



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:32 AM GMT

PDB ID : 2DHF  
Title : CRYSTAL STRUCTURES OF RECOMBINANT HUMAN DIHYDROFOLATE REDUCTASE COMPLEXED WITH FOLATE AND 5-DEAZOFOLATE  
Authors : Davies /II, J.F.; Kraut, J.  
Deposited on : 1989-10-25  
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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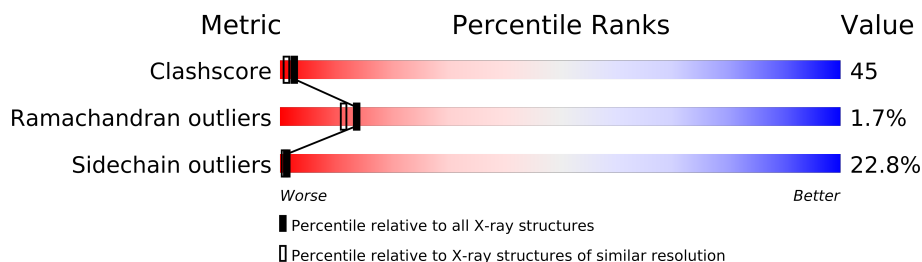
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 Å.


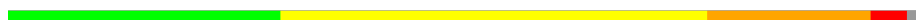
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	186	
1	B	186	

## 2 Entry composition i

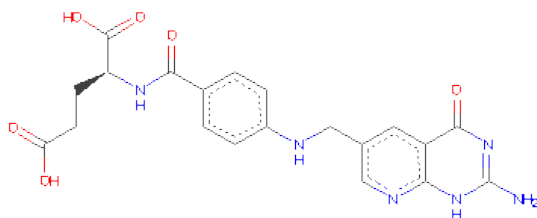
There are 3 unique types of molecules in this entry. The entry contains 3123 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DIHYDROFOLATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1476	949	249	271	7			
1	B	182	Total	C	N	O	S	0	0	0
			1472	947	249	269	7			

- Molecule 2 is 5-DEAZAFOLIC ACID (three-letter code: DZF) (formula: C<sub>20</sub>H<sub>20</sub>N<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	20	6	6		
2	B	1	Total	C	N	O	0	0
			32	20	6	6		

- Molecule 3 is water.

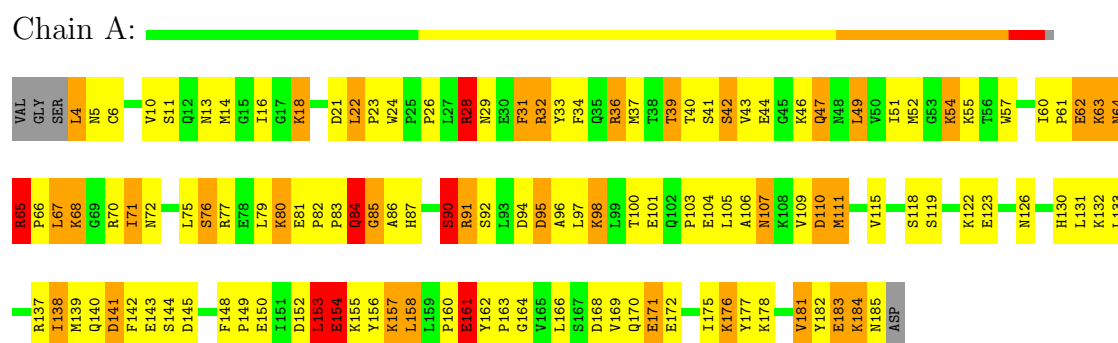
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total 52	O 52	0	0
3	B	59	Total 59	O 59	0	0

### 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.

Note EDS was not executed.

#### • Molecule 1: DIHYDROFOLATE REDUCTASE



#### • Molecule 1: DIHYDROFOLATE REDUCTASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.10Å 38.50Å 76.80Å 93.90° 91.40° 111.50°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.194 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3123	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.12	2/1511 (0.1%)	1.84	28/2039 (1.4%)
1	B	1.20	1/1507 (0.1%)	1.96	41/2034 (2.0%)
All	All	1.16	3/3018 (0.1%)	1.90	69/4073 (1.7%)

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	A	1	4
1	B	0	5
All	All	1	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	ARG	CD-NE	-6.88	1.34	1.46
1	A	92	SER	CB-OG	-6.82	1.33	1.42
1	A	144	SER	CB-OG	5.53	1.49	1.42

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	ARG	CD-NE-CZ	17.64	148.30	123.60
1	A	65	ARG	NE-CZ-NH2	-16.75	111.92	120.30
1	A	28	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	B	95	ASP	CB-CG-OD1	9.64	126.98	118.30
1	B	70	ARG	NE-CZ-NH2	9.39	124.99	120.30
1	B	36	ARG	NE-CZ-NH1	9.30	124.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	ASP	CB-CG-OD1	9.21	126.59	118.30
1	B	30	GLU	CA-CB-CG	8.55	132.22	113.40
1	B	36	ARG	NE-CZ-NH2	-8.29	116.15	120.30
1	B	65	ARG	NE-CZ-NH1	-8.28	116.16	120.30
1	A	110	ASP	CB-CG-OD1	8.15	125.64	118.30
1	B	144	SER	N-CA-CB	-7.96	98.56	110.50
1	A	4	LEU	CA-CB-CG	7.53	132.62	115.30
1	B	95	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	B	9	ALA	CB-CA-C	-7.12	99.42	110.10
1	B	65	ARG	NE-CZ-NH2	7.07	123.84	120.30
1	B	93	LEU	CB-CA-C	6.95	123.40	110.20
1	B	93	LEU	CA-CB-CG	6.67	130.65	115.30
1	A	67	LEU	CB-CA-C	6.66	122.85	110.20
1	B	182	TYR	N-CA-CB	6.61	122.50	110.60
1	B	44	GLU	CA-CB-CG	6.54	127.78	113.40
1	A	153	LEU	CB-CA-C	6.50	122.56	110.20
1	A	65	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	161	GLU	CA-CB-CG	6.39	127.46	113.40
1	B	111	MET	CA-CB-CG	6.22	123.88	113.30
1	A	28	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	97	LEU	CB-CA-C	6.18	121.94	110.20
1	A	84	GLN	CB-CA-C	-6.14	98.12	110.40
1	B	145	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	62	GLU	CA-CB-CG	6.07	126.75	113.40
1	B	77	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	181	VAL	CA-CB-CG2	6.06	119.99	110.90
1	A	31	PHE	CB-CG-CD2	-6.04	116.57	120.80
1	B	168	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	95	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	90	SER	N-CA-CB	6.02	119.53	110.50
1	A	111	MET	CA-CB-CG	5.99	123.48	113.30
1	B	159	LEU	CA-CB-CG	5.88	128.81	115.30
1	A	21	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	172	GLU	CA-CB-CG	5.84	126.25	113.40
1	B	76	SER	N-CA-CB	5.76	119.14	110.50
1	B	29	ASN	CA-CB-CG	5.74	126.02	113.40
1	B	171	GLU	CB-CA-C	-5.72	98.96	110.40
1	B	154	GLU	CA-CB-CG	5.70	125.94	113.40
1	B	65	ARG	N-CA-CB	5.69	120.84	110.60
1	B	118	SER	N-CA-CB	5.65	118.97	110.50
1	B	59	SER	N-CA-CB	5.62	118.93	110.50
1	A	39	THR	CA-CB-CG2	-5.54	104.64	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156	TYR	CB-CG-CD2	-5.54	117.67	121.00
1	A	22	LEU	CB-CA-C	5.54	120.72	110.20
1	B	30	GLU	CB-CA-C	5.53	121.46	110.40
1	A	171	GLU	OE1-CD-OE2	5.44	129.82	123.30
1	B	99	LEU	CB-CA-C	5.41	120.49	110.20
1	A	110	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	183	GLU	N-CA-CB	5.36	120.24	110.60
1	A	171	GLU	CG-CD-OE2	-5.30	107.69	118.30
1	B	110	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	B	129	GLY	C-N-CA	5.22	134.75	121.70
1	B	185	ASN	CA-C-O	5.16	130.93	120.10
1	B	71	ILE	N-CA-C	-5.15	97.08	111.00
1	B	141	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	B	79	LEU	O-C-N	5.14	130.92	122.70
1	A	182	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	B	142	PHE	CB-CA-C	5.11	120.61	110.40
1	A	21	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	B	153	LEU	CB-CA-C	5.04	119.77	110.20
1	A	154	GLU	CA-CB-CG	5.01	124.42	113.40
1	A	60	ILE	CB-CA-C	-5.00	101.59	111.60
1	A	92	SER	N-CA-CB	-5.00	102.99	110.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	4	LEU	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	ARG	Sidechain
1	A	32	ARG	Sidechain
1	A	36	ARG	Sidechain
1	A	91	ARG	Sidechain
1	B	137	ARG	Sidechain
1	B	28	ARG	Sidechain
1	B	32	ARG	Sidechain
1	B	65	ARG	Sidechain
1	B	91	ARG	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1476	0	1487	140	1
1	B	1472	0	1483	135	1
2	A	32	0	18	0	0
2	B	32	0	17	4	0
3	A	52	0	0	6	0
3	B	59	0	0	16	0
All	All	3123	0	3005	270	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 45.

All (270) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:171:GLU:OE2	1:A:176:LYS:HE2	1.38	1.22
1:B:80:LYS:NZ	1:B:80:LYS:HA	1.56	1.19
1:B:80:LYS:NZ	1:B:80:LYS:CA	2.10	1.15
1:B:80:LYS:HZ2	1:B:80:LYS:HA	1.08	1.13
1:B:80:LYS:HZ2	1:B:80:LYS:CA	1.63	1.11
1:A:66:PRO:O	1:A:68:LYS:HD2	1.51	1.09
1:B:80:LYS:HE3	1:B:80:LYS:C	1.74	1.08
1:B:130:HIS:HE1	1:B:183:GLU:OE1	1.35	1.07
1:A:156:TYR:C	1:A:157:LYS:HD3	1.76	1.05
1:A:14:MET:HA	1:A:14:MET:HE2	1.40	1.02
1:B:76:SER:O	1:B:91:ARG:HD3	1.59	1.01
1:B:107:ASN:HB3	3:B:493:HOH:O	1.58	1.01
1:A:64:ASN:HD22	1:A:64:ASN:N	1.58	1.01
1:A:77:ARG:HA	1:A:91:ARG:HD2	1.44	0.99
1:A:156:TYR:O	1:A:157:LYS:HD3	1.65	0.96
1:B:130:HIS:CE1	1:B:183:GLU:OE1	2.19	0.96
1:B:80:LYS:C	1:B:80:LYS:CE	2.35	0.95
1:B:104:GLU:HA	3:B:468:HOH:O	1.66	0.94
1:A:153:LEU:CD1	1:A:153:LEU:O	2.15	0.94
1:A:153:LEU:O	1:A:153:LEU:HD13	1.67	0.94
1:B:146:THR:HG21	3:B:408:HOH:O	1.65	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:64:ASN:N	1:A:64:ASN:ND2	2.11	0.92
1:B:23:PRO:HG2	1:B:24:TRP:CZ3	2.05	0.92
1:B:146:THR:HG23	3:B:421:HOH:O	1.70	0.91
1:B:81:GLU:HB3	1:B:82:PRO:HD2	1.52	0.90
1:B:22:LEU:HD12	3:B:428:HOH:O	1.70	0.90
1:B:80:LYS:HE3	1:B:80:LYS:O	1.72	0.89
1:A:160:PRO:HG2	1:A:161:GLU:OE2	1.71	0.89
1:A:171:GLU:OE2	1:A:176:LYS:CE	2.25	0.84
1:A:54:LYS:HG3	1:A:79:LEU:HD11	1.60	0.84
1:B:139:MET:HG2	3:B:501:HOH:O	1.78	0.84
1:B:24:TRP:HB2	1:B:25:PRO:HD2	1.60	0.83
1:B:99:LEU:HD11	1:B:105:LEU:CD2	2.07	0.83
1:B:99:LEU:HD11	1:B:105:LEU:HD21	1.60	0.82
1:B:104:GLU:HG2	3:B:468:HOH:O	1.80	0.80
1:A:14:MET:CE	1:A:14:MET:HA	2.10	0.80
1:B:99:LEU:CD1	1:B:105:LEU:CD2	2.60	0.79
1:A:98:LYS:O	1:A:101:GLU:CB	2.31	0.78
1:B:80:LYS:HZ1	1:B:80:LYS:HA	1.46	0.78
1:A:94:ASP:O	1:A:98:LYS:HD3	1.83	0.78
1:B:89:LEU:HD21	1:B:91:ARG:NH2	1.99	0.77
1:B:118:SER:HB2	3:B:440:HOH:O	1.84	0.77
1:B:80:LYS:NZ	1:B:80:LYS:C	2.36	0.77
1:B:80:LYS:O	1:B:80:LYS:CE	2.32	0.77
1:A:64:ASN:HD22	1:A:64:ASN:H	1.31	0.76
1:B:99:LEU:O	1:B:105:LEU:HD23	1.85	0.75
1:B:76:SER:O	1:B:91:ARG:CD	2.34	0.75
1:A:171:GLU:HG3	1:A:176:LYS:HD3	1.69	0.75
1:A:98:LYS:O	1:A:101:GLU:HB2	1.86	0.75
1:B:40:THR:O	1:B:111:MET:HE1	1.86	0.75
1:B:81:GLU:CB	1:B:82:PRO:HD2	2.16	0.75
1:A:80:LYS:HA	1:A:80:LYS:HE2	1.69	0.75
1:A:68:LYS:N	1:A:70:ARG:HH11	1.86	0.74
1:A:54:LYS:HG3	1:A:79:LEU:CD1	2.18	0.73
1:A:66:PRO:O	1:A:68:LYS:CD	2.33	0.73
1:A:6:CYS:HB2	1:A:133:LEU:HD23	1.70	0.72
1:A:84:GLN:CG	1:A:85:GLY:N	2.49	0.72
1:A:153:LEU:O	1:A:153:LEU:HD12	1.88	0.72
1:A:68:LYS:H	1:A:70:ARG:HH11	1.34	0.71
1:B:89:LEU:HD21	1:B:91:ARG:HH22	1.53	0.71
1:B:114:ILE:HD13	1:B:124:ALA:CB	2.18	0.71
1:B:154:GLU:CD	3:B:487:HOH:O	2.28	0.71
1:B:78:GLU:O	1:B:79:LEU:C	2.27	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:154:GLU:OE1	1:A:155:LYS:HD3	1.92	0.70
1:A:80:LYS:HE2	1:A:80:LYS:O	1.91	0.70
1:A:152:ASP:OD1	1:A:154:GLU:N	2.25	0.70
1:B:136:THR:HG22	1:B:138:ILE:CD1	2.22	0.69
1:B:23:PRO:HG2	1:B:24:TRP:CE3	2.27	0.69
1:B:81:GLU:HB3	1:B:82:PRO:CD	2.22	0.69
1:A:76:SER:O	1:A:91:ARG:HD3	1.93	0.69
1:B:62:GLU:CG	1:B:62:GLU:O	2.39	0.69
1:A:14:MET:HE1	3:A:426:HOH:O	1.92	0.69
1:A:111:MET:HE1	3:A:404:HOH:O	1.93	0.69
1:B:79:LEU:HD13	1:B:83:PRO:HD3	1.74	0.69
1:B:159:LEU:HD21	1:B:183:GLU:HB3	1.73	0.68
1:B:40:THR:O	1:B:111:MET:CE	2.42	0.68
1:A:84:GLN:HG2	1:A:84:GLN:O	1.76	0.68
1:B:79:LEU:CD1	1:B:83:PRO:HD3	2.24	0.67
1:A:95:ASP:HA	1:A:98:LYS:HZ3	1.59	0.67
1:A:18:LYS:HD2	1:A:143:GLU:O	1.95	0.67
1:B:122:LYS:NZ	3:B:440:HOH:O	2.26	0.67
1:A:61:PRO:HB2	1:A:64:ASN:HD21	1.58	0.67
1:B:80:LYS:HZ1	1:B:80:LYS:CA	1.99	0.67
1:B:114:ILE:HD13	1:B:124:ALA:HB2	1.76	0.67
1:A:137:ARG:O	1:A:177:TYR:HA	1.97	0.65
1:B:76:SER:HB3	1:B:79:LEU:HB2	1.79	0.65
1:A:171:GLU:HG3	1:A:176:LYS:CD	2.27	0.64
1:A:80:LYS:CE	1:A:80:LYS:O	2.45	0.64
1:B:80:LYS:CE	1:B:80:LYS:CA	2.76	0.64
1:B:62:GLU:O	1:B:62:GLU:HG2	1.98	0.63
1:A:71:ILE:N	1:A:71:ILE:CD1	2.62	0.63
1:A:80:LYS:HE2	1:A:80:LYS:CA	2.28	0.63
1:A:183:GLU:HG2	1:A:184:LYS:N	2.13	0.63
1:A:139:MET:HE2	1:A:177:TYR:HA	1.80	0.62
1:A:171:GLU:HA	1:A:175:ILE:O	1.99	0.62
1:A:95:ASP:HA	1:A:98:LYS:NZ	2.13	0.62
1:A:18:LYS:HA	1:A:145:ASP:OD1	1.98	0.62
1:B:61:PRO:O	1:B:63:LYS:N	2.30	0.61
1:A:68:LYS:H	1:A:70:ARG:NH1	1.99	0.61
1:A:14:MET:CE	1:A:14:MET:CA	2.78	0.61
1:A:170:GLN:O	1:A:176:LYS:HA	2.01	0.61
1:A:139:MET:CE	1:A:177:TYR:HA	2.30	0.61
1:B:151:ILE:O	1:B:153:LEU:HD22	2.00	0.61
1:A:61:PRO:O	1:A:64:ASN:ND2	2.34	0.61
1:B:99:LEU:CD1	1:B:105:LEU:HD23	2.30	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:83:PRO:O	1:A:84:GLN:O	2.19	0.61
1:B:81:GLU:CB	1:B:82:PRO:CD	2.78	0.61
1:B:24:TRP:HB2	1:B:25:PRO:CD	2.29	0.61
1:A:71:ILE:HD13	1:A:71:ILE:N	2.15	0.60
1:B:30:GLU:OE1	2:B:187:DZF:NA2	2.30	0.60
1:A:104:GLU:HA	1:A:104:GLU:OE1	2.01	0.60
1:A:139:MET:CE	1:A:177:TYR:CA	2.79	0.60
1:B:139:MET:HB2	1:B:176:LYS:O	2.01	0.60
1:A:14:MET:HE2	1:A:14:MET:CA	2.23	0.60
1:A:63:LYS:O	1:A:63:LYS:CD	2.49	0.59
1:B:5:ASN:O	1:B:113:TRP:HA	2.02	0.59
1:B:98:LYS:O	1:B:101:GLU:HG2	2.02	0.59
1:B:171:GLU:HA	1:B:175:ILE:O	2.03	0.58
1:A:81:GLU:HB3	1:A:82:PRO:HD2	1.85	0.58
1:B:80:LYS:NZ	1:B:80:LYS:O	2.33	0.58
1:B:180:GLU:OE1	1:B:182:TYR:OH	2.15	0.58
1:B:22:LEU:HD12	3:B:454:HOH:O	2.03	0.58
1:A:130:HIS:NE2	1:A:183:GLU:OE1	2.24	0.58
1:A:98:LYS:O	1:A:101:GLU:HB3	2.04	0.58
1:A:63:LYS:O	1:A:63:LYS:HD3	2.04	0.57
1:A:23:PRO:HD2	1:A:24:TRP:CE3	2.40	0.57
1:A:157:LYS:HD3	1:A:157:LYS:N	2.12	0.57
1:A:161:GLU:N	1:A:161:GLU:OE2	2.38	0.56
1:B:176:LYS:NZ	3:B:445:HOH:O	2.38	0.56
1:A:84:GLN:C	1:A:86:ALA:H	2.08	0.56
1:B:93:LEU:HD23	1:B:123:GLU:HB3	1.88	0.56
1:A:36:ARG:HH12	1:A:164:GLY:C	2.10	0.55
1:B:73:LEU:HG	1:B:88:PHE:HB2	1.87	0.55
1:A:80:LYS:HE2	1:A:80:LYS:C	2.26	0.55
1:A:77:ARG:HG3	1:A:91:ARG:HB3	1.86	0.55
1:A:77:ARG:HA	1:A:91:ARG:CD	2.29	0.55
1:A:84:GLN:O	1:A:86:ALA:N	2.38	0.55
1:B:148:PHE:CD2	1:B:149:PRO:O	2.59	0.55
1:B:130:HIS:HE1	1:B:183:GLU:CD	2.07	0.55
1:A:75:LEU:HA	1:A:90:SER:O	2.06	0.54
1:A:72:ASN:O	1:A:87:HIS:HB2	2.07	0.54
1:A:57:TRP:CE2	1:A:65:ARG:HD3	2.42	0.54
1:A:10:VAL:HG12	1:A:16:ILE:CG2	2.38	0.54
1:B:22:LEU:CD1	3:B:454:HOH:O	2.53	0.54
1:B:52:MET:HB3	1:B:115:VAL:CG2	2.38	0.54
1:B:80:LYS:HZ1	1:B:80:LYS:C	2.03	0.53
1:B:34:PHE:O	1:B:38:THR:HG23	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:26:PRO:HA	3:A:488:HOH:O	2.08	0.53
1:B:72:ASN:O	1:B:87:HIS:HB2	2.09	0.53
1:A:84:GLN:HG2	1:A:85:GLY:N	1.93	0.52
1:A:29:ASN:HB2	1:A:172:GLU:OE1	2.10	0.52
1:B:61:PRO:HB2	1:B:63:LYS:HE3	1.92	0.51
1:A:158:LEU:HD23	1:A:181:VAL:O	2.09	0.51
1:A:43:VAL:HG11	1:A:46:LYS:HG3	1.92	0.51
1:A:6:CYS:HB2	1:A:133:LEU:CD2	2.40	0.51
1:B:4:LEU:HB3	1:B:131:LEU:HG	1.91	0.51
1:A:40:THR:O	1:A:111:MET:CE	2.58	0.51
1:A:11:SER:O	1:A:14:MET:HE2	2.10	0.51
1:A:154:GLU:OE1	1:A:154:GLU:O	2.28	0.51
1:A:140:GLN:HG2	1:A:141:ASP:N	2.25	0.50
1:B:104:GLU:CA	3:B:468:HOH:O	2.42	0.50
1:A:183:GLU:HG2	1:A:184:LYS:H	1.77	0.50
1:A:13:ASN:ND2	3:A:411:HOH:O	2.44	0.50
1:B:60:ILE:O	1:B:65:ARG:NH2	2.38	0.50
1:B:99:LEU:HD12	1:B:105:LEU:HD23	1.94	0.50
1:B:31:PHE:HB3	2:B:187:DZF:CD	2.42	0.50
1:B:56:THR:O	1:B:57:TRP:C	2.50	0.50
1:A:47:GLN:O	1:A:109:VAL:HA	2.12	0.50
1:A:51:ILE:CG2	1:A:75:LEU:HD11	2.42	0.50
1:B:104:GLU:CG	3:B:468:HOH:O	2.48	0.49
1:B:152:ASP:OD1	1:B:154:GLU:CB	2.60	0.49
1:B:161:GLU:OE1	1:B:163:PRO:HD3	2.12	0.49
1:A:139:MET:HE3	1:A:176:LYS:C	2.32	0.49
1:B:114:ILE:HD13	1:B:124:ALA:HB1	1.94	0.49
1:B:8:VAL:HG11	1:B:148:PHE:CE1	2.47	0.49
1:A:10:VAL:HG12	1:A:16:ILE:HG22	1.94	0.49
1:B:153:LEU:HD13	1:B:153:LEU:HA	1.48	0.49
1:B:66:PRO:HB2	1:B:72:ASN:ND2	2.27	0.49
1:A:11:SER:O	1:A:14:MET:CE	2.61	0.49
1:A:80:LYS:HE3	1:A:91:ARG:NH1	2.27	0.49
1:A:160:PRO:HG2	1:A:161:GLU:CD	2.32	0.48
1:B:114:ILE:CD1	1:B:124:ALA:HB1	2.43	0.48
1:B:66:PRO:HB2	1:B:72:ASN:CG	2.33	0.48
1:B:49:LEU:HD23	1:B:112:VAL:HG13	1.95	0.48
1:B:63:LYS:CD	1:B:63:LYS:C	2.82	0.48
1:B:4:LEU:HA	1:B:4:LEU:HD23	1.49	0.48
1:B:70:ARG:O	3:B:465:HOH:O	2.20	0.48
1:B:27:LEU:HD22	1:B:172:GLU:HG2	1.95	0.48
1:B:102:GLN:HB2	1:B:105:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:52:MET:HB3	1:A:115:VAL:CG2	2.45	0.47
1:B:99:LEU:HD12	1:B:105:LEU:CD2	2.42	0.47
1:A:148:PHE:CD1	1:A:149:PRO:HD2	2.50	0.47
1:B:158:LEU:HD23	1:B:158:LEU:HA	1.62	0.47
1:B:80:LYS:HE3	1:B:81:GLU:N	2.26	0.47
1:A:119:SER:N	3:A:456:HOH:O	2.49	0.46
1:B:117:GLY:O	1:B:118:SER:C	2.52	0.46
1:A:158:LEU:CD2	1:A:158:LEU:C	2.83	0.46
1:B:60:ILE:HG23	1:B:61:PRO:HD2	1.98	0.46
1:A:169:VAL:CG2	1:A:176:LYS:HG3	2.45	0.46
1:A:24:TRP:O	3:A:477:HOH:O	2.20	0.46
1:A:162:TYR:HA	1:A:163:PRO:HD2	1.69	0.46
1:A:96:ALA:O	1:A:100:THR:HG23	2.15	0.46
1:B:12:GLN:HB3	1:B:141:ASP:OD1	2.16	0.45
1:B:22:LEU:HD11	1:B:31:PHE:CZ	2.51	0.45
1:B:152:ASP:OD1	1:B:154:GLU:HB2	2.16	0.45
1:B:127:HIS:HA	1:B:128:PRO:HD3	1.81	0.45
1:A:33:TYR:O	1:A:37:MET:HG2	2.16	0.45
1:A:68:LYS:N	1:A:70:ARG:NH1	2.57	0.45
1:A:46:LYS:NZ	1:A:106:ALA:O	2.49	0.45
1:B:24:TRP:CB	1:B:25:PRO:CD	2.94	0.45
1:A:5:ASN:OD1	1:A:132:LYS:HB2	2.17	0.45
1:A:107:ASN:OD1	1:A:107:ASN:O	2.34	0.45
1:B:105:LEU:HD12	1:B:105:LEU:HA	1.65	0.45
1:B:78:GLU:O	1:B:79:LEU:O	2.34	0.45
1:A:40:THR:O	1:A:111:MET:HE3	2.17	0.45
1:A:183:GLU:CG	1:A:184:LYS:N	2.77	0.45
1:B:14:MET:O	1:B:147:PHE:HA	2.17	0.45
1:A:172:GLU:N	1:A:175:ILE:O	2.44	0.44
1:A:42:SER:N	1:A:110:ASP:OD2	2.49	0.44
1:A:139:MET:HE2	1:A:177:TYR:CA	2.44	0.44
1:B:33:TYR:O	1:B:37:MET:HG2	2.17	0.44
1:A:14:MET:CE	1:A:14:MET:N	2.80	0.44
1:A:83:PRO:O	1:A:84:GLN:C	2.56	0.44
1:A:138:ILE:HG22	1:A:138:ILE:O	2.18	0.44
1:A:166:LEU:N	1:A:166:LEU:HD23	2.33	0.44
1:A:152:ASP:OD1	1:A:152:ASP:C	2.55	0.44
1:A:155:LYS:C	1:A:157:LYS:HE2	2.39	0.43
1:B:125:MET:HE1	1:B:151:ILE:HA	2.00	0.43
1:B:157:LYS:HB2	1:B:157:LYS:HE3	1.61	0.43
1:A:171:GLU:CG	1:A:176:LYS:CD	2.96	0.43
1:A:87:HIS:ND1	1:B:104:GLU:CG	2.82	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:171:GLU:HB2	1:A:176:LYS:HD2	2.01	0.43
1:B:62:GLU:HA	1:B:65:ARG:HG3	2.00	0.43
1:A:67:LEU:HB3	1:A:70:ARG:CZ	2.49	0.43
1:A:80:LYS:NZ	1:B:98:LYS:CE	2.82	0.43
1:B:89:LEU:HD21	1:B:91:ARG:CZ	2.48	0.43
1:A:153:LEU:CD1	1:A:153:LEU:C	2.76	0.43
1:B:52:MET:HB2	1:B:56:THR:HB	2.01	0.43
1:A:49:LEU:HD12	1:A:71:ILE:HB	2.01	0.43
1:A:66:PRO:O	1:A:67:LEU:C	2.57	0.42
1:B:52:MET:HA	1:B:116:GLY:O	2.19	0.42
1:B:57:TRP:O	1:B:65:ARG:HD3	2.19	0.42
1:B:162:TYR:HA	1:B:163:PRO:HD2	1.81	0.42
1:A:107:ASN:C	1:A:107:ASN:OD1	2.56	0.42
1:B:43:VAL:HB	1:B:46:LYS:HB2	2.00	0.42
1:A:23:PRO:HB2	1:A:142:PHE:HB3	2.02	0.42
1:B:36:ARG:HH21	1:B:36:ARG:HD3	1.54	0.42
1:A:80:LYS:NZ	1:B:98:LYS:HE2	2.34	0.42
1:B:16:ILE:CG2	1:B:148:PHE:HB2	2.50	0.42
1:B:115:VAL:O	2:B:187:DZF:H7	2.19	0.41
1:B:21:ASP:OD2	1:B:22:LEU:N	2.51	0.41
1:B:170:GLN:O	1:B:176:LYS:HA	2.19	0.41
1:A:183:GLU:CG	1:A:184:LYS:H	2.33	0.41
1:A:158:LEU:HD22	1:A:158:LEU:C	2.40	0.41
1:A:22:LEU:HA	1:A:23:PRO:HD3	1.86	0.41
1:A:103:PRO:HG2	1:B:87:HIS:O	2.19	0.41
1:A:97:LEU:HA	1:A:97:LEU:HD23	1.78	0.41
1:A:80:LYS:HZ2	1:B:98:LYS:CE	2.33	0.41
1:B:178:LYS:HE3	1:B:178:LYS:HB3	1.79	0.41
1:A:43:VAL:CG1	1:A:46:LYS:HG3	2.50	0.41
1:A:83:PRO:C	1:A:84:GLN:O	2.59	0.41
1:B:34:PHE:CD2	1:B:34:PHE:C	2.94	0.41
1:A:169:VAL:HG23	1:A:176:LYS:HG3	2.02	0.41
1:B:31:PHE:HB3	2:B:187:DZF:CG	2.50	0.41
1:B:156:TYR:CZ	1:B:184:LYS:HD3	2.56	0.41
1:B:124:ALA:O	1:B:131:LEU:HD11	2.21	0.40
1:B:159:LEU:HA	1:B:160:PRO:HD2	1.82	0.40
1:A:154:GLU:C	1:A:154:GLU:OE1	2.59	0.40
1:A:94:ASP:C	1:A:98:LYS:HD3	2.40	0.40
1:B:10:VAL:HG12	1:B:16:ILE:HG22	2.03	0.40

All (1) 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	Distance(Å)	Clash(Å)
1:A:141:ASP:OD1	1:B:32:ARG:NH1[1_554]	2.08	0.12

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	180/186 (97%)	165 (92%)	12 (7%)	3 (2%)	14	11
1	B	180/186 (97%)	167 (93%)	10 (6%)	3 (2%)	14	11
All	All	360/372 (97%)	332 (92%)	22 (6%)	6 (2%)	14	11

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	85	GLY
1	B	62	GLU
1	A	62	GLU
1	B	79	LEU
1	B	163	PRO

### 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	165/168 (98%)	121 (73%)	44 (27%)	1	0
1	B	164/168 (98%)	133 (81%)	31 (19%)	2	2
All	All	329/336 (98%)	254 (77%)	75 (23%)	1	1

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	18	LYS
1	A	28	ARG
1	A	31	PHE
1	A	32	ARG
1	A	34	PHE
1	A	39	THR
1	A	41	SER
1	A	42	SER
1	A	44	GLU
1	A	47	GLN
1	A	49	LEU
1	A	54	LYS
1	A	55	LYS
1	A	63	LYS
1	A	64	ASN
1	A	65	ARG
1	A	68	LYS
1	A	71	ILE
1	A	76	SER
1	A	80	LYS
1	A	84	GLN
1	A	90	SER
1	A	98	LYS
1	A	105	LEU
1	A	107	ASN
1	A	118	SER
1	A	122	LYS
1	A	123	GLU
1	A	126	ASN
1	A	131	LEU
1	A	138	ILE
1	A	141	ASP
1	A	150	GLU
1	A	153	LEU
1	A	154	GLU
1	A	157	LYS
1	A	158	LEU
1	A	161	GLU
1	A	168	ASP
1	A	176	LYS
1	A	178	LYS
1	A	184	LYS

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Mol	Chain	Res	Type
1	A	185	ASN
1	B	12	GLN
1	B	18	LYS
1	B	30	GLU
1	B	32	ARG
1	B	63	LYS
1	B	70	ARG
1	B	77	ARG
1	B	80	LYS
1	B	84	GLN
1	B	89	LEU
1	B	95	ASP
1	B	101	GLU
1	B	103	PRO
1	B	105	LEU
1	B	107	ASN
1	B	108	LYS
1	B	119	SER
1	B	122	LYS
1	B	131	LEU
1	B	133	LEU
1	B	138	ILE
1	B	146	THR
1	B	150	GLU
1	B	153	LEU
1	B	155	LYS
1	B	157	LYS
1	B	158	LEU
1	B	159	LEU
1	B	161	GLU
1	B	178	LYS
1	B	184	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	126	ASN
1	B	12	GLN
1	B	107	ASN
1	B	130	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	DZF	A	187	-	34,34,34	1.92	12 (35%)	45,47,47	2.45	16 (35%)
2	DZF	B	187	-	34,34,34	2.25	12 (35%)	45,47,47	2.95	24 (53%)

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	DZF	A	187	-	-	0/22/22/22	0/1/3/3
2	DZF	B	187	-	-	0/22/22/22	0/1/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	187	DZF	C2-N3	7.54	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	DZF	C2-N3	5.05	1.39	1.33
2	B	187	DZF	C4A-C8A	-3.88	1.35	1.41
2	A	187	DZF	CA-N	3.76	1.54	1.45
2	B	187	DZF	C7-C6	3.29	1.43	1.38
2	B	187	DZF	CB-CG	3.22	1.63	1.52
2	A	187	DZF	C4A-C8A	-3.16	1.36	1.41
2	B	187	DZF	CG-CD	3.13	1.58	1.50
2	A	187	DZF	CG-CD	3.06	1.58	1.50
2	B	187	DZF	C8A-N8	2.81	1.38	1.34
2	A	187	DZF	CB-CG	2.75	1.61	1.52
2	B	187	DZF	C5-C4A	-2.65	1.36	1.42
2	A	187	DZF	C2-NA2	-2.63	1.28	1.32
2	B	187	DZF	C2-NA2	-2.55	1.28	1.32
2	B	187	DZF	C15-C14	2.53	1.43	1.39
2	A	187	DZF	C8A-N8	-2.49	1.31	1.34
2	B	187	DZF	C-N	-2.49	1.28	1.34
2	A	187	DZF	C5-C4A	-2.46	1.37	1.42
2	A	187	DZF	C13-C14	-2.43	1.35	1.39
2	B	187	DZF	C4-C4A	2.29	1.48	1.39
2	B	187	DZF	C13-C14	-2.28	1.35	1.39
2	A	187	DZF	OE2-CD	-2.13	1.22	1.30
2	A	187	DZF	C4-C4A	2.04	1.47	1.39
2	A	187	DZF	C5-C6	-2.00	1.33	1.37

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	187	DZF	NA2-C2-N1	7.58	126.20	117.86
2	B	187	DZF	C4A-C4-N3	-6.80	115.77	123.72
2	A	187	DZF	C4A-C4-N3	-6.55	116.06	123.72
2	B	187	DZF	C4-N3-C2	6.33	123.75	116.91
2	A	187	DZF	C4-N3-C2	5.54	122.89	116.91
2	B	187	DZF	O-C-N	-5.48	112.55	122.44
2	A	187	DZF	OE1-CD-CG	-5.21	105.09	123.03
2	A	187	DZF	NA2-C2-N1	5.21	123.59	117.86
2	B	187	DZF	C11-C-N	4.64	124.62	116.89
2	B	187	DZF	CB-CA-N	4.50	119.40	110.83
2	A	187	DZF	CB-CA-N	-3.92	103.36	110.83
2	B	187	DZF	C5-C4A-C8A	3.88	123.09	116.65
2	B	187	DZF	C7-N8-C8A	-3.83	111.19	116.62
2	B	187	DZF	OE1-CD-CG	-3.82	109.89	123.03
2	A	187	DZF	C5-C4A-C8A	3.72	122.82	116.65

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	187	DZF	CB-CG-CD	-3.67	103.98	112.88
2	B	187	DZF	CA-N-C	3.58	129.78	121.80
2	A	187	DZF	C4A-C8A-N1	3.25	123.50	119.36
2	B	187	DZF	NA2-C2-N3	-3.07	116.14	120.30
2	A	187	DZF	NA2-C2-N3	-3.04	116.18	120.30
2	A	187	DZF	C6-C5-C4A	-3.03	115.43	122.10
2	B	187	DZF	C13-C12-C11	2.98	124.32	120.76
2	B	187	DZF	N1-C2-N3	-2.96	117.63	121.75
2	A	187	DZF	OE2-CD-CG	2.93	124.58	114.22
2	B	187	DZF	CB-CG-CD	-2.89	105.87	112.88
2	B	187	DZF	C6-C7-N8	2.76	128.60	123.73
2	A	187	DZF	OE2-CD-OE1	2.73	130.23	123.30
2	B	187	DZF	C6-C5-C4A	-2.71	116.13	122.10
2	A	187	DZF	C12-C13-C14	-2.66	117.18	120.27
2	B	187	DZF	C16-C11-C12	-2.58	114.95	118.63
2	A	187	DZF	C7-N8-C8A	-2.47	113.11	116.62
2	B	187	DZF	C15-C14-N10	-2.33	116.27	121.02
2	B	187	DZF	C6-C9-N10	2.31	118.89	113.73
2	A	187	DZF	C13-C12-C11	2.26	123.45	120.76
2	B	187	DZF	C9-C6-C5	-2.25	118.78	122.27
2	B	187	DZF	C5-C4A-C4	-2.24	117.67	121.95
2	A	187	DZF	C15-C14-N10	-2.23	116.47	121.02
2	B	187	DZF	C16-C11-C	2.19	127.34	120.56
2	B	187	DZF	OE2-CD-CG	2.07	121.54	114.22
2	B	187	DZF	OE2-CD-OE1	2.06	128.53	123.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.