



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:14 AM UTC

PDB ID : 1OGK / pdb_00001ogk
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	:	4-5-2 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

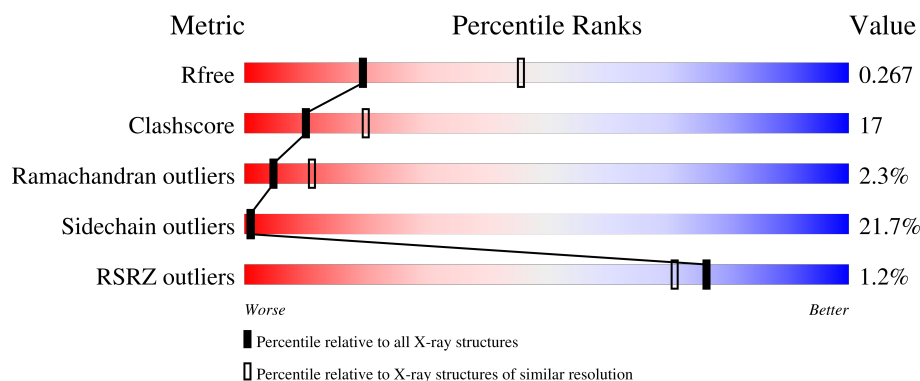
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	283	% 48% 25% 7% 19%
1	B	283	48% 26% 10% 15%
1	D	283	% 43% 32% 7% • 16%
1	E	283	% 45% 31% 7% • 14%

2 Entry composition [i](#)

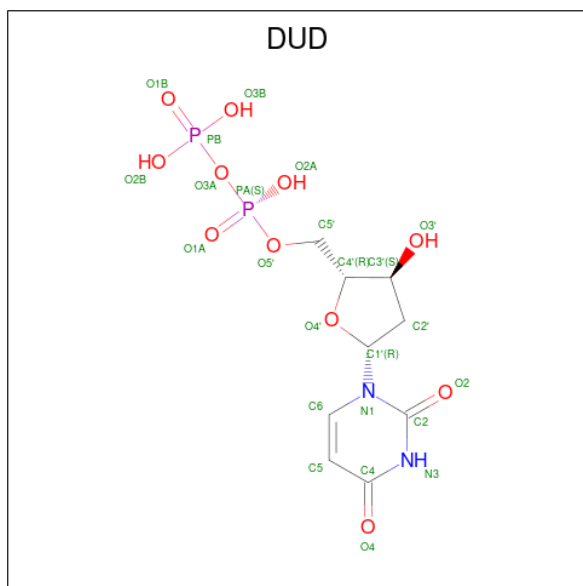
There are 2 unique types of molecules in this entry. The entry contains 7784 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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		

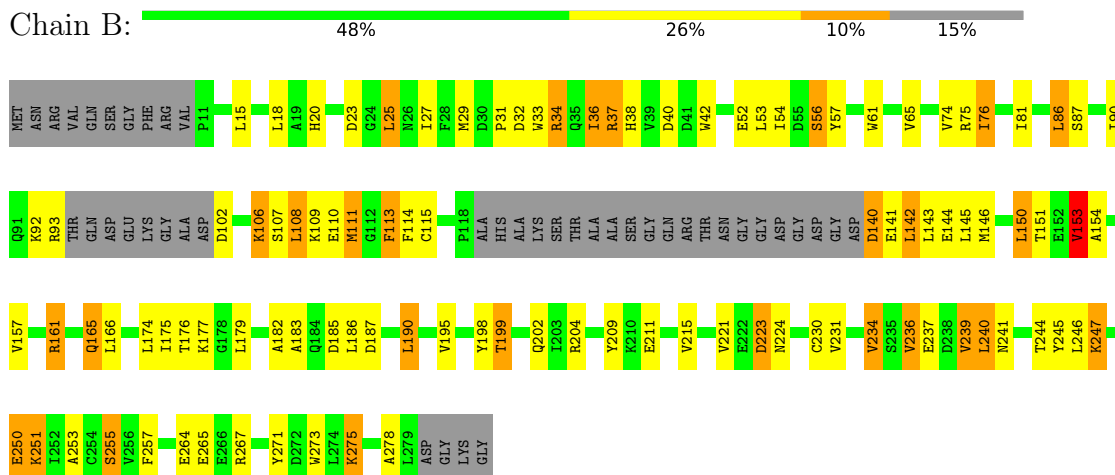
3 Residue-property plots

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.

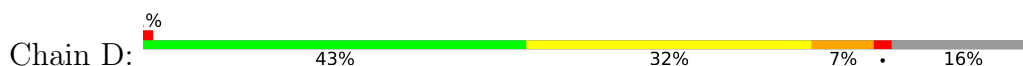
• Molecule 1: DEOXYURIDINE TRIPHOSPHATASE

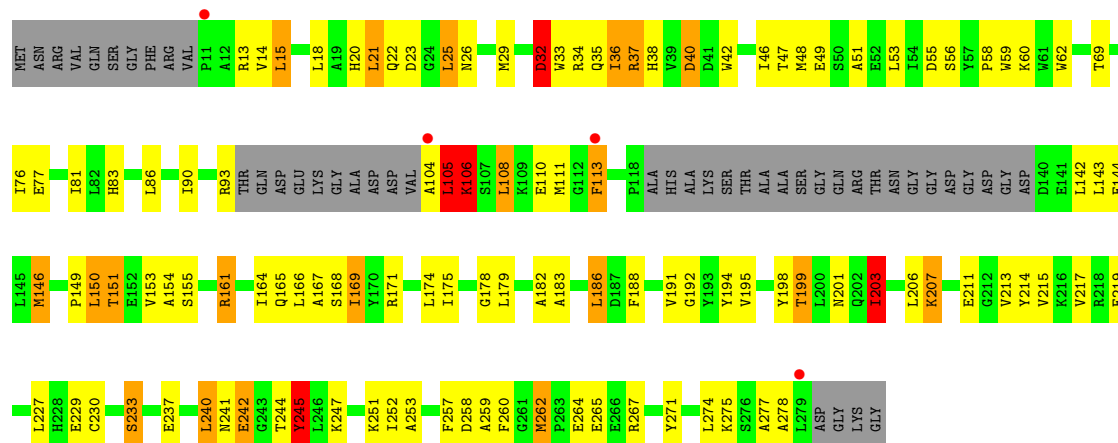


• Molecule 1: DEOXYURIDINE TRIPHOSPHATASE

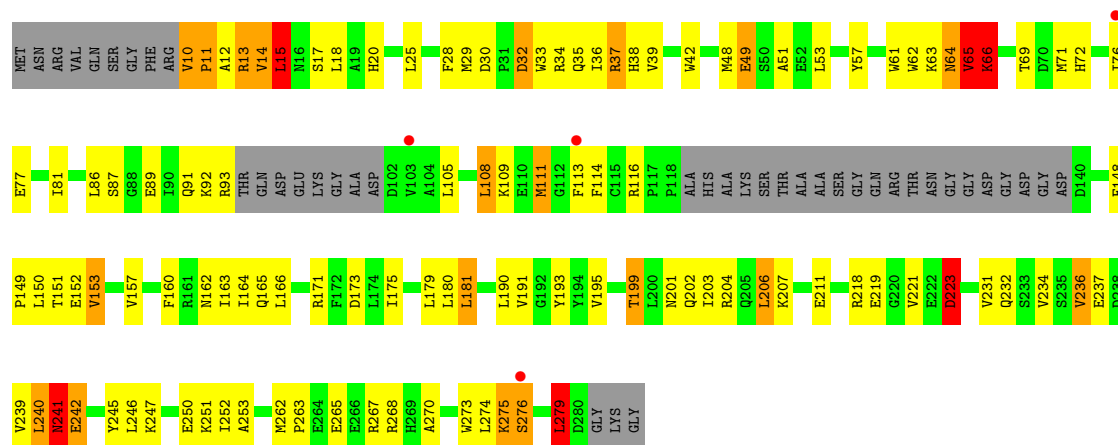


• Molecule 1: DEOXYURIDINE TRIPHOSPHATASE





• Molecule 1: DEOXYURIDINE TRIPHOSPHATASE



4 Data and refinement statistics

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 – 2.85 109.21 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.1 (111.80-2.85) 99.1 (109.21-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.83Å)	Xtriage
Refinement program	REFMAC 5.1.13	Depositor
R, R_{free}	0.205 , 0.273 0.210 , 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 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.020 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	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.*

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: 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	1.21	2/1906 (0.1%)	1.28	9/2584 (0.3%)
1	B	1.22	5/1993 (0.3%)	1.28	10/2698 (0.4%)
1	D	0.99	4/1978 (0.2%)	1.19	5/2677 (0.2%)
1	E	1.18	4/2008 (0.2%)	1.32	11/2720 (0.4%)
All	All	1.15	15/7885 (0.2%)	1.27	35/10679 (0.3%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	278	ALA	C-N	-7.50	1.22	1.33
1	E	276	SER	CA-C	-7.48	1.49	1.53
1	D	203	ILE	CA-CB	7.33	1.63	1.54
1	B	278	ALA	C-N	-6.95	1.23	1.33
1	E	279	LEU	C-N	-6.87	1.23	1.33
1	B	239	VAL	CA-CB	6.36	1.61	1.54
1	D	146	MET	SD-CE	-5.92	1.64	1.79
1	A	29	MET	SD-CE	5.74	1.94	1.79
1	E	275	LYS	N-CA	5.71	1.53	1.46
1	B	65	VAL	CA-CB	5.25	1.61	1.54
1	B	146	MET	CG-SD	-5.24	1.67	1.80
1	D	29	MET	SD-CE	-5.22	1.66	1.79
1	B	154	ALA	CA-CB	-5.11	1.45	1.53
1	A	191	VAL	CA-CB	5.08	1.61	1.54
1	E	223	ASP	CB-CG	-5.05	1.39	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	276	SER	CA-C-O	11.89	124.84	117.94
1	E	276	SER	N-CA-C	10.76	117.60	108.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	276	SER	CB-CA-C	-9.30	103.67	117.07
1	A	166	LEU	N-CA-C	-7.84	102.82	111.36
1	E	12	ALA	N-CA-C	-7.31	103.83	112.89
1	E	276	SER	O-C-N	7.05	126.76	121.47
1	A	153	VAL	N-CA-C	6.38	116.86	110.23
1	E	86	LEU	N-CA-C	-6.19	104.53	111.28
1	D	113	PHE	N-CA-C	-6.18	103.66	112.13
1	B	113	PHE	N-CA-C	-6.17	105.58	113.23
1	B	86	LEU	N-CA-C	-6.11	104.53	111.07
1	E	66	LYS	N-CA-C	-6.03	99.89	109.59
1	E	11	PRO	CB-CA-C	6.02	118.94	111.23
1	B	236	VAL	CB-CA-C	-5.99	104.20	112.04
1	B	278	ALA	O-C-N	-5.97	113.45	123.00
1	B	198	TYR	N-CA-C	-5.83	104.83	111.07
1	A	153	VAL	CB-CA-C	-5.81	104.26	111.70
1	E	234	VAL	CB-CA-C	-5.69	103.05	111.19
1	D	106	LYS	N-CA-C	5.65	118.98	111.75
1	D	105	LEU	CA-C-N	5.61	128.57	120.38
1	D	105	LEU	C-N-CA	5.61	128.57	120.38
1	B	153	VAL	CB-CA-C	-5.47	102.31	111.29
1	B	52	GLU	CA-CB-CG	5.36	124.83	114.10
1	A	163	ILE	CB-CA-C	-5.31	104.97	112.14
1	B	234	VAL	CB-CA-C	-5.30	103.92	111.19
1	D	213	VAL	N-CA-C	5.18	119.35	111.89
1	B	250	GLU	N-CA-C	-5.17	106.23	112.54
1	A	151	THR	N-CA-C	-5.14	106.85	113.23
1	A	152	GLU	CA-C-N	5.12	127.48	120.77
1	A	152	GLU	C-N-CA	5.12	127.48	120.77
1	A	41	ASP	N-CA-C	-5.12	104.67	112.04
1	B	115	CYS	N-CA-C	5.11	116.75	109.14
1	E	252	ILE	N-CA-C	-5.11	105.86	110.82
1	E	105	LEU	N-CA-C	5.08	116.51	110.97
1	A	80	ASP	N-CA-C	-5.08	105.74	111.28

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	1865	0	1826	59	0
1	B	1949	0	1922	66	0
1	D	1934	0	1909	76	0
1	E	1964	0	1941	82	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	265	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 17.

All (265) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:48:MET:HE1	1:E:51:ALA:O	1.93	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:A:48:MET:HE1	1:B:54:ILE:HB	1.75	0.66
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:113:PHE:CD1	1:A:113:PHE:C	2.74	0.64
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:A:142:LEU:C	1:A:142:LEU:HD13	2.23	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:A:108:LEU:HD11	1:B:111:MET:HE2	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:257:PHE:HB3	1:D:267:ARG:HE	1.68	0.58
1:E:66:LYS:HB3	1:E:66:LYS:HZ3	1.68	0.58
1:D:33:TRP:O	1:D:34:ARG:C	2.46	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: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:D:146:MET:HE1	1:D:178:GLY:O	2.07	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:A:63:LYS:O	1:A:64:ASN:C	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:GLU:O	1:E:153:VAL:C	2.50	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:D:105:LEU:C	1:D:105:LEU:HD12	2.35	0.52
1:A:71:MET:HE2	1:A:186:LEU:HD21	1.91	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
1:A:181:LEU:O	1:A:182:ALA:C	2.52	0.52
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:B:140:ASP:C	1:B:142:LEU:N	2.67	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:D:149:PRO:C	1:D:151:THR:H	2.19	0.50
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:153:VAL:O	1:D:154:ALA:C	2.55	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:D:111:MET:HE3	1:E:108:LEU:HD22	1.93	0.49
1:D:244:THR:O	1:D:245:TYR:C	2.56	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:14:VAL:O	1:E:15:LEU:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:ALA:O	1:E:48:MET:HE1	2.14	0.48
1:E:153:VAL:O	1:E:157:VAL:HG23	2.13	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:A:263:PRO:O	1:A:264:GLU:C	2.58	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:207:LYS:HB3	1:D:214:TYR:CD1	2.49	0.47
1:B:186:LEU:O	1:B:187:ASP:C	2.58	0.47
1:E:148:PHE:HB3	1:E:149:PRO:HA	1.96	0.47
1:B:57:TYR:OH	1:B:150:LEU:O	2.31	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
1:A:12:ALA:O	1:A:13:ARG:C	2.59	0.46
1:A:201:ASN:O	1:A:205:GLN:HG3	2.15	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: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:A:108:LEU:HD11	1:B:111:MET:CE	2.46	0.46
1:B:244:THR:O	1:B:245:TYR:C	2.59	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:25:LEU:HD22	1:B:29:MET:HE3	1.97	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:A:102:ASP:C	1:A:104:ALA:H	2.23	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:B:38:HIS:CD2	1:B:40:ASP:H	2.34	0.45
1:B:110:GLU:O	1:B:111:MET:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:194:TYR:CD2	1:D:194:TYR:C	2.95	0.44
1:E:57:TYR:CE2	1:E:71:MET:HE1	2.53	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:149:PRO:C	1:D:151:THR:N	2.75	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
1:D:227:LEU:O	1:D:230:CYS:HB2	2.18	0.43
1:A:267:ARG:O	1:A:268:ARG:C	2.60	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:B:175:ILE:O	1:B:176:THR:C	2.61	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:A:142:LEU:C	1:A:142:LEU:CD1	2.91	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:57:TYR:OH	1:A:150:LEU:O	2.26	0.42
1:E:162:ASN:O	1:E:163:ILE:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:ARG:O	1:E:219:GLU:CB	2.61	0.42
1:B:111:MET:HE3	1:B:111:MET:HB3	1.88	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:E:91:GLN:C	1:E:93:ARG:H	2.28	0.42
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:14:VAL:O	1:D:15:LEU:C	2.62	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: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: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
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:53:LEU:C	1:E:53:LEU:HD23	2.46	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:74:VAL:O	1:B:75:ARG:C	2.64	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:E:111:MET:HA	1:E:111:MET:HE3	2.03	0.40

There are no symmetry-related clashes.

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	222/283 (78%)	200 (90%)	18 (8%)	4 (2%)	6	15
1	B	234/283 (83%)	211 (90%)	20 (8%)	3 (1%)	9	21
1	D	232/283 (82%)	197 (85%)	29 (12%)	6 (3%)	4	9
1	E	236/283 (83%)	209 (89%)	19 (8%)	8 (3%)	3	6
All	All	924/1132 (82%)	817 (88%)	86 (9%)	21 (2%)	5	11

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
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 ⓘ

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%)	159 (80%)	41 (20%)	1	1
1	B	208/238 (87%)	164 (79%)	44 (21%)	1	1
1	D	206/238 (87%)	163 (79%)	43 (21%)	1	1
1	E	210/238 (88%)	159 (76%)	51 (24%)	1	0
All	All	824/952 (87%)	645 (78%)	179 (22%)	1	1

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	25	LEU
1	A	27	ILE
1	A	32	ASP
1	A	38	HIS
1	A	40	ASP
1	A	54	ILE
1	A	55	ASP
1	A	56	SER
1	A	63	LYS
1	A	68	GLN
1	A	76	ILE
1	A	92	LYS
1	A	101	ASP
1	A	111	MET
1	A	113	PHE
1	A	116	ARG
1	A	142	LEU
1	A	143	LEU
1	A	150	LEU
1	A	153	VAL
1	A	161	ARG
1	A	166	LEU
1	A	168	SER

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Mol	Chain	Res	Type
1	A	176	THR
1	A	181	LEU
1	A	187	ASP
1	A	190	LEU
1	A	191	VAL
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	246	LEU
1	A	251	LYS
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	76	ILE
1	B	87	SER
1	B	93	ARG
1	B	106	LYS
1	B	107	SER
1	B	108	LEU
1	B	109	LYS
1	B	111	MET
1	B	140	ASP
1	B	142	LEU
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

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Mol	Chain	Res	Type
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	231	VAL
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	251	LYS
1	B	255	SER
1	B	264	GLU
1	B	265	GLU
1	B	275	LYS
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	36	ILE
1	D	37	ARG
1	D	40	ASP
1	D	47	THR
1	D	55	ASP
1	D	76	ILE
1	D	93	ARG
1	D	105	LEU
1	D	106	LYS
1	D	108	LEU
1	D	110	GLU
1	D	143	LEU
1	D	150	LEU
1	D	151	THR
1	D	155	SER
1	D	161	ARG

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Mol	Chain	Res	Type
1	D	164	ILE
1	D	166	LEU
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	229	GLU
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	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	29	MET
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	64	ASN
1	E	65	VAL
1	E	66	LYS
1	E	69	THR
1	E	72	HIS
1	E	76	ILE
1	E	87	SER
1	E	108	LEU
1	E	109	LYS

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Mol	Chain	Res	Type
1	E	111	MET
1	E	116	ARG
1	E	150	LEU
1	E	151	THR
1	E	166	LEU
1	E	171	ARG
1	E	181	LEU
1	E	190	LEU
1	E	191	VAL
1	E	199	THR
1	E	202	GLN
1	E	206	LEU
1	E	211	GLU
1	E	221	VAL
1	E	223	ASP
1	E	232	GLN
1	E	236	VAL
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	267	ARG
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 (21) 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	A	269	HIS
1	B	20	HIS
1	B	38	HIS
1	B	72	HIS

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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
1	E	269	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	D	1280	-	24,25,25	1.13	2 (8%)	36,38,38	1.75	7 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DUD	E	1281	-	24,25,25	1.97	7 (29%)	36,38,38	2.07	10 (27%)
2	DUD	B	1280	-	24,25,25	1.85	7 (29%)	36,38,38	2.07	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	D	1280	-	-	1/16/28/28	0/2/2/2
2	DUD	E	1281	-	-	1/16/28/28	0/2/2/2
2	DUD	B	1280	-	-	2/16/28/28	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1281	DUD	PA-O3A	-5.92	1.53	1.59
2	B	1280	DUD	PA-O3A	-4.39	1.54	1.59
2	E	1281	DUD	C4-N3	-3.50	1.32	1.38
2	B	1280	DUD	C4-N3	-3.38	1.32	1.38
2	D	1280	DUD	C6-C5	2.95	1.41	1.35
2	E	1281	DUD	PA-O5'	-2.92	1.48	1.59
2	B	1280	DUD	C2-N3	-2.82	1.33	1.38
2	B	1280	DUD	PA-O5'	-2.75	1.48	1.59
2	E	1281	DUD	C2-N3	-2.64	1.33	1.38
2	B	1280	DUD	O4'-C4'	-2.61	1.39	1.45
2	D	1280	DUD	PA-O3A	-2.61	1.56	1.59
2	E	1281	DUD	C5-C4	-2.34	1.38	1.43
2	E	1281	DUD	C2-N1	-2.28	1.34	1.38
2	B	1280	DUD	C6-N1	-2.25	1.32	1.38
2	B	1280	DUD	C6-C5	2.23	1.40	1.35
2	E	1281	DUD	C6-C5	2.17	1.40	1.35

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1280	DUD	N3-C2-N1	6.79	123.73	114.89
2	E	1281	DUD	N3-C2-N1	6.20	122.97	114.89
2	E	1281	DUD	C4-N3-C2	-5.59	119.67	126.61
2	B	1280	DUD	C4-N3-C2	-5.00	120.40	126.61
2	D	1280	DUD	N3-C2-N1	4.80	121.14	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1280	DUD	C4-N3-C2	-4.47	121.06	126.61
2	B	1280	DUD	O4'-C1'-N1	3.75	114.52	107.86
2	B	1280	DUD	O2B-PB-O3A	3.73	117.13	104.64
2	D	1280	DUD	O2B-PB-O3A	3.59	116.68	104.64
2	E	1281	DUD	C5-C4-N3	3.53	119.75	114.80
2	B	1280	DUD	O2-C2-N3	-3.30	115.41	121.49
2	D	1280	DUD	O4'-C1'-N1	3.27	113.66	107.86
2	E	1281	DUD	O2B-PB-O3A	3.26	115.57	104.64
2	E	1281	DUD	O4'-C1'-C2'	-3.26	100.15	106.25
2	D	1280	DUD	C5-C4-N3	3.19	119.27	114.80
2	D	1280	DUD	O4-C4-C5	-2.92	120.13	125.16
2	E	1281	DUD	C4'-O4'-C1'	2.63	115.77	109.51
2	B	1280	DUD	C4'-O4'-C1'	2.61	115.71	109.51
2	E	1281	DUD	O4'-C1'-N1	2.59	112.47	107.86
2	B	1280	DUD	O4'-C1'-C2'	-2.58	101.43	106.25
2	E	1281	DUD	O4-C4-C5	-2.48	120.88	125.16
2	E	1281	DUD	O2-C2-N3	-2.46	116.96	121.49
2	D	1280	DUD	O2-C2-N1	-2.24	119.88	122.80
2	B	1280	DUD	C5-C4-N3	2.18	117.85	114.80
2	E	1281	DUD	O2-C2-N1	-2.10	120.07	122.80

There are no chirality outliers.

All (4) 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
2	B	1280	DUD	PB-O3A-PA-O2A

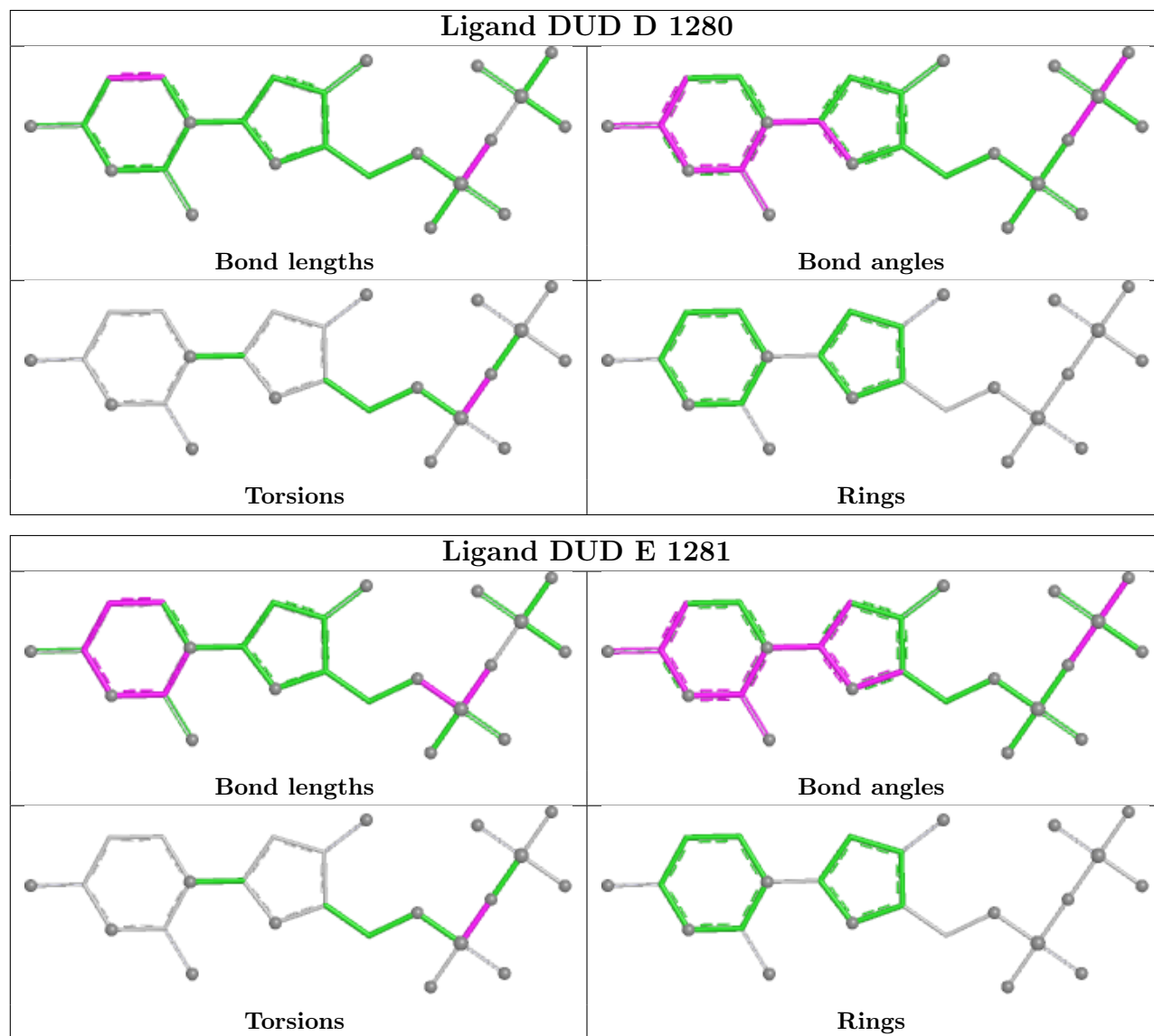
There are no ring outliers.

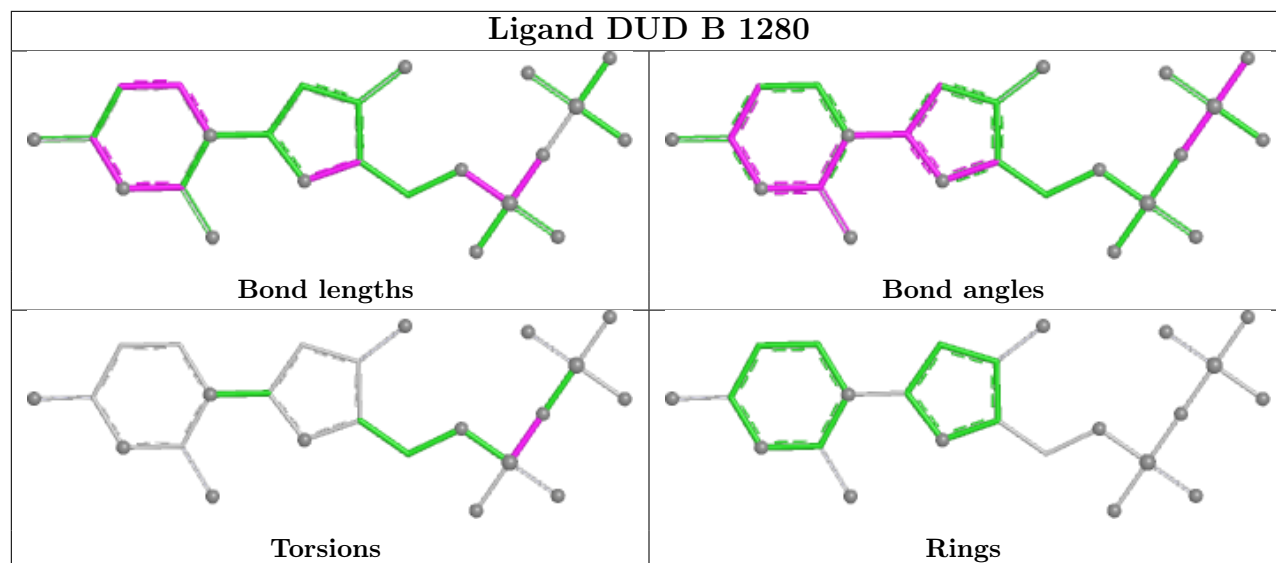
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1280	DUD	3	0
2	E	1281	DUD	2	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	230/283 (81%)	-0.30	3 (1%) 75 68	22, 34, 50, 78	0
1	B	240/283 (84%)	-0.23	0 100 100	24, 34, 45, 61	0
1	D	238/283 (84%)	0.08	4 (1%) 69 63	23, 36, 47, 84	0
1	E	242/283 (85%)	-0.19	4 (1%) 69 63	27, 34, 45, 64	0
All	All	950/1132 (83%)	-0.16	11 (1%) 76 71	22, 35, 48, 84	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	113	PHE	3.8
1	D	104	ALA	3.2
1	E	276	SER	3.1
1	D	11	PRO	2.4
1	D	279	LEU	2.4
1	A	139	ASP	2.2
1	E	103	VAL	2.2
1	A	101	ASP	2.2
1	E	113	PHE	2.1
1	E	76	ILE	2.1
1	A	235	SER	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

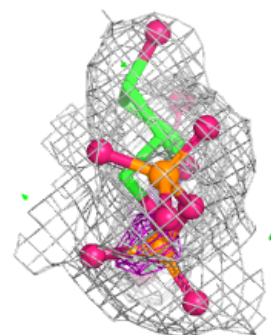
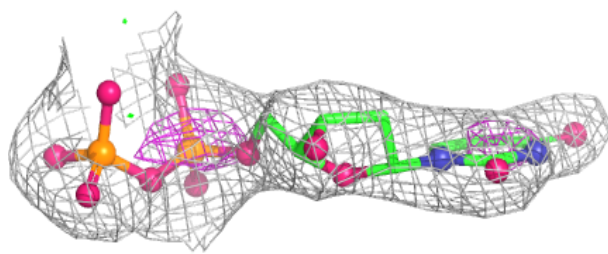
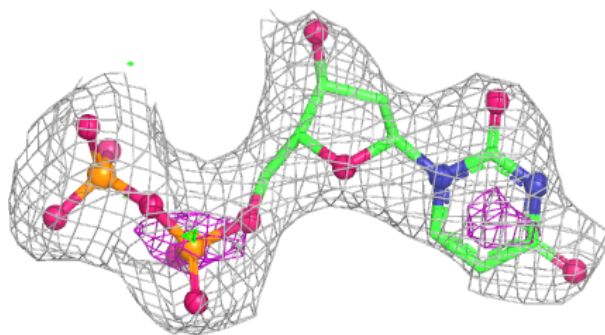
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DUD	D	1280	24/24	0.92	0.09	56,61,63,64	0
2	DUD	E	1281	24/24	0.95	0.09	55,61,63,63	0
2	DUD	B	1280	24/24	0.96	0.09	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.

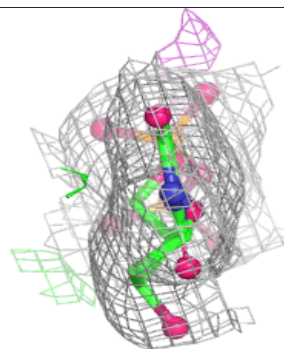
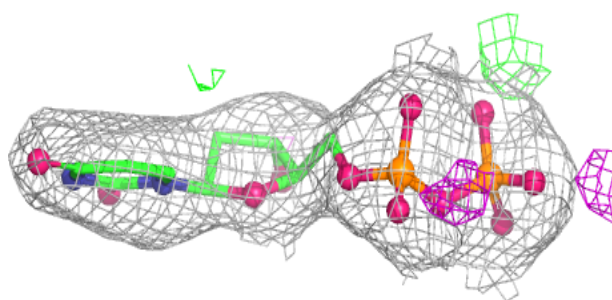
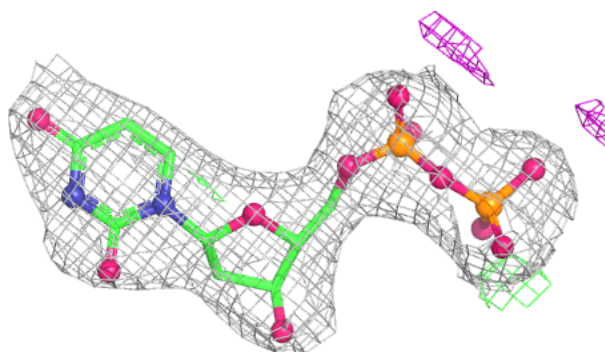
Electron density around DUD D 1280:

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

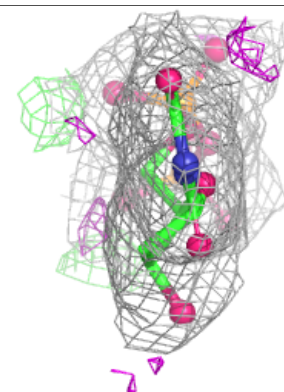
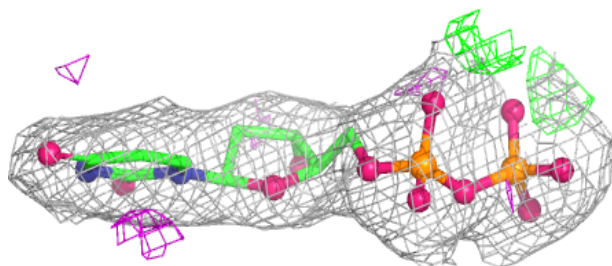
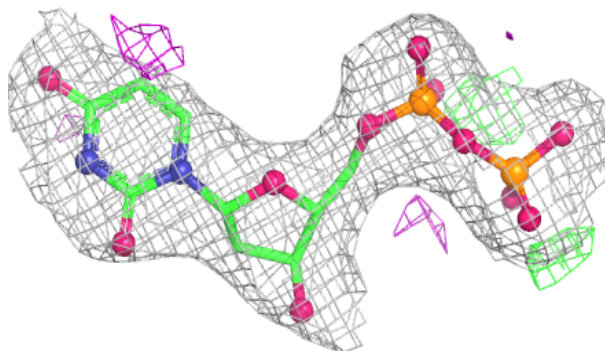


Electron density around DUD E 1281:

$2mF_o-DF_c$ (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.