



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:17 AM UTC

PDB ID : 7W5P / pdb_00007w5p
Title : Crystal Structure of the dioxygenase CcTet from Coprinopsis cinerea bound to 12bp N6-methyldeoxyadenine (6mA) containing duplex DNA
Authors : Mu, Y.J.; Zhang, L.; Zhang, L.
Deposited on : 2021-11-30
Resolution : 2.30 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
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

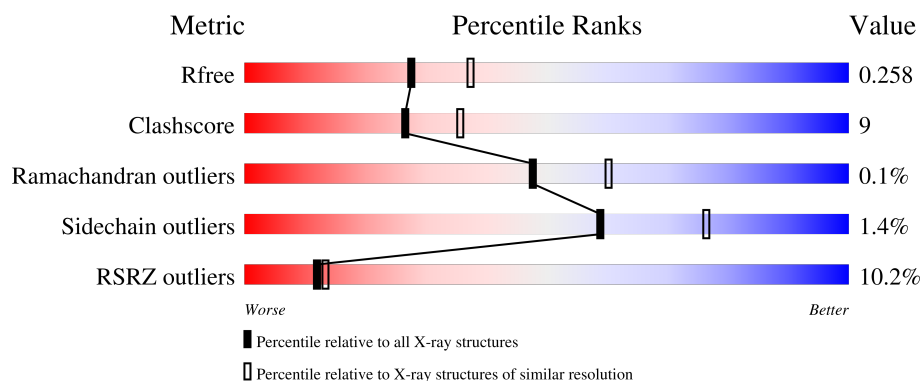
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	430	9% 71% 17% 11%
1	D	430	12% 66% 20% 12%
1	G	430	5% 70% 16% 12%
1	H	430	9% 67% 17% 13%
2	B	12	67% 25% 8%

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Mol	Chain	Length	Quality of chain
2	E	12	25% 50% 50%
3	C	12	33% 33% 67%
3	F	12	33% 75% 25%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13728 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 CcTet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2992	1912	532	534	14			
1	D	377	Total	C	N	O	S	0	0	0
			2953	1887	524	528	14			
1	G	378	Total	C	N	O	S	0	0	0
			2966	1895	526	531	14			
1	H	372	Total	C	N	O	S	0	0	0
			2917	1867	514	522	14			

- Molecule 2 is a DNA chain called DNA (12-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	P	0	0	0
			246	117	46	71	12			
2	E	12	Total	C	N	O	P	0	0	0
			246	117	46	71	12			

- Molecule 3 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			249	117	48	72	12			
3	F	12	Total	C	N	O	P	0	0	0
			249	117	48	72	12			

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

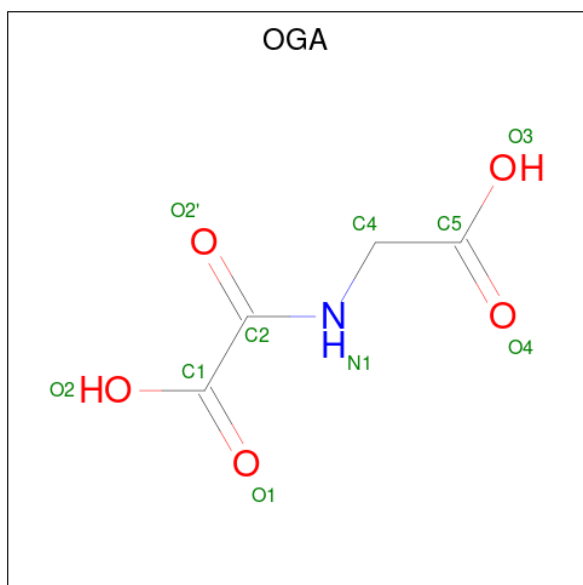
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	D	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mn	0	0
			1	1		
4	H	1	Total	Mn	0	0
			1	1		

- Molecule 5 is N-OXALYLGLYCINE (CCD ID: OGA) (formula: $C_4H_5NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	4	1	5		
5	D	1	Total	C	N	O	0	0
			10	4	1	5		
5	G	1	Total	C	N	O	0	0
			10	4	1	5		
5	H	1	Total	C	N	O	0	0
			10	4	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	186	Total	O	0	0
			186	186		
6	B	26	Total	O	0	0
			26	26		
6	C	21	Total	O	0	0
			21	21		

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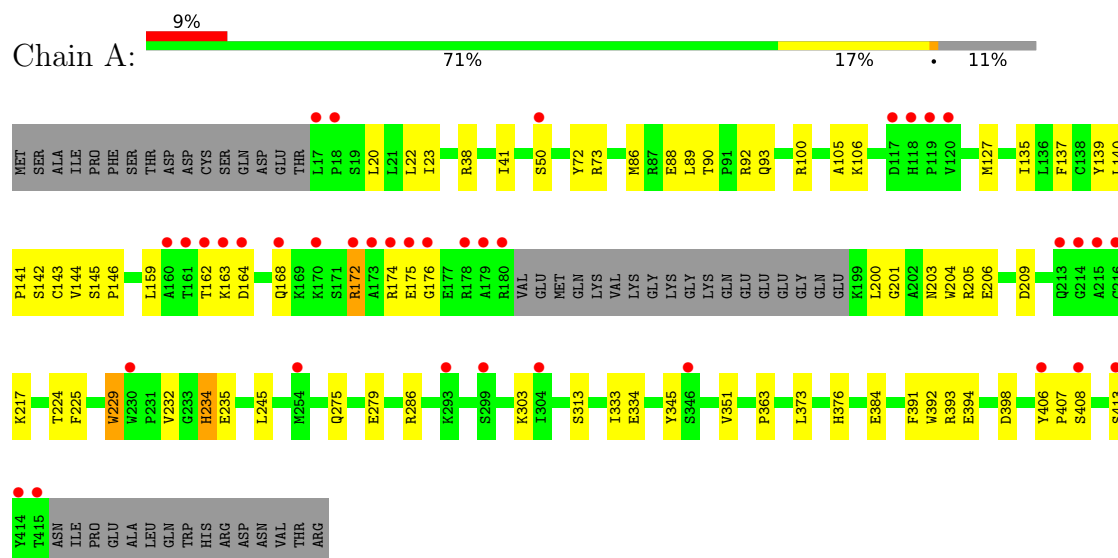
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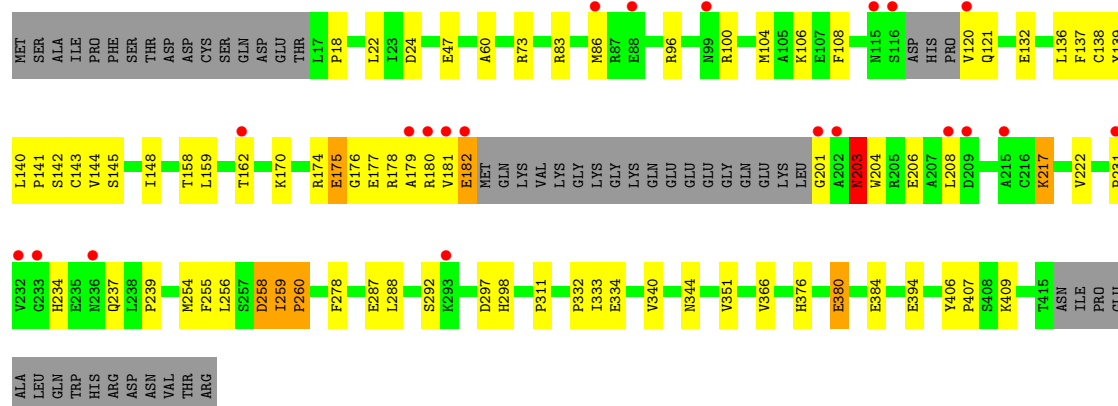
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	207	Total 207	O 207	0	0
6	E	27	Total 27	O 27	0	0
6	F	24	Total 24	O 24	0	0
6	G	214	Total 214	O 214	0	0
6	H	161	Total 161	O 161	0	0

3 Residue-property plots [i](#)

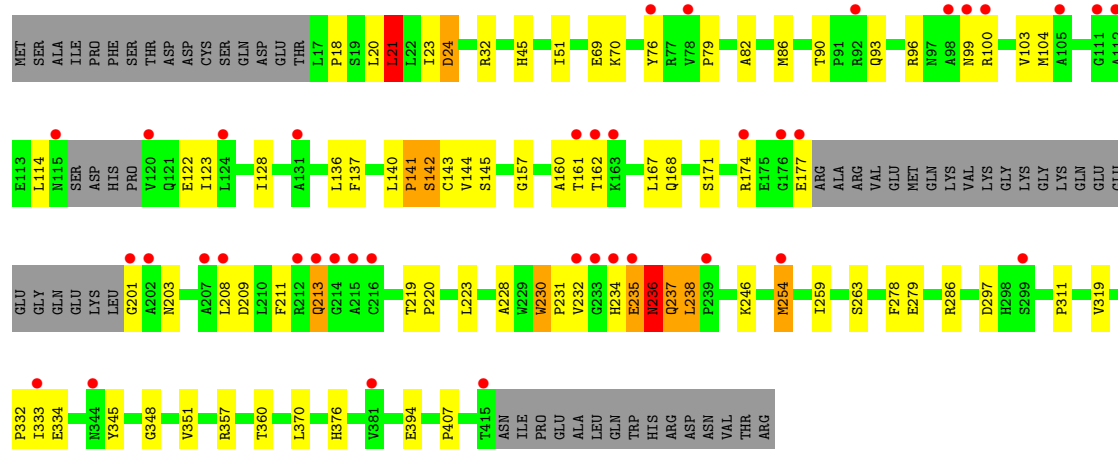
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CcTet





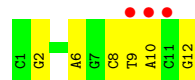
• Molecule 1: CcTet



• Molecule 2: DNA (12-MER)

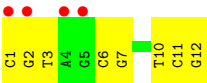


• Molecule 2: DNA (12-MER)



• Molecule 3: DNA





● Molecule 3: DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.79Å 105.20Å 196.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.18 – 2.30 49.18 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.18-2.30) 99.1 (49.18-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.52 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.228 , 0.257 0.228 , 0.258	Depositor DCC
R_{free} test set	4829 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.068 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13728	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: MN, OGA, 6MA

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	0.75	19/3070 (0.6%)	0.64	6/4176 (0.1%)
1	D	0.95	27/3030 (0.9%)	1.06	26/4123 (0.6%)
1	G	0.85	22/3041 (0.7%)	0.93	22/4135 (0.5%)
1	H	0.86	21/2992 (0.7%)	0.88	21/4070 (0.5%)
2	B	0.33	0/249	0.61	0/379
2	E	0.32	0/249	0.68	0/379
3	C	0.35	0/279	0.65	0/429
3	F	0.31	0/279	0.65	0/429
All	All	0.83	89/13189 (0.7%)	0.87	75/18120 (0.4%)

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	141	PRO	N-CA	17.45	1.68	1.47
1	D	141	PRO	N-CA	16.70	1.67	1.47
1	G	141	PRO	N-CA	16.08	1.66	1.47
1	H	238	LEU	C-N	15.16	1.51	1.33
1	A	137	PHE	C-O	-11.70	1.09	1.23
1	G	145	SER	C-N	11.27	1.48	1.33
1	H	145	SER	C-N	11.18	1.48	1.33
1	G	258	ASP	C-N	-11.10	1.20	1.33
1	D	137	PHE	C-O	-11.08	1.11	1.23
1	D	145	SER	C-N	10.27	1.48	1.33
1	D	142	SER	C-O	-9.87	1.10	1.23
1	A	139	TYR	C-O	-9.68	1.12	1.24
1	H	143	CYS	C-O	-9.48	1.12	1.24
1	A	204	TRP	C-O	-9.14	1.12	1.24
1	A	201	GLY	C-O	-8.96	1.14	1.24
1	H	21	LEU	C-O	-8.95	1.13	1.24
1	G	143	CYS	C-O	-8.86	1.13	1.24
1	D	118	HIS	CE1-NE2	-8.69	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	142	SER	C-O	-8.64	1.12	1.23
1	G	204	TRP	C-O	-8.64	1.13	1.24
1	A	141	PRO	C-O	-8.34	1.14	1.23
1	D	122	GLU	C-O	-8.30	1.13	1.23
1	G	141	PRO	C-O	-8.27	1.13	1.23
1	A	142	SER	C-O	-8.15	1.13	1.23
1	G	140	LEU	C-N	8.13	1.43	1.33
1	H	24	ASP	C-O	-7.88	1.15	1.24
1	D	144	VAL	C-O	-7.83	1.15	1.24
1	H	137	PHE	C-O	-7.77	1.14	1.23
1	H	230	TRP	C-O	-7.77	1.15	1.24
1	D	259	ILE	C-N	-7.70	1.24	1.34
1	H	142	SER	C-O	-7.67	1.13	1.23
1	D	140	LEU	C-N	7.61	1.42	1.33
1	D	139	TYR	C-O	-7.56	1.15	1.24
1	H	235	GLU	C-O	-7.56	1.14	1.24
1	G	259	ILE	C-N	-7.51	1.25	1.34
1	D	121	GLN	C-O	-7.45	1.14	1.23
1	A	229	TRP	C-O	-7.35	1.15	1.23
1	G	137	PHE	C-O	-7.29	1.15	1.23
1	D	167	LEU	C-O	-7.29	1.15	1.24
1	G	203	ASN	C-O	-7.27	1.17	1.24
1	D	258	ASP	C-N	-7.25	1.25	1.33
1	A	303	LYS	C-O	-7.14	1.15	1.24
1	H	254	MET	C-O	-7.14	1.15	1.24
1	H	140	LEU	C-N	7.12	1.42	1.33
1	A	234	HIS	CE1-NE2	-7.11	1.25	1.32
1	G	175	GLU	C-O	-7.11	1.15	1.24
1	G	136	LEU	C-O	-7.00	1.14	1.23
1	A	146	PRO	C-O	-6.90	1.15	1.24
1	A	209	ASP	C-O	-6.85	1.15	1.24
1	D	122	GLU	CD-OE2	-6.83	1.12	1.25
1	D	114	LEU	C-O	-6.77	1.14	1.23
1	A	144	VAL	C-O	-6.68	1.16	1.24
1	G	260	PRO	C-O	-6.66	1.16	1.24
1	D	229	TRP	C-O	-6.64	1.15	1.23
1	D	236	ASN	C-O	-6.64	1.14	1.24
1	A	143	CYS	C-O	-6.48	1.16	1.24
1	D	234	HIS	CE1-NE2	-6.46	1.26	1.32
1	A	205	ARG	C-O	-6.45	1.15	1.24
1	H	140	LEU	C-O	-6.44	1.16	1.24
1	G	179	ALA	C-O	-6.42	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	ASN	C-O	-6.38	1.14	1.23
1	G	140	LEU	C-O	-6.33	1.16	1.24
1	H	228	ALA	C-O	-6.29	1.16	1.24
1	D	136	LEU	C-O	-6.25	1.15	1.23
1	G	139	TYR	C-O	-6.21	1.16	1.24
1	D	119	PRO	C-O	-6.19	1.16	1.23
1	H	231	PRO	C-O	-6.19	1.16	1.23
1	D	234	HIS	C-O	-6.16	1.15	1.23
1	G	239	PRO	C-O	-6.16	1.16	1.23
1	D	118	HIS	C-O	-6.13	1.19	1.24
1	D	143	CYS	C-O	-6.13	1.16	1.24
1	H	237	GLN	C-O	-5.95	1.16	1.23
1	H	24	ASP	CG-OD2	-5.89	1.14	1.25
1	D	350	LEU	C-O	-5.85	1.17	1.24
1	H	32	ARG	C-O	-5.83	1.17	1.24
1	A	145	SER	CA-CB	-5.77	1.44	1.53
1	H	144	VAL	C-O	-5.71	1.17	1.24
1	D	201	GLY	C-O	-5.57	1.16	1.23
1	A	140	LEU	C-O	-5.48	1.17	1.24
1	A	200	LEU	C-O	-5.40	1.17	1.24
1	G	259	ILE	C-O	-5.30	1.17	1.24
1	H	24	ASP	CG-OD1	-5.27	1.15	1.25
1	G	144	VAL	C-O	-5.25	1.17	1.24
1	D	217	LYS	C-O	-5.24	1.17	1.24
1	A	234	HIS	C-O	-5.23	1.16	1.23
1	G	176	GLY	C-O	-5.15	1.17	1.23
1	H	234	HIS	C-O	-5.13	1.17	1.24
1	G	138	CYS	C-O	-5.06	1.18	1.24
1	D	141	PRO	C-O	-5.04	1.17	1.23

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	117	ASP	N-CA-C	17.79	137.00	111.56
1	D	140	LEU	CA-C-N	15.91	137.02	119.83
1	D	140	LEU	C-N-CA	15.91	137.02	119.83
1	G	140	LEU	CA-C-N	15.61	136.69	119.83
1	G	140	LEU	C-N-CA	15.61	136.69	119.83
1	H	140	LEU	CA-C-N	15.51	135.74	119.76
1	H	140	LEU	C-N-CA	15.51	135.74	119.76
1	D	116	SER	CA-C-N	15.05	144.48	122.36
1	D	116	SER	C-N-CA	15.05	144.48	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	238	LEU	O-C-N	-12.57	108.28	121.60
1	D	163	LYS	CA-CB-CG	10.98	136.07	114.10
1	D	163	LYS	CB-CG-CD	9.90	134.06	111.30
1	D	145	SER	CA-C-N	9.32	130.28	119.47
1	D	145	SER	C-N-CA	9.32	130.28	119.47
1	H	140	LEU	O-C-N	-9.17	113.18	121.34
1	G	140	LEU	O-C-N	-8.79	113.52	121.34
1	D	163	LYS	CG-CD-CE	-8.74	91.20	111.30
1	G	259	ILE	CA-C-N	8.62	128.25	118.85
1	G	259	ILE	C-N-CA	8.62	128.25	118.85
1	H	145	SER	CA-C-N	8.56	128.69	119.28
1	H	145	SER	C-N-CA	8.56	128.69	119.28
1	D	140	LEU	O-C-N	-8.52	113.76	121.34
1	G	145	SER	CA-C-N	8.46	128.58	119.28
1	G	145	SER	C-N-CA	8.46	128.58	119.28
1	H	286	ARG	CG-CD-NE	-7.93	94.55	112.00
1	D	118	HIS	N-CA-CB	-7.85	98.52	109.82
1	H	24	ASP	CB-CA-C	-7.68	98.03	110.79
1	H	235	GLU	CB-CG-CD	7.68	125.67	112.60
1	G	141	PRO	CA-N-CD	-7.56	101.41	112.00
1	G	145	SER	O-C-N	-7.36	113.19	121.43
1	H	24	ASP	CA-CB-CG	-7.29	105.31	112.60
1	G	141	PRO	CB-CA-C	7.20	120.71	111.64
1	A	229	TRP	CA-CB-CG	7.08	127.06	113.60
1	A	229	TRP	N-CA-CB	-7.05	100.84	111.56
1	H	213	GLN	CA-CB-CG	-7.00	100.10	114.10
1	D	201	GLY	CA-C-O	-6.88	117.48	122.23
1	D	141	PRO	CB-CA-C	6.81	120.22	111.64
1	G	181	VAL	CA-C-O	-6.76	113.92	120.95
1	G	181	VAL	CA-C-N	-6.76	109.54	121.70
1	G	181	VAL	C-N-CA	-6.76	109.54	121.70
1	D	141	PRO	CA-N-CD	-6.75	102.56	112.00
1	H	145	SER	O-C-N	-6.74	113.88	121.43
1	D	115	ASN	CB-CA-C	6.58	122.03	110.85
1	H	141	PRO	CA-N-CD	-6.42	103.02	112.00
1	D	145	SER	O-C-N	-6.40	114.70	121.30
1	D	117	ASP	CB-CA-C	-6.30	103.76	111.82
1	G	258	ASP	CA-C-N	-6.24	110.58	122.13
1	G	258	ASP	C-N-CA	-6.24	110.58	122.13
1	G	217	LYS	CB-CG-CD	6.20	125.57	111.30
1	D	116	SER	O-C-N	6.20	130.58	123.27
1	A	172	ARG	CA-CB-CG	6.07	126.25	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	380	GLU	CB-CG-CD	6.06	122.91	112.60
1	G	106	LYS	CB-CA-C	-6.06	99.61	110.70
1	G	141	PRO	N-CA-C	-5.91	101.93	111.03
1	D	141	PRO	N-CA-C	-5.88	101.97	111.03
1	D	115	ASN	CA-C-N	-5.79	114.95	123.05
1	D	115	ASN	C-N-CA	-5.79	114.95	123.05
1	H	234	HIS	N-CA-C	-5.78	103.81	112.54
1	D	229	TRP	N-CA-CB	-5.70	101.42	111.39
1	G	177	GLU	CB-CA-C	5.63	120.43	110.85
1	A	209	ASP	CB-CA-C	-5.50	99.79	110.46
1	H	237	GLN	CA-C-N	5.46	129.76	121.03
1	H	237	GLN	C-N-CA	5.46	129.76	121.03
1	D	116	SER	N-CA-C	5.37	117.28	108.52
1	D	177	GLU	N-CA-C	-5.32	105.48	111.28
1	H	144	VAL	CA-C-N	5.30	128.71	120.60
1	H	144	VAL	C-N-CA	5.30	128.71	120.60
1	H	236	ASN	CB-CA-C	5.25	120.35	110.63
1	H	137	PHE	CA-CB-CG	5.23	119.03	113.80
1	G	182	GLU	N-CA-CB	5.20	119.33	110.50
1	D	119	PRO	CB-CA-C	-5.16	104.19	110.95
1	G	181	VAL	N-CA-CB	5.12	117.50	110.54
1	A	209	ASP	N-CA-CB	-5.08	102.11	110.14
1	H	32	ARG	CG-CD-NE	5.06	123.14	112.00
1	A	234	HIS	CA-C-O	-5.02	114.95	121.17

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	2992	0	3009	44	0
1	D	2953	0	2967	69	0
1	G	2966	0	2981	47	0
1	H	2917	0	2930	58	0
2	B	246	0	137	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	246	0	137	8	0
3	C	249	0	135	6	0
3	F	249	0	135	5	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	10	0	3	0	0
5	D	10	0	3	0	0
5	G	10	0	3	0	0
5	H	10	0	3	0	0
6	A	186	0	0	13	2
6	B	26	0	0	2	0
6	C	21	0	0	1	0
6	D	207	0	0	16	2
6	E	27	0	0	3	0
6	F	24	0	0	2	0
6	G	214	0	0	10	3
6	H	161	0	0	9	1
All	All	13728	0	12443	235	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 9.

All (235) 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:H:141:PRO:N	1:H:141:PRO:CA	1.68	1.36
1:D:33:MET:HE2	1:D:62:TRP:CE2	1.89	1.08
1:G:234:HIS:HB3	1:G:237:GLN:CD	1.79	1.07
1:D:167:LEU:HD22	1:D:223:LEU:HD11	1.38	1.05
1:H:171:SER:HA	1:H:174:ARG:HE	1.32	0.94
1:D:73:ARG:NE	6:D:602:HOH:O	1.98	0.93
2:E:9:DT:H2"	2:E:10:DA:C8	2.08	0.88
1:G:203:ASN:O	1:G:203:ASN:ND2	2.06	0.87
1:D:56:ILE:O	6:D:601:HOH:O	1.93	0.86
1:G:344:ASN:ND2	1:G:344:ASN:O	2.08	0.85
1:G:234:HIS:HB3	1:G:237:GLN:OE1	1.77	0.84
1:D:99:ASN:ND2	6:D:604:HOH:O	2.11	0.83
1:A:394:GLU:OE1	6:A:601:HOH:O	1.97	0.82
1:A:164:ASP:OD1	1:A:172:ARG:NH1	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:86:MET:SD	1:H:333:ILE:CG2	2.70	0.80
1:D:167:LEU:CD2	1:D:223:LEU:HD11	2.12	0.79
1:A:162:THR:O	1:A:168:GLN:NE2	2.15	0.79
1:D:20:LEU:HB3	1:D:286:ARG:NH1	1.98	0.78
1:G:182:GLU:OE1	1:G:182:GLU:N	2.17	0.77
1:G:334:GLU:HB3	1:G:407:PRO:HD3	1.66	0.77
1:G:24:ASP:OD2	6:G:601:HOH:O	2.03	0.77
1:H:236:ASN:HD22	1:H:236:ASN:H	1.29	0.77
1:G:203:ASN:HD21	1:G:206:GLU:HB2	1.49	0.77
1:D:320:ASN:HD21	1:D:384:GLU:HA	1.50	0.76
1:A:174:ARG:NH1	1:A:206:GLU:O	2.19	0.76
2:B:9:DT:H2''	2:B:10:DA:N7	2.01	0.76
1:D:17:LEU:HD12	1:D:18:PRO:HD2	1.68	0.76
1:H:279:GLU:OE1	6:H:601:HOH:O	2.03	0.75
1:H:236:ASN:H	1:H:236:ASN:ND2	1.80	0.75
3:C:3:DT:OP2	6:C:101:HOH:O	2.04	0.74
3:F:5:DG:OP2	6:F:101:HOH:O	2.05	0.74
1:A:232:VAL:O	1:A:234:HIS:HD2	1.71	0.73
1:D:248:PRO:HA	1:D:253:ARG:NH2	2.04	0.73
2:E:9:DT:OP2	6:E:101:HOH:O	2.05	0.73
2:B:10:DA:OP1	6:B:101:HOH:O	2.07	0.72
1:A:135:ILE:O	6:A:603:HOH:O	2.08	0.71
1:G:231:PRO:HG2	1:G:234:HIS:HB2	1.72	0.71
1:A:235:GLU:OE2	6:A:604:HOH:O	2.09	0.70
1:H:86:MET:SD	1:H:333:ILE:HG21	2.31	0.70
1:D:33:MET:HE2	1:D:62:TRP:CD2	2.25	0.70
1:A:334:GLU:HB3	1:A:407:PRO:HD3	1.73	0.70
1:H:174:ARG:HH11	1:H:208:LEU:HD22	1.55	0.70
1:H:177:GLU:O	6:H:602:HOH:O	2.08	0.70
1:G:83:ARG:NH1	6:G:605:HOH:O	2.25	0.69
1:A:398:ASP:OD2	6:A:605:HOH:O	2.11	0.68
1:H:259:ILE:C	1:H:259:ILE:HD12	2.18	0.68
1:H:86:MET:HE3	1:H:333:ILE:HG21	1.74	0.68
1:H:86:MET:CE	1:H:333:ILE:HG21	2.23	0.68
1:D:33:MET:HE2	1:D:62:TRP:NE1	2.08	0.68
1:D:167:LEU:HD22	1:D:223:LEU:CD1	2.19	0.68
2:B:9:DT:H4'	6:B:101:HOH:O	1.93	0.67
1:H:141:PRO:N	1:H:141:PRO:C	2.52	0.67
1:H:174:ARG:HD2	1:H:208:LEU:HD21	1.75	0.67
1:D:163:LYS:O	6:D:606:HOH:O	2.14	0.65
1:D:29:VAL:HG21	1:D:51:ILE:HG13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ARG:NH2	6:A:613:HOH:O	2.30	0.65
2:E:2:DG:OP2	6:E:102:HOH:O	2.14	0.65
1:G:234:HIS:ND1	1:G:237:GLN:OE1	2.30	0.64
1:H:171:SER:HA	1:H:174:ARG:NE	2.09	0.64
1:A:100:ARG:HD3	1:H:21:LEU:HD11	1.80	0.64
1:H:203:ASN:N	6:H:611:HOH:O	2.29	0.64
2:B:9:DT:H2''	2:B:10:DA:C8	2.32	0.64
3:F:12:DG:H8	1:G:18:PRO:HB2	1.61	0.64
1:D:246:LYS:HE3	1:D:297:ASP:OD2	1.98	0.63
1:H:259:ILE:O	1:H:259:ILE:CD1	2.45	0.63
1:D:300:THR:O	1:D:304:ILE:HG12	1.98	0.63
3:C:12:DG:H8	1:H:18:PRO:HB2	1.63	0.63
1:D:17:LEU:HD11	1:D:306:GLU:HG2	1.81	0.63
1:D:245:LEU:HB3	1:D:304:ILE:HD12	1.82	0.62
1:D:20:LEU:HB3	1:D:286:ARG:HH12	1.64	0.62
1:G:108:PHE:O	6:G:602:HOH:O	2.16	0.62
1:G:259:ILE:N	1:G:260:PRO:CD	2.63	0.61
1:H:259:ILE:HD12	1:H:259:ILE:O	2.00	0.61
1:D:167:LEU:CD2	1:D:223:LEU:CD1	2.76	0.61
1:D:146:PRO:O	6:D:607:HOH:O	2.16	0.61
1:A:106:LYS:NZ	6:A:615:HOH:O	2.33	0.60
1:H:246:LYS:NZ	1:H:297:ASP:OD2	2.30	0.60
1:D:20:LEU:CD2	1:D:286:ARG:HG3	2.32	0.60
2:E:9:DT:H4'	2:E:10:DA:OP1	2.03	0.59
3:F:12:DG:C8	1:G:18:PRO:HB2	2.37	0.59
1:H:174:ARG:HD2	1:H:208:LEU:CD2	2.32	0.59
1:H:334:GLU:HB3	1:H:407:PRO:HD3	1.85	0.58
1:A:41:ILE:O	6:A:606:HOH:O	2.17	0.58
1:G:120:VAL:N	6:G:611:HOH:O	2.36	0.58
1:D:393:ARG:NH1	6:D:612:HOH:O	2.22	0.58
1:H:96:ARG:NH2	1:H:201:GLY:O	2.37	0.58
1:H:100:ARG:HD2	6:H:676:HOH:O	2.03	0.57
1:D:86:MET:HE2	1:D:333:ILE:HG23	1.87	0.57
1:D:232:VAL:O	1:D:234:HIS:HD2	1.87	0.57
1:G:96:ARG:NH2	1:G:201:GLY:O	2.35	0.56
1:A:88:GLU:OE1	6:A:608:HOH:O	2.18	0.56
2:B:8:DC:H2''	2:B:9:DT:C6	2.41	0.56
1:D:115:ASN:ND2	6:D:621:HOH:O	2.39	0.56
1:H:79:PRO:O	6:H:603:HOH:O	2.18	0.56
1:D:20:LEU:HD23	1:D:286:ARG:HG3	1.86	0.56
1:A:105:ALA:O	6:A:607:HOH:O	2.17	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:70:LYS:NZ	6:H:617:HOH:O	2.38	0.55
1:G:86:MET:HG2	1:G:333:ILE:HD11	1.90	0.53
1:A:72:TYR:HA	1:A:127:MET:HE3	1.89	0.53
1:D:259:ILE:N	1:D:260:PRO:CD	2.71	0.53
1:G:47:GLU:OE2	6:G:603:HOH:O	2.18	0.53
1:G:159:LEU:HG	1:G:255:PHE:HB2	1.90	0.53
1:G:234:HIS:CB	1:G:237:GLN:OE1	2.51	0.53
3:C:12:DG:C8	1:H:18:PRO:HB2	2.42	0.53
1:H:162:THR:O	1:H:168:GLN:HG3	2.09	0.53
1:D:248:PRO:HA	1:D:253:ARG:HH21	1.73	0.52
1:G:287:GLU:OE1	6:G:604:HOH:O	2.19	0.52
1:D:22:LEU:HD12	1:D:50:SER:HB3	1.92	0.52
1:H:259:ILE:C	1:H:259:ILE:CD1	2.83	0.52
1:D:152:ILE:HD11	1:D:262:ALA:HB1	1.91	0.51
1:D:19:SER:HA	1:D:309:PHE:CE2	2.46	0.51
1:D:163:LYS:HB3	1:D:164:ASP:CG	2.36	0.51
1:D:20:LEU:HD23	1:D:286:ARG:CG	2.41	0.50
1:D:255:PHE:O	1:D:259:ILE:HG13	2.12	0.50
1:G:217:LYS:H	1:G:384:GLU:CD	2.19	0.50
3:C:10:DT:H2"	3:C:11:DC:C6	2.47	0.49
1:D:238:LEU:O	6:D:609:HOH:O	2.19	0.49
1:D:107:GLU:OE2	6:D:610:HOH:O	2.20	0.49
1:D:224:THR:HG21	1:D:229:TRP:CZ2	2.48	0.49
1:D:329:THR:HA	1:D:372:LYS:HD3	1.94	0.49
1:D:76:TYR:HB2	1:D:128:ILE:HD13	1.95	0.49
1:D:334:GLU:HB3	1:D:407:PRO:HD3	1.95	0.49
1:H:123:ILE:HG12	1:H:360:THR:OG1	2.13	0.49
1:H:160:ALA:HB1	1:H:219:THR:H	1.79	0.48
1:H:259:ILE:HD13	1:H:263:SER:OG	2.13	0.48
1:D:288:LEU:O	1:D:298:HIS:HE1	1.97	0.48
1:G:259:ILE:O	1:G:259:ILE:HG13	2.12	0.48
1:A:406:TYR:CG	1:A:407:PRO:HD2	2.47	0.48
1:H:82:ALA:HB2	1:H:136:LEU:HD21	1.95	0.48
1:D:271:ALA:O	1:D:275:GLN:HG3	2.13	0.48
1:G:132:GLU:HB3	6:G:606:HOH:O	2.13	0.48
1:A:174:ARG:NH2	1:A:206:GLU:HB2	2.30	0.47
2:E:8:DC:H2"	2:E:9:DT:C5	2.49	0.47
2:E:9:DT:H2"	2:E:10:DA:N7	2.30	0.47
1:D:20:LEU:CB	1:D:286:ARG:NH1	2.74	0.47
1:H:20:LEU:HA	1:H:23:ILE:HG12	1.96	0.47
1:D:320:ASN:ND2	6:D:623:HOH:O	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:PRO:HB3	6:A:603:HOH:O	2.15	0.46
1:D:33:MET:HE2	1:D:62:TRP:CD1	2.49	0.46
1:D:313:SER:HB2	1:D:392:TRP:HA	1.97	0.46
1:G:158:THR:O	1:G:162:THR:HG23	2.16	0.46
1:A:275:GLN:O	1:A:279:GLU:HG3	2.15	0.46
1:A:92:ARG:NH1	6:A:629:HOH:O	2.49	0.46
1:D:212:ARG:NH2	6:D:628:HOH:O	2.49	0.46
3:F:12:DG:C4	1:G:22:LEU:HD12	2.51	0.46
1:A:86:MET:HE2	1:A:333:ILE:HG23	1.98	0.46
1:D:170:LYS:HE3	6:D:639:HOH:O	2.17	0.45
1:A:163:LYS:O	1:A:168:GLN:OE1	2.35	0.45
1:H:136:LEU:HD23	1:H:370:LEU:HD12	1.97	0.45
1:G:351:VAL:O	1:G:376:HIS:HA	2.17	0.45
1:H:160:ALA:HB1	1:H:219:THR:N	2.32	0.45
1:A:224:THR:HG21	1:A:229:TRP:CZ2	2.52	0.45
1:A:334:GLU:CB	1:A:407:PRO:HD3	2.43	0.44
1:D:225:PHE:HB3	1:D:245:LEU:HD11	2.00	0.44
1:G:278:PHE:CD1	1:G:311:PRO:HG3	2.52	0.44
1:A:217:LYS:HE2	1:A:384:GLU:OE1	2.18	0.44
1:G:170:LYS:HE3	1:G:222:VAL:O	2.18	0.44
1:H:209:ASP:OD1	1:H:209:ASP:N	2.51	0.44
1:D:230:TRP:CZ3	1:D:395:ARG:HB3	2.53	0.44
1:D:396:LEU:HA	1:D:396:LEU:HD23	1.46	0.44
1:G:259:ILE:N	1:G:260:PRO:HD2	2.33	0.44
1:H:345:TYR:HE2	1:H:348:GLY:HA3	1.82	0.44
1:G:73:ARG:NH1	6:G:622:HOH:O	2.51	0.44
1:G:100:ARG:O	1:G:104:MET:HG2	2.18	0.44
1:A:176:GLY:N	6:A:618:HOH:O	2.40	0.44
1:D:294:LEU:O	6:D:611:HOH:O	2.20	0.44
1:D:229:TRP:HD1	2:E:8:DC:OP1	2.01	0.43
1:G:292:SER:HA	1:G:298:HIS:CE1	2.53	0.43
1:G:258:ASP:C	1:G:259:ILE:HG23	2.44	0.43
1:H:100:ARG:O	1:H:104:MET:HG2	2.18	0.43
1:A:38:ARG:NH2	1:A:413:SER:OG	2.48	0.43
1:A:86:MET:SD	1:A:373:LEU:HD12	2.58	0.43
1:D:351:VAL:O	1:D:376:HIS:HA	2.18	0.43
1:H:69:GLU:OE2	6:H:604:HOH:O	2.21	0.43
1:H:230:TRP:HB3	1:H:235:GLU:HG2	2.00	0.43
1:A:391:PHE:HB3	2:B:6:6MA:H13	2.01	0.43
1:H:104:MET:HB2	6:H:624:HOH:O	2.17	0.43
1:D:20:LEU:HD21	1:D:286:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:MET:HE3	6:D:673:HOH:O	2.18	0.43
1:A:225:PHE:HB3	1:A:245:LEU:HD11	2.00	0.43
1:D:178:ARG:HA	1:D:178:ARG:HD2	1.84	0.43
1:D:224:THR:HG21	1:D:229:TRP:HZ2	1.83	0.43
1:D:271:ALA:HB2	1:D:278:PHE:CG	2.54	0.43
1:A:20:LEU:HA	1:A:23:ILE:HG12	2.01	0.43
1:A:90:THR:OG1	1:A:93:GLN:HB2	2.19	0.43
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.93	0.42
3:C:6:DC:H2'	3:C:7:DG:C5	2.54	0.42
1:G:288:LEU:O	1:G:298:HIS:HE1	2.02	0.42
1:H:76:TYR:HB2	1:H:128:ILE:HD13	2.01	0.42
1:H:332:PRO:HB3	1:H:394:GLU:HB2	1.99	0.42
1:G:409:LYS:NZ	6:G:606:HOH:O	2.52	0.42
1:A:393:ARG:HH22	2:B:6:6MA:H8	1.84	0.42
1:H:211:PHE:O	1:H:213:GLN:HG2	2.20	0.42
1:A:172:ARG:O	1:A:175:GLU:HB3	2.18	0.42
1:D:46:THR:N	6:D:603:HOH:O	1.98	0.42
1:A:22:LEU:HD23	1:A:50:SER:HB2	2.02	0.42
1:H:45:HIS:NE2	1:H:51:ILE:HB	2.34	0.42
1:H:220:PRO:HA	1:H:319:VAL:O	2.20	0.42
1:D:33:MET:CE	1:D:62:TRP:CD1	3.03	0.42
1:D:234:HIS:C	1:D:236:ASN:H	2.27	0.42
1:G:297:ASP:N	6:G:623:HOH:O	2.53	0.42
1:G:406:TYR:CG	1:G:407:PRO:HD2	2.55	0.42
1:D:92:ARG:NE	6:D:631:HOH:O	2.53	0.42
1:G:60:ALA:CB	1:G:148:ILE:HD12	2.50	0.42
1:G:159:LEU:HD12	1:G:255:PHE:CD1	2.55	0.42
1:H:230:TRP:CB	1:H:235:GLU:HG2	2.50	0.42
1:H:122:GLU:HA	6:H:616:HOH:O	2.20	0.42
1:A:313:SER:HB2	1:A:392:TRP:HA	2.02	0.41
1:D:20:LEU:HD23	1:D:286:ARG:NH1	2.35	0.41
1:H:157:GLY:O	1:H:161:THR:OG1	2.25	0.41
1:A:393:ARG:HH22	2:B:6:6MA:C8	2.33	0.41
1:G:340:VAL:HG22	1:G:366:VAL:HG22	2.02	0.41
1:H:99:ASN:O	1:H:103:VAL:HG23	2.19	0.41
1:H:167:LEU:HG	1:H:223:LEU:HD11	2.02	0.41
3:C:1:DC:H2'	3:C:2:DG:C8	2.55	0.41
1:D:303:LYS:HD3	1:D:303:LYS:HA	1.80	0.41
1:G:174:ARG:CD	1:G:208:LEU:HG	2.50	0.41
1:H:90:THR:OG1	1:H:93:GLN:HB2	2.20	0.41
1:A:351:VAL:O	1:A:376:HIS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:SER:HA	6:A:611:HOH:O	2.20	0.41
1:G:120:VAL:HG12	1:G:121:GLN:H	1.84	0.41
1:G:234:HIS:HB3	1:G:237:GLN:NE2	2.29	0.41
1:G:254:MET:HE3	1:G:254:MET:HB2	1.85	0.41
1:H:278:PHE:CD1	1:H:311:PRO:HG3	2.56	0.41
1:D:22:LEU:HD12	1:D:50:SER:CB	2.50	0.41
1:H:351:VAL:O	1:H:376:HIS:HA	2.21	0.41
1:D:29:VAL:O	1:D:33:MET:HG3	2.21	0.41
1:H:114:LEU:HD23	1:H:357:ARG:CZ	2.51	0.41
1:A:20:LEU:HD12	1:A:286:ARG:HG3	2.03	0.40
2:E:12:DG:OP2	6:E:103:HOH:O	2.22	0.40
1:A:86:MET:SD	1:A:89:LEU:HD12	2.62	0.40
3:F:6:DC:OP2	6:F:102:HOH:O	2.22	0.40
1:G:332:PRO:HB3	1:G:394:GLU:HB2	2.02	0.40
1:H:232:VAL:O	1:H:232:VAL:HG13	2.20	0.40
1:A:345:TYR:CZ	1:A:363:PRO:HD3	2.56	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)
6:A:758:HOH:O	6:G:757:HOH:O[4_565]	1.97	0.23
6:A:783:HOH:O	6:G:801:HOH:O[4_555]	1.98	0.22
6:D:787:HOH:O	6:G:814:HOH:O[3_454]	2.07	0.13
6:D:803:HOH:O	6:H:757:HOH:O[3_454]	2.11	0.09

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	377/430 (88%)	366 (97%)	11 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	373/430 (87%)	358 (96%)	14 (4%)	1 (0%)	36	46
1	G	372/430 (86%)	362 (97%)	10 (3%)	0	100	100
1	H	366/430 (85%)	355 (97%)	11 (3%)	0	100	100
All	All	1488/1720 (86%)	1441 (97%)	46 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	163	LYS

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	318/362 (88%)	318 (100%)	0	100	100
1	D	314/362 (87%)	310 (99%)	4 (1%)	61	77
1	G	315/362 (87%)	309 (98%)	6 (2%)	50	69
1	H	310/362 (86%)	303 (98%)	7 (2%)	44	63
All	All	1257/1448 (87%)	1240 (99%)	17 (1%)	59	76

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	116	SER
1	D	167	LEU
1	D	175	GLU
1	D	229	TRP
1	G	175	GLU
1	G	178	ARG
1	G	180	ARG
1	G	203	ASN
1	G	256	LEU
1	G	380	GLU

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Mol	Chain	Res	Type
1	H	21	LEU
1	H	24	ASP
1	H	142	SER
1	H	236	ASN
1	H	237	GLN
1	H	238	LEU
1	H	254	MET

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	35	GLN
1	A	134	HIS
1	A	168	GLN
1	A	213	GLN
1	A	234	HIS
1	D	48	ASN
1	D	115	ASN
1	D	118	HIS
1	D	121	GLN
1	D	234	HIS
1	D	320	ASN
1	D	356	ASN
1	G	99	ASN
1	G	203	ASN
1	H	48	ASN
1	H	115	ASN
1	H	213	GLN
1	H	234	HIS
1	H	236	ASN
1	H	237	GLN
1	H	275	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	6MA	B	6	2	21,24,25	1.84	3 (14%)	27,34,37	3.13	7 (25%)
2	6MA	E	6	2	21,24,25	1.82	4 (19%)	27,34,37	3.34	7 (25%)

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	6MA	B	6	2	-	0/9/23/24	0/3/3/3
2	6MA	E	6	2	-	0/9/23/24	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	6MA	C6-N1	5.55	1.43	1.35
2	E	6	6MA	C6-N1	5.50	1.43	1.35
2	B	6	6MA	C6-N6	3.63	1.38	1.34
2	E	6	6MA	C6-N6	3.49	1.38	1.34
2	B	6	6MA	C1'-N9	-2.45	1.41	1.46
2	E	6	6MA	C1'-N9	-2.38	1.42	1.46
2	E	6	6MA	O4'-C4'	-2.12	1.40	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	6	6MA	C1-N6-C6	-14.23	109.65	122.85
2	B	6	6MA	C1-N6-C6	-13.28	110.53	122.85
2	E	6	6MA	O4'-C1'-N9	5.26	117.41	107.96
2	B	6	6MA	C4-C5-C6	5.17	121.08	116.78
2	E	6	6MA	C4-C5-C6	5.04	120.97	116.78
2	B	6	6MA	O4'-C1'-N9	4.00	115.15	107.96
2	B	6	6MA	C6-C5-N7	-3.12	129.03	132.43
2	B	6	6MA	C5-C6-N1	-3.06	114.87	118.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	6	6MA	C6-C5-N7	-2.91	129.25	132.43
2	E	6	6MA	C2'-C1'-N9	-2.76	108.14	114.63
2	E	6	6MA	C5-C6-N1	-2.74	115.21	118.15
2	B	6	6MA	C2'-C1'-N9	-2.67	108.36	114.63
2	E	6	6MA	O3'-C3'-C4'	2.13	118.14	110.07
2	B	6	6MA	O3'-C3'-C4'	2.11	118.08	110.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6	6MA	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
5	OGA	D	502	4	9,9,9	1.28	0	8,11,11	1.55	1 (12%)
5	OGA	A	502	4	9,9,9	1.26	0	8,11,11	1.43	1 (12%)
5	OGA	G	502	4	9,9,9	1.32	0	8,11,11	1.35	1 (12%)
5	OGA	H	502	4	9,9,9	1.21	0	8,11,11	1.48	1 (12%)

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
5	OGA	D	502	4	-	0/8/9/9	-
5	OGA	A	502	4	-	0/8/9/9	-
5	OGA	G	502	4	-	0/8/9/9	-
5	OGA	H	502	4	-	0/8/9/9	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	502	OGA	O2'-C2-C1	-3.14	117.23	121.36
5	D	502	OGA	O2'-C2-C1	-3.09	117.29	121.36
5	G	502	OGA	O2'-C2-C1	-2.86	117.60	121.36
5	A	502	OGA	O2'-C2-C1	-2.45	118.13	121.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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, 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	381/430 (88%)	0.53	37 (9%) 13 15	14, 29, 54, 83	0
1	D	377/430 (87%)	0.74	51 (13%) 7 8	14, 32, 55, 77	0
1	G	378/430 (87%)	0.46	21 (5%) 30 32	12, 29, 56, 72	0
1	H	372/430 (86%)	0.82	39 (10%) 11 13	15, 35, 59, 77	0
2	B	11/12 (91%)	0.57	0 100 100	23, 33, 58, 59	0
2	E	11/12 (91%)	1.10	3 (27%) 1 1	25, 34, 70, 71	0
3	C	12/12 (100%)	0.98	4 (33%) 1 1	24, 33, 71, 114	0
3	F	12/12 (100%)	1.08	4 (33%) 1 1	24, 38, 86, 123	0
All	All	1554/1768 (87%)	0.65	159 (10%) 12 13	12, 31, 58, 123	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	120	VAL	9.2
1	D	116	SER	6.2
1	A	179	ALA	5.4
1	A	215	ALA	5.4
1	D	413	SER	5.4
1	H	233	GLY	4.8
1	H	215	ALA	4.6
1	A	415	THR	4.5
1	H	232	VAL	4.4
1	H	214	GLY	4.4
3	F	1	DC	4.4
1	G	116	SER	4.4
1	G	120	VAL	4.4
3	C	1	DC	4.3
1	H	201	GLY	4.3
1	H	213	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	215	ALA	4.1
1	A	180	ARG	4.0
1	A	413	SER	4.0
1	H	161	THR	3.9
1	D	163	LYS	3.9
1	G	180	ARG	3.8
1	D	118	HIS	3.8
1	H	162	THR	3.7
1	G	179	ALA	3.7
1	D	117	ASP	3.7
1	A	119	PRO	3.7
1	A	163	LYS	3.6
1	A	176	GLY	3.6
3	F	2	DG	3.5
1	H	176	GLY	3.4
1	D	408	SER	3.4
1	A	117	ASP	3.4
1	H	115	ASN	3.4
1	D	301	VAL	3.3
1	H	234	HIS	3.3
1	G	202	ALA	3.3
1	G	208	LEU	3.3
1	A	214	GLY	3.3
1	D	19	SER	3.2
1	H	112	ALA	3.2
1	D	162	THR	3.1
1	D	410	TRP	3.1
1	G	232	VAL	3.1
1	G	201	GLY	3.0
1	A	120	VAL	3.0
1	D	18	PRO	3.0
1	A	162	THR	3.0
1	D	20	LEU	3.0
1	A	173	ALA	2.9
3	C	5	DG	2.9
1	G	233	GLY	2.9
1	A	168	GLN	2.9
2	E	9	DT	2.9
1	D	179	ALA	2.9
3	C	2	DG	2.9
1	D	176	GLY	2.9
1	H	163	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
3	F	3	DT	2.8
1	D	304	ILE	2.8
1	D	164	ASP	2.8
1	G	181	VAL	2.8
1	A	216	CYS	2.8
1	H	299	SER	2.8
1	H	105	ALA	2.8
1	D	229	TRP	2.8
1	G	99	ASN	2.8
1	H	99	ASN	2.7
1	G	231	PRO	2.7
1	H	111	GLY	2.7
1	D	299	SER	2.7
1	D	154	ALA	2.7
1	G	215	ALA	2.7
1	A	414	TYR	2.7
1	G	115	ASN	2.7
1	H	333	ILE	2.7
1	A	18	PRO	2.7
1	D	406	TYR	2.6
1	H	78	VAL	2.6
1	D	256	LEU	2.6
1	D	214	GLY	2.6
1	D	248	PRO	2.6
1	G	182	GLU	2.5
2	E	11	DC	2.5
1	D	172	ARG	2.5
1	H	207	ALA	2.5
1	H	344	ASN	2.5
3	C	4	DA	2.5
1	D	302	SER	2.5
1	A	172	ARG	2.5
1	H	100	ARG	2.4
1	A	174	ARG	2.4
1	D	155	ALA	2.4
1	A	408	SER	2.4
1	H	98	ALA	2.4
1	G	293	LYS	2.4
1	A	213	GLN	2.4
1	H	76	TYR	2.4
1	A	175	GLU	2.4
2	E	10	DA	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	4	DA	2.4
1	A	160	ALA	2.4
1	D	120	VAL	2.4
1	A	293	LYS	2.3
1	D	209	ASP	2.3
1	D	300	THR	2.3
1	G	86	MET	2.3
1	H	254	MET	2.3
1	A	299	SER	2.3
1	D	412	GLU	2.3
1	H	235	GLU	2.3
1	A	304	ILE	2.3
1	H	124	LEU	2.2
1	H	216	CYS	2.2
1	H	239	PRO	2.2
1	H	202	ALA	2.2
1	H	208	LEU	2.2
1	H	92	ARG	2.2
1	H	212	ARG	2.2
1	G	88	GLU	2.2
1	D	246	LYS	2.2
1	H	131	ALA	2.2
1	A	17	LEU	2.2
1	D	307	ILE	2.2
1	D	254	MET	2.2
1	D	298	HIS	2.2
1	G	162	THR	2.2
1	A	254	MET	2.1
1	H	381	VAL	2.1
1	A	406	TYR	2.1
1	D	223	LEU	2.1
1	D	175	GLU	2.1
1	D	177	GLU	2.1
1	G	209	ASP	2.1
1	D	208	LEU	2.1
1	D	344	ASN	2.1
1	D	166	HIS	2.1
1	A	230	TRP	2.1
1	A	50	SER	2.1
1	A	170	LYS	2.1
1	A	164	ASP	2.1
1	A	178	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	346	SER	2.0
1	D	295	THR	2.0
1	D	160	ALA	2.0
1	H	177	GLU	2.0
1	A	118	HIS	2.0
1	D	168	GLN	2.0
1	D	115	ASN	2.0
1	D	382	ASP	2.0
1	D	259	ILE	2.0
1	D	407	PRO	2.0
1	A	161	THR	2.0
1	D	292	SER	2.0
1	H	415	THR	2.0
1	G	236	ASN	2.0
1	D	174	ARG	2.0
1	H	174	ARG	2.0
1	D	249	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	6MA	B	6	22/23	0.96	0.07	13,24,33,36	0
2	6MA	E	6	22/23	0.96	0.07	16,23,27,44	0

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($\text{\AA}^2$)	Q<0.9
5	OGA	D	502	10/10	0.93	0.08	19,23,28,29	0
5	OGA	H	502	10/10	0.94	0.08	22,27,30,31	0
5	OGA	G	502	10/10	0.96	0.07	14,22,24,27	0
5	OGA	A	502	10/10	0.96	0.06	17,21,25,25	0
4	MN	H	501	1/1	0.98	0.05	32,32,32,32	0
4	MN	G	501	1/1	0.99	0.02	24,24,24,24	0
4	MN	D	501	1/1	0.99	0.07	26,26,26,26	0
4	MN	A	501	1/1	1.00	0.10	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.