Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 09:19 AM EST

PDB ID	:	3PKP
Title	:	Q83S Variant of S. Enterica RmlA with dATP
Authors	:	Chang, A.; Moretti, R.; Bingman, C.A.; Thorson, J.S.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on	:	2010-11-11
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:

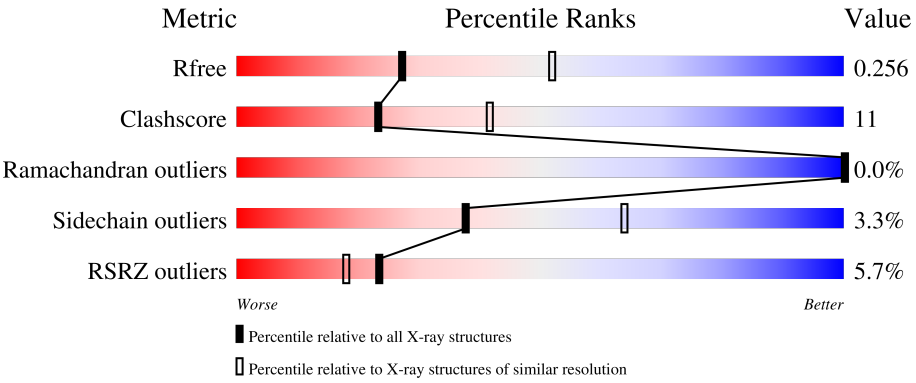
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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	292	% 76% 21%
1	B	292	2% 75% 23%
1	C	292	4% 76% 21%
1	D	292	7% 74% 22%
1	I	292	% 77% 21%

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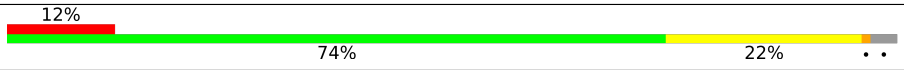
Mol	Chain	Length	Quality of chain
1	J	292	
1	K	292	
1	L	292	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18344 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.

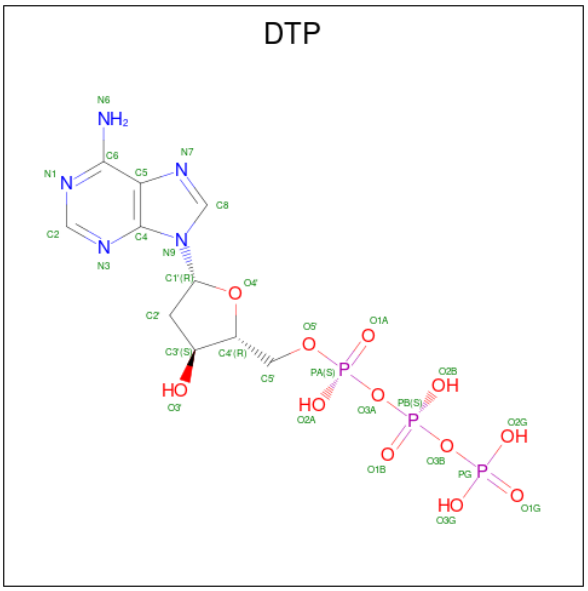
- Molecule 1 is a protein called Glucose-1-phosphate thymidylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2267	1451	377	427	12			
1	B	289	Total	C	N	O	S	0	0	0
			2259	1446	376	426	11			
1	C	282	Total	C	N	O	S	0	0	0
			2208	1415	364	418	11			
1	D	283	Total	C	N	O	S	0	0	0
			2217	1421	366	419	11			
1	I	289	Total	C	N	O	S	0	0	0
			2259	1446	376	426	11			
1	J	289	Total	C	N	O	S	0	0	0
			2259	1446	376	426	11			
1	K	284	Total	C	N	O	S	0	0	0
			2223	1426	369	417	11			
1	L	284	Total	C	N	O	S	0	0	0
			2226	1427	368	420	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	SER	GLN	engineered mutation	UNP P26393
B	83	SER	GLN	engineered mutation	UNP P26393
C	83	SER	GLN	engineered mutation	UNP P26393
D	83	SER	GLN	engineered mutation	UNP P26393
I	83	SER	GLN	engineered mutation	UNP P26393
J	83	SER	GLN	variant	UNP P26393
K	83	SER	GLN	variant	UNP P26393
L	83	SER	GLN	variant	UNP P26393

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O P 30 10 5 12 3	0	0
2	B	1	Total C N O P 30 10 5 12 3	0	0
2	C	1	Total C N O P 30 10 5 12 3	0	0
2	D	1	Total C N O P 30 10 5 12 3	0	0
2	I	1	Total C N O P 30 10 5 12 3	0	0
2	J	1	Total C N O P 30 10 5 12 3	0	0
2	K	1	Total C N O P 30 10 5 12 3	0	0
2	L	1	Total C N O P 30 10 5 12 3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0
3	D	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	2	Total Mg 2 2	0	0
3	J	2	Total Mg 2 2	0	0
3	K	2	Total Mg 2 2	0	0
3	L	2	Total Mg 2 2	0	0

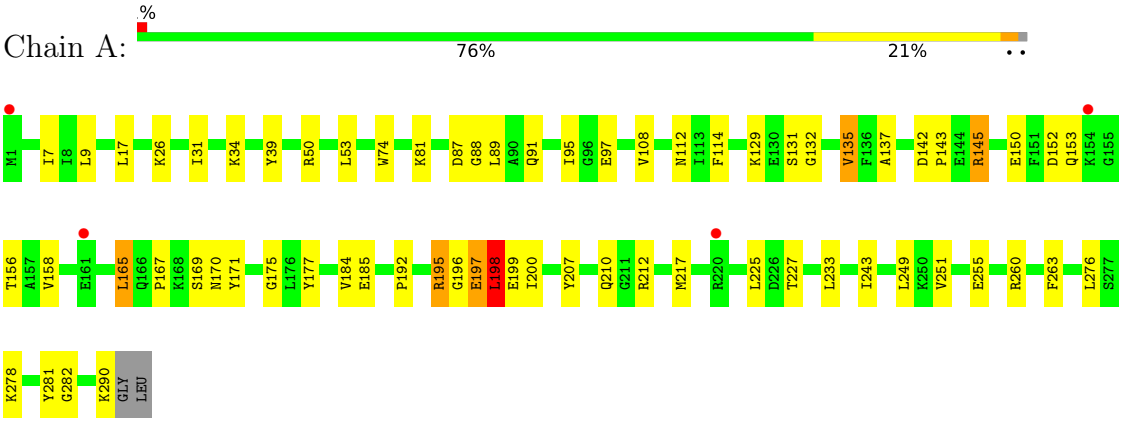
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	45	Total O 45 45	0	0
4	B	31	Total O 31 31	0	0
4	C	11	Total O 11 11	0	0
4	D	10	Total O 10 10	0	0
4	I	35	Total O 35 35	0	0
4	J	30	Total O 30 30	0	0
4	K	4	Total O 4 4	0	0
4	L	4	Total O 4 4	0	0

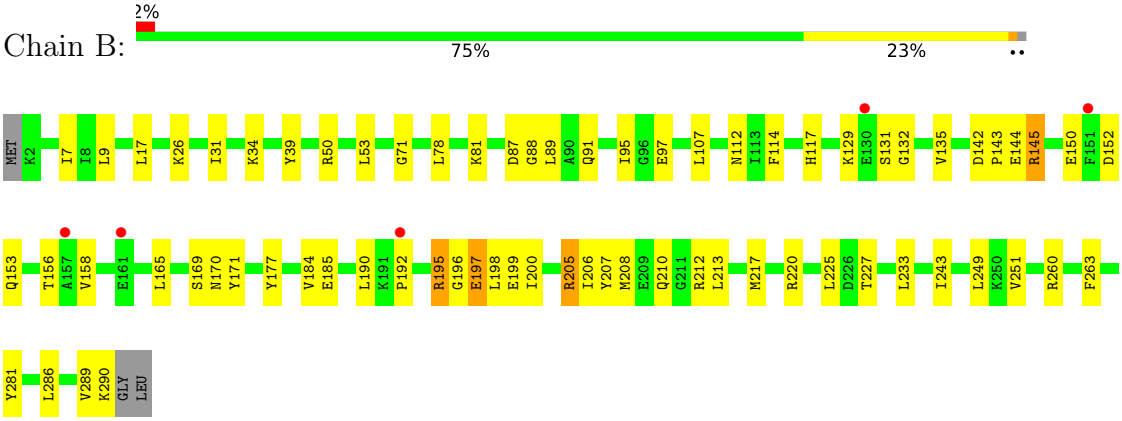
3 Residue-property plots (i)

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.

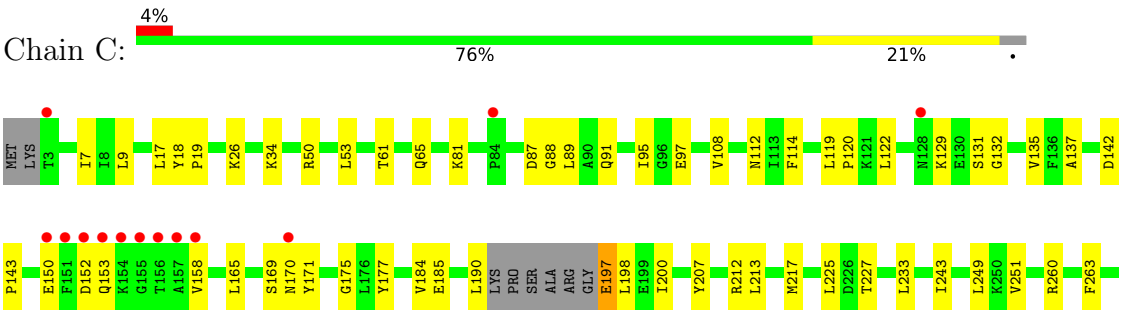
• Molecule 1: Glucose-1-phosphate thymidylyltransferase



• Molecule 1: Glucose-1-phosphate thymidylyltransferase

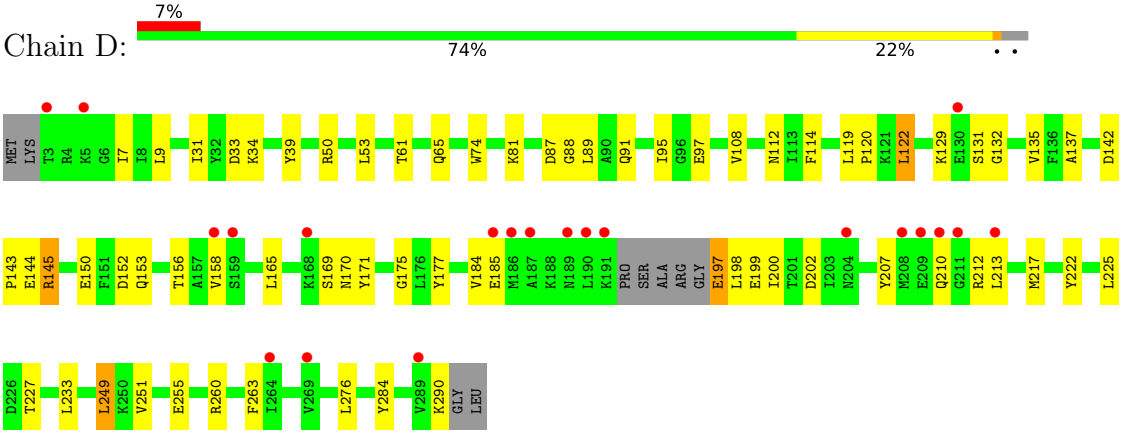


• Molecule 1: Glucose-1-phosphate thymidylyltransferase



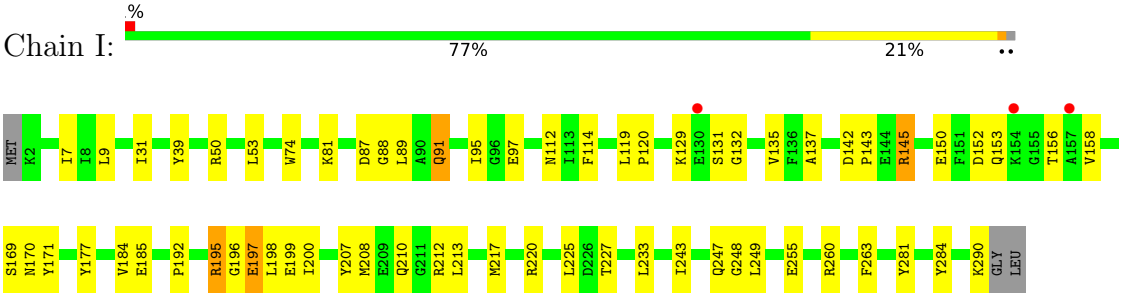
• Molecule 1: Glucose-1-phosphate thymidylyltransferase

Chain D:



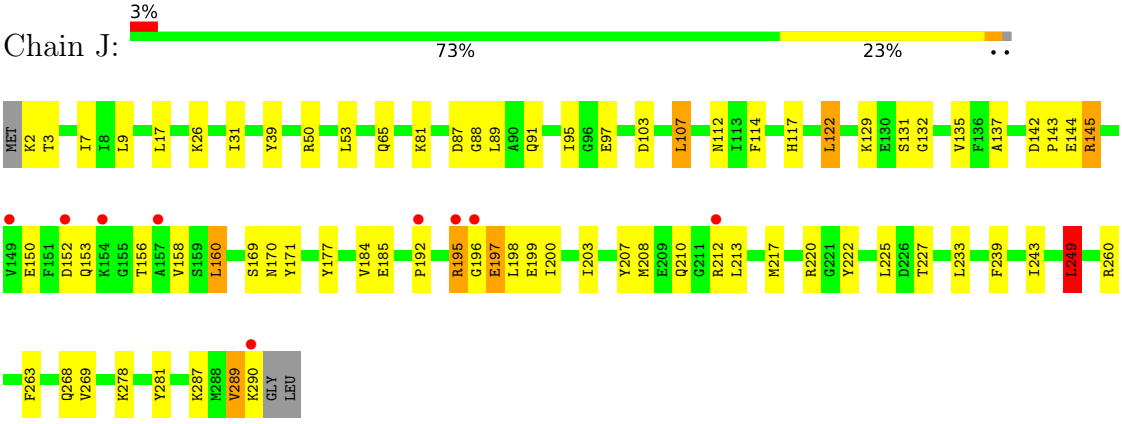
• Molecule 1: Glucose-1-phosphate thymidylyltransferase

Chain I:



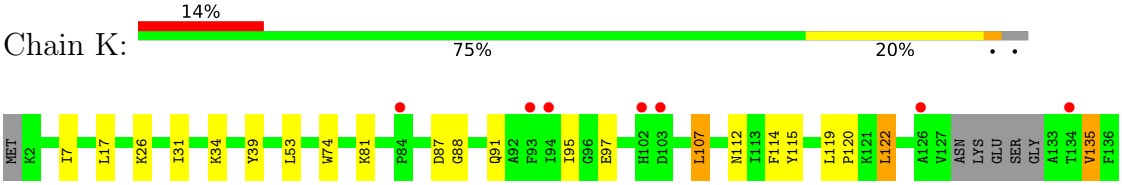
• Molecule 1: Glucose-1-phosphate thymidylyltransferase

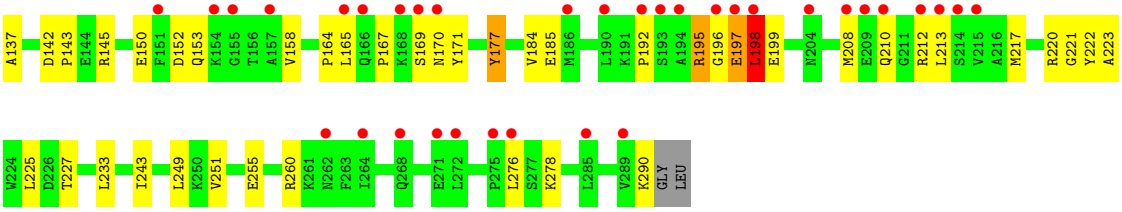
Chain J:



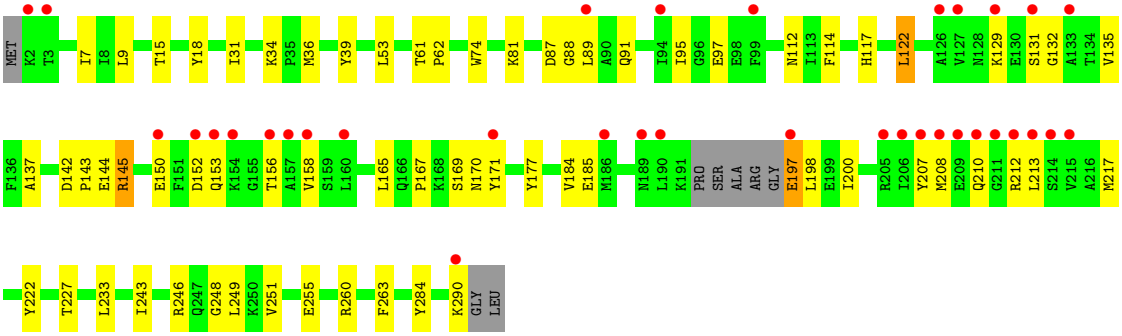
• Molecule 1: Glucose-1-phosphate thymidylyltransferase

Chain K:





• Molecule 1: Glucose-1-phosphate thymidylyltransferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	109.88Å 134.31Å 175.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.39 – 2.60 43.39 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.4 (43.39-2.60) 89.7 (43.39-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.200 , 0.260 0.196 , 0.256	Depositor DCC
R_{free} test set	2000 reflections (2.58%)	wwPDB-VP
Wilson B-factor (Å^2)	50.8	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 64.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18344	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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: DTP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.47	0/2314	0.64	2/3131 (0.1%)
1	B	0.46	0/2306	0.63	1/3121 (0.0%)
1	C	0.39	0/2253	0.60	1/3050 (0.0%)
1	D	0.39	0/2262	0.58	0/3061
1	I	0.45	0/2306	0.61	0/3121
1	J	0.45	0/2306	0.64	3/3121 (0.1%)
1	K	0.43	0/2269	0.65	4/3071 (0.1%)
1	L	0.40	0/2271	0.58	0/3072
All	All	0.43	0/18287	0.62	11/24748 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	225	LEU	CA-CB-CG	5.84	128.74	115.30
1	K	198	LEU	CB-CG-CD2	5.78	120.83	111.00
1	A	135	VAL	CG1-CB-CG2	5.78	120.15	110.90
1	K	135	VAL	CG1-CB-CG2	5.76	120.11	110.90
1	K	225	LEU	CA-CB-CG	5.72	128.47	115.30
1	A	198	LEU	CB-CG-CD2	5.28	119.97	111.00
1	C	225	LEU	CA-CB-CG	5.25	127.36	115.30
1	J	107	LEU	CB-CG-CD2	5.24	119.90	111.00
1	J	249	LEU	CB-CG-CD2	5.24	119.90	111.00
1	K	107	LEU	CB-CG-CD2	5.18	119.80	111.00
1	J	160	LEU	CB-CG-CD1	5.11	119.68	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2267	0	2279	50	0
1	B	2259	0	2267	59	0
1	C	2208	0	2207	44	0
1	D	2217	0	2220	46	0
1	I	2259	0	2267	52	0
1	J	2259	0	2267	69	0
1	K	2223	0	2233	54	0
1	L	2226	0	2233	55	0
2	A	30	0	12	0	0
2	B	30	0	12	0	0
2	C	30	0	12	1	0
2	D	30	0	12	0	0
2	I	30	0	12	0	0
2	J	30	0	12	1	0
2	K	30	0	12	1	0
2	L	30	0	12	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	45	0	0	3	0
4	B	31	0	0	1	0
4	C	11	0	0	0	0
4	D	10	0	0	0	0
4	I	35	0	0	1	0
4	J	30	0	0	2	0
4	K	4	0	0	0	0
4	L	4	0	0	2	0
All	All	18344	0	18069	409	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 11.

All (409) 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:B:205:ARG:HG3	1:B:208:MET:CE	1.50	1.39
1:J:2:LYS:O	1:J:3:THR:HG23	1.39	1.23
1:B:205:ARG:CG	1:B:208:MET:HE2	1.83	1.09
1:B:205:ARG:CG	1:B:208:MET:CE	2.32	1.05
1:J:287:LYS:O	1:J:290:LYS:HG2	1.58	1.02
1:J:2:LYS:O	1:J:3:THR:CG2	2.22	0.85
1:B:205:ARG:HG3	1:B:208:MET:HE2	0.87	0.85
1:L:117:HIS:CD2	4:L:296:HOH:O	2.30	0.83
1:D:260:ARG:HG3	1:D:260:ARG:HH11	1.43	0.82
1:I:260:ARG:HG3	1:I:260:ARG:HH11	1.44	0.82
1:K:260:ARG:HG3	1:K:260:ARG:HH11	1.44	0.81
1:A:260:ARG:HG3	1:A:260:ARG:HH11	1.47	0.80
1:B:260:ARG:HG3	1:B:260:ARG:HH11	1.43	0.80
1:C:260:ARG:HH11	1:C:260:ARG:HG3	1.47	0.80
1:J:260:ARG:HH11	1:J:260:ARG:HG3	1.45	0.80
1:L:129:LYS:HE2	1:L:131:SER:O	1.82	0.80
1:B:129:LYS:HE2	1:B:131:SER:O	1.83	0.79
1:C:129:LYS:HE2	1:C:131:SER:O	1.82	0.78
1:J:287:LYS:O	1:J:290:LYS:CG	2.31	0.78
1:I:129:LYS:HE2	1:I:131:SER:O	1.84	0.78
1:J:129:LYS:HE2	1:J:131:SER:O	1.84	0.78
1:D:129:LYS:HE2	1:D:131:SER:O	1.83	0.77
1:A:129:LYS:HE2	1:A:131:SER:O	1.84	0.77
1:D:198:LEU:HD12	1:D:198:LEU:H	1.51	0.76
1:L:260:ARG:HG3	1:L:260:ARG:HH11	1.50	0.76
1:D:198:LEU:HD12	1:D:198:LEU:N	2.01	0.76
1:B:286:LEU:O	1:B:289:VAL:HG22	1.88	0.73
1:L:198:LEU:N	1:L:198:LEU:HD12	2.05	0.71
1:K:88:GLY:O	1:K:91:GLN:HB2	1.91	0.70
1:L:88:GLY:O	1:L:91:GLN:HB2	1.90	0.70
1:B:143:PRO:HG3	1:B:170:ASN:HA	1.72	0.70
1:B:249:LEU:HD12	1:B:249:LEU:O	1.91	0.69
1:K:97:GLU:HG3	1:K:184:VAL:HG11	1.75	0.69
1:B:198:LEU:N	1:B:198:LEU:HD12	2.06	0.69
1:A:143:PRO:HG3	1:A:170:ASN:HA	1.75	0.69
1:I:143:PRO:HG3	1:I:170:ASN:HA	1.74	0.68
1:C:198:LEU:N	1:C:198:LEU:HD12	2.08	0.68
1:A:249:LEU:HD12	1:A:249:LEU:O	1.92	0.67
1:D:81:LYS:HG2	1:D:95:ILE:CG2	2.24	0.67
1:C:88:GLY:O	1:C:91:GLN:HB2	1.94	0.67
1:J:143:PRO:HG3	1:J:170:ASN:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:198:LEU:N	1:J:198:LEU:HD12	2.08	0.67
1:C:143:PRO:HG3	1:C:170:ASN:HA	1.77	0.67
1:D:88:GLY:O	1:D:91:GLN:HB2	1.95	0.66
1:K:143:PRO:HG3	1:K:170:ASN:HA	1.77	0.66
1:I:284:TYR:CZ	1:K:220:ARG:NH1	2.64	0.66
1:J:97:GLU:HG3	1:J:184:VAL:HG11	1.78	0.66
1:D:260:ARG:HG3	1:D:260:ARG:NH1	2.11	0.65
1:I:88:GLY:O	1:I:91:GLN:HB2	1.95	0.65
2:J:500:DTP:O2G	2:J:500:DTP:O2B	2.13	0.65
1:K:192:PRO:HB3	1:K:196:GLY:C	2.18	0.65
1:A:88:GLY:O	1:A:91:GLN:HB2	1.95	0.64
1:J:220:ARG:HB2	1:L:248:GLY:O	1.98	0.64
1:B:205:ARG:CG	1:B:208:MET:HE3	2.25	0.64
1:L:143:PRO:HG3	1:L:170:ASN:HA	1.79	0.64
1:D:97:GLU:HG3	1:D:184:VAL:HG11	1.79	0.64
1:J:88:GLY:O	1:J:91:GLN:HB2	1.97	0.64
1:J:260:ARG:HG3	1:J:260:ARG:NH1	2.13	0.64
1:K:81:LYS:HG2	1:K:95:ILE:CG2	2.28	0.64
1:B:88:GLY:O	1:B:91:GLN:HB2	1.98	0.63
1:J:287:LYS:HA	1:J:290:LYS:HD3	1.80	0.63
1:I:152:ASP:OD1	1:I:153:GLN:N	2.31	0.63
1:K:249:LEU:HD12	1:K:249:LEU:O	1.98	0.63
1:C:81:LYS:HG2	1:C:95:ILE:CG2	2.27	0.63
2:C:500:DTP:O2G	2:C:500:DTP:O2B	2.14	0.63
1:C:260:ARG:HG3	1:C:260:ARG:NH1	2.14	0.63
1:I:89:LEU:HB3	1:I:200:ILE:HD11	1.80	0.63
1:B:152:ASP:OD1	1:B:153:GLN:N	2.32	0.63
1:B:205:ARG:HG3	1:B:208:MET:HE3	1.68	0.62
1:L:81:LYS:HG2	1:L:95:ILE:CG2	2.30	0.62
1:L:97:GLU:HG3	1:L:184:VAL:HG11	1.80	0.62
1:C:97:GLU:HG3	1:C:184:VAL:HG11	1.81	0.62
1:C:152:ASP:OD1	1:C:153:GLN:N	2.33	0.62
1:D:198:LEU:H	1:D:198:LEU:CD1	2.12	0.62
1:B:192:PRO:HB3	1:B:196:GLY:C	2.20	0.62
1:I:198:LEU:HD12	1:I:198:LEU:N	2.14	0.62
1:J:117:HIS:CD2	4:L:296:HOH:O	2.52	0.62
1:K:260:ARG:HG3	1:K:260:ARG:NH1	2.13	0.62
1:D:143:PRO:HG3	1:D:170:ASN:HA	1.81	0.62
1:J:287:LYS:C	1:J:290:LYS:HG2	2.20	0.61
1:L:152:ASP:OD1	1:L:153:GLN:N	2.33	0.61
1:C:249:LEU:HD12	1:C:249:LEU:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:287:LYS:HA	1:J:290:LYS:CD	2.30	0.61
1:B:97:GLU:HG3	1:B:184:VAL:HG11	1.81	0.61
1:J:89:LEU:HB3	1:J:200:ILE:HD11	1.81	0.61
1:D:152:ASP:OD1	1:D:153:GLN:N	2.33	0.61
1:A:89:LEU:HB3	1:A:200:ILE:HD11	1.81	0.61
1:J:152:ASP:OD1	1:J:153:GLN:N	2.34	0.61
1:I:81:LYS:HG2	1:I:95:ILE:CG2	2.31	0.61
1:I:249:LEU:HD12	1:I:249:LEU:O	2.01	0.61
1:A:198:LEU:H	1:A:198:LEU:HD23	1.66	0.61
1:A:260:ARG:HG3	1:A:260:ARG:NH1	2.15	0.61
1:A:197:GLU:HB3	4:A:322:HOH:O	1.99	0.61
1:J:81:LYS:HG2	1:J:95:ILE:CG2	2.31	0.61
1:I:243:ILE:CD1	1:K:243:ILE:HD11	2.31	0.60
1:J:192:PRO:HB3	1:J:196:GLY:C	2.22	0.60
1:L:260:ARG:HG3	1:L:260:ARG:NH1	2.16	0.60
1:I:97:GLU:HG3	1:I:184:VAL:HG11	1.83	0.60
1:L:89:LEU:HB3	1:L:200:ILE:HD11	1.84	0.60
1:C:198:LEU:HD12	1:C:198:LEU:H	1.67	0.60
1:L:198:LEU:HD12	1:L:198:LEU:H	1.65	0.60
1:C:18:TYR:HB3	1:D:276:LEU:CD2	2.32	0.60
1:A:152:ASP:OD1	1:A:153:GLN:N	2.34	0.59
1:I:192:PRO:HB3	1:I:196:GLY:C	2.22	0.59
1:K:152:ASP:OD1	1:K:153:GLN:N	2.36	0.59
1:B:260:ARG:HG3	1:B:260:ARG:NH1	2.11	0.59
1:K:198:LEU:H	1:K:198:LEU:HD23	1.68	0.59
1:B:81:LYS:HG2	1:B:95:ILE:CG2	2.33	0.58
1:B:198:LEU:HD12	1:B:198:LEU:H	1.66	0.58
1:C:18:TYR:HB3	1:D:276:LEU:HD23	1.85	0.58
1:C:89:LEU:HB3	1:C:200:ILE:HD11	1.85	0.58
1:A:81:LYS:HG2	1:A:95:ILE:CG2	2.33	0.58
1:A:97:GLU:HG3	1:A:184:VAL:HG11	1.84	0.58
1:I:260:ARG:HG3	1:I:260:ARG:NH1	2.11	0.58
1:A:192:PRO:HB3	1:A:196:GLY:C	2.23	0.58
1:C:34:LYS:HE2	1:C:251:VAL:O	2.03	0.58
1:J:243:ILE:HD11	1:L:243:ILE:CD1	2.34	0.58
1:K:122:LEU:HD22	1:K:222:TYR:OH	2.04	0.57
1:J:198:LEU:HD12	1:J:198:LEU:H	1.69	0.57
1:I:249:LEU:HD23	1:K:221:GLY:HA2	1.87	0.57
1:J:2:LYS:N	1:J:103:ASP:OD1	2.38	0.57
1:B:249:LEU:HD12	1:B:249:LEU:C	2.25	0.56
1:K:34:LYS:HE2	1:K:251:VAL:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:N	1:A:198:LEU:CD2	2.70	0.55
1:I:185:GLU:OE1	1:I:185:GLU:HA	2.07	0.55
1:I:243:ILE:HD11	1:K:243:ILE:CD1	2.35	0.55
1:D:185:GLU:OE1	1:D:185:GLU:HA	2.06	0.54
1:I:284:TYR:OH	1:K:220:ARG:NH1	2.40	0.54
1:B:205:ARG:O	1:B:206:ILE:C	2.42	0.54
1:J:243:ILE:CD1	1:L:243:ILE:HD11	2.38	0.54
1:J:268:GLN:HB3	4:J:303:HOH:O	2.07	0.53
1:A:185:GLU:OE1	1:A:185:GLU:HA	2.07	0.53
1:A:249:LEU:HD12	1:A:249:LEU:C	2.29	0.53
1:K:198:LEU:N	1:K:198:LEU:CD2	2.71	0.53
1:L:185:GLU:HA	1:L:185:GLU:OE1	2.09	0.53
1:L:198:LEU:H	1:L:198:LEU:CD1	2.22	0.53
1:B:143:PRO:CG	1:B:170:ASN:HA	2.39	0.52
1:B:185:GLU:OE1	1:B:185:GLU:HA	2.10	0.52
1:B:243:ILE:HG22	1:B:249:LEU:HD11	1.92	0.52
1:C:50:ARG:HD3	1:C:263:PHE:CE1	2.45	0.52
1:D:34:LYS:HE2	1:D:251:VAL:O	2.10	0.52
1:I:243:ILE:HD11	1:K:243:ILE:HD11	1.92	0.52
1:I:243:ILE:HG22	1:I:249:LEU:HD11	1.92	0.52
1:K:185:GLU:OE1	1:K:185:GLU:HA	2.09	0.52
1:J:210:GLN:OE1	1:J:212:ARG:NH1	2.43	0.51
1:K:227:THR:CG2	1:K:233:LEU:HD13	2.40	0.51
1:C:185:GLU:HA	1:C:185:GLU:OE1	2.09	0.51
1:J:132:GLY:HA2	1:J:207:TYR:CE2	2.45	0.51
1:K:249:LEU:HD12	1:K:249:LEU:C	2.31	0.51
1:K:276:LEU:HD23	1:L:18:TYR:HB3	1.91	0.51
1:A:50:ARG:HD3	1:A:263:PHE:CE1	2.45	0.51
1:K:243:ILE:HG22	1:K:249:LEU:HD11	1.93	0.51
1:D:50:ARG:HD3	1:D:263:PHE:CE1	2.46	0.51
1:C:249:LEU:HD12	1:C:249:LEU:C	2.32	0.51
1:K:195:ARG:NH2	1:K:199:GLU:OE2	2.44	0.51
1:L:132:GLY:HA2	1:L:207:TYR:CE2	2.46	0.51
1:J:185:GLU:HA	1:J:185:GLU:OE1	2.10	0.51
1:L:198:LEU:N	1:L:198:LEU:CD1	2.71	0.51
1:J:278:LYS:NZ	4:J:313:HOH:O	2.41	0.50
1:K:171:TYR:CE1	1:K:217:MET:HG3	2.47	0.50
1:A:243:ILE:HG22	1:A:249:LEU:HD11	1.93	0.50
1:K:143:PRO:CG	1:K:170:ASN:HA	2.40	0.50
1:I:248:GLY:O	1:K:220:ARG:HB2	2.11	0.50
1:A:198:LEU:HD23	4:A:297:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:195:ARG:O	1:J:197:GLU:HG2	2.12	0.50
1:J:122:LEU:HD22	1:J:222:TYR:OH	2.12	0.49
1:D:171:TYR:CE1	1:D:217:MET:HG3	2.47	0.49
1:D:227:THR:CG2	1:D:233:LEU:HD13	2.42	0.49
1:J:195:ARG:NH2	1:J:199:GLU:OE2	2.44	0.49
1:K:208:MET:HB2	1:K:213:LEU:HD23	1.94	0.49
1:J:112:ASN:HB3	1:J:114:PHE:CE1	2.47	0.49
1:K:227:THR:HG23	1:K:233:LEU:HA	1.94	0.49
1:D:7:ILE:HG12	1:D:53:LEU:HB3	1.94	0.49
1:I:249:LEU:HD12	1:I:249:LEU:C	2.33	0.49
1:A:143:PRO:CG	1:A:170:ASN:HA	2.40	0.49
1:B:198:LEU:H	1:B:198:LEU:CD1	2.25	0.49
1:D:199:GLU:HB2	1:D:202:ASP:OD2	2.13	0.49
1:K:87:ASP:HB3	1:K:197:GLU:OE1	2.13	0.49
1:L:9:LEU:HD13	1:L:89:LEU:HG	1.95	0.49
1:A:227:THR:HG23	1:A:233:LEU:HA	1.95	0.48
1:B:117:HIS:CD2	4:B:319:HOH:O	2.66	0.48
1:C:198:LEU:H	1:C:198:LEU:CD1	2.26	0.48
1:D:132:GLY:HA2	1:D:207:TYR:CE2	2.48	0.48
1:I:198:LEU:HD12	1:I:198:LEU:H	1.78	0.48
1:J:2:LYS:C	1:J:3:THR:HG23	2.24	0.48
1:A:278:LYS:NZ	4:A:331:HOH:O	2.39	0.48
1:C:132:GLY:HA2	1:C:207:TYR:CE2	2.48	0.48
1:I:132:GLY:HA2	1:I:207:TYR:CE2	2.48	0.48
1:J:198:LEU:N	1:J:198:LEU:CD1	2.75	0.48
1:K:7:ILE:HG12	1:K:53:LEU:HB3	1.96	0.48
1:K:198:LEU:H	1:K:198:LEU:CD2	2.27	0.48
1:K:115:TYR:HB3	1:K:223:ALA:HB3	1.96	0.48
1:J:198:LEU:H	1:J:198:LEU:CD1	2.26	0.48
1:B:208:MET:HB2	1:B:213:LEU:HD23	1.95	0.48
1:C:135:VAL:HG13	1:C:213:LEU:HD11	1.96	0.48
1:J:17:LEU:HD12	1:J:26:LYS:HD3	1.96	0.48
1:J:243:ILE:CD1	1:L:243:ILE:CD1	2.91	0.48
1:L:227:THR:HG23	1:L:233:LEU:HA	1.95	0.48
1:B:132:GLY:HA2	1:B:207:TYR:CE2	2.49	0.48
1:C:143:PRO:CG	1:C:170:ASN:HA	2.44	0.48
1:C:227:THR:HG23	1:C:233:LEU:HA	1.95	0.48
1:A:198:LEU:H	1:A:198:LEU:CD2	2.26	0.48
1:C:198:LEU:N	1:C:198:LEU:CD1	2.75	0.48
1:I:143:PRO:CG	1:I:170:ASN:HA	2.41	0.48
1:L:243:ILE:HG22	1:L:249:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:GLU:HG2	1:D:145:ARG:HG2	1.96	0.47
1:L:249:LEU:O	1:L:249:LEU:HD12	2.14	0.47
1:A:34:LYS:HE2	1:A:251:VAL:O	2.15	0.47
1:B:135:VAL:HG13	1:B:213:LEU:HD11	1.96	0.47
1:D:135:VAL:HG13	1:D:213:LEU:HD11	1.95	0.47
1:I:135:VAL:HG13	1:I:213:LEU:HD11	1.97	0.47
1:I:171:TYR:CE1	1:I:217:MET:HG3	2.49	0.47
1:I:195:ARG:NH2	1:I:199:GLU:OE2	2.47	0.47
1:J:142:ASP:OD1	1:J:142:ASP:N	2.47	0.47
1:I:50:ARG:HD3	1:I:263:PHE:CE1	2.49	0.47
1:I:227:THR:CG2	1:I:233:LEU:HD13	2.45	0.47
1:A:195:ARG:NH2	1:A:199:GLU:OE2	2.47	0.47
1:A:177:TYR:CD1	1:A:177:TYR:N	2.83	0.47
1:B:17:LEU:HD12	1:B:26:LYS:HD3	1.97	0.47
1:D:227:THR:HG23	1:D:233:LEU:HA	1.96	0.47
1:D:9:LEU:HD13	1:D:89:LEU:HD13	1.96	0.47
1:A:87:ASP:HB3	1:A:197:GLU:OE1	2.15	0.47
1:B:192:PRO:HB3	1:B:197:GLU:N	2.30	0.47
1:A:243:ILE:HD11	1:C:243:ILE:CD1	2.45	0.46
1:J:171:TYR:CE1	1:J:217:MET:HG3	2.50	0.46
1:A:210:GLN:OE1	1:A:212:ARG:NH1	2.48	0.46
1:B:195:ARG:NH2	1:B:199:GLU:OE2	2.49	0.46
1:L:87:ASP:HB3	1:L:197:GLU:OE1	2.15	0.46
1:B:87:ASP:HB3	1:B:197:GLU:OE1	2.16	0.46
1:L:135:VAL:HG13	1:L:213:LEU:HD11	1.97	0.46
1:A:112:ASN:HB3	1:A:114:PHE:CE1	2.51	0.46
1:A:171:TYR:CE1	1:A:217:MET:HG3	2.50	0.46
1:C:87:ASP:HB3	1:C:197:GLU:OE1	2.14	0.46
1:D:31:ILE:HB	1:D:39:TYR:CE1	2.51	0.46
1:D:122:LEU:HD22	1:D:222:TYR:OH	2.16	0.46
1:I:220:ARG:NH2	4:I:317:HOH:O	2.47	0.46
1:L:7:ILE:HG12	1:L:53:LEU:HB3	1.98	0.46
1:L:150:GLU:O	1:L:158:VAL:HG22	2.16	0.46
1:I:74:TRP:NE1	1:I:255:GLU:HG3	2.31	0.46
1:J:135:VAL:HG13	1:J:213:LEU:HD11	1.98	0.46
1:A:142:ASP:N	1:A:142:ASP:OD1	2.49	0.46
1:K:17:LEU:HD12	1:K:26:LYS:HD3	1.96	0.46
1:C:177:TYR:CD1	1:C:177:TYR:N	2.84	0.46
1:C:243:ILE:HG22	1:C:249:LEU:HD11	1.98	0.46
1:D:87:ASP:HB3	1:D:197:GLU:OE1	2.15	0.46
1:I:210:GLN:OE1	1:I:212:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASP:HB2	1:A:145:ARG:HG3	1.98	0.46
1:C:150:GLU:O	1:C:158:VAL:HG22	2.16	0.46
1:D:177:TYR:N	1:D:177:TYR:CD1	2.84	0.45
1:I:150:GLU:O	1:I:158:VAL:HG22	2.16	0.45
1:L:31:ILE:HD11	1:L:36:MET:HE2	1.98	0.45
1:L:34:LYS:HE2	1:L:251:VAL:O	2.15	0.45
1:D:50:ARG:HD3	1:D:263:PHE:CZ	2.51	0.45
1:J:50:ARG:HD3	1:J:263:PHE:CE1	2.51	0.45
1:I:9:LEU:HD13	1:I:89:LEU:HG	1.99	0.45
1:J:143:PRO:CG	1:J:170:ASN:HA	2.45	0.45
1:A:243:ILE:CD1	1:C:243:ILE:HD11	2.46	0.45
1:J:9:LEU:HD13	1:J:89:LEU:HG	1.98	0.45
1:C:50:ARG:HD3	1:C:263:PHE:CZ	2.51	0.45
1:I:87:ASP:HB3	1:I:197:GLU:OE1	2.16	0.45
1:I:227:THR:HG23	1:I:233:LEU:HA	1.99	0.45
1:L:177:TYR:N	1:L:177:TYR:CD1	2.84	0.45
1:A:31:ILE:HB	1:A:39:TYR:CE1	2.51	0.45
1:B:50:ARG:HD3	1:B:263:PHE:CE1	2.52	0.45
1:I:31:ILE:HB	1:I:39:TYR:CE1	2.52	0.45
1:J:142:ASP:HB2	1:J:145:ARG:HG3	1.99	0.45
1:D:150:GLU:O	1:D:158:VAL:HG22	2.17	0.45
1:B:195:ARG:O	1:B:197:GLU:HG2	2.16	0.44
1:A:7:ILE:HG12	1:A:53:LEU:HB3	2.00	0.44
1:B:89:LEU:HB3	1:B:200:ILE:HD11	1.98	0.44
1:J:31:ILE:HB	1:J:39:TYR:CE1	2.52	0.44
1:J:152:ASP:HB3	1:J:156:THR:H	1.82	0.44
1:K:177:TYR:CD1	1:K:177:TYR:N	2.84	0.44
1:B:227:THR:HG23	1:B:233:LEU:HA	2.00	0.44
1:J:177:TYR:CD1	1:J:177:TYR:N	2.86	0.44
1:B:171:TYR:CE1	1:B:217:MET:HG3	2.52	0.44
1:C:171:TYR:CE1	1:C:217:MET:HG3	2.52	0.44
1:L:143:PRO:CG	1:L:170:ASN:HA	2.47	0.44
1:I:142:ASP:HB2	1:I:145:ARG:HG3	1.99	0.44
2:K:500:DTP:O2B	2:K:500:DTP:O2G	2.33	0.44
1:A:17:LEU:HD12	1:A:26:LYS:HD3	1.98	0.44
1:A:227:THR:CG2	1:A:233:LEU:HD13	2.47	0.44
1:J:208:MET:HB2	1:J:213:LEU:HD23	2.00	0.44
1:J:260:ARG:NH1	1:J:260:ARG:CG	2.81	0.44
1:C:7:ILE:HG12	1:C:53:LEU:HB3	1.99	0.44
1:D:137:ALA:HB1	1:D:171:TYR:HB3	2.00	0.44
1:J:192:PRO:HB3	1:J:197:GLU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:31:ILE:HB	1:K:39:TYR:CE1	2.53	0.44
1:I:208:MET:HB2	1:I:213:LEU:HD23	2.00	0.44
1:J:87:ASP:HB3	1:J:197:GLU:OE1	2.16	0.44
1:J:239:PHE:CD1	1:L:246:ARG:HG3	2.52	0.44
1:L:171:TYR:CE1	1:L:217:MET:HG3	2.53	0.44
1:C:137:ALA:HB1	1:C:171:TYR:HB3	1.99	0.43
1:D:142:ASP:OD1	1:D:142:ASP:N	2.51	0.43
1:D:210:GLN:OE1	1:D:212:ARG:NH1	2.52	0.43
1:K:31:ILE:HD11	1:K:227:THR:HG21	2.01	0.43
1:A:132:GLY:HA2	1:A:207:TYR:CE2	2.53	0.43
1:C:17:LEU:HD12	1:C:26:LYS:HD3	2.00	0.43
1:L:137:ALA:HB1	1:L:171:TYR:HB3	2.00	0.43
1:L:152:ASP:HB3	1:L:156:THR:H	1.83	0.43
1:L:208:MET:HB2	1:L:213:LEU:HD23	1.99	0.43
1:A:9:LEU:HD13	1:A:89:LEU:HG	2.00	0.43
1:A:276:LEU:O	1:A:282:GLY:HA3	2.18	0.43
1:B:142:ASP:OD1	1:B:142:ASP:N	2.52	0.43
1:C:142:ASP:N	1:C:142:ASP:OD1	2.51	0.43
1:J:249:LEU:HD22	1:J:249:LEU:O	2.18	0.43
1:K:142:ASP:N	1:K:142:ASP:OD1	2.51	0.43
1:L:122:LEU:HD22	1:L:222:TYR:OH	2.19	0.43
1:B:177:TYR:CD1	1:B:177:TYR:N	2.87	0.43
1:C:19:PRO:HD2	1:D:33:ASP:O	2.19	0.43
1:D:112:ASN:HB3	1:D:114:PHE:CE1	2.53	0.43
1:J:150:GLU:O	1:J:158:VAL:HG22	2.19	0.43
1:K:74:TRP:HE1	1:K:255:GLU:HG3	1.83	0.43
1:L:142:ASP:HB2	1:L:145:ARG:HG3	2.00	0.43
1:B:210:GLN:OE1	1:B:212:ARG:NH1	2.52	0.43
1:K:112:ASN:HB3	1:K:114:PHE:CE1	2.54	0.43
1:A:165:LEU:O	1:A:167:PRO:HD3	2.18	0.43
1:B:9:LEU:HG	1:B:107:LEU:HD11	2.00	0.43
1:B:150:GLU:O	1:B:158:VAL:HG22	2.17	0.43
1:B:220:ARG:NH1	1:D:284:TYR:OH	2.52	0.43
1:C:132:GLY:HA3	1:C:212:ARG:HB3	2.01	0.43
1:B:144:GLU:HG2	1:B:145:ARG:HG2	2.01	0.43
1:D:165:LEU:HD12	1:D:165:LEU:HA	1.89	0.43
1:D:249:LEU:O	1:D:249:LEU:HD22	2.19	0.43
1:L:112:ASN:HB3	1:L:114:PHE:CE1	2.54	0.43
1:L:227:THR:CG2	1:L:233:LEU:HD13	2.49	0.43
1:A:192:PRO:HB3	1:A:197:GLU:N	2.34	0.42
1:B:205:ARG:O	1:B:208:MET:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:LEU:HD13	1:C:89:LEU:HG	2.02	0.42
1:I:142:ASP:OD1	1:I:142:ASP:N	2.49	0.42
1:I:192:PRO:HB3	1:I:197:GLU:N	2.34	0.42
1:K:137:ALA:HB1	1:K:171:TYR:HB3	2.00	0.42
1:K:192:PRO:HB3	1:K:197:GLU:N	2.34	0.42
1:B:34:LYS:HE2	1:B:251:VAL:O	2.19	0.42
1:B:165:LEU:HD12	1:B:165:LEU:HA	1.90	0.42
1:I:152:ASP:HB3	1:I:156:THR:H	1.84	0.42
1:K:150:GLU:O	1:K:158:VAL:HG22	2.19	0.42
1:K:195:ARG:O	1:K:197:GLU:HG2	2.20	0.42
1:L:74:TRP:NE1	1:L:255:GLU:HG3	2.35	0.42
1:A:150:GLU:O	1:A:158:VAL:HG22	2.19	0.42
1:B:31:ILE:HB	1:B:39:TYR:CE1	2.55	0.42
1:J:227:THR:CG2	1:J:233:LEU:HD13	2.50	0.42
1:B:205:ARG:CD	1:B:208:MET:CE	2.94	0.42
1:D:61:THR:O	1:D:65:GLN:HG3	2.19	0.42
1:L:263:PHE:N	1:L:263:PHE:CD2	2.88	0.42
1:A:152:ASP:HB3	1:A:156:THR:H	1.84	0.42
1:B:112:ASN:HB3	1:B:114:PHE:CE1	2.55	0.42
1:L:144:GLU:HG2	1:L:145:ARG:HG2	2.00	0.42
1:L:249:LEU:HD12	1:L:249:LEU:C	2.40	0.42
1:A:108:VAL:HA	1:A:175:GLY:O	2.19	0.42
1:B:9:LEU:HD13	1:B:89:LEU:HD13	2.01	0.42
1:L:31:ILE:HB	1:L:39:TYR:CE1	2.55	0.42
1:A:74:TRP:NE1	1:A:255:GLU:HG3	2.35	0.42
1:B:71:GLY:HA3	1:B:78:LEU:HG	2.02	0.42
1:K:165:LEU:HD12	1:K:165:LEU:HA	1.89	0.42
1:B:7:ILE:HG12	1:B:53:LEU:HB3	2.02	0.41
1:J:137:ALA:HB1	1:J:171:TYR:HB3	2.02	0.41
1:K:119:LEU:HB3	1:K:120:PRO:HD3	2.02	0.41
1:K:278:LYS:HD3	1:L:15:THR:OG1	2.20	0.41
1:D:31:ILE:HD11	1:D:227:THR:HG21	2.03	0.41
1:I:7:ILE:HG12	1:I:53:LEU:HB3	2.01	0.41
1:J:31:ILE:HD11	1:J:227:THR:HG21	2.02	0.41
1:J:220:ARG:NH1	1:L:284:TYR:CZ	2.88	0.41
1:J:269:VAL:HG11	1:J:289:VAL:CG1	2.50	0.41
1:K:142:ASP:HB2	1:K:145:ARG:HG3	2.01	0.41
1:A:165:LEU:C	1:A:167:PRO:HD3	2.41	0.41
1:A:195:ARG:O	1:A:197:GLU:HG2	2.21	0.41
1:D:74:TRP:NE1	1:D:255:GLU:HG3	2.35	0.41
1:J:227:THR:HG23	1:J:233:LEU:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:LEU:HB3	1:D:120:PRO:HD3	2.02	0.41
1:I:31:ILE:HD11	1:I:227:THR:HG21	2.03	0.41
1:I:247:GLN:HA	1:K:222:TYR:O	2.20	0.41
1:I:260:ARG:NH1	1:I:260:ARG:CG	2.81	0.41
1:K:74:TRP:NE1	1:K:255:GLU:HG3	2.35	0.41
1:L:210:GLN:OE1	1:L:212:ARG:NH1	2.53	0.41
1:A:137:ALA:HB1	1:A:171:TYR:HB3	2.01	0.41
1:B:152:ASP:HB3	1:B:156:THR:H	1.85	0.41
1:C:112:ASN:HB3	1:C:114:PHE:CE1	2.55	0.41
1:C:119:LEU:HB3	1:C:120:PRO:HD3	2.02	0.41
1:J:132:GLY:HA2	1:J:207:TYR:HE2	1.84	0.41
1:K:164:PRO:CG	1:K:167:PRO:HA	2.51	0.41
1:K:210:GLN:OE1	1:K:212:ARG:NH1	2.54	0.41
1:B:142:ASP:HB2	1:B:145:ARG:HG3	2.03	0.41
1:C:108:VAL:HA	1:C:175:GLY:O	2.21	0.41
1:J:50:ARG:HD3	1:J:263:PHE:CZ	2.56	0.41
1:L:61:THR:N	1:L:62:PRO:CD	2.84	0.41
1:B:198:LEU:N	1:B:198:LEU:CD1	2.73	0.41
1:B:263:PHE:N	1:B:263:PHE:CD2	2.88	0.41
1:I:74:TRP:HE1	1:I:255:GLU:HG3	1.86	0.41
1:I:137:ALA:HB1	1:I:171:TYR:HB3	2.02	0.41
1:I:177:TYR:CD1	1:I:177:TYR:N	2.88	0.41
1:J:7:ILE:HG12	1:J:53:LEU:HB3	2.03	0.41
1:L:31:ILE:HD11	1:L:227:THR:HG21	2.02	0.41
1:L:165:LEU:O	1:L:167:PRO:HD3	2.21	0.41
1:B:196:GLY:HA2	1:J:65:GLN:OE1	2.21	0.40
1:D:108:VAL:HA	1:D:175:GLY:O	2.21	0.40
1:D:152:ASP:HB3	1:D:156:THR:H	1.86	0.40
1:J:132:GLY:HA3	1:J:212:ARG:HB3	2.03	0.40
1:L:142:ASP:OD1	1:L:142:ASP:N	2.54	0.40
1:K:243:ILE:HD13	1:K:243:ILE:HA	1.88	0.40
1:L:165:LEU:HD12	1:L:165:LEU:HA	1.92	0.40
1:C:61:THR:O	1:C:65:GLN:HG3	2.22	0.40
1:C:165:LEU:HD12	1:C:165:LEU:HA	1.92	0.40
1:I:119:LEU:HB3	1:I:120:PRO:HD3	2.03	0.40
1:J:2:LYS:O	1:J:2:LYS:HG2	2.21	0.40
1:J:263:PHE:N	1:J:263:PHE:CD2	2.90	0.40
1:D:89:LEU:HB3	1:D:200:ILE:HD11	2.03	0.40
1:I:112:ASN:HB3	1:I:114:PHE:CE1	2.56	0.40
1:J:144:GLU:HG2	1:J:145:ARG:HG2	2.03	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	288/292 (99%)	280 (97%)	8 (3%)	0	100	100
1	B	287/292 (98%)	278 (97%)	9 (3%)	0	100	100
1	C	278/292 (95%)	273 (98%)	5 (2%)	0	100	100
1	D	279/292 (96%)	273 (98%)	6 (2%)	0	100	100
1	I	287/292 (98%)	279 (97%)	8 (3%)	0	100	100
1	J	287/292 (98%)	278 (97%)	8 (3%)	1 (0%)	41	64
1	K	280/292 (96%)	274 (98%)	6 (2%)	0	100	100
1	L	280/292 (96%)	275 (98%)	5 (2%)	0	100	100
All	All	2266/2336 (97%)	2210 (98%)	55 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	289	VAL

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	244/245 (100%)	234 (96%)	10 (4%)	30	56
1	B	243/245 (99%)	235 (97%)	8 (3%)	38	64
1	C	238/245 (97%)	232 (98%)	6 (2%)	47	73
1	D	239/245 (98%)	232 (97%)	7 (3%)	42	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	243/245 (99%)	235 (97%)	8 (3%)	38	64
1	J	243/245 (99%)	232 (96%)	11 (4%)	27	52
1	K	239/245 (98%)	230 (96%)	9 (4%)	33	59
1	L	240/245 (98%)	235 (98%)	5 (2%)	53	77
All	All	1929/1960 (98%)	1865 (97%)	64 (3%)	38	64

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

Mol	Chain	Res	Type
1	A	135	VAL
1	A	145	ARG
1	A	165	LEU
1	A	169	SER
1	A	195	ARG
1	A	197	GLU
1	A	198	LEU
1	A	225	LEU
1	A	281	TYR
1	A	290	LYS
1	B	145	ARG
1	B	169	SER
1	B	190	LEU
1	B	195	ARG
1	B	197	GLU
1	B	205	ARG
1	B	281	TYR
1	B	290	LYS
1	C	122	LEU
1	C	169	SER
1	C	190	LEU
1	C	197	GLU
1	C	281	TYR
1	C	290	LYS
1	D	122	LEU
1	D	145	ARG
1	D	169	SER
1	D	197	GLU
1	D	225	LEU
1	D	249	LEU
1	D	290	LYS
1	I	91	GLN

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Mol	Chain	Res	Type
1	I	145	ARG
1	I	169	SER
1	I	195	ARG
1	I	197	GLU
1	I	225	LEU
1	I	281	TYR
1	I	290	LYS
1	J	107	LEU
1	J	122	LEU
1	J	145	ARG
1	J	160	LEU
1	J	169	SER
1	J	195	ARG
1	J	197	GLU
1	J	203	ILE
1	J	225	LEU
1	J	249	LEU
1	J	281	TYR
1	K	107	LEU
1	K	122	LEU
1	K	135	VAL
1	K	169	SER
1	K	177	TYR
1	K	195	ARG
1	K	197	GLU
1	K	198	LEU
1	K	290	LYS
1	L	122	LEU
1	L	145	ARG
1	L	169	SER
1	L	197	GLU
1	L	290	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DTP	C	500	3	26,32,32	1.02	2 (7%)	30,50,50	3.51	9 (30%)
2	DTP	B	500	3	26,32,32	1.09	3 (11%)	30,50,50	1.59	7 (23%)
2	DTP	K	500	3	26,32,32	1.03	2 (7%)	30,50,50	3.05	7 (23%)
2	DTP	J	500	3	26,32,32	1.02	1 (3%)	30,50,50	3.47	9 (30%)
2	DTP	A	500	3	26,32,32	0.95	1 (3%)	30,50,50	1.59	6 (20%)
2	DTP	L	500	3	26,32,32	1.06	1 (3%)	30,50,50	1.69	6 (20%)
2	DTP	D	500	3	26,32,32	0.96	1 (3%)	30,50,50	1.63	7 (23%)
2	DTP	I	500	3	26,32,32	1.05	2 (7%)	30,50,50	1.81	6 (20%)

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
2	DTP	C	500	3	-	5/18/34/34	0/3/3/3
2	DTP	B	500	3	-	4/18/34/34	0/3/3/3
2	DTP	K	500	3	-	5/18/34/34	0/3/3/3
2	DTP	J	500	3	-	5/18/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTP	A	500	3	-	5/18/34/34	0/3/3/3
2	DTP	L	500	3	-	4/18/34/34	0/3/3/3
2	DTP	D	500	3	-	6/18/34/34	0/3/3/3
2	DTP	I	500	3	-	6/18/34/34	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	DTP	C5-C4	2.92	1.48	1.40
2	A	500	DTP	C5-C4	2.91	1.48	1.40
2	L	500	DTP	C5-C4	2.84	1.48	1.40
2	J	500	DTP	C5-C4	2.73	1.48	1.40
2	K	500	DTP	C5-C4	2.72	1.48	1.40
2	I	500	DTP	C5-C4	2.56	1.47	1.40
2	C	500	DTP	C5-C4	2.55	1.47	1.40
2	C	500	DTP	PG-O2G	-2.53	1.45	1.54
2	D	500	DTP	C5-C4	2.49	1.47	1.40
2	I	500	DTP	PB-O1B	2.24	1.58	1.50
2	K	500	DTP	PG-O3G	-2.19	1.46	1.54
2	B	500	DTP	C2-N3	2.17	1.35	1.32
2	B	500	DTP	PG-O2G	-2.04	1.47	1.54

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	DTP	O2G-PG-O1G	12.47	159.51	110.68
2	J	500	DTP	O2G-PG-O1G	12.42	159.30	110.68
2	K	500	DTP	O2G-PG-O1G	11.95	157.47	110.68
2	C	500	DTP	O2G-PG-O3B	-10.19	70.45	104.64
2	J	500	DTP	O2G-PG-O3B	-9.63	72.33	104.64
2	K	500	DTP	O2G-PG-O3B	-7.72	78.76	104.64
2	C	500	DTP	O3G-PG-O2G	-5.95	84.90	107.64
2	J	500	DTP	O3G-PG-O2G	-4.92	88.85	107.64
2	K	500	DTP	O3B-PG-O1G	-4.84	84.33	111.19
2	I	500	DTP	O2B-PB-O1B	4.51	134.56	112.24
2	A	500	DTP	O2G-PG-O1G	4.45	128.11	110.68
2	J	500	DTP	O3G-PG-O1G	-4.39	93.51	110.68
2	L	500	DTP	PA-O3A-PB	-4.21	118.38	132.83
2	J	500	DTP	O3B-PG-O1G	-4.16	88.13	111.19
2	I	500	DTP	O2G-PG-O1G	4.10	126.74	110.68
2	D	500	DTP	O2G-PG-O1G	3.97	126.21	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	DTP	O3B-PG-O1G	-3.81	90.08	111.19
2	I	500	DTP	O2G-PG-O3B	-3.78	91.96	104.64
2	I	500	DTP	PA-O3A-PB	-3.77	119.90	132.83
2	B	500	DTP	N3-C2-N1	-3.48	123.24	128.68
2	D	500	DTP	O2G-PG-O3B	-3.36	93.37	104.64
2	L	500	DTP	O2G-PG-O1G	3.21	123.26	110.68
2	L	500	DTP	O3G-PG-O3B	3.19	115.33	104.64
2	C	500	DTP	O3G-PG-O1G	-3.18	98.23	110.68
2	B	500	DTP	O2G-PG-O3B	-3.14	94.10	104.64
2	J	500	DTP	O3G-PG-O3B	3.11	115.07	104.64
2	I	500	DTP	N3-C2-N1	-3.10	123.84	128.68
2	B	500	DTP	O2G-PG-O1G	3.09	122.76	110.68
2	C	500	DTP	O3G-PG-O3B	3.08	114.96	104.64
2	D	500	DTP	PA-O3A-PB	-3.07	122.30	132.83
2	A	500	DTP	O2G-PG-O3B	-3.06	94.37	104.64
2	L	500	DTP	C4-C5-N7	-3.04	106.23	109.40
2	L	500	DTP	O2G-PG-O3B	-3.04	94.44	104.64
2	B	500	DTP	PA-O3A-PB	-3.02	122.45	132.83
2	C	500	DTP	N3-C2-N1	-2.99	124.01	128.68
2	J	500	DTP	N3-C2-N1	-2.96	124.05	128.68
2	K	500	DTP	N3-C2-N1	-2.94	124.08	128.68
2	A	500	DTP	PA-O3A-PB	-2.94	122.75	132.83
2	D	500	DTP	N3-C2-N1	-2.93	124.09	128.68
2	K	500	DTP	O3G-PG-O1G	-2.91	99.30	110.68
2	A	500	DTP	N3-C2-N1	-2.85	124.23	128.68
2	L	500	DTP	N3-C2-N1	-2.79	124.32	128.68
2	I	500	DTP	C4-C5-N7	-2.78	106.50	109.40
2	C	500	DTP	C4-C5-N7	-2.76	106.53	109.40
2	K	500	DTP	C4-C5-N7	-2.70	106.58	109.40
2	J	500	DTP	PA-O3A-PB	-2.63	123.80	132.83
2	A	500	DTP	O3G-PG-O3B	2.55	113.19	104.64
2	C	500	DTP	PA-O3A-PB	-2.53	124.14	132.83
2	J	500	DTP	C4-C5-N7	-2.50	106.79	109.40
2	D	500	DTP	C4-C5-N7	-2.48	106.81	109.40
2	B	500	DTP	O3G-PG-O3B	2.42	112.74	104.64
2	K	500	DTP	PA-O3A-PB	-2.40	124.59	132.83
2	D	500	DTP	O3G-PG-O3B	2.17	111.90	104.64
2	A	500	DTP	O2B-PB-O1B	2.12	122.71	112.24
2	B	500	DTP	C4-C5-N7	-2.09	107.23	109.40
2	B	500	DTP	O2B-PB-O1B	2.03	122.27	112.24
2	D	500	DTP	O2B-PB-O1B	2.02	122.23	112.24

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	DTP	C5'-O5'-PA-O1A
2	A	500	DTP	C5'-O5'-PA-O2A
2	B	500	DTP	C5'-O5'-PA-O1A
2	B	500	DTP	C5'-O5'-PA-O2A
2	C	500	DTP	PB-O3B-PG-O2G
2	C	500	DTP	C5'-O5'-PA-O1A
2	C	500	DTP	C5'-O5'-PA-O2A
2	D	500	DTP	C5'-O5'-PA-O1A
2	D	500	DTP	C5'-O5'-PA-O2A
2	I	500	DTP	PB-O3B-PG-O2G
2	I	500	DTP	C5'-O5'-PA-O1A
2	I	500	DTP	C5'-O5'-PA-O2A
2	J	500	DTP	PB-O3B-PG-O2G
2	J	500	DTP	C5'-O5'-PA-O1A
2	J	500	DTP	C5'-O5'-PA-O2A
2	K	500	DTP	PB-O3B-PG-O2G
2	K	500	DTP	C5'-O5'-PA-O1A
2	K	500	DTP	C5'-O5'-PA-O2A
2	L	500	DTP	C5'-O5'-PA-O1A
2	L	500	DTP	C5'-O5'-PA-O2A
2	I	500	DTP	PB-O3B-PG-O1G
2	I	500	DTP	PA-O3A-PB-O2B
2	J	500	DTP	PA-O3A-PB-O1B
2	K	500	DTP	PA-O3A-PB-O1B
2	A	500	DTP	C5'-O5'-PA-O3A
2	B	500	DTP	C5'-O5'-PA-O3A
2	C	500	DTP	C5'-O5'-PA-O3A
2	D	500	DTP	C5'-O5'-PA-O3A
2	I	500	DTP	C5'-O5'-PA-O3A
2	J	500	DTP	C5'-O5'-PA-O3A
2	K	500	DTP	C5'-O5'-PA-O3A
2	L	500	DTP	C5'-O5'-PA-O3A
2	A	500	DTP	PG-O3B-PB-O1B
2	A	500	DTP	PA-O3A-PB-O2B
2	B	500	DTP	PG-O3B-PB-O1B
2	D	500	DTP	PG-O3B-PB-O1B
2	D	500	DTP	PA-O3A-PB-O1B
2	D	500	DTP	PA-O3A-PB-O2B
2	L	500	DTP	PA-O3A-PB-O2B
2	C	500	DTP	C4'-C5'-O5'-PA

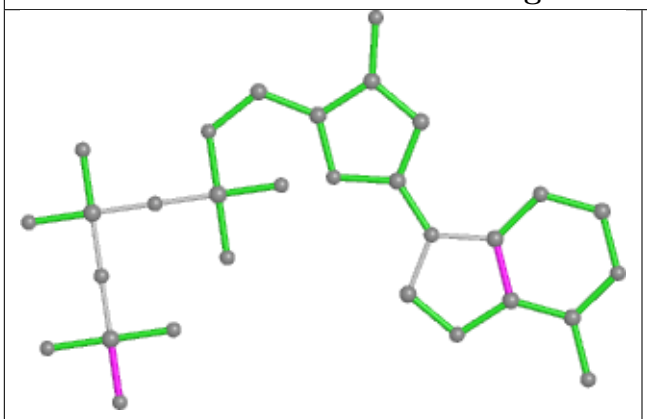
There are no ring outliers.

3 monomers are involved in 3 short contacts:

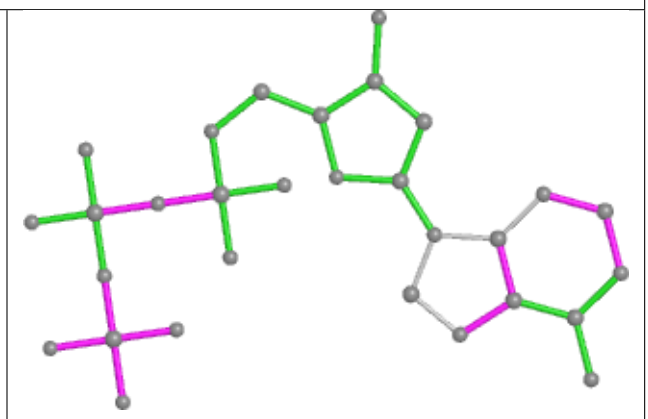
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	DTP	1	0
2	K	500	DTP	1	0
2	J	500	DTP	1	0

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.

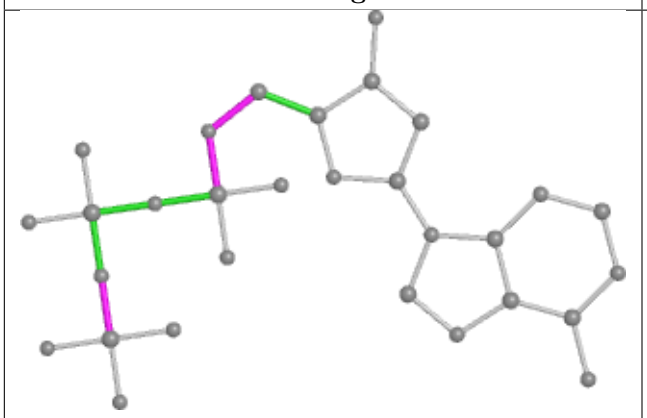
Ligand DTP C 500



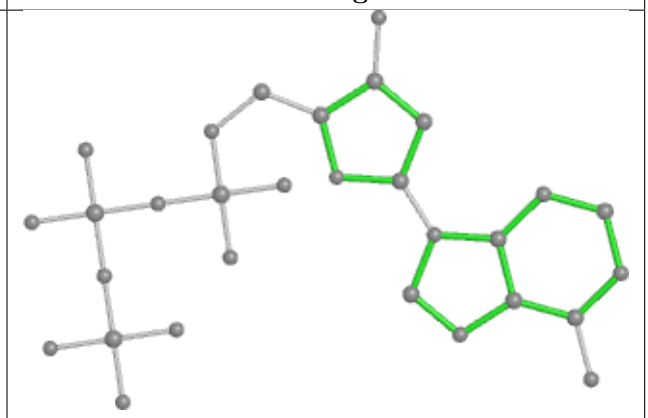
Bond lengths



Bond angles

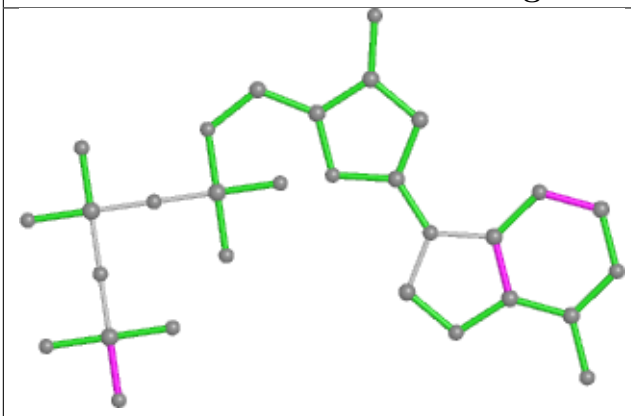


Torsions

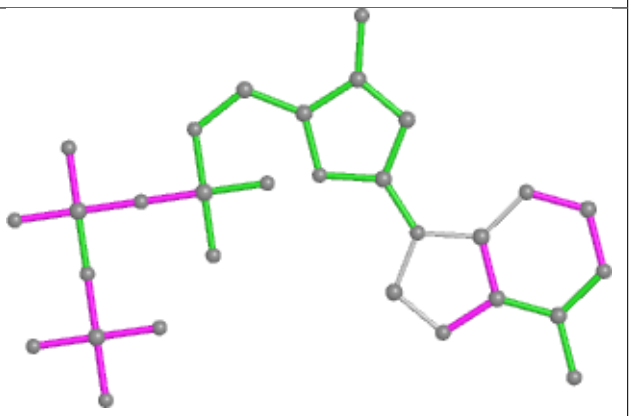


Rings

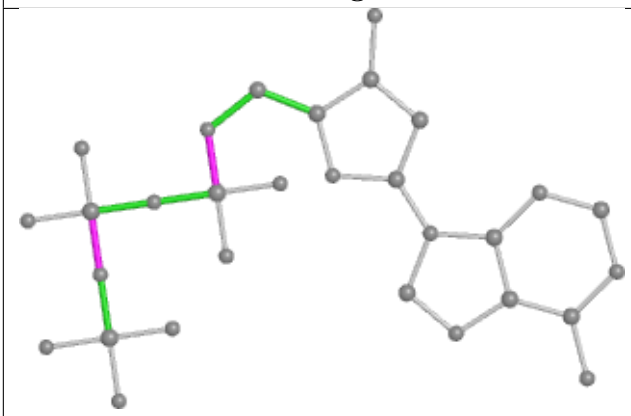
Ligand DTP B 500



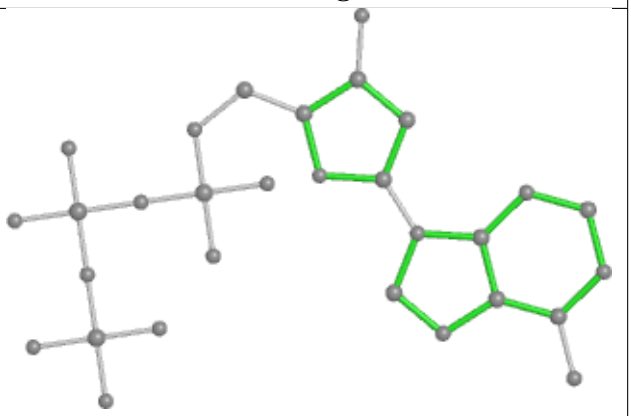
Bond lengths



Bond angles

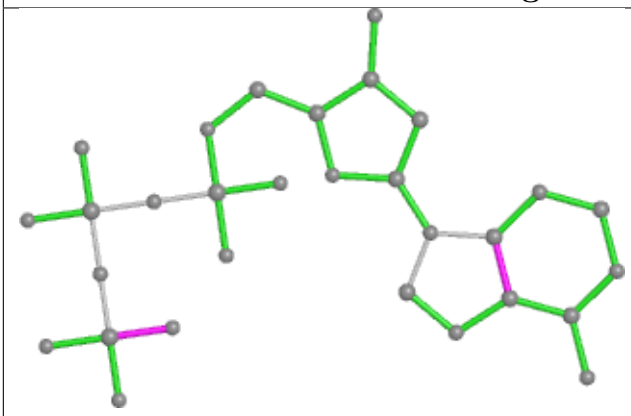


Torsions

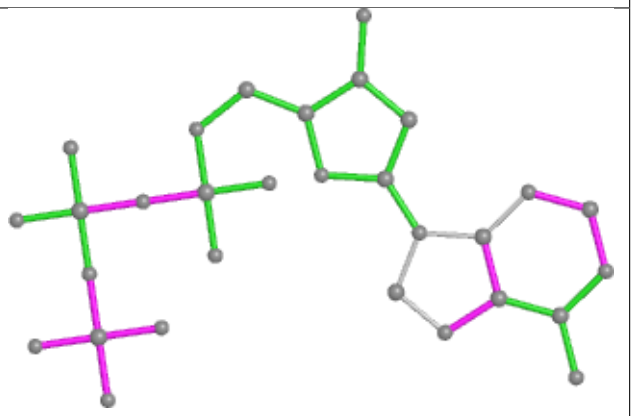


Rings

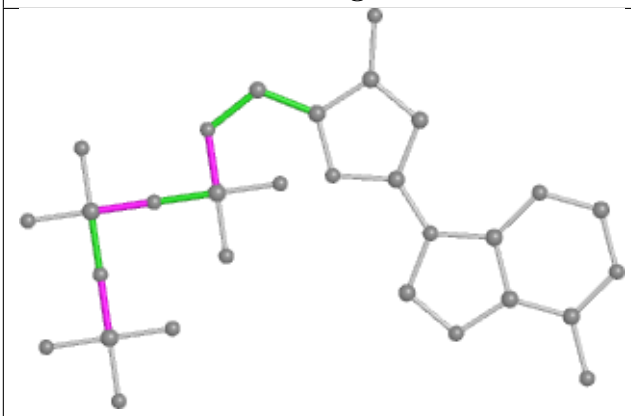
Ligand DTP K 500



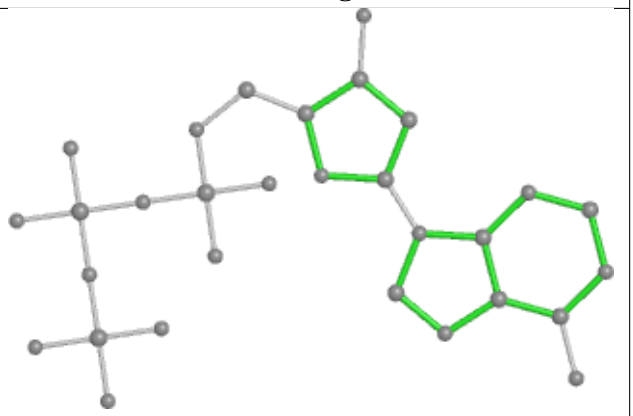
Bond lengths



Bond angles

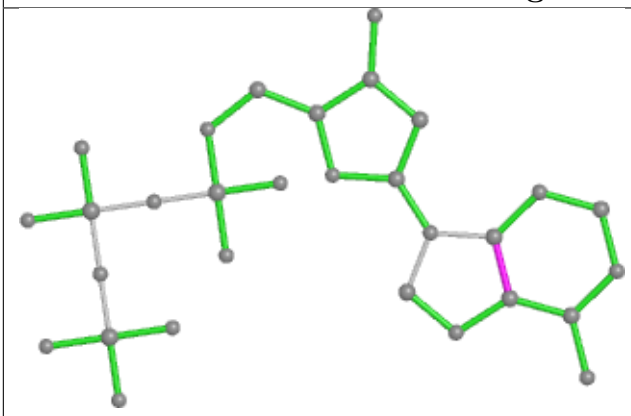


Torsions

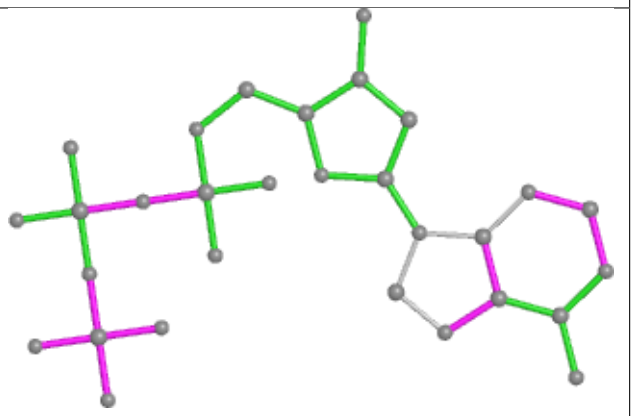


Rings

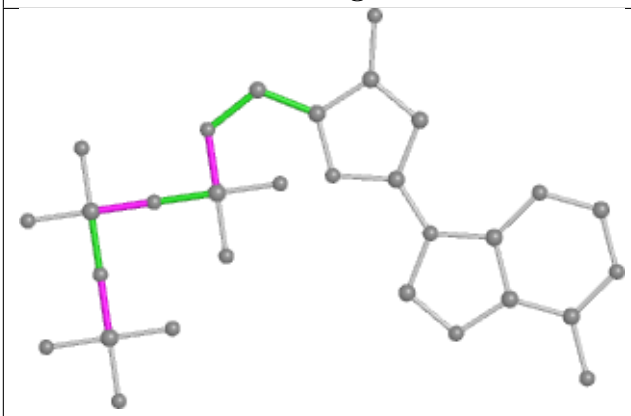
Ligand DTP J 500



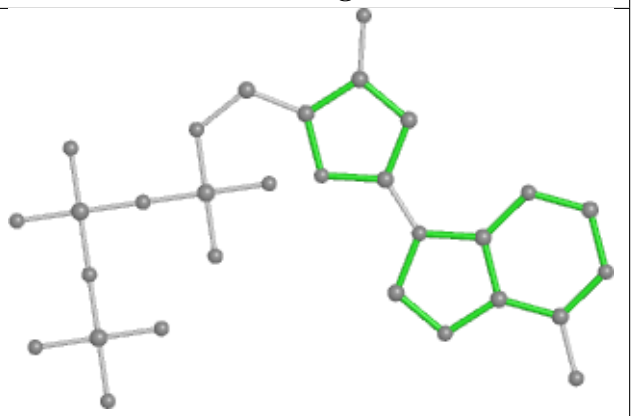
Bond lengths



Bond angles

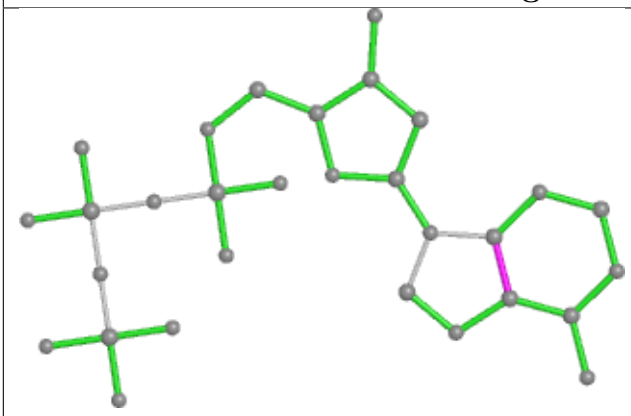


Torsions

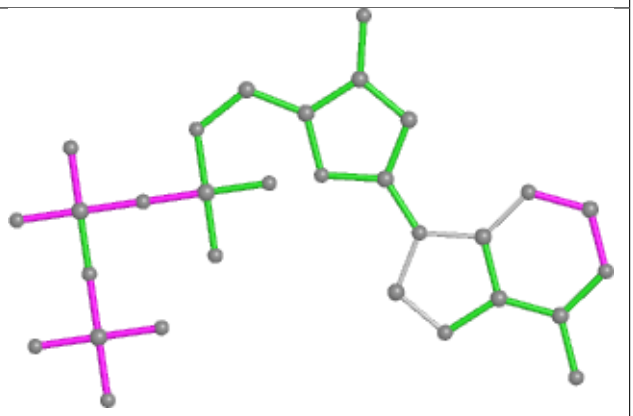


Rings

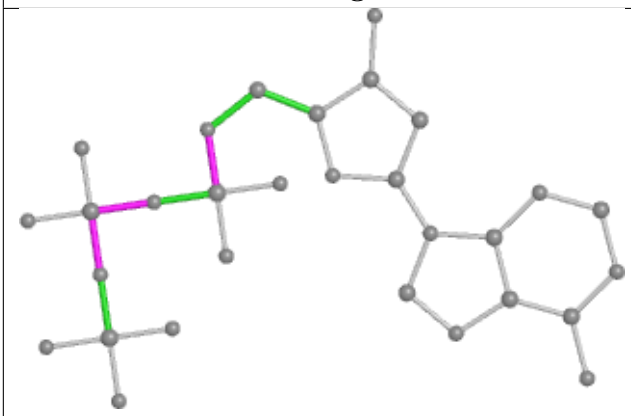
Ligand DTP A 500



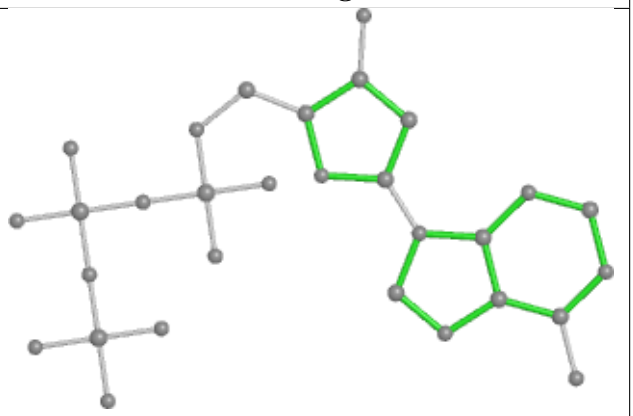
Bond lengths



Bond angles

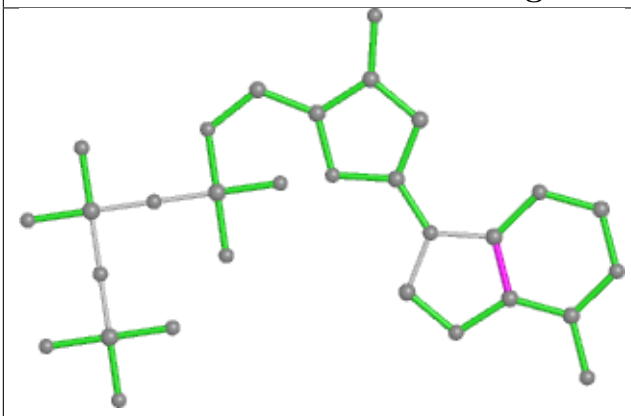


Torsions

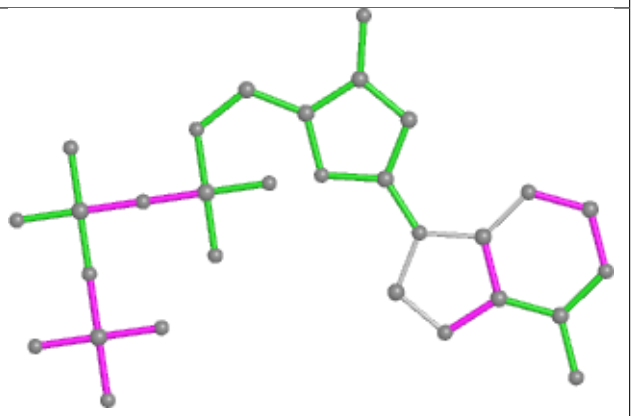


Rings

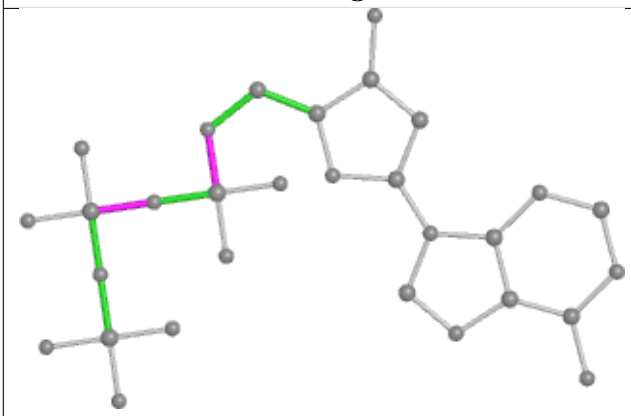
Ligand DTP L 500



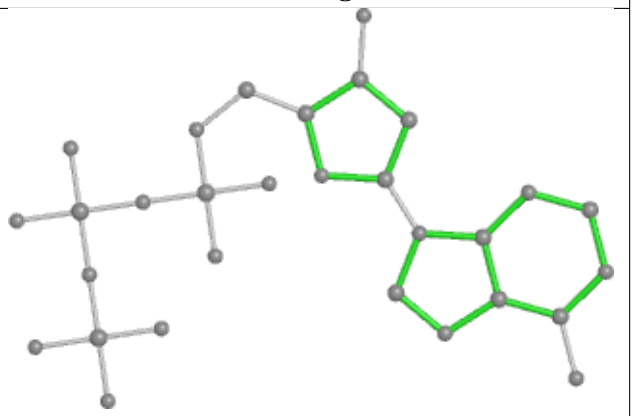
Bond lengths



Bond angles

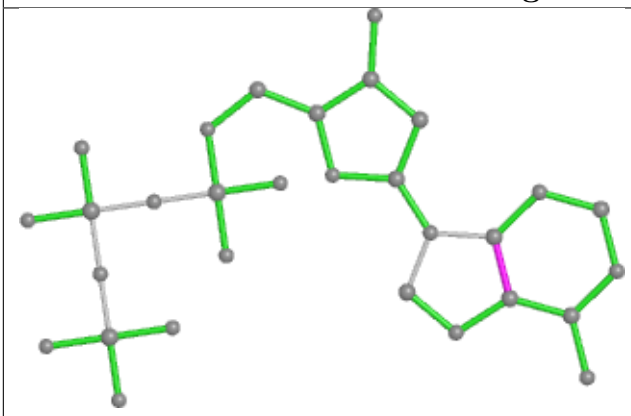


Torsions

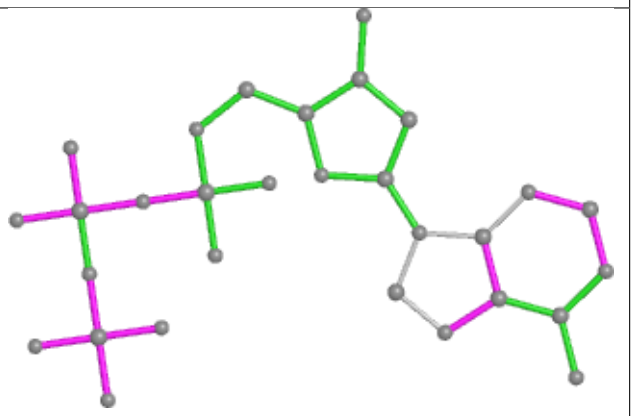


Rings

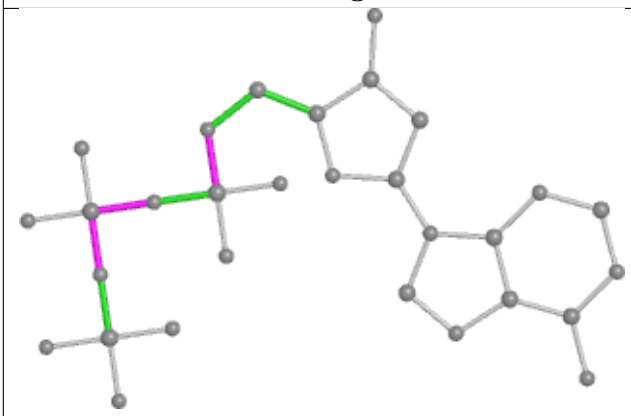
Ligand DTP D 500



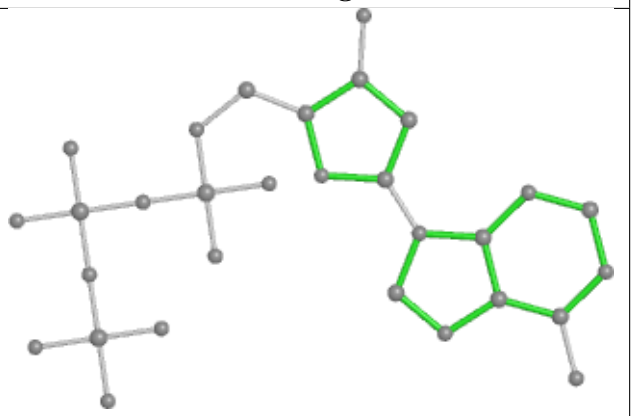
Bond lengths



Bond angles

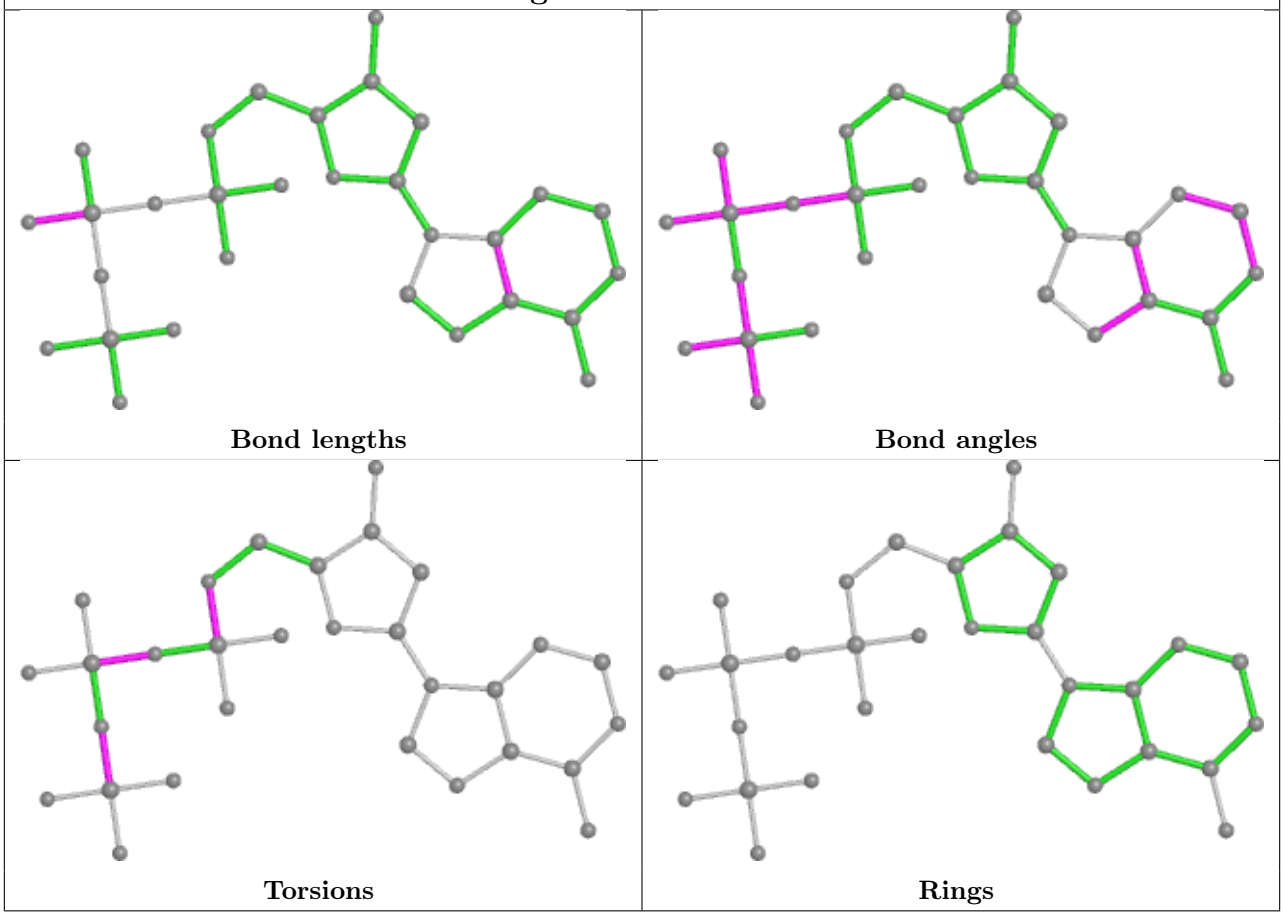


Torsions



Rings

Ligand DTP I 500



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	290/292 (99%)	-0.17	4 (1%) 75 71	28, 58, 116, 148	0
1	B	289/292 (98%)	-0.11	5 (1%) 70 66	32, 64, 120, 161	0
1	C	282/292 (96%)	0.14	13 (4%) 32 26	37, 84, 128, 160	0
1	D	283/292 (96%)	0.32	21 (7%) 14 10	40, 89, 137, 165	0
1	I	289/292 (98%)	-0.18	3 (1%) 82 80	35, 64, 117, 148	0
1	J	289/292 (98%)	0.02	9 (3%) 49 42	34, 64, 124, 163	0
1	K	284/292 (97%)	0.65	41 (14%) 2 1	55, 104, 147, 205	0
1	L	284/292 (97%)	0.56	35 (12%) 4 2	51, 100, 144, 165	0
All	All	2290/2336 (98%)	0.15	131 (5%) 23 18	28, 81, 133, 205	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	193	SER	8.1
1	K	194	ALA	7.5
1	L	211	GLY	6.3
1	L	210	GLN	6.2
1	L	208	MET	5.9
1	J	196	GLY	5.2
1	L	158	VAL	5.2
1	K	289	VAL	5.1
1	C	154	LYS	4.9
1	D	289	VAL	4.9
1	K	275	PRO	4.9
1	K	84	PRO	4.8
1	L	209	GLU	4.6
1	L	212	ARG	4.6
1	K	198	LEU	4.5
1	D	190	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	158	VAL	4.3
1	K	276	LEU	4.3
1	L	214	SER	4.1
1	K	190	LEU	4.0
1	L	154	LYS	4.0
1	L	213	LEU	3.9
1	K	157	ALA	3.8
1	J	192	PRO	3.8
1	K	102	HIS	3.7
1	K	204	ASN	3.7
1	L	153	GLN	3.7
1	L	127	VAL	3.6
1	C	158	VAL	3.6
1	D	187	ALA	3.6
1	L	129	LYS	3.6
1	D	209	GLU	3.5
1	D	3	THR	3.5
1	L	2	LYS	3.5
1	K	154	LYS	3.4
1	K	262	ASN	3.4
1	L	152	ASP	3.4
1	L	157	ALA	3.3
1	C	155	GLY	3.3
1	K	151	PHE	3.3
1	L	94	ILE	3.3
1	J	157	ALA	3.3
1	D	208	MET	3.3
1	K	166	GLN	3.3
1	C	170	ASN	3.3
1	C	152	ASP	3.2
1	K	103	ASP	3.2
1	D	189	ASN	3.2
1	K	214	SER	3.1
1	J	212	ARG	3.1
1	K	208	MET	3.1
1	L	160	LEU	3.0
1	K	197	GLU	3.0
1	L	215	VAL	3.0
1	D	264	ILE	2.9
1	K	134	THR	2.9
1	B	161	GLU	2.8
1	K	93	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	169	SER	2.8
1	D	204	ASN	2.8
1	L	205	ARG	2.8
1	C	3	THR	2.8
1	K	168	LYS	2.8
1	C	157	ALA	2.8
1	K	209	GLU	2.7
1	D	211	GLY	2.7
1	L	190	LEU	2.7
1	K	213	LEU	2.7
1	J	152	ASP	2.6
1	C	153	GLN	2.6
1	L	150	GLU	2.6
1	B	157	ALA	2.6
1	D	130	GLU	2.6
1	K	264	ILE	2.6
1	C	84	PRO	2.6
1	L	207	TYR	2.6
1	D	5	LYS	2.6
1	K	272	LEU	2.6
1	L	131	SER	2.6
1	C	128	ASN	2.5
1	L	99	PHE	2.5
1	D	269	VAL	2.5
1	A	1	MET	2.5
1	D	186	MET	2.5
1	B	130	GLU	2.5
1	K	268	GLN	2.5
1	K	94	ILE	2.4
1	K	215	VAL	2.4
1	K	271	GLU	2.3
1	I	154	LYS	2.3
1	K	192	PRO	2.3
1	D	159	SER	2.3
1	D	213	LEU	2.3
1	L	3	THR	2.3
1	B	151	PHE	2.3
1	K	210	GLN	2.3
1	L	133	ALA	2.3
1	K	212	ARG	2.3
1	K	155	GLY	2.3
1	L	290	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	126	ALA	2.3
1	A	154	LYS	2.3
1	J	154	LYS	2.3
1	K	196	GLY	2.2
1	L	186	MET	2.2
1	J	149	VAL	2.2
1	B	192	PRO	2.2
1	I	157	ALA	2.2
1	K	186	MET	2.2
1	K	285	LEU	2.2
1	D	191	LYS	2.1
1	L	189	ASN	2.1
1	D	210	GLN	2.1
1	A	161	GLU	2.1
1	L	171	TYR	2.1
1	J	290	LYS	2.1
1	L	206	ILE	2.1
1	C	150	GLU	2.1
1	C	156	THR	2.1
1	D	168	LYS	2.1
1	C	151	PHE	2.1
1	D	185	GLU	2.1
1	J	195	ARG	2.1
1	L	197	GLU	2.1
1	K	170	ASN	2.0
1	L	156	THR	2.0
1	K	165	LEU	2.0
1	L	89	LEU	2.0
1	L	126	ALA	2.0
1	A	220	ARG	2.0
1	I	130	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

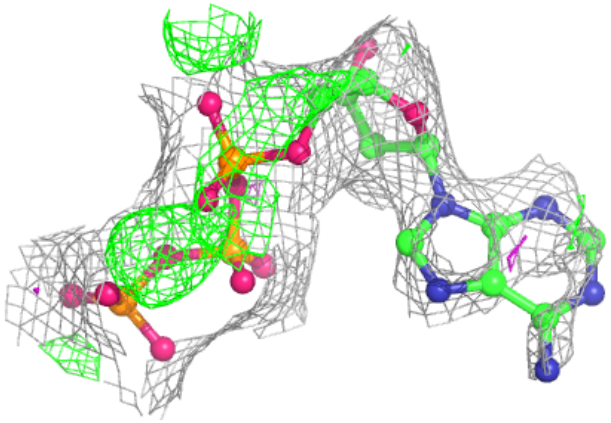
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

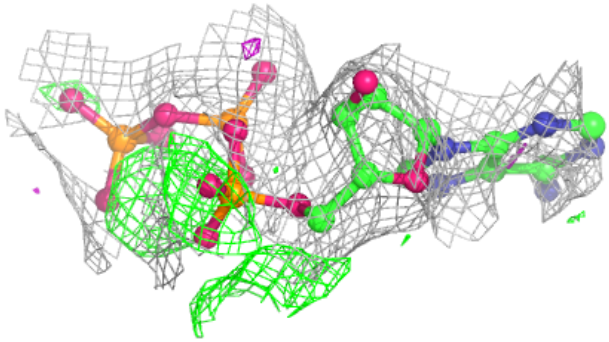
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	K	501	1/1	0.53	0.29	30,30,30,30	0
3	MG	D	501	1/1	0.65	0.21	67,67,67,67	0
3	MG	C	501	1/1	0.68	0.33	61,61,61,61	0
3	MG	L	501	1/1	0.72	0.20	69,69,69,69	0
3	MG	B	501	1/1	0.83	0.19	50,50,50,50	0
3	MG	A	501	1/1	0.84	0.28	61,61,61,61	0
3	MG	C	502	1/1	0.85	0.18	61,61,61,61	0
3	MG	D	502	1/1	0.88	0.19	66,66,66,66	0
3	MG	K	502	1/1	0.89	0.26	30,30,30,30	0
3	MG	I	501	1/1	0.89	0.13	64,64,64,64	0
3	MG	L	502	1/1	0.89	0.19	68,68,68,68	0
2	DTP	L	500	30/30	0.91	0.18	66,96,128,142	0
2	DTP	K	500	30/30	0.91	0.23	51,106,138,154	30
3	MG	A	502	1/1	0.93	0.27	53,53,53,53	0
3	MG	B	502	1/1	0.94	0.18	50,50,50,50	0
2	DTP	B	500	30/30	0.95	0.15	33,68,101,113	0
2	DTP	C	500	30/30	0.96	0.14	42,83,110,146	0
3	MG	J	501	1/1	0.96	0.29	69,69,69,69	0
3	MG	I	502	1/1	0.97	0.22	55,55,55,55	0
2	DTP	J	500	30/30	0.97	0.15	34,66,106,156	0
2	DTP	A	500	30/30	0.97	0.15	38,67,106,141	0
2	DTP	I	500	30/30	0.98	0.13	34,67,110,133	0
3	MG	J	502	1/1	0.98	0.21	57,57,57,57	0
2	DTP	D	500	30/30	0.98	0.14	55,79,110,121	0

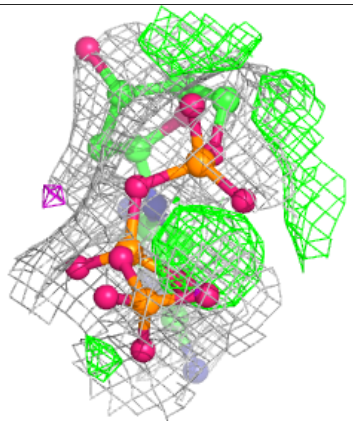
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DTP L 500:

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

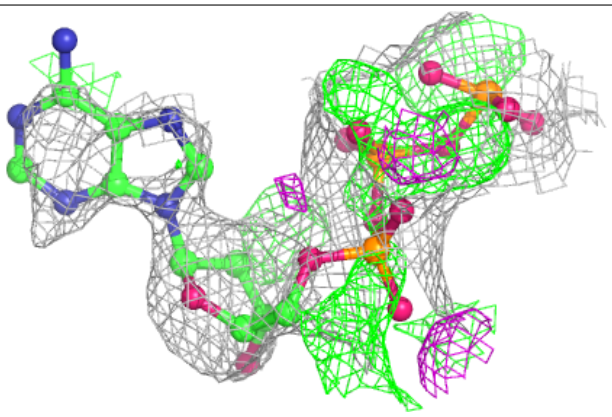


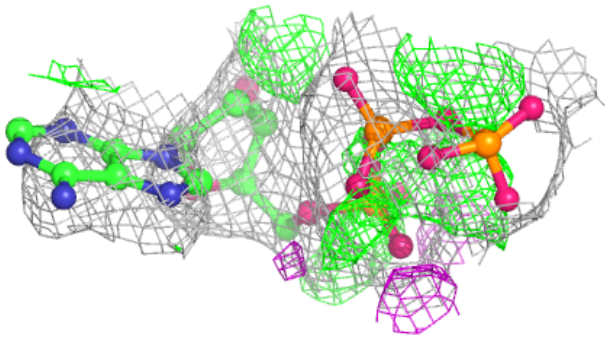


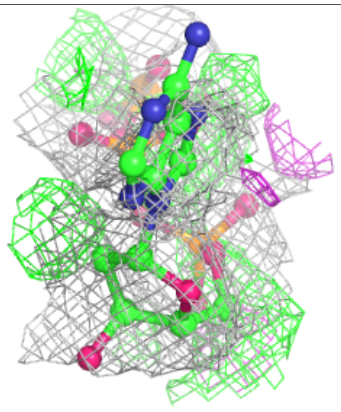


Electron density around DTP K 500:

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

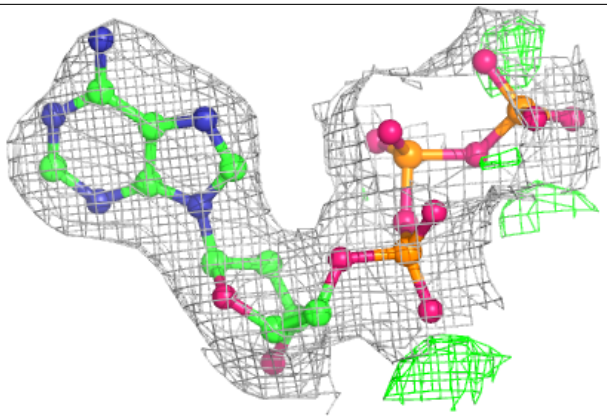


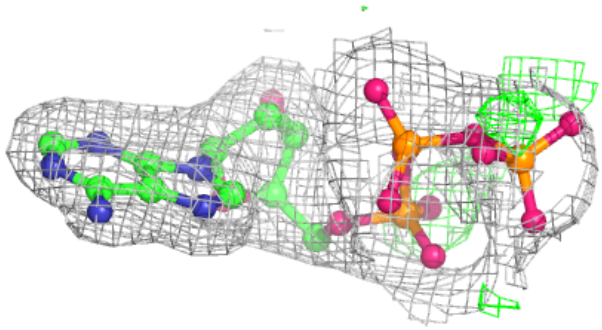




Electron density around DTP B 500:

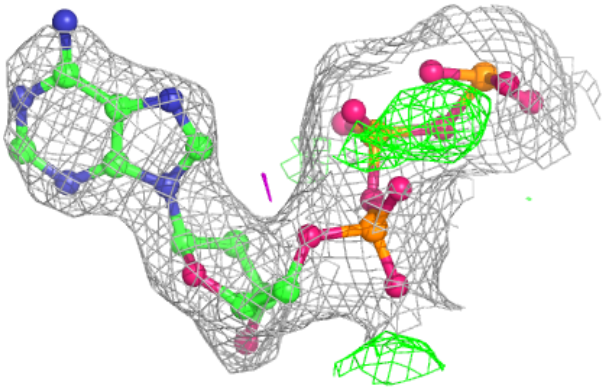
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

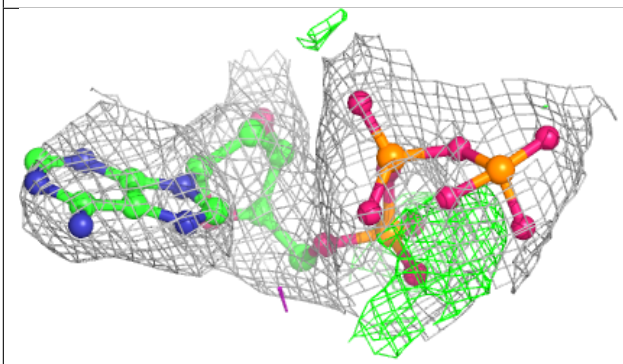


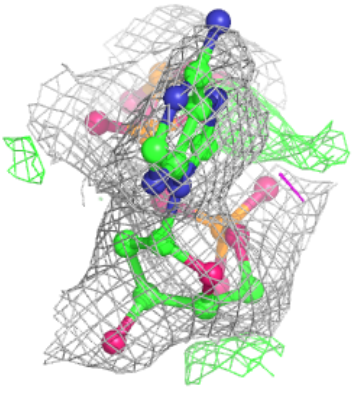


Electron density around DTP C 500:

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

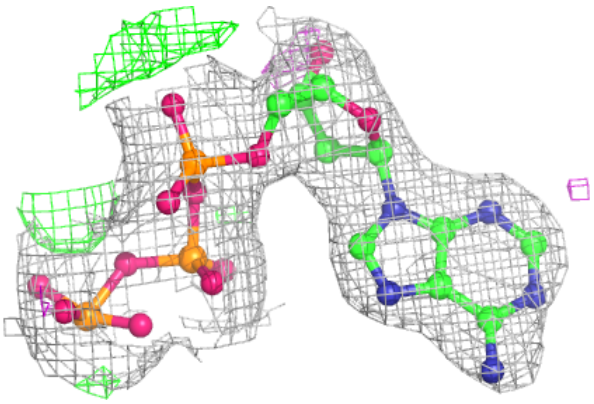


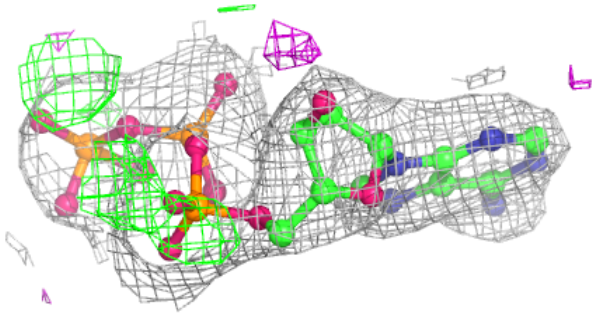


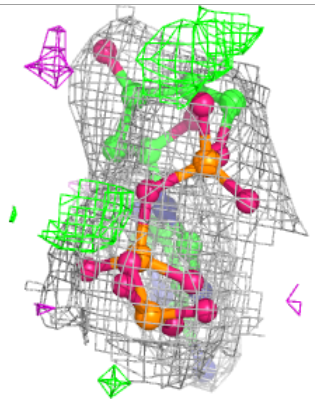


Electron density around DTP J 500:

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

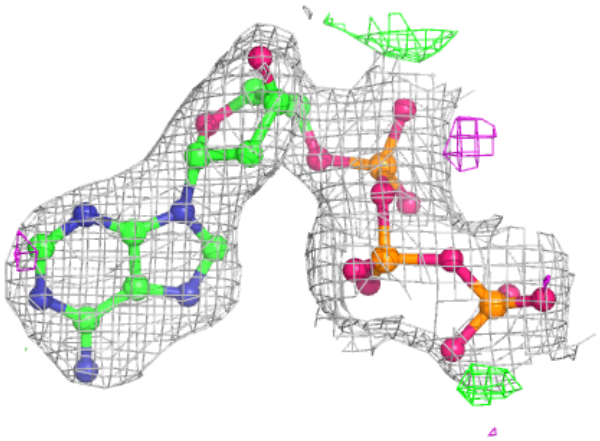


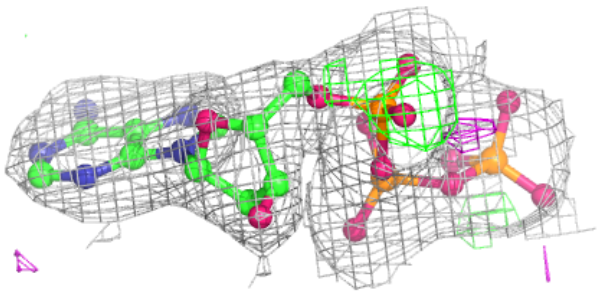




Electron density around DTP A 500:

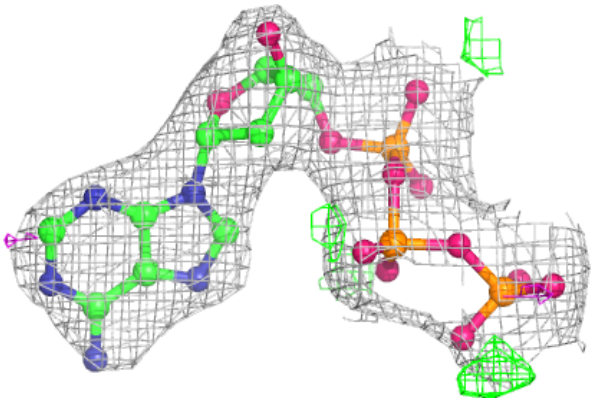
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

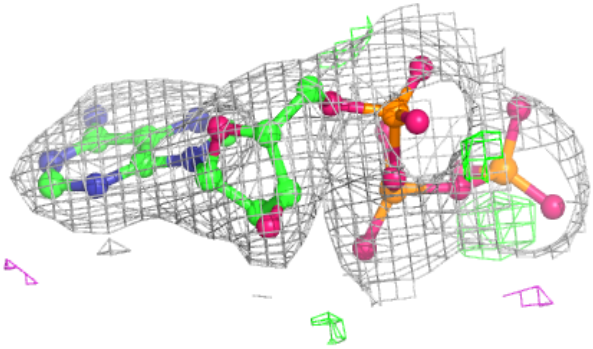


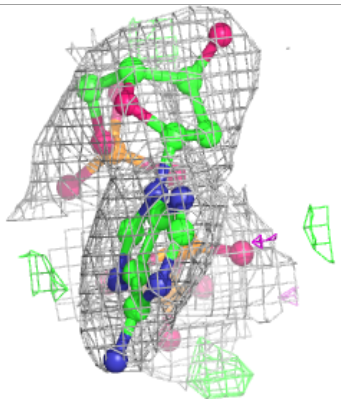


Electron density around DTP I 500:

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

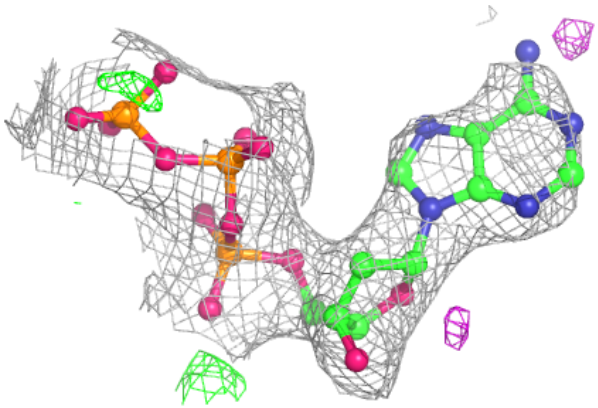


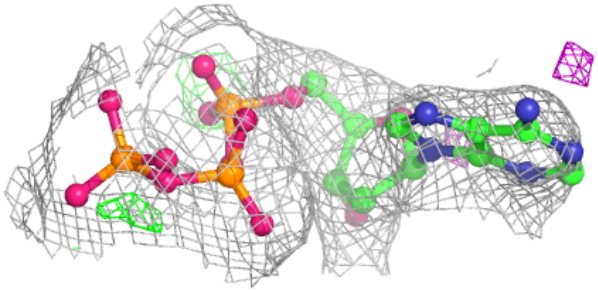


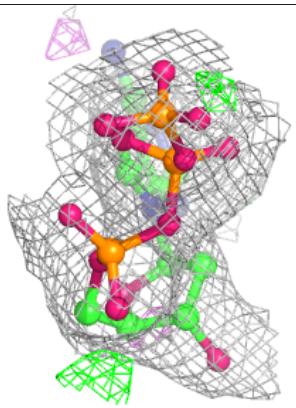


Electron density around DTP D 500:

$2mF_o$-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.