



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:39 PM UTC

PDB ID : 7KQN / pdb_00007kqn
Title : Ternary complex of TERT (telomerase reverse transcriptase) with RNA template, DNA primer, an incoming dGTP and a downstream hybrid duplex
Authors : Choi, W.S.; Weng, P.J.; Yang, W.
Deposited on : 2020-11-17
Resolution : 2.02 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

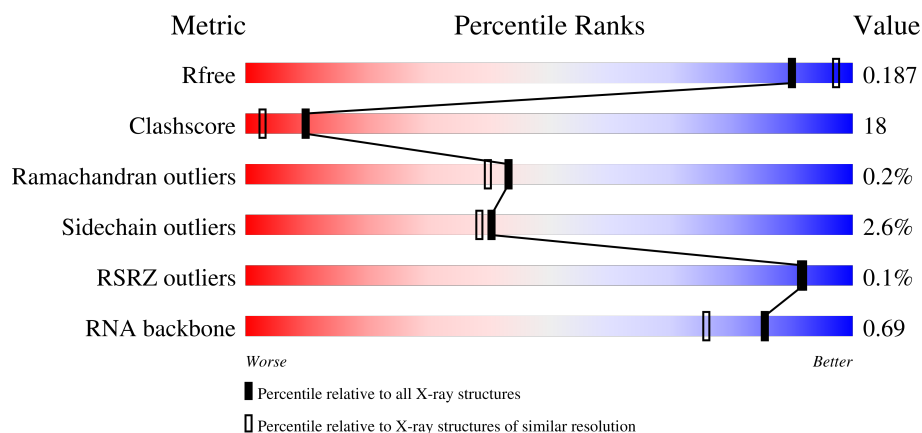
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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.



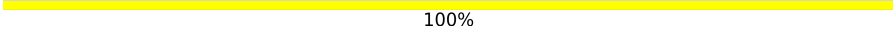
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)
RNA backbone	3983	1000 (2.38-1.66)

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	596	77% 21% .
1	D	596	78% 21% .
2	B	18	72% 28%
2	E	18	61% 39%

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Mol	Chain	Length	Quality of chain
3	C	7	
3	F	7	
4	I	7	
4	J	7	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	605	-	-	X	-
5	EDO	A	606	-	-	X	-
5	EDO	A	607	-	-	X	-
5	EDO	A	609	-	-	X	-
5	EDO	D	604	-	-	X	-
5	EDO	D	607	-	-	X	-
5	EDO	D	608	-	-	X	-
5	EDO	D	609	-	-	X	-
5	EDO	D	610	-	-	X	-
6	MES	A	612	-	-	X	-
7	PEG	A	613	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12874 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 Telomerase reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	14	0
			5059	3307	868	861	23			
1	D	596	Total	C	N	O	S	0	8	0
			5002	3270	858	851	23			

- Molecule 2 is a RNA chain called RNA (5'-R(*CP*AP*AP*AP*GP*AP*AP*AP*UP*CP*CP*AP*GP*GP*UP*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	18	Total	C	N	O	P	0	0	0
			384	174	76	117	17			
2	E	18	Total	C	N	O	P	0	0	0
			385	174	76	118	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	7	Total	C	N	O	P	0	0	0
			139	67	26	40	6			
3	F	7	Total	C	N	O	P	0	0	0
			139	67	26	40	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	7	Total	C	N	O	P	0	0	0
			138	69	18	45	6			
4	J	7	Total	C	N	O	P	0	0	0
			138	69	18	45	6			

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



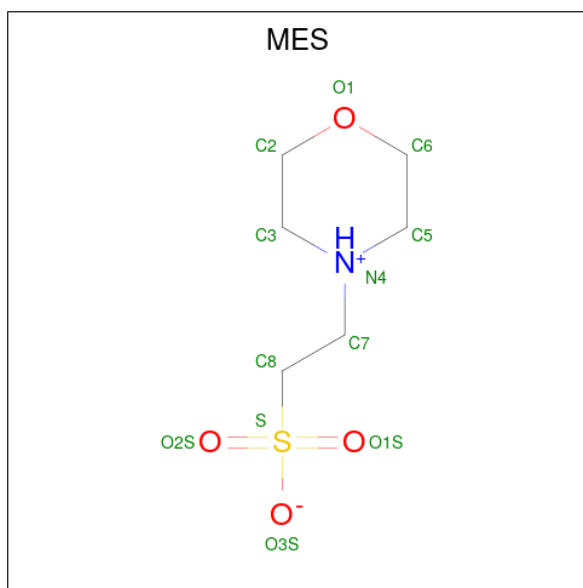
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).

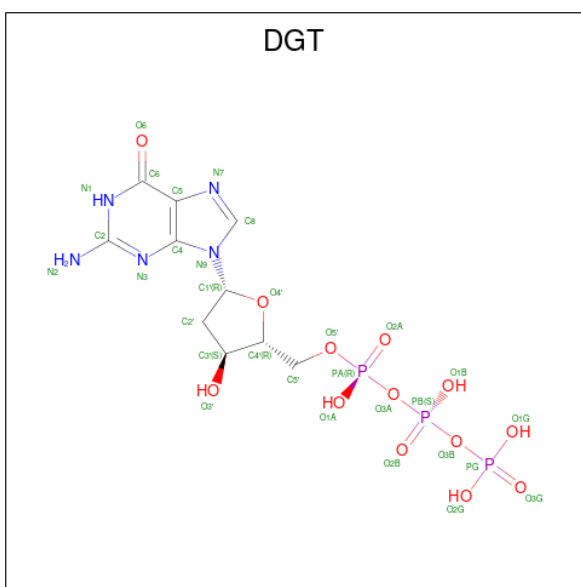


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		
8	D	1	Total	Ca	0	0
			1	1		

- Molecule 9 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
9	D	1	Total 31	C 10	N 5	O 13	P 3	0	0

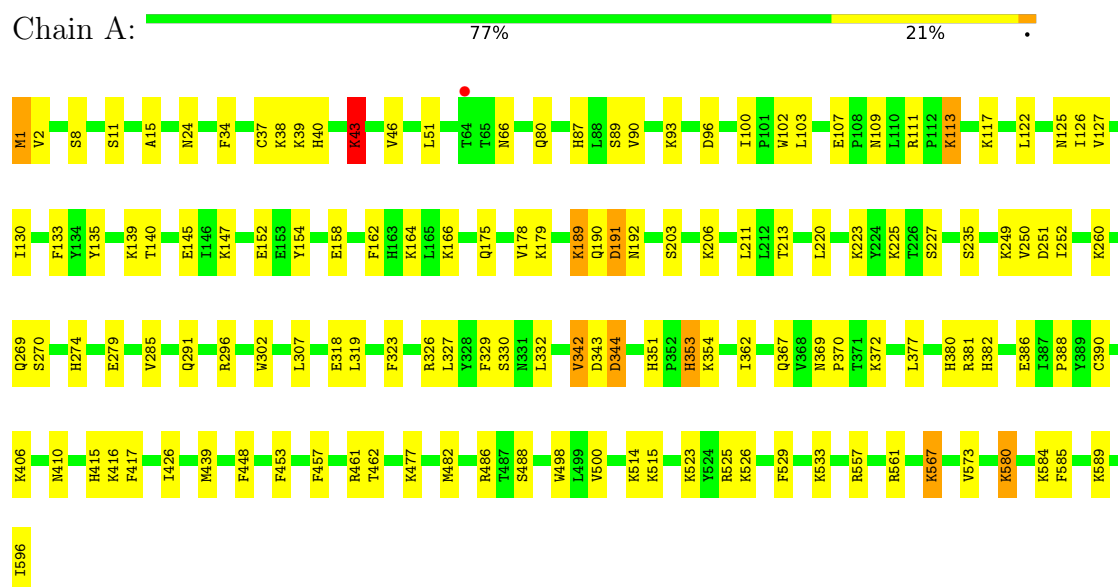
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	571	Total O 571 571	0	0
10	B	80	Total O 80 80	0	0
10	C	39	Total O 39 39	0	0
10	D	496	Total O 496 496	0	0
10	E	83	Total O 83 83	0	0
10	F	32	Total O 32 32	0	0
10	I	2	Total O 2 2	0	0
10	J	1	Total O 1 1	0	0

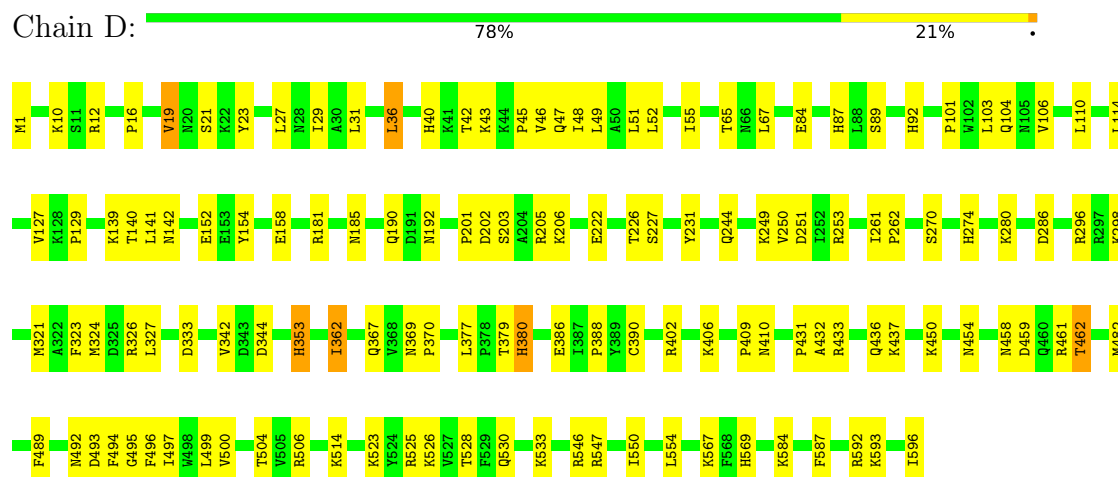
3 Residue-property plots [i](#)

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: Telomerase reverse transcriptase



• Molecule 1: Telomerase reverse transcriptase



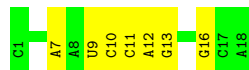
• Molecule 2: RNA (5'-R(*CP*AP*AP*AP*GP*AP*AP*AP*UP*CP*CP*AP*GP*GP*UP*GP*CP*A)-3')

Chain B:  72% 28%



- Molecule 2: RNA (5'-R(*CP*AP*AP*AP*GP*AP*AP*AP*UP*CP*CP*AP*GP*GP*UP*GP*CP*A)-3')

Chain E:  61% 39%



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

Chain C:  86% 14%



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

Chain F:  71% 29%



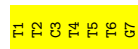
- Molecule 4: DNA (5'-D(*TP*TP*CP*TP*TP*TP*G)-3')

Chain I:  14% 86%



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

Chain J:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.86Å 164.04Å 95.36Å 90.00° 111.91° 90.00°	Depositor
Resolution (Å)	29.65 – 2.02 29.65 – 2.02	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.65-2.02) 98.0 (29.65-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.168 , 0.188 0.168 , 0.187	Depositor DCC
R_{free} test set	1007 reflections (0.75%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.078 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12874	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: DGT, MES, PEG, CA, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	0/5192	0.68	5/7005 (0.1%)
1	D	0.47	0/5134	0.70	4/6930 (0.1%)
2	B	0.35	0/431	0.53	0/671
2	E	0.33	0/432	0.50	0/672
3	C	0.55	0/155	0.64	0/237
3	F	0.52	0/155	0.63	0/237
4	I	0.33	0/152	0.59	0/233
4	J	0.30	0/152	0.58	0/233
All	All	0.45	0/11803	0.68	9/16218 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	D	0	3
All	All	0	9

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	10	LYS	CB-CG-CD	8.98	131.96	111.30
1	A	191	ASP	CB-CA-C	7.13	116.89	109.83
1	A	164	LYS	CA-CB-CG	6.53	127.17	114.10
1	A	279	GLU	CA-CB-CG	6.14	126.38	114.10
1	D	36	LEU	CA-CB-CG	5.78	136.51	116.30
1	D	202	ASP	N-CA-C	-5.55	96.19	107.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	LYS	N-CA-C	-5.35	105.45	111.28
1	D	10	LYS	N-CA-CB	5.14	118.14	110.22
1	A	164	LYS	CB-CA-C	-5.12	102.62	110.81

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	329	PHE	Mainchain
1	A	330[A]	SER	Mainchain
1	A	330[B]	SER	Mainchain
1	A	344[B]	ASP	Mainchain
1	A	353[B]	HIS	Mainchain
1	D	296[A]	ARG	Mainchain
1	D	296[B]	ARG	Mainchain
1	D	462[B]	THR	Mainchain

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	5059	0	5151	144	0
1	D	5002	0	5077	178	1
2	B	384	0	195	2	0
2	E	385	0	198	5	0
3	C	139	0	80	2	0
3	F	139	0	80	3	0
4	I	138	0	84	6	0
4	J	138	0	84	6	0
5	A	40	0	60	25	0
5	D	40	0	60	39	0
5	E	4	0	6	0	0
6	A	24	0	26	9	0
7	A	7	0	10	3	1
7	D	7	0	10	2	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	31	0	12	0	0
9	D	31	0	12	0	0
10	A	571	0	0	118	3
10	B	80	0	0	0	0
10	C	39	0	0	0	0
10	D	496	0	0	138	3
10	E	83	0	0	11	0
10	F	32	0	0	1	0
10	I	2	0	0	2	0
10	J	1	0	0	1	0
All	All	12874	0	11145	399	4

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 18.

All (399) 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)
5:A:605:EDO:H11	10:A:1030:HOH:O	1.31	1.31
1:A:381:ARG:HB3	10:A:1121:HOH:O	1.32	1.30
1:A:525:ARG:NH1	10:A:701:HOH:O	1.67	1.28
1:A:1:MET:HG2	10:A:1203:HOH:O	1.14	1.27
1:A:367:GLN:HG2	10:A:1138:HOH:O	1.30	1.25
5:D:603:EDO:H11	10:D:765:HOH:O	1.26	1.24
1:D:286:ASP:HB2	10:D:956:HOH:O	1.33	1.21
5:D:602:EDO:H22	10:D:993:HOH:O	1.37	1.18
1:D:65:THR:HG21	10:D:1080:HOH:O	1.43	1.18
1:A:381:ARG:HG3	10:A:954:HOH:O	1.39	1.16
1:D:227:SER:HB3	10:D:771:HOH:O	1.41	1.16
5:A:603:EDO:H22	10:A:1065:HOH:O	1.46	1.15
1:D:431:PRO:CD	5:D:609:EDO:H22	1.74	1.15
1:D:192:ASN:HB3	10:D:743:HOH:O	1.50	1.11
1:D:596:ILE:C	10:D:755:HOH:O	1.91	1.10
1:A:498:TRP:HB3	10:A:793:HOH:O	1.51	1.10
1:D:270:SER:CB	10:D:944:HOH:O	1.97	1.09
1:D:142:ASN:HB3	10:D:744:HOH:O	1.54	1.06
1:D:431:PRO:HD2	5:D:609:EDO:C2	1.84	1.06
1:D:326:ARG:HD3	10:D:1038:HOH:O	1.56	1.05
1:D:333:ASP:HB3	10:D:1106:HOH:O	1.57	1.05
5:D:608:EDO:H11	10:D:809:HOH:O	1.54	1.03
1:A:1:MET:HE2	10:E:278:HOH:O	1.56	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:SER:HA	10:D:1005:HOH:O	1.56	1.02
5:A:609:EDO:H21	10:A:761:HOH:O	0.85	1.02
1:A:410:ASN:HA	10:A:713:HOH:O	1.60	1.01
10:E:202:HOH:O	3:F:6:DT:H1'	1.61	1.01
5:D:608:EDO:H22	10:D:1039:HOH:O	1.60	1.00
1:D:270:SER:HB3	10:D:944:HOH:O	1.55	1.00
1:A:353[A]:HIS:HE1	10:A:872:HOH:O	1.45	0.99
1:A:1:MET:HE1	10:E:280:HOH:O	1.63	0.98
1:A:353[B]:HIS:HE1	10:A:998:HOH:O	1.45	0.98
1:D:353[A]:HIS:HE1	10:D:941:HOH:O	1.45	0.97
1:D:142:ASN:CB	10:D:744:HOH:O	2.07	0.95
5:D:601:EDO:H12	10:E:250:HOH:O	1.65	0.94
1:A:353[A]:HIS:CE1	10:A:872:HOH:O	2.20	0.94
1:D:226:THR:HG23	10:D:731:HOH:O	1.67	0.94
1:A:1:MET:N	10:A:705:HOH:O	2.00	0.93
1:D:528:THR:HG21	5:D:604:EDO:H22	1.49	0.93
1:D:492:ASN:N	10:D:703:HOH:O	1.83	0.92
1:A:406:LYS:CD	10:A:723:HOH:O	2.15	0.92
1:A:1:MET:N	10:A:707:HOH:O	2.02	0.92
1:D:525:ARG:HD2	10:D:745:HOH:O	1.69	0.91
1:D:499:LEU:HD23	10:D:1071:HOH:O	1.69	0.91
1:D:584:LYS:HE3	10:D:1032:HOH:O	1.69	0.91
1:A:533:LYS:HE3	10:A:852:HOH:O	1.72	0.90
1:A:192[B]:ASN:OD1	10:A:702:HOH:O	1.89	0.90
1:D:431:PRO:HD2	5:D:609:EDO:H22	0.92	0.90
4:I:2:DT:H4'	10:I:101:HOH:O	1.70	0.90
1:A:514:LYS:HE2	10:A:1022:HOH:O	1.72	0.89
1:A:353[B]:HIS:CE1	10:A:998:HOH:O	2.22	0.88
5:A:604:EDO:H12	10:A:742:HOH:O	1.72	0.88
1:D:353[B]:HIS:HB2	10:D:776:HOH:O	1.72	0.88
1:A:154:TYR:CZ	10:A:710:HOH:O	2.27	0.87
2:E:12:A:OP1	10:E:201:HOH:O	1.92	0.87
1:D:432:ALA:H	5:D:609:EDO:H21	1.38	0.86
1:D:584:LYS:HG2	10:D:721:HOH:O	1.74	0.86
1:A:274:HIS:HD2	10:A:847:HOH:O	1.58	0.85
1:D:222:GLU:HB2	10:D:877:HOH:O	1.75	0.85
1:D:596:ILE:O	10:D:701:HOH:O	1.92	0.85
5:D:608:EDO:C2	10:D:1039:HOH:O	2.19	0.85
1:D:409:PRO:CA	10:D:773:HOH:O	2.25	0.84
1:D:437:LYS:HD3	10:D:726:HOH:O	1.77	0.84
1:D:261:ILE:HB	5:D:610:EDO:H22	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:528:THR:HG21	5:D:604:EDO:C2	2.08	0.83
1:D:274:HIS:HD2	10:D:1037:HOH:O	1.60	0.83
1:D:437:LYS:HG3	10:D:1167:HOH:O	1.78	0.83
1:D:506:ARG:HD3	10:D:823:HOH:O	1.80	0.82
1:D:253:ARG:HD2	10:D:778:HOH:O	1.81	0.81
5:A:605:EDO:H22	10:A:718:HOH:O	1.81	0.80
1:A:580:LYS:NZ	10:A:712:HOH:O	2.14	0.80
1:D:409:PRO:HA	10:D:773:HOH:O	1.82	0.79
1:D:437:LYS:HE2	10:D:726:HOH:O	1.80	0.79
1:A:410:ASN:CA	10:A:713:HOH:O	2.23	0.79
1:D:450:LYS:HE2	10:D:1130:HOH:O	1.82	0.79
5:D:609:EDO:H11	10:D:1033:HOH:O	1.83	0.79
1:D:244:GLN:OE1	10:D:704:HOH:O	1.99	0.79
1:A:410:ASN:N	10:A:713:HOH:O	2.15	0.78
1:A:515:LYS:CE	10:A:1152:HOH:O	2.32	0.77
1:D:593:LYS:CE	10:D:763:HOH:O	2.32	0.77
5:A:603:EDO:C2	10:A:1065:HOH:O	2.14	0.77
5:D:608:EDO:C1	10:D:809:HOH:O	2.20	0.77
1:A:46:VAL:O	10:A:706:HOH:O	2.01	0.77
5:A:605:EDO:C1	10:A:836:HOH:O	2.31	0.77
1:A:351:HIS:ND1	10:A:714:HOH:O	2.17	0.77
1:D:530:GLN:NE2	10:D:710:HOH:O	2.16	0.77
1:A:406:LYS:HD3	10:A:723:HOH:O	1.82	0.76
1:D:353[A]:HIS:CE1	10:D:941:HOH:O	2.26	0.76
1:A:515:LYS:HE3	10:A:1152:HOH:O	1.86	0.76
1:D:353[A]:HIS:HB2	10:D:776:HOH:O	1.85	0.76
1:D:226:THR:CG2	10:D:731:HOH:O	2.30	0.76
5:D:607:EDO:H22	10:D:792:HOH:O	1.85	0.75
5:A:607:EDO:O1	10:A:704:HOH:O	1.98	0.75
1:A:270:SER:OG	10:A:708:HOH:O	2.05	0.74
1:D:139:LYS:CD	10:D:768:HOH:O	2.33	0.74
1:D:437:LYS:CE	10:D:726:HOH:O	2.34	0.74
5:D:607:EDO:C1	10:D:785:HOH:O	2.35	0.74
10:A:1149:HOH:O	7:D:611:PEG:C4	2.37	0.73
10:A:1035:HOH:O	1:D:499:LEU:CD2	2.36	0.73
1:D:251:ASP:OD1	1:D:344:ASP:OD1	2.05	0.73
1:A:406:LYS:NZ	10:A:723:HOH:O	2.22	0.72
6:A:612:MES:H52	10:A:715:HOH:O	1.88	0.72
1:D:437:LYS:CD	10:D:726:HOH:O	2.34	0.72
10:A:1035:HOH:O	1:D:499:LEU:HD21	1.89	0.72
1:D:593:LYS:HD2	10:D:763:HOH:O	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:LYS:HD2	10:D:768:HOH:O	1.90	0.72
1:A:139:LYS:HG3	10:A:993:HOH:O	1.88	0.72
1:D:593:LYS:CD	10:D:763:HOH:O	2.38	0.71
5:A:607:EDO:H21	10:A:737:HOH:O	1.90	0.71
5:A:605:EDO:H11	10:A:836:HOH:O	1.87	0.71
1:D:353[B]:HIS:NE2	10:D:709:HOH:O	2.15	0.70
5:D:609:EDO:C1	10:D:1033:HOH:O	2.38	0.69
1:A:561:ARG:CZ	10:A:740:HOH:O	2.40	0.69
1:A:154:TYR:OH	10:A:710:HOH:O	2.10	0.68
1:D:280:LYS:NZ	10:D:720:HOH:O	2.26	0.68
5:A:605:EDO:C2	10:A:718:HOH:O	2.37	0.68
1:D:262:PRO:HD3	5:D:610:EDO:H22	1.74	0.68
1:A:344[A]:ASP:OD2	3:C:7:DG:H5''	1.93	0.68
1:D:433[B]:ARG:CZ	1:D:437:LYS:HD3	2.25	0.67
1:D:496:PHE:CD1	10:D:789:HOH:O	2.48	0.67
1:A:139:LYS:CE	10:A:779:HOH:O	2.43	0.67
1:A:386:GLU:OE1	10:A:711:HOH:O	2.13	0.66
1:A:406:LYS:HD2	10:A:723:HOH:O	1.84	0.66
1:D:436:GLN:NE2	10:D:724:HOH:O	2.28	0.66
1:D:321:MET:SD	10:D:1139:HOH:O	2.53	0.66
1:D:496:PHE:HD1	10:D:789:HOH:O	1.77	0.66
5:A:605:EDO:C2	10:A:836:HOH:O	2.44	0.65
5:A:607:EDO:C1	10:A:704:HOH:O	2.41	0.65
1:D:323:PHE:CZ	1:D:327:LEU:HD11	2.31	0.65
1:A:381:ARG:CG	10:A:954:HOH:O	2.14	0.65
1:D:436:GLN:OE1	10:D:705:HOH:O	2.15	0.65
1:A:37:CYS:SG	1:A:51:LEU:HD22	2.37	0.65
1:D:227:SER:HB3	10:D:746:HOH:O	1.97	0.65
1:D:546:ARG:NH1	10:D:711:HOH:O	2.18	0.65
1:A:285:VAL:HG11	10:A:1039:HOH:O	1.97	0.65
1:D:593:LYS:N	10:D:718:HOH:O	2.24	0.65
1:D:227:SER:CB	10:D:771:HOH:O	2.18	0.64
1:D:433[B]:ARG:NH2	10:D:726:HOH:O	2.29	0.64
1:D:461:ARG:NH1	10:D:713:HOH:O	2.19	0.64
1:D:270:SER:CA	10:D:944:HOH:O	2.36	0.64
1:D:370:PRO:HA	10:D:876:HOH:O	1.96	0.64
1:A:561:ARG:NH1	10:A:740:HOH:O	2.31	0.64
5:A:606:EDO:C2	10:A:907:HOH:O	2.45	0.63
1:A:175:GLN:HG2	1:A:178:VAL:HG23	1.80	0.63
2:E:13:G:N2	10:E:202:HOH:O	2.26	0.63
1:D:158:GLU:OE2	10:D:706:HOH:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LYS:NZ	10:A:737:HOH:O	2.31	0.63
1:A:274:HIS:CD2	10:A:847:HOH:O	2.40	0.63
1:D:547:ARG:HB3	1:D:550:ILE:HD13	1.80	0.63
1:A:380:HIS:CD2	10:A:802:HOH:O	2.51	0.62
1:D:587:PHE:HB2	10:D:1155:HOH:O	1.98	0.62
1:D:227:SER:N	10:D:731:HOH:O	2.33	0.62
1:A:179:LYS:HD2	10:A:1116:HOH:O	2.00	0.62
1:D:142:ASN:HB2	10:D:744:HOH:O	1.85	0.62
1:D:353[A]:HIS:CB	10:D:776:HOH:O	2.44	0.62
1:A:24:ASN:HD22	1:A:102:TRP:HE3	1.48	0.61
1:A:89:SER:HB2	1:A:93:LYS:HD2	1.82	0.61
1:D:494:PHE:HB3	1:D:497:ILE:HG13	1.82	0.61
1:A:249:LYS:HD2	1:A:388:PRO:O	2.01	0.61
1:D:514:LYS:HB3	10:D:1122:HOH:O	2.01	0.61
6:A:612:MES:C2	10:A:728:HOH:O	2.48	0.61
1:D:370:PRO:CA	10:D:876:HOH:O	2.49	0.61
1:A:107:GLU:HG2	1:A:109:ASN:H	1.66	0.60
1:A:596:ILE:C	10:A:706:HOH:O	2.44	0.60
1:D:45:PRO:HG2	10:D:1104:HOH:O	2.02	0.60
4:I:2:DT:C4'	10:I:101:HOH:O	2.38	0.60
1:A:567:LYS:HE3	10:A:1068:HOH:O	2.00	0.60
1:D:227:SER:CB	10:D:746:HOH:O	2.50	0.60
1:D:504:THR:HG22	10:D:1096:HOH:O	2.00	0.60
1:D:379:THR:OG1	10:D:707:HOH:O	2.15	0.60
1:D:500:VAL:O	1:D:504:THR:HG23	2.01	0.59
1:D:23:TYR:HB3	1:D:27:LEU:HD12	1.85	0.59
5:A:606:EDO:H22	10:A:907:HOH:O	2.03	0.59
1:A:382:HIS:N	10:A:709:HOH:O	2.06	0.59
1:D:432:ALA:H	5:D:609:EDO:C2	2.12	0.59
1:A:260:LYS:NZ	10:A:749:HOH:O	2.35	0.58
1:A:370:PRO:HB3	10:A:1183:HOH:O	2.02	0.58
1:A:162:PHE:CZ	1:A:166:LYS:HD2	2.38	0.58
1:D:406:LYS:NZ	10:D:740:HOH:O	2.36	0.58
1:A:557:ARG:NH1	10:A:732:HOH:O	2.28	0.58
1:D:36:LEU:HD12	1:D:40:HIS:CE1	2.39	0.58
1:D:333:ASP:CB	10:D:1106:HOH:O	2.29	0.58
1:D:499:LEU:CD2	10:D:1071:HOH:O	2.39	0.58
1:A:461[B]:ARG:NE	10:A:736:HOH:O	2.31	0.58
5:D:607:EDO:H11	10:D:785:HOH:O	2.03	0.58
1:A:369[A]:ASN:ND2	1:A:372:LYS:HE3	2.20	0.57
1:D:431:PRO:CD	5:D:609:EDO:C2	2.58	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ALA:HA	1:A:125:ASN:HD22	1.70	0.57
1:D:141:LEU:CD2	2:E:10:C:H41	2.18	0.57
1:A:529:PHE:CD2	5:A:605:EDO:H21	2.41	0.56
1:D:433[B]:ARG:HD3	10:D:724:HOH:O	2.06	0.56
1:D:139:LYS:HE3	10:D:914:HOH:O	2.04	0.56
1:D:253:ARG:CD	10:D:778:HOH:O	2.47	0.56
1:A:500:VAL:HG12	1:D:514:LYS:HE2	1.86	0.56
1:D:410:ASN:C	10:D:719:HOH:O	2.49	0.56
1:D:262:PRO:HD3	5:D:610:EDO:C2	2.36	0.56
5:A:609:EDO:C2	10:A:761:HOH:O	1.72	0.55
5:D:607:EDO:H12	10:D:785:HOH:O	2.01	0.55
1:A:223:LYS:O	1:A:326:ARG:NH2	2.40	0.55
1:A:225:LYS:NZ	10:A:733:HOH:O	2.37	0.55
1:D:51:LEU:O	1:D:55:ILE:HG12	2.06	0.55
10:E:202:HOH:O	3:F:6:DT:C1'	2.36	0.55
1:D:261:ILE:H	5:D:610:EDO:C2	2.19	0.55
1:D:380:HIS:HA	10:D:774:HOH:O	2.07	0.55
6:A:612:MES:H61	10:A:760:HOH:O	2.07	0.54
10:A:1149:HOH:O	7:D:611:PEG:C3	2.54	0.54
1:D:461:ARG:NH2	10:D:748:HOH:O	2.39	0.54
1:A:252:ILE:HB	1:A:343:ASP:HB2	1.89	0.54
1:A:417:PHE:HB3	1:A:477[A]:LYS:HZ3	1.72	0.54
7:A:613:PEG:O2	10:A:715:HOH:O	2.18	0.54
1:D:52:LEU:HD11	1:D:127:VAL:HG22	1.90	0.54
1:D:569:HIS:CE1	10:D:984:HOH:O	2.61	0.54
1:A:152:GLU:HG3	4:J:1:DT:H71	1.89	0.54
1:A:584:LYS:O	10:A:717:HOH:O	2.19	0.54
1:D:592:ARG:HA	10:D:718:HOH:O	2.08	0.54
6:A:611:MES:H21	6:A:612:MES:H21	1.89	0.54
1:D:270:SER:OG	10:D:712:HOH:O	2.19	0.53
1:D:154:TYR:OH	10:D:706:HOH:O	2.19	0.53
6:A:612:MES:H21	10:A:728:HOH:O	2.09	0.53
1:A:103:LEU:HD23	1:A:111:ARG:HB3	1.89	0.53
1:A:461[B]:ARG:HG2	10:A:736:HOH:O	2.08	0.53
5:D:602:EDO:H21	10:D:886:HOH:O	2.08	0.53
5:D:604:EDO:H11	10:D:812:HOH:O	2.08	0.53
1:D:370:PRO:CB	10:D:876:HOH:O	2.55	0.53
1:D:250:VAL:HG21	1:D:362[B]:ILE:HG21	1.91	0.53
2:E:7:A:H1'	10:E:215:HOH:O	2.08	0.53
5:D:605:EDO:C2	10:D:738:HOH:O	2.57	0.53
1:D:353[B]:HIS:CB	10:D:776:HOH:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:VAL:HG21	1:A:362:ILE:HG12	1.90	0.53
1:A:515:LYS:HE2	10:A:1152:HOH:O	2.02	0.52
1:D:129:PRO:HB3	10:D:1107:HOH:O	2.08	0.52
1:D:49:LEU:HB2	10:D:758:HOH:O	2.09	0.52
1:A:410:ASN:HB3	1:A:589:LYS:HE3	1.91	0.52
1:A:66:ASN:HD21	1:A:96:ASP:HB3	1.74	0.52
1:A:448:PHE:HA	1:A:453:PHE:HE2	1.74	0.52
1:D:49:LEU:CB	10:D:758:HOH:O	2.58	0.52
2:B:11:C:H2'	2:B:12:A:C8	2.45	0.52
5:D:605:EDO:H12	10:D:738:HOH:O	2.09	0.52
1:D:181:ARG:NH2	10:D:752:HOH:O	2.40	0.51
1:A:380:HIS:ND1	10:A:744:HOH:O	2.33	0.51
1:A:24:ASN:ND2	1:A:102:TRP:HB2	2.26	0.51
6:A:611:MES:HN4	6:A:612:MES:H31	1.76	0.51
5:D:608:EDO:H21	10:D:1039:HOH:O	2.00	0.51
1:D:353[B]:HIS:CG	10:D:776:HOH:O	2.63	0.51
10:A:726:HOH:O	1:D:499:LEU:HD11	2.09	0.51
1:A:213[A]:THR:HG21	10:A:1006:HOH:O	2.11	0.51
1:D:409:PRO:CB	10:D:773:HOH:O	2.56	0.51
1:A:122:LEU:HD23	1:A:126:ILE:HD12	1.93	0.50
1:A:332:LEU:HB3	10:A:774:HOH:O	2.11	0.50
1:A:381:ARG:HG3	10:A:815:HOH:O	2.11	0.50
1:A:417:PHE:HB3	1:A:477[A]:LYS:NZ	2.26	0.50
1:A:158:GLU:HB2	10:A:710:HOH:O	2.10	0.50
2:E:11:C:H2'	2:E:12:A:C8	2.47	0.50
1:A:369[A]:ASN:HD22	1:A:372:LYS:HE3	1.76	0.50
1:D:49:LEU:HG	10:D:758:HOH:O	2.12	0.50
1:D:495:GLY:N	10:D:764:HOH:O	2.44	0.50
1:A:140:THR:HG21	1:A:147:LYS:HG3	1.94	0.50
1:A:514:LYS:CE	10:A:1022:HOH:O	2.42	0.49
5:A:607:EDO:C2	10:A:737:HOH:O	2.53	0.49
1:A:158:GLU:HG2	1:A:296:ARG:HH21	1.76	0.49
1:D:84:GLU:OE2	1:D:592:ARG:NH2	2.43	0.49
4:J:4:DT:H2''	4:J:5:DT:H5'	1.94	0.49
1:A:416:LYS:NZ	10:A:754:HOH:O	2.41	0.49
1:A:323:PHE:CZ	1:A:327:LEU:HD11	2.48	0.49
1:A:2:VAL:HG22	10:A:1045:HOH:O	2.10	0.49
1:A:139:LYS:HE3	10:A:779:HOH:O	2.09	0.49
1:D:450:LYS:HE3	10:D:811:HOH:O	2.13	0.49
5:A:606:EDO:H21	10:A:907:HOH:O	2.12	0.49
1:D:1:MET:N	10:D:727:HOH:O	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:HIS:HE1	1:D:489:PHE:CE1	2.31	0.49
1:D:110:LEU:HB3	1:D:114:LEU:HD23	1.95	0.49
1:D:593:LYS:NZ	10:D:763:HOH:O	2.44	0.49
1:A:158:GLU:HG2	1:A:296:ARG:NH2	2.28	0.49
5:A:605:EDO:O2	10:A:718:HOH:O	2.19	0.49
1:D:454:ASN:O	1:D:458:ASN:HB2	2.13	0.48
1:A:192[A]:ASN:OD1	10:A:719:HOH:O	2.19	0.48
5:A:609:EDO:H22	10:A:708:HOH:O	2.13	0.48
1:D:367:GLN:HB3	10:D:879:HOH:O	2.12	0.48
1:D:152:GLU:CD	1:D:152:GLU:H	2.21	0.48
5:D:601:EDO:H11	10:E:272:HOH:O	2.13	0.48
1:D:569:HIS:HE1	10:D:1086:HOH:O	1.96	0.48
1:A:291:GLN:HB3	1:A:307:LEU:HD22	1.95	0.48
1:A:353[A]:HIS:HD2	10:A:1102:HOH:O	1.97	0.48
1:A:406:LYS:NZ	10:A:769:HOH:O	2.46	0.48
1:A:461[B]:ARG:CG	10:A:736:HOH:O	2.62	0.48
1:D:87:HIS:HE1	1:D:489:PHE:CZ	2.31	0.48
1:A:269:GLN:NE2	10:A:772:HOH:O	2.47	0.48
6:A:612:MES:C6	10:A:760:HOH:O	2.60	0.48
1:D:103:LEU:O	1:D:106:VAL:HG22	2.13	0.48
1:D:201:PRO:HD2	10:D:780:HOH:O	2.13	0.48
1:A:34:PHE:HE1	1:A:130:ILE:HB	1.79	0.47
1:D:528:THR:HG21	5:D:604:EDO:H21	1.94	0.47
1:A:353[A]:HIS:CD2	10:A:1102:HOH:O	2.66	0.47
4:I:4:DT:H2''	4:I:5:DT:H5'	1.96	0.47
1:D:432:ALA:N	5:D:609:EDO:H21	2.18	0.47
1:A:38:LYS:HD3	1:A:133:PHE:CD2	2.50	0.47
1:A:461[A]:ARG:HA	1:A:573:VAL:HG22	1.96	0.47
1:D:140:THR:C	1:D:141:LEU:HD12	2.40	0.47
5:D:605:EDO:C1	10:D:738:HOH:O	2.63	0.47
4:J:5:DT:H73	10:J:101:HOH:O	2.14	0.47
1:A:100:ILE:HG21	1:A:103:LEU:HD13	1.96	0.47
1:D:596:ILE:C	10:D:701:HOH:O	2.48	0.46
1:A:90:VAL:HG21	1:A:488:SER:HA	1.98	0.46
1:A:189:LYS:HE2	1:A:189:LYS:HB3	1.47	0.46
1:D:49:LEU:CG	10:D:758:HOH:O	2.62	0.46
6:A:612:MES:H81	6:A:612:MES:H51	1.67	0.46
1:D:192:ASN:CB	10:D:743:HOH:O	2.32	0.46
1:D:249:LYS:HD3	1:D:388:PRO:O	2.16	0.46
1:D:46:VAL:HG22	10:D:739:HOH:O	2.15	0.46
1:A:251:ASP:OD2	1:A:344[A]:ASP:OD1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:TRP:CG	1:A:307:LEU:HD13	2.50	0.46
5:A:604:EDO:C1	10:A:742:HOH:O	2.44	0.46
1:A:87:HIS:HE1	1:A:426:ILE:O	1.98	0.46
7:A:613:PEG:C1	10:A:703:HOH:O	2.53	0.46
1:D:433[A]:ARG:NH2	10:D:726:HOH:O	2.49	0.46
1:D:29:ILE:HD12	1:D:29:ILE:H	1.81	0.45
1:D:101:PRO:HA	1:D:104:GLN:HG2	1.97	0.45
4:I:6:DT:H2'	4:I:7:DG:H8	1.81	0.45
1:D:16:PRO:O	1:D:31:LEU:HD22	2.16	0.45
1:D:409:PRO:HB3	10:D:773:HOH:O	2.16	0.45
1:D:461:ARG:NH2	10:D:728:HOH:O	2.31	0.45
1:A:139:LYS:NZ	10:A:779:HOH:O	2.49	0.45
1:A:211:LEU:HD22	5:A:606:EDO:H21	1.99	0.45
1:A:381:ARG:CZ	10:A:815:HOH:O	2.64	0.45
1:A:533:LYS:CE	10:A:852:HOH:O	2.43	0.45
1:D:386:GLU:OE2	10:D:714:HOH:O	2.21	0.45
4:J:4:DT:H2'	4:J:5:DT:C6	2.52	0.45
1:A:145:GLU:HG3	1:A:415:HIS:CD2	2.52	0.45
1:D:48:ILE:HG12	10:D:755:HOH:O	2.17	0.44
1:D:110:LEU:O	1:D:114:LEU:HD23	2.17	0.44
1:D:152:GLU:HG3	4:I:1:DT:H71	1.99	0.44
1:A:448:PHE:HA	1:A:453:PHE:CE2	2.53	0.44
1:D:409:PRO:N	10:D:773:HOH:O	2.48	0.44
1:D:231:TYR:CD2	1:D:450:LYS:HD2	2.53	0.44
1:A:175:GLN:CG	1:A:178:VAL:HG23	2.47	0.43
1:A:235[B]:SER:HG	1:A:457:PHE:HE2	1.65	0.43
1:A:127:VAL:O	1:A:130:ILE:HG22	2.18	0.43
1:A:260:LYS:NZ	10:A:783:HOH:O	2.50	0.43
1:D:450:LYS:CE	10:D:811:HOH:O	2.66	0.43
1:A:1:MET:CE	10:E:280:HOH:O	2.36	0.43
1:A:147:LYS:HE3	10:A:873:HOH:O	2.17	0.43
1:D:377:LEU:HD23	1:D:377:LEU:HA	1.78	0.43
1:A:1:MET:CA	10:A:705:HOH:O	2.61	0.43
1:D:12:ARG:NH1	10:D:760:HOH:O	2.43	0.43
1:D:40:HIS:N	1:D:40:HIS:CD2	2.85	0.43
1:A:318:GLU:HG2	10:A:915:HOH:O	2.19	0.43
2:B:12:A:H2'	2:B:13:G:O4'	2.18	0.43
1:A:135:TYR:CZ	1:A:596:ILE:HB	2.54	0.43
1:A:439:MET:HE2	1:A:439:MET:HA	2.00	0.42
7:A:613:PEG:C3	10:A:715:HOH:O	2.67	0.42
1:D:270:SER:HA	10:D:944:HOH:O	2.11	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:PHE:CE2	5:A:605:EDO:H21	2.54	0.42
1:A:584:LYS:HD2	1:A:585:PHE:CE2	2.55	0.42
1:A:353[A]:HIS:NE2	1:A:354:LYS:HE2	2.35	0.42
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.85	0.42
1:A:113:LYS:HG3	1:A:117:LYS:NZ	2.35	0.42
1:D:261:ILE:N	5:D:610:EDO:O2	2.38	0.42
1:D:19:VAL:HG21	1:D:27:LEU:HB2	2.02	0.42
1:A:342:VAL:HG21	3:C:7:DG:H1'	2.01	0.42
1:D:593:LYS:HE2	10:D:763:HOH:O	2.09	0.42
1:A:8:SER:HA	1:A:80:GLN:OE1	2.20	0.42
1:A:381:ARG:HB2	10:A:815:HOH:O	2.20	0.42
1:D:493:ASP:N	10:D:703:HOH:O	2.48	0.42
1:D:526:LYS:NZ	10:D:765:HOH:O	2.45	0.42
4:I:6:DT:H2'	4:I:7:DG:C8	2.54	0.41
1:A:154:TYR:CE1	10:A:710:HOH:O	2.67	0.41
1:D:185:ASN:HA	10:E:208:HOH:O	2.20	0.41
1:D:436:GLN:HG3	10:D:705:HOH:O	2.20	0.41
1:A:227:SER:HA	10:A:1135:HOH:O	2.20	0.41
1:D:554:LEU:HD12	1:D:554:LEU:HA	1.85	0.41
1:A:584:LYS:NZ	10:A:743:HOH:O	2.42	0.41
1:D:261:ILE:CB	5:D:610:EDO:H22	2.42	0.41
4:J:6:DT:H2''	4:J:7:DG:OP1	2.20	0.41
5:A:609:EDO:C1	10:A:761:HOH:O	2.37	0.41
1:D:47:GLN:NE2	10:D:702:HOH:O	1.71	0.41
4:J:2:DT:H2'	4:J:3:DC:C6	2.56	0.41
1:A:43:LYS:HB2	1:A:43:LYS:HE3	1.88	0.41
5:D:602:EDO:C2	10:D:993:HOH:O	2.21	0.41
1:A:220:LEU:HD21	1:A:319:LEU:HA	2.02	0.41
1:D:250:VAL:HG21	1:D:362[B]:ILE:HD12	2.03	0.41
1:D:323:PHE:CE2	1:D:327:LEU:HD11	2.56	0.41
1:A:353[B]:HIS:HB3	10:A:1102:HOH:O	2.19	0.41
1:A:462[A]:THR:HG22	10:A:834:HOH:O	2.20	0.41
1:D:482:MET:SD	1:D:497:ILE:HD12	2.60	0.41
3:F:7:DG:OP1	10:F:101:HOH:O	2.21	0.41
1:A:102:TRP:CE3	1:A:103:LEU:HD12	2.56	0.41
5:D:609:EDO:C1	10:D:824:HOH:O	2.69	0.41
1:D:89:SER:HA	1:D:92:HIS:CD2	2.56	0.40
1:D:402:ARG:HD2	1:D:462[A]:THR:HG23	2.02	0.40
1:A:526:LYS:HD2	10:A:953:HOH:O	2.22	0.40
6:A:611:MES:H52	6:A:611:MES:H82	1.81	0.40
1:D:369:ASN:CG	10:D:856:HOH:O	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:CE	10:A:873:HOH:O	2.69	0.40
1:D:437:LYS:HA	1:D:437:LYS:HD2	1.90	0.40
5:D:607:EDO:C2	10:D:792:HOH:O	2.55	0.40
1:D:323:PHE:CD2	1:D:324:MET:HE2	2.57	0.40
1:A:482:MET:O	1:A:486:ARG:HG2	2.21	0.40
1:D:250:VAL:HG21	1:D:362[A]:ILE:HG21	2.03	0.40
1:D:459:ASP:OD1	1:D:523:LYS:HD3	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:ARG:CB	10:D:785:HOH:O[1_455]	1.97	0.23
10:A:832:HOH:O	10:D:1121:HOH:O[2_655]	2.13	0.07
7:A:613:PEG:C4	10:A:716:HOH:O[1_455]	2.18	0.02
10:A:1125:HOH:O	10:D:738:HOH:O[2_555]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	608/596 (102%)	584 (96%)	23 (4%)	1 (0%)	43	40
1	D	602/596 (101%)	586 (97%)	15 (2%)	1 (0%)	43	40
All	All	1210/1192 (102%)	1170 (97%)	38 (3%)	2 (0%)	43	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	342	VAL
1	A	342	VAL

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	558/552 (101%)	543 (97%)	15 (3%)	39	37
1	D	549/552 (100%)	533 (97%)	16 (3%)	37	34
All	All	1107/1104 (100%)	1076 (97%)	31 (3%)	40	35

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	11[A]	SER
1	A	11[B]	SER
1	A	39	LYS
1	A	40	HIS
1	A	43	LYS
1	A	113	LYS
1	A	189	LYS
1	A	190	GLN
1	A	191	ASP
1	A	203	SER
1	A	206	LYS
1	A	390	CYS
1	A	567	LYS
1	A	580	LYS
1	D	19	VAL
1	D	21	SER
1	D	42	THR
1	D	43	LYS
1	D	67	LEU
1	D	190	GLN
1	D	206	LYS
1	D	298	LYS
1	D	353[A]	HIS
1	D	353[B]	HIS
1	D	362[A]	ILE
1	D	362[B]	ILE

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Mol	Chain	Res	Type
1	D	380	HIS
1	D	390	CYS
1	D	533	LYS
1	D	567	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	33	ASN
1	A	125	ASN
1	A	163	HIS
1	A	190	GLN
1	A	258	ASN
1	A	274	HIS
1	A	303	ASN
1	D	33	ASN
1	D	40	HIS
1	D	185	ASN
1	D	239	GLN
1	D	290	ASN
1	D	380	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	17/18 (94%)	2 (11%)	0
2	E	17/18 (94%)	2 (11%)	0
All	All	34/36 (94%)	4 (11%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	U
2	B	16	G
2	E	9	U
2	E	16	G

There are no RNA pucker outliers to report.

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 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	MES	A	611	-	12,12,12	0.69	0	15,16,16	0.29	0
9	DGT	A	615	8	32,33,33	3.48	8 (25%)	48,52,52	1.86	12 (25%)
5	EDO	D	602	-	3,3,3	0.59	0	2,2,2	0.28	0
5	EDO	D	603	-	3,3,3	0.07	0	2,2,2	0.10	0
5	EDO	E	101	-	3,3,3	0.47	0	2,2,2	0.40	0
5	EDO	A	603	-	3,3,3	0.52	0	2,2,2	0.38	0
9	DGT	D	613	8	32,33,33	3.70	6 (18%)	48,52,52	1.85	11 (22%)
6	MES	A	612	-	12,12,12	0.70	0	15,16,16	0.29	0
5	EDO	A	608	-	3,3,3	0.06	0	2,2,2	0.08	0
5	EDO	A	604	-	3,3,3	0.53	0	2,2,2	0.24	0
5	EDO	A	601	-	3,3,3	0.49	0	2,2,2	0.37	0
5	EDO	D	607	-	3,3,3	0.07	0	2,2,2	0.09	0
5	EDO	D	605	-	3,3,3	0.07	0	2,2,2	0.09	0
5	EDO	A	605	-	3,3,3	0.06	0	2,2,2	0.10	0
5	EDO	D	610	-	3,3,3	0.08	0	2,2,2	0.06	0
5	EDO	D	609	-	3,3,3	0.08	0	2,2,2	0.05	0
5	EDO	A	610	-	3,3,3	0.08	0	2,2,2	0.07	0
7	PEG	D	611	-	6,6,6	0.11	0	5,5,5	0.08	0
5	EDO	D	606	-	3,3,3	0.06	0	2,2,2	0.09	0
5	EDO	A	606	-	3,3,3	0.07	0	2,2,2	0.09	0
5	EDO	D	601	-	3,3,3	0.38	0	2,2,2	0.96	0
5	EDO	D	608	-	3,3,3	0.06	0	2,2,2	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PEG	A	613	-	6,6,6	0.12	0	5,5,5	0.08	0
5	EDO	A	609	-	3,3,3	0.07	0	2,2,2	0.09	0
5	EDO	A	602	-	3,3,3	0.44	0	2,2,2	0.57	0
5	EDO	A	607	-	3,3,3	0.06	0	2,2,2	0.09	0
5	EDO	D	604	-	3,3,3	0.07	0	2,2,2	0.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MES	A	611	-	-	4/6/14/14	0/1/1/1
9	DGT	A	615	8	-	3/22/34/34	0/3/3/3
5	EDO	D	602	-	-	1/1/1/1	-
5	EDO	D	603	-	-	1/1/1/1	-
5	EDO	E	101	-	-	0/1/1/1	-
5	EDO	A	603	-	-	0/1/1/1	-
9	DGT	D	613	8	-	5/22/34/34	0/3/3/3
6	MES	A	612	-	-	2/6/14/14	0/1/1/1
5	EDO	A	608	-	-	1/1/1/1	-
5	EDO	A	604	-	-	1/1/1/1	-
5	EDO	A	601	-	-	1/1/1/1	-
5	EDO	D	607	-	-	1/1/1/1	-
5	EDO	D	605	-	-	1/1/1/1	-
5	EDO	A	605	-	-	1/1/1/1	-
5	EDO	D	610	-	-	1/1/1/1	-
5	EDO	D	609	-	-	1/1/1/1	-
5	EDO	A	610	-	-	1/1/1/1	-
7	PEG	D	611	-	-	2/4/4/4	-
5	EDO	D	606	-	-	1/1/1/1	-
5	EDO	A	606	-	-	0/1/1/1	-
5	EDO	D	601	-	-	0/1/1/1	-
5	EDO	D	608	-	-	1/1/1/1	-
7	PEG	A	613	-	-	2/4/4/4	-
5	EDO	A	609	-	-	0/1/1/1	-
5	EDO	A	602	-	-	0/1/1/1	-
5	EDO	A	607	-	-	1/1/1/1	-
5	EDO	D	604	-	-	1/1/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	613	DGT	PB-O3A	17.25	1.78	1.59
9	A	615	DGT	PB-O3A	15.76	1.76	1.59
9	A	615	DGT	O6-C6	6.62	1.36	1.23
9	D	613	DGT	O6-C6	6.59	1.36	1.23
9	D	613	DGT	PA-O5'	5.97	1.82	1.59
9	A	615	DGT	PA-O5'	5.74	1.81	1.59
9	A	615	DGT	PA-O3A	-3.15	1.56	1.59
9	A	615	DGT	O5'-C5'	-3.04	1.33	1.44
9	D	613	DGT	O5'-C5'	-3.02	1.33	1.44
9	D	613	DGT	PA-O3A	-2.93	1.56	1.59
9	D	613	DGT	C2-N2	2.50	1.40	1.34
9	A	615	DGT	C2-N2	2.47	1.40	1.34
9	A	615	DGT	PB-O3B	-2.13	1.57	1.59
9	A	615	DGT	O4'-C1'	-2.10	1.37	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	613	DGT	C2-N1-C6	-4.60	116.77	125.11
9	A	615	DGT	C2-N1-C6	-4.49	116.97	125.11
9	D	613	DGT	O3A-PB-O2B	-4.32	97.71	110.70
9	A	615	DGT	O1B-PB-O3A	-3.93	96.64	107.27
9	D	613	DGT	C5-C6-N1	3.76	122.83	113.25
9	A	615	DGT	O5'-PA-O2A	-3.75	94.07	108.94
9	A	615	DGT	C5-C6-N1	3.66	122.56	113.25
9	D	613	DGT	O5'-PA-O2A	-3.65	94.46	108.94
9	A	615	DGT	O3A-PB-O2B	-3.21	101.05	110.70
9	A	615	DGT	C6-C5-N7	3.09	135.92	130.29
9	D	613	DGT	C6-C5-N7	3.04	135.82	130.29
9	A	615	DGT	O1A-PA-O3A	2.91	115.13	107.27
9	D	613	DGT	O1A-PA-O3A	2.91	115.13	107.27
9	D	613	DGT	C6-C5-C4	-2.89	114.48	118.83
9	A	615	DGT	O3A-PA-O2A	2.84	119.25	110.70
9	A	615	DGT	C6-C5-C4	-2.83	114.57	118.83
9	D	613	DGT	O3A-PA-O2A	2.70	118.83	110.70
9	D	613	DGT	O6-C6-C5	-2.70	119.41	126.53
9	A	615	DGT	O6-C6-C5	-2.62	119.63	126.53
9	D	613	DGT	O1A-PA-O5'	-2.57	95.94	107.57
9	D	613	DGT	O1B-PB-O3A	-2.47	100.61	107.27
9	A	615	DGT	O1A-PA-O5'	-2.43	96.57	107.57
9	A	615	DGT	N2-C2-N3	-2.05	115.68	119.67

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	611	MES	C8-C7-N4-C5
6	A	611	MES	N4-C7-C8-S
6	A	612	MES	C8-C7-N4-C5
9	A	615	DGT	PB-O3B-PG-O2G
9	D	613	DGT	PB-O3B-PG-O2G
7	D	611	PEG	O2-C3-C4-O4
5	A	601	EDO	O1-C1-C2-O2
5	D	603	EDO	O1-C1-C2-O2
5	D	604	EDO	O1-C1-C2-O2
6	A	611	MES	C8-C7-N4-C3
6	A	612	MES	C8-C7-N4-C3
7	A	613	PEG	C4-C3-O2-C2
7	D	611	PEG	C1-C2-O2-C3
7	A	613	PEG	C1-C2-O2-C3
5	A	607	EDO	O1-C1-C2-O2
9	D	613	DGT	PA-O3A-PB-O1B
5	D	602	EDO	O1-C1-C2-O2
5	D	607	EDO	O1-C1-C2-O2
5	D	608	EDO	O1-C1-C2-O2
5	D	609	EDO	O1-C1-C2-O2
5	A	604	EDO	O1-C1-C2-O2
5	A	605	EDO	O1-C1-C2-O2
5	A	608	EDO	O1-C1-C2-O2
5	D	606	EDO	O1-C1-C2-O2
5	D	610	EDO	O1-C1-C2-O2
6	A	611	MES	C7-C8-S-O1S
9	A	615	DGT	PB-O3B-PG-O1G
9	D	613	DGT	PB-O3B-PG-O1G
5	D	605	EDO	O1-C1-C2-O2
9	A	615	DGT	PA-O3A-PB-O1B
9	D	613	DGT	PA-O3A-PB-O2B
9	D	613	DGT	PB-O3B-PG-O3G
5	A	610	EDO	O1-C1-C2-O2

There are no ring outliers.

19 monomers are involved in 79 short contacts:

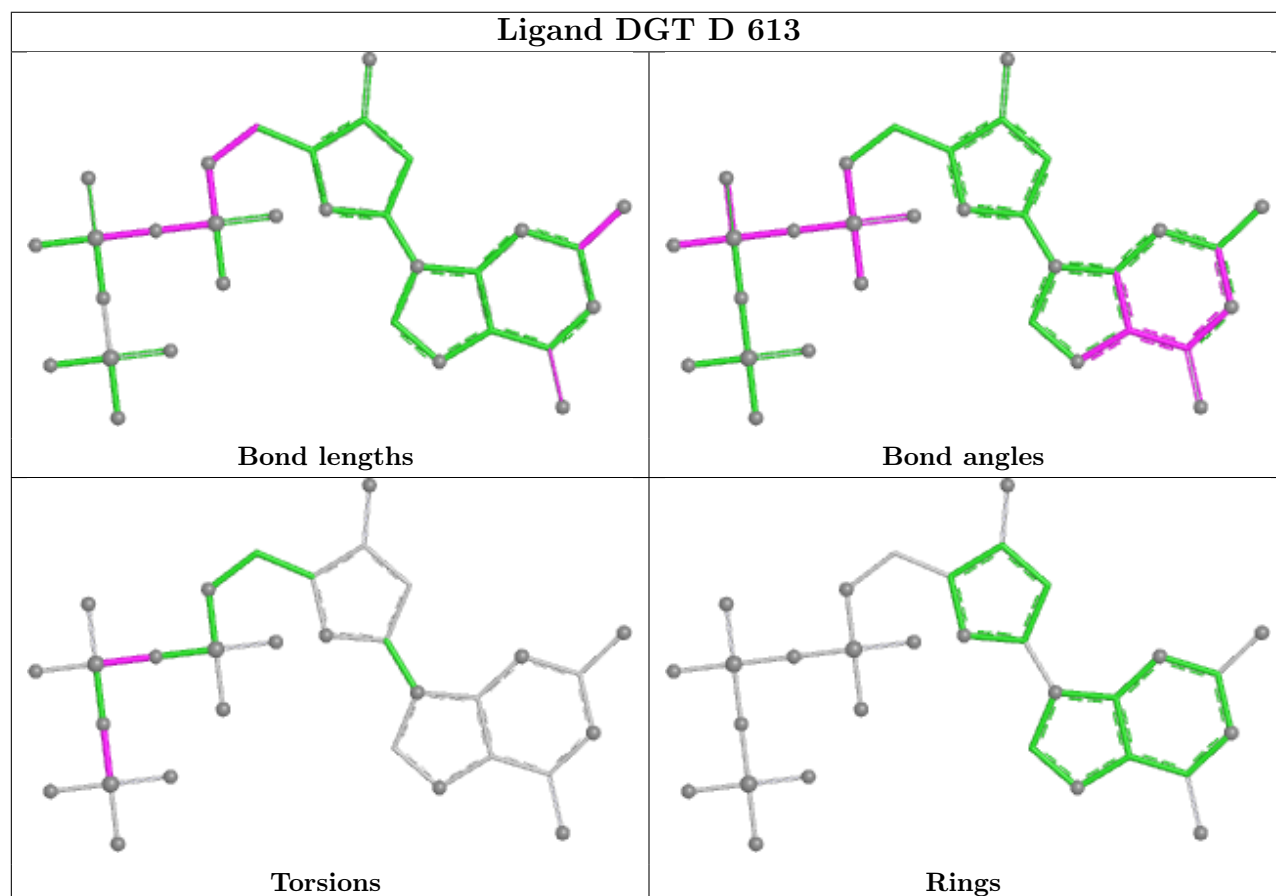
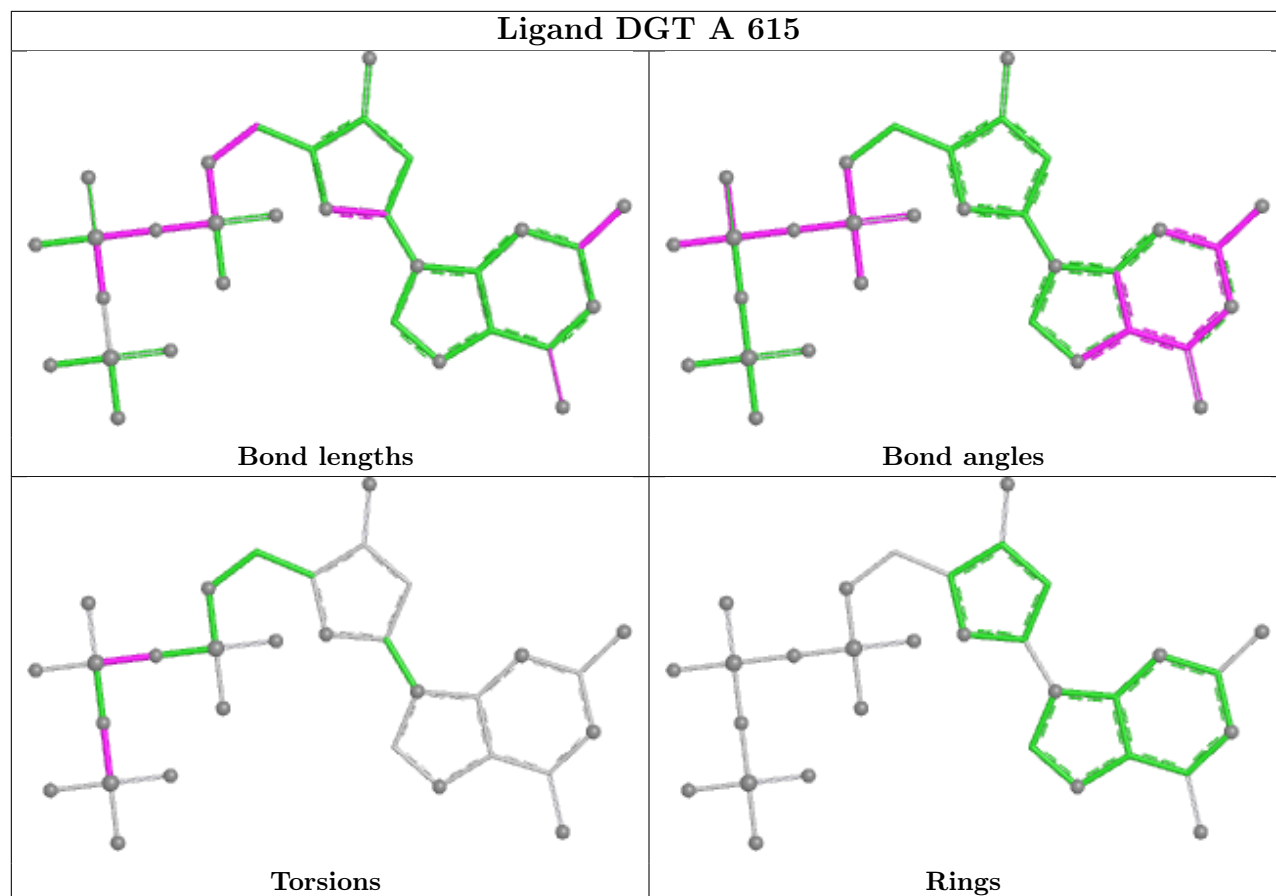
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	611	MES	3	0
5	D	602	EDO	3	0
5	D	603	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	603	EDO	2	0
6	A	612	MES	8	0
5	A	604	EDO	2	0
5	D	607	EDO	5	0
5	D	605	EDO	3	0
5	A	605	EDO	9	0
5	D	610	EDO	6	0
5	D	609	EDO	10	0
7	D	611	PEG	2	0
5	A	606	EDO	4	0
5	D	601	EDO	2	0
5	D	608	EDO	5	0
7	A	613	PEG	3	1
5	A	609	EDO	4	0
5	A	607	EDO	4	0
5	D	604	EDO	4	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	596/596 (100%)	-0.32	1 (0%) 91 91	17, 52, 100, 131	14 (2%)
1	D	596/596 (100%)	-0.26	0 100 100	18, 54, 105, 157	8 (1%)
2	B	18/18 (100%)	-1.12	0 100 100	33, 45, 106, 110	0
2	E	18/18 (100%)	-1.09	0 100 100	33, 53, 82, 83	0
3	C	7/7 (100%)	-1.26	0 100 100	33, 35, 39, 42	0
3	F	7/7 (100%)	-1.02	0 100 100	36, 39, 45, 48	0
4	I	7/7 (100%)	-0.05	0 100 100	92, 95, 101, 106	0
4	J	7/7 (100%)	-0.02	0 100 100	112, 112, 118, 118	0
All	All	1256/1256 (100%)	-0.32	1 (0%) 92 91	17, 53, 106, 157	22 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	64	THR	2.4

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,

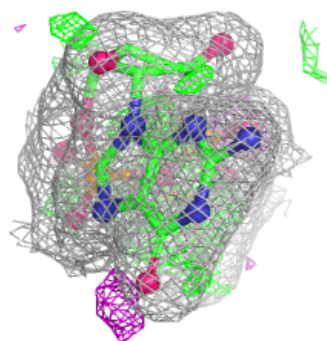
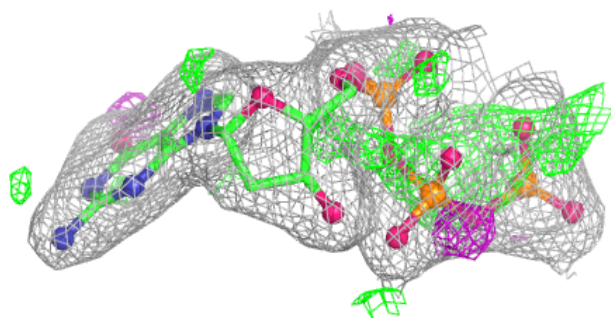
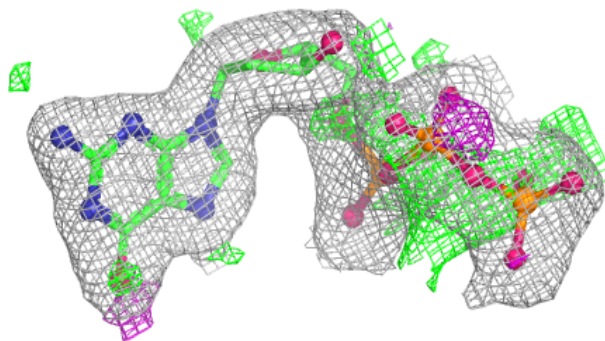
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	A	604	4/4	0.69	0.10	72,79,83,83	0
6	MES	A	612	12/12	0.73	0.13	71,80,98,103	0
6	MES	A	611	12/12	0.79	0.12	59,69,103,122	0
5	EDO	E	101	4/4	0.79	0.12	74,76,80,84	0
7	PEG	D	611	7/7	0.79	0.15	65,71,77,78	0
5	EDO	D	603	4/4	0.82	0.11	72,73,74,75	0
5	EDO	D	607	4/4	0.84	0.10	73,76,81,82	0
5	EDO	D	604	4/4	0.85	0.12	65,65,70,75	0
5	EDO	A	603	4/4	0.86	0.09	61,65,68,71	0
5	EDO	D	606	4/4	0.87	0.17	61,65,65,69	0
5	EDO	A	608	4/4	0.87	0.15	54,59,62,69	0
5	EDO	A	605	4/4	0.88	0.07	67,73,74,76	0
5	EDO	A	609	4/4	0.88	0.10	56,71,73,80	0
5	EDO	D	609	4/4	0.88	0.08	64,65,69,78	0
5	EDO	D	610	4/4	0.88	0.14	51,54,54,65	0
5	EDO	A	606	4/4	0.89	0.08	67,69,72,72	0
7	PEG	A	613	7/7	0.89	0.11	53,63,73,76	0
5	EDO	D	602	4/4	0.89	0.11	63,71,72,72	0
5	EDO	D	608	4/4	0.90	0.07	65,67,70,74	0
5	EDO	A	610	4/4	0.90	0.10	46,52,59,61	0
5	EDO	A	601	4/4	0.90	0.08	64,66,68,75	0
5	EDO	A	607	4/4	0.90	0.15	51,53,64,74	0
5	EDO	D	601	4/4	0.92	0.16	59,61,63,67	0
5	EDO	D	605	4/4	0.93	0.19	55,56,57,59	0
5	EDO	A	602	4/4	0.96	0.10	45,49,51,62	0
9	DGT	A	615	31/31	0.97	0.06	28,33,40,46	0
9	DGT	D	613	31/31	0.97	0.06	29,35,41,47	0
8	CA	D	612	1/1	0.99	0.02	29,29,29,29	0
8	CA	A	614	1/1	1.00	0.02	30,30,30,30	0

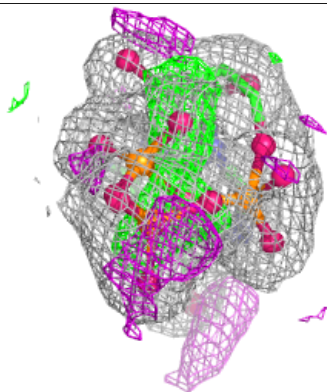
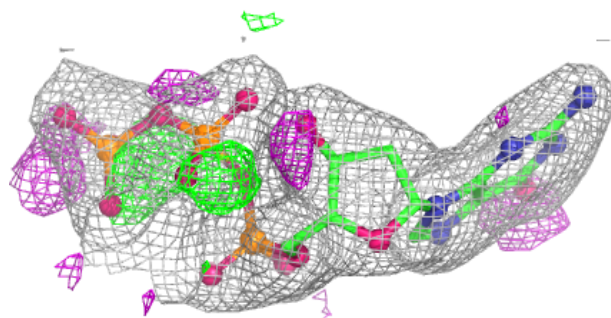
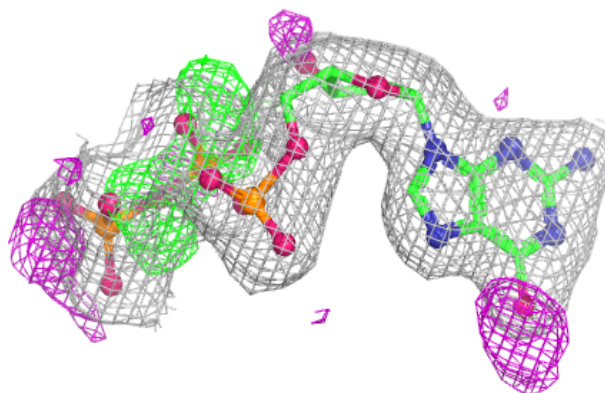
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGT A 615:

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

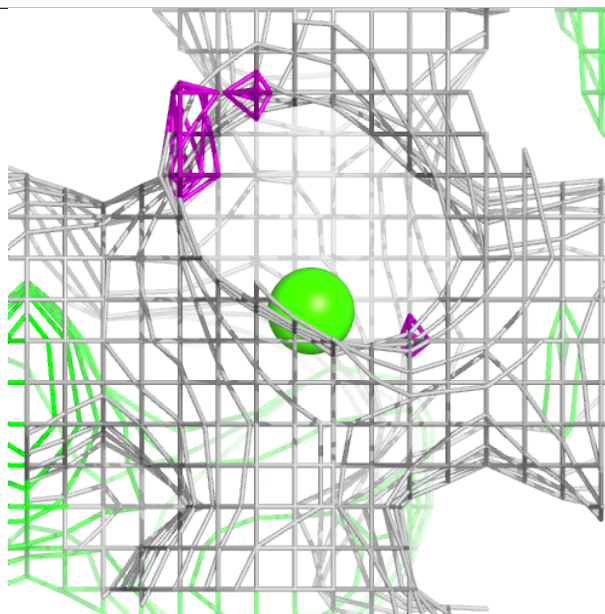
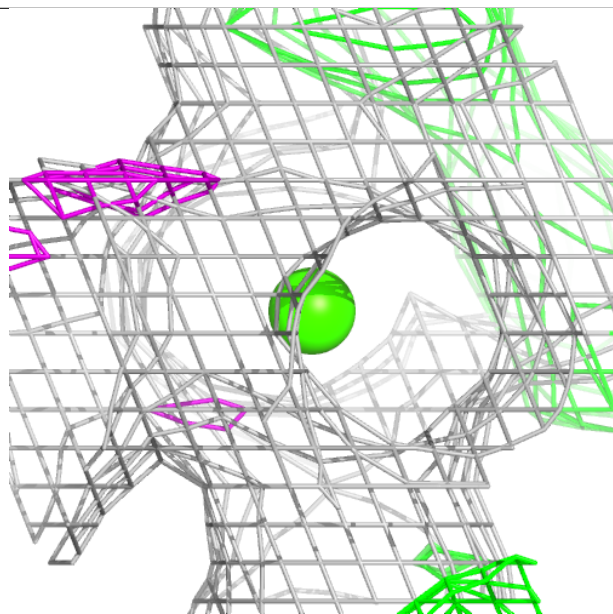
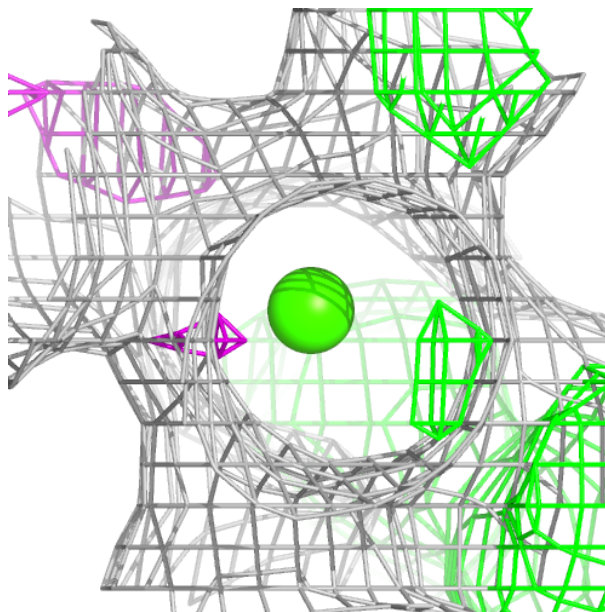
**Electron density around DGT D 613:**

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



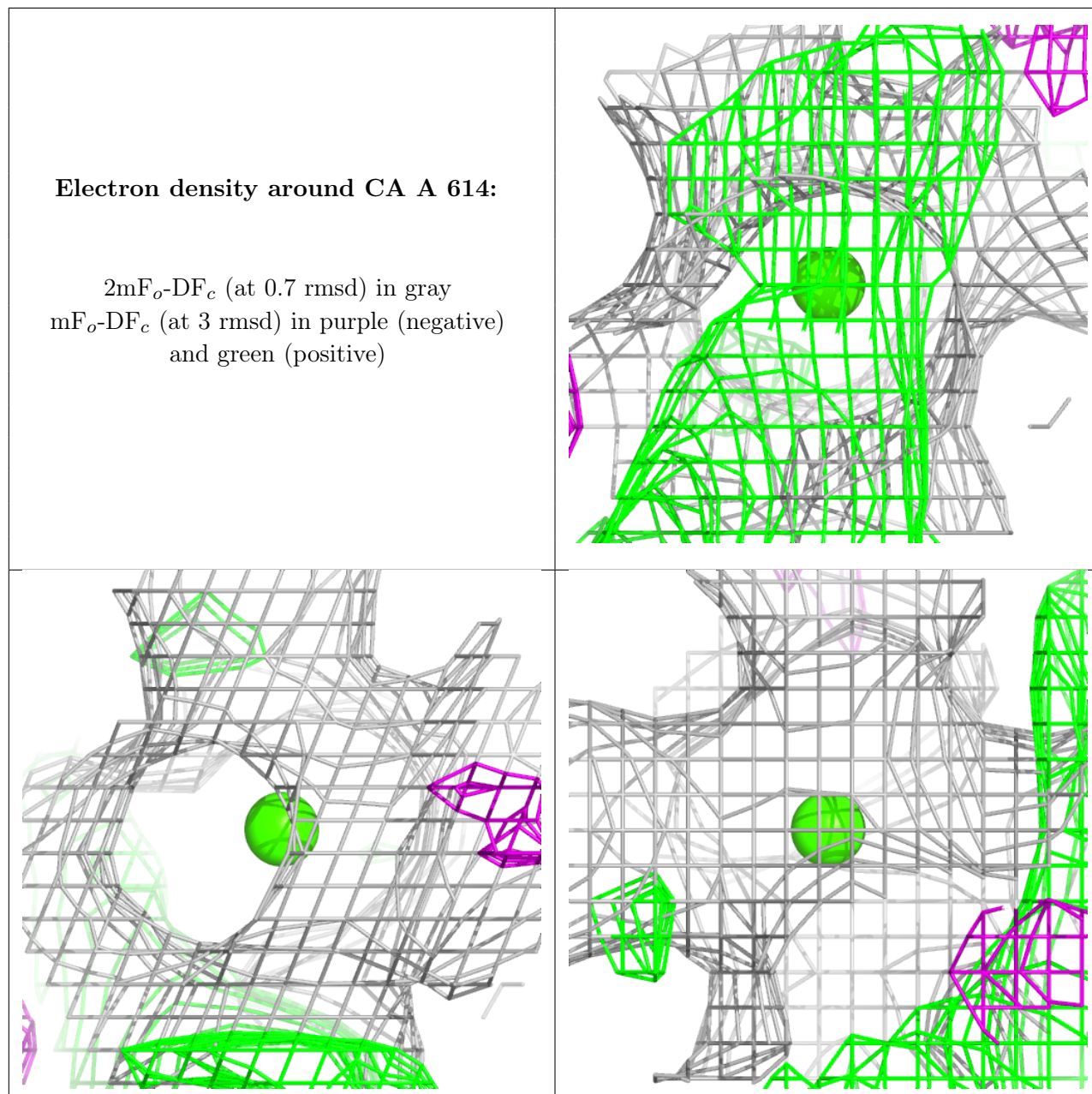
Electron density around CA D 612:

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



Electron density around CA A 614:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.