Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2024 – 12:32 pm BST

PDB ID	:	1OGK
Title	:	The crystal structure of Trypanosoma cruzi dUTPase in complex with dUDP
Authors	:	Harkiolaki, M.; Dodson, E.J.; Bernier-Villamor, V.; Turkenburg, J.P.; Gonzalez-Pacanowska, D.; Wilson, K.S.
Deposited on	:	2003-05-07
Resolution	:	2.85 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

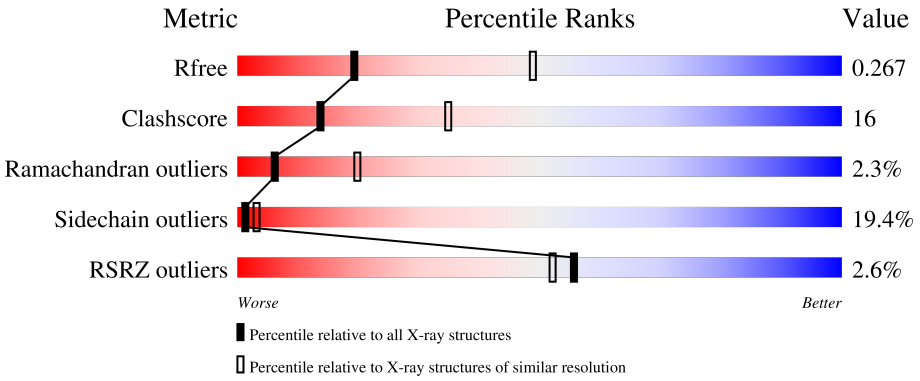
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	283	51% 24% 6% 19%
1	B	283	49% 28% 7% • 15%
1	D	283	6% 45% 31% 8% • 16%
1	E	283	2% 48% 30% 5% • 14%

2 Entry composition (i)

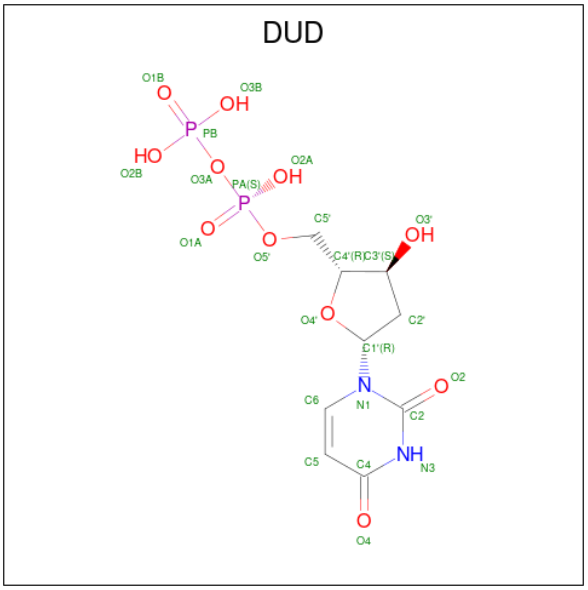
There are 2 unique types of molecules in this entry. The entry contains 7784 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DEOXYURIDINE TRIPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	1
			1865	1200	311	345	9			
1	B	240	Total	C	N	O	S	0	0	1
			1949	1256	327	357	9			
1	D	238	Total	C	N	O	S	0	0	1
			1934	1247	325	353	9			
1	E	242	Total	C	N	O	S	0	0	1
			1964	1267	329	359	9			

- Molecule 2 is DEOXYURIDINE-5'-DIPHOSPHATE (three-letter code: DUD) (formula: $C_9H_{14}N_2O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			24	9	2	11	2		
2	D	1	Total	C	N	O	P	0	0
			24	9	2	11	2		

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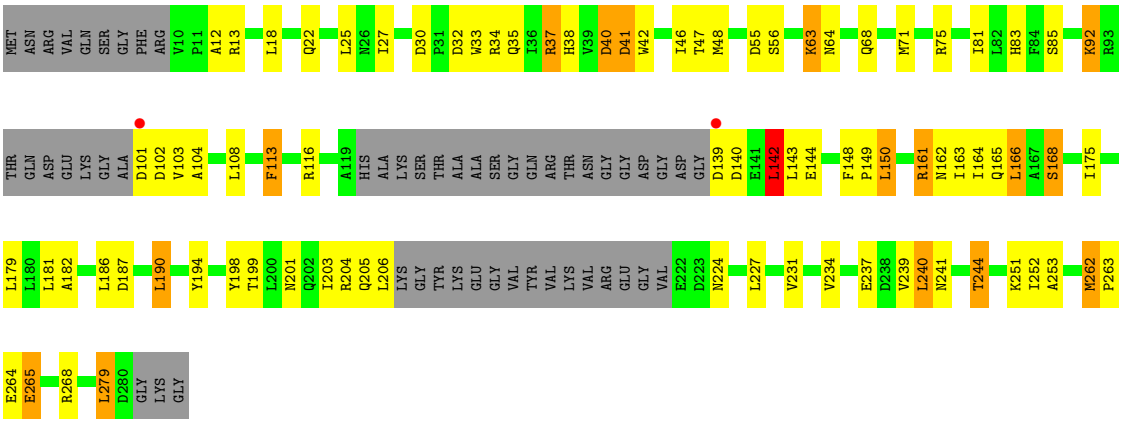
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			24	9	2	11	2		

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.

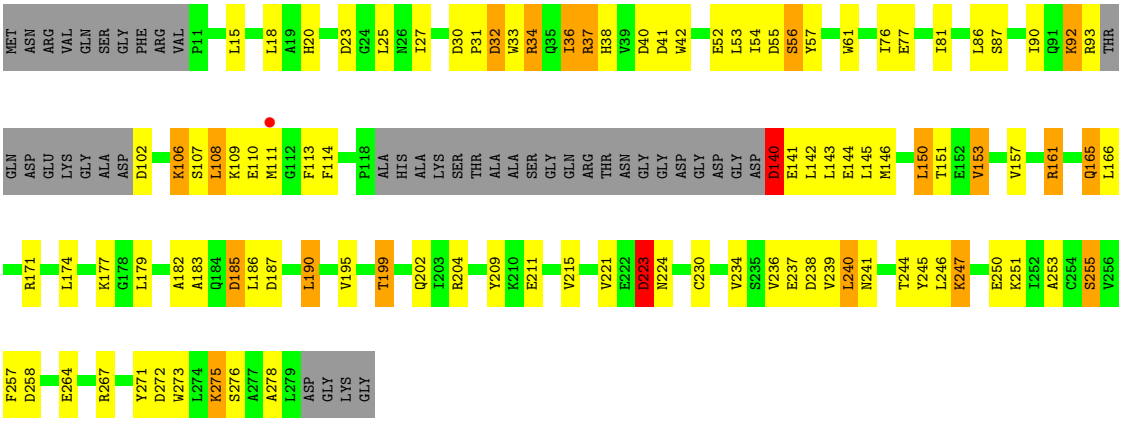
• Molecule 1: DEOXYURIDINE TRIPHOSPHATASE

Chain A:



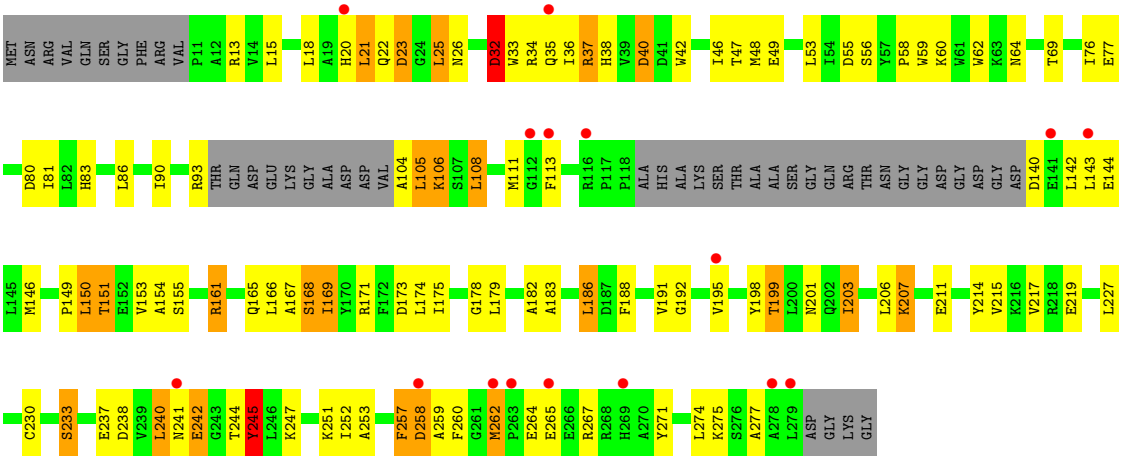
• Molecule 1: DEOXYURIDINE TRIPHOSPHATASE

Chain B:



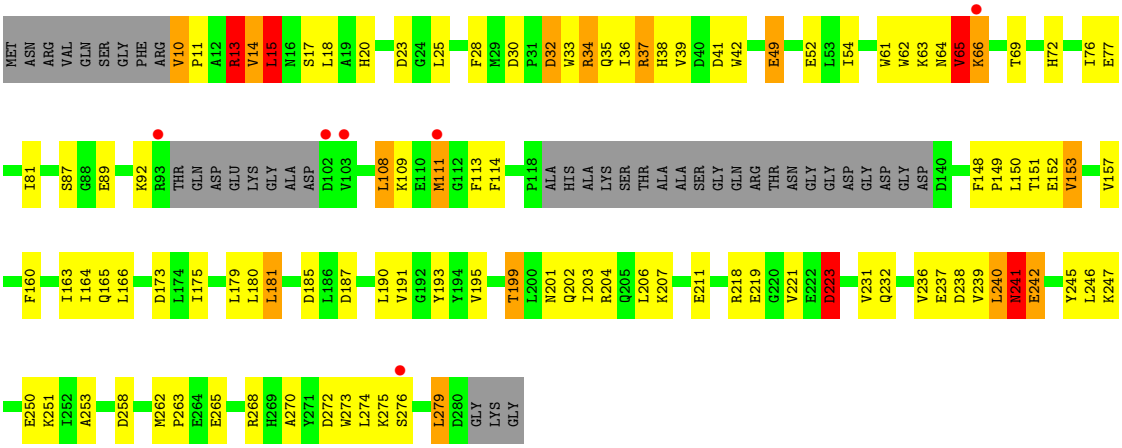
• Molecule 1: DEOXYURIDINE TRIPHOSPHATASE

Chain D:



• Molecule 1: DEOXYURIDINE TRIPHOSPHATASE

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.39Å 50.31Å 111.39Å 90.00° 101.35° 90.00°	Depositor
Resolution (Å)	111.80 – 2.85 20.03 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.1 (111.80-2.85) 99.5 (20.03-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.83Å)	Xtriage
Refinement program	REFMAC 5.1.13	Depositor
R, R_{free}	0.205 , 0.273 0.209 , 0.267	Depositor DCC
R_{free} test set	1362 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	59.5	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 36.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.020 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7784	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.98	0/1906	1.07	7/2584 (0.3%)
1	B	0.98	2/1993 (0.1%)	1.10	15/2698 (0.6%)
1	D	0.75	0/1978	0.96	6/2677 (0.2%)
1	E	0.90	1/2008 (0.0%)	1.07	12/2720 (0.4%)
All	All	0.91	3/7885 (0.0%)	1.05	40/10679 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	77	GLU	CG-CD	6.28	1.61	1.51
1	E	223	ASP	CB-CG	-5.87	1.39	1.51
1	B	146	MET	CG-SD	-5.19	1.67	1.81

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	238	ASP	CB-CG-OD2	11.55	128.69	118.30
1	A	139	ASP	CB-CG-OD2	9.23	126.61	118.30
1	B	77	GLU	OE1-CD-OE2	-8.33	113.30	123.30
1	E	52	GLU	OE1-CD-OE2	-7.88	113.85	123.30
1	A	140	ASP	CB-CG-OD2	7.60	125.14	118.30
1	E	272	ASP	CB-CG-OD2	7.55	125.10	118.30
1	B	30	ASP	CB-CG-OD2	7.52	125.07	118.30
1	E	41	ASP	CB-CG-OD2	7.38	124.94	118.30
1	E	187	ASP	CB-CG-OD2	7.28	124.85	118.30
1	D	23	ASP	CB-CG-OD2	7.28	124.85	118.30
1	B	55	ASP	CB-CG-OD2	7.19	124.77	118.30
1	D	238	ASP	CB-CG-OD2	7.02	124.62	118.30
1	D	80	ASP	CB-CG-OD2	6.95	124.56	118.30
1	B	41	ASP	CB-CG-OD2	6.88	124.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	258	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	75	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	B	52	GLU	OE1-CD-OE2	-6.71	115.25	123.30
1	B	223	ASP	CB-CG-OD2	6.64	124.28	118.30
1	D	258	ASP	CB-CG-OD2	6.57	124.22	118.30
1	B	32	ASP	CB-CG-OD2	6.54	124.18	118.30
1	A	41	ASP	CB-CG-OD2	6.42	124.07	118.30
1	E	238	ASP	CB-CG-OD2	6.21	123.89	118.30
1	B	140	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	238	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	E	34	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	278	ALA	O-C-N	-5.78	113.45	122.70
1	E	223	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	30	ASP	CB-CG-OD1	5.73	123.46	118.30
1	B	258	ASP	CB-CG-OD2	5.62	123.36	118.30
1	E	185	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	40	ASP	CB-CG-OD2	5.52	123.27	118.30
1	E	23	ASP	CB-CG-OD2	5.49	123.25	118.30
1	D	140	ASP	CB-CG-OD2	5.47	123.23	118.30
1	B	185	ASP	CB-CG-OD2	5.46	123.21	118.30
1	D	173	ASP	CB-CG-OD2	5.32	123.09	118.30
1	E	223	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	A	142	LEU	CA-CB-CG	5.21	127.27	115.30
1	B	52	GLU	CA-CB-CG	5.20	124.83	113.40
1	B	272	ASP	CB-CG-OD2	5.20	122.98	118.30
1	E	13	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1865	0	1826	54	0
1	B	1949	0	1922	60	0
1	D	1934	0	1909	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1964	0	1941	75	0
2	B	24	0	11	0	0
2	D	24	0	11	3	0
2	E	24	0	11	2	0
All	All	7784	0	7631	245	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 16.

All (245) 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:E:65:VAL:CG1	1:E:66:LYS:H	1.63	1.11
1:E:65:VAL:HG12	1:E:66:LYS:H	1.06	1.10
1:E:10:VAL:CG2	1:E:180:LEU:HD22	1.81	1.08
1:E:10:VAL:HG21	1:E:180:LEU:CD2	1.95	0.95
1:E:65:VAL:HG12	1:E:66:LYS:N	1.86	0.88
1:E:65:VAL:CG1	1:E:66:LYS:N	2.32	0.88
1:E:199:THR:HG21	1:E:253:ALA:HA	1.61	0.82
1:E:10:VAL:HG21	1:E:180:LEU:HD22	1.51	0.81
1:B:199:THR:HG21	1:B:253:ALA:HA	1.64	0.80
1:D:161:ARG:HG3	1:D:161:ARG:HH11	1.47	0.80
1:E:10:VAL:CG2	1:E:180:LEU:CD2	2.54	0.79
1:D:199:THR:HG21	1:D:253:ALA:HA	1.65	0.79
1:B:140:ASP:OD1	1:B:140:ASP:N	2.16	0.78
1:E:113:PHE:CZ	1:E:165:GLN:HG3	2.20	0.77
1:B:161:ARG:HG3	1:B:161:ARG:HH11	1.50	0.77
1:E:49:GLU:HG3	1:E:77:GLU:OE2	1.86	0.76
1:B:195:VAL:O	1:B:199:THR:HG22	1.85	0.76
1:B:113:PHE:CE1	1:B:165:GLN:HG3	2.22	0.75
1:B:113:PHE:CE2	1:B:165:GLN:NE2	2.55	0.74
1:E:113:PHE:CE2	1:E:165:GLN:HG3	2.22	0.74
1:B:53:LEU:O	1:B:56:SER:HB2	1.89	0.73
1:E:10:VAL:HG21	1:E:180:LEU:HD21	1.70	0.73
1:E:195:VAL:O	1:E:199:THR:HG22	1.88	0.72
1:A:234:VAL:HG22	1:A:251:LYS:HD2	1.72	0.71
1:D:150:LEU:HB2	1:D:186:LEU:CD1	2.20	0.71
1:A:113:PHE:CE1	1:A:165:GLN:HG3	2.26	0.71
1:A:168:SER:OG	1:B:165:GLN:NE2	2.24	0.69
1:E:218:ARG:O	1:E:219:GLU:HB2	1.92	0.69
1:D:104:ALA:N	1:D:106:LYS:HZ3	1.89	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:CYS:O	1:D:233:SER:HB3	1.92	0.69
1:D:271:TYR:O	1:D:275:LYS:HD3	1.94	0.67
1:B:86:LEU:O	1:B:90:ILE:HG13	1.95	0.67
1:A:113:PHE:HE1	1:A:165:GLN:HG3	1.59	0.67
1:D:13:ARG:NH1	1:D:242:GLU:HA	2.10	0.67
1:E:13:ARG:HD2	1:E:242:GLU:HB3	1.77	0.66
1:A:241:ASN:HD22	1:A:244:THR:HG23	1.60	0.66
1:D:105:LEU:O	1:D:108:LEU:HB2	1.95	0.66
1:A:265:GLU:OE1	1:A:265:GLU:HA	1.94	0.66
1:E:28:PHE:HZ	1:E:206:LEU:HD11	1.61	0.65
1:A:108:LEU:HD23	1:A:113:PHE:HE2	1.62	0.65
1:D:113:PHE:HE2	1:E:113:PHE:CE2	2.15	0.65
1:D:264:GLU:HA	1:D:267:ARG:HD2	1.79	0.65
1:D:199:THR:O	1:D:203:ILE:HG23	1.96	0.65
1:A:22:GLN:NE2	1:A:194:TYR:OH	2.29	0.64
1:E:33:TRP:O	1:E:37:ARG:HB2	1.97	0.64
1:E:37:ARG:HG2	1:E:42:TRP:CZ2	2.32	0.64
1:E:108:LEU:HG	1:E:113:PHE:CD1	2.33	0.64
1:E:239:VAL:HG23	1:E:240:LEU:HD13	1.80	0.64
1:D:168:SER:OG	1:E:165:GLN:NE2	2.31	0.63
1:D:59:TRP:CZ2	1:D:60:LYS:HE3	2.33	0.63
1:E:10:VAL:HG23	1:E:180:LEU:HD22	1.75	0.63
1:E:108:LEU:HD12	1:E:113:PHE:HB2	1.82	0.62
2:D:1280:DUD:H5	1:E:62:TRP:CE3	2.34	0.62
1:B:113:PHE:CZ	1:B:165:GLN:NE2	2.68	0.62
1:D:108:LEU:HB3	1:D:113:PHE:CD1	2.35	0.61
1:D:262:MET:O	1:D:262:MET:HG2	2.00	0.61
1:E:20:HIS:CD2	1:E:273:TRP:CZ3	2.88	0.61
1:D:108:LEU:HA	1:D:111:MET:HB3	1.82	0.61
1:A:203:ILE:HG12	1:A:262:MET:HG3	1.81	0.61
1:D:169:ILE:O	1:D:171:ARG:HG2	1.99	0.60
1:B:239:VAL:HG23	1:B:240:LEU:HD13	1.82	0.60
1:D:33:TRP:HA	1:D:36:ILE:HG22	1.84	0.60
1:A:113:PHE:CD1	1:A:113:PHE:C	2.74	0.60
1:E:20:HIS:CD2	1:E:273:TRP:HZ3	2.20	0.59
1:A:25:LEU:HD21	1:A:198:TYR:HD1	1.68	0.59
1:B:37:ARG:HG2	1:B:42:TRP:CZ2	2.37	0.59
1:D:191:VAL:HG21	1:D:240:LEU:HD11	1.84	0.59
1:B:20:HIS:CD2	1:B:273:TRP:CZ3	2.90	0.59
1:A:142:LEU:C	1:A:142:LEU:HD13	2.23	0.58
1:D:257:PHE:HB3	1:D:267:ARG:HE	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:LYS:HB3	1:E:66:LYS:HZ3	1.68	0.58
1:D:150:LEU:HB2	1:D:186:LEU:HD13	1.85	0.58
1:D:37:ARG:HG2	1:D:42:TRP:CZ2	2.38	0.58
1:E:10:VAL:HG23	1:E:180:LEU:HD13	1.86	0.58
1:A:165:GLN:O	1:A:168:SER:HB2	2.03	0.57
1:D:195:VAL:O	1:D:199:THR:HG22	2.03	0.57
1:D:22:GLN:HE21	1:D:26:ASN:HD21	1.51	0.57
1:E:237:GLU:O	1:E:241:ASN:HB2	2.04	0.57
1:D:262:MET:HB2	1:D:267:ARG:NH2	2.19	0.56
1:A:48:MET:HE1	1:B:54:ILE:HB	1.87	0.56
1:B:271:TYR:O	1:B:275:LYS:HD3	2.04	0.56
1:D:22:GLN:HE21	1:D:26:ASN:ND2	2.04	0.56
1:E:65:VAL:HG13	1:E:66:LYS:N	2.20	0.56
1:D:257:PHE:CD2	1:D:267:ARG:HG2	2.41	0.56
1:A:162:ASN:O	1:A:166:LEU:HD22	2.07	0.55
1:E:64:ASN:O	1:E:65:VAL:O	2.23	0.55
1:B:32:ASP:OD1	1:B:32:ASP:N	2.29	0.55
1:E:193:TYR:CE2	1:E:231:VAL:HG21	2.42	0.55
1:D:191:VAL:HG21	1:D:240:LEU:CD1	2.37	0.55
1:E:113:PHE:CD1	1:E:114:PHE:CE2	2.95	0.55
1:A:163:ILE:HD12	1:A:175:ILE:HG23	1.89	0.54
1:A:37:ARG:HG2	1:A:42:TRP:CZ2	2.43	0.54
1:A:227:LEU:O	1:A:231:VAL:HG23	2.08	0.54
1:A:241:ASN:ND2	1:A:244:THR:HG23	2.22	0.54
1:D:21:LEU:HD22	1:D:198:TYR:CZ	2.42	0.54
1:D:38:HIS:CD2	1:D:40:ASP:HB2	2.41	0.54
1:E:20:HIS:HD2	1:E:273:TRP:HZ3	1.55	0.54
1:D:20:HIS:HD2	1:D:277:ALA:HA	1.73	0.54
1:A:41:ASP:HB3	1:B:61:TRP:CZ3	2.43	0.54
1:E:89:GLU:OE1	1:E:173:ASP:HA	2.08	0.54
1:E:30:ASP:O	1:E:33:TRP:HB3	2.08	0.54
1:D:33:TRP:O	1:D:34:ARG:C	2.46	0.54
1:B:108:LEU:O	1:B:111:MET:HB2	2.09	0.53
1:E:66:LYS:HB3	1:E:66:LYS:NZ	2.21	0.53
1:E:236:VAL:O	1:E:240:LEU:HD22	2.09	0.53
1:A:161:ARG:HH11	1:A:161:ARG:HG3	1.73	0.52
1:B:81:ILE:HG22	1:B:179:LEU:HD11	1.92	0.52
1:D:81:ILE:HG22	1:D:179:LEU:HD11	1.92	0.52
1:A:108:LEU:HD23	1:A:113:PHE:CE2	2.44	0.52
1:A:104:ALA:HB1	1:B:111:MET:SD	2.50	0.52
1:B:241:ASN:HB3	1:B:244:THR:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:HIS:CD2	1:B:273:TRP:HZ3	2.28	0.51
1:B:183:ALA:HB2	1:B:190:LEU:HD12	1.91	0.51
1:E:240:LEU:O	1:E:242:GLU:N	2.44	0.51
1:A:33:TRP:O	1:A:37:ARG:HB2	2.11	0.51
1:E:113:PHE:HD1	1:E:114:PHE:CE2	2.30	0.50
1:A:113:PHE:CZ	1:A:165:GLN:OE1	2.64	0.50
1:B:234:VAL:HG12	1:B:251:LYS:NZ	2.26	0.50
1:A:33:TRP:CE2	1:A:34:ARG:HG3	2.47	0.50
1:A:234:VAL:HG21	1:A:252:ILE:HG13	1.94	0.50
1:D:108:LEU:HD23	1:D:113:PHE:CE1	2.47	0.50
1:A:63:LYS:O	1:A:64:ASN:C	2.49	0.49
1:A:63:LYS:HG2	1:B:209:TYR:CE1	2.46	0.49
1:D:53:LEU:O	1:D:56:SER:HB2	2.11	0.49
1:D:183:ALA:HA	1:D:188:PHE:CE2	2.47	0.49
1:E:270:ALA:O	1:E:274:LEU:HG	2.12	0.49
1:E:152:GLU:O	1:E:153:VAL:C	2.50	0.49
1:B:204:ARG:O	1:B:209:TYR:HB2	2.13	0.49
1:D:142:LEU:HB2	1:D:174:LEU:HD22	1.95	0.48
1:B:114:PHE:CD1	1:B:145:LEU:HD22	2.47	0.48
1:B:57:TYR:HB3	1:B:153:VAL:HG13	1.96	0.48
1:A:22:GLN:NE2	1:A:83:HIS:ND1	2.55	0.48
1:D:144:GLU:OE2	1:D:144:GLU:O	2.32	0.48
1:E:160:PHE:CD1	1:E:163:ILE:HG13	2.48	0.48
1:A:83:HIS:CE1	1:A:194:TYR:CE1	3.02	0.48
1:E:153:VAL:O	1:E:157:VAL:HG23	2.13	0.48
1:D:105:LEU:C	1:D:105:LEU:HD12	2.35	0.48
1:A:81:ILE:HG22	1:A:179:LEU:HD11	1.95	0.47
1:B:215:VAL:HG22	1:E:207:LYS:HG2	1.97	0.47
1:D:33:TRP:CG	1:D:34:ARG:N	2.83	0.47
1:B:241:ASN:O	1:B:245:TYR:HB3	2.15	0.47
1:D:113:PHE:HE2	1:E:113:PHE:CD2	2.33	0.47
1:D:146:MET:HE2	1:D:178:GLY:HA2	1.95	0.47
1:D:207:LYS:HB3	1:D:214:TYR:CD1	2.49	0.47
1:A:181:LEU:O	1:A:182:ALA:C	2.52	0.47
1:E:148:PHE:HB3	1:E:149:PRO:HA	1.96	0.47
1:D:42:TRP:CZ3	1:E:61:TRP:HZ2	2.33	0.47
1:D:274:LEU:O	1:D:277:ALA:HB3	2.14	0.47
1:B:247:LYS:HE3	1:B:247:LYS:HA	1.97	0.46
1:A:239:VAL:HG23	1:A:240:LEU:HD13	1.96	0.46
1:D:46:ILE:HD13	1:D:175:ILE:HD13	1.97	0.46
1:E:32:ASP:OD1	1:E:35:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASN:O	1:A:205:GLN:HG3	2.15	0.46
1:B:140:ASP:C	1:B:142:LEU:N	2.67	0.46
1:D:192:GLY:HA2	1:D:252:ILE:CD1	2.44	0.46
1:B:32:ASP:O	1:B:36:ILE:HG22	2.15	0.46
1:D:201:ASN:HD21	2:D:1280:DUD:H4'	1.80	0.46
1:A:63:LYS:CG	1:B:209:TYR:CE1	2.98	0.46
1:A:108:LEU:HD11	1:B:111:MET:CE	2.46	0.46
1:D:83:HIS:CB	2:D:1280:DUD:H2'2	2.45	0.46
1:A:46:ILE:HD11	1:A:85:SER:HA	1.98	0.46
1:E:108:LEU:O	1:E:111:MET:HB3	2.15	0.46
1:B:157:VAL:O	1:B:161:ARG:HB2	2.15	0.45
1:E:195:VAL:O	1:E:199:THR:CG2	2.59	0.45
1:E:113:PHE:CE2	1:E:165:GLN:CG	2.95	0.45
1:E:160:PHE:O	1:E:164:ILE:HG13	2.16	0.45
1:B:114:PHE:CG	1:B:145:LEU:HD22	2.52	0.45
1:D:58:PRO:HD3	1:D:69:THR:HB	1.98	0.45
1:D:149:PRO:C	1:D:151:THR:H	2.19	0.45
1:D:179:LEU:O	1:D:182:ALA:HB3	2.17	0.45
1:A:71:MET:CE	1:A:186:LEU:HD21	2.47	0.45
1:D:48:MET:HE1	1:E:54:ILE:HB	1.99	0.45
1:B:38:HIS:CD2	1:B:40:ASP:H	2.34	0.45
1:A:231:VAL:O	1:A:234:VAL:O	2.34	0.45
1:B:230:CYS:SG	1:B:255:SER:HB3	2.56	0.44
1:D:62:TRP:CE3	2:E:1281:DUD:H5	2.52	0.44
1:D:161:ARG:HG3	1:D:161:ARG:NH1	2.24	0.44
1:A:108:LEU:HG	1:A:113:PHE:HD2	1.82	0.44
1:D:153:VAL:O	1:D:154:ALA:C	2.55	0.44
1:E:181:LEU:HD12	1:E:181:LEU:HA	1.80	0.44
1:E:204:ARG:NE	1:E:223:ASP:OD2	2.42	0.44
1:A:47:THR:HG23	1:A:164:ILE:HG23	1.99	0.44
1:A:113:PHE:CE1	1:A:165:GLN:CG	2.99	0.44
1:D:244:THR:O	1:D:245:TYR:C	2.56	0.44
1:A:190:LEU:HD23	1:A:190:LEU:O	2.18	0.44
1:B:76:ILE:HD13	1:B:224:ASN:HB3	1.98	0.44
1:E:65:VAL:HG13	1:E:66:LYS:HG2	1.98	0.44
1:B:20:HIS:CD2	1:B:273:TRP:CE3	3.05	0.44
1:D:165:GLN:HA	1:D:165:GLN:OE1	2.16	0.44
1:E:20:HIS:HD2	1:E:20:HIS:O	2.01	0.44
1:B:23:ASP:OD1	1:B:34:ARG:NH2	2.51	0.43
1:E:250:GLU:OE1	1:E:275:LYS:HE2	2.17	0.43
1:D:149:PRO:HB2	1:D:151:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:LEU:O	1:D:230:CYS:HB2	2.18	0.43
1:B:165:GLN:OE1	1:B:165:GLN:HA	2.18	0.43
1:E:37:ARG:O	1:E:38:HIS:ND1	2.50	0.43
1:E:175:ILE:O	1:E:179:LEU:HG	2.17	0.43
1:E:201:ASN:HD21	2:E:1281:DUD:H4'	1.83	0.43
1:E:14:VAL:O	1:E:15:LEU:C	2.57	0.43
1:D:271:TYR:HA	1:D:274:LEU:HD12	1.99	0.43
1:E:199:THR:O	1:E:203:ILE:HG13	2.18	0.43
1:D:111:MET:O	1:D:111:MET:HG3	2.18	0.43
1:D:262:MET:HB2	1:D:267:ARG:HH22	1.82	0.43
1:B:27:ILE:HG23	1:B:31:PRO:HA	2.00	0.43
1:A:168:SER:CB	1:B:165:GLN:HE22	2.32	0.43
1:E:262:MET:HA	1:E:263:PRO:HD3	1.89	0.42
1:B:102:ASP:O	1:B:106:LYS:HG2	2.18	0.42
1:A:263:PRO:O	1:A:264:GLU:C	2.58	0.42
1:A:265:GLU:OE1	1:A:265:GLU:CA	2.64	0.42
1:B:33:TRP:O	1:B:37:ARG:HB2	2.19	0.42
1:E:218:ARG:O	1:E:219:GLU:CB	2.61	0.42
1:B:186:LEU:O	1:B:187:ASP:C	2.58	0.42
1:B:257:PHE:CD1	1:B:267:ARG:HG2	2.55	0.42
1:D:167:ALA:HB2	1:D:175:ILE:HD11	2.01	0.42
1:E:10:VAL:HG23	1:E:180:LEU:CD1	2.50	0.42
1:B:161:ARG:HH11	1:B:161:ARG:CG	2.26	0.42
1:A:12:ALA:O	1:A:13:ARG:C	2.59	0.41
1:D:258:ASP:O	1:D:260:PHE:N	2.53	0.41
1:E:11:PRO:HB2	1:E:14:VAL:HG23	2.02	0.41
1:B:234:VAL:HG12	1:B:251:LYS:HZ1	1.85	0.41
1:D:32:ASP:HB3	1:D:36:ILE:CG2	2.49	0.41
1:A:148:PHE:HB3	1:A:149:PRO:HA	2.03	0.41
1:B:142:LEU:HD23	1:B:174:LEU:HB3	2.02	0.41
1:D:49:GLU:OE1	1:D:77:GLU:OE1	2.38	0.41
1:A:102:ASP:C	1:A:104:ALA:H	2.23	0.41
1:E:20:HIS:HD2	1:E:273:TRP:CZ3	2.31	0.41
1:E:28:PHE:CZ	1:E:206:LEU:HD11	2.46	0.41
1:A:108:LEU:HG	1:A:113:PHE:CD2	2.55	0.41
1:B:244:THR:O	1:B:245:TYR:C	2.59	0.41
1:D:25:LEU:HD12	1:D:198:TYR:HD1	1.85	0.41
1:E:173:ASP:OD1	1:E:173:ASP:N	2.52	0.41
1:A:113:PHE:CE2	1:B:113:PHE:HE2	2.39	0.41
1:A:199:THR:HG21	1:A:253:ALA:HA	2.03	0.41
1:B:150:LEU:HD12	1:B:150:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:LYS:H	1:D:106:LYS:HD3	1.85	0.41
1:D:150:LEU:CB	1:D:186:LEU:CD1	2.96	0.41
1:E:14:VAL:O	1:E:17:SER:N	2.54	0.41
1:E:81:ILE:HG22	1:E:179:LEU:HD11	2.03	0.41
1:B:108:LEU:HG	1:B:113:PHE:CD1	2.56	0.40
1:D:86:LEU:O	1:D:90:ILE:HD12	2.20	0.40
1:A:150:LEU:CD2	1:A:182:ALA:HA	2.51	0.40
1:B:150:LEU:CD2	1:B:182:ALA:HB1	2.52	0.40
1:B:195:VAL:O	1:B:199:THR:CG2	2.62	0.40
1:B:177:LYS:HE2	1:B:177:LYS:HB2	1.97	0.40
1:B:110:GLU:O	1:B:111:MET:C	2.59	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	222/283 (78%)	200 (90%)	18 (8%)	4 (2%)	8 25
1	B	234/283 (83%)	211 (90%)	20 (8%)	3 (1%)	12 33
1	D	232/283 (82%)	197 (85%)	29 (12%)	6 (3%)	5 17
1	E	236/283 (83%)	209 (89%)	19 (8%)	8 (3%)	3 12
All	All	924/1132 (82%)	817 (88%)	86 (9%)	21 (2%)	6 20

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	92	LYS
1	B	223	ASP
1	E	65	VAL
1	E	92	LYS

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Mol	Chain	Res	Type
1	E	153	VAL
1	E	241	ASN
1	A	279	LEU
1	D	32	ASP
1	E	15	LEU
1	E	279	LEU
1	D	219	GLU
1	D	242	GLU
1	D	245	TYR
1	E	223	ASP
1	B	141	GLU
1	D	169	ILE
1	D	259	ALA
1	A	92	LYS
1	A	103	VAL
1	A	144	GLU
1	E	14	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	200/238 (84%)	167 (84%)	33 (16%)	2	5
1	B	208/238 (87%)	167 (80%)	41 (20%)	1	3
1	D	206/238 (87%)	164 (80%)	42 (20%)	1	3
1	E	210/238 (88%)	166 (79%)	44 (21%)	1	2
All	All	824/952 (87%)	664 (81%)	160 (19%)	1	3

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	27	ILE
1	A	32	ASP
1	A	35	GLN

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Mol	Chain	Res	Type
1	A	37	ARG
1	A	38	HIS
1	A	40	ASP
1	A	55	ASP
1	A	56	SER
1	A	63	LYS
1	A	68	GLN
1	A	92	LYS
1	A	101	ASP
1	A	113	PHE
1	A	116	ARG
1	A	142	LEU
1	A	143	LEU
1	A	150	LEU
1	A	161	ARG
1	A	166	LEU
1	A	168	SER
1	A	187	ASP
1	A	190	LEU
1	A	204	ARG
1	A	206	LEU
1	A	224	ASN
1	A	237	GLU
1	A	240	LEU
1	A	244	THR
1	A	262	MET
1	A	265	GLU
1	A	268	ARG
1	A	279	LEU
1	B	15	LEU
1	B	18	LEU
1	B	25	LEU
1	B	34	ARG
1	B	36	ILE
1	B	37	ARG
1	B	56	SER
1	B	87	SER
1	B	92	LYS
1	B	93	ARG
1	B	106	LYS
1	B	107	SER
1	B	108	LEU

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Mol	Chain	Res	Type
1	B	109	LYS
1	B	140	ASP
1	B	143	LEU
1	B	144	GLU
1	B	150	LEU
1	B	151	THR
1	B	153	VAL
1	B	161	ARG
1	B	165	GLN
1	B	166	LEU
1	B	171	ARG
1	B	185	ASP
1	B	190	LEU
1	B	199	THR
1	B	202	GLN
1	B	211	GLU
1	B	221	VAL
1	B	223	ASP
1	B	236	VAL
1	B	237	GLU
1	B	240	LEU
1	B	246	LEU
1	B	247	LYS
1	B	250	GLU
1	B	255	SER
1	B	264	GLU
1	B	275	LYS
1	B	276	SER
1	D	15	LEU
1	D	18	LEU
1	D	21	LEU
1	D	23	ASP
1	D	25	LEU
1	D	32	ASP
1	D	35	GLN
1	D	37	ARG
1	D	40	ASP
1	D	47	THR
1	D	55	ASP
1	D	64	ASN
1	D	76	ILE
1	D	93	ARG

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Mol	Chain	Res	Type
1	D	105	LEU
1	D	106	LYS
1	D	108	LEU
1	D	143	LEU
1	D	150	LEU
1	D	151	THR
1	D	155	SER
1	D	161	ARG
1	D	166	LEU
1	D	168	SER
1	D	186	LEU
1	D	199	THR
1	D	203	ILE
1	D	206	LEU
1	D	207	LYS
1	D	211	GLU
1	D	215	VAL
1	D	217	VAL
1	D	233	SER
1	D	237	GLU
1	D	240	LEU
1	D	241	ASN
1	D	245	TYR
1	D	247	LYS
1	D	251	LYS
1	D	257	PHE
1	D	262	MET
1	D	265	GLU
1	E	10	VAL
1	E	13	ARG
1	E	15	LEU
1	E	18	LEU
1	E	25	LEU
1	E	32	ASP
1	E	34	ARG
1	E	36	ILE
1	E	37	ARG
1	E	39	VAL
1	E	49	GLU
1	E	63	LYS
1	E	65	VAL
1	E	66	LYS

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Mol	Chain	Res	Type
1	E	69	THR
1	E	72	HIS
1	E	76	ILE
1	E	87	SER
1	E	108	LEU
1	E	109	LYS
1	E	111	MET
1	E	150	LEU
1	E	151	THR
1	E	166	LEU
1	E	181	LEU
1	E	190	LEU
1	E	191	VAL
1	E	199	THR
1	E	202	GLN
1	E	211	GLU
1	E	221	VAL
1	E	223	ASP
1	E	232	GLN
1	E	240	LEU
1	E	241	ASN
1	E	242	GLU
1	E	245	TYR
1	E	246	LEU
1	E	247	LYS
1	E	251	LYS
1	E	265	GLU
1	E	268	ARG
1	E	276	SER
1	E	279	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	73	ASN
1	A	165	GLN
1	A	205	GLN
1	A	241	ASN
1	B	20	HIS
1	B	38	HIS
1	B	165	GLN

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Mol	Chain	Res	Type
1	B	201	ASN
1	D	20	HIS
1	D	26	ASN
1	D	38	HIS
1	D	64	ASN
1	D	201	ASN
1	D	202	GLN
1	E	20	HIS
1	E	165	GLN
1	E	201	ASN
1	E	232	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DUD	E	1281	-	23,25,25	1.55	6 (26%)	35,38,38	2.02	10 (28%)
2	DUD	D	1280	-	23,25,25	0.99	1 (4%)	35,38,38	1.73	7 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	DUD	B	1280	-	23,25,25	1.60	6 (26%)	35,38,38	2.05	8 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DUD	E	1281	-	-	1/16/28/28	0/2/2/2
2	DUD	D	1280	-	-	1/16/28/28	0/2/2/2
2	DUD	B	1280	-	-	1/16/28/28	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1281	DUD	C4-N3	-3.32	1.32	1.38
2	B	1280	DUD	C4-N3	-3.20	1.32	1.38
2	D	1280	DUD	C6-C5	2.96	1.41	1.35
2	E	1281	DUD	PA-O5'	-2.80	1.48	1.59
2	B	1280	DUD	C2-N3	-2.76	1.33	1.38
2	B	1280	DUD	PA-O5'	-2.63	1.48	1.59
2	B	1280	DUD	O4'-C4'	-2.60	1.39	1.45
2	E	1281	DUD	C2-N3	-2.58	1.33	1.38
2	E	1281	DUD	C5-C4	-2.26	1.38	1.43
2	B	1280	DUD	C6-C5	2.25	1.40	1.35
2	E	1281	DUD	C2-N1	-2.22	1.34	1.38
2	E	1281	DUD	C6-C5	2.19	1.40	1.35
2	B	1280	DUD	C6-N1	-2.17	1.32	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1280	DUD	N3-C2-N1	6.66	123.73	114.89
2	E	1281	DUD	N3-C2-N1	6.08	122.97	114.89
2	E	1281	DUD	C4-N3-C2	-5.24	119.67	126.58
2	D	1280	DUD	N3-C2-N1	4.71	121.14	114.89
2	B	1280	DUD	C4-N3-C2	-4.68	120.40	126.58
2	D	1280	DUD	C4-N3-C2	-4.18	121.06	126.58
2	B	1280	DUD	O2B-PB-O3A	3.73	117.13	104.64
2	B	1280	DUD	O4'-C1'-N1	3.72	114.52	107.86
2	D	1280	DUD	O2B-PB-O3A	3.59	116.68	104.64
2	E	1281	DUD	C5-C4-N3	3.28	119.75	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1280	DUD	O2-C2-N3	-3.27	115.41	121.50
2	E	1281	DUD	O2B-PB-O3A	3.26	115.57	104.64
2	D	1280	DUD	O4'-C1'-N1	3.24	113.66	107.86
2	E	1281	DUD	O4'-C1'-C2'	-3.23	100.15	106.25
2	D	1280	DUD	C5-C4-N3	2.96	119.27	114.84
2	D	1280	DUD	O4-C4-C5	-2.86	120.13	125.16
2	E	1281	DUD	C4'-O4'-C1'	2.61	115.77	109.45
2	B	1280	DUD	C4'-O4'-C1'	2.59	115.71	109.45
2	E	1281	DUD	O4'-C1'-N1	2.58	112.47	107.86
2	B	1280	DUD	O4'-C1'-C2'	-2.55	101.43	106.25
2	E	1281	DUD	O2-C2-N3	-2.44	116.96	121.50
2	E	1281	DUD	O4-C4-C5	-2.43	120.88	125.16
2	D	1280	DUD	O2-C2-N1	-2.19	119.88	122.79
2	E	1281	DUD	O2-C2-N1	-2.05	120.07	122.79
2	B	1280	DUD	C5-C4-N3	2.01	117.85	114.84

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1280	DUD	PB-O3A-PA-O1A
2	D	1280	DUD	PB-O3A-PA-O1A
2	E	1281	DUD	PB-O3A-PA-O1A

There are no ring outliers.

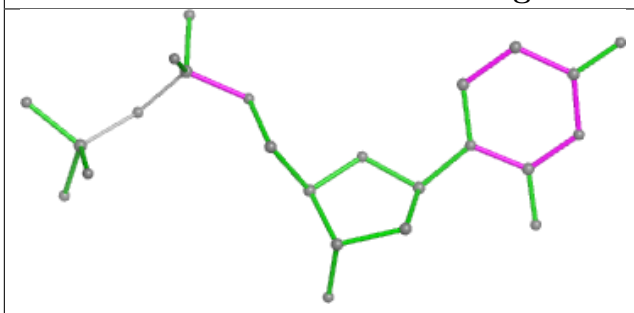
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1281	DUD	2	0
2	D	1280	DUD	3	0

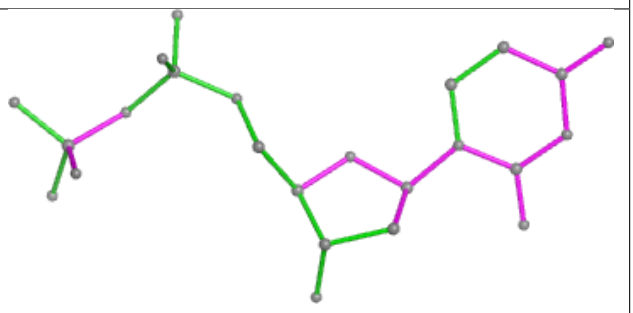
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

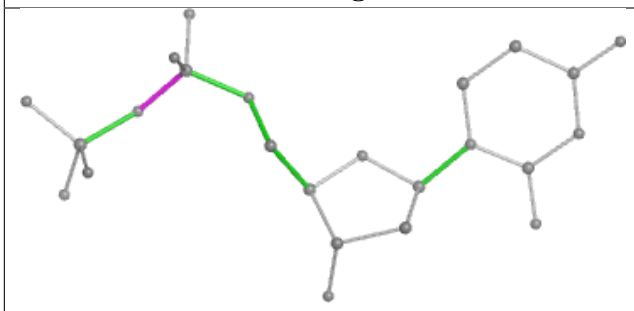
Ligand DUD E 1281



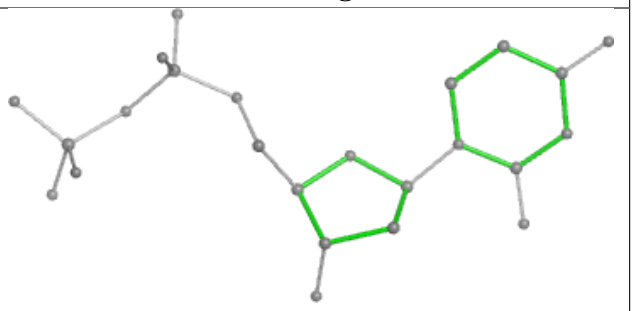
Bond lengths



Bond angles

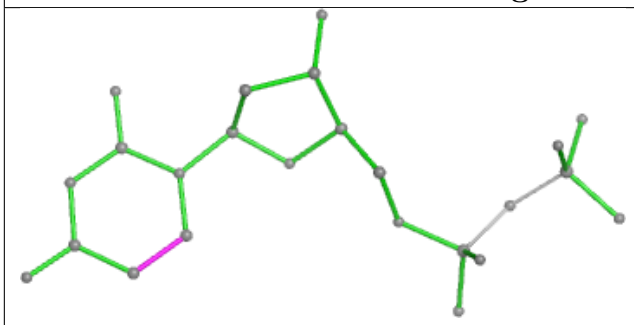


Torsions

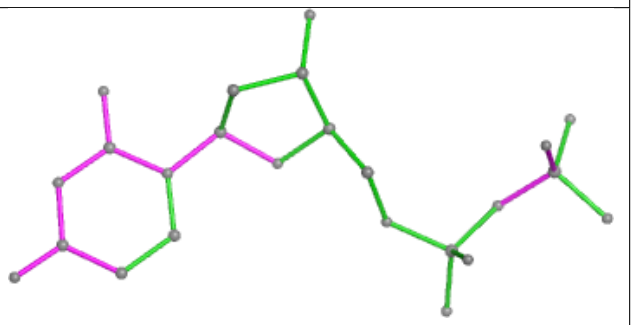


Rings

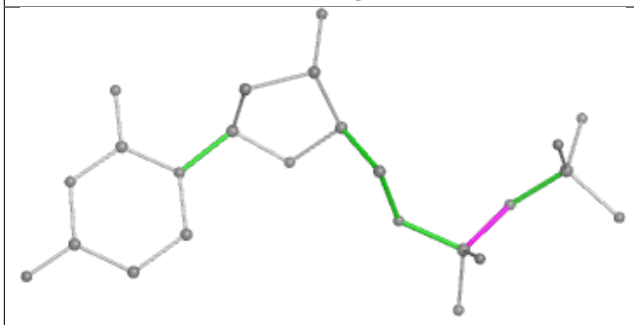
Ligand DUD D 1280



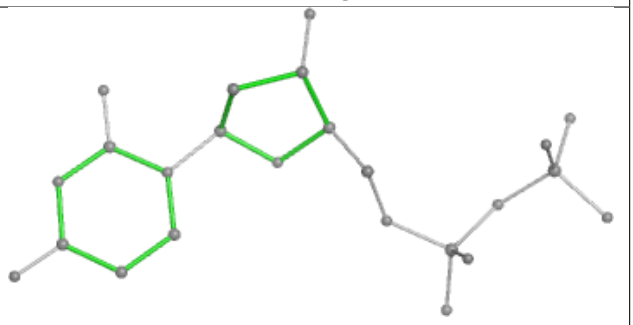
Bond lengths



Bond angles

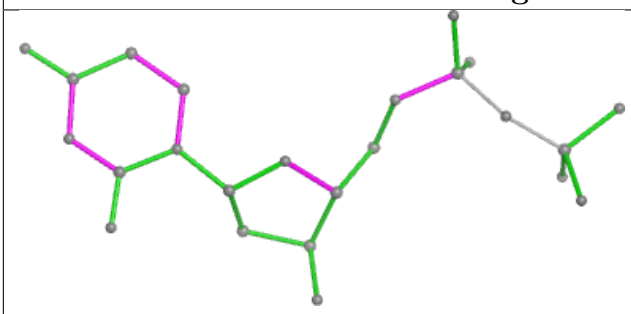


Torsions

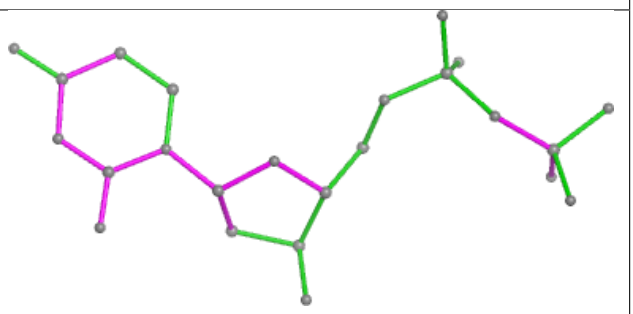


Rings

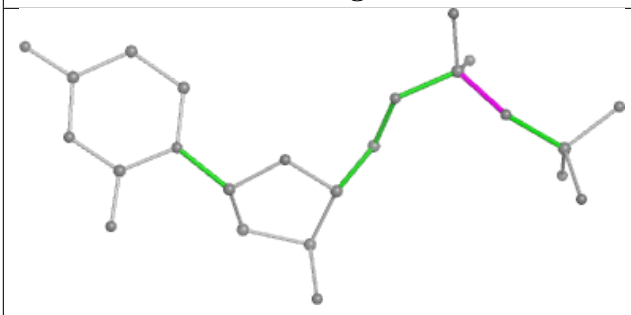
Ligand DUD B 1280



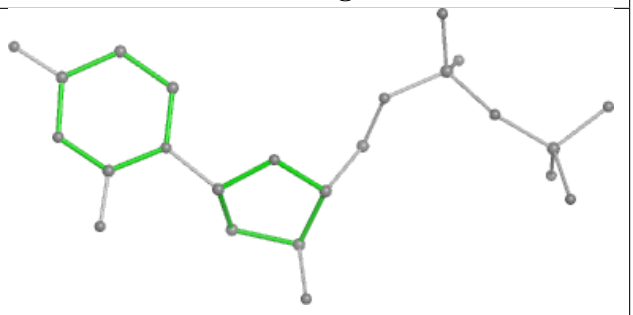
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	230/283 (81%)	-0.35	2 (0%)	84	84	22, 34, 50, 78	0
1	B	240/283 (84%)	-0.45	1 (0%)	92	92	24, 34, 45, 61	0
1	D	238/283 (84%)	0.18	16 (6%)	17	13	23, 36, 47, 84	0
1	E	242/283 (85%)	-0.28	6 (2%)	57	54	27, 34, 45, 64	0
All	All	950/1132 (83%)	-0.22	25 (2%)	56	52	22, 35, 48, 84	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	112	GLY	6.2
1	A	101	ASP	4.7
1	A	139	ASP	4.1
1	E	102	ASP	3.7
1	D	113	PHE	3.7
1	D	265	GLU	3.3
1	E	103	VAL	3.2
1	E	276	SER	3.0
1	E	66	LYS	3.0
1	D	279	LEU	2.8
1	D	241	ASN	2.8
1	D	143	LEU	2.7
1	D	35	GLN	2.6
1	D	141	GLU	2.6
1	E	111	MET	2.5
1	D	20	HIS	2.5
1	E	93	ARG	2.5
1	D	195	VAL	2.5
1	D	116	ARG	2.4
1	D	258	ASP	2.4
1	B	111	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	278	ALA	2.3
1	D	262	MET	2.1
1	D	269	HIS	2.1
1	D	263	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

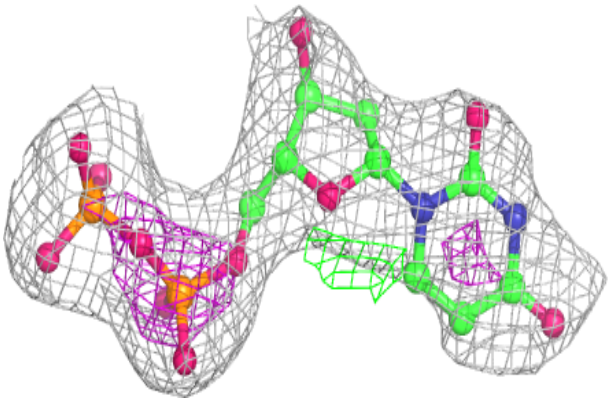
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

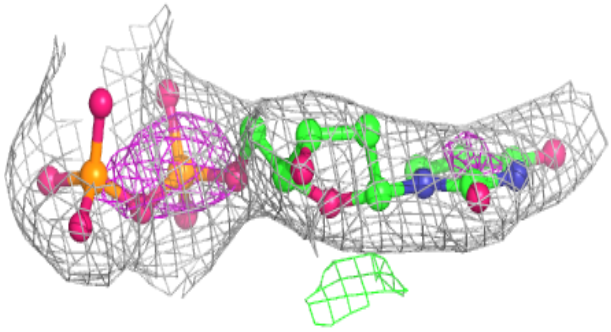
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DUD	D	1280	24/24	0.96	0.12	56,61,63,64	0
2	DUD	E	1281	24/24	0.96	0.14	55,61,63,63	0
2	DUD	B	1280	24/24	0.97	0.17	55,61,63,63	0

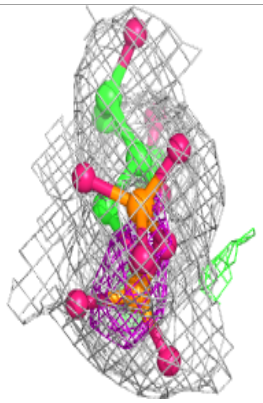
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DUD D 1280:

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

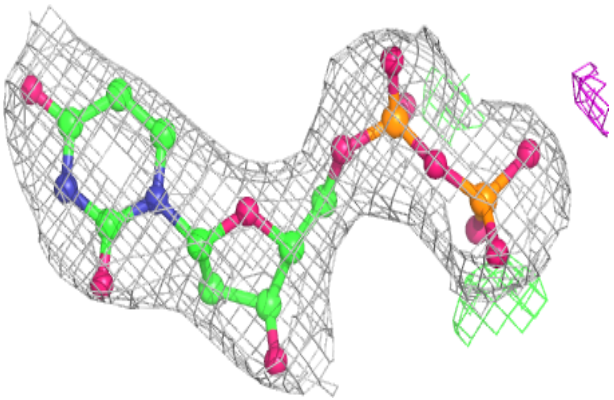


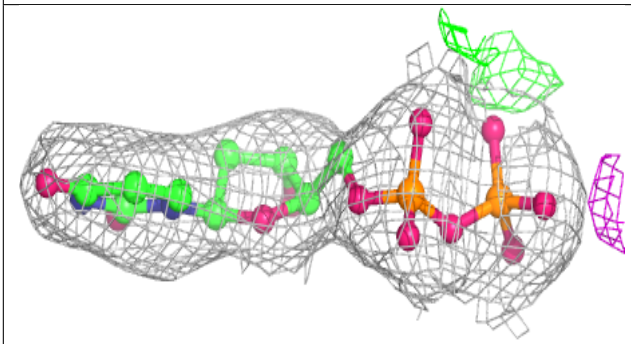


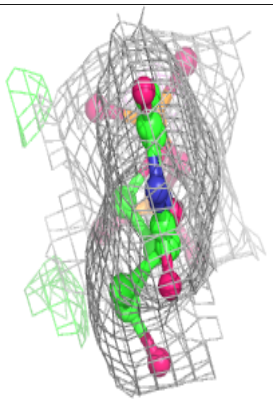


Electron density around DUD E 1281:

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

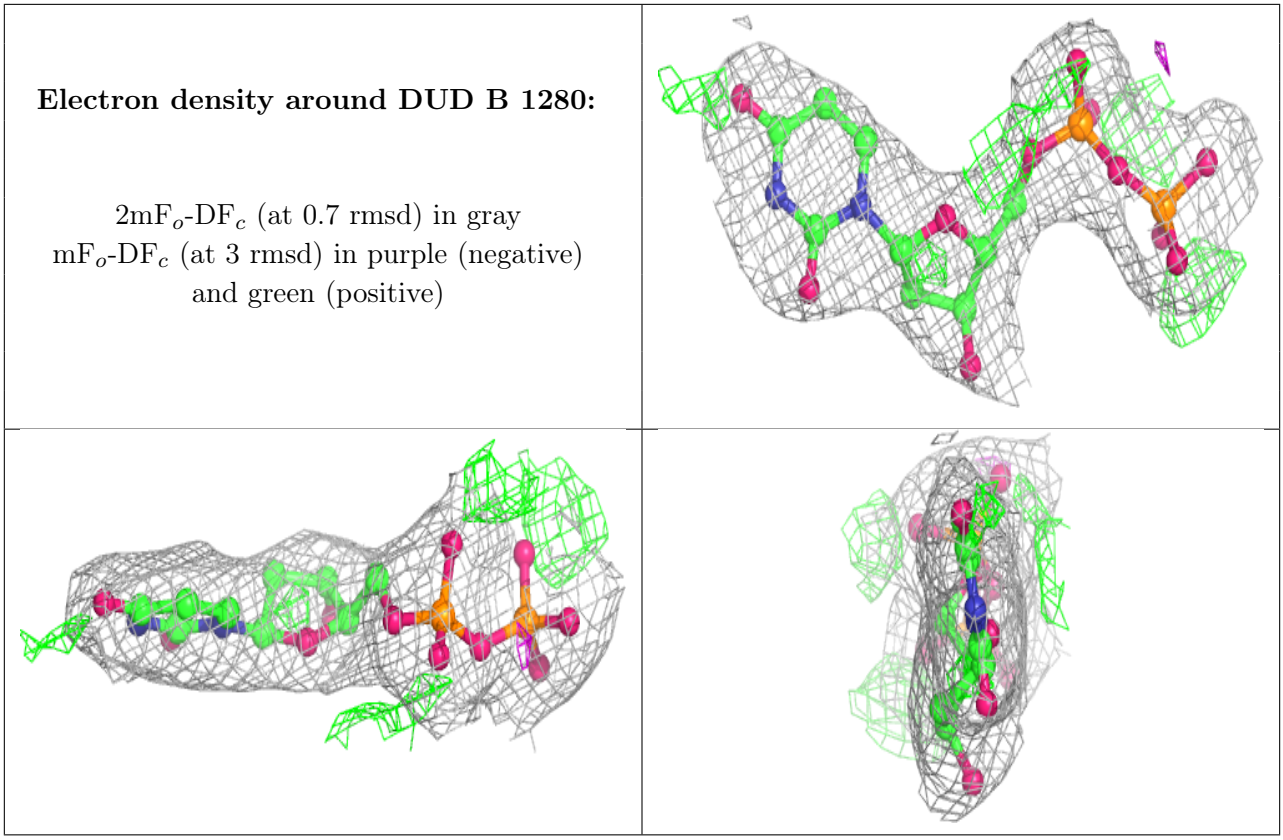






Electron density around DUD B 1280:

$2mF_o$-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.