

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	1TEZ
Title	:	COMPLEX BETWEEN DNA AND THE DNA PHOTOLYASE FROM ANA-
		CYSTIS NIDULANS
Authors	:	Essen, LO.; Carell, T.; Mees, A.; Klar, T.
Deposited on	:	2004-05-26
Resolution	:	1.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
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)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	т	11	18%						
	1	11	36%	27%	36%				
			27%						
1	K	11	36%	27%	36%				
			22%						
2	J	9	56%		44%				
			33%						
2	L	9	44%		56%				
3	М	4		100%					



Mol	Chain	Length	Quality of chain		
			50%		
3	Ο	4	50% 50%		
			100%		
4	Ν	5	100%		
			40%		
4	Р	5	60% 40%		
			3%		
5	А	474	85%	14%	•
			3%		
5	В	474	84%	15%	•
			4%		
5	С	474	84%	15%	•
	-		3%		_
5	D	474	87%	12%	•

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	HDF	А	5486	Х	-	-	-
11	HDF	В	6486	Х	-	-	-
11	HDF	С	7486	Х	-	-	-
11	HDF	D	8486	Х	-	-	-



2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 18206 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 DNA chain called 5'-D(*AP*TP*CP*GP*GP*CP*T*(TCP)P*CP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	т	7	Total	С	Ν	0	Р	0	0	0
	1	1	140	68	25	41	6	0	0	
1	K	7	Total	С	Ν	Ο	Р	0	0	0
	Γ	1	140	68	25	41	6	0	0	0

• Molecule 2 is a DNA chain called 5'-D(P*CP*GP*AP*AP*GP*CP*CP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	т	0	Total	С	Ν	Ο	Р	0	0	0
	1	9	186	87	39	51	9	0	0	
0	т	0	Total	С	Ν	0	Р	0	0	0
		9	186	87	39	51	9	0	U	U

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
3	М	4	Total	С	Ν	Ο	Р	1	0	0	
0	111	4	77	38	$13 \ 23 \ 3$	3	T	0	0		
2	0	1	Total	С	Ν	Ο	Р	0	0	0	
5	0	4	77	38	13	23	3	0	0	0	

• Molecule 4 is a DNA chain called 5'-D(P*GP*CP*CP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	К	Total	С	Ν	Ο	Р	0	0	0
4	4	5	103	48	21	29	5	0	0	
4	D	Б	Total	С	Ν	0	Р	0	0	0
4	1	5	103	48	21	29	5	0	0	0

• Molecule 5 is a protein called Deoxyribodipyrimidine photolyase.



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace	
F	Λ	474	Total	С	Ν	0	\mathbf{S}	2	0	0	
5	A	414	3774	2411	674	679	10	2	0		
5	В	474	Total	С	Ν	0	S	6	0	0	
0	D	414	3782	2414	678	680	10	0	0	0	
5	С	474	Total	С	Ν	0	S	0	0	0	
0	U	414	3773	2409	674	680	10	0	0	0	
5	Л	474	Total	С	Ν	0	S	6	0	0	
5	D	414	3777	2412	675	680	10	0	0		

• Molecule 6 is 5'-METHYLTHYMIDINE (three-letter code: TCP) (formula: $C_{11}H_{16}N_2O_5$).



Ν	Aol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf
	6	Ι	1	Total 18	C 11	N 2	O 5	0	0
	6	K	1	Total 18	C 11	N 2	O 5	0	0

• Molecule 7 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C) (formula: $C_9H_{14}N_3O_8P$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	Т	1	Total	С	Ν	0	Р	0	0
1	1	1	19	9	3	6	1	0	0
7	Т	1	Total	С	Ν	0	Р	0	0
1	1		19	9	3	6	1	0	
7	V	1	Total	С	Ν	Ο	Р	0	0
1	Γ	1	19	9	3	6	1	0	
7	V	1	Total	С	Ν	Ο	Р	0	0
(K	1	19	9	3	6	1	0	0

• Molecule 8 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: G) (formula: $C_{10}H_{14}N_5O_8P$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
0	Т	1	Total	С	Ν	Ο	Р	0	0
0	1	L	22	10	5	6	1	0	
0	K	1	Total	С	Ν	Ο	Р	0	0
0	Γ	L	22	10	5	6	1	0	0

• Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	1	Total Mg 1 1	0	0
9	В	1	Total Mg 1 1	0	0

• Molecule 10 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
10	Λ	1	Total	С	Ν	Ο	Р	0	0
10	Л	1	53	27	9	15	2	0	0
10	Р	1	Total	С	Ν	0	Р	0	0
10 В	D		53	27	9	15	2	0	
10	C	1	Total	С	Ν	0	Р	0	0
10	U	1	53	27	9	15	2	0	0
10	П	1	Total	С	Ν	Ο	Р	0	0
10			53	27	9	15	2	0	0

• Molecule 11 is 8-HYDROXY-10-(D-RIBO-2,3,4,5-TETRAHYDROXYPENTYL)-5-DEAZA



ISOALLOXAZINE (three-letter code: HDF) (formula: $C_{16}H_{17}N_3O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
11	Δ	1	Total	С	Ν	0	0	0	
	Л	T	26	16	3	7	0		
11	В	1	Total	С	Ν	Ο	0	0	
		1	26	16	3	7	0		
11	С	1	Total	С	Ν	0	0	0	
	U	L	26	16	3	7	0	0	
11	Л	1	Total	С	Ν	Ο	0	0	
	D		26	16	3	7	U	0	

• Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	Ι	10	Total O 10 10	0	0
12	J	11	Total O 11 11	0	0
12	K	8	Total O 8 8	0	0
12	L	9	Total O 9 9	0	0
12	М	14	Total O 14 14	0	0
12	N	10	Total O 10 10	0	0
12	Р	5	Total O 5 5	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	А	409	Total O 409 409	0	0
12	В	404	Total O 404 404	0	0
12	С	374	Total O 374 374	0	0
12	D	360	Total O 360 360	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: 5'-D(*AP*TP*CP*GP*GP*CP*T*(TCP)P*CP*GP*C)-3'









• Molecule 5: Deoxyribodipyrimidine photolyase

Chain C:

84%



.

15%

K194 A2 R195 D12 R216 D12 R216 L15 R219 L34 R226 Q43 P2300 Q60 R244 Q63 P2300 Q60 R346 L34 R65 R66 R348 Q63 R309 P12 R346 Q63 R347 Q63 R346 L76 R347 Q63 R348 R65 R349 Q63 R346 L76 R347 P127 R348 Q126 R349 Q126 R347 P141 R348 Q126 R349 R147 R349 R147 R346 L102 R347 P144 R348 R147 R349 R147 R346 R144 R347 R147<



• Molecule 5: Deoxyribodipyrimidine photolyase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	173.81Å 88.50 Å 161.62 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.11° 90.00°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	29.92 - 1.80	Depositor
Resolution (A)	29.92 - 1.80	EDS
% Data completeness	96.1 (29.92-1.80)	Depositor
(in resolution range)	95.8(29.92-1.80)	EDS
R _{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.83 (at 1.80 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
D D.	0.205 , 0.226	Depositor
Π, Π_{free}	0.203 , 0.223	DCC
R_{free} test set	7425 reflections (3.40%)	wwPDB-VP
Wilson B-factor $(Å^2)$	24.7	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35 , 38.4	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.417 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18206	wwPDB-VP
Average B, all atoms $(Å^2)$	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

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).

Mal	Chain	Bond	lengths	Bond	angles
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	Ι	0.25	0/156	0.67	0/239
1	Κ	0.25	0/156	0.68	0/239
2	J	0.42	0/209	0.72	0/320
2	L	0.43	0/209	0.72	0/320
3	М	0.38	0/85	0.85	0/129
3	0	0.34	0/85	0.82	0/129
4	Ν	0.54	0/115	0.76	0/175
4	Р	0.52	0/115	0.76	0/175
5	А	0.32	0/3883	0.54	0/5292
5	В	0.32	0/3891	0.55	0/5302
5	С	0.32	0/3882	0.55	0/5292
5	D	0.32	0/3886	0.56	0/5296
All	All	0.32	0/16672	0.57	0/22908

There are no bond length outliers.

There are no bond angle outliers.

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	Ι	140	0	80	7	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Κ	140	0	80	7	0
2	J	186	0	100	5	0
2	L	186	0	100	5	0
3	М	77	0	47	0	0
3	0	77	0	47	1	0
4	Ν	103	0	56	0	0
4	Р	103	0	56	1	0
5	А	3774	0	3681	60	0
5	В	3782	0	3694	61	0
5	С	3773	0	3674	66	0
5	D	3777	0	3685	56	0
6	Ι	18	0	14	6	0
6	Κ	18	0	14	6	0
7	Ι	38	0	23	0	0
7	Κ	38	0	23	0	0
8	Ι	22	0	11	0	0
8	Κ	22	0	11	0	0
9	А	1	0	0	0	0
9	В	1	0	0	0	0
10	А	53	0	31	0	0
10	В	53	0	31	1	0
10	С	53	0	31	1	0
10	D	53	0	31	1	0
11	А	26	0	15	0	0
11	В	26	0	16	0	0
11	С	26	0	15	0	0
11	D	26	0	15	0	0
12	А	409	0	0	5	0
12	В	404	0	0	7	0
12	С	374	0	0	8	0
12	D	360	0	0	10	0
12	Ι	10	0	0	0	0
12	J	11	0	0	0	0
12	Κ	8	0	0	0	0
12	L	9	0	0	0	0
12	М	14	0	0	0	0
12	N	10	0	0	0	0
12	Р	5	0	0	0	0
All	All	18206	0	15581	255	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 8.



A 1	A 4 - 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:C:401:LYS:HB2	5:C:401:LYS:HB2 5:C:402:PRO:HD2		1.07
5:C:401:LYS:HG2	5:C:404:ARG:HH21	1.29	0.98
5:C:401:LYS:HG2	5:C:404:ARG:NH2	1.88	0.88
5:D:199:ASP:HB2	12:D:8744:HOH:O	1.75	0.85
5:C:226:ALA:HA	12:C:7764:HOH:O	1.78	0.84
1:K:7:DT:H72	6:K:12:TCP:H72	1.61	0.82
5:D:403:LEU:O	5:D:404:ARG:HB2	1.79	0.82
5:A:306:ARG:NH2	5:A:400:PRO:HG3	1.94	0.82
5:C:277:ILE:HG13	12:C:7764:HOH:O	1.80	0.81
1:I:7:DT:H72	6:I:12:TCP:H72	1.63	0.80
5:C:401:LYS:CG	5:C:404:ARG:HH21	1.98	0.77
1:I:1:DA:H2"	1:I:2:DT:C5	2.23	0.74
5:A:86:GLN:HE21	5:C:195:GLN:HG2	1.54	0.73
5:A:459:LEU:O	5:A:463:GLN:HG3	1.89	0.72
2:J:9:DA:C2	5:A:402:PRO:HD3	2.25	0.72
1:K:1:DA:H2"	1:K:2:DT:C5	2.25	0.71
5:B:60:GLN:NE2	12:B:9389:HOH:O	2.25	0.70
5:A:84:ILE:HB	5:A:85:PRO:HD3	1.74	0.70
5:B:195:GLN:HG2	5:D:86:GLN:HE21	1.55	0.69
5:D:84:ILE:HB	5:D:85:PRO:HD3	1.75	0.69
5:A:269:ARG:NH2	5:B:219:GLU:HA	2.09	0.68
5:B:64:GLN:O	5:B:68:GLN:HG3	1.94	0.68
5:B:306:ARG:NH2	5:B:400:PRO:HG3	2.09	0.67
5:A:34:LEU:CD1	5:A:76:LEU:HD13	2.25	0.67
5:C:401:LYS:HB2	5:C:402:PRO:CD	2.20	0.66
5:D:34:LEU:CD1	5:D:76:LEU:HD13	2.26	0.66
5:D:404:ARG:NH2	5:D:465:LYS:NZ	2.44	0.66
5:A:102:ILE:HD13	5:A:102:ILE:H	1.62	0.65
5:A:215:ALA:O	5:A:219:GLU:HG3	1.97	0.65
5:C:192:THR:OG1	5:C:195:GLN:HG3	1.96	0.64
5:C:471:LEU:HD12	12:C:7770:HOH:O	1.96	0.64
5:D:102:ILE:HD13	5:D:102:ILE:H	1.63	0.64
5:D:215:ALA:O	5:D:219:GLU:HG3	1.98	0.64
5:B:102:ILE:HD13	5:B:102:ILE:H	1.62	0.63
5:D:400:PRO:O	5:D:401:LYS:HG3	1.97	0.63
5:B:77:GLN:NE2	12:B:9386:HOH:O	2.32	0.62
5:C:84:ILE:HB	5:C:85:PRO:HD3	1.80	0.62
5:C:102:ILE:HD13	5:C:102:ILE:H	1.65	0.62
5:B:84:ILE:HB	5:B:85:PRO:HD3	1.81	0.62
5:B:215:ALA:O	5:B:219:GLU:HG3	1.99	0.61

All (255) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Interatomic Clash				
Atom-1 Atom-2		distance (Å)	overlap (Å)	
5:C:215:ALA:O	5:C:219:GLU:HG3	2.00	0.61	
6:I:12:TCP:H71	5:A:392:TRP:CD2	2.36	0.61	
5:A:228:TYR:CE2	5:A:232:ARG:HD2	2.36	0.61	
5:C:392:TRP:O	5:C:404:ARG:NH1	2.34	0.60	
5:D:348:HIS:CD2	5:D:350:ARG:H	2.21	0.59	
5:D:403:LEU:O	5:D:404:ARG:CB	2.47	0.59	
5:B:192:THR:OG1	5:B:195:GLN:HG3	2.02	0.59	
5:A:275:ASN:O	5:A:279:VAL:HG23	2.03	0.58	
5:C:348:HIS:CD2	5:C:350:ARG:H	2.20	0.58	
5:B:60:GLN:HG2	5:B:190:LEU:HD23	1.84	0.58	
5:A:348:HIS:CD2	5:A:350:ARG:H	2.20	0.58	
5:C:348:HIS:HD2	5:C:350:ARG:H	1.51	0.58	
5:D:399:ASP:N	5:D:400:PRO:HD3	2.19	0.58	
5:C:60:GLN:HG2	5:C:190:LEU:HD23	1.86	0.57	
5:B:160:PRO:HG2	12:B:9119:HOH:O	2.04	0.57	
5:C:399:ASP:N	5:C:400:PRO:HD3	2.19	0.57	
5:B:348:HIS:CD2	5:B:350:ARG:H	2.21	0.57	
5:A:269:ARG:HH21	5:B:219:GLU:HA	1.67	0.57	
5:D:348:HIS:HD2	5:D:350:ARG:H	1.51	0.57	
5:C:276:SER:HB2	12:C:7764:HOH:O	2.03	0.57	
5:A:192:THR:OG1	5:A:195:GLN:HG3	2.05	0.57	
5:C:34:LEU:CD1	5:C:76:LEU:HD13	2.35	0.56	
5:B:348:HIS:HD2	5:B:350:ARG:H	1.53	0.56	
5:D:192:THR:OG1	5:D:195:GLN:HG3	2.05	0.56	
5:C:321:PHE:HB2	5:C:365:ILE:HD13	1.86	0.56	
5:C:248:LYS:HD3	5:C:248:LYS:C	2.26	0.56	
6:K:12:TCP:H71	5:B:392:TRP:CD2	2.40	0.56	
5:C:400:PRO:O	5:C:401:LYS:HB3	2.06	0.56	
5:D:405:ILE:HD12	5:D:461:GLN:HG3	1.86	0.56	
5:B:427:PRO:HA	5:B:430:ARG:NE	2.21	0.55	
5:C:427:PRO:HA	5:C:430:ARG:NE	2.22	0.55	
5:B:248:LYS:HD3	5:B:248:LYS:C	2.27	0.55	
5:A:43:GLN:NE2	5:C:43:GLN:O	2.40	0.54	
5:C:15:LEU:HD22	5:C:65:ARG:HB3	1.89	0.54	
5:A:305:TYR:CE1	5:A:398:MET:HG2	2.42	0.54	
5:A:348:HIS:HD2	5:A:350:ARG:H	1.54	0.54	
5:D:147:SER:O	5:D:399:ASP:N	2.40	0.54	
5:C:401:LYS:CB	5:C:402:PRO:HD2	2.17	0.54	
5:A:306:ARG:CZ	5:A:400:PRO:HG3	2.38	0.53	
5:B:308:LEU:C	5:B:308:LEU:HD23	2.29	0.53	
5:C:401:LYS:CD	5:C:404:ARG:HH21	2.21	0.53	



Interatomic Clash					
Atom-1	Atom-2	distance (Å)	overlap (Å)		
5:D:321:PHE:HB2	5:D:365:ILE:HD13	1.91	0.53		
2:L:9:DA:C2	5:B:402:PRO:HD3	2.43	0.53		
5:D:472:LYS:O	5:D:475:ILE:HG22	2.09	0.53		
5:C:308:LEU:C	5:C:308:LEU:HD23	2.30	0.52		
5:D:160:PRO:HG2	12:D:8603:HOH:O	2.08	0.52		
5:B:228:TYR:CE2	5:B:232:ARG:HD2	2.44	0.52		
5:B:34:LEU:CD1	5:B:76:LEU:HD13	2.39	0.52		
5:A:321:PHE:HB2	5:A:365:ILE:HD13	1.92	0.52		
5:B:75:LEU:C	5:B:76:LEU:HD12	2.30	0.52		
5:D:232:ARG:HD2	12:D:8648:HOH:O	2.10	0.52		
5:D:248:LYS:HD3	5:D:248:LYS:C	2.29	0.51		
5:D:404:ARG:NH2	5:D:465:LYS:HZ3	2.07	0.51		
5:C:447:ARG:HB2	5:C:450:TYR:HB3	1.91	0.51		
5:C:473:ALA:C	5:C:475:ILE:H	2.14	0.51		
5:C:75:LEU:C	5:C:76:LEU:HD12	2.31	0.51		
5:A:86:GLN:HE21	5:C:195:GLN:CG	2.21	0.51		
5:A:306:ARG:HB2	5:A:397:GLY:O	2.09	0.51		
6:I:12:TCP:H71	5:A:392:TRP:CE2	2.45	0.51		
5:C:64:GLN:O	5:C:68:GLN:HG3	2.11	0.50		
5:B:447:ARG:HB2	5:B:450:TYR:HB3	1.92	0.50		
5:C:445:ILE:HD12	5:C:446:GLU:N	2.26	0.50		
5:D:34:LEU:HD21	5:D:84:ILE:CD1	2.42	0.49		
5:A:445:ILE:HG13	12:A:9409:HOH:O	2.11	0.49		
5:D:459:LEU:HG	5:D:463:GLN:HE21	1.76	0.49		
5:A:40:GLN:HG2	12:A:9283:HOH:O	2.12	0.49		
5:B:445:ILE:HD12	5:B:446:GLU:N	2.27	0.49		
5:A:269:ARG:NH2	5:B:219:GLU:HG2	2.27	0.49		
12:A:9218:HOH:O	5:B:269:ARG:HG2	2.12	0.49		
5:D:308:LEU:C	5:D:308:LEU:HD23	2.32	0.49		
5:A:34:LEU:HD21	5:A:84:ILE:CD1	2.43	0.49		
5:A:98:TRP:CE2	5:A:126:GLN:HG2	2.47	0.49		
5:B:43:GLN:O	5:D:43:GLN:NE2	2.42	0.49		
5:B:401:LYS:HE3	12:B:9267:HOH:O	2.12	0.49		
5:A:175:SER:OG	5:A:177:GLU:HG2	2.13	0.49		
5:B:306:ARG:HB2	5:B:397:GLY:O	2.13	0.49		
6:K:12:TCP:H71	5:B:392:TRP:CE2	2.47	0.49		
5:D:405:ILE:CD1	5:D:461:GLN:HG3	2.41	0.49		
5:A:340:GLN:HG2	5:A:346:TRP:O	2.12	0.48		
6:K:12:TCP:C6	5:B:353:MET:SD	3.01	0.48		
6:I:12:TCP:C6	5:A:353:MET:SD	3.02	0.48		
1:K:7:DT:H2"	6:K:12:TCP:O5'	2.12	0.48		



		Interatomic	Clash
Atom-1 Atom-2		distance (\AA)	overlap (Å)
5:D:85:PRO:O	5:D:89:GLN:HG3	2.14	0.48
5:A:248:LYS:HD3	5:A:248:LYS:C	2.33	0.48
5:B:321:PHE:HB2	5:B:365:ILE:HD13	1.95	0.48
5:D:75:LEU:C	5:D:76:LEU:HD12	2.34	0.48
5:D:340:GLN:HG2	5:D:346:TRP:O	2.13	0.48
5:D:414:LYS:HG3	12:D:8833:HOH:O	2.13	0.48
1:K:7:DT:H72	6:K:12:TCP:C5M	2.39	0.48
2:L:7:DG:H1'	2:L:8:DA:O5'	2.14	0.48
1:I:7:DT:H2"	6:I:12:TCP:O5'	2.14	0.47
5:B:60:GLN:HG2	5:B:190:LEU:CD2	2.44	0.47
1:I:1:DA:H2"	1:I:2:DT:C6	2.49	0.47
5:A:308:LEU:HD23	5:A:308:LEU:C	2.33	0.47
5:B:60:GLN:O	5:B:64:GLN:HG3	2.14	0.47
5:D:183:ALA:N	5:D:184:PRO:HD2	2.28	0.47
5:C:60:GLN:HG2	5:C:190:LEU:CD2	2.44	0.47
5:C:397:GLY:O	5:C:400:PRO:HG3	2.15	0.47
5:A:75:LEU:C	5:A:76:LEU:HD12	2.35	0.47
5:B:472:LYS:O	5:B:475:ILE:HG22	2.14	0.47
5:D:153:TRP:CH2	5:D:282:GLN:HG2	2.50	0.47
5:D:404:ARG:HH21	5:D:465:LYS:HZ3	1.63	0.47
5:B:427:PRO:HB3	5:B:430:ARG:CZ	2.44	0.47
5:D:275:ASN:O	5:D:279:VAL:HG23	2.15	0.47
5:B:43:GLN:OE1	5:B:43:GLN:HA	2.14	0.47
5:B:222:ASP:O	5:B:223:ARG:HD3	2.16	0.46
5:B:176:PRO:HD2	5:B:177:GLU:OE2	2.16	0.46
5:C:153:TRP:CH2	5:C:282:GLN:HG2	2.50	0.46
5:C:472:LYS:O	5:C:475:ILE:HG22	2.15	0.46
5:A:183:ALA:HB3	5:A:184:PRO:HD3	1.97	0.46
5:B:339:ARG:HD3	12:B:9357:HOH:O	2.16	0.46
5:D:404:ARG:NH2	5:D:465:LYS:HZ1	2.14	0.46
5:B:63:GLN:O	5:B:67:GLN:HG3	2.15	0.46
5:D:194:LYS:NZ	12:D:8744:HOH:O	2.48	0.46
5:D:98:TRP:CE2	5:D:126:GLN:HG2	2.50	0.46
5:A:82:HIS:ND1	5:C:194:LYS:NZ	2.51	0.46
5:A:145:PRO:HB3	5:A:296:HIS:CD2	2.51	0.46
5:B:15:LEU:HD22	5:B:65:ARG:HB3	1.97	0.46
5:C:20:GLY:HA2	5:C:127:LEU:HD12	1.97	0.46
5:D:445:ILE:HG13	12:D:8837:HOH:O	2.16	0.46
1:K:1:DA:H2"	1:K:2:DT:C6	2.50	0.45
1:K:1:DA:H2"	1:K:2:DT:H72	1.99	0.45
5:A:153:TRP:CH2	5:A:282:GLN:HG2	2.51	0.45



Interatomic C				
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:J:7:DG:H1'	2:J:8:DA:O5'	2.15	0.45	
5:A:177:GLU:CD	5:A:177:GLU:H	2.20	0.45	
5:A:305:TYR:CD1	5:A:398:MET:HG2	2.51	0.45	
5:A:311:GLN:CD	5:A:475:ILE:HD11	2.36	0.45	
5:C:401:LYS:CG	5:C:404:ARG:NH2	2.67	0.45	
5:C:443:THR:HG23	12:C:7767:HOH:O	2.16	0.45	
5:C:401:LYS:HD2	5:C:404:ARG:HE	1.80	0.45	
5:B:183:ALA:HB3	5:B:184:PRO:HD3	1.97	0.45	
5:D:404:ARG:NH1	5:D:461:GLN:OE1	2.49	0.45	
5:A:348:HIS:HE1	12:A:9025:HOH:O	2.00	0.45	
1:I:1:DA:H2"	1:I:2:DT:H72	1.98	0.44	
5:D:404:ARG:HD3	5:D:405:ILE:N	2.31	0.44	
5:A:234:PHE:HA	5:A:235:PRO:HD2	1.94	0.44	
5:B:175:SER:OG	5:B:177:GLU:HG2	2.17	0.44	
5:C:340:GLN:HG2	5:C:346:TRP:O	2.16	0.44	
5:C:63:GLN:O	5:C:67:GLN:HG3	2.18	0.44	
5:A:435:LYS:HB2	5:A:435:LYS:HE3	1.85	0.44	
2:J:8:DA:H2"	5:A:402:PRO:HG3	1.99	0.44	
5:B:177:GLU:CD	5:B:177:GLU:H	2.21	0.44	
5:B:306:ARG:CZ	5:B:400:PRO:HG3	2.48	0.44	
5:C:98:TRP:CE2	5:C:126:GLN:HG2	2.52	0.44	
5:C:244:SER:HB3	10:C:7485:FAD:C5'	2.47	0.43	
2:J:7:DG:H2"	2:J:8:DA:O5'	2.18	0.43	
5:C:176:PRO:HD2	5:C:177:GLU:OE2	2.18	0.43	
5:D:456:ASN:O	5:D:460:ARG:HG2	2.18	0.43	
5:B:194:LYS:NZ	5:D:82:HIS:ND1	2.53	0.43	
5:C:401:LYS:HB3	5:C:401:LYS:NZ	2.33	0.43	
5:C:459:LEU:O	5:C:463:GLN:HG3	2.18	0.43	
1:I:1:DA:H2"	1:I:2:DT:C7	2.48	0.43	
5:B:473:ALA:C	5:B:475:ILE:H	2.22	0.43	
5:B:64:GLN:HB3	12:B:9210:HOH:O	2.18	0.43	
5:D:404:ARG:HH22	5:D:465:LYS:HZ1	1.67	0.43	
5:B:340:GLN:HG2	5:B:346:TRP:O	2.17	0.43	
5:D:244:SER:HB3	10:D:8485:FAD:C5'	2.48	0.43	
5:A:405:ILE:HG21	5:A:461:GLN:HG3	2.00	0.43	
5:A:471:LEU:O	5:A:475:ILE:HB	2.19	0.43	
5:B:315:GLU:HG2	5:B:317:ARG:HG3	2.01	0.43	
5:C:64:GLN:HB3	12:C:7727:HOH:O	2.17	0.43	
5:B:275:ASN:O	5:B:279:VAL:HG23	2.19	0.43	
5:B:305:TYR:CD1	5:B:398:MET:HB3	2.53	0.43	
5:C:83:LEU:HD22	12:C:7779:HOH:O	2.18	0.43	



Interatomic Clash				
Atom-1	Atom-2	distance (Å)	overlap (Å)	
5:C:401:LYS:CG	5:C:404:ARG:HE	2.32	0.43	
5:D:158:ALA:HB3	12:D:8776:HOH:O	2.19	0.43	
1:K:1:DA:H2"	1:K:2:DT:C7	2.49	0.43	
5:B:244:SER:HB3	10:B:6485:FAD:C5'	2.49	0.43	
3:O:9:DC:H2"	3:O:10:DG:OP2	2.17	0.42	
5:C:183:ALA:N	5:C:184:PRO:HD2	2.34	0.42	
5:C:214:ILE:O	5:C:218:GLN:HG3	2.19	0.42	
5:D:194:LYS:CD	12:D:8744:HOH:O	2.66	0.42	
5:D:459:LEU:O	5:D:463:GLN:HG3	2.19	0.42	
5:A:76:LEU:HD23	5:A:83:LEU:HB3	2.00	0.42	
1:I:7:DT:H72	6:I:12:TCP:C5M	2.42	0.42	
5:A:60:GLN:HG2	5:A:190:LEU:HD23	2.01	0.42	
5:A:305:TYR:O	5:A:310:GLN:NE2	2.52	0.42	
5:A:433:HIS:ND1	5:A:434:PRO:HD2	2.34	0.42	
2:L:9:DA:H2"	2:L:10:DG:O5'	2.19	0.42	
2:L:13:DG:C5'	5:B:151:PRO:HG2	2.49	0.42	
5:D:5:ILE:HD12	5:D:28:SER:HB3	2.02	0.42	
5:D:219:GLU:HG3	12:D:8642:HOH:O	2.19	0.42	
5:A:85:PRO:O	5:A:89:GLN:HG3	2.20	0.42	
5:A:475:ILE:HG23	5:A:475:ILE:OXT	2.19	0.42	
5:A:471:LEU:HD11	5:A:475:ILE:HD12	2.02	0.42	
5:D:187:LEU:HD12	5:D:187:LEU:HA	1.95	0.42	
4:P:11:DC:H2"	4:P:12:DC:C5	2.55	0.42	
5:C:34:LEU:HD21	5:C:84:ILE:CD1	2.49	0.42	
5:C:147:SER:O	5:C:399:ASP:N	2.50	0.42	
5:D:34:LEU:HD21	5:D:84:ILE:HD12	2.00	0.42	
5:D:404:ARG:HD3	5:D:405:ILE:H	1.84	0.42	
5:C:447:ARG:O	5:C:448:ARG:C	2.58	0.42	
2:L:7:DG:H2"	2:L:8:DA:O5'	2.20	0.41	
5:C:392:TRP:HD1	12:C:7668:HOH:O	2.03	0.41	
5:A:219:GLU:HG3	12:A:9159:HOH:O	2.20	0.41	
5:C:427:PRO:HB3	5:C:430:ARG:CZ	2.50	0.41	
5:A:306:ARG:HH22	5:A:308:LEU:HD13	1.85	0.41	
5:B:85:PRO:O	5:B:89:GLN:HG3	2.21	0.41	
5:C:12:ASP:N	5:C:12:ASP:OD1	2.54	0.41	
5:C:177:GLU:CD	5:C:177:GLU:H	2.23	0.41	
5:A:443:THR:OG1	5:A:446:GLU:HG3	2.21	0.41	
5:A:456:ASN:O	5:A:460:ARG:HG2	2.21	0.41	
5:B:447:ARG:O	5:B:448:ARG:C	2.59	0.41	
5:C:34:LEU:HD21	5:C:84:ILE:HD12	2.03	0.41	
5:D:398:MET:HE2	5:D:398:MET:HA	2.03	0.41	



Atom-1	Atom-2	Interatomic	Clash
	1100111-2	distance $(Å)$	overlap (Å)
5:C:190:LEU:HD12	5:C:191:PRO:HD2	2.03	0.40
2:J:9:DA:H2"	2:J:10:DG:O5'	2.21	0.40
5:B:20:GLY:HA2	5:B:127:LEU:HD12	2.03	0.40
5:B:145:PRO:HB3	5:B:296:HIS:CD2	2.56	0.40
5:D:145:PRO:HB3	5:D:296:HIS:CD2	2.55	0.40
5:A:187:LEU:HD12	5:A:187:LEU:HA	1.96	0.40
5:D:126:GLN:NE2	12:D:8518:HOH:O	2.55	0.40
5:A:358:PHE:O	5:A:362:ASP:HB2	2.22	0.40
5:B:443:THR:HG23	12:B:9276:HOH:O	2.21	0.40
5:C:175:SER:OG	5:C:177:GLU:HG2	2.22	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	Perce	ntiles
5	А	472/474~(100%)	457 (97%)	15 (3%)	0	100	100
5	В	472/474~(100%)	458 (97%)	14 (3%)	0	100	100
5	С	472/474~(100%)	454 (96%)	15 (3%)	3~(1%)	25	12
5	D	472/474~(100%)	453~(96%)	18 (4%)	1 (0%)	47	33
All	All	1888/1896~(100%)	1822 (96%)	62 (3%)	4 (0%)	47	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	404	ARG
5	С	474	ALA
5	С	402	PRO
5	С	401	LYS



5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
5	А	383/385~(100%)	377~(98%)	6~(2%)	62	54
5	В	385/385~(100%)	377~(98%)	8 (2%)	53	42
5	С	383/385~(100%)	376~(98%)	7~(2%)	59	48
5	D	384/385~(100%)	378~(98%)	6 (2%)	62	54
All	All	1535/1540~(100%)	1508~(98%)	27~(2%)	59	48

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
5	А	102	ILE
5	А	157	GLN
5	А	230	PRO
5	А	248	LYS
5	А	306	ARG
5	А	475	ILE
5	В	43	GLN
5	В	90	GLN
5	В	102	ILE
5	В	157	GLN
5	В	230	PRO
5	В	248	LYS
5	В	271	ASP
5	В	306	ARG
5	С	90	GLN
5	С	102	ILE
5	С	157	GLN
5	С	230	PRO
5	С	248	LYS
5	С	398	MET
5	С	401	LYS
5	D	102	ILE
5	D	157	GLN
5	D	230	PRO



 $Continued \ from \ previous \ page...$

Mol	Chain	Res	Type
5	D	248	LYS
5	D	398	MET
5	D	404	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
5	А	63	GLN
5	А	77	GLN
5	А	86	GLN
5	А	112	GLN
5	А	126	GLN
5	А	157	GLN
5	А	310	GLN
5	А	328	GLN
5	А	348	HIS
5	А	372	GLN
5	А	376	GLN
5	А	386	ASN
5	А	461	GLN
5	А	463	GLN
5	В	60	GLN
5	В	63	GLN
5	В	77	GLN
5	В	90	GLN
5	В	112	GLN
5	В	126	GLN
5	В	157	GLN
5	В	218	GLN
5	В	259	GLN
5	В	348	HIS
5	В	372	GLN
5	В	376	GLN
5	В	386	ASN
5	В	461	GLN
5	С	63	GLN
5	С	77	GLN
5	С	90	GLN
5	С	112	GLN
5	С	126	GLN
5	С	157	GLN
5	С	348	HIS



Mol	Chain	Res	Type
5	С	372	GLN
5	С	376	GLN
5	С	386	ASN
5	С	461	GLN
5	D	63	GLN
5	D	77	GLN
5	D	86	GLN
5	D	126	GLN
5	D	157	GLN
5	D	328	GLN
5	D	348	HIS
5	D	372	GLN
5	D	376	GLN
5	D	386	ASN
5	D	463	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	Bos	Link	Bo	ond leng	ths	E	ond ang	gles
WIOI	Type	Ullalli	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
10	FAD	С	7485	-	$53,\!58,\!58$	1.22	5 (9%)	68,89,89	1.08	5 (7%)
11	HDF	С	7486	-	$25,\!28,\!28$	2.56	4 (16%)	29,41,41	4.41	10 (34%)
10	FAD	D	8485	-	$53,\!58,\!58$	1.28	6 (11%)	68,89,89	1.06	5 (7%)
6	TCP	K	12	1	19,19,19	0.27	0	27,27,27	0.63	0
6	TCP	Ι	12	1	19,19,19	0.24	0	27,27,27	0.61	0
8	G	Κ	14	-	18,24,26	1.01	2 (11%)	19,35,40	0.66	1 (5%)
7	С	К	15	-	17,20,22	0.32	0	24,28,33	0.48	0
8	G	Ι	14	-	18,24,26	1.01	2 (11%)	19,35,40	0.66	1 (5%)
11	HDF	В	6486	-	25,28,28	2.48	4 (16%)	29,41,41	4.42	9 (31%)
11	HDF	А	5486	-	25,28,28	2.61	4 (16%)	29,41,41	4.46	10 (34%)
10	FAD	В	6485	-	$53,\!58,\!58$	1.28	5 (9%)	68,89,89	1.06	5 (7%)
11	HDF	D	8486	-	25,28,28	2.67	4 (16%)	29,41,41	4.40	9 (31%)
7	С	Ι	15	-	17,20,22	0.33	0	24,28,33	0.48	0
10	FAD	А	5485	-	53,58,58	1.23	6 (11%)	68,89,89	1.04	5 (7%)
7	С	Ι	13	-	17,20,22	0.33	0	24,28,33	0.31	0
7	С	K	13	-	17,20,22	0.36	0	24,28,33	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	FAD	С	7485	-	-	5/30/50/50	0/6/6/6
11	HDF	С	7486	-	2/2/3/3	6/14/14/14	0/3/3/3
10	FAD	D	8485	-	-	5/30/50/50	0/6/6/6
6	TCP	Κ	12	1	-	4/7/19/19	0/2/2/2
7	С	Ι	15	-	-	4/7/21/26	0/2/2/2
8	G	Κ	14	-	-	0/3/21/26	0/3/3/3
7	С	К	15	-	-	4/7/21/26	0/2/2/2
11	HDF	В	6486	-	2/2/3/3	5/14/14/14	0/3/3/3
8	G	Ι	14	-	-	0/3/21/26	0/3/3/3
11	HDF	А	5486	-	2/2/3/3	5/14/14/14	0/3/3/3
11	HDF	D	8486	-	2/2/3/3	5/14/14/14	0/3/3/3
10	FAD	В	6485	-	-	5/30/50/50	0/6/6/6
6	TCP	Ι	12	1	-	4/7/19/19	0/2/2/2
10	FAD	А	5485	-	-	5/30/50/50	0/6/6/6



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	С	Ι	13	-	-	0/7/21/26	0/2/2/2
7	С	Κ	13	-	-	0/7/21/26	0/2/2/2

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	8486	HDF	C1'-N10	-10.40	1.37	1.48
11	А	5486	HDF	C1'-N10	-10.22	1.37	1.48
11	С	7486	HDF	C1'-N10	-9.69	1.38	1.48
11	В	6486	HDF	C1'-N10	-9.38	1.38	1.48
11	D	8486	HDF	C10-N1	5.25	1.40	1.33
11	А	5486	HDF	C10-N1	5.03	1.39	1.33
11	С	7486	HDF	C4-N3	5.02	1.41	1.33
10	D	8485	FAD	C4X-N5	4.91	1.40	1.30
10	В	6485	FAD	C4X-N5	4.90	1.40	1.30
11	С	7486	HDF	C10-N1	4.86	1.39	1.33
10	А	5485	FAD	C4X-N5	4.84	1.40	1.30
11	В	6486	HDF	C10-N1	4.76	1.39	1.33
11	В	6486	HDF	C4-N3	4.72	1.41	1.33
11	D	8486	HDF	C4-N3	4.62	1.41	1.33
10	С	7485	FAD	C4X-N5	4.47	1.39	1.30
11	А	5486	HDF	C4-N3	4.37	1.40	1.33
10	В	6485	FAD	O4B-C1B	2.72	1.44	1.41
10	А	5485	FAD	C9A-C5X	2.70	1.45	1.41
11	А	5486	HDF	C4A-C10	2.57	1.43	1.41
10	С	7485	FAD	C9A-C5X	2.57	1.45	1.41
10	D	8485	FAD	C9A-C5X	2.52	1.45	1.41
10	В	6485	FAD	C9A-C5X	2.47	1.45	1.41
8	Ι	14	G	C8-N7	-2.44	1.30	1.35
8	K	14	G	C5-C6	-2.42	1.42	1.47
11	D	8486	HDF	C4A-C10	2.41	1.43	1.41
8	Ι	14	G	C5-C6	-2.40	1.42	1.47
10	В	6485	FAD	C2A-N3A	2.38	1.35	1.32
10	А	5485	FAD	O4B-C1B	2.37	1.44	1.41
10	D	8485	FAD	C2A-N3A	2.37	1.35	1.32
8	K	14	G	C8-N7	-2.34	1.31	1.35
10	С	7485	FAD	O4B-C1B	2.32	1.44	1.41
10	С	7485	FAD	C2A-N3A	2.32	1.35	1.32
11	В	6486	HDF	C4A-C10	2.31	1.43	1.41
11	С	7486	HDF	C4A-C10	2.21	1.43	1.41
10	D	8485	FAD	C10-N1	2.21	1.37	1.33
10	С	7485	FAD	C2A-N1A	2.16	1.37	1.33



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
10	А	5485	FAD	C2A-N3A	2.15	1.35	1.32
10	В	6485	FAD	C10-N1	2.12	1.37	1.33
10	А	5485	FAD	C10-N1	2.12	1.37	1.33
10	D	8485	FAD	C2A-N1A	2.09	1.37	1.33
10	D	8485	FAD	O4B-C1B	2.08	1.44	1.41
10	А	5485	FAD	C2A-N1A	2.03	1.37	1.33

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
11	С	7486	HDF	C4A-C4-N3	-15.45	113.63	124.40
11	А	5486	HDF	C4A-C4-N3	-15.36	113.69	124.40
11	В	6486	HDF	C4A-C4-N3	-15.34	113.70	124.40
11	D	8486	HDF	C4A-C4-N3	-15.12	113.86	124.40
11	А	5486	HDF	C2-N3-C4	13.27	126.35	115.14
11	D	8486	HDF	C2-N3-C4	13.04	126.15	115.14
11	В	6486	HDF	C2-N3-C4	12.80	125.95	115.14
11	С	7486	HDF	C2-N3-C4	12.61	125.79	115.14
11	А	5486	HDF	C1'-N10-C9A	7.79	124.42	118.29
11	D	8486	HDF	C1'-N10-C9A	7.77	124.41	118.29
11	В	6486	HDF	C1'-N10-C9A	7.67	124.33	118.29
11	С	7486	HDF	C1'-N10-C9A	7.56	124.24	118.29
11	D	8486	HDF	C1'-C2'-C3'	4.24	121.65	109.79
11	В	6486	HDF	C1'-C2'-C3'	4.24	121.64	109.79
11	С	7486	HDF	C1'-C2'-C3'	4.22	121.58	109.79
11	А	5486	HDF	C1'-C2'-C3'	4.20	121.52	109.79
11	В	6486	HDF	C9A-N10-C10	-4.07	116.57	121.91
11	С	7486	HDF	C9A-N10-C10	-4.05	116.60	121.91
11	D	8486	HDF	C9A-N10-C10	-4.03	116.63	121.91
11	С	7486	HDF	C5A-C9A-N10	4.00	122.63	118.71
11	А	5486	HDF	C9A-N10-C10	-3.99	116.69	121.91
11	В	6486	HDF	C5A-C9A-N10	3.91	122.54	118.71
11	D	8486	HDF	C5A-C9A-N10	3.83	122.46	118.71
11	А	5486	HDF	C5A-C9A-N10	3.81	122.45	118.71
11	С	7486	HDF	C10-C4A-C4	3.80	124.08	119.99
11	А	5486	HDF	C10-C4A-C4	3.77	124.05	119.99
11	D	8486	HDF	C10-C4A-C4	3.73	124.01	119.99
11	В	6486	HDF	C10-C4A-C4	3.72	124.00	119.99
11	С	7486	HDF	O3'-C3'-C2'	3.29	116.76	108.81
11	В	6486	HDF	O3'-C3'-C2'	3.22	116.60	108.81
11	D	8486	HDF	O3'-C3'-C2'	3.02	116.12	108.81
11	А	5486	HDF	O3'-C3'-C2'	2.98	116.02	108.81



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
11	В	6486	HDF	O2'-C2'-C1'	2.94	116.68	109.59
10	D	8485	FAD	C9A-C5X-N5	-2.86	119.32	122.43
11	С	7486	HDF	O2'-C2'-C1'	2.84	116.44	109.59
10	В	6485	FAD	C9A-C5X-N5	-2.81	119.38	122.43
11	А	5486	HDF	O2'-C2'-C1'	2.74	116.19	109.59
10	А	5485	FAD	C9A-C5X-N5	-2.73	119.47	122.43
11	D	8486	HDF	O2'-C2'-C1'	2.69	116.08	109.59
10	С	7485	FAD	C9A-C5X-N5	-2.67	119.53	122.43
10	С	7485	FAD	C4-C4X-N5	2.49	121.78	118.23
10	А	5485	FAD	C4-C4X-N5	2.43	121.68	118.23
10	D	8485	FAD	C4-C4X-N5	2.40	121.65	118.23
10	А	5485	FAD	C5A-C6A-N6A	2.38	123.97	120.35
10	D	8485	FAD	C5A-C6A-N6A	2.31	123.87	120.35
10	С	7485	FAD	C5A-C6A-N6A	2.27	123.81	120.35
10	В	6485	FAD	C4-C4X-N5	2.26	121.44	118.23
10	С	7485	FAD	C10-C4X-N5	-2.24	120.10	124.86
10	В	6485	FAD	C5A-C6A-N6A	2.17	123.65	120.35
10	D	8485	FAD	N3A-C2A-N1A	-2.14	125.34	128.68
10	А	5485	FAD	N3A-C2A-N1A	-2.13	125.35	128.68
10	В	6485	FAD	N3A-C2A-N1A	-2.13	125.35	128.68
8	Ι	14	G	O6-C6-C5	2.12	128.52	124.37
10	D	8485	FAD	C10-C4X-N5	-2.11	120.38	124.86
8	K	14	G	O6-C6-C5	2.10	128.48	124.37
10	С	7485	FAD	N3A-C2A-N1A	-2.10	125.39	128.68
10	В	6485	FAD	C10-C4X-N5	-2.10	120.41	124.86
10	А	5485	FAD	C10-C4X-N5	-2.06	120.49	124.86
11	А	5486	HDF	C4'-C3'-C2'	2.04	117.60	113.36
11	С	7486	HDF	C4'-C3'-C2'	2.02	117.56	113.36

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All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	А	5486	HDF	C4'
11	А	5486	HDF	C2'
11	В	6486	HDF	C4'
11	В	6486	HDF	C2'
11	С	7486	HDF	C4'
11	С	7486	HDF	C2'
11	D	8486	HDF	C4'
11	D	8486	HDF	C2'

All (57) torsion outliers are listed below:



1TEZ

Mol	Chain	Res	Type	Atoms
10	А	5485	FAD	C5B-O5B-PA-O1A
10	В	6485	FAD	C5B-O5B-PA-O1A
11	А	5486	HDF	N10-C1'-C2'-O2'
11	А	5486	HDF	N10-C1'-C2'-C3'
11	А	5486	HDF	O2'-C2'-C3'-O3'
11	А	5486	HDF	O2'-C2'-C3'-C4'
11	В	6486	HDF	N10-C1'-C2'-O2'
11	В	6486	HDF	N10-C1'-C2'-C3'
11	В	6486	HDF	O2'-C2'-C3'-O3'
11	В	6486	HDF	O2'-C2'-C3'-C4'
11	С	7486	HDF	N10-C1'-C2'-O2'
11	С	7486	HDF	N10-C1'-C2'-C3'
11	С	7486	HDF	O2'-C2'-C3'-O3'
11	С	7486	HDF	O2'-C2'-C3'-C4'
11	D	8486	HDF	N10-C1'-C2'-O2'
11	D	8486	HDF	N10-C1'-C2'-C3'
11	D	8486	HDF	O2'-C2'-C3'-O3'
11	D	8486	HDF	O2'-C2'-C3'-C4'
11	С	7486	HDF	C2'-C3'-C4'-O4'
11	В	6486	HDF	C2'-C3'-C4'-O4'
6	Ι	12	TCP	C2'-C1'-N1-C6
6	Κ	12	TCP	C2'-C1'-N1-C6
7	Ι	15	С	C2'-C1'-N1-C6
7	K	15	С	C2'-C1'-N1-C6
10	С	7485	FAD	C4'-C5'-O5'-P
6	Ι	12	TCP	O4'-C1'-N1-C6
6	Κ	12	TCP	O4'-C1'-N1-C6
10	В	6485	FAD	C5B-O5B-PA-O3P
10	В	6485	FAD	P-O3P-PA-O1A
10	С	7485	FAD	P-O3P-PA-O1A
10	D	8485	FAD	P-O3P-PA-O1A
10	В	6485	FAD	C4'-C5'-O5'-P
10	С	7485	FAD	C5B-O5B-PA-O1A
7	Ι	15	С	O4'-C1'-N1-C6
7	K	15	С	C2'-C1'-N1-C2
7	K	15	С	O4'-C1'-N1-C6
6	Ι	12	TCP	C2'-C1'-N1-C2
6	K	12	TCP	C2'-C1'-N1-C2
7	Ι	15	C	C2'-C1'-N1-C2
6	Ι	12	TCP	O4'-C1'-N1-C2
10	А	5485	FAD	P-O3P-PA-O1A
10	А	5485	FAD	C4'-C5'-O5'-P
10	D	8485	FAD	C4'-C5'-O5'-P



11	$\mathbf{P}\mathbf{P}\mathbf{Z}$
Τ.	$\Gamma \Gamma \Delta$

Mol	Chain	Res	Type	Atoms
7	Ι	15	С	O4'-C1'-N1-C2
7	Κ	15	С	O4'-C1'-N1-C2
6	Κ	12	TCP	O4'-C1'-N1-C2
11	А	5486	HDF	C2'-C3'-C4'-O4'
11	D	8486	HDF	C2'-C3'-C4'-O4'
10	А	5485	FAD	C5B-O5B-PA-O3P
10	С	7485	FAD	C5B-O5B-PA-O3P
10	D	8485	FAD	C5B-O5B-PA-O3P
10	А	5485	FAD	C5'-O5'-P-O1P
10	В	6485	FAD	C5'-O5'-P-O1P
10	С	7485	FAD	C5'-O5'-P-O1P
10	D	8485	FAD	C5B-O5B-PA-O1A
10	D	8485	FAD	C5'-O5'-P-O1P
11	С	7486	HDF	C2'-C3'-C4'-C5'

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There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	С	7485	FAD	1	0
10	D	8485	FAD	1	0
6	Κ	12	TCP	6	0
6	Ι	12	TCP	6	0
10	В	6485	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.















































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, 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	Ι	7/11~(63%)	1.36	2(28%) 0	0	41, 52, 58, 60	7 (100%)
1	Κ	7/11~(63%)	1.76	3~(42%) 0	0	42, 52, 60, 60	7 (100%)
2	J	9/9~(100%)	1.37	2(22%) 0	0	37, 48, 62, 63	9 (100%)
2	L	9/9~(100%)	1.38	3~(33%)~0	0	42, 50, 62, 64	9 (100%)
3	М	4/4~(100%)	0.99	0 100 10	0	39, 47, 48, 51	4 (100%)
3	Ο	4/4 (100%)	2.30	2~(50%) 0	0	47, 52, 55, 56	4 (100%)
4	Ν	5/5~(100%)	5.23	5 (100%) 0	0	51, 53, 56, 59	5 (100%)
4	Р	5/5~(100%)	3.23	2 (40%) 0	0	43, 47, 55, 60	5 (100%)
5	А	474/474~(100%)	0.07	16 (3%) 45	39	15, 27, 48, 63	1 (0%)
5	В	474/474~(100%)	-0.03	14 (2%) 50	44	14, 26, 47, 65	2~(0%)
5	С	474/474~(100%)	0.06	19 (4%) 38	32	14, 25, 48, 65	0
5	D	474/474~(100%)	0.07	16 (3%) 45	39	16, 27, 48, 63	2(0%)
All	All	$194\overline{6/1954}\ (99\%)$	0.09	84 (4%) 35	29	14, 27, 50, 65	55 (2%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	А	2	ALA	8.1
5	С	2	ALA	7.9
4	Ν	10	DG	7.4
4	Р	10	DG	6.5
4	Ν	11	DC	5.9
5	D	2	ALA	5.9
5	В	475	ILE	5.9
5	В	305	TYR	5.7
5	С	404	ARG	5.6
4	Р	11	DC	5.2
5	С	475	ILE	5.2



Mol	Chain	Res	Type	RSRZ
5	А	475	ILE	5.2
4	N	13	DG	4.8
1	K	1	DA	4.6
4	N	14	DA	4.4
2	J	6	DC	4.3
5	D	305	TYR	4.3
5	А	305	TYR	4.0
5	С	392	TRP	3.9
5	D	405	ILE	3.9
5	В	2	ALA	3.8
5	А	308	LEU	3.7
5	D	404	ARG	3.7
4	N	12	DC	3.7
3	0	8	DT	3.6
5	D	475	ILE	3.5
5	А	396	SER	3.4
5	С	402	PRO	3.4
5	А	3	ALA	3.4
1	K	2	DT	3.3
5	В	473	ALA	3.3
1	Ι	1	DA	3.2
5	С	474	ALA	3.2
5	D	3	ALA	3.1
2	L	9	DA	3.1
5	В	177	GLU	2.9
5	В	474	ALA	2.9
5	D	403	LEU	2.9
5	В	396	SER	2.9
5	А	471	LEU	2.9
5	А	307	SER	2.9
5	С	269	ARG	2.8
5	С	473	ALA	2.8
5	C	443	THR	2.7
2	L	6	DC	2.7
5	C	445	ILE	2.7
5	С	177	GLU	2.7
5	D	445	ILE	2.6
5	D	311	GLN	2.6
3	0	11	DC	2.6
5	С	141	GLY	2.6
5	С	147	SER	2.6
5	D	395	SER	2.6



17	ΓEΖ

Mol	Chain	Res	Type	RSRZ
5	D	222	ASP	2.6
5	А	403	LEU	2.5
5	D	392	TRP	2.5
5	В	403	LEU	2.5
5	А	474	ALA	2.5
5	С	154	LYS	2.4
2	L	7	DG	2.4
5	В	445	ILE	2.4
5	А	466	ALA	2.4
5	С	268	SER	2.4
5	А	472	LYS	2.3
5	А	269	ARG	2.3
5	С	142	SER	2.2
5	С	151	PRO	2.2
5	D	472	LYS	2.2
1	Ι	2	DT	2.2
5	В	223	ARG	2.1
5	В	444	PRO	2.1
5	D	473	ALA	2.1
5	D	140	SER	2.1
5	А	468	TYR	2.1
5	А	222	ASP	2.1
5	А	469	ASN	2.1
5	В	222	ASP	2.1
5	С	307	SER	2.1
5	В	470	GLN	2.1
5	В	398	MET	2.0
5	D	142	SER	2.0
1	K	3	DC	2.0
2	J	9	DA	2.0
5	С	472	LYS	2.0

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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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
6	TCP	K	12	18/18	0.85	0.17	33,35,39,42	18
7	С	Ι	15	19/21	0.89	0.19	40,50,51,55	19
7	С	K	15	19/21	0.89	0.21	35,49,51,54	19
7	С	K	13	19/21	0.91	0.19	35,44,53,53	19
6	TCP	Ι	12	18/18	0.92	0.14	32,34,37,40	18
11	HDF	А	5486	26/26	0.92	0.10	13,18,25,29	0
11	HDF	D	8486	26/26	0.92	0.11	14,18,24,30	0
11	HDF	С	7486	26/26	0.93	0.10	12,16,19,23	0
7	С	Ι	13	19/21	0.94	0.17	35,43,52,55	19
11	HDF	В	6486	26/26	0.94	0.10	12,16,19,25	0
9	MG	А	9002	1/1	0.94	0.04	50,50,50,50	0
9	MG	В	9001	1/1	0.94	0.06	$51,\!51,\!51,\!51$	0
8	G	Ι	14	22/24	0.95	0.14	26,41,46,47	22
8	G	K	14	22/24	0.95	0.17	26,42,50,51	22
10	FAD	А	5485	53/53	0.97	0.09	13,16,18,19	0
10	FAD	В	6485	53/53	0.97	0.09	11,16,19,20	0
10	FAD	С	7485	53/53	0.97	0.09	12,16,19,19	0
10	FAD	D	8485	53/53	0.97	0.09	12,16,19,21	0

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



















































6.5 Other polymers (i)

There are no such residues in this entry.

