	2.35	0.41
1:A:254:ILE:HG13	1:A:322:ILE:CG2	2.50	0.41
1:B:42:LYS:O	1:B:45:LEU:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:LEU:C	1:B:357:LEU:HD23	2.45	0.41
1:F:126:PHE:CD1	10:F:605:TTP:H2'1	2.55	0.41
1:G:287:ALA:O	1:G:314:GLU:HG2	2.19	0.41
1:G:378:ILE:CD1	6:G:601:DIO:H2'1	2.50	0.41
1:G:277:ILE:HD12	1:G:277:ILE:HA	1.91	0.41
1:G:394:GLY:C	1:G:395:ASN:OD1	2.64	0.41
1:F:528:GLU:HB2	12:F:736:HOH:O	2.20	0.41
1:A:435:PRO:HB2	1:A:437:THR:HG23	2.02	0.41
1:A:477:TYR:CE1	1:A:483:ARG:HB3	2.56	0.41
1:F:199:LEU:HD23	1:F:199:LEU:C	2.45	0.41
1:G:298:ASP:HA	6:G:605:DIO:H12	2.02	0.41
1:G:337:GLN:N	1:G:337:GLN:CD	2.78	0.41
1:G:448:TRP:CD1	1:G:448:TRP:N	2.88	0.41
1:B:419:TRP:CE2	1:B:423:LEU:CD1	3.03	0.41
1:F:131:LEU:HD11	1:F:160:LEU:HA	2.02	0.41
1:F:164:MET:HB3	1:F:167:SER:OG	2.20	0.41
2:H:14:DC:H2''	2:H:15:DG:C8	2.55	0.41
1:A:242:MET:HE2	1:A:251:PRO:HA	2.02	0.41
1:B:205:LYS:NZ	1:B:206:ASP:CG	2.78	0.41
1:F:83:ARG:HD3	1:F:85:LEU:HD21	2.03	0.41
1:F:120:ILE:HG13	1:F:226:ILE:HG23	2.02	0.41
2:H:23:DA:C2	2:H:24:DA:C4	3.09	0.41
1:A:68:TRP:O	1:A:140:ALA:HB3	2.21	0.41
1:A:236:PRO:HB2	1:A:243:GLN:HE22	1.86	0.41
1:A:368:VAL:HG11	3:E:13:DC:OP2	2.20	0.41
1:B:249:ILE:O	1:B:251:PRO:HD3	2.20	0.41
1:F:472:ASN:O	1:F:486:LYS:NZ	2.54	0.41
1:A:199:LEU:HD23	1:A:200[B]:CYS:N	2.36	0.41
1:B:107:SER:HB2	1:B:108:PRO:HD2	2.03	0.41
3:I:16:DT:C6	3:I:17:DT:H72	2.55	0.40
1:A:347:PRO:HD3	1:A:374:TYR:CE1	2.56	0.40
1:A:524:THR:HB	1:A:560:ILE:HD13	2.02	0.40
1:B:64:SER:HB2	1:B:156:GLN:HG2	2.02	0.40
1:G:231:ILE:HG22	1:G:232:GLN:N	2.36	0.40
1:G:338:LEU:HD12	1:G:338:LEU:C	2.47	0.40
1:A:75:ILE:HG12	1:A:85:LEU:HD11	2.03	0.40
1:B:346:SER:OG	1:B:347:PRO:HD2	2.22	0.40
1:F:77:LYS:HE3	1:F:82:TRP:O	2.20	0.40
1:G:149:LYS:HG2	1:G:150:GLU:N	2.36	0.40
2:H:22:DA:H2''	2:H:23:DA:OP2	2.21	0.40
1:A:387:LEU:HD11	1:B:39:PRO:HD2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:LEU:HD21	6:B:602:DIO:H22	2.02	0.40
2:D:8:DT:H2'	2:D:9:DG:C8	2.56	0.40
1:B:180:GLN:HB3	1:B:181:PRO:HD3	2.04	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	567/618 (92%)	548 (97%)	19 (3%)	0	100	100
1	B	432/618 (70%)	418 (97%)	14 (3%)	0	100	100
1	F	568/618 (92%)	543 (96%)	24 (4%)	1 (0%)	43	64
1	G	434/618 (70%)	417 (96%)	17 (4%)	0	100	100
All	All	2001/2472 (81%)	1926 (96%)	74 (4%)	1 (0%)	48	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	195	ILE

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	500/549 (91%)	485 (97%)	15 (3%)	36	62
1	B	370/549 (67%)	356 (96%)	14 (4%)	29	54
1	F	500/549 (91%)	477 (95%)	23 (5%)	24	47
1	G	374/549 (68%)	362 (97%)	12 (3%)	34	60
All	All	1744/2196 (79%)	1680 (96%)	64 (4%)	30	55

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ASP
1	A	148	ASN
1	A	149	LYS
1	A	179	LEU
1	A	184	GLU
1	A	211	CYS
1	A	216	GLN
1	A	254	ILE
1	A	255	GLU
1	A	258	LYS
1	A	350	ILE
1	A	437	THR
1	A	452	LYS
1	A	457	GLU
1	A	461	ASN
1	B	57	GLU
1	B	114	ASP
1	B	134	GLN
1	B	196	ASP
1	B	207	LYS
1	B	242	MET
1	B	260	THR
1	B	285	THR
1	B	318	VAL
1	B	369	LYS
1	B	372	THR
1	B	390	THR
1	B	404	LEU
1	B	437	THR
1	F	46	GLU
1	F	120	ILE
1	F	148	ASN
1	F	165	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	206	ASP
1	F	209	ILE
1	F	229	ASP
1	F	235	THR
1	F	260	THR
1	F	262	LYS
1	F	280	THR
1	F	295	LEU
1	F	301	LEU
1	F	333	LEU
1	F	369	LYS
1	F	384	GLN
1	F	406	LYS
1	F	410	ARG
1	F	427	VAL
1	F	437	THR
1	F	491	SER
1	F	493	GLN
1	F	525	ARG
1	G	78	LYS
1	G	196	ASP
1	G	200	CYS
1	G	207	LYS
1	G	235	THR
1	G	246	ASN
1	G	259	ASP
1	G	315	ILE
1	G	361	SER
1	G	380	THR
1	G	396	ASP
1	G	423	LEU

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

Mol	Chain	Res	Type
1	A	148	ASN
1	A	193	HIS
1	A	243	GLN
1	A	265	ASN
1	A	539	GLN
1	A	566	HIS
1	B	49	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	156	GLN
1	B	238	HIS
1	B	275	ASN
1	B	425	ASN
1	F	53	ASN
1	F	60	HIS
1	F	243	GLN
1	F	326	GLN
1	F	328	ASN
1	F	354	ASN
1	G	43	GLN
1	G	55	GLN
1	G	162	GLN
1	G	275	ASN
1	G	384	GLN
1	G	441	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 63 ligands modelled in this entry, 18 are monoatomic - leaving 45 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	DIO	F	603	-	6,6,6	0.33	0	6,6,6	0.19	0
6	DIO	A	607	-	6,6,6	0.24	0	6,6,6	0.12	0
7	EDO	A	608	-	3,3,3	0.08	0	2,2,2	0.13	0
6	DIO	F	604	-	6,6,6	0.17	0	6,6,6	0.23	0
7	EDO	F	615	-	3,3,3	0.14	0	2,2,2	0.23	0
6	DIO	B	606	-	6,6,6	0.39	0	6,6,6	0.19	0
6	DIO	B	610	-	6,6,6	0.46	0	6,6,6	0.39	0
6	DIO	G	603	-	6,6,6	0.31	0	6,6,6	0.18	0
6	DIO	G	604	-	6,6,6	0.29	0	6,6,6	0.12	0
7	EDO	F	606	-	3,3,3	0.09	0	2,2,2	0.09	0
6	DIO	B	608	-	6,6,6	0.20	0	6,6,6	0.30	0
6	DIO	F	619	-	6,6,6	0.37	0	6,6,6	0.23	0
6	DIO	F	612	-	6,6,6	0.24	0	6,6,6	0.23	0
6	DIO	A	603	-	6,6,6	0.26	0	6,6,6	0.24	0
6	DIO	B	602	-	6,6,6	0.19	0	6,6,6	0.29	0
6	DIO	A	604	-	6,6,6	0.50	0	6,6,6	0.25	0
6	DIO	F	613	-	6,6,6	0.12	0	6,6,6	0.20	0
6	DIO	B	607	-	6,6,6	0.31	0	6,6,6	0.30	0
5	DCP	A	602	4	28,29,29	0.60	0	41,45,45	0.82	1 (2%)
9	PG6	G	602	-	17,17,17	0.41	0	16,16,16	0.23	0
6	DIO	F	609	-	6,6,6	0.19	0	6,6,6	0.34	0
6	DIO	F	618	-	6,6,6	0.33	0	6,6,6	0.26	0
6	DIO	B	603	-	6,6,6	0.22	0	6,6,6	0.21	0
6	DIO	F	617	-	6,6,6	0.11	0	6,6,6	0.18	0
6	DIO	F	611	-	6,6,6	0.22	0	6,6,6	0.30	0
6	DIO	G	605	-	6,6,6	0.41	0	6,6,6	0.16	0
7	EDO	F	608	-	3,3,3	0.36	0	2,2,2	0.27	0
6	DIO	G	601	-	6,6,6	0.36	0	6,6,6	0.49	0
6	DIO	F	616	-	6,6,6	0.09	0	6,6,6	0.25	0
9	PG6	B	605	-	17,17,17	0.37	0	16,16,16	0.21	0
6	DIO	B	601	-	6,6,6	0.43	0	6,6,6	0.22	0
6	DIO	G	606	-	6,6,6	0.26	0	6,6,6	0.24	0
6	DIO	A	606	-	6,6,6	0.32	0	6,6,6	0.17	0
6	DIO	B	604	-	6,6,6	0.19	0	6,6,6	0.19	0
6	DIO	B	611	-	6,6,6	0.23	0	6,6,6	0.25	0
6	DIO	A	605	-	6,6,6	0.28	0	6,6,6	0.10	0
10	TTP	F	605	4	29,30,30	0.70	1 (3%)	43,47,47	0.73	0
6	DIO	F	610	-	6,6,6	0.14	0	6,6,6	0.18	0
6	DIO	B	609	-	6,6,6	0.05	0	6,6,6	0.24	0
6	DIO	B	612	-	6,6,6	0.31	0	6,6,6	0.18	0
6	DIO	F	614	-	6,6,6	0.19	0	6,6,6	0.15	0
7	EDO	B	613	-	3,3,3	0.10	0	2,2,2	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	F	607	-	3,3,3	0.07	0	2,2,2	0.05	0
6	DIO	F	601	-	6,6,6	0.17	0	6,6,6	0.24	0
7	EDO	G	607	-	3,3,3	0.15	0	2,2,2	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DIO	F	603	-	-	-	0/1/1/1
7	EDO	A	608	-	-	0/1/1/1	-
6	DIO	A	607	-	-	-	0/1/1/1
6	DIO	F	604	-	-	-	0/1/1/1
7	EDO	F	615	-	-	1/1/1/1	-
6	DIO	B	606	-	-	-	0/1/1/1
7	EDO	F	606	-	-	0/1/1/1	-
6	DIO	B	610	-	-	-	0/1/1/1
6	DIO	G	603	-	-	-	0/1/1/1
6	DIO	G	604	-	-	-	0/1/1/1
6	DIO	B	608	-	-	-	0/1/1/1
6	DIO	F	619	-	-	-	0/1/1/1
6	DIO	F	612	-	-	-	0/1/1/1
6	DIO	A	603	-	-	-	0/1/1/1
6	DIO	B	602	-	-	-	0/1/1/1
6	DIO	A	604	-	-	-	0/1/1/1
6	DIO	F	613	-	-	-	0/1/1/1
6	DIO	B	607	-	-	-	0/1/1/1
9	PG6	G	602	-	-	8/15/15/15	-
5	DCP	A	602	4	-	3/22/34/34	0/2/2/2
6	DIO	F	609	-	-	-	0/1/1/1
6	DIO	F	618	-	-	-	0/1/1/1
6	DIO	B	603	-	-	-	0/1/1/1
6	DIO	F	617	-	-	-	0/1/1/1
6	DIO	F	611	-	-	-	0/1/1/1
6	DIO	G	605	-	-	-	0/1/1/1
7	EDO	F	608	-	-	1/1/1/1	-
6	DIO	G	601	-	-	-	0/1/1/1
6	DIO	F	616	-	-	-	0/1/1/1
9	PG6	B	605	-	-	11/15/15/15	-
6	DIO	B	601	-	-	-	0/1/1/1
6	DIO	G	606	-	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DIO	A	606	-	-	-	0/1/1/1
6	DIO	B	604	-	-	-	0/1/1/1
6	DIO	B	611	-	-	-	0/1/1/1
6	DIO	A	605	-	-	-	0/1/1/1
10	TTP	F	605	4	-	4/22/34/34	0/2/2/2
6	DIO	F	610	-	-	-	0/1/1/1
6	DIO	B	609	-	-	-	0/1/1/1
6	DIO	B	612	-	-	-	0/1/1/1
6	DIO	F	614	-	-	-	0/1/1/1
7	EDO	B	613	-	-	1/1/1/1	-
7	EDO	F	607	-	-	0/1/1/1	-
6	DIO	F	601	-	-	-	0/1/1/1
7	EDO	G	607	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	605	TTP	PA-O3A	2.16	1.61	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	DCP	O3B-PB-O1B	-2.13	104.30	110.70

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	G	602	PG6	O2-C4-C5-O3
9	B	605	PG6	O5-C10-C11-O6
9	G	602	PG6	O4-C8-C9-O5
9	B	605	PG6	O2-C4-C5-O3
9	G	602	PG6	O3-C6-C7-O4
9	G	602	PG6	O1-C2-C3-O2
7	F	608	EDO	O1-C1-C2-O2
9	G	602	PG6	O5-C10-C11-O6
10	F	605	TTP	PA-O3A-PB-O1B
10	F	605	TTP	O4'-C4'-C5'-O5'
9	B	605	PG6	O3-C6-C7-O4
9	G	602	PG6	C9-C8-O4-C7
9	G	602	PG6	C5-C4-O2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	F	605	TTP	PB-O3B-PG-O2G
9	B	605	PG6	C6-C7-O4-C8
9	B	605	PG6	C9-C8-O4-C7
9	B	605	PG6	C4-C5-O3-C6
9	B	605	PG6	C3-C2-O1-C1
9	G	602	PG6	C6-C7-O4-C8
9	B	605	PG6	O4-C8-C9-O5
10	F	605	TTP	PA-O3A-PB-O2B
7	G	607	EDO	O1-C1-C2-O2
7	B	613	EDO	O1-C1-C2-O2
5	A	602	DCP	PG-O3B-PB-O1B
9	B	605	PG6	C10-C11-O6-C12
9	B	605	PG6	C2-C3-O2-C4
5	A	602	DCP	PG-O3B-PB-O2B
9	B	605	PG6	C11-C10-O5-C9
7	F	615	EDO	O1-C1-C2-O2
5	A	602	DCP	PB-O3A-PA-O2A

There are no ring outliers.

21 monomers are involved in 39 short contacts:

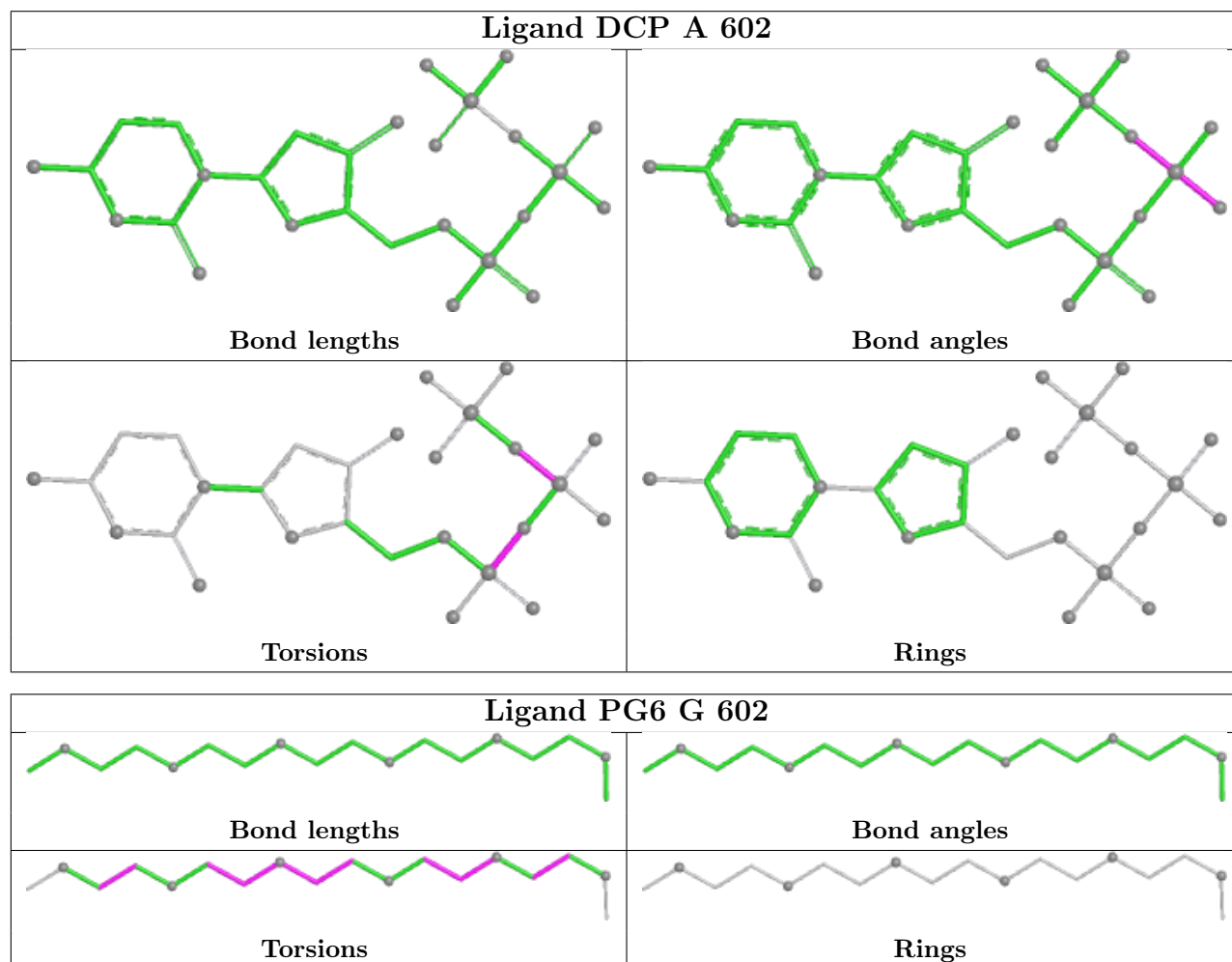
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	604	DIO	3	0
6	B	606	DIO	1	0
6	G	604	DIO	1	0
6	B	608	DIO	1	0
6	A	603	DIO	1	0
6	B	602	DIO	1	0
6	F	613	DIO	2	0
6	B	607	DIO	2	0
5	A	602	DCP	1	0
9	G	602	PG6	2	0
6	B	603	DIO	1	0
6	F	617	DIO	1	0
6	F	611	DIO	1	0
6	G	605	DIO	1	0
6	G	601	DIO	7	0
6	F	616	DIO	3	0
9	B	605	PG6	2	0
6	G	606	DIO	3	0
6	B	604	DIO	3	0
6	B	611	DIO	1	0

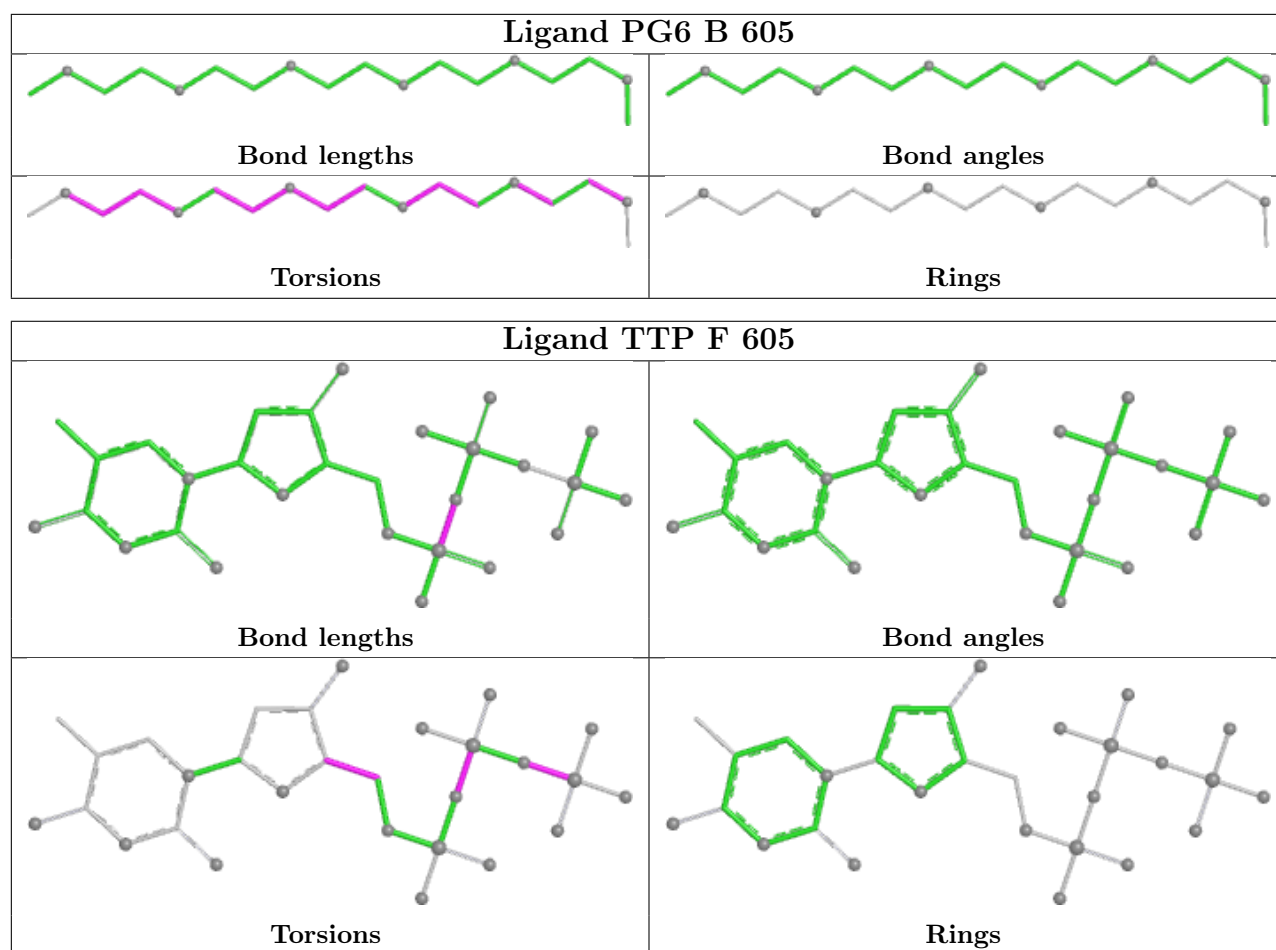
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	605	TTP	4	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	566/618 (91%)	-0.02	6 (1%) 78 74	36, 72, 101, 127	18 (3%)
1	B	432/618 (69%)	0.19	16 (3%) 45 40	28, 74, 139, 173	18 (4%)
1	F	566/618 (91%)	-0.06	5 (0%) 81 78	25, 72, 98, 129	12 (2%)
1	G	432/618 (69%)	0.18	19 (4%) 39 33	35, 74, 134, 165	15 (3%)
2	D	23/24 (95%)	-0.05	0 100 100	47, 77, 137, 158	0
2	H	23/24 (95%)	-0.05	1 (4%) 40 34	57, 75, 131, 186	0
3	E	20/21 (95%)	0.01	0 100 100	52, 78, 183, 187	0
3	I	20/21 (95%)	-0.14	0 100 100	53, 82, 140, 163	0
All	All	2082/2562 (81%)	0.05	47 (2%) 61 56	25, 73, 125, 187	63 (3%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	239	TYR	4.5
1	G	367	THR	3.7
1	B	367	THR	3.7
1	G	345[A]	HIS	3.6
1	G	368	VAL	3.4
1	A	254	ILE	3.2
1	B	212	TYR	3.1
1	G	372	THR	3.1
1	A	536	MET	3.0
1	F	38	TRP	3.0
2	H	25	DC	3.0
1	B	195	ILE	2.8
1	B	201	ALA	2.8
1	G	20	PRO	2.7
1	B	368	VAL	2.7
1	G	111	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	195	ILE	2.6
1	B	100	PRO	2.6
1	B	108	PRO	2.6
1	B	111	ILE	2.5
1	G	103	PRO	2.5
1	G	65	PHE	2.5
1	G	201	ALA	2.5
1	B	372	THR	2.5
1	G	369	LYS	2.5
1	F	254	ILE	2.4
1	G	231	ILE	2.4
1	G	100	PRO	2.4
1	F	333	LEU	2.4
1	B	200	CYS	2.4
1	B	244	ILE	2.3
1	G	244	ILE	2.3
1	B	238	HIS	2.3
1	G	232	GLN	2.3
1	G	371	PHE	2.3
1	G	240	LEU	2.2
1	G	105	LEU	2.2
1	A	302	ASN	2.2
1	A	535	SER	2.2
1	F	456	CYS	2.1
1	A	586	SER	2.1
1	B	213	THR	2.1
1	B	369	LYS	2.1
1	B	190	TYR	2.1
1	A	463	LEU	2.1
1	F	70	SER	2.0
1	G	366	SER	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	DIO	F	617	6/6	0.88	0.21	48,56,61,61	6
6	DIO	B	608	6/6	0.89	0.21	30,37,39,40	6
6	DIO	A	605	6/6	0.89	0.22	52,57,65,69	6
7	EDO	B	613	4/4	0.89	0.27	87,89,92,92	0
6	DIO	F	616	6/6	0.90	0.21	48,57,60,61	6
6	DIO	F	601	6/6	0.90	0.14	54,57,63,68	0
6	DIO	F	618	6/6	0.90	0.22	48,54,55,62	6
7	EDO	A	608	4/4	0.90	0.25	61,68,68,71	4
6	DIO	F	610	6/6	0.90	0.16	41,48,50,51	6
7	EDO	F	615	4/4	0.90	0.15	52,58,58,63	4
6	DIO	A	607	6/6	0.91	0.20	45,53,58,65	6
6	DIO	G	606	6/6	0.91	0.18	44,51,53,61	6
6	DIO	F	611	6/6	0.91	0.17	32,38,42,42	6
6	DIO	B	603	6/6	0.91	0.21	44,51,65,69	6
6	DIO	F	609	6/6	0.91	0.18	42,45,56,59	6
8	K	B	614	1/1	0.91	0.21	92,92,92,92	0
8	K	F	621	1/1	0.91	0.12	95,95,95,95	0
9	PG6	G	602	18/18	0.91	0.15	63,80,91,94	0
6	DIO	B	610	6/6	0.92	0.18	57,62,74,75	0
6	DIO	G	603	6/6	0.92	0.19	57,62,69,69	0
6	DIO	G	604	6/6	0.92	0.15	53,58,65,68	6
7	EDO	F	607	4/4	0.92	0.17	74,77,82,83	0
4	MG	G	611	1/1	0.93	0.13	69,69,69,69	0
9	PG6	B	605	18/18	0.93	0.14	56,74,100,108	0
6	DIO	A	604	6/6	0.93	0.15	60,62,70,70	0
6	DIO	B	607	6/6	0.94	0.10	60,70,77,81	0
6	DIO	G	605	6/6	0.94	0.13	57,60,72,74	0
6	DIO	F	614	6/6	0.94	0.17	41,51,54,60	6
6	DIO	F	619	6/6	0.94	0.17	22,25,27,27	6
6	DIO	B	606	6/6	0.94	0.12	60,69,77,81	0
7	EDO	F	606	4/4	0.94	0.18	72,72,73,80	0
6	DIO	F	604	6/6	0.95	0.14	51,59,70,71	0
6	DIO	B	609	6/6	0.95	0.14	39,46,51,52	6
7	EDO	G	607	4/4	0.95	0.18	55,56,63,71	4
6	DIO	B	604	6/6	0.95	0.14	39,44,53,56	6
6	DIO	A	606	6/6	0.95	0.15	43,46,54,55	6
6	DIO	G	601	6/6	0.95	0.15	23,25,27,29	6

Continued on next page...

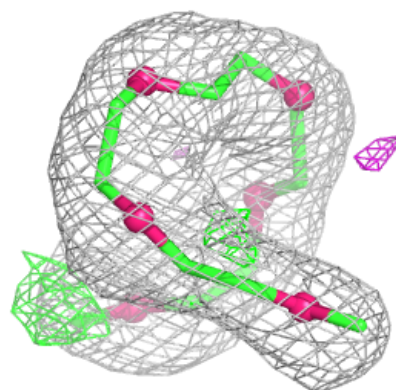
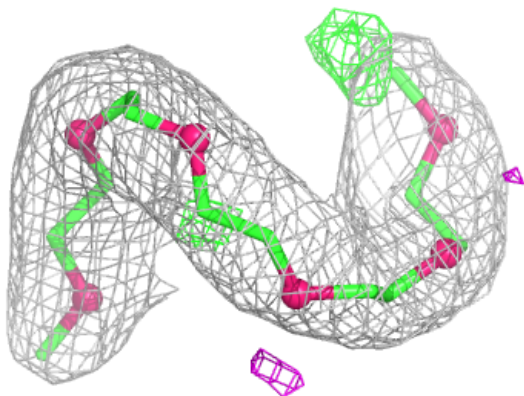
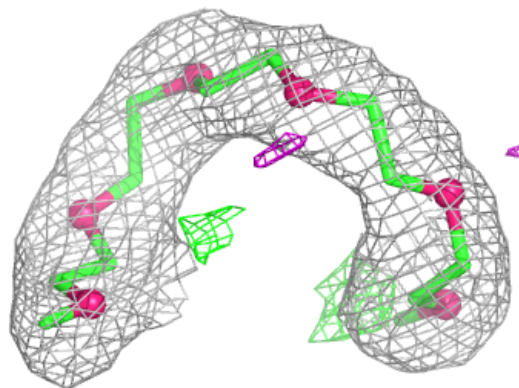
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	DIO	F	603	6/6	0.95	0.14	39,53,62,63	6
11	CL	F	620	1/1	0.95	0.10	85,85,85,85	0
6	DIO	A	603	6/6	0.96	0.09	46,59,65,70	0
6	DIO	B	602	6/6	0.96	0.17	32,37,39,43	6
8	K	A	610	1/1	0.96	0.10	71,71,71,71	0
6	DIO	F	612	6/6	0.96	0.14	38,42,43,46	6
6	DIO	F	613	6/6	0.96	0.14	40,45,52,53	6
8	K	G	609	1/1	0.96	0.11	81,81,81,81	0
8	K	G	610	1/1	0.96	0.07	85,85,85,85	0
4	MG	A	612	1/1	0.96	0.11	45,45,45,45	1
6	DIO	B	612	6/6	0.96	0.11	57,64,77,77	0
7	EDO	F	608	4/4	0.96	0.09	48,52,53,57	0
6	DIO	B	611	6/6	0.97	0.10	60,65,70,74	0
5	DCP	A	602	28/28	0.97	0.06	43,57,85,100	0
8	K	D	101	1/1	0.97	0.06	64,64,64,64	0
4	MG	D	103	1/1	0.97	0.06	67,67,67,67	0
8	K	F	622	1/1	0.97	0.12	84,84,84,84	0
11	CL	G	608	1/1	0.97	0.06	71,71,71,71	0
8	K	A	611	1/1	0.98	0.08	101,101,101,101	0
8	K	A	609	1/1	0.98	0.19	92,92,92,92	0
10	TTP	F	605	29/29	0.98	0.05	48,69,82,89	0
8	K	B	615	1/1	0.98	0.06	84,84,84,84	0
6	DIO	B	601	6/6	0.98	0.10	54,56,69,72	0
8	K	D	102	1/1	0.99	0.06	60,60,60,60	0
4	MG	A	601	1/1	0.99	0.05	62,62,62,62	0
4	MG	F	602	1/1	1.00	0.03	60,60,60,60	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.

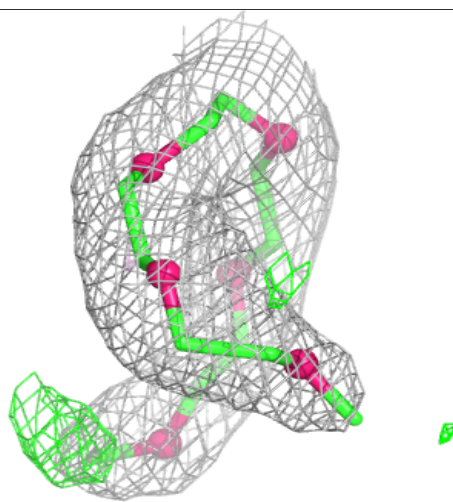
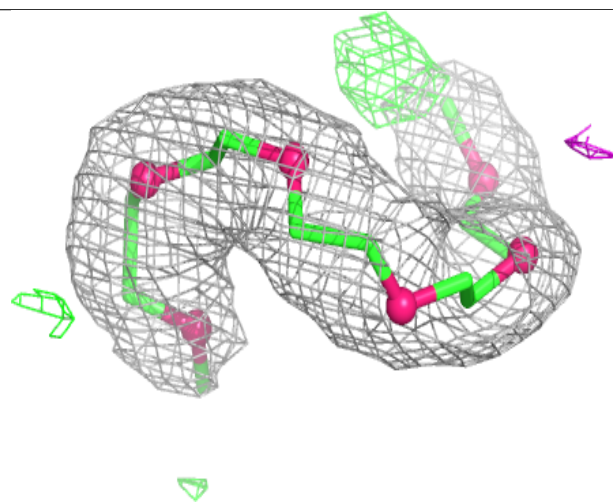
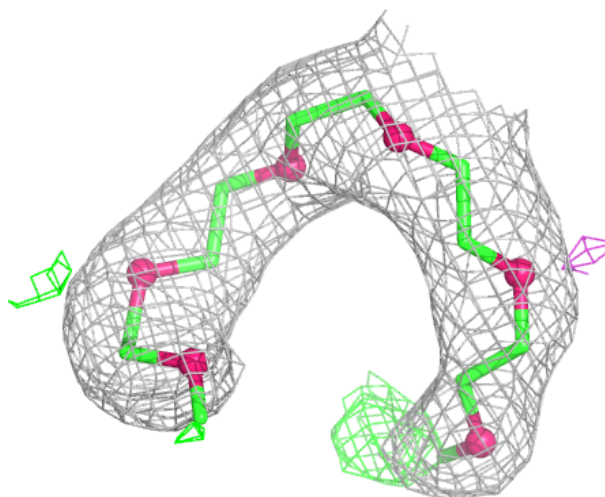
Electron density around PG6 G 602:

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



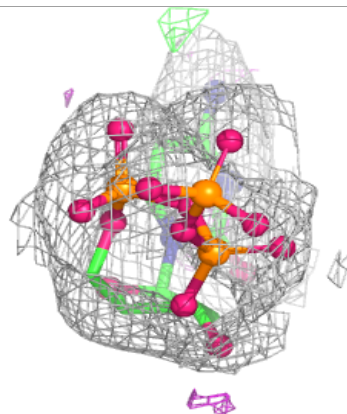
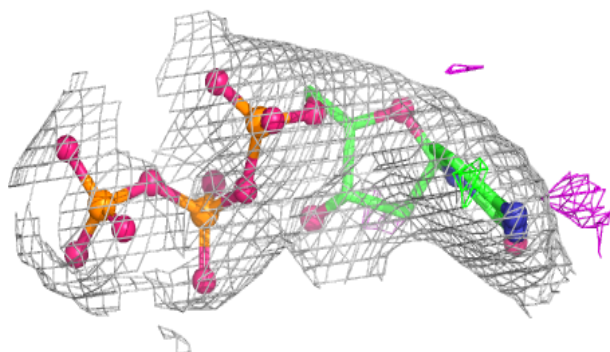
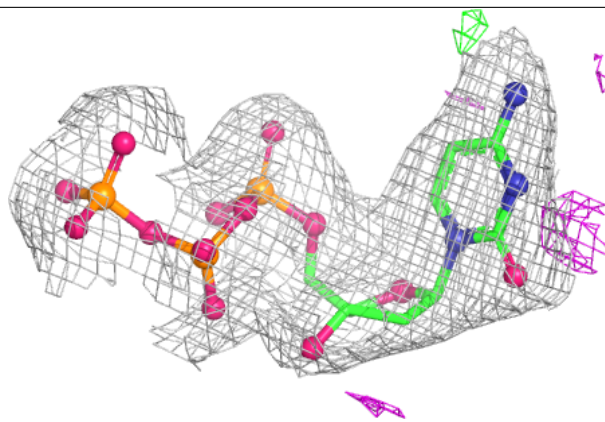
Electron density around PG6 B 605:

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

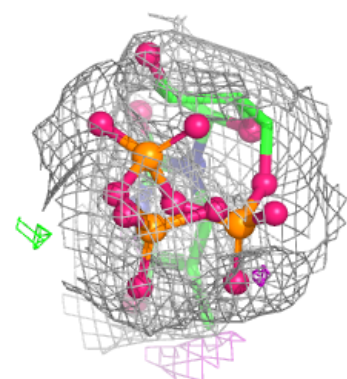
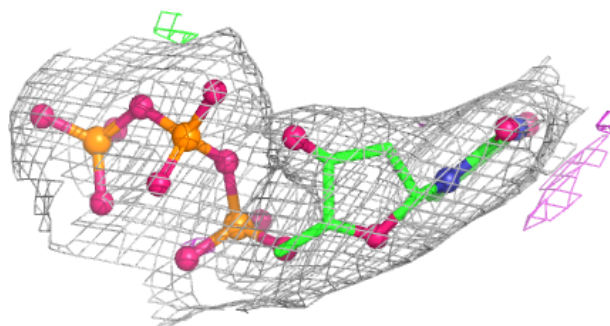
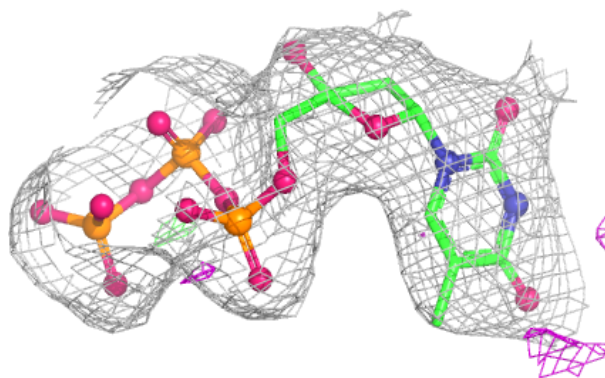


Electron density around DCP A 602:

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

**Electron density around TTP F 605:**

$2mF_o-DF_c$ (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.