



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 05:36 AM EST

PDB ID : 4K4H
Title : Ternary crystal structures of a human DNA POLYMERASE LAMBDA IN COMPLEX WITH DNA AND (-)3TC-TP.
Authors : Vyas, R.; Suo, Z.
Deposited on : 2013-04-12
Resolution : 2.10 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

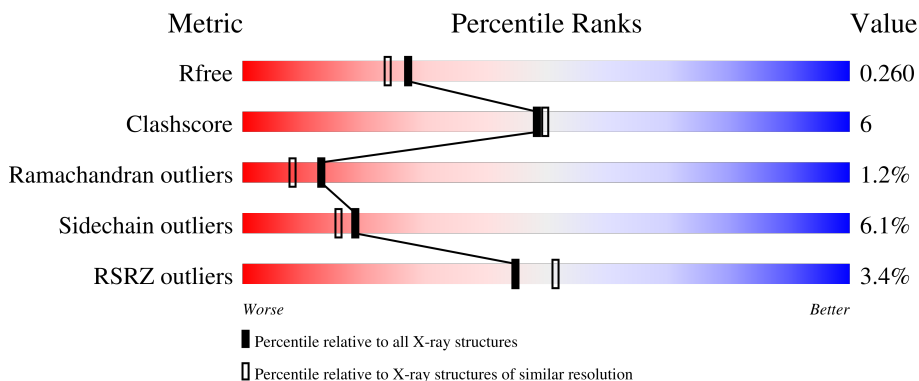
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	340	 3% 81% 13% . .
1	E	340	 4% 78% 14% . .
1	I	340	 5% 81% 15% . .
1	M	340	 2% 76% 16% . .
2	B	11	 73% 27%

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Mol	Chain	Length	Quality of chain
2	F	11	 55% 36% 9%
2	J	11	 82% 18%
2	N	11	 64% 27% 9%
3	C	6	 100%
3	G	6	 83% 17%
3	K	6	 100%
3	O	6	 83% 17%
4	D	4	 50% 25% 25%
4	H	4	 25% 50% 25%
4	L	4	 50% 50%
4	P	4	 75% 25%

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 12678 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 DNA polymerase lambda.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	327	Total 2578	C 1621	N 473	O 473	S 11	0	0	0
1	E	326	Total 2563	C 1612	N 470	O 469	S 12	0	0	0
1	I	332	Total 2623	C 1647	N 483	O 481	S 12	0	1	0
1	M	325	Total 2564	C 1614	N 467	O 471	S 12	0	1	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	MET	-	expression tag	UNP Q9UGP5
A	576	LEU	-	expression tag	UNP Q9UGP5
A	577	GLU	-	expression tag	UNP Q9UGP5
A	578	HIS	-	expression tag	UNP Q9UGP5
A	579	HIS	-	expression tag	UNP Q9UGP5
A	580	HIS	-	expression tag	UNP Q9UGP5
A	581	HIS	-	expression tag	UNP Q9UGP5
A	582	HIS	-	expression tag	UNP Q9UGP5
A	583	HIS	-	expression tag	UNP Q9UGP5
E	244	MET	-	expression tag	UNP Q9UGP5
E	576	LEU	-	expression tag	UNP Q9UGP5
E	577	GLU	-	expression tag	UNP Q9UGP5
E	578	HIS	-	expression tag	UNP Q9UGP5
E	579	HIS	-	expression tag	UNP Q9UGP5
E	580	HIS	-	expression tag	UNP Q9UGP5
E	581	HIS	-	expression tag	UNP Q9UGP5
E	582	HIS	-	expression tag	UNP Q9UGP5
E	583	HIS	-	expression tag	UNP Q9UGP5
I	244	MET	-	expression tag	UNP Q9UGP5
I	576	LEU	-	expression tag	UNP Q9UGP5
I	577	GLU	-	expression tag	UNP Q9UGP5

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Chain	Residue	Modelled	Actual	Comment	Reference
I	578	HIS	-	expression tag	UNP Q9UGP5
I	579	HIS	-	expression tag	UNP Q9UGP5
I	580	HIS	-	expression tag	UNP Q9UGP5
I	581	HIS	-	expression tag	UNP Q9UGP5
I	582	HIS	-	expression tag	UNP Q9UGP5
I	583	HIS	-	expression tag	UNP Q9UGP5
M	244	MET	-	expression tag	UNP Q9UGP5
M	576	LEU	-	expression tag	UNP Q9UGP5
M	577	GLU	-	expression tag	UNP Q9UGP5
M	578	HIS	-	expression tag	UNP Q9UGP5
M	579	HIS	-	expression tag	UNP Q9UGP5
M	580	HIS	-	expression tag	UNP Q9UGP5
M	581	HIS	-	expression tag	UNP Q9UGP5
M	582	HIS	-	expression tag	UNP Q9UGP5
M	583	HIS	-	expression tag	UNP Q9UGP5

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	B	11	Total	C	N	O	P	0	0	0
			225	107	43	65	10			
2	F	11	Total	C	N	O	P	0	0	0
			225	107	43	65	10			
2	J	11	Total	C	N	O	P	0	0	0
			225	107	43	65	10			
2	N	11	Total	C	N	O	P	0	0	0
			225	107	43	65	10			

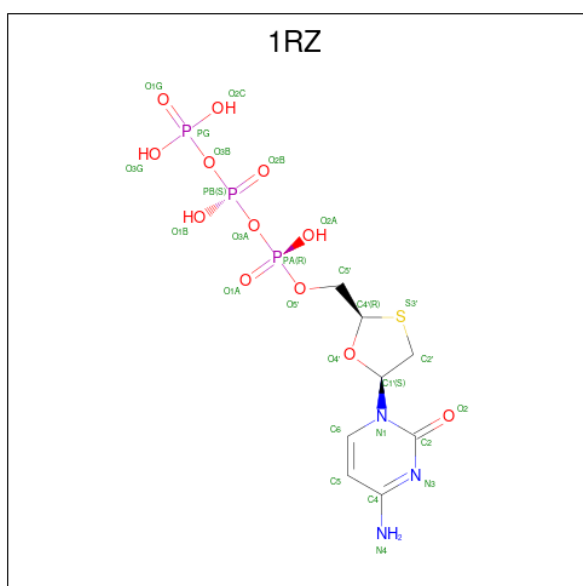
- Molecule 3 is a DNA chain called DNA (5'-D(*CP*AP*GP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	C	6	Total	C	N	O	P	0	0	0
			119	58	23	33	5			
3	G	6	Total	C	N	O	P	0	0	0
			119	58	23	33	5			
3	K	6	Total	C	N	O	P	0	0	0
			119	58	23	33	5			
3	O	6	Total	C	N	O	P	0	0	0
			119	58	23	33	5			

- Molecule 4 is a DNA chain called DNA (5'-D(P*GP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
4	D	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			
4	H	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			
4	L	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			
4	P	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			

- Molecule 5 is Lamivudine Triphosphate (three-letter code: 1RZ) (formula: $C_8H_{14}N_3O_{12}P_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	N	O	P	S	0	0
			27	8	3	12	3	1		
5	E	1	Total	C	N	O	P	S	0	0
			27	8	3	12	3	1		
5	I	1	Total	C	N	O	P	S	0	0
			27	8	3	12	3	1		
5	M	1	Total	C	N	O	P	S	0	0
			27	8	3	12	3	1		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

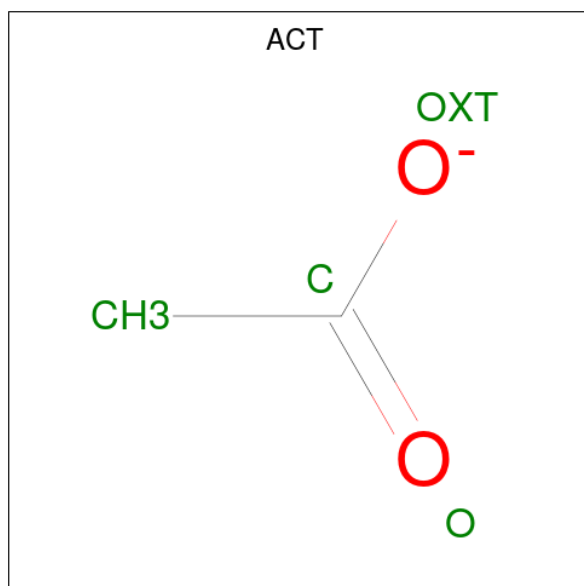
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	Ca	0	0
			6	6		
6	B	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	4	Total Ca 4 4	0	0
6	F	1	Total Ca 1 1	0	0
6	I	4	Total Ca 4 4	0	0
6	J	1	Total Ca 1 1	0	0
6	M	5	Total Ca 5 5	0	0
6	N	1	Total Ca 1 1	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

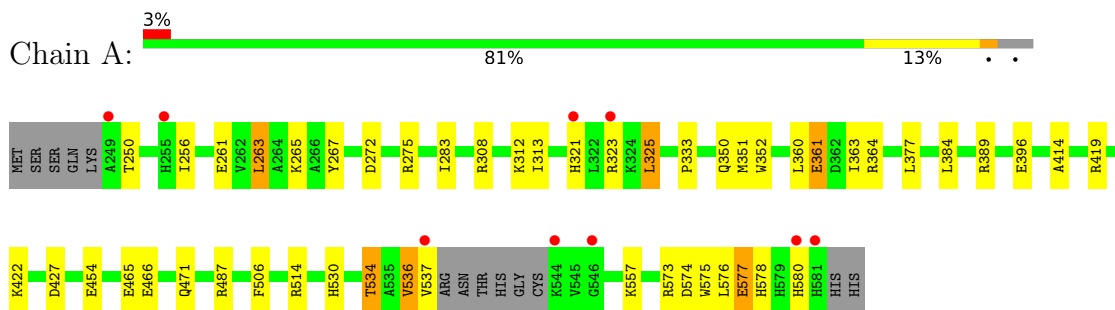
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	120	Total 120	O 120	0	0
8	B	19	Total 19	O 19	0	0
8	C	11	Total 11	O 11	0	0
8	D	1	Total 1	O 1	0	0
8	E	82	Total 82	O 82	0	0
8	F	7	Total 7	O 7	0	0
8	G	2	Total 2	O 2	0	0
8	H	2	Total 2	O 2	0	0
8	I	81	Total 81	O 81	0	0
8	J	6	Total 6	O 6	0	0
8	K	5	Total 5	O 5	0	0
8	M	143	Total 143	O 143	0	0
8	N	6	Total 6	O 6	0	0
8	O	5	Total 5	O 5	0	0
8	P	1	Total 1	O 1	0	0

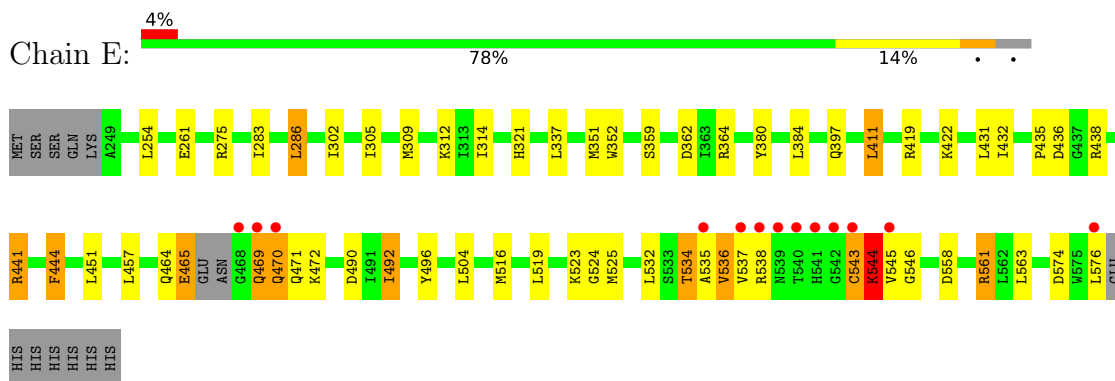
3 Residue-property plots i

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.

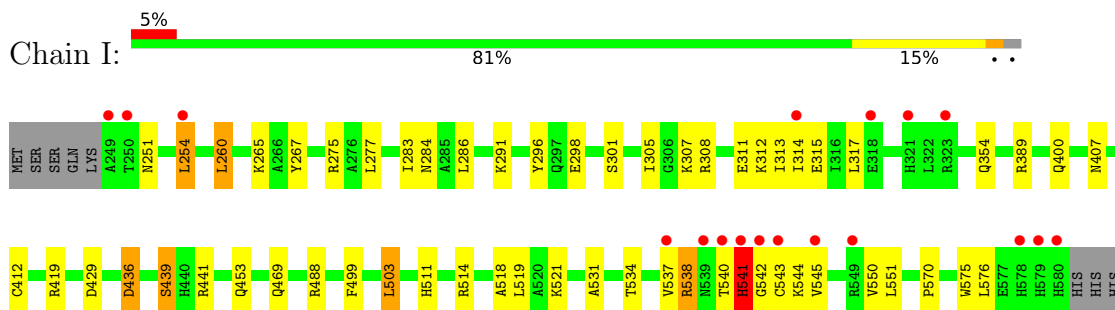
- Molecule 1: DNA polymerase lambda



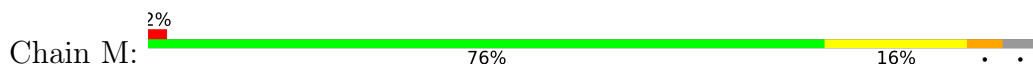
- Molecule 1: DNA polymerase lambda

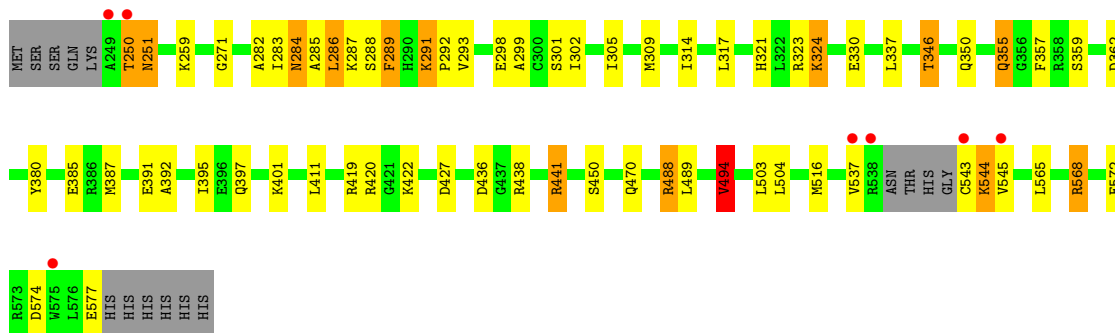


- Molecule 1: DNA polymerase lambda



- Molecule 1: DNA polymerase lambda





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

Chain B: 73% 27%



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

Chain F: 55% 36% 9%



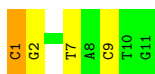
- Molecule 2: DNA (5'-D(*CP*GP*GP*CP*GP*GP*TP*AP*CP*TP*G)-3')

Chain J: 82% 18%



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

Chain N: 64% 27% 9%



- Molecule 3: DNA (5'-D(*CP*AP*GP*TP*AP*C)-3')

Chain C: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: DNA (5'-D(*CP*AP*GP*TP*AP*C)-3')

Chain G: 83% 17%



- Molecule 3: DNA (5'-D(*CP*AP*GP*TP*AP*C)-3')

Chain K: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: DNA (5'-D(*CP*AP*GP*TP*AP*C)-3')

Chain O: 83% 17%



- Molecule 4: DNA (5'-D(P*GP*CP*CP*G)-3')

Chain D: 50% 25% 25%



- Molecule 4: DNA (5'-D(P*GP*CP*CP*G)-3')

Chain H: 25% 50% 25%



- Molecule 4: DNA (5'-D(P*GP*CP*CP*G)-3')

Chain L: 50% 50%



- Molecule 4: DNA (5'-D(P*GP*CP*CP*G)-3')

Chain P: 75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	194.95Å 97.44Å 105.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.88 – 2.10 40.88 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.1 (40.88-2.10) 95.2 (40.88-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.204 , 0.260 0.209 , 0.260	Depositor DCC
R_{free} test set	5588 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtrriage
Anisotropy	0.235	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12678	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 1RZ, ACT, CA

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	0.95	2/2633 (0.1%)	0.97	9/3554 (0.3%)
1	E	0.86	1/2615 (0.0%)	0.92	6/3528 (0.2%)
1	I	0.83	1/2682 (0.0%)	0.93	5/3621 (0.1%)
1	M	0.92	1/2618 (0.0%)	1.11	11/3532 (0.3%)
2	B	0.78	0/252	1.02	0/388
2	F	0.58	0/252	1.05	2/388 (0.5%)
2	J	0.76	1/252 (0.4%)	1.19	1/388 (0.3%)
2	N	0.71	0/252	1.01	3/388 (0.8%)
3	C	0.84	0/133	0.95	0/203
3	G	0.76	1/133 (0.8%)	0.80	0/203
3	K	0.83	0/133	0.97	0/203
3	O	0.68	0/133	0.97	1/203 (0.5%)
4	D	1.27	1/92 (1.1%)	1.07	2/138 (1.4%)
4	H	1.31	1/92 (1.1%)	0.78	0/138
4	L	1.26	1/92 (1.1%)	0.87	0/138
4	P	1.13	1/92 (1.1%)	0.96	1/138 (0.7%)
All	All	0.89	11/12456 (0.1%)	0.99	41/17151 (0.2%)

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	E	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	DG	OP3-P	-10.90	1.48	1.61
4	L	1	DG	OP3-P	-10.41	1.48	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	DG	OP3-P	-10.20	1.49	1.61
4	P	1	DG	OP3-P	-9.43	1.49	1.61
1	I	429	ASP	CB-CG	6.44	1.65	1.51
1	E	490	ASP	CB-CG	6.43	1.65	1.51
3	G	3	DG	O3'-P	-5.30	1.54	1.61
1	A	575	TRP	CB-CG	-5.25	1.40	1.50
2	J	8	DA	O3'-P	-5.21	1.54	1.61
1	A	465	GLU	CD-OE2	5.20	1.31	1.25
1	M	450	SER	CB-OG	-5.17	1.35	1.42

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	488	ARG	NE-CZ-NH2	-20.73	109.94	120.30
1	M	488	ARG	NE-CZ-NH1	16.06	128.33	120.30
2	J	9	DC	O5'-P-OP1	-12.46	94.49	105.70
1	M	441	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	M	427	ASP	CB-CG-OD1	9.84	127.16	118.30
1	I	429	ASP	CB-CG-OD2	9.63	126.97	118.30
1	A	427	ASP	CB-CG-OD1	7.85	125.36	118.30
1	A	419	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	I	389	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	E	436	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	E	436	ASP	CB-CG-OD1	6.72	124.35	118.30
4	D	3	DC	O5'-P-OP1	6.64	118.67	110.70
2	F	4	DC	C1'-O4'-C4'	-6.27	103.83	110.10
1	M	488	ARG	CD-NE-CZ	6.12	132.17	123.60
4	P	1	DG	O5'-P-OP1	-6.00	100.30	105.70
1	M	494	VAL	N-CA-CB	-5.90	98.53	111.50
1	M	441	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	308	ARG	NE-CZ-NH1	5.85	123.23	120.30
3	O	4	DT	O5'-P-OP1	-5.82	100.46	105.70
1	M	420	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	E	490	ASP	CB-CG-OD2	5.75	123.47	118.30
1	I	419	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	419	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	M	503	LEU	CA-CB-CG	5.64	128.27	115.30
1	A	272	ASP	CB-CG-OD2	-5.61	113.25	118.30
2	N	9	DC	O5'-P-OP2	-5.59	100.67	105.70
1	A	487	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	M	494	VAL	CG1-CB-CG2	5.44	119.61	110.90
2	N	1	DC	C5'-C4'-O4'	5.40	119.55	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	286	LEU	CA-CB-CG	5.36	127.64	115.30
1	A	574	ASP	CB-CG-OD1	5.35	123.11	118.30
4	D	1	DG	O5'-P-OP1	-5.29	100.94	105.70
1	M	419	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	E	419	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	I	488	ARG	NE-CZ-NH2	-5.17	117.71	120.30
2	N	1	DC	C5'-C4'-C3'	5.17	123.40	114.10
2	F	1	DC	C5'-C4'-O4'	5.17	119.11	109.30
1	A	272	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	573	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	I	419	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	E	561	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	469	GLN	Peptide

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	2578	0	2564	25	0
1	E	2563	0	2570	43	0
1	I	2623	0	2617	31	0
1	M	2564	0	2575	37	0
2	B	225	0	125	2	0
2	F	225	0	125	7	0
2	J	225	0	125	0	0
2	N	225	0	125	2	0
3	C	119	0	68	0	0
3	G	119	0	69	0	0
3	K	119	0	69	0	0
3	O	119	0	69	0	0
4	D	83	0	45	1	0
4	H	83	0	45	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	83	0	45	1	0
4	P	83	0	45	0	0
5	A	27	0	12	0	0
5	E	27	0	11	0	0
5	I	27	0	12	0	0
5	M	27	0	11	0	0
6	A	6	0	0	0	0
6	B	1	0	0	0	0
6	E	4	0	0	0	0
6	F	1	0	0	0	0
6	I	4	0	0	0	0
6	J	1	0	0	0	0
6	M	5	0	0	0	0
6	N	1	0	0	0	0
7	A	4	0	3	0	0
7	F	4	0	3	0	0
7	I	4	0	3	0	0
7	M	8	0	6	0	0
8	A	120	0	0	6	0
8	B	19	0	0	0	0
8	C	11	0	0	0	0
8	D	1	0	0	0	0
8	E	82	0	0	3	0
8	F	7	0	0	1	0
8	G	2	0	0	0	0
8	H	2	0	0	0	0
8	I	81	0	0	2	0
8	J	6	0	0	0	0
8	K	5	0	0	0	0
8	M	143	0	0	4	0
8	N	6	0	0	1	0
8	O	5	0	0	0	0
8	P	1	0	0	0	0
All	All	12678	0	11342	142	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (142) 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)
2:F:8:DA:OP2	8:F:201:HOH:O	1.89	0.89
1:M:321:HIS:ND1	8:M:760:HOH:O	2.13	0.81
1:A:333:PRO:O	8:A:721:HOH:O	2.00	0.80
1:M:387:MET:HE1	1:M:395:ILE:HD12	1.64	0.79
1:E:464:GLN:HG3	2:F:8:DA:O3'	1.82	0.78
1:E:444:PHE:CD2	1:E:465:GLU:OE1	2.38	0.77
1:M:537:VAL:HB	1:M:545:VAL:O	1.85	0.76
1:M:422:LYS:NZ	1:M:574:ASP:OD2	2.19	0.76
1:E:464:GLN:CD	2:F:8:DA:H4'	2.06	0.76
1:M:271:GLY:CA	1:M:346:THR:HG21	2.16	0.74
1:M:438:ARG:O	1:M:441:ARG:HD3	1.89	0.73
1:I:441:ARG:NH2	8:I:739:HOH:O	2.19	0.70
1:E:464:GLN:CG	2:F:8:DA:H4'	2.23	0.69
1:I:537:VAL:HA	1:I:538:ARG:CB	2.23	0.68
1:E:321:HIS:HB2	8:E:782:HOH:O	1.95	0.67
1:M:271:GLY:HA3	1:M:346:THR:HG21	1.76	0.67
1:A:364:ARG:HG2	1:A:377:LEU:HD21	1.75	0.66
1:I:540:THR:HG23	1:I:541:HIS:CD2	2.30	0.66
1:M:284:ASN:N	1:M:284:ASN:HD22	1.93	0.66
1:A:396:GLU:HG3	1:A:414:ALA:HB2	1.77	0.66
1:A:536:VAL:HG22	8:A:810:HOH:O	1.95	0.65
1:A:534:THR:C	8:A:810:HOH:O	2.36	0.64
2:N:7:DT:OP2	8:N:202:HOH:O	2.16	0.63
1:I:537:VAL:HA	1:I:538:ARG:HB3	1.80	0.62
1:M:346:THR:HG22	1:M:350:GLN:HE21	1.65	0.62
1:M:438:ARG:O	1:M:441:ARG:CD	2.48	0.61
1:I:267:TYR:CZ	1:I:275:ARG:HD3	2.36	0.61
1:A:361:GLU:OE1	1:A:364:ARG:NH1	2.35	0.59
1:M:387:MET:CE	1:M:395:ILE:HD12	2.33	0.59
1:E:523:LYS:O	1:E:525:MET:HG3	2.03	0.58
1:M:287:LYS:C	8:M:755:HOH:O	2.41	0.58
1:A:471:GLN:HE22	1:A:530:HIS:HE1	1.51	0.56
1:I:307:LYS:O	1:I:311:GLU:HG3	2.05	0.56
1:M:288:SER:O	1:M:289:PHE:C	2.42	0.56
1:E:305:ILE:HG23	1:E:309:MET:HB3	1.86	0.56
2:B:1:DC:H2'	2:B:2:DG:C8	2.40	0.56
1:E:544:LYS:O	1:E:546:GLY:N	2.39	0.55
1:A:312:LYS:NZ	4:D:1:DG:OP3	2.40	0.55
1:A:263:LEU:CD1	1:A:267:TYR:CE2	2.89	0.55
1:M:324:LYS:O	1:M:324:LYS:NZ	2.40	0.54
1:E:312:LYS:NZ	4:H:1:DG:OP3	2.39	0.54
1:E:525:MET:HE1	1:E:563:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:283:ILE:O	1:M:287:LYS:HB2	2.08	0.54
1:M:251:ASN:HA	8:M:755:HOH:O	2.06	0.54
1:I:314:ILE:HD12	1:I:315:GLU:N	2.23	0.54
1:E:364:ARG:NH2	8:E:766:HOH:O	2.42	0.53
1:E:438:ARG:O	1:E:441:ARG:HD2	2.09	0.53
1:M:305:ILE:HG23	1:M:309:MET:HB3	1.90	0.53
2:N:1:DC:H2''	2:N:2:DG:C8	2.43	0.53
1:E:558:ASP:OD1	1:E:561:ARG:NH2	2.42	0.53
1:A:557:LYS:HD2	8:A:779:HOH:O	2.08	0.52
1:A:466:GLU:OE2	1:M:438:ARG:NH2	2.43	0.52
1:E:275:ARG:HG3	4:H:1:DG:C8	2.44	0.52
1:A:537:VAL:N	8:A:768:HOH:O	2.42	0.52
1:I:400:GLN:HG3	1:I:412:CYS:HB2	1.92	0.52
1:M:359:SER:OG	1:M:362:ASP:OD1	2.28	0.52
1:I:540:THR:HG23	1:I:541:HIS:NE2	2.25	0.52
1:E:525:MET:CE	1:E:563:LEU:HD23	2.40	0.51
1:M:282:ALA:O	1:M:286:LEU:HD22	2.11	0.51
1:E:422:LYS:NZ	1:E:574:ASP:OD2	2.43	0.51
1:E:444:PHE:CD2	1:E:471:GLN:HB3	2.45	0.51
1:M:568:ARG:HG2	1:M:572:GLU:HB2	1.93	0.51
1:I:267:TYR:CE2	1:I:275:ARG:HD3	2.46	0.50
1:A:263:LEU:CD1	1:A:267:TYR:HE2	2.25	0.50
1:I:531:ALA:HB1	1:I:550:VAL:HG13	1.92	0.50
1:E:523:LYS:NZ	1:E:563:LEU:O	2.41	0.50
8:I:745:HOH:O	4:L:2:DC:H4'	2.12	0.49
1:I:511:HIS:CD2	1:I:514:ARG:HH21	2.31	0.49
1:E:464:GLN:CG	2:F:8:DA:O3'	2.56	0.49
1:M:291:LYS:HB2	1:M:292:PRO:HD2	1.94	0.48
1:E:444:PHE:CD2	1:E:471:GLN:CB	2.96	0.48
1:A:514:ARG:HD2	2:B:5:DG:OP2	2.13	0.48
1:M:293:VAL:HG11	1:M:299:ALA:HB2	1.95	0.48
1:I:518:ALA:O	1:I:521:LYS:HB3	2.13	0.48
1:I:540:THR:O	1:I:542:GLY:N	2.45	0.48
1:A:360:LEU:O	1:A:363:ILE:HB	2.14	0.48
1:E:537:VAL:O	1:E:544:LYS:O	2.32	0.48
1:I:436:ASP:C	1:I:436:ASP:OD1	2.52	0.47
1:E:451:LEU:HB3	1:E:457:LEU:HG	1.95	0.47
1:M:504:LEU:HD21	1:M:516:MET:CE	2.45	0.47
1:E:524:GLY:O	1:E:535:ALA:O	2.32	0.47
1:I:286:LEU:HD11	1:I:313:ILE:HD11	1.96	0.47
1:M:250:THR:O	1:M:251:ASN:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:499:PHE:CZ	1:I:503:LEU:HD21	2.50	0.46
1:A:263:LEU:HD23	1:A:325:LEU:CD2	2.45	0.46
1:M:337:LEU:HD12	1:M:380:TYR:OH	2.15	0.46
1:E:464:GLN:HB3	1:E:472:LYS:HB3	1.98	0.46
1:A:267:TYR:CZ	1:A:275:ARG:HD3	2.51	0.46
1:E:411:LEU:O	1:E:432:ILE:HA	2.16	0.45
1:I:286:LEU:HG	1:I:305:ILE:HD11	1.99	0.45
1:I:538:ARG:HH11	1:I:543:CYS:HA	1.81	0.45
1:I:284:ASN:HB2	1:I:575:TRP:CE2	2.51	0.45
2:F:1:DC:H2''	2:F:2:DG:H5'	1.98	0.45
1:E:261:GLU:HG3	1:E:283:ILE:HD13	1.98	0.45
1:E:504:LEU:HD21	1:E:516:MET:CE	2.46	0.45
1:I:298:GLU:O	1:I:301:SER:OG	2.26	0.45
1:M:387:MET:HE2	1:M:391:GLU:HB3	1.98	0.45
1:E:561:ARG:HG2	1:E:561:ARG:HH11	1.82	0.45
1:E:431:LEU:HA	1:E:492:ILE:HG22	2.00	0.44
1:I:251:ASN:ND2	1:I:254:LEU:HA	2.32	0.44
1:E:337:LEU:HD12	1:E:380:TYR:OH	2.18	0.44
4:H:3:DC:H2''	4:H:4:DG:C8	2.52	0.44
1:M:250:THR:HG23	8:M:748:HOH:O	2.18	0.43
1:M:436:ASP:C	1:M:436:ASP:OD1	2.56	0.43
1:E:321:HIS:ND1	8:E:780:HOH:O	2.35	0.43
1:E:435:PRO:HA	1:E:496:TYR:CD1	2.54	0.43
1:I:407:ASN:C	1:I:407:ASN:OD1	2.56	0.43
1:E:351:MET:CE	1:E:352:TRP:CD1	3.02	0.43
1:M:470:GLN:HG2	1:M:494:VAL:HG22	2.01	0.42
1:A:389:ARG:HD2	1:A:422:LYS:O	2.19	0.42
1:M:250:THR:O	1:M:251:ASN:HB2	2.19	0.42
1:A:578:HIS:HA	8:A:815:HOH:O	2.19	0.42
1:I:260:LEU:HB3	1:I:283:ILE:HD11	2.02	0.42
1:A:256:ILE:HD13	1:A:313:ILE:HG23	2.01	0.42
1:E:519:LEU:C	1:E:519:LEU:HD23	2.41	0.42
1:M:355:GLN:HG2	1:M:357:PHE:CZ	2.54	0.42
1:I:436:ASP:OD2	1:I:439:SER:HB2	2.20	0.42
1:E:464:GLN:HG3	2:F:9:DC:P	2.59	0.41
1:E:535:ALA:O	1:E:536:VAL:HB	2.20	0.41
1:E:543:CYS:O	1:E:544:LYS:HB2	2.20	0.41
1:E:302:ILE:HB	1:E:305:ILE:HD12	2.02	0.41
1:M:284:ASN:O	1:M:285:ALA:C	2.58	0.41
1:A:263:LEU:HD23	1:A:325:LEU:HD23	2.03	0.41
1:E:534:THR:O	1:E:536:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:291:LYS:HE3	1:I:298:GLU:OE2	2.20	0.41
1:I:296:TYR:HB2	1:I:314:ILE:HG21	2.02	0.41
1:A:351:MET:HE2	1:A:352:TRP:CD1	2.55	0.41
1:A:577:GLU:H	1:A:577:GLU:CD	2.24	0.41
1:M:284:ASN:N	1:M:284:ASN:ND2	2.64	0.41
1:A:471:GLN:HE22	1:A:530:HIS:CE1	2.35	0.41
1:E:359:SER:O	1:E:362:ASP:HB2	2.21	0.41
1:M:289:PHE:HE2	1:M:298:GLU:OE2	2.04	0.41
1:M:397:GLN:O	1:M:401:LYS:HG3	2.20	0.41
1:I:308:ARG:O	1:I:312:LYS:HD3	2.21	0.40
1:E:469:GLN:C	1:E:470:GLN:O	2.59	0.40
1:M:387:MET:HE2	1:M:392:ALA:N	2.36	0.40
1:A:261:GLU:HG3	1:A:283:ILE:HD13	2.03	0.40
1:E:444:PHE:CD2	1:E:471:GLN:HB2	2.56	0.40
1:I:534:THR:HG23	1:I:551:LEU:HD21	2.02	0.40
1:I:541:HIS:ND1	1:I:541:HIS:N	2.69	0.40
1:E:435:PRO:HA	1:E:496:TYR:CG	2.56	0.40
1:I:538:ARG:NH1	1:I:543:CYS:HA	2.36	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	323/340 (95%)	309 (96%)	12 (4%)	2 (1%)	25 21
1	E	322/340 (95%)	304 (94%)	12 (4%)	6 (2%)	8 3
1	I	331/340 (97%)	316 (96%)	13 (4%)	2 (1%)	25 21
1	M	322/340 (95%)	304 (94%)	13 (4%)	5 (2%)	9 5
All	All	1298/1360 (95%)	1233 (95%)	50 (4%)	15 (1%)	13 8

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	470	GLN
1	I	538	ARG
1	I	541	HIS
1	M	251	ASN
1	A	250	THR
1	E	544	LYS
1	E	545	VAL
1	M	289	PHE
1	M	250	THR
1	E	543	CYS
1	A	580	HIS
1	E	538	ARG
1	M	301	SER
1	E	536	VAL
1	M	544	LYS

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	274/287 (96%)	260 (95%)	14 (5%)	24	22
1	E	273/287 (95%)	259 (95%)	14 (5%)	24	22
1	I	280/287 (98%)	263 (94%)	17 (6%)	18	16
1	M	274/287 (96%)	252 (92%)	22 (8%)	12	8
All	All	1101/1148 (96%)	1034 (94%)	67 (6%)	18	16

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	LEU
1	A	265	LYS
1	A	321	HIS
1	A	323	ARG
1	A	325	LEU
1	A	350	GLN
1	A	361	GLU

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Mol	Chain	Res	Type
1	A	384	LEU
1	A	454	GLU
1	A	506	PHE
1	A	534	THR
1	A	536	VAL
1	A	576	LEU
1	A	577	GLU
1	E	254	LEU
1	E	286	LEU
1	E	314	ILE
1	E	384	LEU
1	E	397	GLN
1	E	411	LEU
1	E	441	ARG
1	E	444	PHE
1	E	465	GLU
1	E	492	ILE
1	E	532	LEU
1	E	534	THR
1	E	544	LYS
1	E	576	LEU
1	I	254	LEU
1	I	260	LEU
1	I	265	LYS
1	I	277	LEU
1	I	317	LEU
1	I	354	GLN
1	I	436	ASP
1	I	439	SER
1	I	453	GLN
1	I	469	GLN
1	I	503	LEU
1	I	519	LEU
1	I	541	HIS
1	I	544	LYS
1	I	545	VAL
1	I	570	PRO
1	I	576	LEU
1	M	259	LYS
1	M	284	ASN
1	M	286	LEU
1	M	291	LYS

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Mol	Chain	Res	Type
1	M	302	ILE
1	M	314	ILE
1	M	317	LEU
1	M	323	ARG
1	M	324	LYS
1	M	330	GLU
1	M	346	THR
1	M	355	GLN
1	M	385	GLU
1	M	411	LEU
1	M	488	ARG
1	M	489	LEU
1	M	494	VAL
1	M	543	CYS
1	M	544	LYS
1	M	565	LEU
1	M	568	ARG
1	M	577	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	GLN
1	A	350	GLN
1	A	354	GLN
1	A	471	GLN
1	E	290	HIS
1	I	270	GLN
1	I	372	GLN
1	I	434	HIS
1	I	453	GLN
1	I	511	HIS
1	M	284	ASN
1	M	350	GLN

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 32 ligands modelled in this entry, 23 are monoatomic - leaving 9 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
5	1RZ	M	601	6	24,28,28	1.21	2 (8%)	34,43,43	2.53	16 (47%)
7	ACT	M	607	-	3,3,3	1.11	0	3,3,3	0.44	0
7	ACT	I	606	-	3,3,3	0.63	0	3,3,3	0.94	0
7	ACT	M	608	-	3,3,3	0.86	0	3,3,3	1.09	0
7	ACT	F	102	-	3,3,3	0.74	0	3,3,3	0.96	0
5	1RZ	I	601	6	24,28,28	1.76	2 (8%)	34,43,43	1.98	10 (29%)
5	1RZ	E	601	6	24,28,28	1.80	3 (12%)	34,43,43	1.45	5 (14%)
7	ACT	A	608	-	3,3,3	0.64	0	3,3,3	1.65	1 (33%)
5	1RZ	A	601	6	24,28,28	1.61	4 (16%)	34,43,43	1.36	4 (11%)

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
5	1RZ	E	601	6	-	5/22/31/31	0/2/2/2
5	1RZ	M	601	6	-	9/22/31/31	0/2/2/2
5	1RZ	A	601	6	-	3/22/31/31	0/2/2/2
5	1RZ	I	601	6	-	8/22/31/31	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	601	1RZ	O2-C2	7.49	1.37	1.23
5	E	601	1RZ	O2-C2	6.92	1.36	1.23
5	A	601	1RZ	O2-C2	4.84	1.32	1.23
5	M	601	1RZ	O2-C2	3.43	1.30	1.23
5	A	601	1RZ	C2-N1	-3.35	1.32	1.40
5	A	601	1RZ	O4'-C1'	-2.39	1.37	1.42
5	E	601	1RZ	C2-N1	-2.33	1.34	1.40
5	I	601	1RZ	C6-C5	2.22	1.40	1.35
5	A	601	1RZ	C2'-S3'	-2.07	1.75	1.81
5	E	601	1RZ	PG-O3G	-2.06	1.46	1.54
5	M	601	1RZ	C4-N4	2.01	1.38	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	601	1RZ	O4'-C1'-N1	7.42	121.12	107.86
5	I	601	1RZ	O2-C2-N3	-6.16	112.30	122.33
5	M	601	1RZ	O2-C2-N3	-5.83	112.84	122.33
5	A	601	1RZ	O2-C2-N3	-4.31	115.32	122.33
5	E	601	1RZ	O2-C2-N3	-4.14	115.59	122.33
5	M	601	1RZ	N1-C2-N3	4.05	126.19	118.81
5	I	601	1RZ	O2-C2-N1	3.88	126.90	118.89
5	I	601	1RZ	PA-O3A-PB	-3.82	119.72	132.83
5	M	601	1RZ	C6-C5-C4	3.59	123.29	117.50
5	A	601	1RZ	N1-C2-N3	3.00	124.28	118.81
5	M	601	1RZ	O4'-C1'-C2'	-2.81	102.74	109.29
5	M	601	1RZ	O1B-PB-O2B	2.77	125.92	112.24
5	E	601	1RZ	C1'-C2'-S3'	2.66	110.35	104.03
5	M	601	1RZ	C1'-C2'-S3'	2.63	110.28	104.03
5	I	601	1RZ	PB-O3B-PG	-2.58	123.97	132.83
5	I	601	1RZ	O2C-PG-O3G	2.58	117.48	107.64
5	M	601	1RZ	C4'-O4'-C1'	-2.55	107.20	112.59
5	M	601	1RZ	O3G-PG-O3B	-2.52	96.18	104.64
5	I	601	1RZ	O1B-PB-O2B	2.50	124.58	112.24
5	M	601	1RZ	C1'-N1-C2	2.45	122.03	117.74
5	M	601	1RZ	C5-C4-N3	-2.44	117.17	121.33
5	I	601	1RZ	C5-C4-N4	2.42	124.38	120.57
5	E	601	1RZ	O2C-PG-O3G	2.38	116.72	107.64
5	A	601	1RZ	O3G-PG-O1G	2.33	119.81	110.68
5	I	601	1RZ	O2C-PG-O3B	2.32	112.40	104.64
5	E	601	1RZ	PA-O3A-PB	-2.31	124.89	132.83
5	M	601	1RZ	O5'-PA-O1A	2.29	118.02	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	601	1RZ	O3G-PG-O1G	2.26	119.52	110.68
7	A	608	ACT	OXT-C-CH3	2.20	124.27	115.18
5	M	601	1RZ	PA-O5'-C5'	2.18	134.48	121.68
5	M	601	1RZ	O4'-C4'-S3'	2.17	110.90	106.44
5	I	601	1RZ	C1'-N1-C2	2.16	121.53	117.74
5	A	601	1RZ	C4-N3-C2	-2.11	116.85	120.25
5	M	601	1RZ	C6-N1-C2	-2.07	116.91	120.49
5	E	601	1RZ	PB-O3B-PG	-2.03	125.85	132.83
5	I	601	1RZ	C1'-C2'-S3'	2.02	108.83	104.03

There are no chirality outliers.

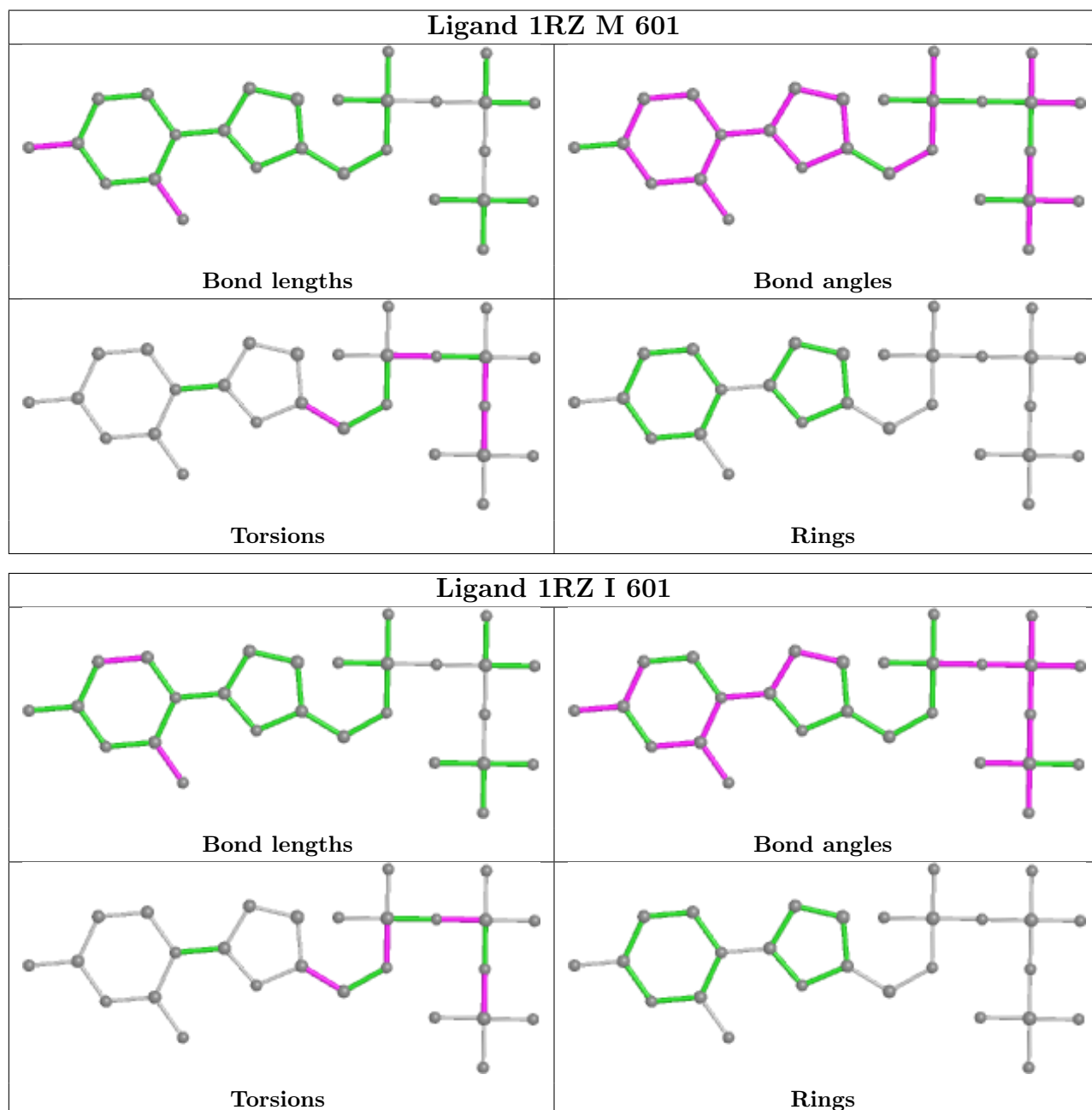
All (25) torsion outliers are listed below:

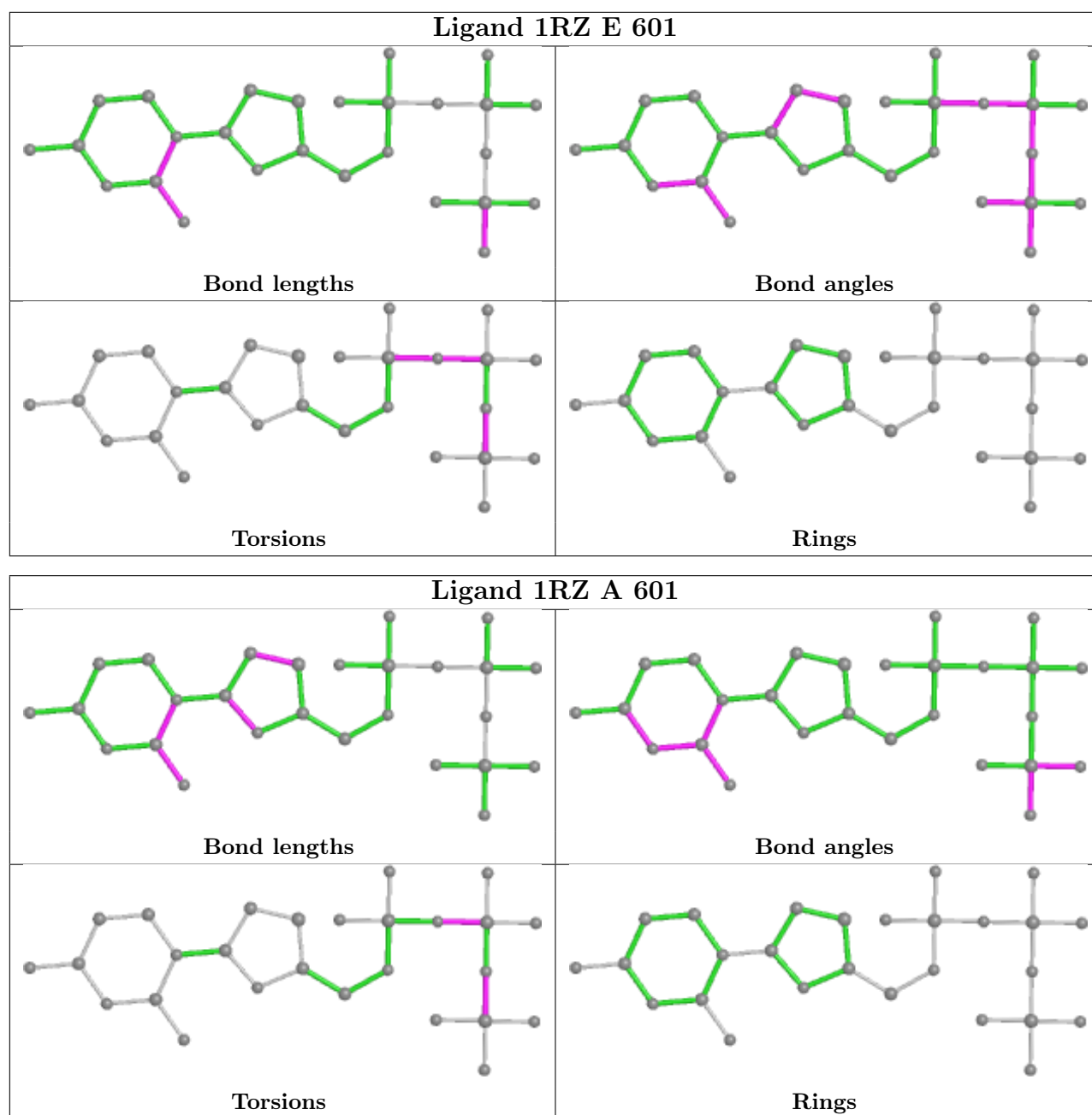
Mol	Chain	Res	Type	Atoms
5	A	601	1RZ	PB-O3B-PG-O2C
5	E	601	1RZ	PB-O3B-PG-O2C
5	I	601	1RZ	PB-O3B-PG-O2C
5	I	601	1RZ	C5'-O5'-PA-O3A
5	I	601	1RZ	O4'-C4'-C5'-O5'
5	I	601	1RZ	S3'-C4'-C5'-O5'
5	M	601	1RZ	PB-O3B-PG-O2C
5	M	601	1RZ	O4'-C4'-C5'-O5'
5	M	601	1RZ	S3'-C4'-C5'-O5'
5	I	601	1RZ	PA-O3A-PB-O2B
5	M	601	1RZ	PB-O3A-PA-O5'
5	I	601	1RZ	PA-O3A-PB-O1B
5	M	601	1RZ	PG-O3B-PB-O1B
5	I	601	1RZ	PB-O3B-PG-O1G
5	A	601	1RZ	PA-O3A-PB-O2B
5	A	601	1RZ	PB-O3B-PG-O1G
5	E	601	1RZ	PB-O3B-PG-O1G
5	M	601	1RZ	PB-O3B-PG-O1G
5	E	601	1RZ	PB-O3B-PG-O3G
5	I	601	1RZ	PB-O3B-PG-O3G
5	M	601	1RZ	PB-O3B-PG-O3G
5	E	601	1RZ	PA-O3A-PB-O1B
5	E	601	1RZ	PB-O3A-PA-O2A
5	M	601	1RZ	PB-O3A-PA-O1A
5	M	601	1RZ	PB-O3A-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	327/340 (96%)	-0.17	9 (2%) 53 59	18, 33, 62, 116	0
1	E	326/340 (95%)	-0.07	13 (3%) 38 44	22, 38, 70, 130	0
1	I	332/340 (97%)	-0.05	18 (5%) 25 31	22, 39, 70, 132	0
1	M	325/340 (95%)	-0.20	7 (2%) 62 66	17, 35, 55, 90	0
2	B	11/11 (100%)	-0.27	0 100 100	24, 27, 46, 46	0
2	F	11/11 (100%)	-0.40	0 100 100	37, 43, 52, 68	0
2	J	11/11 (100%)	-0.52	0 100 100	33, 38, 43, 45	0
2	N	11/11 (100%)	-0.56	0 100 100	26, 32, 45, 46	0
3	C	6/6 (100%)	-0.37	0 100 100	21, 26, 39, 42	0
3	G	6/6 (100%)	-0.24	0 100 100	30, 34, 59, 73	0
3	K	6/6 (100%)	-0.25	0 100 100	25, 29, 59, 61	0
3	O	6/6 (100%)	-0.43	0 100 100	28, 31, 50, 55	0
4	D	4/4 (100%)	-0.71	0 100 100	33, 33, 38, 42	0
4	H	4/4 (100%)	-0.70	0 100 100	30, 33, 36, 41	0
4	L	4/4 (100%)	-0.60	0 100 100	38, 42, 45, 46	0
4	P	4/4 (100%)	-0.71	0 100 100	34, 36, 44, 45	0
All	All	1394/1444 (96%)	-0.14	47 (3%) 45 51	17, 36, 64, 132	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	539	ASN	8.6
1	E	540	THR	7.7
1	I	542	GLY	7.1
1	E	542	GLY	7.1
1	I	541	HIS	6.4

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Mol	Chain	Res	Type	RSRZ
1	E	541	HIS	6.3
1	E	539	ASN	5.3
1	E	543	CYS	5.3
1	M	249	ALA	5.2
1	I	540	THR	5.1
1	I	543	CYS	5.0
1	I	249	ALA	4.8
1	A	581	HIS	4.7
1	E	537	VAL	4.3
1	A	544	LYS	4.2
1	E	469	GLN	4.1
1	E	468	GLY	4.0
1	M	250	THR	3.6
1	I	537	VAL	3.6
1	M	543	CYS	3.5
1	M	538	ARG	3.3
1	A	321	HIS	3.2
1	I	578	HIS	3.1
1	I	250	THR	3.1
1	I	321	HIS	3.0
1	A	255	HIS	2.9
1	I	323	ARG	2.9
1	M	575	TRP	2.8
1	E	538	ARG	2.7
1	I	579	HIS	2.6
1	I	545	VAL	2.6
1	E	545	VAL	2.6
1	M	545	VAL	2.5
1	I	580	HIS	2.5
1	I	314	ILE	2.5
1	E	535	ALA	2.4
1	A	249	ALA	2.4
1	E	576	LEU	2.3
1	A	546	GLY	2.3
1	M	537	VAL	2.2
1	I	254	LEU	2.2
1	I	549	ARG	2.2
1	I	318	GLU	2.1
1	E	470	GLN	2.0
1	A	580	HIS	2.0
1	A	323	ARG	2.0
1	A	537	VAL	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, 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.

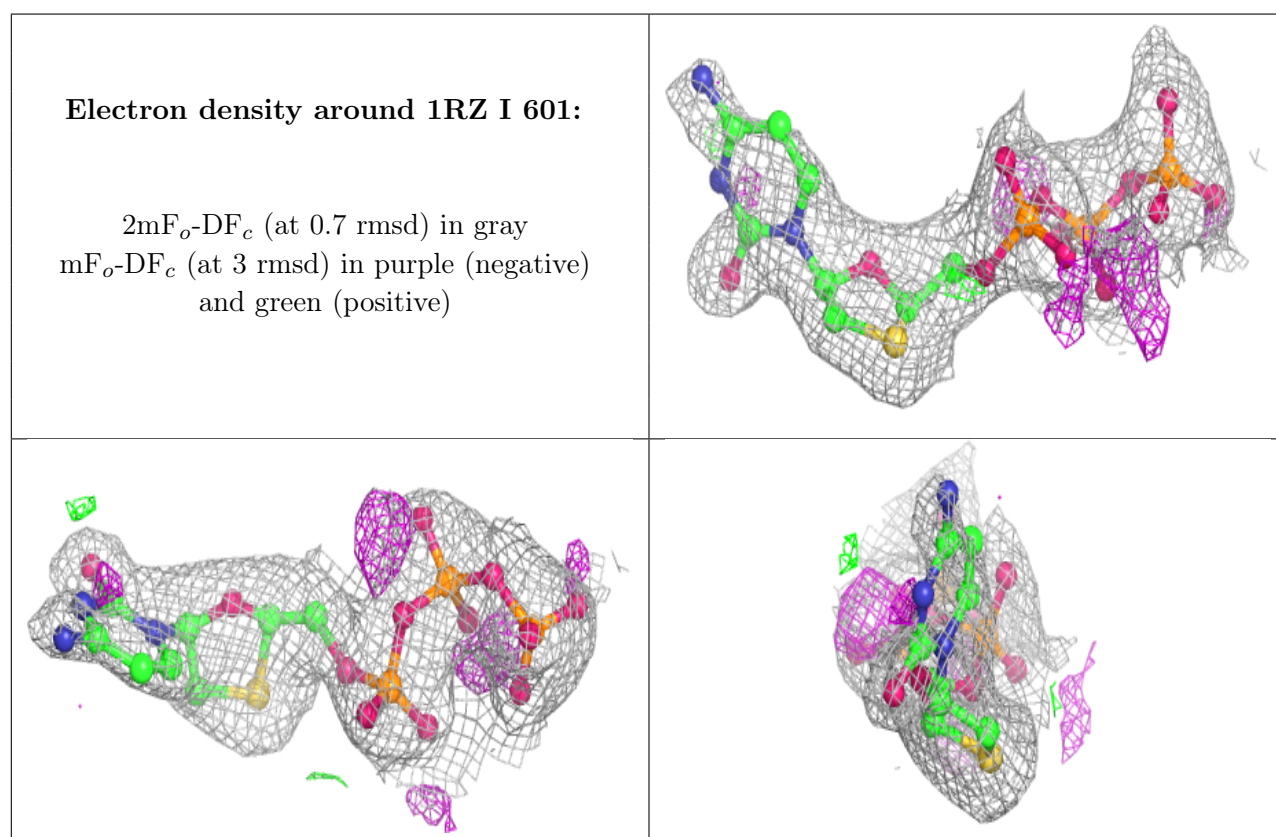
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	ACT	M	607	4/4	0.61	0.24	53,54,58,61	0
6	CA	E	604	1/1	0.71	0.10	53,53,53,53	0
6	CA	N	101	1/1	0.80	0.18	60,60,60,60	0
6	CA	I	604	1/1	0.80	0.13	59,59,59,59	0
6	CA	J	101	1/1	0.81	0.08	68,68,68,68	0
6	CA	M	605	1/1	0.82	0.09	66,66,66,66	0
6	CA	M	602	1/1	0.84	0.12	55,55,55,55	0
6	CA	B	101	1/1	0.85	0.13	65,65,65,65	0
6	CA	A	606	1/1	0.86	0.11	62,62,62,62	0
7	ACT	M	608	4/4	0.87	0.18	34,40,45,46	0
6	CA	M	603	1/1	0.88	0.06	64,64,64,64	0
6	CA	A	607	1/1	0.89	0.17	51,51,51,51	0
6	CA	I	602	1/1	0.89	0.10	46,46,46,46	0
7	ACT	I	606	4/4	0.91	0.24	44,47,51,56	0
6	CA	F	101	1/1	0.91	0.11	52,52,52,52	0
7	ACT	A	608	4/4	0.91	0.12	43,46,47,51	0
6	CA	E	605	1/1	0.92	0.11	67,67,67,67	0
7	ACT	F	102	4/4	0.93	0.17	42,44,45,49	0
5	1RZ	I	601	27/27	0.94	0.13	40,49,68,75	0
5	1RZ	M	601	27/27	0.94	0.11	23,38,51,54	0
6	CA	A	603	1/1	0.94	0.06	46,46,46,46	0
6	CA	I	603	1/1	0.95	0.05	49,49,49,49	0
6	CA	E	603	1/1	0.96	0.14	39,39,39,39	0
6	CA	M	606	1/1	0.96	0.04	45,45,45,45	0
6	CA	A	604	1/1	0.96	0.05	29,29,29,29	0
6	CA	M	604	1/1	0.96	0.11	39,39,39,39	0
6	CA	A	605	1/1	0.97	0.07	33,33,33,33	0

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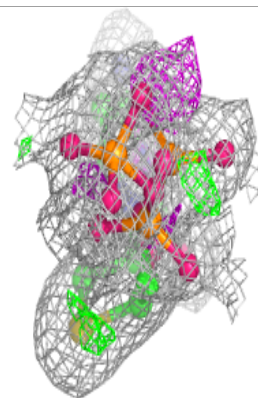
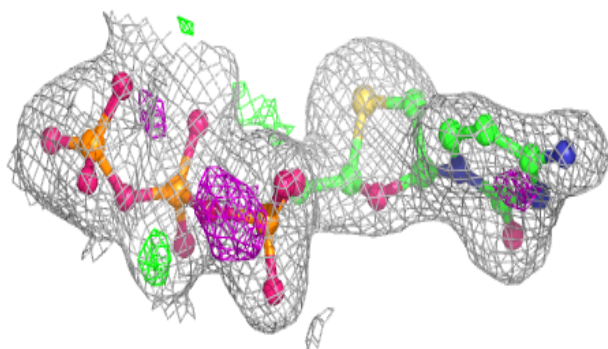
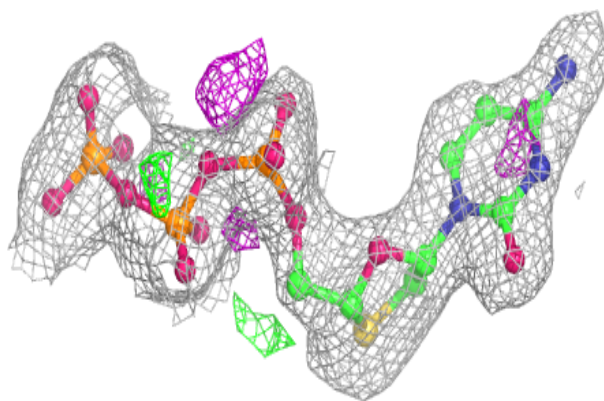
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	1RZ	E	601	27/27	0.98	0.11	22,28,39,42	0
6	CA	E	602	1/1	0.98	0.10	26,26,26,26	0
5	1RZ	A	601	27/27	0.98	0.11	18,22,25,26	0
6	CA	I	605	1/1	0.99	0.04	34,34,34,34	0
6	CA	A	602	1/1	1.00	0.09	24,24,24,24	0

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.

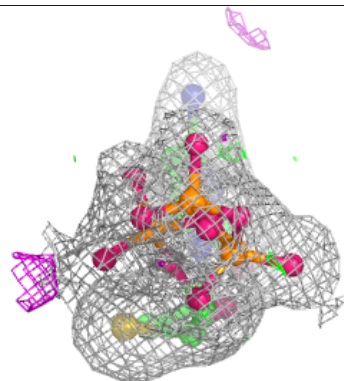
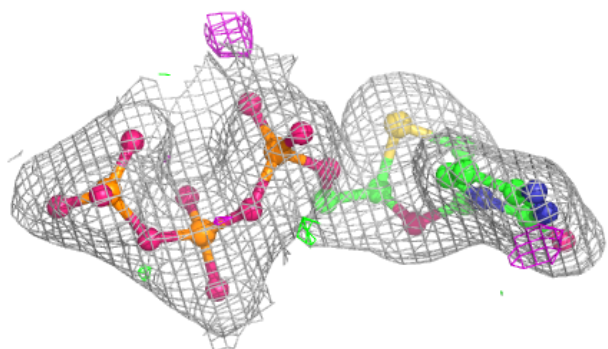
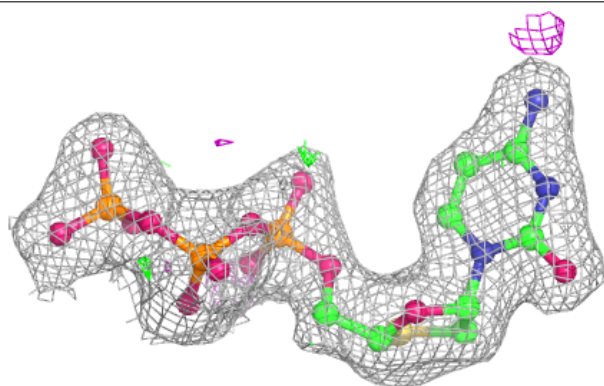


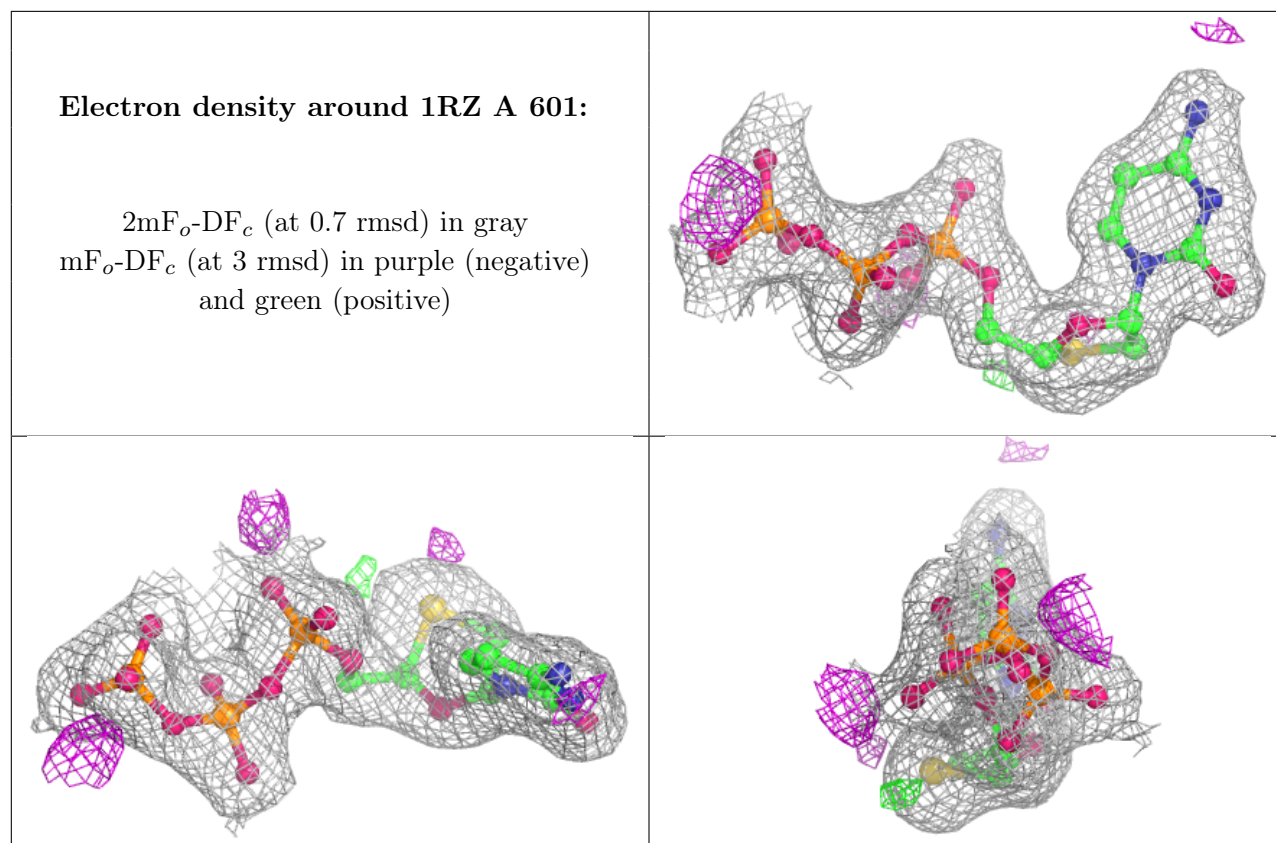
Electron density around 1RZ M 601:

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

**Electron density around 1RZ E 601:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.