



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:22 pm BST

PDB ID : 1XS1
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 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 : 2.11
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) : 2.11

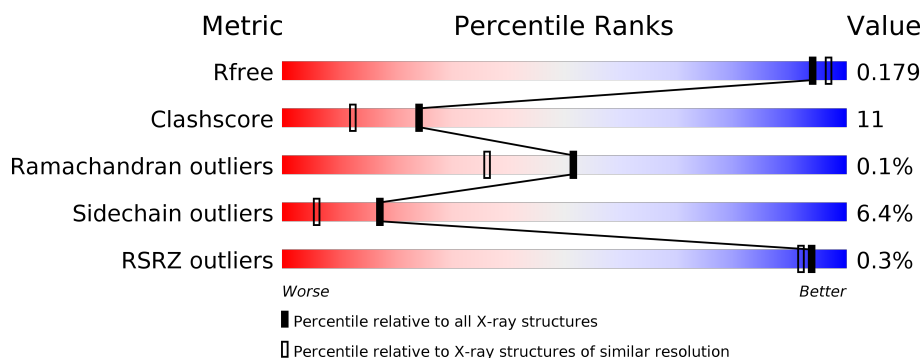
1 Overall quality at a glance

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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 on 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	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>32%</div> <div>.</div> </div> </div>
1	B	193	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>..</div> </div> </div>
1	C	193	<div> <div></div> <div> <div>72%</div> <div>25%</div> <div>.</div> </div> </div>
1	D	193	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>.</div> </div> </div>
1	E	193	<div> <div></div> <div> <div>80%</div> <div>17%</div> <div>.</div> </div> </div>
1	F	193	<div> <div></div> <div> <div>69%</div> <div>28%</div> <div>..</div> </div> </div>

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.

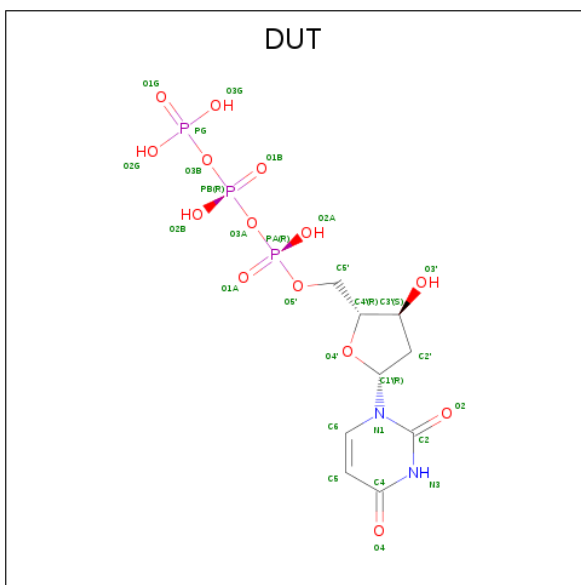
- Molecule 1 is a protein called Deoxycytidine triphosphate deaminase.

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is DEOXYURIDINE-5'-TRIPHOSPHATE (three-letter code: DUT) (formula: $C_9H_{15}N_2O_{14}P_3$).



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		

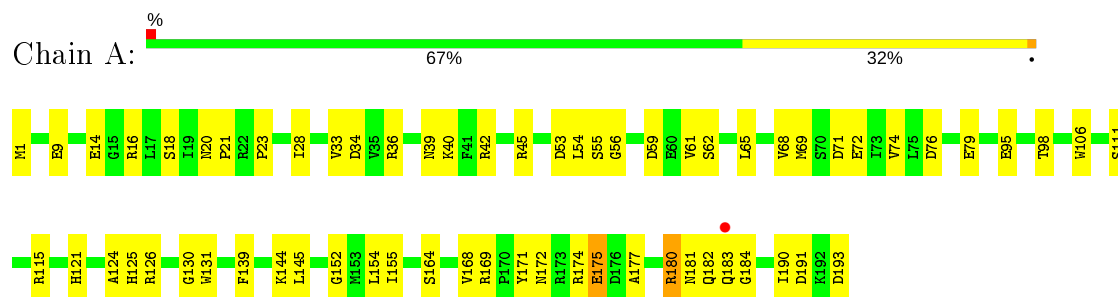
- Molecule 4 is water.

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		

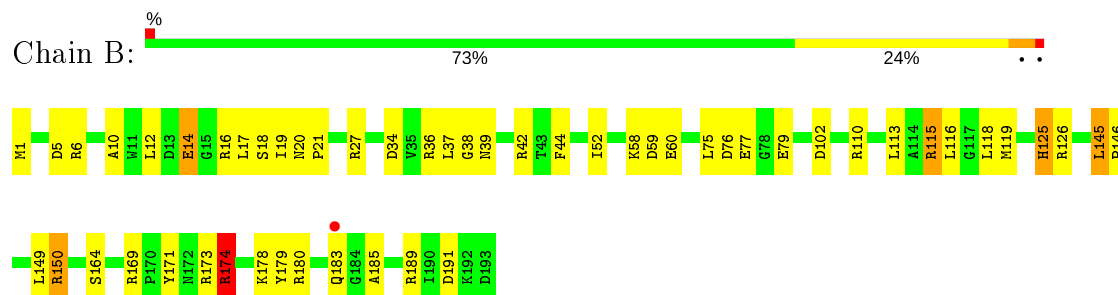
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

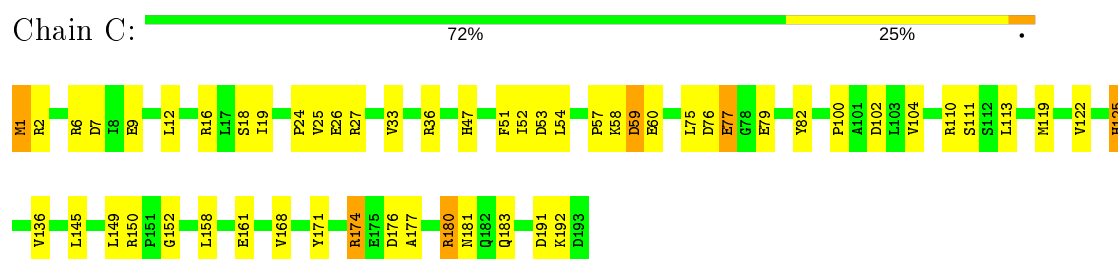
• Molecule 1: Deoxycytidine triphosphate deaminase



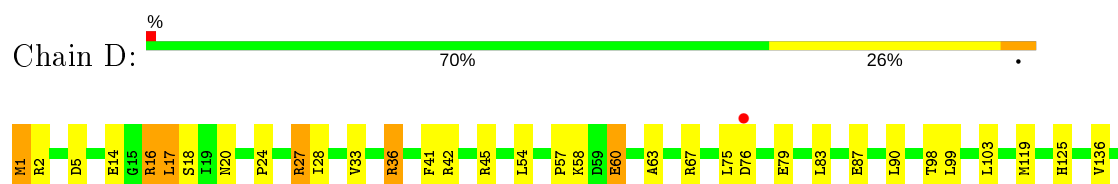
• Molecule 1: Deoxycytidine triphosphate deaminase



• Molecule 1: Deoxycytidine triphosphate deaminase

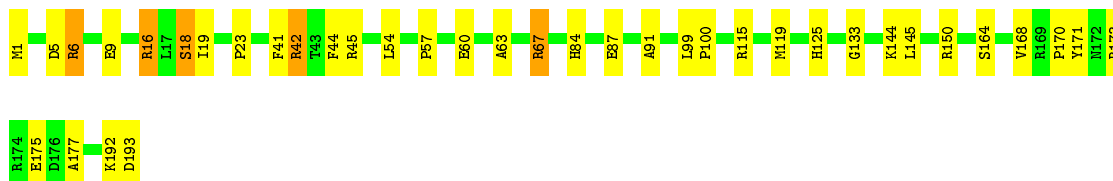
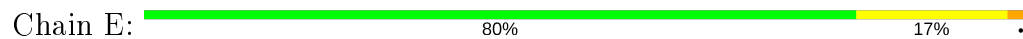


• Molecule 1: Deoxycytidine triphosphate deaminase

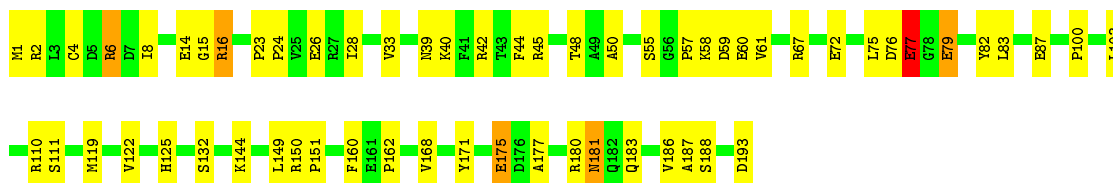




- Molecule 1: Deoxycytidine triphosphate deaminase



- 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	63.03 Å 97.46 Å 95.47 Å 90.00° 109.23° 90.00°	Depositor
Resolution (Å)	25.00 – 1.80 24.37 – 1.80	Depositor EDS
% Data completeness (in resolution range)	90.1 (25.00-1.80) 94.7 (24.37-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.45 (at 1.80 Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.164 , 0.195 0.151 , 0.179	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)	0.32 , 31.7	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	0.97	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	1/1564 (0.1%)	1.03	2/2119 (0.1%)
1	B	0.38	0/1535	1.02	8/2081 (0.4%)
1	C	0.41	0/1536	1.16	3/2082 (0.1%)
1	D	0.41	1/1533 (0.1%)	1.03	6/2078 (0.3%)
1	E	0.40	1/1543 (0.1%)	0.96	1/2091 (0.0%)
1	F	0.42	1/1535 (0.1%)	1.03	3/2081 (0.1%)
All	All	0.41	4/9246 (0.0%)	1.04	23/12532 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	ASP	C-OXT	10.66	1.43	1.23
1	F	193	ASP	C-OXT	7.54	1.37	1.23
1	D	193	ASP	C-OXT	-7.00	1.10	1.23
1	E	193	ASP	C-OXT	5.38	1.33	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	ARG	CD-NE-CZ	26.63	160.88	123.60
1	C	174	ARG	NE-CZ-NH1	11.38	125.99	120.30
1	D	150	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	D	150	ARG	CD-NE-CZ	8.47	135.46	123.60
1	D	174	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	C	174	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	A	174	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	D	36	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	D	16	ARG	NE-CZ-NH1	-7.22	116.69	120.30
1	B	174	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	B	150	ARG	NE-CZ-NH1	-6.84	116.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	ARG	CD-NE-CZ	6.50	132.69	123.60
1	B	126	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	B	173	ARG	NE-CZ-NH2	5.75	123.18	120.30
1	F	180	ARG	CD-NE-CZ	5.75	131.65	123.60
1	F	150	ARG	NE-CZ-NH1	-5.65	117.48	120.30
1	F	110	ARG	CD-NE-CZ	5.62	131.47	123.60
1	A	180	ARG	CD-NE-CZ	5.62	131.46	123.60
1	B	174	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	B	115	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	E	42	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	D	27	ARG	CD-NE-CZ	5.29	131.01	123.60
1	B	34	ASP	CB-CG-OD1	5.05	122.85	118.30

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	48	0
1	B	1500	0	1497	35	0
1	C	1501	0	1497	43	0
1	D	1498	0	1496	46	0
1	E	1504	0	1509	36	0
1	F	1500	0	1497	46	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4	0
All	All	9621	0	9082	201	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 (201) 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
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:E:119:MET:HE1	4:F:6202:HOH:O	1.83	0.78
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:B:1:MET:H1	1:C:1:MET:N	1.85	0.74
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:B:1:MET:H1	1:C:1:MET:H2	1.38	0.71
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:58:LYS:HD2	1:D:191:ASP:O	1.96	0.66
1:D:5:ASP:OD1	1:E:168[A]:VAL:HG22	1.95	0.66
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:E:1:MET:H3	1:F:1:MET:H3	1.51	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
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:A:1:MET:CE	1:B:164:SER:HA	2.34	0.57
1:D:1:MET:SD	1:E:164:SER:HB3	2.44	0.57
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:178:LYS:HE3	3:D:4194:DUT:O1G	2.07	0.55
1:D:144:LYS:HE3	1:E:44:PHE:HD1	1.72	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: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:B:39[A]:ASN:OD1	1:B:75:LEU:HB2	2.10	0.52
1:C:16:ARG:HB3	1:C:100:PRO:HB3	1.91	0.51
1:F:1:MET:O	1:F:162:PRO:HD2	2.10	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:E:171:TYR:CZ	1:E:177:ALA:HB1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HB2	4:A:2239:HOH:O	2.11	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:164:SER:HA	1:F:1:MET:HE1	1.93	0.49
1:A:106:TRP:CH2	1:A:126:ARG:HG3	2.47	0.49
1:D:63:ALA:O	1:D:67:ARG:HG3	2.13	0.49
1:D:144:LYS:HZ2	1:E:44:PHE:H	1.61	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: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:144[B]:LYS:HE3	1:F:87:GLU:OE1	2.14	0.48
1:E:18:SER:HB2	4:E:6204:HOH:O	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: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:D:147:LEU:HD22	1:E:54:LEU:HD21	1.96	0.47
1:F:40:LYS:HD3	1:F:72:GLU:CD	2.35	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: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:1:MET:H3	1:F:1:MET:N	2.12	0.47
1:E:19:ILE:HG22	1:E:23:PRO:HD3	1.98	0.46
1:C:24:PRO:HB2	1:C:26:GLU:CD	2.35	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:C:77:GLU:HG2	1:C:77:GLU:O	2.11	0.46
1:A:164:SER:OG	1:C:7:ASP:OD2	2.30	0.46
1:E:63:ALA:O	1:E:67:ARG:HG2	2.15	0.46
1:A:1:MET:HE1	1:B:164:SER:HA	1.98	0.46
1:F:23:PRO:HG2	1:F:33:VAL:CG1	2.46	0.46
1:E:119:MET:HE3	1:F:119:MET:SD	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:E:5:ASP:O	1:E:9:GLU:HG3	2.16	0.45
1:D:168:VAL:HG23	1:F:6:ARG:HB2	1.98	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:76:ASP:O	1:A:79:GLU:HB2	2.17	0.45
1:A:36[B]:ARG:HD3	1:A:95:GLU:OE2	2.16	0.45
1:D:18[B]:SER:OG	1:D:20:ASN:ND2	2.50	0.45
1:D:161:GLU:CD	1:F:2:ARG:HE	2.20	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:E:99:LEU:N	1:E:99:LEU:HD23	2.31	0.44
1:D:54:LEU:HD12	1:F:149:LEU:CD2	2.47	0.44
1:F:45:ARG:NH2	4:F:6226:HOH:O	2.50	0.44
1:B:113:LEU:HD22	1:B:118:LEU:HD23	1.98	0.44
1:B:58:LYS:HE3	1:B:191:ASP:O	2.17	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:103:LEU:HD21	1:F:160:PHE:HB3	2.00	0.44
1:F:76:ASP:O	1:F:79:GLU:HB2	2.18	0.44
1:C:33:VAL:HG22	1:C:158:LEU:HB2	1.99	0.44
1:A:9:GLU:OE2	1:B:169:ARG:NH2	2.50	0.43
1:B:119:MET:HE3	1:C:119:MET:SD	2.59	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:D:119:MET:SD	1:F:119:MET:HE1	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:GLU:HG2	1:F:77:GLU:H	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
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:180:ARG:O	1:A:181:ASN:HB3	2.18	0.42
1:A:144:LYS:HG3	1:B:44:PHE:HB2	2.01	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:NE	1:C:27:ARG:HA	2.35	0.42
1:F:175:GLU:HG3	4:F:6199:HOH:O	2.20	0.42
1:A:111:SER:O	1:A:115:ARG:HG3	2.19	0.42
1:A:39:ASN:O	1:A:74:VAL:HA	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:ND2	1:F:75:LEU:HB2	2.34	0.42
1:F:39[B]:ASN:OD1	1:F:75:LEU:N	2.53	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:D:175:GLU:HA	1:D:180:ARG:HH22	1.86	0.41
1:D:1:MET:N	1:E:1:MET:H3	2.17	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:176:ASP:N	1:C:176:ASP:OD1	2.53	0.41
1:C:58:LYS:NZ	1:C:191:ASP:O	2.50	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:171:TYR:O	1:B:180:ARG:HD3	2.21	0.40
1:B:36:ARG:HD3	4:B:3242:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:41:PHE:CD2	1:E:91:ALA:HB2	2.57	0.40
1:E:1:MET:N	1:F:1:MET:N	2.69	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%)	29	15
All	All	1156/1158 (100%)	1103 (95%)	52 (4%)	1 (0%)	51	36

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%)	21	8
1	B	159/158 (101%)	148 (93%)	11 (7%)	15	5
1	C	159/158 (101%)	149 (94%)	10 (6%)	18	6
1	D	159/158 (101%)	150 (94%)	9 (6%)	20	8
1	E	160/158 (101%)	151 (94%)	9 (6%)	21	8
1	F	159/158 (101%)	146 (92%)	13 (8%)	11	3
All	All	958/948 (101%)	897 (94%)	61 (6%)	17	6

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	16	ARG
1	A	42	ARG
1	A	55	SER
1	A	59	ASP
1	A	62	SER
1	A	71	ASP
1	A	145	LEU
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	125	HIS
1	B	145	LEU
1	B	174	ARG
1	B	183	GLN
1	C	1	MET
1	C	18	SER

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Mol	Chain	Res	Type
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	125	HIS
1	C	180	ARG
1	D	1	MET
1	D	17	LEU
1	D	42	ARG
1	D	45	ARG
1	D	60	GLU
1	D	125	HIS
1	D	145	LEU
1	D	181	ASN
1	D	192	LYS
1	E	6	ARG
1	E	16	ARG
1	E	18	SER
1	E	42	ARG
1	E	67	ARG
1	E	125	HIS
1	E	145	LEU
1	E	175	GLU
1	E	192	LYS
1	F	6	ARG
1	F	14	GLU
1	F	16	ARG
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	125	HIS
1	F	175	GLU
1	F	181	ASN
1	F	183	GLN

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

Mol	Chain	Res	Type
1	A	20	ASN
1	B	125	HIS
1	C	20	ASN
1	C	125	HIS
1	C	183	GLN
1	D	20	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 carbohydrates 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	E	5194	2	22,29,29	1.26	3 (13%)	27,45,45	1.64	3 (11%)
3	DUT	A	1194	2	22,29,29	1.21	2 (9%)	27,45,45	1.49	2 (7%)
3	DUT	F	6194	2	22,29,29	1.15	3 (13%)	27,45,45	1.45	1 (3%)
3	DUT	D	4194	2	22,29,29	1.20	3 (13%)	27,45,45	1.47	3 (11%)
3	DUT	C	3194	2	22,29,29	1.28	3 (13%)	27,45,45	1.44	3 (11%)
3	DUT	B	2194	2	22,29,29	1.21	3 (13%)	27,45,45	1.60	2 (7%)

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	E	5194	2	-	3/19/34/34	0/2/2/2
3	DUT	A	1194	2	-	3/19/34/34	0/2/2/2
3	DUT	F	6194	2	-	3/19/34/34	0/2/2/2
3	DUT	D	4194	2	-	3/19/34/34	0/2/2/2
3	DUT	C	3194	2	-	4/19/34/34	0/2/2/2
3	DUT	B	2194	2	-	3/19/34/34	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3194	DUT	C4-N3	2.54	1.37	1.33
3	D	4194	DUT	PA-O5'	-2.54	1.49	1.59
3	B	2194	DUT	PG-O2G	-2.53	1.45	1.54
3	B	2194	DUT	C4-N3	2.47	1.37	1.33
3	C	3194	DUT	C2'-C1'	2.43	1.59	1.52
3	C	3194	DUT	PA-O5'	-2.41	1.49	1.59
3	E	5194	DUT	C2'-C1'	2.40	1.59	1.52
3	A	1194	DUT	C4-N3	2.39	1.37	1.33
3	E	5194	DUT	PA-O5'	-2.39	1.49	1.59
3	E	5194	DUT	C4-N3	2.26	1.37	1.33
3	A	1194	DUT	C2'-C1'	2.25	1.58	1.52
3	F	6194	DUT	PA-O5'	-2.15	1.50	1.59
3	D	4194	DUT	PG-O2G	-2.14	1.46	1.54
3	F	6194	DUT	C4-N3	2.12	1.36	1.33
3	B	2194	DUT	C2'-C1'	2.12	1.58	1.52
3	F	6194	DUT	C2'-C1'	2.07	1.58	1.52
3	D	4194	DUT	C4-N3	2.05	1.36	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5194	DUT	C2'-C1'-N1	-5.80	100.89	114.27
3	A	1194	DUT	C2'-C1'-N1	-5.47	101.66	114.27
3	B	2194	DUT	C2'-C1'-N1	-5.38	101.85	114.27
3	C	3194	DUT	C2'-C1'-N1	-4.93	102.91	114.27
3	F	6194	DUT	C2'-C1'-N1	-4.74	103.33	114.27
3	D	4194	DUT	C2'-C1'-N1	-4.69	103.45	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2194	DUT	O3G-PG-O2G	4.18	123.60	107.64
3	D	4194	DUT	O3G-PG-O2G	3.68	121.72	107.64
3	A	1194	DUT	O3'-C3'-C4'	2.64	120.20	110.10
3	E	5194	DUT	O5'-PA-O1A	2.30	118.04	109.07
3	C	3194	DUT	O2G-PG-O1G	2.26	119.54	110.68
3	D	4194	DUT	PB-O3B-PG	-2.22	125.22	132.83
3	E	5194	DUT	O3'-C3'-C4'	2.21	118.55	110.10
3	C	3194	DUT	O3G-PG-O2G	2.12	115.74	107.64

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	5194	DUT	O4'-C1'-N1-C6
3	A	1194	DUT	O4'-C1'-N1-C6
3	D	4194	DUT	O4'-C1'-N1-C6
3	F	6194	DUT	O4'-C1'-N1-C6
3	B	2194	DUT	O4'-C1'-N1-C6
3	C	3194	DUT	O4'-C1'-N1-C6
3	D	4194	DUT	PG-O3B-PB-O2B
3	F	6194	DUT	PB-O3A-PA-O1A
3	B	2194	DUT	PG-O3B-PB-O1B
3	C	3194	DUT	PG-O3B-PB-O1B
3	E	5194	DUT	PG-O3B-PB-O1B
3	E	5194	DUT	PG-O3B-PB-O2B
3	A	1194	DUT	PG-O3B-PB-O1B
3	A	1194	DUT	PG-O3B-PB-O2B
3	D	4194	DUT	PA-O3A-PB-O1B
3	F	6194	DUT	PG-O3B-PB-O2B
3	B	2194	DUT	PG-O3B-PB-O2B
3	C	3194	DUT	PG-O3B-PB-O2B
3	C	3194	DUT	PB-O3A-PA-O1A

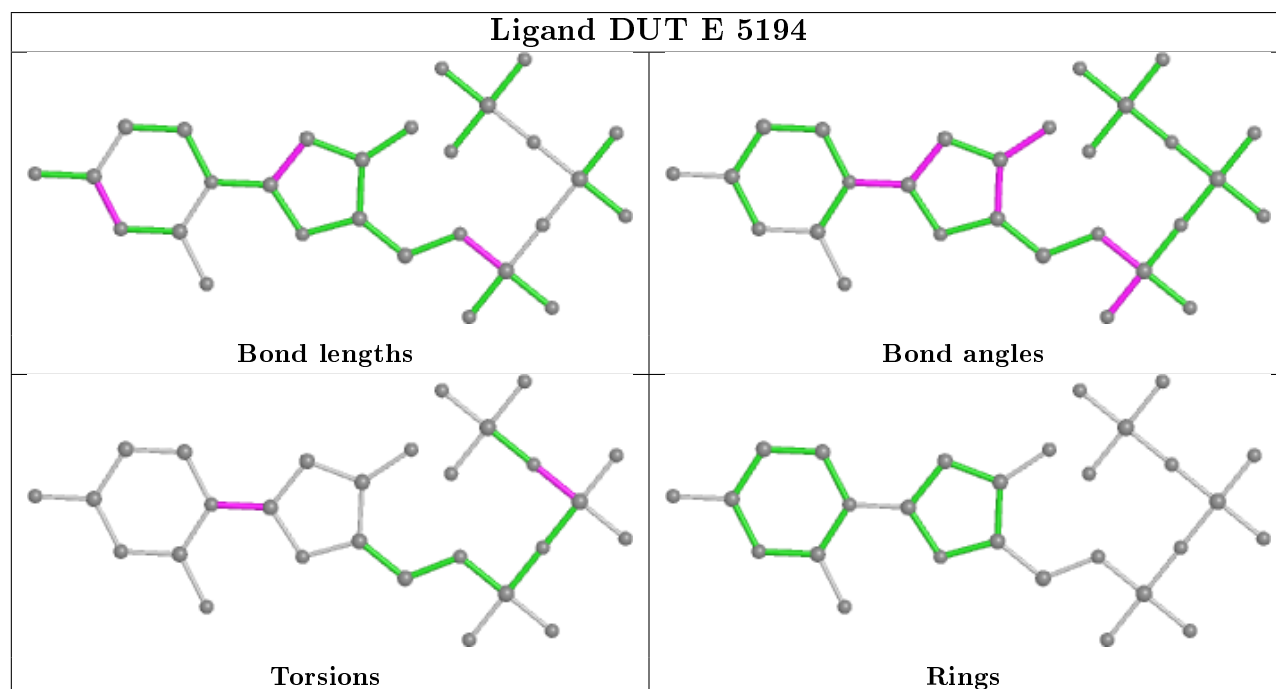
There are no ring outliers.

2 monomers are involved in 2 short contacts:

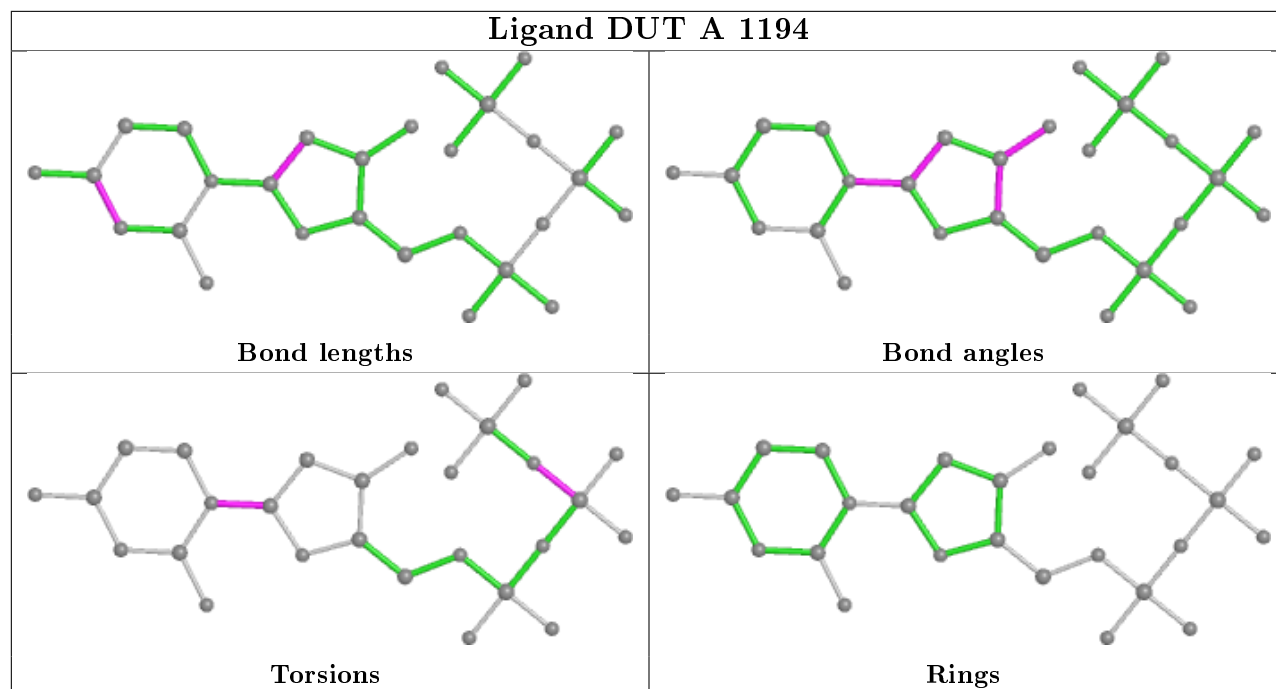
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	4194	DUT	1	0
3	B	2194	DUT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

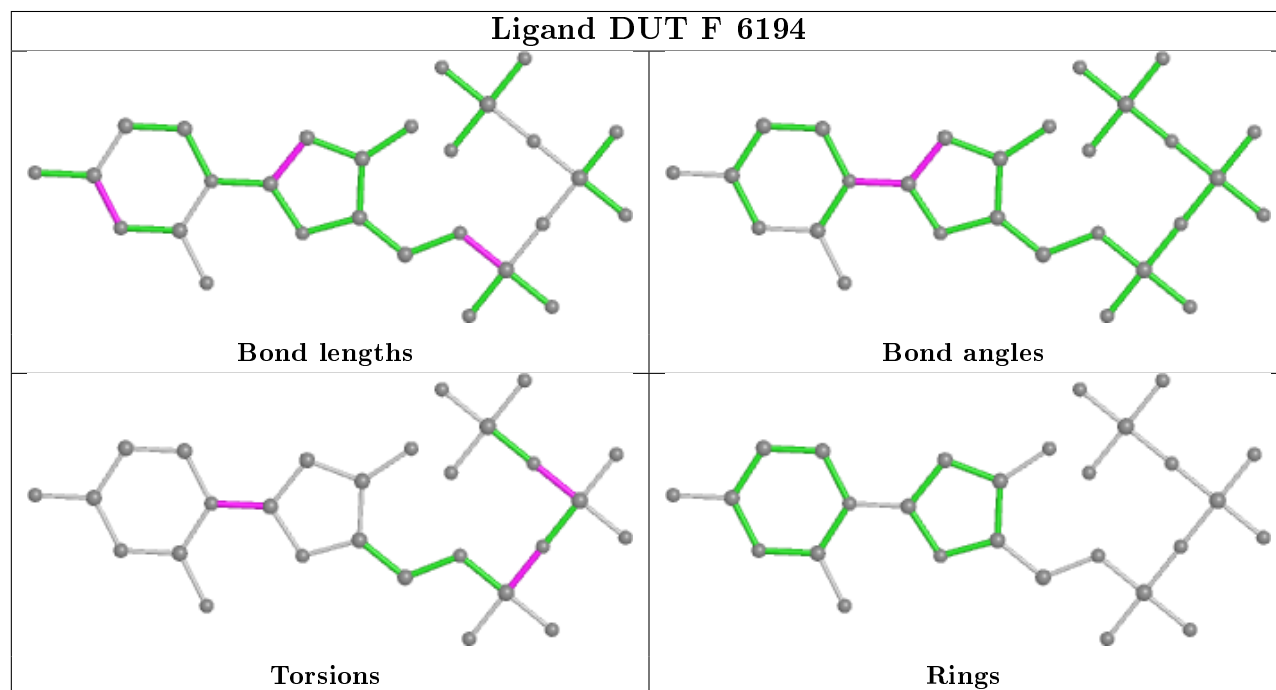
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



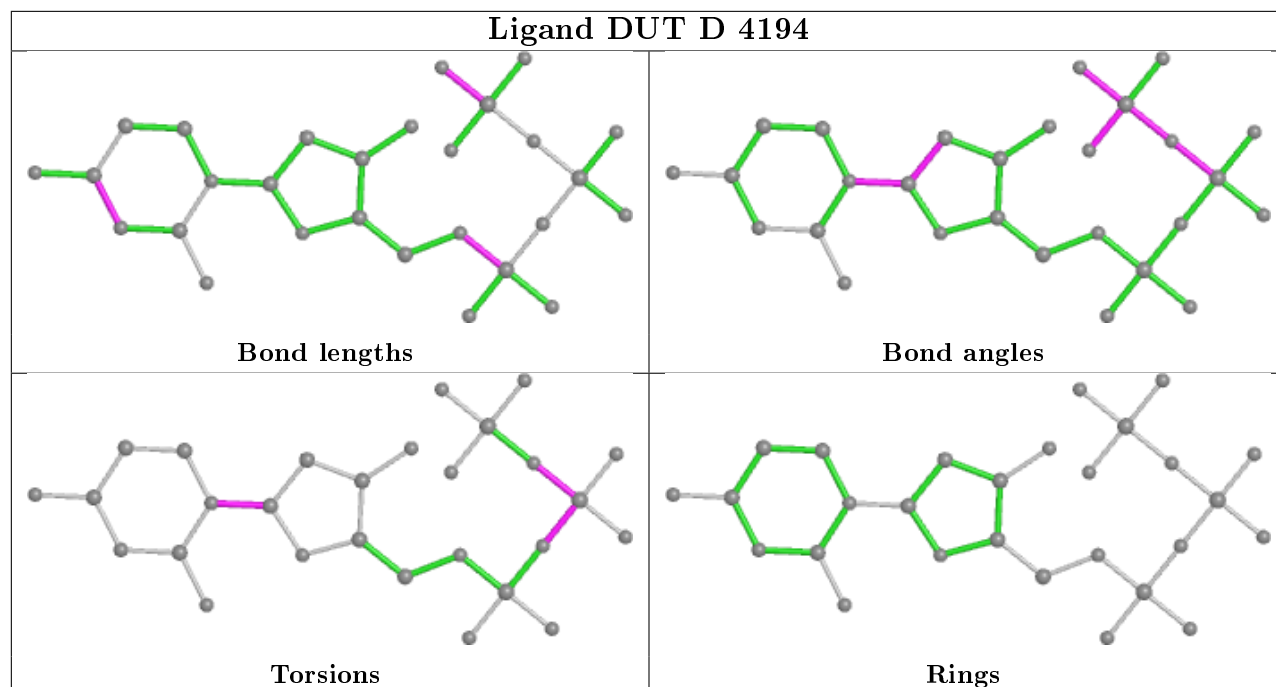
Ligand DUT A 1194



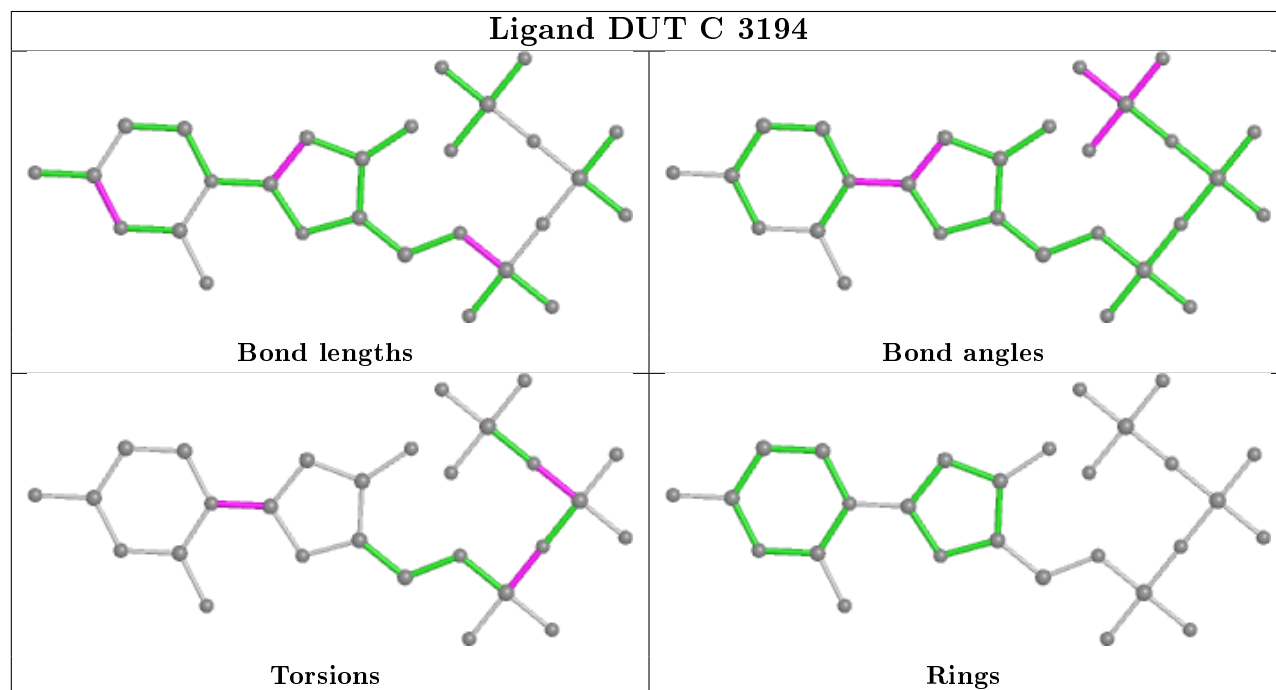
Ligand DUT F 6194

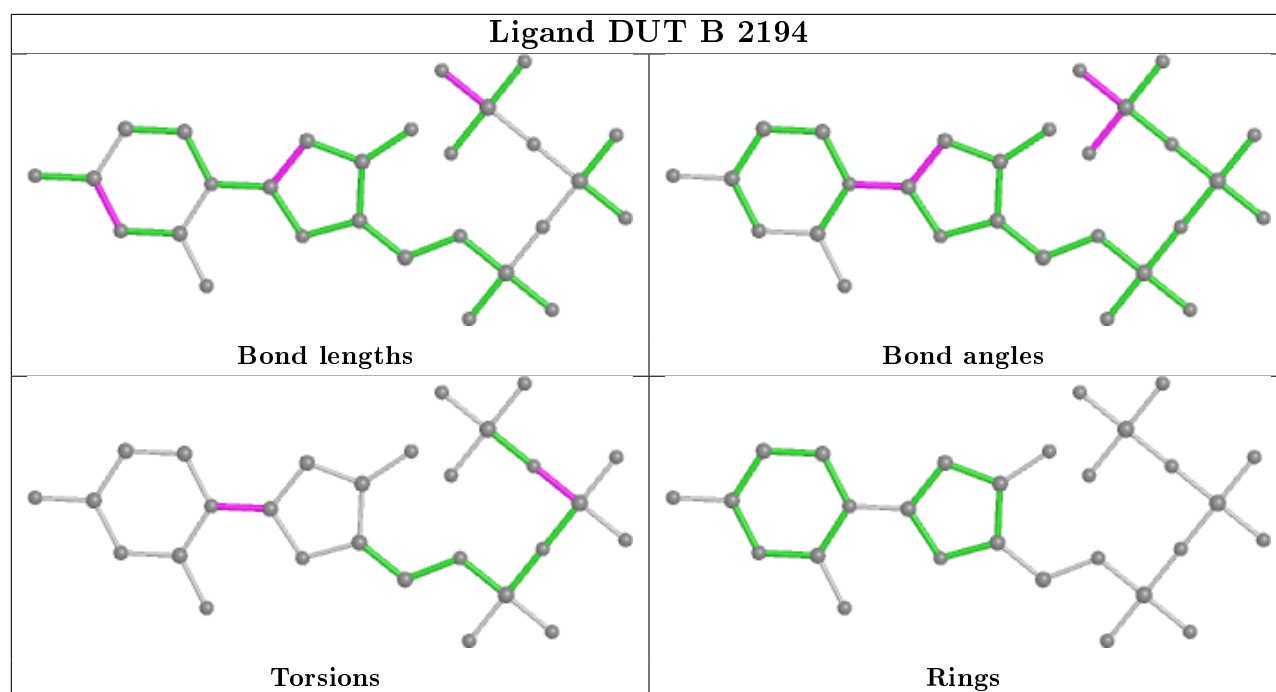


Ligand DUT D 4194



Ligand DUT C 3194





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%)	-0.71	1 (0%) 91 89	17, 25, 49, 64	0
1	B	193/193 (100%)	-0.74	1 (0%) 91 89	16, 25, 49, 96	0
1	C	193/193 (100%)	-0.77	0 100 100	17, 26, 45, 66	0
1	D	193/193 (100%)	-0.73	2 (1%) 82 80	16, 26, 50, 65	0
1	E	193/193 (100%)	-0.80	0 100 100	16, 25, 43, 61	0
1	F	193/193 (100%)	-0.79	0 100 100	14, 25, 48, 61	0
All	All	1158/1158 (100%)	-0.76	4 (0%) 94 92	14, 25, 48, 96	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	183	GLN	3.0
1	A	183	GLN	2.6
1	B	183	GLN	2.3
1	D	76	ASP	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 carbohydrates in this entry.

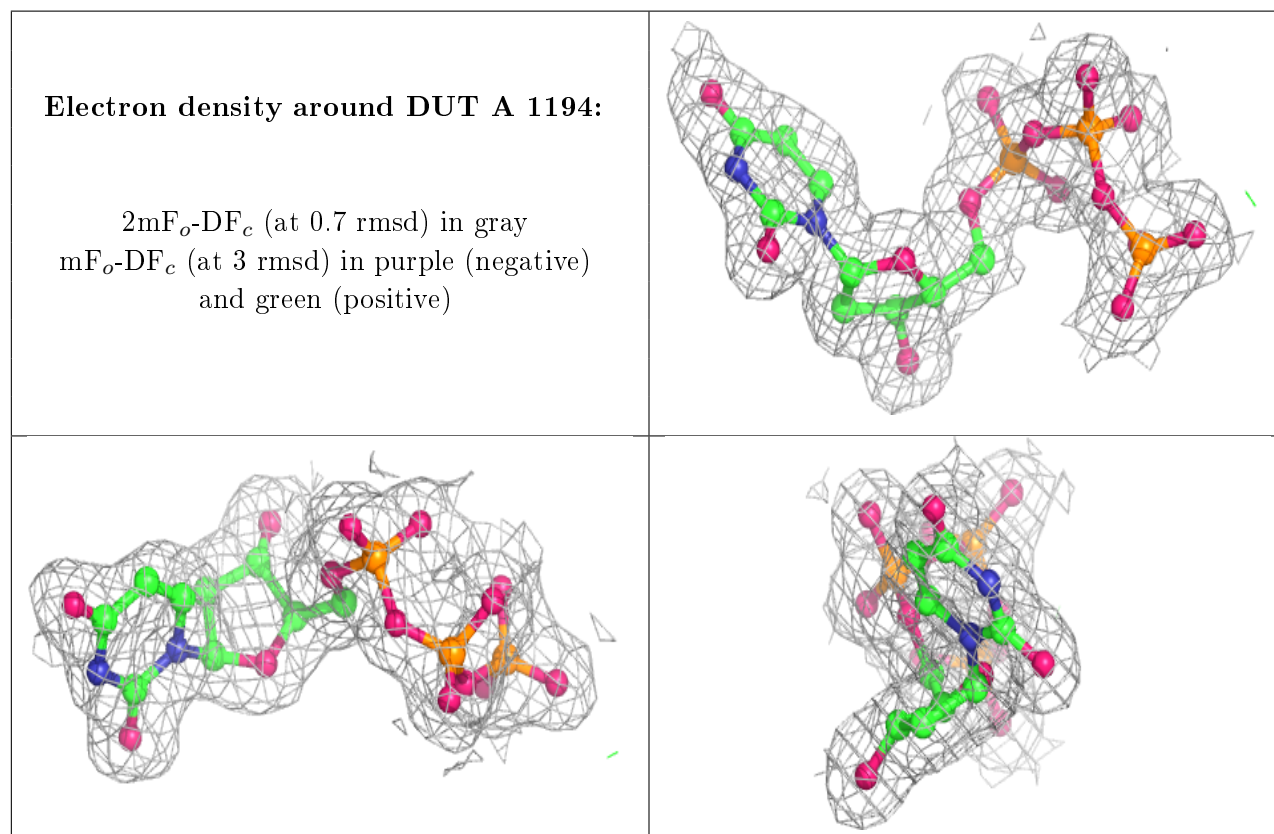
6.4 Ligands [i](#)

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.

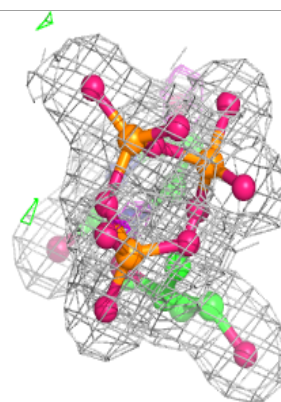
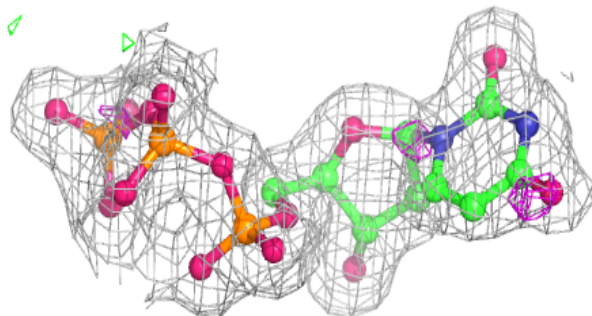
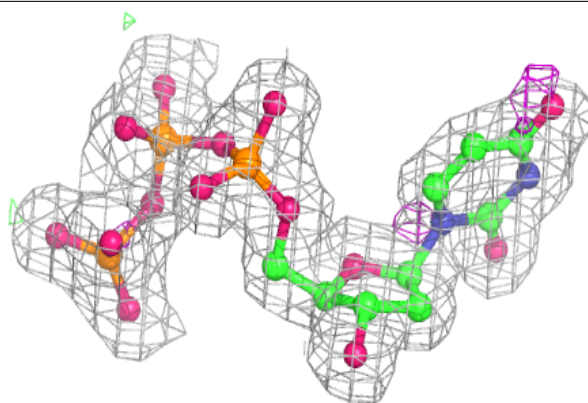
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	F	4195	1/1	0.97	0.06	28,28,28,28	0
3	DUT	A	1194	28/28	0.98	0.06	17,22,25,26	0
2	MG	B	3195	1/1	0.98	0.04	23,23,23,23	0
2	MG	E	6195	1/1	0.98	0.05	25,25,25,25	0
3	DUT	D	4194	28/28	0.98	0.06	17,22,28,30	0
3	DUT	B	2194	28/28	0.98	0.05	14,21,27,29	0
3	DUT	E	5194	28/28	0.98	0.07	14,20,27,28	0
3	DUT	F	6194	28/28	0.99	0.06	15,21,25,30	0
2	MG	C	1195	1/1	0.99	0.04	24,24,24,24	0
2	MG	A	2195	1/1	0.99	0.02	14,14,14,14	0
3	DUT	C	3194	28/28	0.99	0.06	16,20,24,24	0
2	MG	D	5195	1/1	0.99	0.05	21,21,21,21	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.

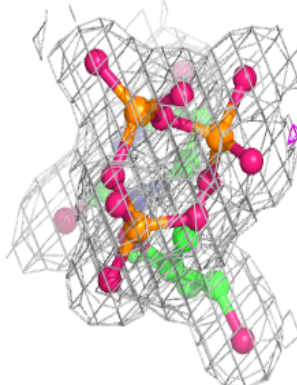
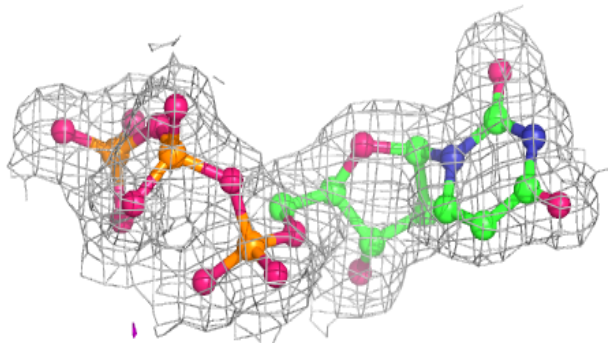
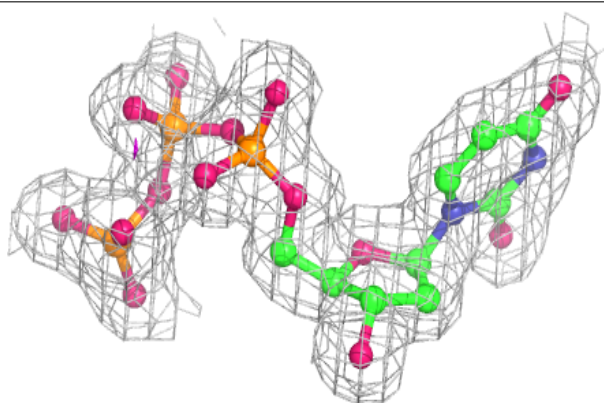


Electron density around DUT D 4194:

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

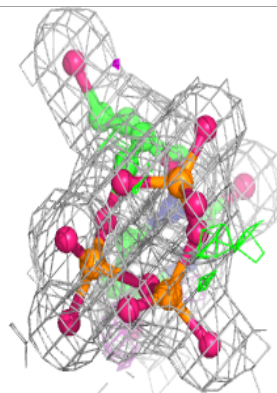
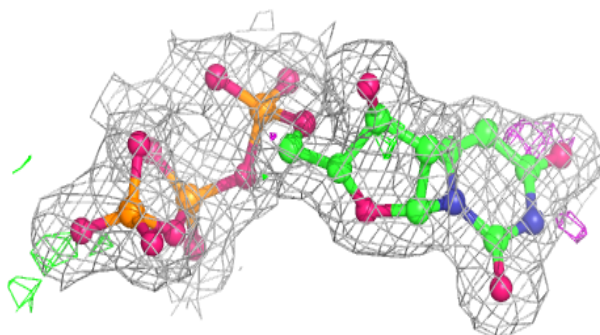
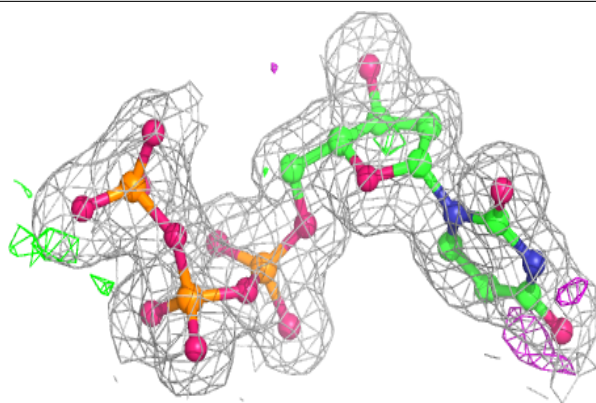
**Electron density around DUT B 2194:**

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

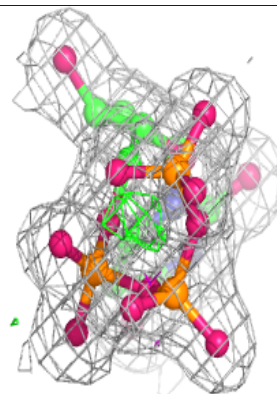
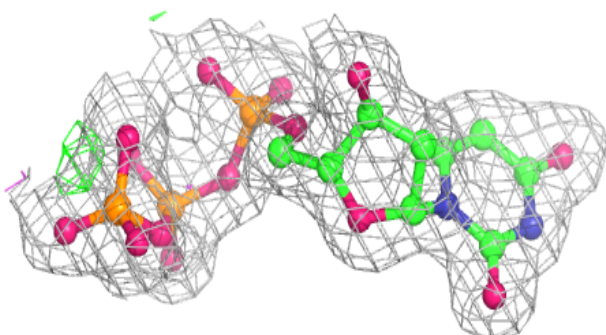
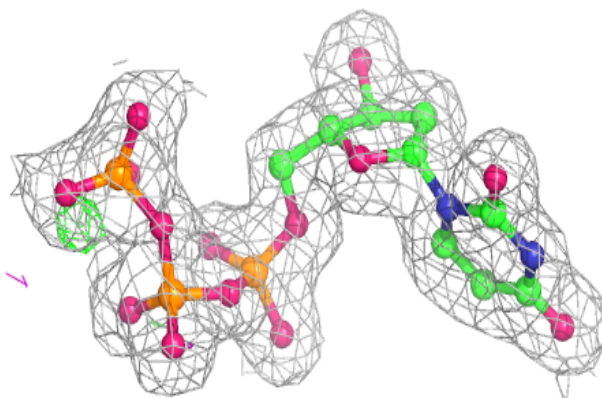


Electron density around DUT E 5194:

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

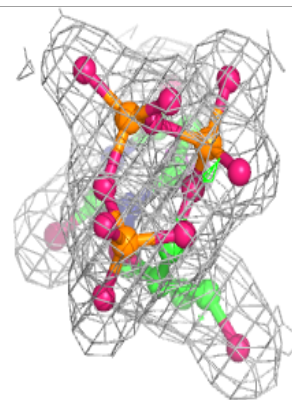
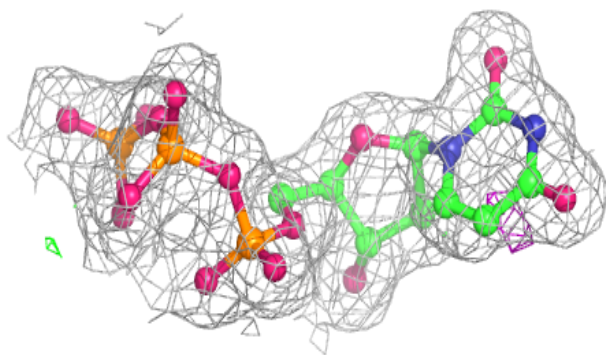
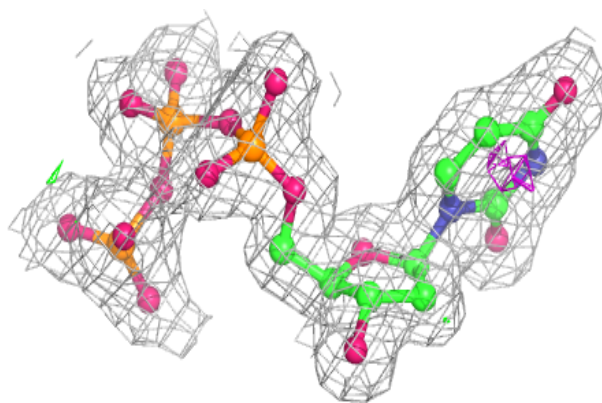
**Electron density around DUT F 6194:**

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.