



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:09 AM GMT

PDB ID : 3DFR  
Title : CRYSTAL STRUCTURES OF ESCHERICHIA COLI AND LACTO-  
BACILLUS CASEI DIHYDROFOLATE REDUCTASE REFINED AT 1.7  
ANGSTROMS RESOLUTION. I. GENERAL FEATURES AND BINDING  
OF METHOTREXATE  
Authors : Filman, D.J.; Matthews, D.A.; Bolin, J.T.; Kraut, J.  
Deposited on : 1982-06-25  
Resolution : 1.70 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>

---

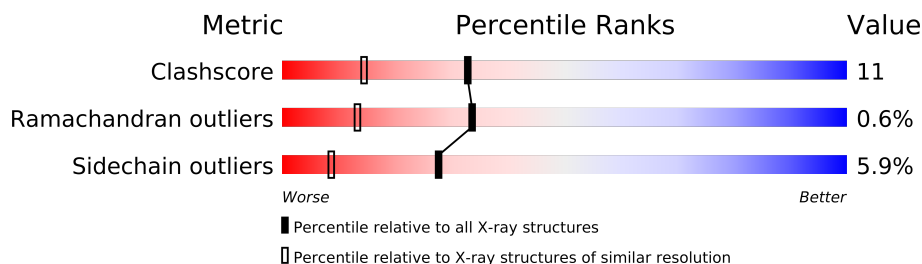
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.70 Å.

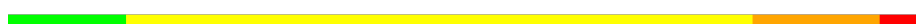
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)

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	162	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 1639 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.

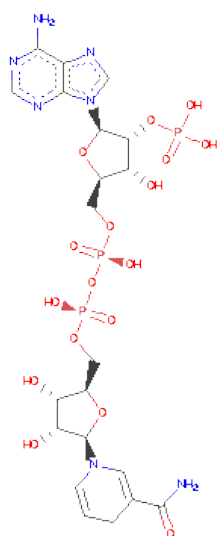
- Molecule 1 is a protein called DIHYDROFOLATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	162	1294	826	226	240	2	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

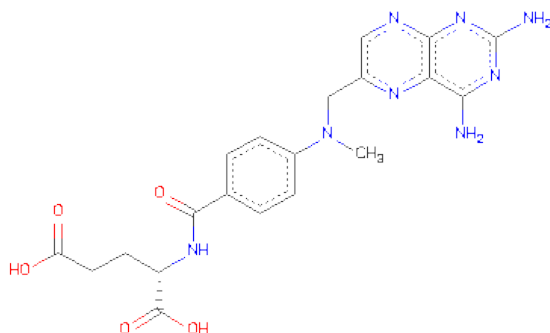
Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ASN	ASP	CONFLICT	UNP P00381
A	10	ASN	ASP	CONFLICT	UNP P00381
A	90	LEU	PRO	CONFLICT	UNP P00381

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0

- Molecule 3 is METHOTREXATE (three-letter code: MTX) (formula:  $C_{20}H_{22}N_8O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	20	8	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	264	Total	O	0	0
			264	264		

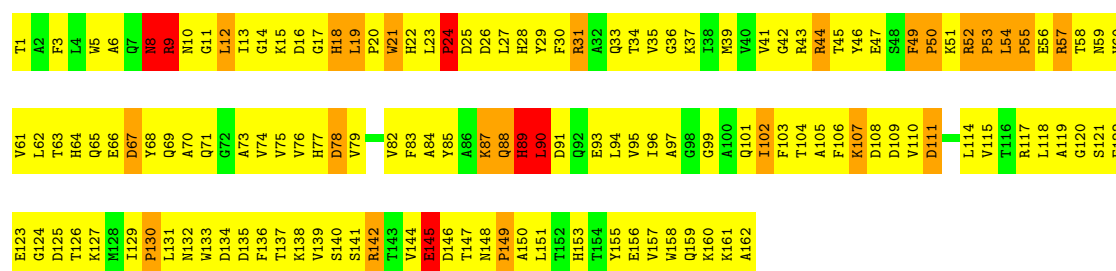
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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

Chain A: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.86Å 71.86Å 93.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	unknown	Depositor
R, $R_{free}$	0.152 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1639	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	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: NDP, MTX

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	3.65	157/1328 (11.8%)	5.35	361/1809 (20.0%)

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	8

All (157) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	PRO	N-CD	22.11	1.78	1.47
1	A	145	GLU	CD-OE2	22.01	1.49	1.25
1	A	24	PRO	N-CD	21.82	1.78	1.47
1	A	130	PRO	N-CD	18.06	1.73	1.47
1	A	89	HIS	C-O	18.04	1.57	1.23
1	A	142	ARG	NE-CZ	16.83	1.54	1.33
1	A	149	PRO	N-CD	16.21	1.70	1.47
1	A	89	HIS	C-N	-16.15	0.96	1.34
1	A	52	ARG	C-N	16.06	1.64	1.34
1	A	55	PRO	N-CD	15.24	1.69	1.47
1	A	67	ASP	CA-CB	15.22	1.87	1.53
1	A	53	PRO	N-CD	15.00	1.68	1.47
1	A	145	GLU	CD-OE1	14.48	1.41	1.25
1	A	145	GLU	CB-CG	13.38	1.77	1.52
1	A	117	ARG	NE-CZ	-13.30	1.15	1.33
1	A	20	PRO	N-CD	12.98	1.66	1.47
1	A	54	LEU	C-N	12.30	1.57	1.34
1	A	140	SER	CA-CB	11.89	1.70	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	ARG	CZ-NH1	11.59	1.48	1.33
1	A	90	LEU	CG-CD2	11.50	1.94	1.51
1	A	19	LEU	C-N	11.41	1.55	1.34
1	A	49	PHE	CG-CD2	11.02	1.55	1.38
1	A	31	ARG	NE-CZ	10.94	1.47	1.33
1	A	121	SER	CB-OG	-10.90	1.28	1.42
1	A	67	ASP	CG-OD1	10.82	1.50	1.25
1	A	129	ILE	C-N	10.79	1.54	1.34
1	A	108	ASP	CB-CG	10.54	1.73	1.51
1	A	10	ASN	CG-OD1	10.39	1.46	1.24
1	A	90	LEU	CG-CD1	9.98	1.88	1.51
1	A	10	ASN	CB-CG	9.87	1.73	1.51
1	A	123	GLU	CD-OE1	9.80	1.36	1.25
1	A	105	ALA	C-O	9.77	1.42	1.23
1	A	67	ASP	CG-OD2	9.76	1.47	1.25
1	A	28	HIS	CG-CD2	9.54	1.51	1.35
1	A	44	ARG	CZ-NH1	9.48	1.45	1.33
1	A	18	HIS	CD2-NE2	9.46	1.61	1.42
1	A	145	GLU	CG-CD	9.42	1.66	1.51
1	A	90	LEU	N-CA	9.20	1.64	1.46
1	A	109	ASP	CB-CG	9.15	1.71	1.51
1	A	93	GLU	CD-OE1	9.12	1.35	1.25
1	A	140	SER	CB-OG	-9.06	1.30	1.42
1	A	142	ARG	CZ-NH1	8.97	1.44	1.33
1	A	148	ASN	C-N	8.88	1.51	1.34
1	A	23	LEU	C-N	8.77	1.50	1.34
1	A	162	ALA	C-O	8.45	1.39	1.23
1	A	44	ARG	CD-NE	-8.44	1.32	1.46
1	A	49	PHE	C-N	8.34	1.50	1.34
1	A	56	GLU	CB-CG	8.17	1.67	1.52
1	A	134	ASP	CG-OD1	8.15	1.44	1.25
1	A	78	ASP	C-O	8.08	1.38	1.23
1	A	90	LEU	CB-CG	-7.96	1.29	1.52
1	A	133	TRP	CD2-CE2	7.84	1.50	1.41
1	A	78	ASP	CG-OD2	7.83	1.43	1.25
1	A	91	ASP	CA-CB	7.78	1.71	1.53
1	A	50	PRO	CA-CB	7.78	1.69	1.53
1	A	134	ASP	CG-OD2	7.74	1.43	1.25
1	A	158	TRP	CZ3-CH2	7.73	1.52	1.40
1	A	99	GLY	CA-C	-7.63	1.39	1.51
1	A	3	PHE	CG-CD1	7.63	1.50	1.38
1	A	106	PHE	CE1-CZ	7.50	1.51	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	GLY	N-CA	7.50	1.57	1.46
1	A	23	LEU	C-O	-7.41	1.09	1.23
1	A	162	ALA	C-OXT	7.40	1.37	1.23
1	A	50	PRO	N-CA	7.33	1.59	1.47
1	A	14	GLY	CA-C	7.31	1.63	1.51
1	A	85	TYR	CG-CD2	7.24	1.48	1.39
1	A	87	LYS	CD-CE	7.22	1.69	1.51
1	A	56	GLU	CD-OE1	7.16	1.33	1.25
1	A	9	ARG	CZ-NH2	7.15	1.42	1.33
1	A	159	GLN	CB-CG	7.12	1.71	1.52
1	A	68	TYR	CE1-CZ	7.09	1.47	1.38
1	A	20	PRO	N-CA	7.09	1.59	1.47
1	A	135	ASP	CA-C	7.05	1.71	1.52
1	A	134	ASP	CA-CB	6.93	1.69	1.53
1	A	65	GLN	CD-NE2	6.91	1.50	1.32
1	A	22	HIS	CG-CD2	6.89	1.47	1.35
1	A	51	LYS	CA-CB	6.89	1.69	1.53
1	A	31	ARG	CZ-NH2	6.88	1.42	1.33
1	A	52	ARG	N-CA	6.85	1.60	1.46
1	A	19	LEU	C-O	-6.84	1.10	1.23
1	A	16	ASP	CA-CB	6.83	1.69	1.53
1	A	107	LYS	CD-CE	6.80	1.68	1.51
1	A	132	ASN	N-CA	6.77	1.59	1.46
1	A	13	ILE	C-N	6.76	1.45	1.33
1	A	9	ARG	CZ-NH1	6.75	1.41	1.33
1	A	66	GLU	CD-OE2	6.69	1.33	1.25
1	A	9	ARG	CG-CD	6.69	1.68	1.51
1	A	66	GLU	CB-CG	6.61	1.64	1.52
1	A	148	ASN	C-O	-6.43	1.11	1.23
1	A	18	HIS	CG-ND1	6.30	1.52	1.38
1	A	135	ASP	CB-CG	6.28	1.65	1.51
1	A	123	GLU	CA-CB	6.21	1.67	1.53
1	A	46	TYR	CG-CD1	6.18	1.47	1.39
1	A	67	ASP	C-N	6.18	1.48	1.34
1	A	108	ASP	CG-OD2	6.17	1.39	1.25
1	A	132	ASN	CB-CG	6.17	1.65	1.51
1	A	77	HIS	CA-CB	6.12	1.67	1.53
1	A	137	THR	C-O	6.12	1.34	1.23
1	A	44	ARG	CZ-NH2	6.10	1.41	1.33
1	A	29	TYR	CE2-CZ	6.02	1.46	1.38
1	A	125	ASP	CG-OD1	6.01	1.39	1.25
1	A	24	PRO	CA-CB	5.99	1.65	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	ARG	CB-CG	-5.98	1.36	1.52
1	A	47	GLU	CD-OE1	-5.96	1.19	1.25
1	A	144	VAL	CB-CG2	-5.92	1.40	1.52
1	A	57	ARG	CZ-NH1	5.88	1.40	1.33
1	A	95	VAL	CA-C	5.86	1.68	1.52
1	A	91	ASP	CG-OD2	5.85	1.38	1.25
1	A	91	ASP	C-O	5.82	1.34	1.23
1	A	149	PRO	C-O	5.78	1.34	1.23
1	A	162	ALA	CA-C	5.78	1.68	1.52
1	A	132	ASN	C-O	5.73	1.34	1.23
1	A	158	TRP	CG-CD1	5.71	1.44	1.36
1	A	111	ASP	CG-OD1	5.71	1.38	1.25
1	A	8	ASN	N-CA	5.69	1.57	1.46
1	A	83	PHE	CE1-CZ	5.65	1.48	1.37
1	A	122	PHE	CG-CD1	5.57	1.47	1.38
1	A	106	PHE	CB-CG	-5.56	1.42	1.51
1	A	43	ARG	NE-CZ	5.54	1.40	1.33
1	A	131	LEU	C-O	5.52	1.33	1.23
1	A	54	LEU	C-O	-5.51	1.12	1.23
1	A	64	HIS	CG-ND1	-5.50	1.26	1.38
1	A	139	VAL	CA-CB	5.50	1.66	1.54
1	A	79	VAL	CB-CG1	-5.48	1.41	1.52
1	A	156	GLU	CB-CG	5.45	1.62	1.52
1	A	25	ASP	CB-CG	-5.44	1.40	1.51
1	A	46	TYR	CG-CD2	5.42	1.46	1.39
1	A	79	VAL	CA-CB	5.42	1.66	1.54
1	A	57	ARG	CA-CB	5.42	1.65	1.53
1	A	70	ALA	C-O	5.36	1.33	1.23
1	A	123	GLU	CD-OE2	5.35	1.31	1.25
1	A	63	THR	C-O	5.35	1.33	1.23
1	A	68	TYR	CE2-CZ	5.35	1.45	1.38
1	A	108	ASP	CG-OD1	5.31	1.37	1.25
1	A	36	GLY	CA-C	-5.28	1.43	1.51
1	A	118	LEU	CB-CG	5.26	1.67	1.52
1	A	88	GLN	C-N	5.21	1.46	1.34
1	A	120	GLY	N-CA	-5.21	1.38	1.46
1	A	58	THR	CA-CB	5.20	1.66	1.53
1	A	107	LYS	CA-CB	5.19	1.65	1.53
1	A	109	ASP	CG-OD2	5.19	1.37	1.25
1	A	83	PHE	C-N	-5.14	1.22	1.34
1	A	11	GLY	C-N	5.13	1.45	1.34
1	A	46	TYR	CE2-CZ	-5.13	1.31	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	ASP	C-O	-5.13	1.13	1.23
1	A	138	LYS	CE-NZ	5.11	1.61	1.49
1	A	146	ASP	CA-C	5.10	1.66	1.52
1	A	91	ASP	C-N	5.08	1.45	1.34
1	A	69	GLN	CD-NE2	5.08	1.45	1.32
1	A	49	PHE	CD2-CE2	5.06	1.49	1.39
1	A	77	HIS	CE1-NE2	5.05	1.44	1.32
1	A	6	ALA	N-CA	5.03	1.56	1.46
1	A	46	TYR	CD2-CE2	5.02	1.46	1.39
1	A	55	PRO	N-CA	5.02	1.55	1.47
1	A	148	ASN	CA-C	5.01	1.66	1.52
1	A	115	VAL	CB-CG1	-5.01	1.42	1.52
1	A	146	ASP	CG-OD2	5.01	1.36	1.25

All (361) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	ARG	NE-CZ-NH2	82.60	161.60	120.30
1	A	117	ARG	NE-CZ-NH1	-43.88	98.36	120.30
1	A	111	ASP	CB-CG-OD1	-35.84	86.04	118.30
1	A	142	ARG	NE-CZ-NH2	-31.48	104.56	120.30
1	A	56	GLU	OE1-CD-OE2	30.53	159.94	123.30
1	A	9	ARG	CD-NE-CZ	30.11	165.75	123.60
1	A	31	ARG	NE-CZ-NH2	-26.68	106.96	120.30
1	A	67	ASP	CB-CG-OD2	-25.60	95.26	118.30
1	A	67	ASP	CB-CG-OD1	-25.14	95.67	118.30
1	A	67	ASP	OD1-CG-OD2	24.09	169.06	123.30
1	A	117	ARG	CD-NE-CZ	22.78	155.49	123.60
1	A	66	GLU	OE1-CD-OE2	22.43	150.21	123.30
1	A	49	PHE	CB-CG-CD1	21.73	136.01	120.80
1	A	44	ARG	NE-CZ-NH2	-21.35	109.62	120.30
1	A	111	ASP	OD1-CG-OD2	19.45	160.26	123.30
1	A	3	PHE	CG-CD2-CE2	19.43	142.17	120.80
1	A	123	GLU	OE1-CD-OE2	18.95	146.04	123.30
1	A	68	TYR	CB-CG-CD1	-18.78	109.73	121.00
1	A	49	PHE	CB-CG-CD2	-18.76	107.67	120.80
1	A	91	ASP	CB-CG-OD1	18.68	135.11	118.30
1	A	125	ASP	CB-CG-OD2	18.33	134.79	118.30
1	A	155	TYR	CB-CG-CD1	-18.21	110.07	121.00
1	A	109	ASP	CB-CG-OD2	-18.15	101.97	118.30
1	A	134	ASP	CB-CG-OD2	-18.11	102.00	118.30
1	A	135	ASP	CB-CG-OD2	-18.02	102.09	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	ARG	NH1-CZ-NH2	-17.64	99.99	119.40
1	A	57	ARG	NE-CZ-NH2	17.59	129.10	120.30
1	A	83	PHE	CB-CG-CD2	-17.23	108.73	120.80
1	A	25	ASP	CB-CG-OD1	16.00	132.70	118.30
1	A	118	LEU	CB-CG-CD2	-15.88	84.00	111.00
1	A	108	ASP	CB-CG-OD2	-15.79	104.09	118.30
1	A	106	PHE	CB-CG-CD1	14.98	131.29	120.80
1	A	10	ASN	OD1-CG-ND2	14.63	155.55	121.90
1	A	29	TYR	CB-CG-CD2	14.52	129.71	121.00
1	A	66	GLU	CG-CD-OE2	-14.47	89.36	118.30
1	A	31	ARG	NE-CZ-NH1	14.27	127.44	120.30
1	A	78	ASP	CB-CG-OD2	-14.16	105.56	118.30
1	A	10	ASN	CB-CG-OD1	-13.97	93.65	121.60
1	A	3	PHE	CB-CG-CD1	13.97	130.58	120.80
1	A	142	ARG	CD-NE-CZ	-13.96	104.05	123.60
1	A	52	ARG	O-C-N	-13.79	94.89	121.10
1	A	134	ASP	CB-CG-OD1	13.08	130.07	118.30
1	A	146	ASP	CB-CG-OD1	13.05	130.05	118.30
1	A	158	TRP	NE1-CE2-CD2	13.03	120.33	107.30
1	A	161	LYS	CD-CE-NZ	13.03	141.66	111.70
1	A	62	LEU	CB-CG-CD2	-12.93	89.02	111.00
1	A	49	PHE	C-N-CD	12.81	155.30	128.40
1	A	29	TYR	CG-CD2-CE2	12.76	131.51	121.30
1	A	23	LEU	C-N-CD	12.13	153.88	128.40
1	A	52	ARG	NE-CZ-NH2	-12.08	114.26	120.30
1	A	44	ARG	NE-CZ-NH1	11.93	126.26	120.30
1	A	54	LEU	C-N-CD	11.79	153.16	128.40
1	A	103	PHE	CB-CG-CD1	-11.79	112.55	120.80
1	A	105	ALA	CA-C-N	11.78	143.10	117.20
1	A	52	ARG	CA-C-O	11.77	144.82	120.10
1	A	56	GLU	CG-CD-OE2	-11.52	95.25	118.30
1	A	142	ARG	NE-CZ-NH1	11.49	126.04	120.30
1	A	19	LEU	C-N-CD	11.47	152.50	128.40
1	A	131	LEU	CD1-CG-CD2	11.32	144.46	110.50
1	A	68	TYR	CB-CG-CD2	11.25	127.75	121.00
1	A	105	ALA	O-C-N	-11.23	104.73	122.70
1	A	67	ASP	CB-CA-C	-11.16	88.07	110.40
1	A	148	ASN	C-N-CD	11.12	151.75	128.40
1	A	90	LEU	CA-CB-CG	-11.09	89.78	115.30
1	A	140	SER	CA-CB-OG	-10.84	81.94	111.20
1	A	3	PHE	CD1-CG-CD2	-10.82	104.23	118.30
1	A	44	ARG	CG-CD-NE	10.82	134.53	111.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	TRP	CB-CG-CD1	10.75	140.98	127.00
1	A	52	ARG	CG-CD-NE	-10.58	89.58	111.80
1	A	91	ASP	OD1-CG-OD2	-10.46	103.43	123.30
1	A	108	ASP	OD1-CG-OD2	10.40	143.07	123.30
1	A	88	GLN	CA-CB-CG	10.34	136.14	113.40
1	A	89	HIS	CA-C-O	-10.28	98.51	120.10
1	A	158	TRP	CE2-CD2-CG	-10.28	99.08	107.30
1	A	44	ARG	N-CA-CB	-10.18	92.28	110.60
1	A	16	ASP	CB-CG-OD1	10.17	127.46	118.30
1	A	52	ARG	C-N-CD	10.10	149.60	128.40
1	A	78	ASP	OD1-CG-OD2	10.09	142.48	123.30
1	A	78	ASP	CA-CB-CG	10.01	135.42	113.40
1	A	162	ALA	CB-CA-C	-9.99	95.11	110.10
1	A	88	GLN	C-N-CA	9.88	146.41	121.70
1	A	73	ALA	O-C-N	-9.85	106.94	122.70
1	A	21	TRP	CB-CG-CD2	-9.75	113.92	126.60
1	A	9	ARG	CG-CD-NE	-9.65	91.53	111.80
1	A	62	LEU	O-C-N	-9.55	107.42	122.70
1	A	34	THR	O-C-N	9.52	137.94	122.70
1	A	26	ASP	CB-CG-OD1	9.45	126.80	118.30
1	A	83	PHE	CD1-CE1-CZ	-9.43	108.78	120.10
1	A	158	TRP	CD1-NE1-CE2	-9.43	100.52	109.00
1	A	136	PHE	CB-CG-CD1	9.42	127.39	120.80
1	A	19	LEU	CA-C-O	9.38	139.81	120.10
1	A	49	PHE	O-C-N	9.36	138.88	121.10
1	A	158	TRP	CE2-CD2-CE3	9.35	129.92	118.70
1	A	26	ASP	O-C-N	-9.27	107.86	122.70
1	A	24	PRO	CA-N-CD	-9.20	98.62	111.50
1	A	123	GLU	O-C-N	-9.19	107.59	123.20
1	A	142	ARG	NH1-CZ-NH2	9.09	129.40	119.40
1	A	129	ILE	C-N-CD	9.04	147.40	128.40
1	A	90	LEU	CB-CG-CD1	9.02	126.34	111.00
1	A	5	TRP	CE3-CZ3-CH2	9.02	131.12	121.20
1	A	135	ASP	OD1-CG-OD2	8.99	140.38	123.30
1	A	43	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	A	88	GLN	CA-C-O	8.96	138.91	120.10
1	A	47	GLU	O-C-N	-8.94	108.39	122.70
1	A	30	PHE	CB-CG-CD1	-8.88	114.58	120.80
1	A	110	VAL	O-C-N	-8.83	108.57	122.70
1	A	65	GLN	O-C-N	-8.80	108.62	122.70
1	A	149	PRO	N-CD-CG	-8.79	90.01	103.20
1	A	123	GLU	CG-CD-OE2	-8.66	100.98	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	HIS	CA-C-N	8.61	136.14	117.20
1	A	78	ASP	CB-CG-OD1	-8.54	110.61	118.30
1	A	53	PRO	CA-N-CD	-8.53	99.56	111.50
1	A	106	PHE	CB-CG-CD2	-8.52	114.84	120.80
1	A	123	GLU	N-CA-CB	-8.52	95.27	110.60
1	A	106	PHE	CG-CD1-CE1	8.50	130.15	120.80
1	A	9	ARG	NE-CZ-NH2	8.49	124.55	120.30
1	A	106	PHE	CD1-CE1-CZ	-8.41	110.01	120.10
1	A	109	ASP	N-CA-CB	-8.39	95.49	110.60
1	A	103	PHE	CG-CD1-CE1	-8.38	111.59	120.80
1	A	131	LEU	CB-CG-CD1	-8.35	96.80	111.00
1	A	110	VAL	CA-C-O	8.34	137.61	120.10
1	A	107	LYS	CB-CG-CD	8.32	133.25	111.60
1	A	31	ARG	CD-NE-CZ	-8.32	111.95	123.60
1	A	29	TYR	CG-CD1-CE1	8.31	127.95	121.30
1	A	108	ASP	O-C-N	8.31	135.99	122.70
1	A	22	HIS	CA-C-O	8.28	137.48	120.10
1	A	25	ASP	OD1-CG-OD2	-8.26	107.61	123.30
1	A	52	ARG	N-CA-C	-8.24	88.75	111.00
1	A	109	ASP	OD1-CG-OD2	8.23	138.94	123.30
1	A	29	TYR	CD1-CG-CD2	-8.20	108.88	117.90
1	A	85	TYR	CB-CG-CD2	8.14	125.89	121.00
1	A	148	ASN	CB-CG-OD1	8.14	137.87	121.60
1	A	89	HIS	N-CA-CB	8.10	125.18	110.60
1	A	149	PRO	N-CA-CB	8.07	112.98	103.30
1	A	63	THR	CA-C-N	8.06	134.94	117.20
1	A	54	LEU	CB-CG-CD1	-8.04	97.32	111.00
1	A	69	GLN	CG-CD-OE1	8.04	137.68	121.60
1	A	148	ASN	CA-C-O	8.04	136.98	120.10
1	A	132	ASN	CA-C-N	8.03	134.87	117.20
1	A	55	PRO	CA-N-CD	-7.98	100.33	111.50
1	A	67	ASP	N-CA-CB	-7.95	96.29	110.60
1	A	132	ASN	CB-CA-C	7.91	126.23	110.40
1	A	51	LYS	O-C-N	-7.89	110.08	122.70
1	A	161	LYS	CA-C-N	7.81	134.39	117.20
1	A	58	THR	CA-CB-OG1	-7.80	92.61	109.00
1	A	127	LYS	CB-CG-CD	-7.76	91.41	111.60
1	A	46	TYR	CG-CD2-CE2	-7.76	115.09	121.30
1	A	5	TRP	CZ3-CH2-CZ2	-7.74	112.32	121.60
1	A	88	GLN	O-C-N	-7.72	110.34	122.70
1	A	88	GLN	CG-CD-OE1	7.72	137.04	121.60
1	A	89	HIS	CB-CA-C	7.71	125.82	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ILE	CG1-CB-CG2	-7.67	94.53	111.40
1	A	78	ASP	O-C-N	-7.64	110.48	122.70
1	A	54	LEU	CA-C-O	7.64	136.14	120.10
1	A	59	ASN	O-C-N	-7.64	110.48	122.70
1	A	37	LYS	CD-CE-NZ	7.62	129.22	111.70
1	A	107	LYS	CD-CE-NZ	-7.61	94.19	111.70
1	A	90	LEU	N-CA-CB	7.59	125.58	110.40
1	A	35	VAL	CA-CB-CG1	-7.57	99.55	110.90
1	A	94	LEU	CB-CG-CD2	7.54	123.81	111.00
1	A	65	GLN	CG-CD-NE2	-7.50	98.69	116.70
1	A	90	LEU	CA-C-O	7.47	135.79	120.10
1	A	87	LYS	N-CA-CB	7.46	124.03	110.60
1	A	129	ILE	CA-C-O	7.46	135.76	120.10
1	A	137	THR	CA-C-N	7.43	133.54	117.20
1	A	144	VAL	CA-CB-CG2	-7.42	99.78	110.90
1	A	46	TYR	CB-CG-CD1	-7.41	116.56	121.00
1	A	93	GLU	CG-CD-OE1	-7.41	103.48	118.30
1	A	50	PRO	N-CD-CG	-7.38	92.13	103.20
1	A	149	PRO	CA-CB-CG	-7.37	90.00	104.00
1	A	121	SER	N-CA-CB	-7.34	99.48	110.50
1	A	3	PHE	CD1-CE1-CZ	7.30	128.87	120.10
1	A	90	LEU	O-C-N	-7.30	111.02	122.70
1	A	76	VAL	CA-C-O	7.28	135.39	120.10
1	A	90	LEU	C-N-CA	7.27	139.87	121.70
1	A	28	HIS	CA-C-N	7.25	133.16	117.20
1	A	119	ALA	N-CA-CB	-7.22	99.99	110.10
1	A	101	GLN	CA-CB-CG	-7.21	97.54	113.40
1	A	19	LEU	CB-CG-CD1	-7.20	98.77	111.00
1	A	89	HIS	ND1-CG-CD2	-7.16	95.98	106.00
1	A	145	GLU	CG-CD-OE1	-7.14	104.01	118.30
1	A	52	ARG	CB-CA-C	-7.13	96.14	110.40
1	A	122	PHE	CG-CD2-CE2	-7.12	112.97	120.80
1	A	24	PRO	CA-C-N	7.10	132.82	117.20
1	A	43	ARG	NE-CZ-NH1	-7.09	116.75	120.30
1	A	50	PRO	CA-N-CD	-7.08	101.59	111.50
1	A	66	GLU	CA-CB-CG	-7.07	97.84	113.40
1	A	56	GLU	CG-CD-OE1	-7.06	104.18	118.30
1	A	8	ASN	CB-CA-C	7.06	124.52	110.40
1	A	147	THR	CA-CB-CG2	-7.01	102.59	112.40
1	A	125	ASP	OD1-CG-OD2	-7.00	110.00	123.30
1	A	45	THR	CA-CB-OG1	-6.99	94.32	109.00
1	A	50	PRO	CB-CA-C	-6.96	94.61	112.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	TYR	CZ-CE2-CD2	-6.91	113.58	119.80
1	A	20	PRO	CA-N-CD	-6.90	101.85	111.50
1	A	136	PHE	CG-CD1-CE1	6.89	128.38	120.80
1	A	161	LYS	CB-CG-CD	-6.89	93.69	111.60
1	A	23	LEU	CA-C-N	-6.88	97.84	117.10
1	A	47	GLU	CA-CB-CG	-6.88	98.28	113.40
1	A	77	HIS	CG-ND1-CE1	6.87	117.82	108.20
1	A	119	ALA	CA-C-N	6.85	129.91	116.20
1	A	114	LEU	CB-CG-CD1	-6.85	99.36	111.00
1	A	57	ARG	NH1-CZ-NH2	-6.84	111.87	119.40
1	A	150	ALA	O-C-N	-6.83	111.77	122.70
1	A	65	GLN	CA-C-N	6.83	132.22	117.20
1	A	23	LEU	CA-C-O	6.83	134.44	120.10
1	A	133	TRP	CE2-CD2-CG	-6.82	101.85	107.30
1	A	8	ASN	CA-C-O	6.78	134.33	120.10
1	A	78	ASP	CB-CA-C	6.75	123.90	110.40
1	A	62	LEU	N-CA-CB	6.74	123.89	110.40
1	A	161	LYS	CG-CD-CE	-6.74	91.69	111.90
1	A	12	LEU	CB-CG-CD1	-6.72	99.57	111.00
1	A	142	ARG	CG-CD-NE	6.72	125.91	111.80
1	A	83	PHE	CD1-CG-CD2	6.70	127.01	118.30
1	A	49	PHE	CG-CD1-CE1	6.69	128.16	120.80
1	A	141	SER	N-CA-CB	-6.68	100.48	110.50
1	A	157	VAL	O-C-N	6.67	133.37	122.70
1	A	135	ASP	N-CA-CB	6.66	122.59	110.60
1	A	132	ASN	C-N-CA	6.64	138.30	121.70
1	A	137	THR	CA-C-O	-6.53	106.39	120.10
1	A	155	TYR	CB-CG-CD2	6.52	124.91	121.00
1	A	62	LEU	CD1-CG-CD2	-6.51	90.98	110.50
1	A	71	GLN	OE1-CD-NE2	-6.50	106.95	121.90
1	A	159	GLN	CB-CG-CD	-6.48	94.75	111.60
1	A	148	ASN	CB-CG-ND2	-6.46	101.19	116.70
1	A	27	LEU	CA-C-O	-6.43	106.59	120.10
1	A	1	THR	CA-CB-CG2	6.40	121.36	112.40
1	A	69	GLN	OE1-CD-NE2	-6.39	107.19	121.90
1	A	83	PHE	CE1-CZ-CE2	6.39	131.50	120.00
1	A	20	PRO	O-C-N	-6.39	112.48	122.70
1	A	99	GLY	O-C-N	-6.38	112.50	122.70
1	A	131	LEU	CB-CG-CD2	-6.37	100.17	111.00
1	A	22	HIS	CA-C-N	-6.36	103.22	117.20
1	A	141	SER	CA-CB-OG	-6.35	94.05	111.20
1	A	159	GLN	CG-CD-OE1	6.34	134.28	121.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	TYR	CG-CD1-CE1	-6.30	116.26	121.30
1	A	44	ARG	O-C-N	-6.28	112.65	122.70
1	A	158	TRP	NE1-CE2-CZ2	-6.28	123.49	130.40
1	A	26	ASP	CA-C-O	6.28	133.28	120.10
1	A	157	VAL	CA-C-O	-6.27	106.94	120.10
1	A	157	VAL	CG1-CB-CG2	6.26	120.92	110.90
1	A	103	PHE	CD1-CG-CD2	6.25	126.42	118.30
1	A	132	ASN	CA-CB-CG	-6.22	99.72	113.40
1	A	141	SER	O-C-N	-6.18	112.81	122.70
1	A	3	PHE	CB-CG-CD2	6.18	125.13	120.80
1	A	31	ARG	CG-CD-NE	6.17	124.76	111.80
1	A	108	ASP	C-N-CA	-6.16	106.30	121.70
1	A	19	LEU	CA-C-N	-6.11	99.98	117.10
1	A	108	ASP	CB-CG-OD1	-6.11	112.80	118.30
1	A	155	TYR	CD1-CG-CD2	6.08	124.59	117.90
1	A	118	LEU	CB-CA-C	6.07	121.72	110.20
1	A	73	ALA	CA-C-N	6.05	130.51	117.20
1	A	129	ILE	CA-C-N	-6.01	100.27	117.10
1	A	46	TYR	O-C-N	-6.00	113.09	122.70
1	A	19	LEU	N-CA-CB	5.96	122.32	110.40
1	A	47	GLU	C-N-CA	5.95	136.58	121.70
1	A	136	PHE	CD1-CE1-CZ	-5.94	112.97	120.10
1	A	25	ASP	CA-C-N	-5.91	104.19	117.20
1	A	132	ASN	CA-C-O	-5.90	107.70	120.10
1	A	43	ARG	NH1-CZ-NH2	5.90	125.89	119.40
1	A	63	THR	CA-C-O	-5.88	107.75	120.10
1	A	74	VAL	O-C-N	-5.88	113.29	122.70
1	A	9	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	A	8	ASN	CB-CG-ND2	5.88	130.80	116.70
1	A	93	GLU	CA-CB-CG	5.87	126.31	113.40
1	A	153	HIS	ND1-CG-CD2	-5.86	97.80	106.00
1	A	140	SER	CB-CA-C	-5.85	98.98	110.10
1	A	135	ASP	O-C-N	5.83	132.03	122.70
1	A	1	THR	OG1-CB-CG2	-5.83	96.59	110.00
1	A	27	LEU	CB-CG-CD2	5.83	120.91	111.00
1	A	13	ILE	C-N-CA	-5.82	110.08	122.30
1	A	64	HIS	O-C-N	5.80	131.98	122.70
1	A	82	VAL	O-C-N	-5.80	113.42	122.70
1	A	54	LEU	N-CA-C	-5.80	95.35	111.00
1	A	85	TYR	CD1-CE1-CZ	5.79	125.01	119.80
1	A	8	ASN	CA-C-N	-5.79	104.46	117.20
1	A	54	LEU	CA-C-N	-5.76	100.97	117.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ALA	C-N-CA	5.75	136.09	121.70
1	A	64	HIS	CG-CD2-NE2	-5.74	98.29	109.20
1	A	30	PHE	CB-CG-CD2	5.74	124.82	120.80
1	A	64	HIS	CB-CG-CD2	-5.74	113.02	130.80
1	A	61	VAL	O-C-N	-5.71	113.56	122.70
1	A	44	ARG	CB-CG-CD	-5.70	96.79	111.60
1	A	151	LEU	CB-CG-CD1	-5.70	101.32	111.00
1	A	125	ASP	N-CA-CB	-5.69	100.35	110.60
1	A	145	GLU	CB-CG-CD	-5.69	98.83	114.20
1	A	57	ARG	CB-CG-CD	-5.69	96.81	111.60
1	A	49	PHE	CA-C-N	-5.67	101.22	117.10
1	A	148	ASN	N-CA-C	-5.66	95.72	111.00
1	A	111	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	A	49	PHE	CG-CD2-CE2	-5.65	114.58	120.80
1	A	83	PHE	CA-C-O	-5.64	108.25	120.10
1	A	31	ARG	NH1-CZ-NH2	5.63	125.59	119.40
1	A	76	VAL	CA-C-N	-5.62	104.84	117.20
1	A	20	PRO	CB-CA-C	-5.58	98.05	112.00
1	A	148	ASN	CA-C-N	-5.56	101.52	117.10
1	A	130	PRO	CA-N-CD	-5.56	103.72	111.50
1	A	96	ILE	CA-CB-CG1	5.54	121.52	111.00
1	A	96	ILE	CA-CB-CG2	-5.53	99.83	110.90
1	A	107	LYS	CA-C-N	5.52	129.35	117.20
1	A	88	GLN	CB-CG-CD	5.52	125.94	111.60
1	A	102	ILE	CA-CB-CG2	5.51	121.92	110.90
1	A	119	ALA	O-C-N	-5.50	113.85	123.20
1	A	28	HIS	CB-CG-ND1	5.49	136.94	123.20
1	A	90	LEU	CB-CA-C	5.49	120.63	110.20
1	A	57	ARG	N-CA-C	-5.48	96.20	111.00
1	A	142	ARG	N-CA-C	-5.47	96.22	111.00
1	A	59	ASN	CB-CG-ND2	5.46	129.80	116.70
1	A	78	ASP	N-CA-CB	-5.45	100.79	110.60
1	A	135	ASP	CB-CA-C	-5.45	99.50	110.40
1	A	122	PHE	CB-CG-CD1	-5.44	116.99	120.80
1	A	134	ASP	O-C-N	-5.44	114.00	122.70
1	A	61	VAL	CG1-CB-CG2	5.42	119.58	110.90
1	A	70	ALA	CB-CA-C	5.42	118.23	110.10
1	A	42	GLY	CA-C-O	5.42	130.35	120.60
1	A	137	THR	CA-CB-OG1	-5.41	97.63	109.00
1	A	159	GLN	OE1-CD-NE2	-5.41	109.47	121.90
1	A	49	PHE	C-N-CA	-5.40	99.31	122.00
1	A	149	PRO	C-N-CA	5.39	135.19	121.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	THR	CA-CB-OG1	-5.39	97.69	109.00
1	A	144	VAL	CG1-CB-CG2	5.38	119.51	110.90
1	A	71	GLN	CA-CB-CG	-5.37	101.59	113.40
1	A	122	PHE	CD1-CG-CD2	5.35	125.26	118.30
1	A	63	THR	OG1-CB-CG2	5.32	122.23	110.00
1	A	117	ARG	O-C-N	5.30	131.19	122.70
1	A	22	HIS	CA-CB-CG	-5.30	104.59	113.60
1	A	42	GLY	O-C-N	-5.30	114.22	122.70
1	A	139	VAL	CG1-CB-CG2	-5.30	102.42	110.90
1	A	67	ASP	N-CA-C	5.29	125.27	111.00
1	A	43	ARG	C-N-CA	-5.27	108.52	121.70
1	A	127	LYS	CA-C-N	-5.27	105.61	117.20
1	A	104	THR	N-CA-CB	-5.26	100.31	110.30
1	A	122	PHE	CG-CD1-CE1	-5.26	115.01	120.80
1	A	122	PHE	CZ-CE2-CD2	5.22	126.36	120.10
1	A	28	HIS	N-CA-C	-5.20	96.96	111.00
1	A	39	MET	CG-SD-CE	5.19	108.51	100.20
1	A	50	PRO	C-N-CA	5.18	134.64	121.70
1	A	151	LEU	N-CA-CB	5.16	120.73	110.40
1	A	114	LEU	CA-CB-CG	-5.16	103.44	115.30
1	A	99	GLY	CA-C-O	5.15	129.87	120.60
1	A	158	TRP	CD2-CE2-CZ2	-5.13	116.14	122.30
1	A	97	ALA	CA-C-O	-5.13	109.33	120.10
1	A	30	PHE	CA-C-N	-5.12	105.93	117.20
1	A	24	PRO	CA-CB-CG	-5.12	94.27	104.00
1	A	33	GLN	CG-CD-NE2	-5.12	104.41	116.70
1	A	77	HIS	ND1-CE1-NE2	-5.12	98.64	109.90
1	A	39	MET	CA-C-N	5.11	128.44	117.20
1	A	75	VAL	CG1-CB-CG2	5.11	119.08	110.90
1	A	37	LYS	N-CA-CB	-5.11	101.41	110.60
1	A	91	ASP	CA-CB-CG	-5.11	102.16	113.40
1	A	95	VAL	CA-CB-CG1	-5.11	103.24	110.90
1	A	75	VAL	O-C-N	-5.09	114.55	122.70
1	A	25	ASP	CA-C-O	5.08	130.76	120.10
1	A	84	ALA	O-C-N	-5.06	114.60	122.70
1	A	87	LYS	O-C-N	-5.06	114.60	122.70
1	A	104	THR	OG1-CB-CG2	-5.05	98.38	110.00
1	A	3	PHE	CE1-CZ-CE2	-5.05	110.90	120.00
1	A	134	ASP	CA-C-N	5.02	128.24	117.20
1	A	30	PHE	CD1-CE1-CZ	-5.01	114.08	120.10
1	A	93	GLU	CG-CD-OE2	5.00	128.31	118.30
1	A	97	ALA	O-C-N	5.00	131.70	123.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	89	HIS	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	GLU	Mainchain
1	A	21	TRP	Mainchain
1	A	31	ARG	Sidechain
1	A	44	ARG	Sidechain
1	A	52	ARG	Sidechain
1	A	57	ARG	Sidechain
1	A	78	ASP	Mainchain
1	A	9	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	1294	0	1254	30	5
2	A	48	0	26	0	0
3	A	33	0	20	1	0
4	A	264	0	0	2	5
All	All	1639	0	1300	30	5

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 11.

All (30) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:145:GLU:CG	1:A:145:GLU:CB	1.77	1.58
1:A:90:LEU:CG	1:A:90:LEU:CD1	1.88	1.50
1:A:67:ASP:CB	1:A:67:ASP:CA	1.87	1.48
1:A:90:LEU:CG	1:A:90:LEU:CD2	1.94	1.44
1:A:50:PRO:N	1:A:50:PRO:CD	1.78	1.38

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:149:PRO:N	1:A:149:PRO:CD	1.70	1.37
1:A:55:PRO:N	1:A:55:PRO:CD	1.69	1.35
1:A:130:PRO:N	1:A:130:PRO:CD	1.73	1.33
1:A:53:PRO:CD	1:A:53:PRO:N	1.68	1.33
1:A:24:PRO:CD	1:A:24:PRO:N	1.78	1.29
1:A:67:ASP:CB	1:A:67:ASP:C	2.34	0.95
1:A:90:LEU:CB	1:A:90:LEU:CD2	2.60	0.78
1:A:89:HIS:O	1:A:90:LEU:HB2	1.83	0.77
1:A:67:ASP:N	1:A:67:ASP:CB	2.49	0.76
1:A:89:HIS:O	1:A:90:LEU:CB	2.37	0.73
1:A:145:GLU:CB	1:A:145:GLU:CD	2.60	0.69
1:A:8:ASN:ND2	1:A:12:LEU:H	1.96	0.62
1:A:67:ASP:CG	1:A:67:ASP:CA	2.69	0.56
1:A:145:GLU:CG	1:A:145:GLU:CA	2.83	0.52
1:A:19:LEU:HD11	3:A:164:MTX:H7	1.92	0.51
1:A:67:ASP:CB	1:A:67:ASP:H	2.23	0.49
1:A:18:HIS:HB3	4:A:403:HOH:O	2.13	0.47
1:A:15:LYS:HG3	1:A:124:GLY:HA2	1.97	0.46
1:A:67:ASP:OD1	1:A:67:ASP:CA	2.62	0.46
1:A:87:LYS:O	1:A:90:LEU:HD12	2.15	0.46
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.92	0.43
1:A:160:LYS:NZ	4:A:319:HOH:O	2.53	0.42
1:A:107:LYS:HE3	1:A:130:PRO:O	2.20	0.41
1:A:41:VAL:HG11	1:A:49:PHE:HZ	1.85	0.41
1:A:142:ARG:HH11	1:A:142:ARG:HD2	1.74	0.41

All (5) 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:60:VAL:CG2	4:A:525:HOH:O[2_665]	0.73	1.47
1:A:60:VAL:CB	4:A:525:HOH:O[2_665]	1.24	0.96
1:A:149:PRO:CG	4:A:410:HOH:O[3_564]	1.31	0.89
1:A:149:PRO:CB	4:A:410:HOH:O[3_564]	1.59	0.61
1:A:149:PRO:CD	4:A:410:HOH:O[3_564]	1.61	0.59

## 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	160/162 (99%)	158 (99%)	1 (1%)	1 (1%)	33	13

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	LEU

### 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	136/137 (99%)	128 (94%)	8 (6%)	28	9

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	9	ARG
1	A	24	PRO
1	A	88	GLN
1	A	89	HIS
1	A	90	LEU
1	A	102	ILE
1	A	111	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	101	GLN

### 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	NDP	A	163	-	52,52,52	2.15	21 (40%)	80,80,80	3.13	36 (45%)
3	MTX	A	164	-	35,35,35	3.33	13 (37%)	49,49,49	5.10	33 (67%)

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	NDP	A	163	-	-	0/35/77/77	0/3/5/5
3	MTX	A	164	-	-	0/25/25/25	0/1/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	164	MTX	C11-C	-9.28	1.30	1.50
3	A	164	MTX	C13-C14	7.89	1.55	1.39
3	A	164	MTX	CG-CD	6.50	1.67	1.50
3	A	164	MTX	C7-N8	-5.62	1.21	1.31
2	A	163	NDP	O4B-C4B	-5.60	1.31	1.45
3	A	164	MTX	C16-C15	-5.22	1.28	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	164	MTX	C15-C14	5.11	1.49	1.39
3	A	164	MTX	C9-N10	-5.04	1.38	1.46
2	A	163	NDP	O4B-C1B	4.67	1.48	1.41
3	A	164	MTX	OE1-CD	4.23	1.37	1.22
3	A	164	MTX	CA-N	-4.22	1.36	1.45
3	A	164	MTX	CM-N10	4.12	1.52	1.46
2	A	163	NDP	C4A-N3A	4.07	1.41	1.35
2	A	163	NDP	C8A-N7A	-3.97	1.26	1.34
2	A	163	NDP	C1D-N1N	3.56	1.53	1.46
2	A	163	NDP	C2A-N1A	3.17	1.40	1.33
2	A	163	NDP	C3B-C2B	2.98	1.60	1.53
2	A	163	NDP	C6N-C5N	2.96	1.39	1.33
2	A	163	NDP	O7N-C7N	2.85	1.31	1.24
2	A	163	NDP	C2N-C3N	-2.78	1.29	1.34
2	A	163	NDP	C6N-N1N	2.77	1.45	1.37
2	A	163	NDP	C6A-C5A	2.73	1.58	1.42
2	A	163	NDP	C5B-C4B	2.71	1.60	1.51
2	A	163	NDP	P2B-O2B	2.45	1.67	1.59
2	A	163	NDP	C6A-N1A	-2.44	1.26	1.37
2	A	163	NDP	C3B-C4B	2.36	1.59	1.53
2	A	163	NDP	O3B-C3B	2.34	1.48	1.43
3	A	164	MTX	O2-CT	2.31	1.38	1.30
2	A	163	NDP	C4N-C5N	-2.30	1.44	1.49
2	A	163	NDP	C1B-N9A	-2.09	1.42	1.48
2	A	163	NDP	C2A-N3A	2.08	1.36	1.32
2	A	163	NDP	C4A-N9A	-2.08	1.34	1.37
3	A	164	MTX	CB-CA	2.07	1.58	1.53
3	A	164	MTX	C9-C6	2.02	1.54	1.51

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	164	MTX	O-C-N	-15.58	94.31	122.44
2	A	163	NDP	C8A-N9A-C4A	-10.00	99.26	106.90
3	A	164	MTX	CA-N-C	9.84	143.75	121.80
2	A	163	NDP	O7N-C7N-C3N	-9.50	102.66	120.51
3	A	164	MTX	OE2-CD-OE1	9.31	146.99	123.30
3	A	164	MTX	CB-CG-CD	9.29	135.44	112.88
3	A	164	MTX	O-C-C11	9.19	137.13	121.01
3	A	164	MTX	C13-C12-C11	8.98	131.48	120.76
3	A	164	MTX	OE2-CD-CG	-8.30	84.90	114.22
3	A	164	MTX	C12-C13-C14	-8.20	109.42	120.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	164	MTX	CB-CA-N	7.88	125.85	110.83
2	A	163	NDP	O4B-C1B-C2B	-7.55	99.89	106.95
3	A	164	MTX	C6-C7-N8	7.54	131.10	123.16
2	A	163	NDP	O2X-P2B-O1X	6.78	132.60	110.44
3	A	164	MTX	C9-N10-C14	6.61	133.11	119.36
3	A	164	MTX	C11-C-N	6.55	127.81	116.89
2	A	163	NDP	N3A-C2A-N1A	6.53	134.16	128.71
2	A	163	NDP	C3N-C7N-N7N	6.29	129.59	117.48
3	A	164	MTX	CB-CA-CT	-5.56	98.74	110.71
2	A	163	NDP	C4N-C3N-C2N	-5.51	114.97	121.68
2	A	163	NDP	C1D-N1N-C2N	5.34	130.12	121.02
2	A	163	NDP	C1D-N1N-C6N	-4.98	109.75	120.79
2	A	163	NDP	C2B-C3B-C4B	-4.88	90.35	101.94
2	A	163	NDP	N6A-C6A-N1A	4.71	128.61	119.36
2	A	163	NDP	C4N-C3N-C7N	4.61	130.96	118.38
3	A	164	MTX	C7-N8-C8A	-4.36	111.94	116.85
3	A	164	MTX	N1-C2-N3	-4.01	121.20	127.54
2	A	163	NDP	C5N-C6N-N1N	-3.99	114.88	123.03
3	A	164	MTX	C16-C15-C14	3.98	125.79	120.44
3	A	164	MTX	C4-C4A-C8A	3.94	120.16	116.87
2	A	163	NDP	C4A-C5A-N7A	-3.90	106.18	109.52
2	A	163	NDP	C2A-N3A-C4A	-3.86	103.04	114.01
2	A	163	NDP	C2N-C3N-C7N	-3.85	108.66	118.49
3	A	164	MTX	CG-CB-CA	3.67	120.19	112.99
3	A	164	MTX	C15-C14-N10	-3.62	116.62	121.61
3	A	164	MTX	C7-C6-N5	-3.62	118.22	120.75
2	A	163	NDP	O3B-C3B-C4B	-3.53	100.67	111.08
3	A	164	MTX	C9-C6-C7	3.46	127.68	121.49
3	A	164	MTX	NA2-C2-N3	3.42	123.09	117.19
3	A	164	MTX	O1-CT-CA	3.41	134.34	121.86
3	A	164	MTX	C13-C14-N10	3.34	126.22	121.61
2	A	163	NDP	O3X-P2B-O2B	-3.31	97.56	107.09
2	A	163	NDP	O2N-PN-O1N	3.20	130.07	112.21
2	A	163	NDP	O4D-C1D-N1N	3.12	114.66	108.05
2	A	163	NDP	C8A-N9A-C1B	3.12	132.52	126.38
2	A	163	NDP	C5A-C6A-N1A	-3.11	108.82	119.27
3	A	164	MTX	O2-CT-O1	-3.09	117.09	124.07
3	A	164	MTX	C2-N3-C4	3.07	127.41	116.50
2	A	163	NDP	O3B-C3B-C2B	3.01	120.05	111.20
2	A	163	NDP	O4B-C4B-C5B	-2.97	98.74	109.36
2	A	163	NDP	C5A-C4A-N9A	2.97	111.45	107.16
2	A	163	NDP	P2B-O2B-C2B	2.86	127.98	121.96

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	163	NDP	C5B-C4B-C3B	-2.79	104.05	115.21
2	A	163	NDP	C2A-N1A-C6A	2.71	123.66	118.77
3	A	164	MTX	NA4-C4-N3	2.68	125.62	116.23
3	A	164	MTX	C15-C16-C11	-2.67	117.57	120.76
2	A	163	NDP	N3A-C4A-N9A	-2.59	120.76	125.43
3	A	164	MTX	CM-N10-C14	-2.58	114.79	119.58
2	A	163	NDP	C4B-O4B-C1B	2.53	112.50	109.75
2	A	163	NDP	C3N-C2N-N1N	2.43	126.49	123.05
2	A	163	NDP	N7A-C8A-N9A	2.39	121.13	114.36
2	A	163	NDP	O2B-P2B-O1X	-2.34	100.27	106.79
2	A	163	NDP	O2X-P2B-O2B	-2.33	100.39	107.09
3	A	164	MTX	C9-C6-N5	-2.24	113.20	116.97
2	A	163	NDP	O2N-PN-O5D	-2.16	97.60	108.51
2	A	163	NDP	C6A-C5A-C4A	2.13	121.16	117.25
3	A	164	MTX	C4A-C4-N3	-2.11	112.17	119.27
3	A	164	MTX	C8A-C4A-N5	-2.11	120.07	122.66
3	A	164	MTX	C12-C11-C	-2.08	114.11	120.56

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.