



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:41 AM UTC

PDB ID : 1XS1 / pdb_00001xs1
Title : dCTP deaminase from Escherichia coli in complex with dUTP
Authors : Johansson, E.; Fano, M.; Bynck, J.H.; Neuhard, J.; Larsen, S.; Sigurskjold, B.W.; Christensen, U.; Willemoes, M.
Deposited on : 2004-10-18
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

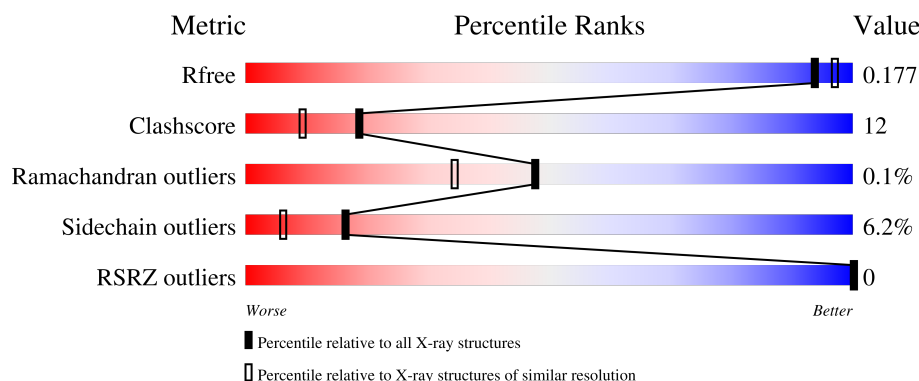
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	193	 65% 33% 0.177
1	B	193	 70% 27% 0.12
1	C	193	 70% 24% 6% 0.01
1	D	193	 71% 25% 0.062
1	E	193	 79% 18% 0.0

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Mol	Chain	Length	Quality of chain
1	F	193	68% 27% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9621 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.

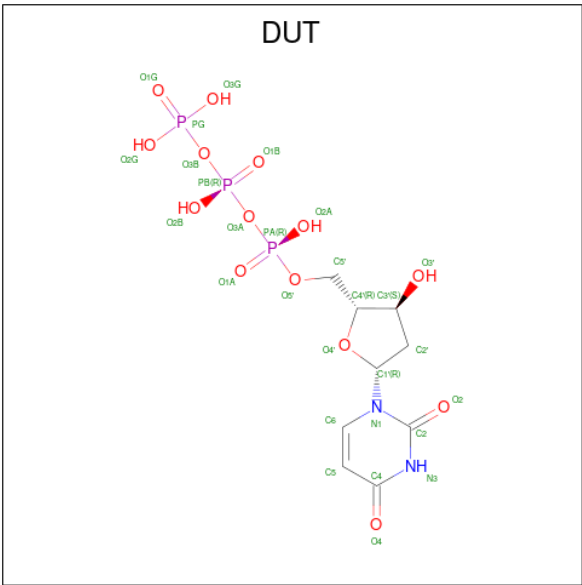
- Molecule 1 is a protein called Deoxycytidine triphosphate deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	4	0
			1517	954	278	279	6			
1	B	193	Total	C	N	O	S	0	1	0
			1500	943	272	279	6			
1	C	193	Total	C	N	O	S	0	1	0
			1501	944	271	280	6			
1	D	193	Total	C	N	O	S	0	1	0
			1498	942	271	279	6			
1	E	193	Total	C	N	O	S	0	2	0
			1504	948	272	278	6			
1	F	193	Total	C	N	O	S	0	1	0
			1500	943	272	279	6			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is DEOXYURIDINE-5'-TRIPHOSPHATE (CCD ID: DUT) (formula: C₉H₁₅N₂O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	9	2	14	3		
3	B	1	Total	C	N	O	P	0	0
			28	9	2	14	3		
3	C	1	Total	C	N	O	P	0	0
			28	9	2	14	3		
3	D	1	Total	C	N	O	P	0	0
			28	9	2	14	3		
3	E	1	Total	C	N	O	P	0	0
			28	9	2	14	3		
3	F	1	Total	C	N	O	P	0	0
			28	9	2	14	3		

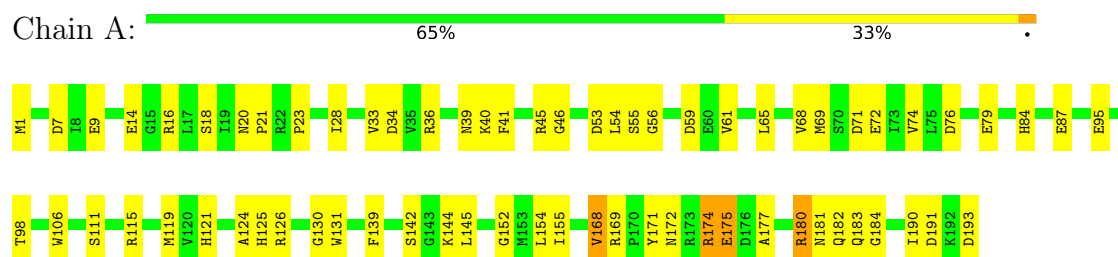
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	78	Total	O	0	0
			78	78		
4	B	79	Total	O	0	0
			79	79		
4	C	60	Total	O	0	0
			60	60		
4	D	64	Total	O	0	0
			64	64		
4	E	79	Total	O	0	0
			79	79		
4	F	67	Total	O	0	0
			67	67		

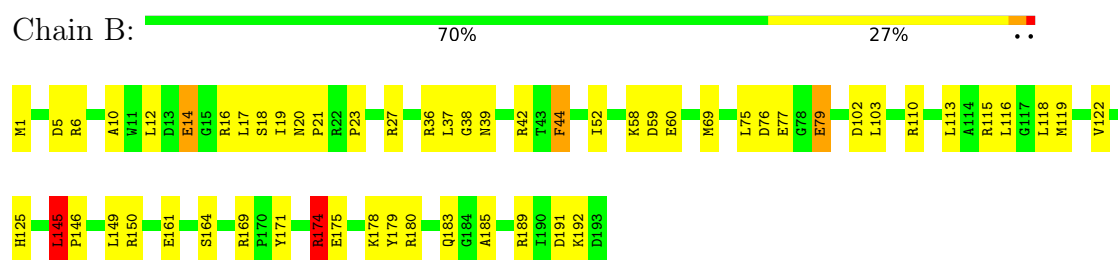
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

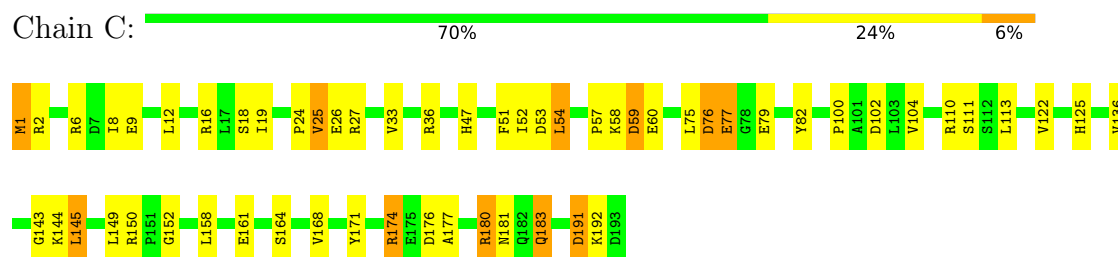
• Molecule 1: Deoxycytidine triphosphate deaminase



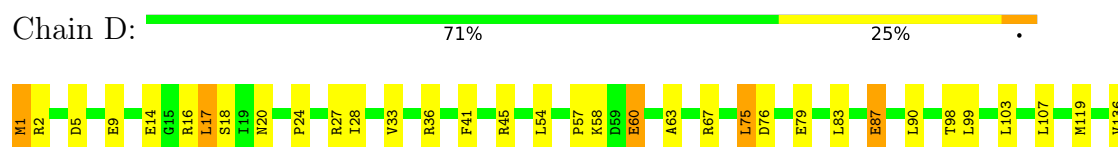
• Molecule 1: Deoxycytidine triphosphate deaminase



• Molecule 1: Deoxycytidine triphosphate deaminase

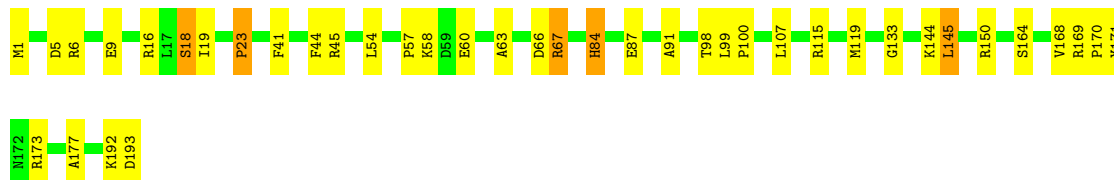
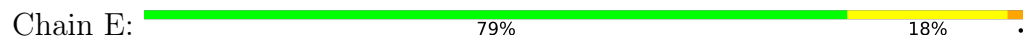


• Molecule 1: Deoxycytidine triphosphate deaminase

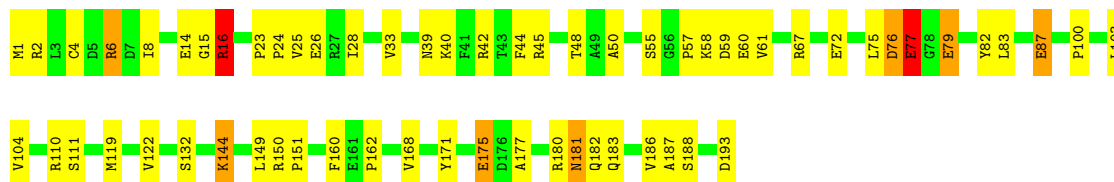




- Molecule 1: Deoxycytidine triphosphate deaminase



- Molecule 1: Deoxycytidine triphosphate deaminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.03Å 97.46Å 95.47Å 90.00° 109.23° 90.00°	Depositor
Resolution (Å)	25.00 – 1.80 25.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	90.1 (25.00-1.80) 94.8 (25.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.45 (at 1.80Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.164 , 0.195 0.149 , 0.177	Depositor DCC
R_{free} test set	4789 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 22.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.469 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9621	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DUT, 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	0.55	1/1564 (0.1%)	1.35	8/2119 (0.4%)
1	B	0.50	0/1535	1.34	9/2081 (0.4%)
1	C	0.51	0/1536	1.46	11/2082 (0.5%)
1	D	0.51	1/1533 (0.1%)	1.30	4/2078 (0.2%)
1	E	0.50	1/1543 (0.1%)	1.31	6/2091 (0.3%)
1	F	0.52	1/1535 (0.1%)	1.37	13/2081 (0.6%)
All	All	0.52	4/9246 (0.0%)	1.35	51/12532 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	ASP	C-OXT	10.03	1.43	1.23
1	F	193	ASP	C-OXT	7.06	1.37	1.23
1	D	193	ASP	C-OXT	-6.75	1.10	1.23
1	E	193	ASP	C-OXT	5.01	1.33	1.23

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	ARG	CD-NE-CZ	26.06	160.88	124.40
1	F	150	ARG	O-C-N	8.17	129.34	121.66
1	D	150	ARG	CD-NE-CZ	7.90	135.46	124.40
1	F	180	ARG	CA-C-N	7.41	132.67	122.07
1	F	180	ARG	C-N-CA	7.41	132.67	122.07
1	B	23	PRO	O-C-N	6.89	124.48	121.31
1	E	145	LEU	O-C-N	6.61	127.87	121.66
1	B	145	LEU	O-C-N	6.48	128.07	121.72
1	B	175	GLU	CA-C-N	-6.48	112.30	122.73
1	B	175	GLU	C-N-CA	-6.48	112.30	122.73
1	D	173	ARG	CA-C-N	6.45	131.72	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	173	ARG	C-N-CA	6.45	131.72	121.66
1	B	122	VAL	CA-C-N	6.35	131.41	122.46
1	B	122	VAL	C-N-CA	6.35	131.41	122.46
1	C	25	VAL	CA-C-N	6.07	129.24	120.38
1	C	25	VAL	C-N-CA	6.07	129.24	120.38
1	A	174	ARG	CA-C-N	5.97	128.88	120.28
1	A	174	ARG	C-N-CA	5.97	128.88	120.28
1	B	174	ARG	CD-NE-CZ	5.92	132.69	124.40
1	F	16	ARG	CA-C-N	5.86	130.81	122.72
1	F	16	ARG	C-N-CA	5.86	130.81	122.72
1	A	84	HIS	CA-C-O	-5.83	115.35	120.60
1	C	8	ILE	CA-C-N	5.79	128.04	120.28
1	C	8	ILE	C-N-CA	5.79	128.04	120.28
1	F	182	GLN	CA-C-N	-5.66	113.33	121.98
1	F	182	GLN	C-N-CA	-5.66	113.33	121.98
1	A	87	GLU	CA-C-N	5.58	129.02	121.05
1	A	87	GLU	C-N-CA	5.58	129.02	121.05
1	F	76	ASP	O-C-N	5.57	129.50	123.10
1	C	183	GLN	CA-C-O	5.41	126.92	120.53
1	C	76	ASP	O-C-N	5.40	128.99	122.94
1	E	23	PRO	O-C-N	5.38	123.78	121.31
1	C	191	ASP	CA-C-N	-5.38	112.65	122.38
1	C	191	ASP	C-N-CA	-5.38	112.65	122.38
1	A	46	GLY	O-C-N	-5.36	116.64	122.54
1	F	104	VAL	CA-C-N	-5.35	117.71	122.47
1	F	104	VAL	C-N-CA	-5.35	117.71	122.47
1	F	87	GLU	CA-C-O	5.29	126.32	120.71
1	A	41	PHE	CA-CB-CG	5.27	119.07	113.80
1	C	54	LEU	CA-C-N	-5.24	114.96	122.67
1	C	54	LEU	C-N-CA	-5.24	114.96	122.67
1	F	180	ARG	CD-NE-CZ	5.18	131.65	124.40
1	B	44	PHE	CA-C-N	5.15	131.81	123.37
1	B	44	PHE	C-N-CA	5.15	131.81	123.37
1	E	66	ASP	CA-C-N	-5.14	111.95	120.68
1	E	66	ASP	C-N-CA	-5.14	111.95	120.68
1	E	84	HIS	CA-CB-CG	-5.13	108.67	113.80
1	D	87	GLU	N-CA-C	5.12	117.97	107.69
1	E	169	ARG	O-C-N	5.11	125.89	121.34
1	F	110	ARG	CD-NE-CZ	5.05	131.47	124.40
1	A	180	ARG	CD-NE-CZ	5.04	131.46	124.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1517	0	1520	52	0
1	B	1500	0	1497	43	0
1	C	1501	0	1497	45	0
1	D	1498	0	1496	49	0
1	E	1504	0	1509	38	0
1	F	1500	0	1497	50	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	28	0	11	0	0
3	B	28	0	11	1	0
3	C	28	0	11	0	0
3	D	28	0	11	1	0
3	E	28	0	11	0	0
3	F	28	0	11	0	0
4	A	78	0	0	8	0
4	B	79	0	0	2	0
4	C	60	0	0	2	0
4	D	64	0	0	1	0
4	E	79	0	0	2	0
4	F	67	0	0	3	0
All	All	9621	0	9082	217	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 12.

All (217) 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:C:58:LYS:HZ2	1:C:192:LYS:HA	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HE2	1:B:164:SER:HA	1.55	0.88
1:C:75:LEU:HD22	1:C:79[B]:GLU:HG2	1.56	0.85
1:D:144:LYS:HD2	1:E:44:PHE:HB2	1.62	0.82
1:F:4:CYS:O	1:F:8:ILE:HG13	1.84	0.78
1:E:119:MET:HG2	1:F:122:VAL:HG13	1.67	0.77
1:C:58:LYS:NZ	1:C:192:LYS:HA	2.04	0.73
1:C:174:ARG:HD3	4:C:3197:HOH:O	1.88	0.72
1:D:164:SER:HA	1:F:1:MET:HE2	1.73	0.68
1:A:45[A]:ARG:NH2	1:E:45:ARG:HG2	2.08	0.68
1:B:76:ASP:O	1:B:79:GLU:HB2	1.93	0.67
1:A:45[A]:ARG:HH22	1:E:45:ARG:HG2	1.59	0.67
1:C:6:ARG:O	1:C:9:GLU:HB2	1.95	0.67
1:A:175:GLU:HG3	4:A:2211:HOH:O	1.95	0.66
1:D:5:ASP:OD1	1:E:168[A]:VAL:HG22	1.95	0.66
1:D:58:LYS:HD2	1:D:191:ASP:O	1.96	0.66
1:B:1:MET:H1	1:C:1:MET:N	1.94	0.65
1:A:36[A]:ARG:HD3	1:A:152:GLY:O	1.95	0.65
1:D:172:ASN:ND2	1:D:173:ARG:HE	1.95	0.65
1:A:36[B]:ARG:HD2	4:A:2255:HOH:O	1.96	0.64
1:E:1:MET:H3	1:F:1:MET:H3	1.44	0.64
1:F:24:PRO:HB2	1:F:26:GLU:OE1	1.98	0.63
1:B:179:TYR:CE2	1:B:189:ARG:HD2	2.34	0.63
1:C:24:PRO:HB2	1:C:26:GLU:OE1	1.98	0.63
1:E:115:ARG:HB2	1:F:188:SER:HB2	1.80	0.63
1:C:36:ARG:HD3	1:C:152:GLY:O	1.98	0.62
1:B:10:ALA:O	1:B:14:GLU:HG3	1.99	0.62
1:B:76:ASP:HB2	1:B:79:GLU:OE1	2.00	0.62
1:F:171:TYR:CZ	1:F:177:ALA:HB1	2.34	0.62
1:B:1:MET:H1	1:C:1:MET:H2	1.46	0.61
1:D:144:LYS:NZ	1:E:44:PHE:H	1.98	0.61
1:A:168:VAL:HG12	1:A:169:ARG:HG3	1.81	0.61
1:D:28:ILE:HG12	1:D:33:VAL:HG13	1.84	0.60
1:A:18:SER:OG	1:A:98:THR:HB	2.01	0.59
1:C:57:PRO:HB2	1:C:59:ASP:OD2	2.02	0.59
1:D:144:LYS:HZ1	1:E:44:PHE:H	1.48	0.59
1:D:1:MET:HG2	1:D:2:ARG:N	2.17	0.59
1:A:171:TYR:O	1:A:180:ARG:HD3	2.03	0.59
1:D:162:PRO:HD2	4:D:5210:HOH:O	2.02	0.58
1:E:57:PRO:HB2	1:E:60:GLU:HB2	1.84	0.58
1:D:144:LYS:CD	1:E:44:PHE:HB2	2.33	0.58
1:D:57:PRO:HB2	1:D:60:GLU:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144[A]:LYS:HD2	1:F:44:PHE:HB2	1.85	0.58
4:B:3260:HOH:O	1:C:125:HIS:HD2	1.87	0.57
1:D:1:MET:SD	1:E:164:SER:HB3	2.44	0.57
1:E:119:MET:HE1	1:F:119:MET:CE	2.35	0.57
1:D:119:MET:HE1	1:F:119:MET:HE1	1.87	0.56
1:D:87:GLU:OE1	1:F:144:LYS:HE3	2.06	0.56
1:A:40:LYS:HD2	1:A:184:GLY:HA2	1.88	0.56
1:F:132:SER:O	1:F:181:ASN:HA	2.06	0.56
1:E:6:ARG:HB2	1:F:168:VAL:CG2	2.36	0.55
1:D:144:LYS:HE3	1:E:44:PHE:HD1	1.72	0.55
1:D:178:LYS:HE3	3:D:4194:DUT:O1G	2.07	0.55
1:F:28:ILE:HG12	1:F:33:VAL:HG22	1.89	0.54
1:C:47:HIS:O	1:F:82:TYR:HD1	1.90	0.54
1:B:116:LEU:HD22	1:C:52:ILE:HD13	1.89	0.54
1:A:121:HIS:CD2	1:A:125:HIS:HB3	2.42	0.54
1:F:48:THR:HB	1:F:67:ARG:HG2	1.91	0.53
1:E:119:MET:HE1	1:F:119:MET:HE1	1.90	0.53
1:E:6:ARG:HB2	1:F:168:VAL:HG23	1.90	0.53
1:F:15:GLY:O	1:F:16:ARG:HD2	2.09	0.53
1:D:164:SER:HA	1:F:1:MET:CE	2.39	0.52
1:F:40:LYS:HD3	1:F:72:GLU:CD	2.35	0.52
1:B:39[A]:ASN:OD1	1:B:75:LEU:HB2	2.10	0.52
1:C:24:PRO:HB2	1:C:26:GLU:CD	2.35	0.52
1:C:16:ARG:HB3	1:C:100:PRO:HB3	1.91	0.51
1:E:58:LYS:HZ1	1:E:192:LYS:HE3	1.74	0.51
1:F:1:MET:O	1:F:162:PRO:HD2	2.10	0.51
1:A:1:MET:H1	1:B:1:MET:H1	1.57	0.51
1:B:149:LEU:HD23	1:C:54:LEU:HD12	1.93	0.50
1:D:76:ASP:OD2	1:D:79:GLU:OE1	2.29	0.50
1:A:124:ALA:HA	4:A:2217:HOH:O	2.12	0.50
1:D:36:ARG:HD3	1:D:152:GLY:O	2.12	0.50
1:A:61:VAL:HG12	1:A:191:ASP:HB3	1.93	0.50
1:D:119:MET:CE	1:F:119:MET:HE1	2.41	0.50
1:E:171:TYR:CZ	1:E:177:ALA:HB1	2.47	0.50
1:A:54:LEU:HB2	4:A:2239:HOH:O	2.11	0.50
1:B:1:MET:HE3	1:C:164:SER:HB3	1.94	0.50
1:B:12:LEU:HD21	1:B:19:ILE:HD12	1.94	0.50
1:B:6:ARG:HB2	1:C:168:VAL:CG2	2.42	0.49
1:B:119:MET:HG3	1:C:122:VAL:HG13	1.94	0.49
1:D:161:GLU:CD	1:F:2:ARG:HE	2.20	0.49
1:A:106:TRP:CH2	1:A:126:ARG:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ALA:O	1:D:67:ARG:HG3	2.13	0.49
1:D:24:PRO:HD2	1:D:27:ARG:HG3	1.95	0.49
1:F:83:LEU:HG	4:F:6220:HOH:O	2.13	0.49
1:A:1:MET:CE	1:B:164:SER:HA	2.34	0.49
1:A:39:ASN:OD1	1:A:39:ASN:O	2.31	0.48
1:B:110:ARG:HB2	1:B:113:LEU:HD12	1.95	0.48
1:D:76:ASP:O	1:D:79:GLU:HB3	2.13	0.48
1:D:170:PRO:HG2	1:D:173:ARG:HG2	1.94	0.48
1:E:18:SER:HB2	4:E:6204:HOH:O	2.14	0.48
1:E:144[B]:LYS:HE3	1:F:87:GLU:OE1	2.14	0.48
1:A:182:GLN:O	1:A:183:GLN:HG3	2.13	0.48
1:A:180:ARG:HG2	4:A:2240:HOH:O	2.13	0.48
1:D:75:LEU:HD12	1:D:151:PRO:HD3	1.96	0.48
1:A:28:ILE:HG12	1:A:33[A]:VAL:HG13	1.96	0.47
1:A:65:LEU:O	1:A:69:MET:HG2	2.14	0.47
1:E:1:MET:H3	1:F:1:MET:N	2.11	0.47
1:A:1:MET:N	1:C:1:MET:H2	2.12	0.47
1:A:34:ASP:HB3	1:A:154:LEU:HD22	1.95	0.47
1:A:40:LYS:HD3	1:A:72:GLU:OE1	2.14	0.47
1:C:171:TYR:CZ	1:C:177:ALA:HB1	2.49	0.47
1:D:147:LEU:HD22	1:E:54:LEU:HD21	1.96	0.47
1:B:20:ASN:OD1	1:B:21:PRO:HA	2.15	0.47
1:A:65:LEU:HD11	1:A:190:ILE:HG22	1.95	0.47
1:E:19:ILE:HG22	1:E:23:PRO:HD3	1.98	0.46
1:B:1:MET:N	1:C:1:MET:H2	2.14	0.46
1:D:83:LEU:CD2	1:D:141:ASN:HB2	2.45	0.46
1:E:84:HIS:O	1:E:87:GLU:HB2	2.15	0.46
1:F:16:ARG:O	1:F:100:PRO:HD3	2.15	0.46
1:A:1:MET:N	1:B:1:MET:H1	2.14	0.46
1:C:77:GLU:O	1:C:77:GLU:HG2	2.11	0.46
1:E:63:ALA:O	1:E:67:ARG:HG2	2.15	0.46
1:F:23:PRO:HG2	1:F:33:VAL:CG1	2.46	0.46
1:A:40:LYS:HD2	1:A:184:GLY:CA	2.46	0.46
1:F:16:ARG:HD2	1:F:16:ARG:HA	1.55	0.46
1:E:170:PRO:CG	1:E:173:ARG:HD2	2.46	0.45
1:A:23:PRO:HG3	4:A:2254:HOH:O	2.15	0.45
1:D:1:MET:HB3	1:D:1:MET:HE3	1.77	0.45
1:A:106:TRP:CZ3	1:A:126:ARG:HG3	2.51	0.45
1:F:57:PRO:O	1:F:61:VAL:HG23	2.17	0.45
1:A:119:MET:HE3	1:A:142:SER:HB3	1.98	0.45
1:B:69:MET:HE3	1:B:69:MET:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:LEU:HD22	1:D:103:LEU:HD23	1.98	0.45
1:A:130:GLY:HA2	1:A:172[A]:ASN:ND2	2.31	0.45
1:B:1:MET:N	1:C:161:GLU:OE2	2.50	0.45
1:D:168:VAL:HG23	1:F:6:ARG:HB2	1.98	0.45
1:E:5:ASP:O	1:E:9:GLU:HG3	2.16	0.45
1:A:98:THR:HA	1:A:131:TRP:O	2.16	0.45
1:B:16:ARG:NH2	1:B:102:ASP:OD2	2.50	0.45
1:C:12:LEU:HD21	1:C:19:ILE:HD12	1.99	0.45
1:A:36[B]:ARG:HD3	1:A:95:GLU:OE2	2.16	0.45
1:A:76:ASP:O	1:A:79:GLU:HB2	2.17	0.45
1:D:18[B]:SER:OG	1:D:20:ASN:ND2	2.50	0.45
1:B:145:LEU:HA	1:B:146:PRO:HD3	1.86	0.45
1:C:16:ARG:NH2	1:C:102:ASP:OD1	2.50	0.45
1:C:183:GLN:NE2	4:C:3252:HOH:O	2.51	0.44
1:A:7:ASP:OD2	1:B:164:SER:OG	2.30	0.44
1:D:54:LEU:HD12	1:F:149:LEU:CD2	2.47	0.44
1:E:99:LEU:N	1:E:99:LEU:HD23	2.31	0.44
1:F:45:ARG:NH2	4:F:6226:HOH:O	2.50	0.44
1:B:58:LYS:HE3	1:B:191:ASP:O	2.17	0.44
1:B:113:LEU:HD22	1:B:118:LEU:HD23	1.98	0.44
1:C:104:VAL:HG12	1:C:161:GLU:HB3	2.00	0.44
1:B:5:ASP:OD1	1:B:6:ARG:N	2.51	0.44
1:A:61:VAL:CG1	1:A:191:ASP:HB3	2.47	0.44
1:B:42:ARG:NE	1:B:185:ALA:O	2.51	0.44
1:D:54:LEU:HD12	1:F:149:LEU:HD23	1.98	0.44
1:F:76:ASP:O	1:F:79:GLU:HB2	2.18	0.44
1:F:103:LEU:HD21	1:F:160:PHE:HB3	2.00	0.44
1:C:33:VAL:HG22	1:C:158:LEU:HB2	1.99	0.44
1:F:39[B]:ASN:CG	1:F:75:LEU:HB2	2.42	0.44
1:A:9:GLU:OE2	1:B:169:ARG:NH2	2.50	0.43
1:A:68:VAL:HG11	1:C:145:LEU:CD2	2.49	0.43
1:D:18[B]:SER:HB3	1:D:98:THR:HB	2.00	0.43
1:A:53:ASP:OD1	1:A:56:GLY:N	2.50	0.43
1:D:41:PHE:HA	1:D:90:LEU:O	2.18	0.43
1:F:39[B]:ASN:ND2	1:F:151:PRO:HG2	2.33	0.43
1:F:77:GLU:H	1:F:77:GLU:HG2	1.65	0.43
1:A:53:ASP:OD1	1:C:150:ARG:NH1	2.51	0.43
1:A:54:LEU:HD12	1:C:149:LEU:CD2	2.49	0.43
1:C:104:VAL:CG1	1:C:161:GLU:HB3	2.49	0.43
1:D:144:LYS:HE3	1:E:44:PHE:CD1	2.51	0.43
1:A:20:ASN:HA	1:A:21:PRO:HA	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:TYR:HA	4:A:2208:HOH:O	2.18	0.43
1:B:178:LYS:HG3	3:B:2194:DUT:O1G	2.19	0.43
1:A:144:LYS:HG3	1:B:44:PHE:HB2	2.01	0.42
1:A:180:ARG:O	1:A:181:ASN:HB3	2.18	0.42
1:B:150:ARG:NH1	1:C:53:ASP:OD2	2.49	0.42
1:D:161:GLU:OE1	1:F:2:ARG:NE	2.50	0.42
1:F:59:ASP:OD1	1:F:60:GLU:N	2.50	0.42
1:D:83:LEU:HD23	1:D:141:ASN:HB2	2.01	0.42
1:C:27:ARG:HA	1:C:27:ARG:NE	2.35	0.42
1:D:161:GLU:CD	1:F:2:ARG:HG2	2.45	0.42
1:F:175:GLU:HG3	4:F:6199:HOH:O	2.20	0.42
1:A:39:ASN:O	1:A:74:VAL:HA	2.19	0.42
1:A:111:SER:O	1:A:115:ARG:HG3	2.19	0.42
1:B:115:ARG:NH1	1:C:136:VAL:HG21	2.34	0.42
1:B:145:LEU:HD23	1:C:51:PHE:HA	2.02	0.42
1:C:2:ARG:HD3	1:C:161:GLU:HB2	2.01	0.42
1:C:180:ARG:O	1:C:181:ASN:HB2	2.19	0.42
1:E:150:ARG:HH11	1:E:150:ARG:HD3	1.66	0.42
1:C:110:ARG:HB2	1:C:113:LEU:HG	2.01	0.42
1:F:39[B]:ASN:OD1	1:F:75:LEU:N	2.53	0.42
1:F:39[B]:ASN:ND2	1:F:75:LEU:HB2	2.34	0.42
1:B:76:ASP:H	1:B:79:GLU:CD	2.26	0.42
1:F:186:VAL:HG12	1:F:187:ALA:O	2.20	0.42
4:A:2196:HOH:O	1:B:125:HIS:HD2	2.02	0.41
1:C:82:TYR:CE2	1:F:50:ALA:HB2	2.56	0.41
1:A:40:LYS:HD3	1:A:72:GLU:CD	2.45	0.41
1:D:175:GLU:HA	1:D:180:ARG:HH22	1.86	0.41
1:D:67:ARG:HG3	1:D:67:ARG:HH11	1.86	0.41
1:E:16:ARG:O	1:E:100:PRO:HD3	2.20	0.41
1:A:139:PHE:HZ	1:A:155:ILE:HG12	1.84	0.41
1:D:18[A]:SER:HB2	1:D:98:THR:HB	2.02	0.41
1:C:143:GLY:C	1:C:144:LYS:HD2	2.46	0.41
1:C:176:ASP:OD1	1:C:176:ASP:N	2.53	0.41
1:C:58:LYS:NZ	1:C:191:ASP:O	2.50	0.41
1:B:103:LEU:HD12	1:B:161:GLU:C	2.45	0.41
1:B:171:TYR:HA	1:B:174:ARG:CG	2.50	0.41
1:E:133:GLY:HA2	4:E:6247:HOH:O	2.21	0.40
1:B:36:ARG:HD3	4:B:3242:HOH:O	2.21	0.40
1:B:171:TYR:O	1:B:180:ARG:HD3	2.21	0.40
1:D:136:VAL:HG23	1:D:182:GLN:NE2	2.35	0.40
1:D:150:ARG:O	1:D:153:MET:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:N	1:C:1:MET:N	2.69	0.40
1:B:27:ARG:HA	1:B:27:ARG:NE	2.36	0.40
1:B:37:LEU:HG	1:B:38:GLY:O	2.21	0.40
1:D:1:MET:N	1:E:1:MET:H3	2.19	0.40
1:E:1:MET:N	1:F:1:MET:N	2.69	0.40
1:E:41:PHE:CD2	1:E:91:ALA:HB2	2.57	0.40
1:E:98:THR:C	1:E:99:LEU:HD23	2.47	0.40
1:A:171:TYR:CZ	1:A:177:ALA:HB1	2.57	0.40
1:D:14:GLU:OE2	1:D:16:ARG:NE	2.50	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	195/193 (101%)	188 (96%)	7 (4%)	0	100	100
1	B	192/193 (100%)	179 (93%)	13 (7%)	0	100	100
1	C	192/193 (100%)	183 (95%)	9 (5%)	0	100	100
1	D	192/193 (100%)	182 (95%)	10 (5%)	0	100	100
1	E	193/193 (100%)	188 (97%)	5 (3%)	0	100	100
1	F	192/193 (100%)	183 (95%)	8 (4%)	1 (0%)	24	14
All	All	1156/1158 (100%)	1103 (95%)	52 (4%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	77	GLU

5.3.2 Protein sidechains ⓘ

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	162/158 (102%)	153 (94%)	9 (6%)	19	8
1	B	159/158 (101%)	147 (92%)	12 (8%)	12	4
1	C	159/158 (101%)	149 (94%)	10 (6%)	16	6
1	D	159/158 (101%)	149 (94%)	10 (6%)	16	6
1	E	160/158 (101%)	156 (98%)	4 (2%)	42	30
1	F	159/158 (101%)	145 (91%)	14 (9%)	9	2
All	All	958/948 (101%)	899 (94%)	59 (6%)	16	6

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	16	ARG
1	A	55	SER
1	A	59	ASP
1	A	71	ASP
1	A	145	LEU
1	A	168	VAL
1	A	174	ARG
1	A	175	GLU
1	B	14	GLU
1	B	17	LEU
1	B	18	SER
1	B	52	ILE
1	B	59	ASP
1	B	60	GLU
1	B	77	GLU
1	B	79	GLU
1	B	145	LEU
1	B	174	ARG
1	B	183	GLN
1	B	192	LYS
1	C	1	MET

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Mol	Chain	Res	Type
1	C	18	SER
1	C	25	VAL
1	C	59	ASP
1	C	60	GLU
1	C	76	ASP
1	C	77	GLU
1	C	111	SER
1	C	145	LEU
1	C	180	ARG
1	D	1	MET
1	D	9	GLU
1	D	17	LEU
1	D	45	ARG
1	D	60	GLU
1	D	75	LEU
1	D	107	LEU
1	D	145	LEU
1	D	174	ARG
1	D	182	GLN
1	E	18	SER
1	E	67	ARG
1	E	107	LEU
1	E	145	LEU
1	F	6	ARG
1	F	14	GLU
1	F	16	ARG
1	F	25	VAL
1	F	42	ARG
1	F	55	SER
1	F	58	LYS
1	F	77	GLU
1	F	79	GLU
1	F	111	SER
1	F	144	LYS
1	F	175	GLU
1	F	181	ASN
1	F	183	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	125	HIS

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Mol	Chain	Res	Type
1	B	181	ASN
1	C	20	ASN
1	C	183	GLN
1	D	20	ASN
1	D	172	ASN
1	E	20	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DUT	D	4194	2	28,29,29	1.49	7 (25%)	41,45,45	2.04	10 (24%)
3	DUT	C	3194	2	28,29,29	1.55	7 (25%)	41,45,45	1.99	12 (29%)
3	DUT	B	2194	2	28,29,29	1.47	7 (25%)	41,45,45	2.09	11 (26%)
3	DUT	F	6194	2	28,29,29	1.42	5 (17%)	41,45,45	2.04	10 (24%)
3	DUT	E	5194	2	28,29,29	1.66	7 (25%)	41,45,45	1.93	10 (24%)
3	DUT	A	1194	2	28,29,29	1.48	5 (17%)	41,45,45	2.10	9 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DUT	D	4194	2	-	4/22/34/34	0/2/2/2
3	DUT	C	3194	2	-	4/22/34/34	0/2/2/2
3	DUT	B	2194	2	-	2/22/34/34	0/2/2/2
3	DUT	F	6194	2	-	4/22/34/34	0/2/2/2
3	DUT	E	5194	2	-	2/22/34/34	0/2/2/2
3	DUT	A	1194	2	-	3/22/34/34	0/2/2/2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5194	DUT	PA-O3A	3.78	1.63	1.59
3	A	1194	DUT	O2-C2	3.65	1.29	1.23
3	F	6194	DUT	O2-C2	3.47	1.29	1.23
3	B	2194	DUT	O2-C2	3.42	1.29	1.23
3	C	3194	DUT	O2-C2	3.30	1.28	1.23
3	E	5194	DUT	O2-C2	2.96	1.28	1.23
3	D	4194	DUT	O2-C2	2.88	1.28	1.23
3	E	5194	DUT	C5-C4	-2.72	1.37	1.43
3	F	6194	DUT	C5-C4	-2.66	1.37	1.43
3	D	4194	DUT	PA-O5'	-2.65	1.49	1.59
3	A	1194	DUT	C5-C4	-2.64	1.38	1.43
3	B	2194	DUT	PG-O2G	-2.62	1.45	1.54
3	D	4194	DUT	C5-C4	-2.60	1.38	1.43
3	C	3194	DUT	PA-O3A	2.54	1.62	1.59
3	B	2194	DUT	C5-C4	-2.53	1.38	1.43
3	C	3194	DUT	C5-C4	-2.52	1.38	1.43
3	C	3194	DUT	PA-O5'	-2.52	1.49	1.59
3	C	3194	DUT	C2'-C1'	2.50	1.59	1.52
3	E	5194	DUT	PA-O5'	-2.49	1.49	1.59
3	E	5194	DUT	C2'-C1'	2.47	1.59	1.52
3	E	5194	DUT	PB-O3B	2.44	1.62	1.59
3	D	4194	DUT	C2-N1	2.34	1.42	1.38
3	D	4194	DUT	C2-N3	2.34	1.42	1.38
3	C	3194	DUT	C2-N3	2.34	1.42	1.38
3	B	2194	DUT	C2-N1	2.33	1.42	1.38
3	A	1194	DUT	C2'-C1'	2.31	1.58	1.52
3	F	6194	DUT	C2-N1	2.28	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1194	DUT	C2-N3	2.26	1.41	1.38
3	F	6194	DUT	PA-O5'	-2.25	1.50	1.59
3	D	4194	DUT	PG-O2G	-2.20	1.46	1.54
3	B	2194	DUT	C2'-C1'	2.18	1.58	1.52
3	E	5194	DUT	C2-N3	2.14	1.41	1.38
3	F	6194	DUT	C2'-C1'	2.12	1.58	1.52
3	A	1194	DUT	PB-O3B	2.10	1.61	1.59
3	B	2194	DUT	C2-N3	2.08	1.41	1.38
3	D	4194	DUT	C2'-C1'	2.04	1.57	1.52
3	C	3194	DUT	PG-O2G	-2.04	1.47	1.54
3	B	2194	DUT	PA-O5'	-2.00	1.51	1.59

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	6194	DUT	O4'-C1'-N1	7.28	120.79	107.86
3	A	1194	DUT	O4'-C1'-N1	7.12	120.50	107.86
3	B	2194	DUT	O4'-C1'-N1	5.34	117.33	107.86
3	E	5194	DUT	C2'-C1'-N1	-5.17	100.89	113.81
3	D	4194	DUT	O4'-C1'-N1	4.93	116.62	107.86
3	A	1194	DUT	C2'-C1'-N1	-4.86	101.66	113.81
3	B	2194	DUT	C2'-C1'-N1	-4.78	101.85	113.81
3	B	2194	DUT	O4-C4-C5	-4.71	117.04	125.16
3	D	4194	DUT	O4-C4-C5	-4.69	117.08	125.16
3	E	5194	DUT	O4'-C1'-N1	4.63	116.07	107.86
3	D	4194	DUT	C4-N3-C2	-4.53	120.99	126.61
3	C	3194	DUT	C4-N3-C2	-4.43	121.12	126.61
3	C	3194	DUT	O4'-C1'-N1	4.38	115.63	107.86
3	C	3194	DUT	C2'-C1'-N1	-4.36	102.91	113.81
3	D	4194	DUT	C5-C4-N3	4.22	120.72	114.80
3	B	2194	DUT	O3G-PG-O2G	4.21	123.60	107.80
3	F	6194	DUT	C2'-C1'-N1	-4.19	103.33	113.81
3	A	1194	DUT	O4-C4-C5	-4.17	117.97	125.16
3	E	5194	DUT	C4-N3-C2	-4.16	121.45	126.61
3	D	4194	DUT	C2'-C1'-N1	-4.14	103.45	113.81
3	E	5194	DUT	C5-C4-N3	4.06	120.49	114.80
3	B	2194	DUT	C5-C4-N3	4.04	120.45	114.80
3	B	2194	DUT	C4-N3-C2	-3.97	121.69	126.61
3	A	1194	DUT	C5-C4-N3	3.80	120.12	114.80
3	C	3194	DUT	C5-C4-N3	3.80	120.12	114.80
3	C	3194	DUT	O4-C4-C5	-3.76	118.67	125.16
3	A	1194	DUT	C4-N3-C2	-3.75	121.95	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4194	DUT	O3G-PG-O2G	3.71	121.72	107.80
3	F	6194	DUT	O4-C4-C5	-3.53	119.07	125.16
3	F	6194	DUT	C5-C4-N3	3.36	119.51	114.80
3	C	3194	DUT	O2-C2-N1	-3.30	118.50	122.80
3	F	6194	DUT	O2-C2-N1	-3.28	118.52	122.80
3	B	2194	DUT	O2-C2-N1	-3.20	118.63	122.80
3	D	4194	DUT	C1'-N1-C6	-3.01	115.60	121.53
3	C	3194	DUT	O2A-PA-O3A	-2.95	99.30	107.27
3	F	6194	DUT	C4-N3-C2	-2.93	122.98	126.61
3	E	5194	DUT	O3A-PB-O1B	-2.78	102.33	110.70
3	A	1194	DUT	C1'-N1-C6	-2.73	116.17	121.53
3	E	5194	DUT	O2B-PB-O3A	2.71	114.61	107.27
3	E	5194	DUT	O4-C4-C5	-2.71	120.48	125.16
3	A	1194	DUT	O3'-C3'-C4'	2.67	120.20	110.07
3	C	3194	DUT	O3A-PB-O1B	-2.59	102.90	110.70
3	A	1194	DUT	C1'-N1-C2	2.56	122.67	117.66
3	F	6194	DUT	C1'-N1-C6	-2.48	116.65	121.53
3	F	6194	DUT	O2A-PA-O3A	-2.43	100.69	107.27
3	C	3194	DUT	C1'-N1-C6	-2.40	116.82	121.53
3	E	5194	DUT	C1'-N1-C6	-2.39	116.83	121.53
3	C	3194	DUT	O2B-PB-O3A	2.33	113.57	107.27
3	B	2194	DUT	C1'-N1-C6	-2.33	116.95	121.53
3	E	5194	DUT	O5'-PA-O1A	2.30	118.04	108.94
3	A	1194	DUT	O2-C2-N1	-2.28	119.83	122.80
3	E	5194	DUT	O3'-C3'-C4'	2.24	118.55	110.07
3	C	3194	DUT	O2G-PG-O1G	2.23	119.54	110.83
3	B	2194	DUT	O4-C4-N3	2.23	122.50	119.27
3	F	6194	DUT	O2-C2-N3	2.22	125.58	121.49
3	D	4194	DUT	O2-C2-N1	-2.15	120.00	122.80
3	C	3194	DUT	O3G-PG-O2G	2.12	115.74	107.80
3	B	2194	DUT	O3A-PB-O1B	-2.05	104.54	110.70
3	B	2194	DUT	O2-C2-N3	2.04	125.25	121.49
3	D	4194	DUT	O3A-PB-O1B	-2.03	104.60	110.70
3	D	4194	DUT	O4-C4-N3	2.02	122.20	119.27
3	F	6194	DUT	O3'-C3'-C4'	2.02	117.73	110.07

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2194	DUT	PG-O3B-PB-O1B
3	C	3194	DUT	PG-O3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
3	D	4194	DUT	PG-O3B-PB-O2B
3	F	6194	DUT	PB-O3A-PA-O1A
3	A	1194	DUT	PG-O3B-PB-O1B
3	A	1194	DUT	PG-O3B-PB-O2B
3	B	2194	DUT	PG-O3B-PB-O2B
3	C	3194	DUT	PG-O3B-PB-O2B
3	D	4194	DUT	PA-O3A-PB-O1B
3	E	5194	DUT	PG-O3B-PB-O1B
3	E	5194	DUT	PG-O3B-PB-O2B
3	F	6194	DUT	PG-O3B-PB-O2B
3	C	3194	DUT	PB-O3A-PA-O1A
3	A	1194	DUT	PB-O3A-PA-O2A
3	C	3194	DUT	PB-O3A-PA-O2A
3	D	4194	DUT	PB-O3A-PA-O2A
3	D	4194	DUT	PG-O3B-PB-O1B
3	F	6194	DUT	PB-O3A-PA-O2A
3	F	6194	DUT	PG-O3B-PB-O1B

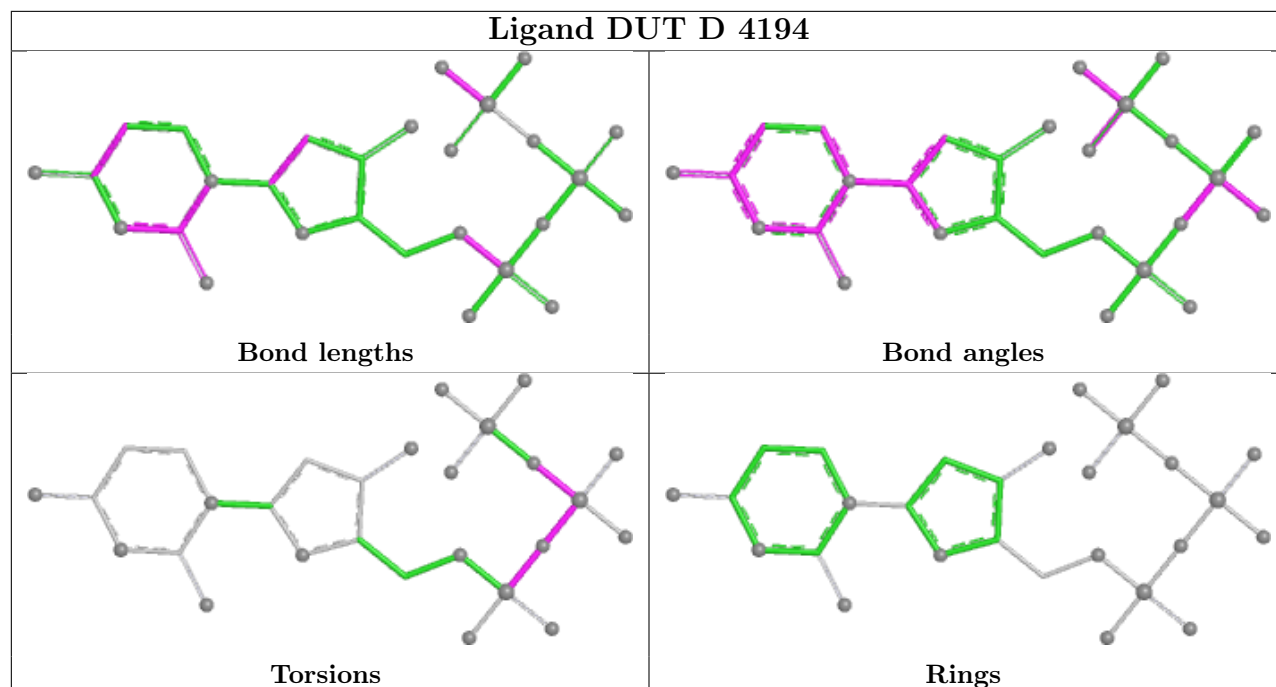
There are no ring outliers.

2 monomers are involved in 2 short contacts:

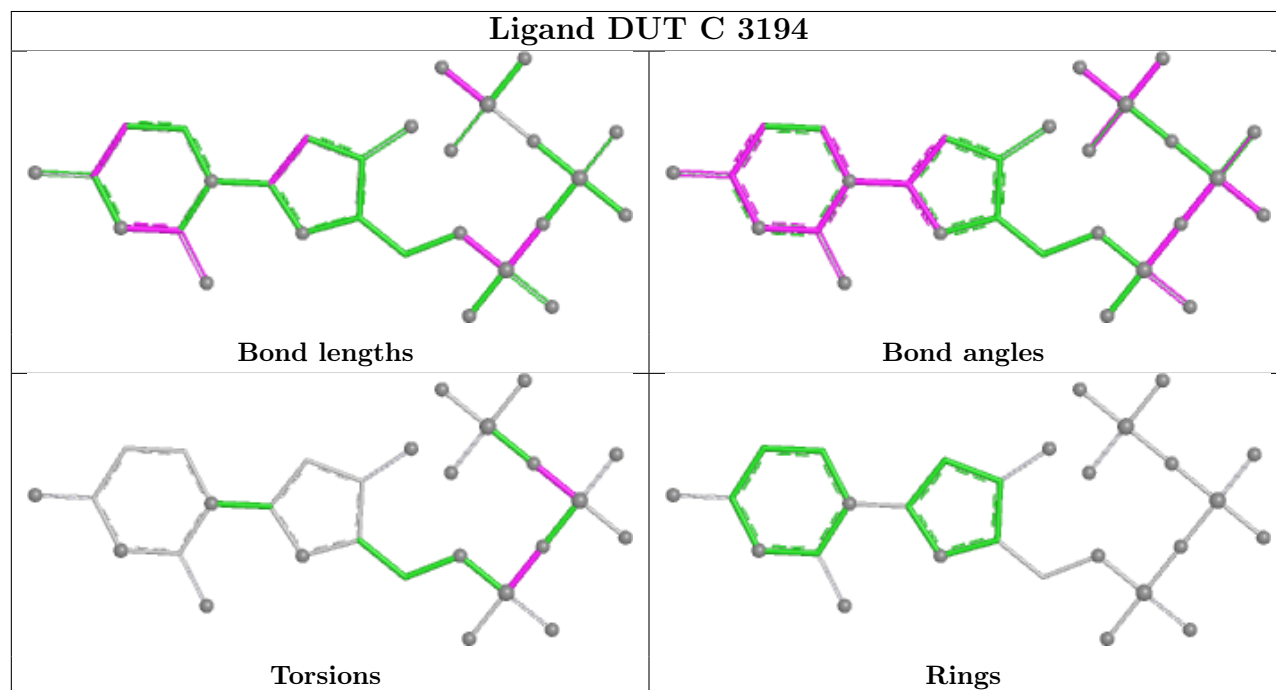
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	4194	DUT	1	0
3	B	2194	DUT	1	0

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 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.

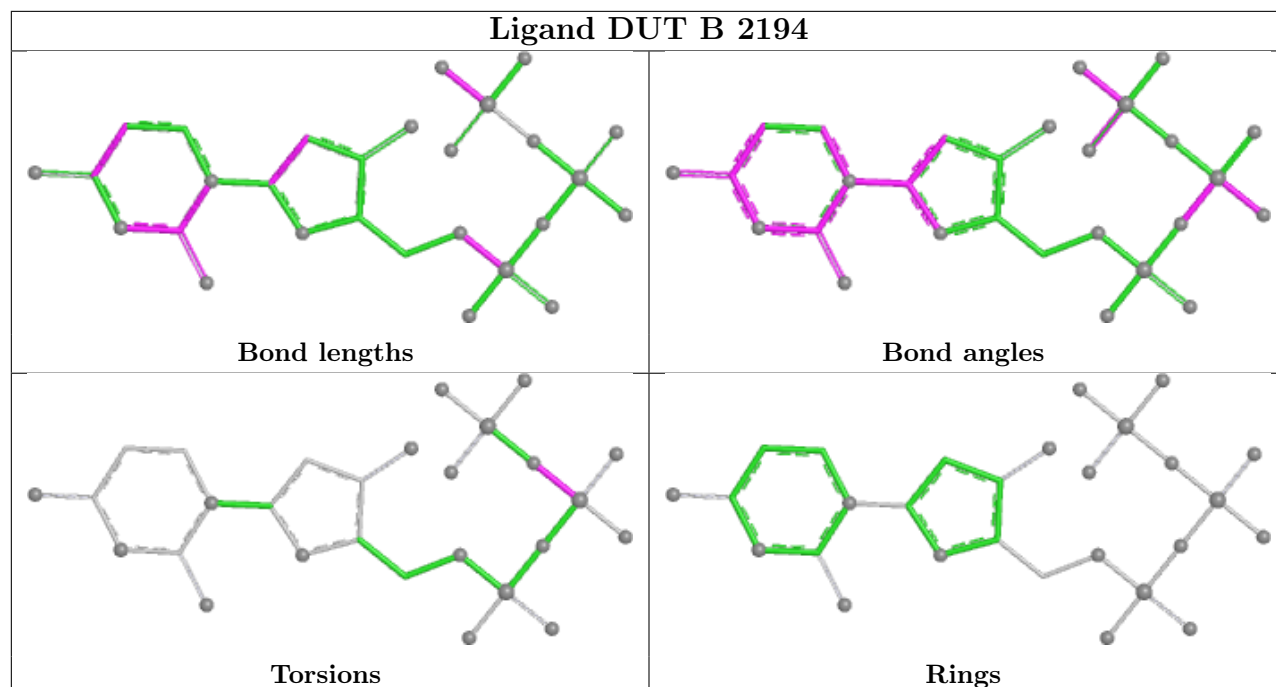
Ligand DUT D 4194



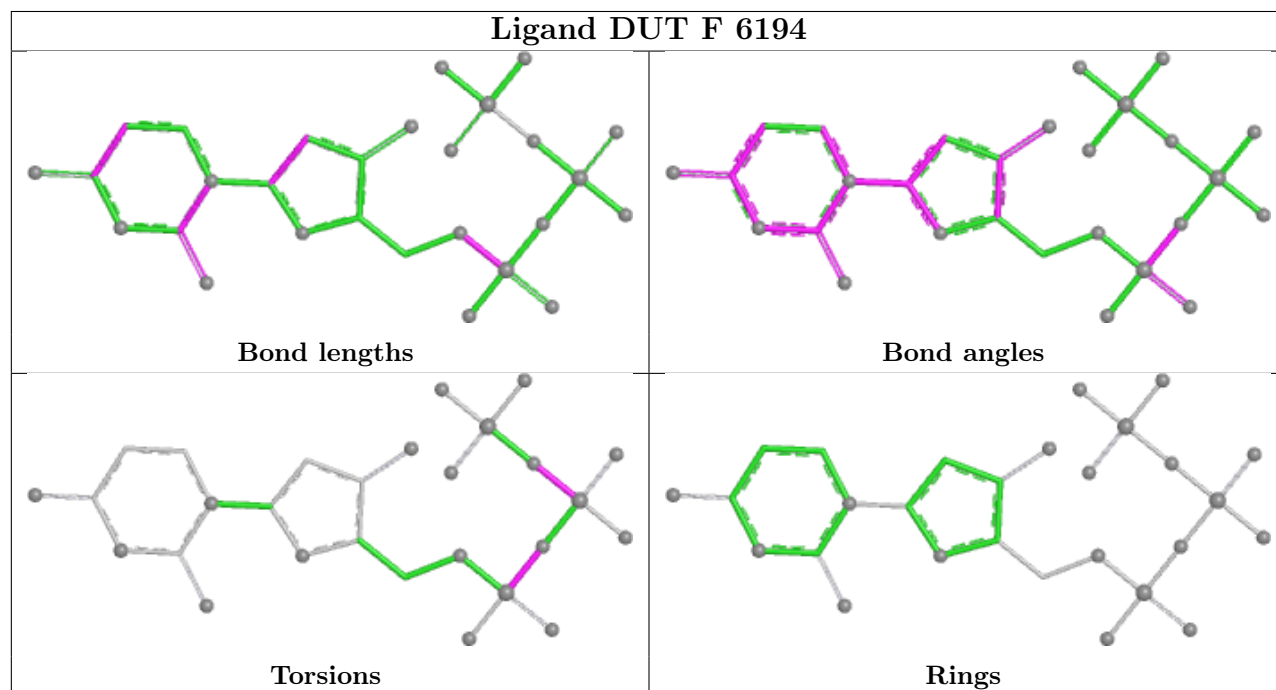
Ligand DUT C 3194

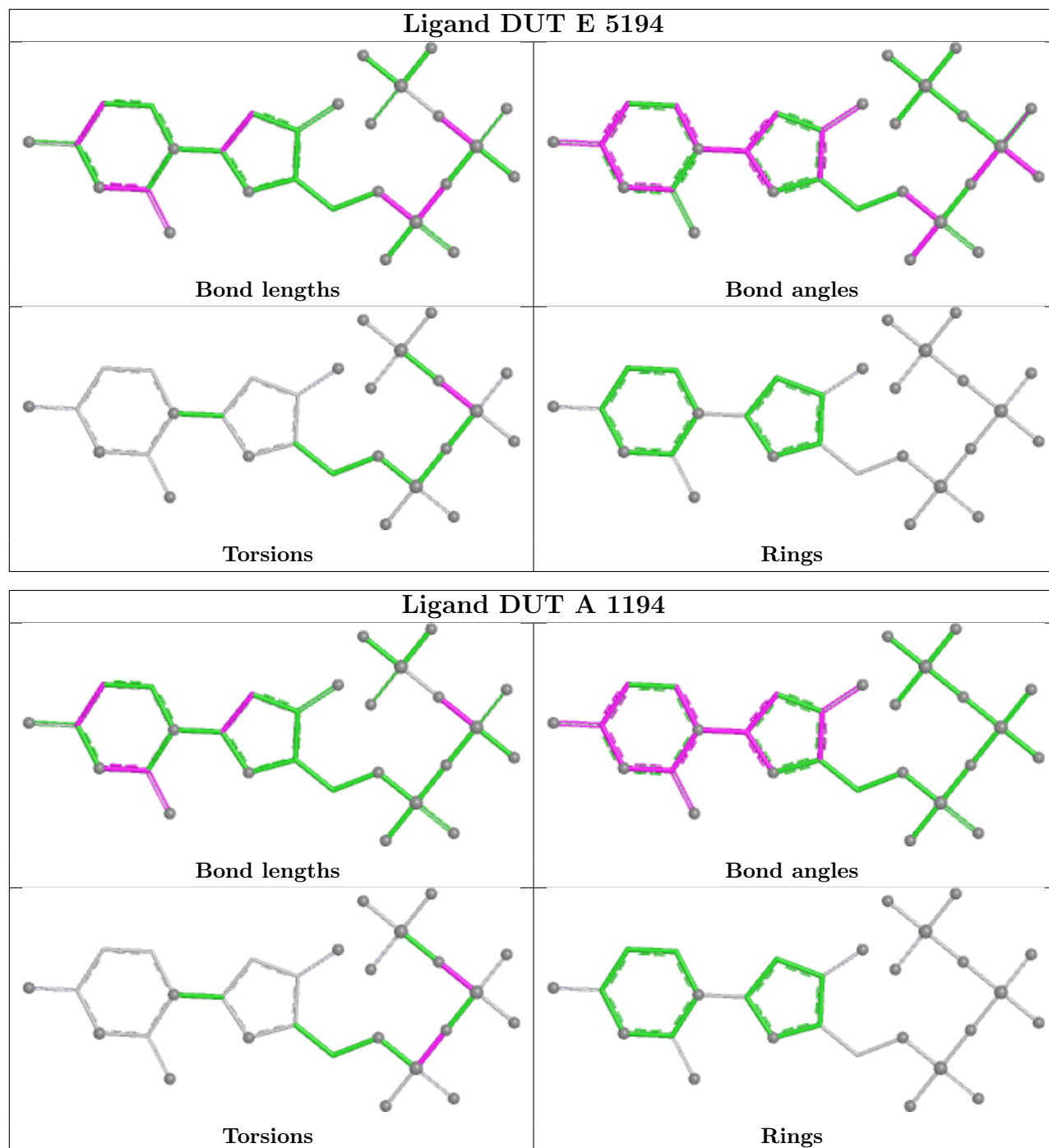


Ligand DUT B 2194



Ligand DUT F 6194





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	193/193 (100%)	-1.43	0 100 100	14, 25, 49, 64	4 (2%)
1	B	193/193 (100%)	-1.44	0 100 100	16, 25, 49, 96	1 (0%)
1	C	193/193 (100%)	-1.44	0 100 100	17, 26, 45, 66	1 (0%)
1	D	193/193 (100%)	-1.42	0 100 100	16, 26, 50, 65	1 (0%)
1	E	193/193 (100%)	-1.48	0 100 100	12, 25, 43, 61	2 (1%)
1	F	193/193 (100%)	-1.45	0 100 100	14, 25, 48, 61	1 (0%)
All	All	1158/1158 (100%)	-1.44	0 100 100	12, 25, 48, 96	10 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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
2	MG	F	4195	1/1	0.99	0.04	28,28,28,28	0

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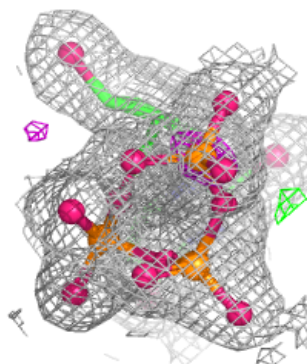
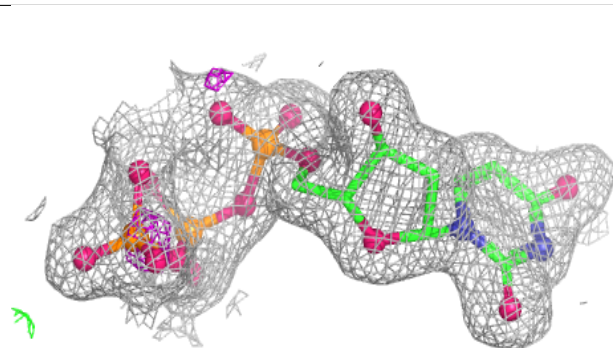
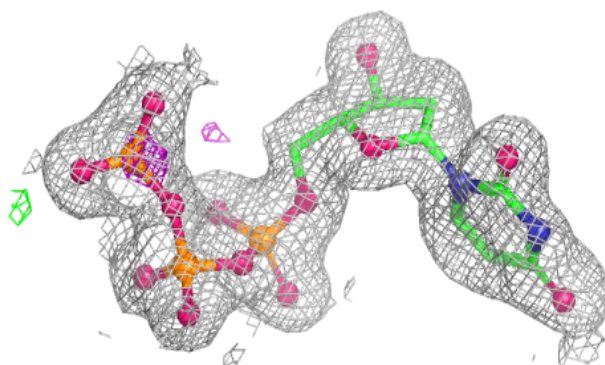
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	3195	1/1	1.00	0.03	23,23,23,23	0
2	MG	C	1195	1/1	1.00	0.02	24,24,24,24	0
2	MG	D	5195	1/1	1.00	0.01	21,21,21,21	0
2	MG	E	6195	1/1	1.00	0.03	25,25,25,25	0
2	MG	A	2195	1/1	1.00	0.04	14,14,14,14	0
3	DUT	A	1194	28/28	1.00	0.02	17,22,25,26	0
3	DUT	B	2194	28/28	1.00	0.02	14,21,27,29	0
3	DUT	C	3194	28/28	1.00	0.02	16,20,24,24	0
3	DUT	D	4194	28/28	1.00	0.02	17,22,28,30	0
3	DUT	E	5194	28/28	1.00	0.02	14,20,27,28	0
3	DUT	F	6194	28/28	1.00	0.02	15,21,25,30	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.

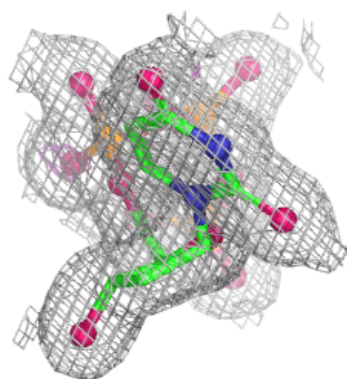
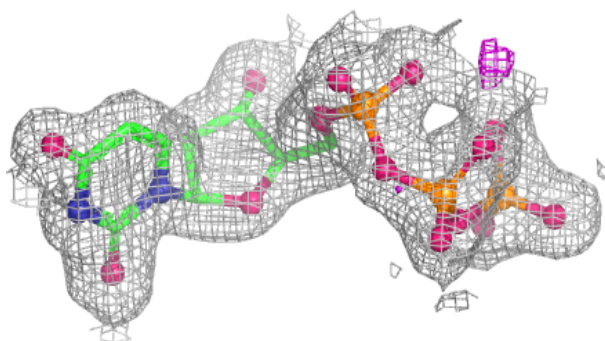
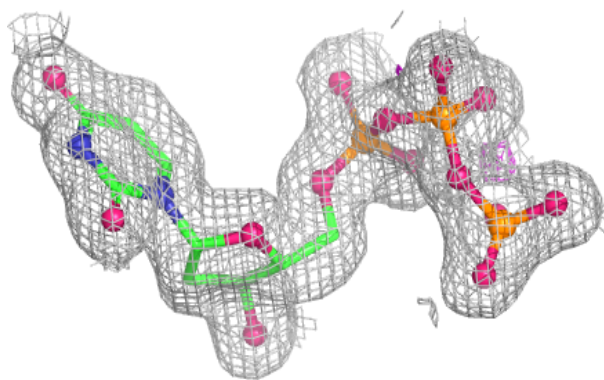
Electron density around DUT A 1194:

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

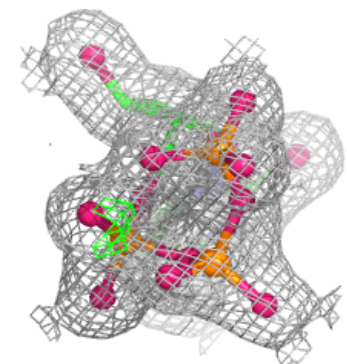
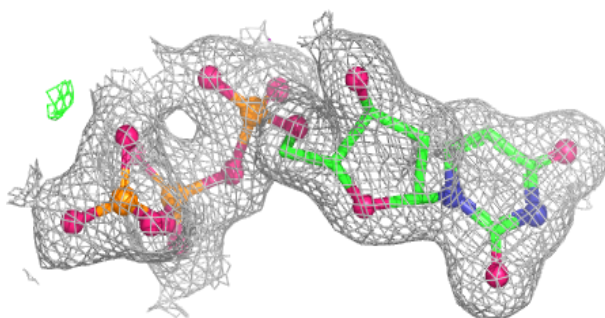
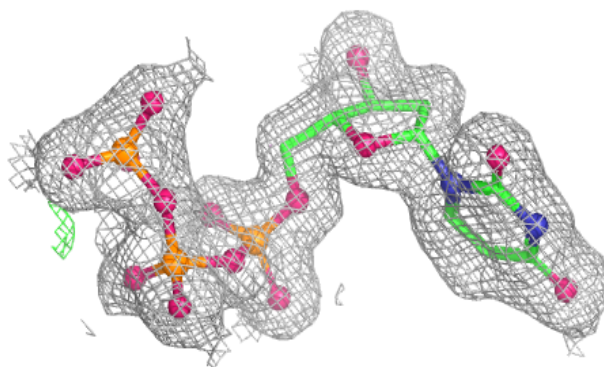


Electron density around DUT B 2194:

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

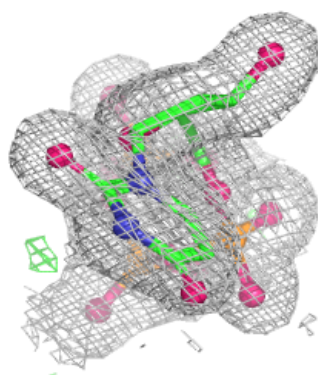
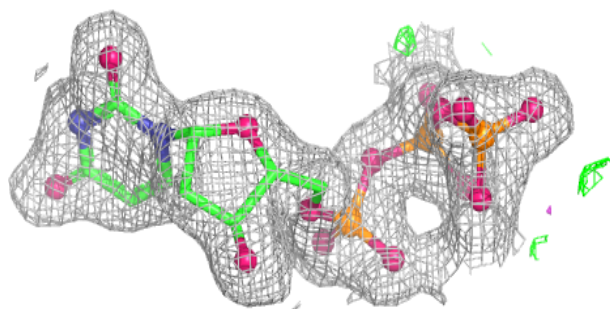
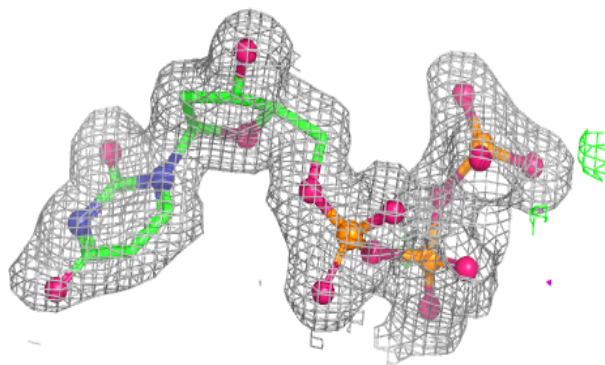
**Electron density around DUT C 3194:**

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

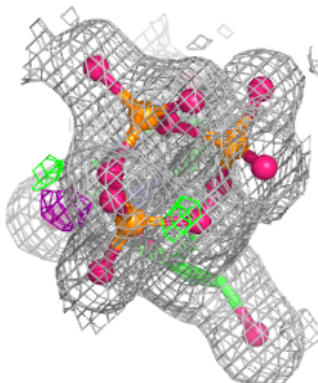
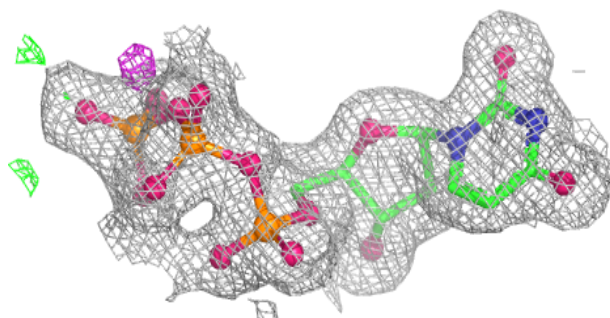
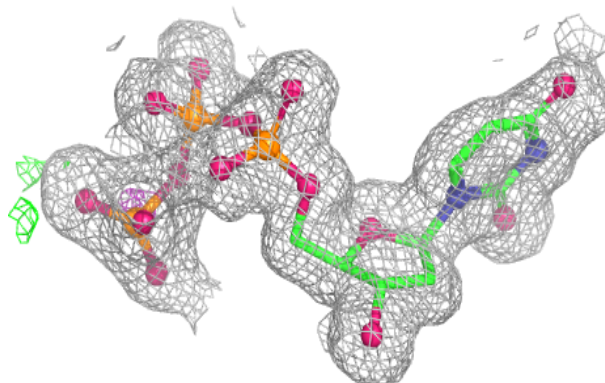


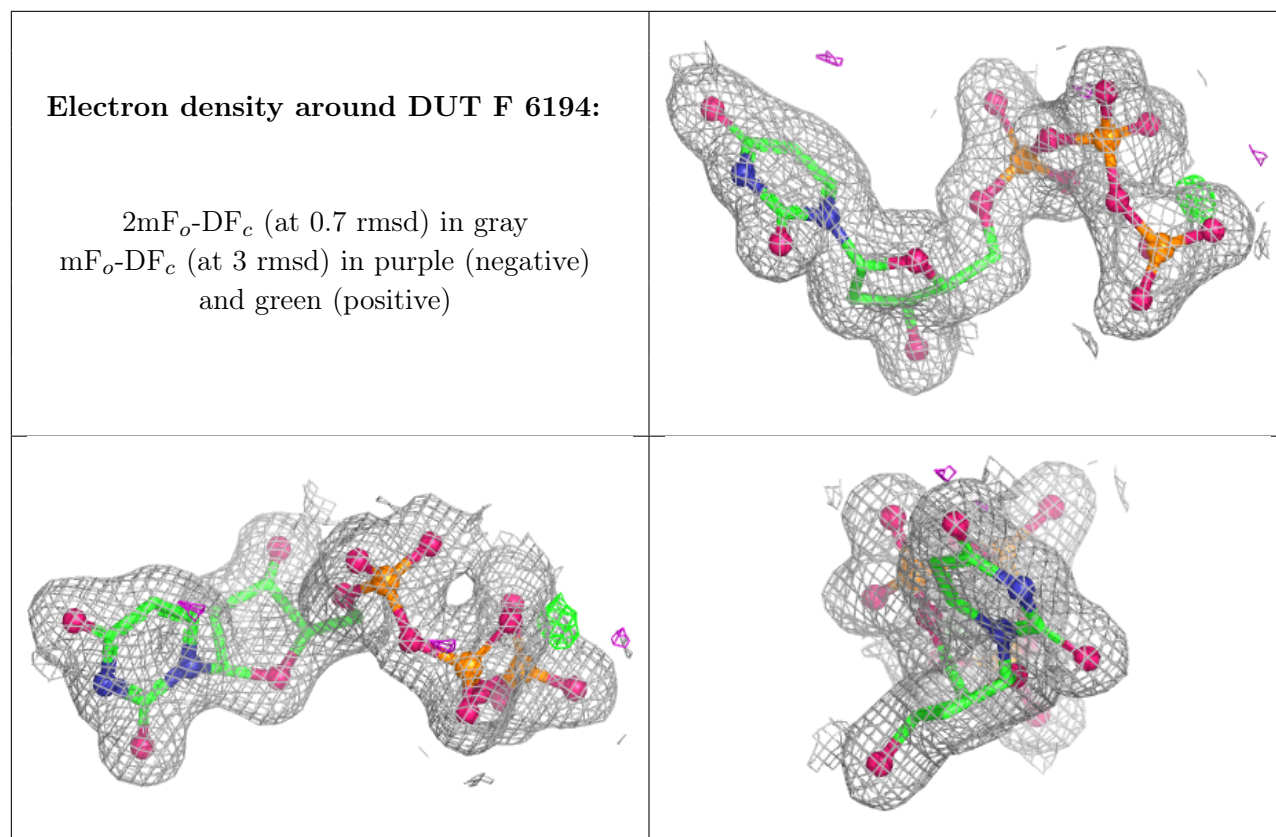
Electron density around DUT D 4194:

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

**Electron density around DUT E 5194:**

$2mF_o-DF_c$ (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.