



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:05 AM GMT

PDB ID : 2VTB
Title : STRUCTURE OF CRYPTOCHROME 3 - DNA COMPLEX
Authors : Pokorny, R.; Klar, T.; Hennecke, U.; Carell, T.; Batschauer, A.; Essen, L.-O.
Deposited on : 2008-05-13
Resolution : 2.01 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

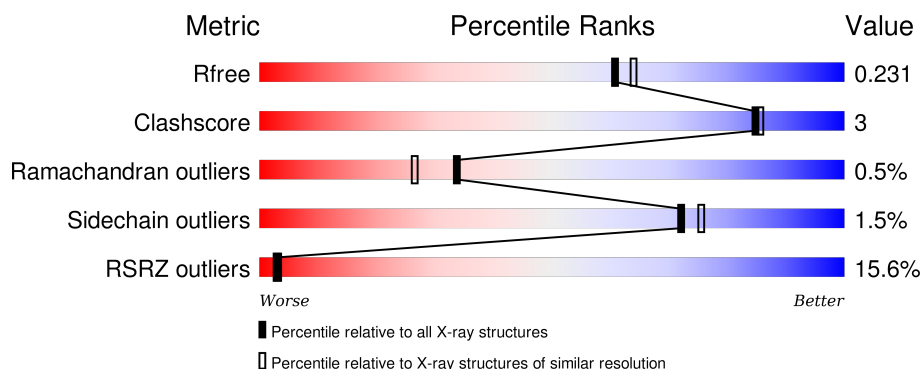
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	526	<div> <div>11%</div> <div>90%</div> <div>5%</div> </div>
1	C	526	<div> <div>14%</div> <div>89%</div> <div>5% 6%</div> </div>
1	D	526	<div> <div>13%</div> <div>87%</div> <div>8%</div> </div>
1	E	526	<div> <div>11%</div> <div>88%</div> <div>6% 6%</div> </div>
1	F	526	<div> <div>24%</div> <div>85%</div> <div>6% 9%</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	525	<div><div></div><div>13%</div><div>88%</div><div>6%</div><div>6%</div></div>
3	G	5	<div><div></div><div>40%</div><div>60%</div></div>
3	H	5	<div><div></div><div>40%</div><div>40%</div><div>20%</div></div>
3	I	5	<div><div></div><div>100%</div></div>
3	J	5	<div><div></div><div>20%</div><div>40%</div><div>40%</div><div>20%</div></div>
3	K	5	<div><div></div><div>20%</div><div>60%</div><div>20%</div></div>
3	L	5	<div><div></div><div>40%</div><div>40%</div><div>20%</div><div>20%</div></div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 26329 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 CRYPTOCHROME DASH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	1	0
			4068	2603	707	738	20			
1	C	495	Total	C	N	O	S	0	1	0
			4042	2593	699	730	20			
1	D	484	Total	C	N	O	S	43	7	0
			3933	2523	674	715	21			
1	E	496	Total	C	N	O	S	0	0	0
			4042	2591	700	731	20			
1	F	480	Total	C	N	O	S	0	1	0
			3896	2503	667	705	21			

- Molecule 2 is a protein called CRYPTOCHROME DASH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	491	Total	C	N	O	S	9	1	0
			3995	2564	688	723	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	353	ASN	GLN	CONFLICT	UNP Q84KJ5

- Molecule 3 is a DNA chain called 5'-D(*DT*DT*DT*DT*DTP)-3'.

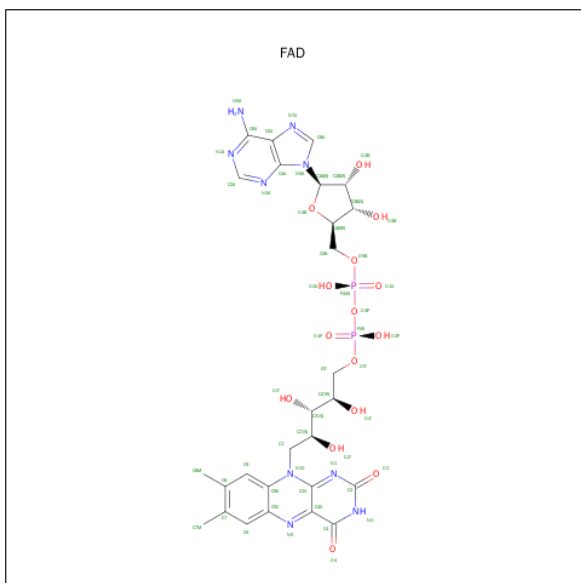
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	5	Total	C	N	O	P	0	0	0
			95	51	10	31	3			
3	H	5	Total	C	N	O	P	0	0	0
			95	51	10	31	3			
3	I	5	Total	C	N	O	P	0	0	0
			95	51	10	31	3			

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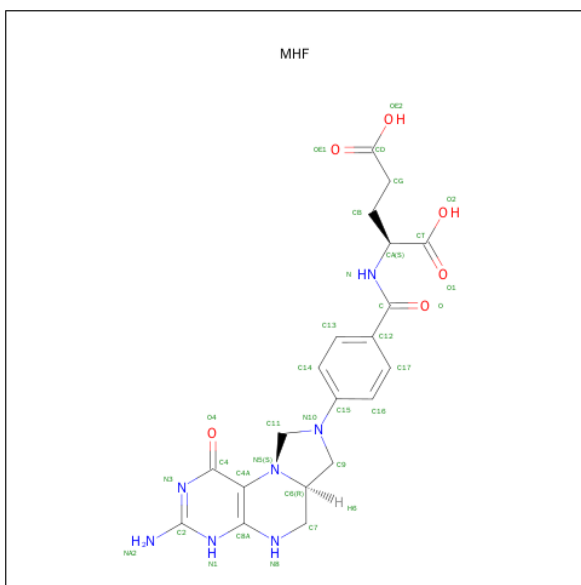
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	5	Total	C	N	O	P	9	0	0
			95	51	10	31	3			
3	K	4	Total	C	N	O	P	0	0	0
			78	41	8	26	3			
3	L	4	Total	C	N	O	P	0	0	0
			62	31	6	22	3			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is 5,10-METHENYL-6,7,8-TRIHYDROFOLIC ACID (three-letter code: MHF) (formula: $C_{20}H_{23}N_7O_6$).

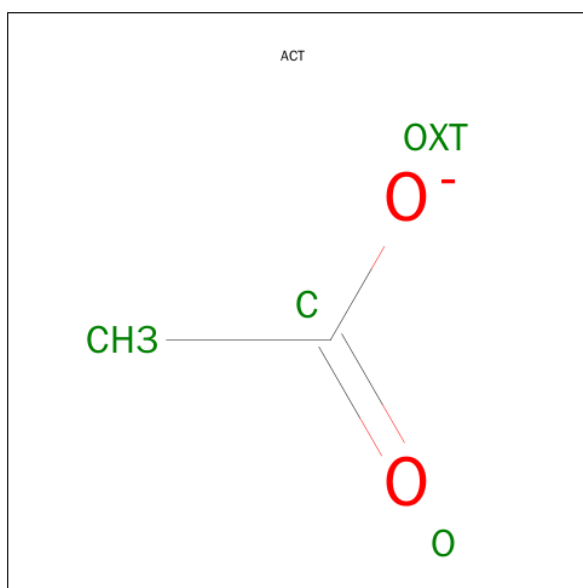


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			33	20	7	6		
5	B	1	Total	C	N	O	0	0
			33	20	7	6		
5	C	1	Total	C	N	O	0	0
			33	20	7	6		
5	D	1	Total	C	N	O	0	0
			33	20	7	6		
5	E	1	Total	C	N	O	0	0
			33	20	7	6		
5	F	1	Total	C	N	O	0	0
			33	20	7	6		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Cl	0	0
			1	1		
6	E	1	Total	Cl	0	0
			1	1		
6	B	2	Total	Cl	0	0
			2	2		
6	C	2	Total	Cl	0	0
			2	2		
6	A	1	Total	Cl	0	0
			1	1		
6	F	1	Total	Cl	0	0
			1	1		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	274	Total	O	0	0
			274	274		
8	B	178	Total	O	0	0
			178	178		
8	C	257	Total	O	0	0
			257	257		
8	D	209	Total	O	0	0
			209	209		
8	E	233	Total	O	0	0
			233	233		
8	F	120	Total	O	0	0
			120	120		
8	G	7	Total	O	0	0
			7	7		
8	H	4	Total	O	0	0
			4	4		
8	I	10	Total	O	0	0
			10	10		
8	J	5	Total	O	0	0
			5	5		

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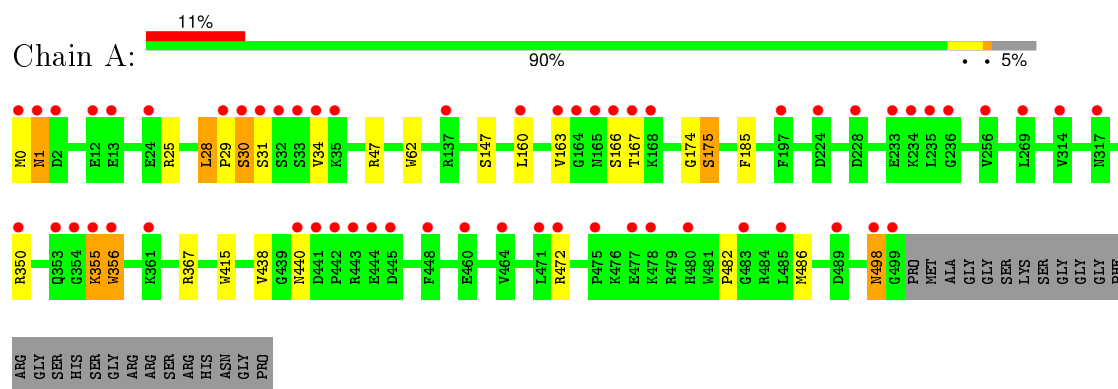
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	K	7	Total	O	0	0
			7	7		
8	L	1	Total	O	0	0
			1	1		

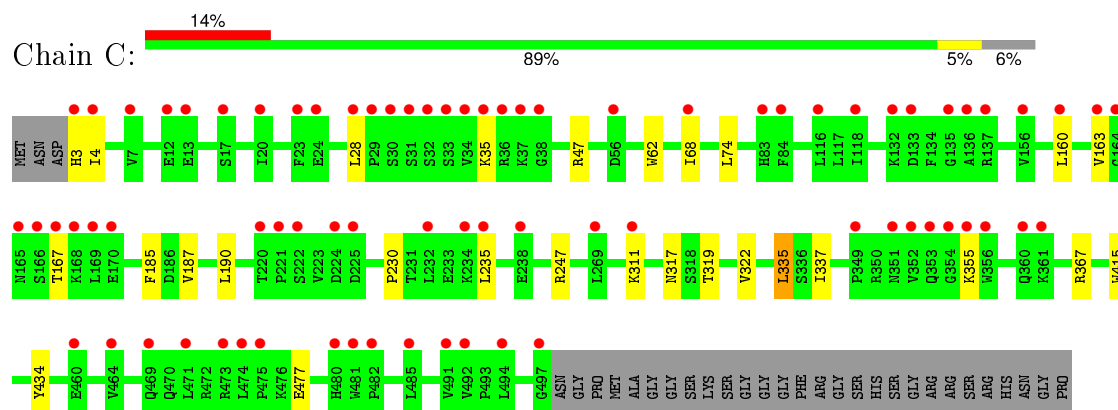
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

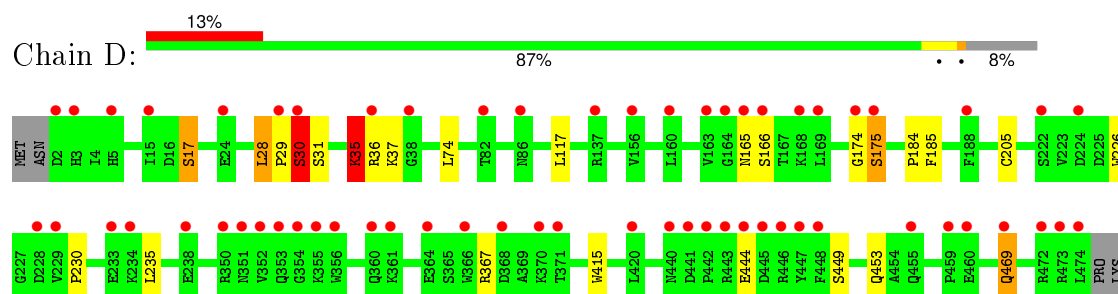
• Molecule 1: CRYPTOCHROME DASH

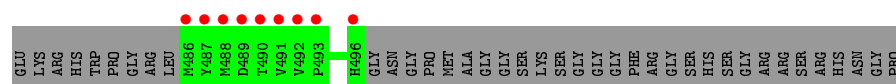


• Molecule 1: CRYPTOCHROME DASH

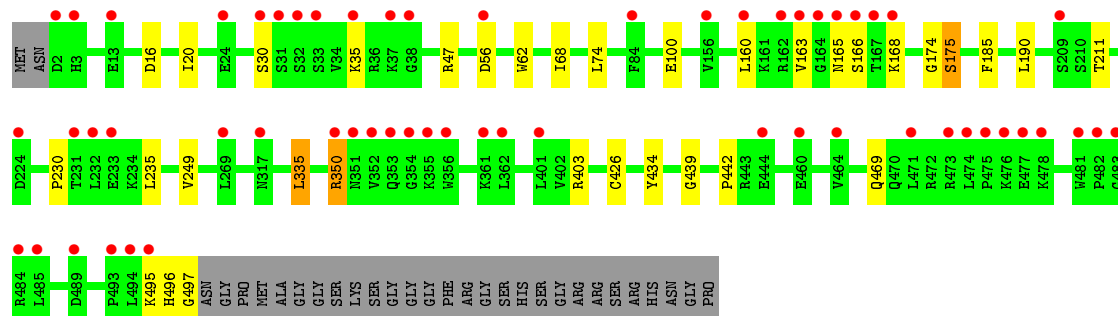
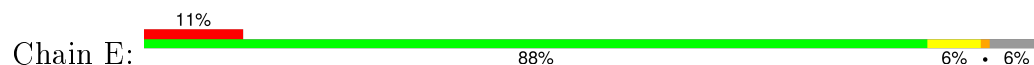


• Molecule 1: CRYPTOCHROME DASH

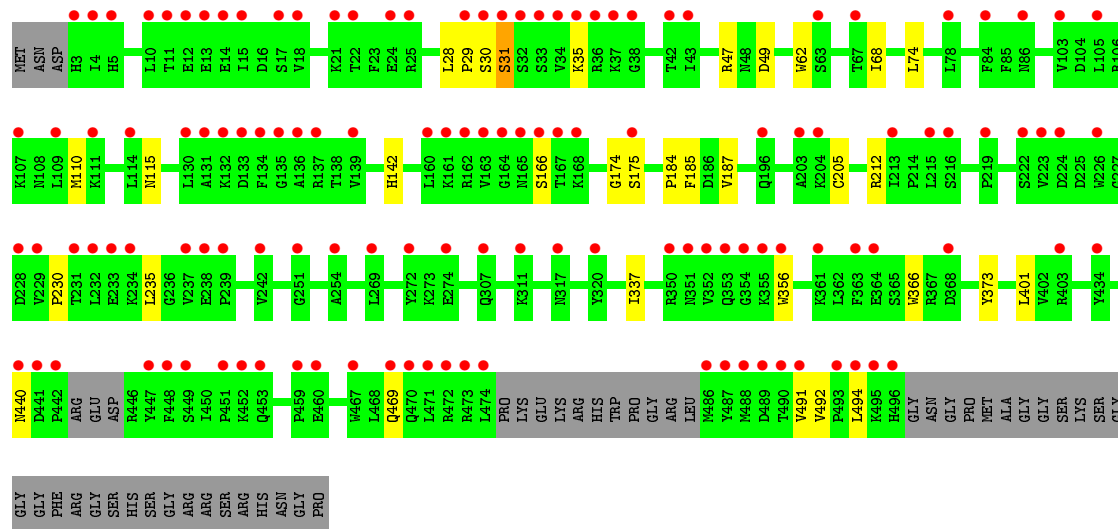
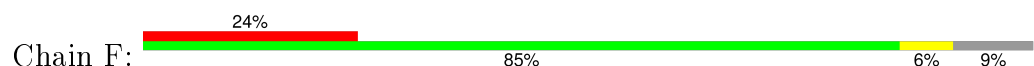




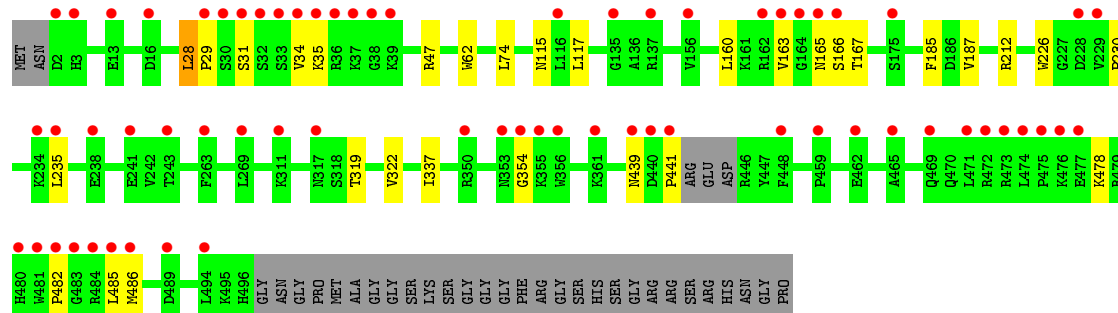
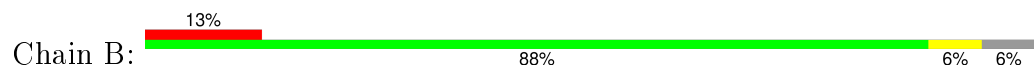
● Molecule 1: CRYPTOCHROME DASH



● Molecule 1: CRYPTOCHROME DASH

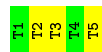


● Molecule 2: CRYPTOCHROME DASH



- Molecule 3: 5'-D(*DT*DT*DT*DT*DTP)-3'

Chain G: 



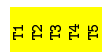
- Molecule 3: 5'-D(*DT*DT*DT*DT*DTP)-3'

Chain H: 




- Molecule 3: 5'-D(*DT*DT*DT*DT*DTP)-3'

Chain I: 



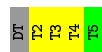
- Molecule 3: 5'-D(*DT*DT*DT*DT*DTP)-3'

Chain J: 



- Molecule 3: 5'-D(*DT*DT*DT*DT*DTP)-3'

Chain K: 



- Molecule 3: 5'-D(*DT*DT*DT*DT*DTP)-3'

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.73Å 136.08Å 211.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.03 – 2.01 15.02 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.2 (15.03-2.01) 99.2 (15.02-2.01)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.184 , 0.222 0.195 , 0.231	Depositor DCC
R_{free} test set	1518 reflections (0.67%)	DCC
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 63.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 229104 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26329	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.07 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.5360e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MHF, ACT, FAD, TCP, CL

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	0.40	0/4181	0.54	0/5656
1	C	0.40	0/4157	0.55	0/5625
1	D	0.57	4/4042 (0.1%)	0.73	8/5471 (0.1%)
1	E	0.40	0/4154	0.55	0/5622
1	F	0.35	0/4004	0.49	0/5419
2	B	0.37	0/4106	0.52	0/5561
3	G	0.68	0/83	1.58	1/124 (0.8%)
3	H	0.71	0/83	1.79	1/124 (0.8%)
3	I	0.81	0/83	1.86	3/124 (2.4%)
3	J	0.98	0/83	8.87	7/124 (5.6%)
3	K	0.74	0/64	1.67	1/94 (1.1%)
3	L	0.78	0/46	1.73	1/67 (1.5%)
All	All	0.43	4/25086 (0.0%)	0.81	22/34011 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
3	J	1	0
All	All	1	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	35[A]	LYS	C-N	-18.77	0.90	1.34
1	D	37[A]	LYS	C-N	-15.39	1.05	1.33
1	D	36	ARG	C-N	9.70	1.56	1.34
1	D	30	SER	C-N	5.17	1.46	1.34

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1	DT	O4'-C1'-N1	90.06	171.04	108.00
1	D	30	SER	O-C-N	-31.84	71.76	122.70
3	J	1	DT	C6-N1-C1'	-22.21	87.08	120.40
3	J	1	DT	C2-N1-C1'	19.79	149.86	118.20
3	J	1	DT	N1-C1'-C2'	-18.01	78.39	112.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	J	1	DT	C1'

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	30	SER	Mainchain
1	D	35[A]	LYS	Mainchain

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	4068	0	3988	21	0
1	C	4042	0	3967	20	0
1	D	3933	0	3840	18	0
1	E	4042	0	3957	27	0
1	F	3896	0	3812	20	0
2	B	3995	0	3896	24	0
3	G	95	0	64	2	0
3	H	95	0	64	3	0
3	I	95	0	64	4	0
3	J	95	0	64	3	0
3	K	78	0	51	3	0
3	L	62	0	38	2	0
4	A	53	0	31	0	0
4	B	53	0	31	0	0
4	C	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	53	0	31	0	0
4	E	53	0	31	0	0
4	F	53	0	31	0	0
5	A	33	0	21	0	0
5	B	33	0	21	0	0
5	C	33	0	21	0	0
5	D	33	0	21	0	0
5	E	33	0	21	0	0
5	F	33	0	21	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	B	4	0	3	0	0
8	A	274	0	0	3	0
8	B	178	0	0	1	0
8	C	257	0	0	1	0
8	D	209	0	0	3	0
8	E	233	0	0	2	0
8	F	120	0	0	1	0
8	G	7	0	0	0	0
8	H	4	0	0	0	0
8	I	10	0	0	0	0
8	J	5	0	0	0	0
8	K	7	0	0	0	0
8	L	1	0	0	0	0
All	All	26329	0	24120	141	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 3.

The worst 5 of 141 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:D:74:LEU:HD21	1:D:235:LEU:HD11	1.40	0.99
3:I:2:DT:H72	3:I:3:TCP:H72	1.49	0.95
1:A:34:VAL:HG11	1:A:62:TRP:CH2	2.06	0.90
1:D:17:SER:CB	8:D:2004:HOH:O	2.21	0.89
2:B:74:LEU:HD21	2:B:235:LEU:HD11	1.55	0.88

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/526 (95%)	479 (96%)	14 (3%)	6 (1%)	16	8
1	C	494/526 (94%)	475 (96%)	19 (4%)	0	100	100
1	D	481/526 (91%)	460 (96%)	19 (4%)	2 (0%)	39	33
1	E	494/526 (94%)	472 (96%)	20 (4%)	2 (0%)	39	33
1	F	475/526 (90%)	456 (96%)	16 (3%)	3 (1%)	30	22
2	B	487/525 (93%)	465 (96%)	19 (4%)	3 (1%)	30	22
All	All	2930/3155 (93%)	2807 (96%)	107 (4%)	16 (0%)	34	26

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	ASN
1	A	30	SER
1	E	30	SER
1	A	355	LYS
1	A	356	TRP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/459 (96%)	435 (99%)	5 (1%)	80	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	438/459 (95%)	429 (98%)	9 (2%)	61	63
1	D	426/459 (93%)	420 (99%)	6 (1%)	74	77
1	E	437/459 (95%)	429 (98%)	8 (2%)	66	69
1	F	422/459 (92%)	417 (99%)	5 (1%)	78	81
2	B	432/459 (94%)	427 (99%)	5 (1%)	78	81
All	All	2595/2754 (94%)	2557 (98%)	38 (2%)	72	75

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	355	LYS
1	D	31[A]	SER
1	F	212	ARG
1	D	17	SER
1	D	35[A]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	277	ASN
1	D	360	GLN
1	F	142	HIS
1	D	86	ASN
1	F	86	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	$\# Z > 2$
3	TCP	G	3	3	14,19,19	1.55	4 (28%)	17,27,27	4.11	4 (23%)
3	TCP	H	3	3	14,19,19	1.56	3 (21%)	17,27,27	4.11	4 (23%)
3	TCP	I	3	3	14,19,19	1.61	3 (21%)	17,27,27	4.24	5 (29%)
3	TCP	J	3	3	14,19,19	1.62	4 (28%)	17,27,27	4.12	5 (29%)
3	TCP	K	3	3	14,19,19	1.54	3 (21%)	17,27,27	4.38	4 (23%)
3	TCP	L	3	3	14,19,19	1.58	3 (21%)	17,27,27	3.96	3 (17%)

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
3	TCP	G	3	3	-	0/3/19/19	0/2/2/2
3	TCP	H	3	3	-	0/3/19/19	0/2/2/2
3	TCP	I	3	3	-	0/3/19/19	0/2/2/2
3	TCP	J	3	3	-	0/3/19/19	0/2/2/2
3	TCP	K	3	3	-	0/3/19/19	0/2/2/2
3	TCP	L	3	3	-	0/3/19/19	0/2/2/2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3	TCP	C6-C5	-2.09	1.34	1.40
3	J	3	TCP	C6-C5	-2.01	1.34	1.40
3	G	3	TCP	C6-N1	2.63	1.38	1.35
3	G	3	TCP	C4-N3	2.83	1.38	1.33
3	K	3	TCP	C4-N3	2.88	1.38	1.33

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	TCP	C5-C4-N3	-8.24	115.97	125.14
3	L	3	TCP	C5-C4-N3	-8.19	116.02	125.14
3	K	3	TCP	C5-C4-N3	-8.18	116.03	125.14
3	G	3	TCP	C5-C4-N3	-7.99	116.24	125.14
3	J	3	TCP	C5-C4-N3	-7.89	116.35	125.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	3	TCP	2	0
3	H	3	TCP	2	0
3	I	3	TCP	4	0
3	J	3	TCP	2	0
3	K	3	TCP	3	0
3	L	3	TCP	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 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	$\# Z > 2$
4	FAD	A	998	-	48,58,58	1.26	6 (12%)	54,89,89	2.03	8 (14%)
5	MHF	A	999	-	25,36,36	0.97	1 (4%)	29,52,52	1.76	7 (24%)
7	ACT	B	1500	-	1,3,3	1.53	0	0,3,3	0.00	-
4	FAD	B	998	-	48,58,58	1.23	7 (14%)	54,89,89	2.05	8 (14%)
5	MHF	B	999	-	25,36,36	0.91	1 (4%)	29,52,52	1.82	8 (27%)
4	FAD	C	998	-	48,58,58	1.27	6 (12%)	54,89,89	2.09	7 (12%)
5	MHF	C	999	-	25,36,36	1.00	1 (4%)	29,52,52	1.77	6 (20%)
4	FAD	D	998	-	48,58,58	1.25	6 (12%)	54,89,89	2.00	8 (14%)
5	MHF	D	999	-	25,36,36	0.91	1 (4%)	29,52,52	1.70	7 (24%)
4	FAD	E	998	-	48,58,58	1.34	6 (12%)	54,89,89	1.97	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MHF	E	999	-	25,36,36	0.93	1 (4%)	29,52,52	1.69	6 (20%)
4	FAD	F	998	-	48,58,58	1.21	6 (12%)	54,89,89	1.94	7 (12%)
5	MHF	F	999	-	25,36,36	0.90	1 (4%)	29,52,52	1.73	7 (24%)

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
4	FAD	A	998	-	-	0/30/50/50	0/6/6/6
5	MHF	A	999	-	-	0/15/42/42	0/4/4/4
7	ACT	B	1500	-	-	0/0/0/0	0/0/0/0
4	FAD	B	998	-	-	0/30/50/50	0/6/6/6
5	MHF	B	999	-	-	0/15/42/42	0/4/4/4
4	FAD	C	998	-	-	0/30/50/50	0/6/6/6
5	MHF	C	999	-	-	0/15/42/42	0/4/4/4
4	FAD	D	998	-	-	0/30/50/50	0/6/6/6
5	MHF	D	999	-	-	0/15/42/42	0/4/4/4
4	FAD	E	998	-	-	0/30/50/50	0/6/6/6
5	MHF	E	999	-	-	0/15/42/42	0/4/4/4
4	FAD	F	998	-	-	0/30/50/50	0/6/6/6
5	MHF	F	999	-	-	0/15/42/42	0/4/4/4

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	998	FAD	C10-N1	2.04	1.39	1.35
4	A	998	FAD	C2A-N1A	2.16	1.38	1.33
4	D	998	FAD	C2A-N1A	2.19	1.38	1.33
4	B	998	FAD	C2A-N1A	2.41	1.38	1.33
4	F	998	FAD	C5X-N5	2.42	1.39	1.35

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	998	FAD	N3A-C2A-N1A	-11.57	120.03	128.89
4	A	998	FAD	N3A-C2A-N1A	-11.35	120.20	128.89
4	D	998	FAD	N3A-C2A-N1A	-11.11	120.39	128.89
4	C	998	FAD	N3A-C2A-N1A	-10.96	120.50	128.89
4	E	998	FAD	N3A-C2A-N1A	-10.92	120.53	128.89

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	500/526 (95%)	0.88	58 (11%) 6 7	36, 41, 59, 67	0
1	C	495/526 (94%)	1.04	76 (15%) 3 3	35, 41, 57, 68	0
1	D	478/526 (90%)	0.93	70 (14%) 3 4	36, 41, 57, 64	0
1	E	496/526 (94%)	0.86	58 (11%) 6 7	35, 41, 59, 69	0
1	F	480/526 (91%)	1.43	128 (26%) 1 1	35, 41, 56, 65	0
2	B	491/525 (93%)	0.98	66 (13%) 4 5	36, 41, 58, 69	1 (0%)
3	G	4/5 (80%)	0.72	0 100 100	40, 45, 47, 52	0
3	H	4/5 (80%)	2.85	2 (50%) 0 1	50, 59, 61, 62	0
3	I	4/5 (80%)	0.37	0 100 100	34, 36, 44, 45	0
3	J	4/5 (80%)	1.49	1 (25%) 1 1	47, 56, 61, 66	1 (25%)
3	K	3/5 (60%)	0.24	0 100 100	40, 40, 40, 49	0
3	L	3/5 (60%)	2.54	2 (66%) 0 1	70, 70, 74, 76	0
All	All	2962/3185 (92%)	1.02	461 (15%) 3 3	34, 41, 58, 76	2 (0%)

The worst 5 of 461 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	32	SER	14.7
2	B	32	SER	14.6
1	F	31	SER	11.7
2	B	483	GLY	11.3
1	F	166	SER	11.2

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	TCP	G	3	18/18	0.89	0.15	-	37,39,42,43	0
3	TCP	K	3	18/18	0.92	0.14	-	37,38,39,41	0
3	TCP	L	3	18/18	0.69	0.31	-	72,73,73,73	0
3	TCP	I	3	18/18	0.91	0.14	-	33,34,35,38	0
3	TCP	J	3	18/18	0.81	0.20	-	45,46,50,51	0
3	TCP	H	3	18/18	0.81	0.21	-	45,46,51,52	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	MHF	A	999	33/33	0.84	0.17	1.31	35,36,44,47	0
5	MHF	E	999	33/33	0.84	0.18	0.95	35,36,45,48	0
7	ACT	B	1500	4/4	0.71	0.19	0.64	63,64,64,64	0
5	MHF	F	999	33/33	0.86	0.16	0.54	35,36,44,47	0
5	MHF	C	999	33/33	0.86	0.16	0.01	34,37,45,49	0
4	FAD	A	998	53/53	0.95	0.14	-0.07	34,35,36,37	0
4	FAD	D	998	53/53	0.94	0.14	-0.13	34,34,36,37	0
5	MHF	B	999	33/33	0.87	0.15	-0.14	35,37,44,48	0
5	MHF	D	999	33/33	0.89	0.14	-0.32	35,37,44,47	0
4	FAD	C	998	53/53	0.95	0.13	-0.35	34,35,37,38	0
4	FAD	E	998	53/53	0.96	0.12	-0.51	34,35,37,37	0
4	FAD	F	998	53/53	0.94	0.13	-0.55	34,34,36,37	0
4	FAD	B	998	53/53	0.95	0.12	-0.69	34,35,36,36	0
6	CL	F	1498	1/1	0.88	0.10	-1.11	69,69,69,69	0
6	CL	B	1498	1/1	0.96	0.06	-1.65	52,52,52,52	0
6	CL	B	1499	1/1	0.96	0.07	-2.20	70,70,70,70	0
6	CL	D	1498	1/1	0.99	0.05	-2.31	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	CL	E	1499	1/1	0.99	0.04	-2.40	44,44,44,44	0
6	CL	C	1500	1/1	0.99	0.04	-2.50	53,53,53,53	0
6	CL	A	1501	1/1	0.99	0.06	-2.60	46,46,46,46	0
6	CL	C	1499	1/1	0.98	0.06	-2.84	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.