



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:43 AM GMT

PDB ID : 2CBF  
Title : THE X-RAY STRUCTURE OF A COBALAMIN BIOSYNTHETIC ENZYME, COBALT PRECORRIN-4 METHYLTRANSFERASE, CBIF, FROM BACILLUS MEGATERIUM, WITH THE HIS-TAG CLEAVED OFF  
Authors : Schubert, H.L.; Raux, E.; Woodcock, S.C.; Warren, M.J.; Wilson, K.S.  
Deposited on : 1998-05-01  
Resolution : 3.10 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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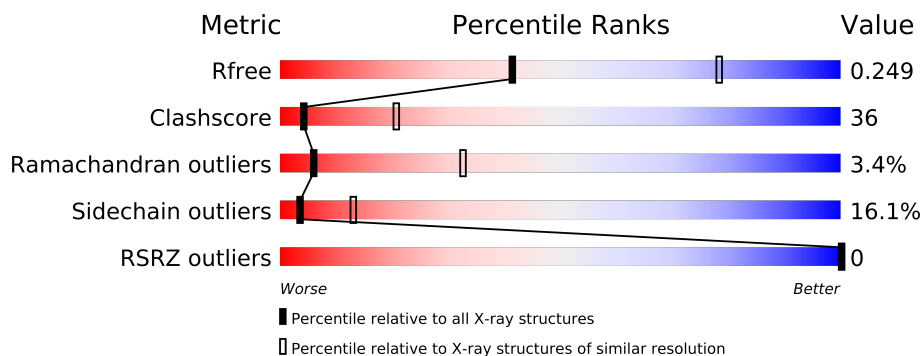
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
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 3.10 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))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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.

Mol	Chain	Length	Quality of chain
1	A	234	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 1807 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.

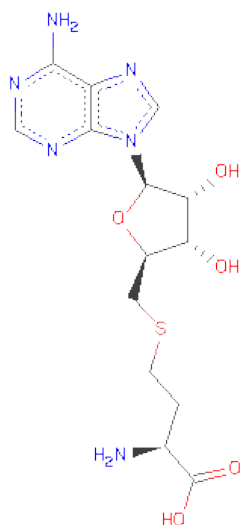
- Molecule 1 is a protein called COBALT-PRECORRIN-4 TRANSMETHYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	234	1781	1135	298	335	13	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	SER	ALA	CONFLICT	UNP O87696

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).



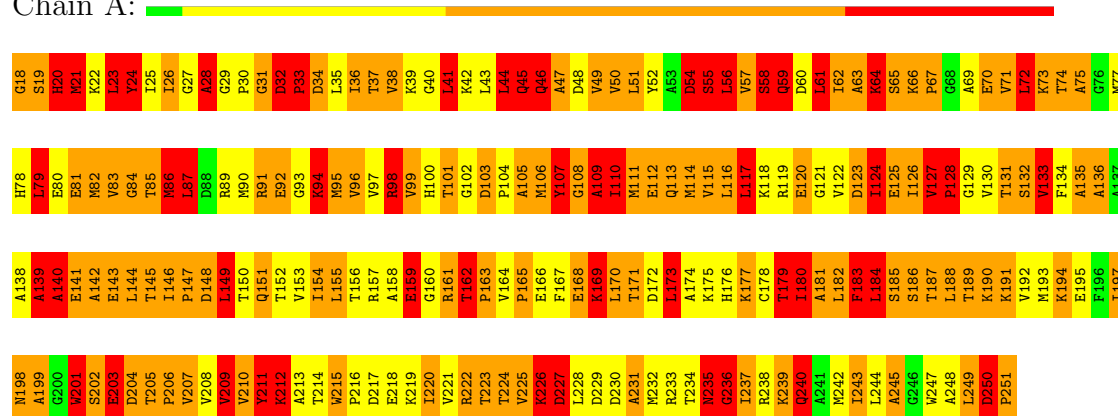
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	26	14	6	5	1	0	0

### 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.

#### • Molecule 1: COBALT-PRECORRIN-4 TRANSMETHYLASE

Chain A:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.04Å 80.04Å 77.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10 22.15 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-3.10) 93.1 (22.15-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 3.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.183 , 0.281 0.181 , 0.249	Depositor DCC
$R_{free}$ test set	225 reflections (4.61%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.3	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.4	EDS
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 5106 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	1807	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	2.46	95/1809 (5.3%)	5.85	662/2451 (27.0%)

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	0	59

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	GLU	CD-OE2	14.93	1.42	1.25
1	A	19	SER	CB-OG	13.47	1.59	1.42
1	A	161	ARG	C-O	11.12	1.44	1.23
1	A	216	PRO	CA-CB	-10.32	1.32	1.53
1	A	121	GLY	N-CA	-9.74	1.31	1.46
1	A	134	PHE	CE2-CZ	-9.64	1.19	1.37
1	A	109	ALA	CA-CB	-9.63	1.32	1.52
1	A	70	GLU	CD-OE1	9.38	1.35	1.25
1	A	177	LYS	C-O	9.09	1.40	1.23
1	A	50	VAL	CB-CG2	-8.58	1.34	1.52
1	A	98	ARG	CZ-NH1	8.44	1.44	1.33
1	A	143	GLU	CD-OE1	8.35	1.34	1.25
1	A	215	TRP	CD2-CE2	-8.17	1.31	1.41
1	A	236	GLY	N-CA	-8.16	1.33	1.46
1	A	213	ALA	CA-CB	-8.10	1.35	1.52
1	A	141	GLU	CD-OE2	7.93	1.34	1.25
1	A	18	GLY	N-CA	7.63	1.57	1.46
1	A	97	VAL	CB-CG1	-7.30	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	ALA	CA-CB	-7.20	1.37	1.52
1	A	251	PRO	N-CD	7.19	1.57	1.47
1	A	81	GLU	CD-OE1	7.15	1.33	1.25
1	A	91	ARG	C-O	-7.15	1.09	1.23
1	A	93	GLY	N-CA	-7.10	1.35	1.46
1	A	168	GLU	CG-CD	-6.93	1.41	1.51
1	A	93	GLY	CA-C	-6.88	1.40	1.51
1	A	36	ILE	N-CA	6.86	1.60	1.46
1	A	71	VAL	C-O	-6.69	1.10	1.23
1	A	107	TYR	CG-CD2	6.61	1.47	1.39
1	A	132	SER	CB-OG	-6.59	1.33	1.42
1	A	215	TRP	CD2-CE3	-6.59	1.30	1.40
1	A	139	ALA	C-O	-6.47	1.11	1.23
1	A	129	GLY	C-N	6.43	1.48	1.34
1	A	115	VAL	CB-CG1	-6.30	1.39	1.52
1	A	128	PRO	N-CD	-6.27	1.39	1.47
1	A	125	GLU	CD-OE2	6.20	1.32	1.25
1	A	43	LEU	CA-C	-6.14	1.36	1.52
1	A	104	PRO	N-CD	-6.11	1.39	1.47
1	A	203	GLU	CD-OE2	6.09	1.32	1.25
1	A	208	VAL	CB-CG2	-6.04	1.40	1.52
1	A	168	GLU	CD-OE1	-6.04	1.19	1.25
1	A	119	ARG	C-O	-6.03	1.11	1.23
1	A	124	ILE	N-CA	-5.99	1.34	1.46
1	A	120	GLU	CD-OE2	5.99	1.32	1.25
1	A	123	ASP	CA-CB	-5.90	1.41	1.53
1	A	215	TRP	CE3-CZ3	-5.80	1.28	1.38
1	A	107	TYR	CE1-CZ	-5.76	1.31	1.38
1	A	61	LEU	N-CA	-5.72	1.34	1.46
1	A	100	HIS	CB-CG	-5.70	1.39	1.50
1	A	43	LEU	CB-CG	5.70	1.69	1.52
1	A	20	HIS	N-CA	5.67	1.57	1.46
1	A	23	LEU	N-CA	-5.67	1.35	1.46
1	A	27	GLY	CA-C	5.66	1.60	1.51
1	A	214	THR	CB-OG1	-5.64	1.31	1.43
1	A	71	VAL	N-CA	-5.64	1.35	1.46
1	A	64	LYS	CA-CB	-5.63	1.41	1.53
1	A	166	GLU	CD-OE1	5.62	1.31	1.25
1	A	251	PRO	C-O	5.60	1.34	1.23
1	A	69	ALA	C-N	-5.59	1.21	1.34
1	A	201	TRP	CG-CD1	-5.57	1.28	1.36
1	A	180	ILE	CA-CB	-5.57	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	GLN	CB-CG	-5.54	1.37	1.52
1	A	101	THR	C-N	-5.50	1.23	1.33
1	A	44	LEU	C-N	-5.49	1.21	1.34
1	A	83	VAL	C-N	-5.48	1.23	1.33
1	A	211	TYR	CE2-CZ	-5.43	1.31	1.38
1	A	240	GLN	CA-CB	-5.43	1.42	1.53
1	A	80	GLU	CD-OE1	5.42	1.31	1.25
1	A	50	VAL	CB-CG1	-5.42	1.41	1.52
1	A	158	ALA	N-CA	5.41	1.57	1.46
1	A	116	LEU	C-O	-5.40	1.13	1.23
1	A	220	ILE	C-N	-5.39	1.21	1.34
1	A	97	VAL	C-N	-5.32	1.21	1.34
1	A	39	LYS	CE-NZ	5.32	1.62	1.49
1	A	222	ARG	CZ-NH1	5.31	1.40	1.33
1	A	168	GLU	CD-OE2	-5.30	1.19	1.25
1	A	19	SER	C-O	5.30	1.33	1.23
1	A	123	ASP	N-CA	-5.30	1.35	1.46
1	A	249	LEU	C-O	5.29	1.33	1.23
1	A	27	GLY	C-O	5.29	1.32	1.23
1	A	170	LEU	C-O	5.27	1.33	1.23
1	A	21	MET	CA-CB	-5.27	1.42	1.53
1	A	110	ILE	N-CA	-5.26	1.35	1.46
1	A	89	ARG	CA-CB	-5.24	1.42	1.53
1	A	160	GLY	C-O	5.23	1.32	1.23
1	A	43	LEU	C-O	-5.21	1.13	1.23
1	A	56	LEU	CA-CB	-5.18	1.41	1.53
1	A	121	GLY	C-O	-5.17	1.15	1.23
1	A	234	THR	CB-OG1	5.16	1.53	1.43
1	A	242	MET	CG-SD	5.12	1.94	1.81
1	A	131	THR	CB-OG1	-5.02	1.33	1.43
1	A	157	ARG	CZ-NH2	5.01	1.39	1.33
1	A	50	VAL	N-CA	5.01	1.56	1.46
1	A	247	TRP	CD2-CE2	-5.01	1.35	1.41
1	A	143	GLU	CG-CD	5.01	1.59	1.51
1	A	60	ASP	CA-CB	-5.00	1.43	1.53

All (662) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ARG	NE-CZ-NH1	66.23	153.41	120.30
1	A	217	ASP	CB-CG-OD2	-60.24	64.08	118.30
1	A	222	ARG	NE-CZ-NH2	-50.63	94.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ARG	NE-CZ-NH2	-42.79	98.91	120.30
1	A	238	ARG	NE-CZ-NH1	36.64	138.62	120.30
1	A	89	ARG	NE-CZ-NH2	-36.46	102.07	120.30
1	A	229	ASP	CB-CG-OD2	32.48	147.53	118.30
1	A	204	ASP	CB-CG-OD2	31.42	146.58	118.30
1	A	123	ASP	CB-CG-OD2	-30.94	90.46	118.30
1	A	211	TYR	CB-CG-CD1	30.00	139.00	121.00
1	A	222	ARG	NH1-CZ-NH2	28.75	151.02	119.40
1	A	183	PHE	CB-CG-CD1	26.84	139.59	120.80
1	A	60	ASP	CB-CG-OD2	-26.29	94.64	118.30
1	A	123	ASP	CB-CG-OD1	23.94	139.85	118.30
1	A	134	PHE	CG-CD2-CE2	23.72	146.90	120.80
1	A	71	VAL	O-C-N	-23.52	85.07	122.70
1	A	211	TYR	CB-CG-CD2	-23.17	107.10	121.00
1	A	139	ALA	N-CA-CB	-22.52	78.58	110.10
1	A	32	ASP	CB-CG-OD2	21.90	138.01	118.30
1	A	217	ASP	OD1-CG-OD2	21.16	163.51	123.30
1	A	251	PRO	CA-N-CD	-20.52	82.77	111.50
1	A	167	PHE	CB-CG-CD1	-19.60	107.08	120.80
1	A	100	HIS	O-C-N	-19.57	91.40	122.70
1	A	105	ALA	N-CA-CB	-19.40	82.94	110.10
1	A	63	ALA	CB-CA-C	-19.12	81.43	110.10
1	A	235	ASN	OD1-CG-ND2	18.79	165.12	121.90
1	A	183	PHE	CB-CG-CD2	-18.61	107.77	120.80
1	A	47	ALA	N-CA-CB	-18.58	84.09	110.10
1	A	172	ASP	CB-CG-OD2	17.70	134.23	118.30
1	A	121	GLY	O-C-N	-17.34	94.96	122.70
1	A	172	ASP	CB-CG-OD1	-17.27	102.75	118.30
1	A	64	LYS	CA-C-N	17.24	155.12	117.20
1	A	89	ARG	NH1-CZ-NH2	16.88	137.97	119.40
1	A	93	GLY	O-C-N	-16.80	95.82	122.70
1	A	87	LEU	CB-CG-CD2	-16.52	82.91	111.00
1	A	131	THR	CA-CB-CG2	16.45	135.43	112.40
1	A	203	GLU	OE1-CD-OE2	16.43	143.01	123.30
1	A	167	PHE	CB-CG-CD2	16.41	132.29	120.80
1	A	221	VAL	CA-CB-CG1	15.94	134.81	110.90
1	A	64	LYS	CA-C-O	-15.73	87.06	120.10
1	A	217	ASP	CB-CG-OD1	15.67	132.40	118.30
1	A	221	VAL	CG1-CB-CG2	-15.49	86.12	110.90
1	A	45	GLN	OE1-CD-NE2	15.39	157.29	121.90
1	A	73	LYS	O-C-N	-15.31	98.21	122.70
1	A	57	VAL	CG1-CB-CG2	-15.30	86.41	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	GLU	OE1-CD-OE2	15.28	141.63	123.30
1	A	48	ASP	CB-CG-OD2	-15.23	104.59	118.30
1	A	227	ASP	CB-CG-OD2	15.21	131.99	118.30
1	A	61	LEU	N-CA-CB	15.15	140.71	110.40
1	A	22	LYS	O-C-N	15.12	146.89	122.70
1	A	134	PHE	CB-CG-CD1	15.03	131.32	120.80
1	A	180	ILE	CG1-CB-CG2	-14.95	78.52	111.40
1	A	250	ASP	CB-CG-OD1	-14.84	104.94	118.30
1	A	222	ARG	CD-NE-CZ	-14.79	102.90	123.60
1	A	148	ASP	CB-CG-OD2	14.72	131.55	118.30
1	A	189	THR	O-C-N	-14.67	99.22	122.70
1	A	218	GLU	OE1-CD-OE2	14.34	140.50	123.30
1	A	94	LYS	O-C-N	-14.05	100.22	122.70
1	A	107	TYR	O-C-N	-13.97	99.45	123.20
1	A	190	LYS	N-CA-CB	13.93	135.66	110.60
1	A	87	LEU	CB-CG-CD1	13.89	134.62	111.00
1	A	139	ALA	CA-C-O	-13.88	90.95	120.10
1	A	230	ASP	CB-CG-OD1	13.85	130.77	118.30
1	A	32	ASP	OD1-CG-OD2	-13.85	96.99	123.30
1	A	238	ARG	NE-CZ-NH2	-13.83	113.38	120.30
1	A	133	VAL	CA-CB-CG2	-13.71	90.33	110.90
1	A	222	ARG	NE-CZ-NH1	-13.61	113.50	120.30
1	A	155	LEU	N-CA-CB	-13.60	83.21	110.40
1	A	47	ALA	CB-CA-C	13.52	130.37	110.10
1	A	106	MET	N-CA-CB	13.50	134.91	110.60
1	A	38	VAL	CG1-CB-CG2	-13.45	89.37	110.90
1	A	94	LYS	CD-CE-NZ	13.33	142.35	111.70
1	A	134	PHE	CD1-CG-CD2	-13.32	100.98	118.30
1	A	103	ASP	CB-CG-OD2	-13.21	106.41	118.30
1	A	195	GLU	CA-CB-CG	13.21	142.46	113.40
1	A	151	GLN	O-C-N	-13.04	101.84	122.70
1	A	103	ASP	CB-CG-OD1	-13.02	106.58	118.30
1	A	213	ALA	CB-CA-C	-13.01	90.59	110.10
1	A	191	LYS	CA-CB-CG	12.90	141.78	113.40
1	A	221	VAL	CA-C-O	-12.87	93.06	120.10
1	A	71	VAL	CA-C-N	12.84	145.45	117.20
1	A	72	LEU	CB-CG-CD2	-12.82	89.20	111.00
1	A	190	LYS	CG-CD-CE	12.72	150.06	111.90
1	A	94	LYS	N-CA-CB	-12.66	87.81	110.60
1	A	113	GLN	CG-CD-OE1	-12.57	96.46	121.60
1	A	108	GLY	CA-C-O	12.54	143.17	120.60
1	A	146	ILE	CA-C-O	-12.51	93.83	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	THR	CA-CB-OG1	-12.48	82.80	109.00
1	A	28	ALA	N-CA-CB	12.31	127.34	110.10
1	A	103	ASP	OD1-CG-OD2	12.30	146.68	123.30
1	A	209	VAL	CA-CB-CG2	12.28	129.32	110.90
1	A	235	ASN	CB-CG-OD1	-12.11	97.37	121.60
1	A	180	ILE	CA-CB-CG1	12.05	133.90	111.00
1	A	229	ASP	CB-CG-OD1	-12.03	107.47	118.30
1	A	107	TYR	CG-CD2-CE2	11.98	130.88	121.30
1	A	173	LEU	CB-CG-CD2	-11.97	90.65	111.00
1	A	193	MET	CG-SD-CE	-11.96	81.07	100.20
1	A	189	THR	CA-CB-CG2	-11.87	95.78	112.40
1	A	107	TYR	CG-CD1-CE1	11.77	130.72	121.30
1	A	133	VAL	CG1-CB-CG2	-11.74	92.11	110.90
1	A	26	ILE	CA-C-N	11.73	139.66	116.20
1	A	129	GLY	N-CA-C	11.73	142.42	113.10
1	A	79	LEU	O-C-N	11.69	141.41	122.70
1	A	190	LYS	CB-CG-CD	11.63	141.85	111.60
1	A	183	PHE	CG-CD1-CE1	11.46	133.40	120.80
1	A	22	LYS	CA-C-O	-11.45	96.05	120.10
1	A	168	GLU	CB-CG-CD	11.42	145.04	114.20
1	A	120	GLU	C-N-CA	11.35	146.13	122.30
1	A	107	TYR	CD1-CG-CD2	-11.32	105.44	117.90
1	A	177	LYS	CA-C-O	-11.31	96.34	120.10
1	A	195	GLU	N-CA-CB	-11.21	90.41	110.60
1	A	168	GLU	CG-CD-OE1	-11.18	95.94	118.30
1	A	108	GLY	O-C-N	-11.15	104.86	122.70
1	A	140	ALA	N-CA-CB	-11.14	94.51	110.10
1	A	64	LYS	CG-CD-CE	11.09	145.18	111.90
1	A	100	HIS	CA-C-O	11.09	143.39	120.10
1	A	23	LEU	CB-CG-CD1	11.07	129.81	111.00
1	A	41	LEU	CB-CG-CD2	-11.06	92.20	111.00
1	A	134	PHE	CZ-CE2-CD2	-11.05	106.84	120.10
1	A	249	LEU	CB-CG-CD2	-11.02	92.27	111.00
1	A	204	ASP	OD1-CG-OD2	-11.02	102.37	123.30
1	A	34	ASP	CB-CG-OD2	-11.01	108.39	118.30
1	A	115	VAL	CA-CB-CG1	-10.99	94.41	110.90
1	A	184	LEU	CB-CG-CD1	10.93	129.57	111.00
1	A	194	LYS	CD-CE-NZ	10.83	136.60	111.70
1	A	250	ASP	CB-CA-C	-10.78	88.85	110.40
1	A	183	PHE	CD1-CE1-CZ	-10.74	107.21	120.10
1	A	91	ARG	CA-C-O	10.70	142.57	120.10
1	A	107	TYR	CB-CG-CD2	10.67	127.40	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ARG	NH1-CZ-NH2	-10.66	107.67	119.40
1	A	139	ALA	O-C-N	10.66	139.75	122.70
1	A	212	LYS	N-CA-CB	-10.65	91.44	110.60
1	A	65	SER	O-C-N	10.62	139.69	122.70
1	A	72	LEU	CA-CB-CG	10.61	139.70	115.30
1	A	173	LEU	O-C-N	-10.60	105.75	122.70
1	A	221	VAL	CA-C-N	10.50	140.30	117.20
1	A	215	TRP	CB-CG-CD1	-10.48	113.37	127.00
1	A	238	ARG	NH1-CZ-NH2	-10.43	107.93	119.40
1	A	229	ASP	OD1-CG-OD2	-10.41	103.53	123.30
1	A	83	VAL	CA-CB-CG2	-10.39	95.31	110.90
1	A	106	MET	CA-C-O	10.32	141.78	120.10
1	A	25	ILE	O-C-N	10.31	139.19	122.70
1	A	155	LEU	CB-CG-CD2	10.31	128.52	111.00
1	A	37	THR	CA-C-O	10.28	141.69	120.10
1	A	250	ASP	CB-CG-OD2	10.27	127.54	118.30
1	A	199	ALA	CB-CA-C	-10.24	94.74	110.10
1	A	73	LYS	N-CA-CB	10.23	129.02	110.60
1	A	73	LYS	CA-C-O	10.22	141.57	120.10
1	A	59	GLN	N-CA-CB	10.15	128.88	110.60
1	A	56	LEU	CA-CB-CG	9.96	138.21	115.30
1	A	20	HIS	O-C-N	9.93	138.59	122.70
1	A	84	GLY	O-C-N	-9.93	106.82	122.70
1	A	19	SER	N-CA-CB	-9.90	95.64	110.50
1	A	225	VAL	CA-CB-CG2	-9.90	96.05	110.90
1	A	192	VAL	CG1-CB-CG2	-9.89	95.07	110.90
1	A	198	ASN	N-CA-CB	9.89	128.41	110.60
1	A	230	ASP	CB-CG-OD2	-9.89	109.40	118.30
1	A	223	THR	OG1-CB-CG2	-9.80	87.46	110.00
1	A	227	ASP	OD1-CG-OD2	-9.77	104.73	123.30
1	A	134	PHE	CB-CG-CD2	9.68	127.57	120.80
1	A	167	PHE	CD1-CE1-CZ	-9.66	108.51	120.10
1	A	92	GLU	OE1-CD-OE2	9.62	134.85	123.30
1	A	243	ILE	O-C-N	9.61	138.07	122.70
1	A	24	TYR	CG-CD2-CE2	-9.57	113.64	121.30
1	A	173	LEU	CB-CG-CD1	9.57	127.26	111.00
1	A	198	ASN	O-C-N	-9.54	107.44	122.70
1	A	226	LYS	CG-CD-CE	9.48	140.35	111.90
1	A	58	SER	CA-CB-OG	-9.46	85.66	111.20
1	A	183	PHE	O-C-N	-9.43	107.61	122.70
1	A	60	ASP	OD1-CG-OD2	9.43	141.21	123.30
1	A	180	ILE	O-C-N	-9.43	107.62	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	GLU	OE1-CD-OE2	9.42	134.60	123.30
1	A	240	GLN	CG-CD-NE2	9.41	139.27	116.70
1	A	47	ALA	O-C-N	-9.40	107.67	122.70
1	A	95	MET	N-CA-CB	9.40	127.51	110.60
1	A	92	GLU	CA-C-O	-9.37	100.43	120.10
1	A	96	VAL	O-C-N	-9.37	107.72	122.70
1	A	36	ILE	CA-C-O	-9.36	100.44	120.10
1	A	82	MET	CA-C-O	9.35	139.73	120.10
1	A	104	PRO	CA-C-O	-9.35	97.76	120.20
1	A	171	THR	CA-CB-CG2	-9.34	99.32	112.40
1	A	212	LYS	O-C-N	-9.22	107.95	122.70
1	A	106	MET	O-C-N	-9.21	107.97	122.70
1	A	107	TYR	CB-CG-CD1	9.20	126.52	121.00
1	A	32	ASP	O-C-N	-9.19	103.64	121.10
1	A	91	ARG	CA-C-N	-9.19	96.98	117.20
1	A	142	ALA	N-CA-CB	-9.19	97.24	110.10
1	A	102	GLY	CA-C-O	-9.18	104.07	120.60
1	A	251	PRO	N-CD-CG	-9.18	89.42	103.20
1	A	122	VAL	CB-CA-C	9.15	128.79	111.40
1	A	238	ARG	CG-CD-NE	9.15	131.02	111.80
1	A	233	ARG	CA-C-O	-9.14	100.91	120.10
1	A	211	TYR	CG-CD2-CE2	9.13	128.61	121.30
1	A	148	ASP	OD1-CG-OD2	-9.13	105.96	123.30
1	A	182	LEU	CB-CG-CD1	-9.11	95.52	111.00
1	A	102	GLY	O-C-N	9.08	137.22	122.70
1	A	65	SER	CA-C-O	-9.07	101.05	120.10
1	A	212	LYS	CD-CE-NZ	-9.07	90.84	111.70
1	A	138	ALA	N-CA-CB	9.06	122.79	110.10
1	A	86	MET	N-CA-CB	-9.05	94.31	110.60
1	A	24	TYR	CZ-CE2-CD2	9.05	127.94	119.80
1	A	209	VAL	CA-C-O	-9.05	101.10	120.10
1	A	126	ILE	CA-CB-CG1	-9.02	93.86	111.00
1	A	240	GLN	CA-CB-CG	9.02	133.24	113.40
1	A	204	ASP	O-C-N	-9.02	108.27	122.70
1	A	166	GLU	C-N-CA	-8.98	99.24	121.70
1	A	45	GLN	CG-CD-OE1	-8.98	103.64	121.60
1	A	107	TYR	CZ-CE2-CD2	-8.97	111.72	119.80
1	A	118	LYS	O-C-N	-8.96	108.36	122.70
1	A	235	ASN	N-CA-CB	-8.95	94.48	110.60
1	A	35	LEU	CB-CG-CD2	8.93	126.19	111.00
1	A	239	LYS	CA-CB-CG	8.91	133.00	113.40
1	A	220	ILE	CA-C-N	8.90	136.78	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	ASP	CB-CG-OD1	-8.88	110.31	118.30
1	A	98	ARG	CD-NE-CZ	8.87	136.02	123.60
1	A	165	PRO	O-C-N	-8.87	108.50	122.70
1	A	184	LEU	N-CA-CB	-8.85	92.71	110.40
1	A	73	LYS	CB-CG-CD	8.81	134.51	111.60
1	A	148	ASP	O-C-N	-8.81	108.60	122.70
1	A	237	ILE	O-C-N	-8.81	108.60	122.70
1	A	26	ILE	CA-C-O	-8.76	101.70	120.10
1	A	238	ARG	O-C-N	-8.72	108.75	122.70
1	A	23	LEU	CA-C-N	8.69	136.31	117.20
1	A	123	ASP	CA-CB-CG	8.67	132.48	113.40
1	A	215	TRP	O-C-N	-8.67	104.62	121.10
1	A	222	ARG	CA-C-N	8.63	136.18	117.20
1	A	56	LEU	CB-CG-CD2	-8.62	96.35	111.00
1	A	114	MET	CG-SD-CE	8.59	113.95	100.20
1	A	178	CYS	CA-C-N	8.59	136.09	117.20
1	A	23	LEU	CA-C-O	-8.58	102.08	120.10
1	A	23	LEU	CB-CG-CD2	-8.53	96.50	111.00
1	A	72	LEU	O-C-N	-8.53	109.05	122.70
1	A	127	VAL	CA-CB-CG1	-8.52	98.11	110.90
1	A	215	TRP	NE1-CE2-CD2	8.49	115.79	107.30
1	A	164	VAL	O-C-N	8.46	137.18	121.10
1	A	165	PRO	C-N-CA	8.46	142.85	121.70
1	A	248	ALA	N-CA-CB	-8.45	98.27	110.10
1	A	71	VAL	C-N-CA	8.45	142.81	121.70
1	A	144	LEU	CB-CG-CD1	-8.43	96.67	111.00
1	A	18	GLY	CA-C-O	8.41	135.75	120.60
1	A	150	THR	CA-CB-CG2	-8.41	100.62	112.40
1	A	49	VAL	O-C-N	-8.39	109.27	122.70
1	A	101	THR	CA-C-O	-8.39	102.48	120.10
1	A	112	GLU	CA-CB-CG	8.38	131.84	113.40
1	A	130	VAL	CA-CB-CG1	8.38	123.46	110.90
1	A	127	VAL	CG1-CB-CG2	-8.31	97.60	110.90
1	A	129	GLY	C-N-CA	-8.30	100.96	121.70
1	A	240	GLN	CG-CD-OE1	-8.30	105.01	121.60
1	A	203	GLU	N-CA-CB	8.29	125.51	110.60
1	A	152	THR	CA-CB-CG2	-8.27	100.82	112.40
1	A	92	GLU	CA-C-N	8.27	132.74	116.20
1	A	207	VAL	CA-CB-CG2	-8.24	98.53	110.90
1	A	50	VAL	CA-C-N	8.23	135.30	117.20
1	A	120	GLU	O-C-N	-8.22	109.23	123.20
1	A	106	MET	CB-CA-C	-8.17	94.06	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	MET	CG-SD-CE	8.17	113.27	100.20
1	A	83	VAL	CA-CB-CG1	8.15	123.13	110.90
1	A	251	PRO	N-CA-CB	-8.15	93.52	103.30
1	A	146	ILE	O-C-N	8.15	136.58	121.10
1	A	235	ASN	CB-CG-ND2	-8.08	97.31	116.70
1	A	213	ALA	N-CA-CB	8.07	121.39	110.10
1	A	119	ARG	CA-C-N	8.04	134.89	117.20
1	A	158	ALA	O-C-N	-8.04	109.84	122.70
1	A	163	PRO	O-C-N	8.03	135.55	122.70
1	A	236	GLY	O-C-N	-8.03	109.85	122.70
1	A	164	VAL	CA-CB-CG2	-8.02	98.87	110.90
1	A	202	SER	O-C-N	-8.02	109.87	122.70
1	A	107	TYR	N-CA-CB	8.02	125.03	110.60
1	A	215	TRP	CZ3-CH2-CZ2	-8.01	111.99	121.60
1	A	33	PRO	CA-CB-CG	-7.99	88.83	104.00
1	A	154	ILE	CG1-CB-CG2	-7.97	93.86	111.40
1	A	219	LYS	CA-C-O	-7.97	103.37	120.10
1	A	231	ALA	CB-CA-C	7.96	122.05	110.10
1	A	163	PRO	N-CA-CB	7.94	112.83	103.30
1	A	18	GLY	O-C-N	-7.92	110.02	122.70
1	A	190	LYS	CD-CE-NZ	7.90	129.88	111.70
1	A	60	ASP	N-CA-C	7.90	132.33	111.00
1	A	97	VAL	CA-CB-CG1	7.87	122.70	110.90
1	A	59	GLN	CB-CG-CD	7.86	132.04	111.60
1	A	112	GLU	CB-CA-C	7.85	126.09	110.40
1	A	195	GLU	CG-CD-OE2	-7.84	102.61	118.30
1	A	132	SER	O-C-N	7.84	135.24	122.70
1	A	142	ALA	O-C-N	-7.83	110.17	122.70
1	A	218	GLU	CA-CB-CG	7.83	130.63	113.40
1	A	161	ARG	CA-C-O	7.83	136.53	120.10
1	A	161	ARG	O-C-N	-7.82	110.19	122.70
1	A	143	GLU	OE1-CD-OE2	7.81	132.67	123.30
1	A	46	GLN	CB-CG-CD	-7.80	91.31	111.60
1	A	50	VAL	C-N-CA	7.80	141.20	121.70
1	A	186	SER	CA-CB-OG	-7.80	90.14	111.20
1	A	79	LEU	C-N-CA	-7.79	102.23	121.70
1	A	37	THR	O-C-N	-7.75	110.30	122.70
1	A	185	SER	O-C-N	-7.70	110.38	122.70
1	A	242	MET	N-CA-C	-7.70	90.21	111.00
1	A	96	VAL	C-N-CA	7.70	140.94	121.70
1	A	111	MET	O-C-N	-7.68	110.42	122.70
1	A	247	TRP	CH2-CZ2-CE2	7.67	125.07	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	VAL	N-CA-CB	-7.66	94.65	111.50
1	A	73	LYS	CA-CB-CG	7.66	130.25	113.40
1	A	45	GLN	CG-CD-NE2	-7.66	98.33	116.70
1	A	80	GLU	CG-CD-OE1	7.65	133.60	118.30
1	A	183	PHE	CZ-CE2-CD2	-7.64	110.93	120.10
1	A	237	ILE	CA-CB-CG1	-7.64	96.48	111.00
1	A	55	SER	O-C-N	-7.63	110.49	122.70
1	A	98	ARG	CB-CG-CD	7.60	131.36	111.60
1	A	135	ALA	N-CA-CB	-7.60	99.46	110.10
1	A	139	ALA	CB-CA-C	-7.60	98.70	110.10
1	A	156	THR	CA-CB-CG2	7.60	123.04	112.40
1	A	216	PRO	N-CA-CB	-7.58	94.20	103.30
1	A	154	ILE	CA-C-O	-7.57	104.19	120.10
1	A	197	ILE	CB-CG1-CD1	7.57	135.09	113.90
1	A	166	GLU	OE1-CD-OE2	-7.55	114.24	123.30
1	A	235	ASN	C-N-CA	7.55	138.15	122.30
1	A	187	THR	CA-CB-CG2	-7.54	101.84	112.40
1	A	62	ILE	O-C-N	-7.54	110.64	122.70
1	A	131	THR	CA-CB-OG1	-7.52	93.20	109.00
1	A	97	VAL	CA-CB-CG2	-7.52	99.62	110.90
1	A	32	ASP	CB-CA-C	-7.52	95.36	110.40
1	A	62	ILE	CA-C-O	7.51	135.88	120.10
1	A	30	PRO	C-N-CA	-7.51	106.53	122.30
1	A	35	LEU	CA-CB-CG	-7.51	98.03	115.30
1	A	35	LEU	CB-CG-CD1	-7.50	98.26	111.00
1	A	47	ALA	C-N-CA	7.49	140.43	121.70
1	A	153	VAL	CG1-CB-CG2	-7.48	98.94	110.90
1	A	129	GLY	O-C-N	-7.47	110.75	122.70
1	A	36	ILE	N-CA-CB	7.47	127.97	110.80
1	A	140	ALA	O-C-N	-7.43	110.81	122.70
1	A	205	THR	N-CA-CB	-7.41	96.22	110.30
1	A	165	PRO	CA-CB-CG	7.39	118.84	104.80
1	A	226	LYS	O-C-N	-7.38	110.90	122.70
1	A	119	ARG	C-N-CA	7.36	140.09	121.70
1	A	103	ASP	N-CA-CB	7.35	123.84	110.60
1	A	212	LYS	C-N-CA	7.35	140.07	121.70
1	A	38	VAL	CA-C-O	7.33	135.49	120.10
1	A	239	LYS	CB-CA-C	-7.32	95.75	110.40
1	A	203	GLU	O-C-N	-7.31	111.01	122.70
1	A	206	PRO	O-C-N	-7.31	111.01	122.70
1	A	48	ASP	OD1-CG-OD2	7.30	137.16	123.30
1	A	67	PRO	C-N-CA	-7.24	107.10	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	VAL	CA-CB-CG1	-7.23	100.06	110.90
1	A	202	SER	CA-CB-OG	-7.21	91.73	111.20
1	A	215	TRP	CE2-CD2-CG	-7.19	101.54	107.30
1	A	67	PRO	O-C-N	7.18	135.41	123.20
1	A	32	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	211	TYR	CZ-CE2-CD2	-7.17	113.34	119.80
1	A	80	GLU	CA-C-N	7.16	132.94	117.20
1	A	123	ASP	CA-C-N	7.14	132.92	117.20
1	A	223	THR	CA-CB-CG2	7.14	122.40	112.40
1	A	214	THR	CA-CB-CG2	7.12	122.36	112.40
1	A	201	TRP	CA-C-O	-7.11	105.17	120.10
1	A	114	MET	N-CA-CB	7.10	123.38	110.60
1	A	25	ILE	CA-C-O	-7.08	105.22	120.10
1	A	133	VAL	CA-C-O	7.07	134.95	120.10
1	A	93	GLY	CA-C-N	7.07	132.75	117.20
1	A	250	ASP	C-N-CD	7.07	143.24	128.40
1	A	33	PRO	CA-C-N	-7.06	101.66	117.20
1	A	175	LYS	O-C-N	-7.06	111.41	122.70
1	A	59	GLN	O-C-N	-7.05	111.42	122.70
1	A	20	HIS	C-N-CA	-7.04	104.09	121.70
1	A	61	LEU	CB-CA-C	-7.00	96.90	110.20
1	A	33	PRO	CA-N-CD	-7.00	101.70	111.50
1	A	83	VAL	O-C-N	-6.99	111.32	123.20
1	A	133	VAL	CA-CB-CG1	-6.99	100.41	110.90
1	A	73	LYS	CD-CE-NZ	6.95	127.69	111.70
1	A	112	GLU	OE1-CD-OE2	-6.95	114.96	123.30
1	A	162	THR	CA-CB-CG2	-6.95	102.67	112.40
1	A	49	VAL	N-CA-CB	-6.95	96.22	111.50
1	A	238	ARG	C-N-CA	6.94	139.05	121.70
1	A	228	LEU	CB-CG-CD1	6.94	122.79	111.00
1	A	91	ARG	C-N-CA	-6.93	104.36	121.70
1	A	20	HIS	CA-CB-CG	-6.93	101.82	113.60
1	A	71	VAL	CG1-CB-CG2	-6.92	99.82	110.90
1	A	188	LEU	N-CA-CB	6.92	124.25	110.40
1	A	132	SER	CA-C-O	-6.90	105.61	120.10
1	A	109	ALA	CA-C-O	-6.87	105.67	120.10
1	A	231	ALA	N-CA-CB	-6.86	100.49	110.10
1	A	69	ALA	CB-CA-C	-6.86	99.81	110.10
1	A	44	LEU	O-C-N	-6.85	111.74	122.70
1	A	192	VAL	CA-CB-CG1	6.84	121.17	110.90
1	A	220	ILE	CA-C-O	-6.84	105.74	120.10
1	A	44	LEU	CB-CG-CD2	-6.83	99.40	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	SER	N-CA-CB	-6.78	100.33	110.50
1	A	59	GLN	N-CA-C	-6.78	92.70	111.00
1	A	190	LYS	CB-CA-C	-6.76	96.88	110.40
1	A	187	THR	OG1-CB-CG2	-6.76	94.46	110.00
1	A	121	GLY	CA-C-N	6.75	132.06	117.20
1	A	179	THR	CA-CB-CG2	6.75	121.85	112.40
1	A	113	GLN	CB-CA-C	6.72	123.84	110.40
1	A	177	LYS	CA-C-N	6.71	131.97	117.20
1	A	202	SER	N-CA-CB	-6.68	100.49	110.50
1	A	162	THR	OG1-CB-CG2	6.67	125.33	110.00
1	A	121	GLY	CA-C-O	6.66	132.59	120.60
1	A	59	GLN	CG-CD-OE1	-6.64	108.31	121.60
1	A	20	HIS	CA-C-O	-6.63	106.17	120.10
1	A	37	THR	CA-CB-CG2	-6.61	103.15	112.40
1	A	92	GLU	CG-CD-OE2	-6.60	105.09	118.30
1	A	243	ILE	CB-CG1-CD1	-6.60	95.42	113.90
1	A	21	MET	CB-CG-SD	6.60	132.19	112.40
1	A	93	GLY	C-N-CA	6.59	138.19	121.70
1	A	244	LEU	CB-CG-CD1	-6.58	99.81	111.00
1	A	35	LEU	N-CA-CB	-6.58	97.25	110.40
1	A	151	GLN	CA-C-O	6.58	133.91	120.10
1	A	215	TRP	CB-CG-CD2	6.57	135.14	126.60
1	A	128	PRO	C-N-CA	6.56	136.07	122.30
1	A	42	LYS	CD-CE-NZ	-6.54	96.66	111.70
1	A	245	ALA	CB-CA-C	-6.53	100.30	110.10
1	A	207	VAL	CA-C-N	6.52	131.54	117.20
1	A	32	ASP	C-N-CD	-6.52	106.26	120.60
1	A	141	GLU	N-CA-CB	-6.51	98.88	110.60
1	A	24	TYR	CE1-CZ-OH	6.51	137.67	120.10
1	A	216	PRO	N-CD-CG	-6.50	93.45	103.20
1	A	127	VAL	CA-CB-CG2	6.50	120.64	110.90
1	A	118	LYS	CB-CA-C	-6.49	97.42	110.40
1	A	179	THR	O-C-N	-6.47	112.34	122.70
1	A	215	TRP	CD1-CG-CD2	6.47	111.47	106.30
1	A	171	THR	O-C-N	6.46	133.04	122.70
1	A	171	THR	CA-CB-OG1	-6.46	95.44	109.00
1	A	33	PRO	CA-C-O	6.44	135.66	120.20
1	A	82	MET	CA-CB-CG	-6.42	102.38	113.30
1	A	39	LYS	CA-C-O	-6.42	106.62	120.10
1	A	95	MET	CA-CB-CG	6.42	124.21	113.30
1	A	197	ILE	O-C-N	-6.42	112.44	122.70
1	A	109	ALA	CB-CA-C	-6.41	100.48	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ASP	O-C-N	-6.41	112.44	122.70
1	A	85	THR	O-C-N	6.41	132.96	122.70
1	A	59	GLN	CB-CA-C	6.40	123.20	110.40
1	A	198	ASN	CA-C-N	6.39	131.27	117.20
1	A	30	PRO	CB-CA-C	-6.39	96.03	112.00
1	A	191	LYS	CB-CA-C	-6.38	97.64	110.40
1	A	236	GLY	C-N-CA	6.38	137.66	121.70
1	A	176	HIS	CA-CB-CG	-6.38	102.75	113.60
1	A	226	LYS	CA-CB-CG	6.38	127.43	113.40
1	A	101	THR	O-C-N	6.37	134.03	123.20
1	A	141	GLU	CA-C-N	-6.36	103.20	117.20
1	A	203	GLU	CG-CD-OE1	-6.34	105.61	118.30
1	A	156	THR	N-CA-CB	-6.34	98.26	110.30
1	A	238	ARG	CB-CG-CD	6.33	128.07	111.60
1	A	138	ALA	CA-C-O	6.29	133.30	120.10
1	A	219	LYS	N-CA-CB	6.28	121.90	110.60
1	A	124	ILE	CA-C-N	-6.27	103.40	117.20
1	A	122	VAL	N-CA-CB	-6.27	97.71	111.50
1	A	131	THR	OG1-CB-CG2	-6.27	95.58	110.00
1	A	188	LEU	O-C-N	6.26	132.72	122.70
1	A	172	ASP	N-CA-CB	-6.25	99.35	110.60
1	A	217	ASP	CA-CB-CG	-6.24	99.67	113.40
1	A	178	CYS	CA-C-O	-6.23	107.01	120.10
1	A	151	GLN	N-CA-CB	-6.23	99.39	110.60
1	A	249	LEU	N-CA-CB	-6.23	97.94	110.40
1	A	207	VAL	C-N-CA	-6.23	106.13	121.70
1	A	181	ALA	O-C-N	-6.20	112.79	122.70
1	A	48	ASP	CA-C-N	6.19	130.82	117.20
1	A	215	TRP	N-CA-CB	-6.18	99.47	110.60
1	A	26	ILE	C-N-CA	6.18	135.28	122.30
1	A	145	THR	OG1-CB-CG2	6.18	124.21	110.00
1	A	140	ALA	CB-CA-C	6.18	119.36	110.10
1	A	45	GLN	CA-CB-CG	-6.17	99.83	113.40
1	A	143	GLU	O-C-N	-6.16	112.84	122.70
1	A	157	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	A	238	ARG	CA-C-N	6.16	130.74	117.20
1	A	126	ILE	CA-C-O	-6.15	107.19	120.10
1	A	86	MET	O-C-N	-6.14	112.87	122.70
1	A	77	MET	CG-SD-CE	6.14	110.02	100.20
1	A	183	PHE	CE1-CZ-CE2	6.13	131.04	120.00
1	A	211	TYR	N-CA-CB	6.13	121.64	110.60
1	A	230	ASP	CA-CB-CG	-6.13	99.92	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	THR	CA-C-O	-6.12	107.24	120.10
1	A	222	ARG	CG-CD-NE	-6.12	98.95	111.80
1	A	70	GLU	CA-C-O	-6.12	107.25	120.10
1	A	21	MET	CA-C-O	-6.11	107.27	120.10
1	A	89	ARG	CA-C-O	6.11	132.93	120.10
1	A	173	LEU	CA-C-O	-6.11	107.28	120.10
1	A	183	PHE	N-CA-CB	6.10	121.58	110.60
1	A	33	PRO	CB-CA-C	-6.08	96.80	112.00
1	A	136	ALA	N-CA-CB	6.08	118.61	110.10
1	A	40	GLY	O-C-N	6.08	132.43	122.70
1	A	215	TRP	NE1-CE2-CZ2	-6.08	123.72	130.40
1	A	164	VAL	CG1-CB-CG2	6.07	120.61	110.90
1	A	80	GLU	O-C-N	-6.07	112.99	122.70
1	A	194	LYS	CB-CA-C	6.07	122.53	110.40
1	A	120	GLU	CG-CD-OE1	6.06	130.43	118.30
1	A	195	GLU	OE1-CD-OE2	6.04	130.55	123.30
1	A	81	GLU	CG-CD-OE2	-6.04	106.22	118.30
1	A	99	VAL	CA-C-O	-6.04	107.42	120.10
1	A	125	GLU	CG-CD-OE2	6.02	130.33	118.30
1	A	189	THR	CA-C-N	6.01	130.42	117.20
1	A	195	GLU	O-C-N	-6.00	113.10	122.70
1	A	209	VAL	CA-C-N	6.00	130.40	117.20
1	A	128	PRO	N-CD-CG	-6.00	94.21	103.20
1	A	36	ILE	CA-CB-CG1	5.99	122.39	111.00
1	A	211	TYR	C-N-CA	-5.99	106.72	121.70
1	A	233	ARG	O-C-N	5.98	132.27	122.70
1	A	104	PRO	CA-C-N	5.97	130.35	117.20
1	A	151	GLN	CG-CD-OE1	-5.97	109.65	121.60
1	A	111	MET	CA-CB-CG	5.97	123.44	113.30
1	A	164	VAL	CA-C-O	-5.96	107.59	120.10
1	A	242	MET	CB-CA-C	5.96	122.31	110.40
1	A	221	VAL	N-CA-C	-5.95	94.93	111.00
1	A	93	GLY	CA-C-O	5.95	131.31	120.60
1	A	197	ILE	CG1-CB-CG2	-5.95	98.32	111.40
1	A	66	LYS	CA-C-O	5.94	132.57	120.10
1	A	83	VAL	CB-CA-C	-5.93	100.12	111.40
1	A	94	LYS	CA-C-O	5.93	132.56	120.10
1	A	230	ASP	C-N-CA	5.92	136.50	121.70
1	A	173	LEU	N-CA-CB	5.92	122.23	110.40
1	A	148	ASP	CA-C-N	5.91	130.21	117.20
1	A	65	SER	N-CA-CB	5.91	119.36	110.50
1	A	226	LYS	CD-CE-NZ	5.90	125.27	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ILE	CB-CG1-CD1	-5.89	97.40	113.90
1	A	61	LEU	CD1-CG-CD2	5.88	128.13	110.50
1	A	144	LEU	CA-C-O	-5.87	107.77	120.10
1	A	128	PRO	N-CA-C	-5.87	96.84	112.10
1	A	132	SER	N-CA-CB	-5.86	101.70	110.50
1	A	171	THR	CB-CA-C	-5.86	95.77	111.60
1	A	170	LEU	CB-CA-C	5.86	121.34	110.20
1	A	79	LEU	CA-C-N	-5.86	104.31	117.20
1	A	151	GLN	C-N-CA	5.84	136.31	121.70
1	A	26	ILE	N-CA-C	5.84	126.77	111.00
1	A	35	LEU	O-C-N	-5.84	113.36	122.70
1	A	39	LYS	N-CA-CB	-5.84	100.09	110.60
1	A	166	GLU	CB-CG-CD	5.83	129.95	114.20
1	A	48	ASP	CA-CB-CG	-5.83	100.58	113.40
1	A	235	ASN	CA-CB-CG	-5.82	100.59	113.40
1	A	205	THR	N-CA-C	-5.81	95.31	111.00
1	A	36	ILE	N-CA-C	-5.81	95.31	111.00
1	A	183	PHE	CD1-CG-CD2	-5.80	110.76	118.30
1	A	28	ALA	O-C-N	-5.79	113.35	123.20
1	A	166	GLU	CG-CD-OE1	5.79	129.89	118.30
1	A	170	LEU	CB-CG-CD1	-5.79	101.16	111.00
1	A	147	PRO	CB-CA-C	-5.79	97.53	112.00
1	A	60	ASP	CA-C-N	5.79	129.93	117.20
1	A	207	VAL	CA-C-O	-5.74	108.05	120.10
1	A	80	GLU	CA-CB-CG	-5.74	100.78	113.40
1	A	104	PRO	O-C-N	5.73	131.87	122.70
1	A	208	VAL	CA-CB-CG1	-5.73	102.30	110.90
1	A	235	ASN	O-C-N	-5.72	113.47	123.20
1	A	133	VAL	CA-C-N	-5.72	104.62	117.20
1	A	224	THR	OG1-CB-CG2	5.71	123.13	110.00
1	A	119	ARG	CA-C-O	-5.71	108.11	120.10
1	A	131	THR	O-C-N	-5.69	113.59	122.70
1	A	142	ALA	CA-C-N	5.69	129.72	117.20
1	A	144	LEU	CA-CB-CG	-5.69	102.22	115.30
1	A	169	LYS	O-C-N	-5.68	113.61	122.70
1	A	240	GLN	C-N-CA	-5.68	107.49	121.70
1	A	236	GLY	N-CA-C	5.66	127.26	113.10
1	A	61	LEU	N-CA-C	-5.65	95.73	111.00
1	A	112	GLU	CB-CG-CD	5.65	129.46	114.20
1	A	115	VAL	O-C-N	-5.64	113.68	122.70
1	A	126	ILE	CB-CG1-CD1	-5.63	98.13	113.90
1	A	219	LYS	O-C-N	5.63	131.70	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	VAL	CA-CB-CG1	-5.61	102.48	110.90
1	A	60	ASP	CB-CA-C	-5.61	99.19	110.40
1	A	44	LEU	N-CA-CB	5.60	121.61	110.40
1	A	135	ALA	CA-C-N	5.60	129.52	117.20
1	A	99	VAL	N-CA-C	-5.60	95.88	111.00
1	A	193	MET	CB-CA-C	-5.60	99.21	110.40
1	A	183	PHE	C-N-CA	5.59	135.68	121.70
1	A	141	GLU	CB-CG-CD	5.58	129.26	114.20
1	A	139	ALA	N-CA-C	-5.58	95.94	111.00
1	A	237	ILE	N-CA-C	-5.58	95.95	111.00
1	A	208	VAL	CG1-CB-CG2	5.57	119.81	110.90
1	A	69	ALA	CA-C-O	-5.56	108.42	120.10
1	A	203	GLU	CA-C-O	5.56	131.77	120.10
1	A	38	VAL	CA-C-N	-5.56	104.97	117.20
1	A	23	LEU	CB-CA-C	5.54	120.72	110.20
1	A	175	LYS	CB-CA-C	-5.53	99.34	110.40
1	A	208	VAL	CA-CB-CG2	-5.52	102.61	110.90
1	A	106	MET	CA-CB-CG	-5.52	103.92	113.30
1	A	29	GLY	CA-C-O	5.52	130.53	120.60
1	A	24	TYR	N-CA-CB	-5.51	100.68	110.60
1	A	220	ILE	CG1-CB-CG2	-5.49	99.33	111.40
1	A	210	VAL	CG1-CB-CG2	-5.48	102.13	110.90
1	A	58	SER	C-N-CA	5.47	135.39	121.70
1	A	42	LYS	N-CA-C	-5.47	96.22	111.00
1	A	207	VAL	N-CA-C	5.47	125.78	111.00
1	A	82	MET	CA-C-N	-5.47	105.17	117.20
1	A	135	ALA	CA-C-O	-5.46	108.63	120.10
1	A	237	ILE	CA-C-N	5.46	129.21	117.20
1	A	89	ARG	N-CA-CB	-5.46	100.78	110.60
1	A	153	VAL	N-CA-CB	-5.46	99.50	111.50
1	A	205	THR	OG1-CB-CG2	5.45	122.53	110.00
1	A	158	ALA	N-CA-CB	-5.44	102.49	110.10
1	A	229	ASP	CA-CB-CG	-5.43	101.45	113.40
1	A	162	THR	CB-CA-C	-5.43	96.94	111.60
1	A	113	GLN	OE1-CD-NE2	5.43	134.39	121.90
1	A	118	LYS	C-N-CA	5.43	135.27	121.70
1	A	37	THR	CA-C-N	-5.43	105.26	117.20
1	A	89	ARG	CD-NE-CZ	5.43	131.20	123.60
1	A	177	LYS	O-C-N	5.42	131.38	122.70
1	A	227	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	229	ASP	C-N-CA	-5.39	108.22	121.70
1	A	67	PRO	CA-C-O	-5.38	107.28	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	ILE	O-C-N	5.38	131.31	122.70
1	A	50	VAL	O-C-N	-5.38	114.09	122.70
1	A	159	GLU	O-C-N	5.37	132.34	123.20
1	A	168	GLU	C-N-CA	-5.37	108.27	121.70
1	A	144	LEU	O-C-N	5.37	131.29	122.70
1	A	149	LEU	CB-CA-C	5.37	120.40	110.20
1	A	172	ASP	N-CA-C	5.37	125.49	111.00
1	A	25	ILE	CB-CA-C	5.36	122.31	111.60
1	A	103	ASP	N-CA-C	-5.35	96.55	111.00
1	A	215	TRP	CG-CD1-NE1	-5.35	104.75	110.10
1	A	92	GLU	C-N-CA	5.34	133.51	122.30
1	A	123	ASP	O-C-N	-5.34	114.16	122.70
1	A	167	PHE	CG-CD2-CE2	-5.34	114.93	120.80
1	A	168	GLU	CG-CD-OE2	5.34	128.97	118.30
1	A	194	LYS	CA-C-O	-5.34	108.89	120.10
1	A	215	TRP	CA-C-O	5.33	131.30	120.10
1	A	231	ALA	O-C-N	5.33	131.23	122.70
1	A	20	HIS	N-CA-CB	5.33	120.19	110.60
1	A	248	ALA	O-C-N	-5.32	114.19	122.70
1	A	206	PRO	CA-C-O	5.32	132.96	120.20
1	A	112	GLU	O-C-N	-5.31	114.20	122.70
1	A	113	GLN	N-CA-CB	-5.31	101.04	110.60
1	A	141	GLU	CA-C-O	5.31	131.25	120.10
1	A	150	THR	CA-C-O	5.31	131.24	120.10
1	A	219	LYS	CD-CE-NZ	5.30	123.89	111.70
1	A	31	GLY	O-C-N	-5.30	114.22	122.70
1	A	64	LYS	O-C-N	-5.30	114.22	122.70
1	A	114	MET	O-C-N	-5.29	114.23	122.70
1	A	71	VAL	CA-CB-CG1	-5.29	102.96	110.90
1	A	99	VAL	N-CA-CB	5.26	123.07	111.50
1	A	178	CYS	CA-CB-SG	-5.25	104.54	114.00
1	A	222	ARG	CA-C-O	-5.25	109.07	120.10
1	A	133	VAL	C-N-CA	5.25	134.82	121.70
1	A	99	VAL	CA-C-N	5.24	128.73	117.20
1	A	69	ALA	CA-C-N	5.24	128.73	117.20
1	A	183	PHE	CA-C-O	5.24	131.10	120.10
1	A	70	GLU	CA-CB-CG	5.24	124.92	113.40
1	A	167	PHE	CG-CD1-CE1	5.22	126.55	120.80
1	A	174	ALA	CA-C-O	-5.22	109.14	120.10
1	A	243	ILE	CB-CA-C	-5.22	101.17	111.60
1	A	19	SER	CA-C-O	-5.21	109.16	120.10
1	A	97	VAL	CA-C-O	-5.21	109.17	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	VAL	CA-CB-CG2	-5.20	103.11	110.90
1	A	251	PRO	CB-CG-CD	-5.19	86.27	106.50
1	A	210	VAL	C-N-CA	5.18	134.66	121.70
1	A	175	LYS	CA-C-N	5.18	128.59	117.20
1	A	49	VAL	CG1-CB-CG2	-5.17	102.63	110.90
1	A	211	TYR	CA-C-O	-5.17	109.25	120.10
1	A	130	VAL	CA-C-N	5.16	128.55	117.20
1	A	208	VAL	C-N-CA	-5.12	108.89	121.70
1	A	186	SER	CB-CA-C	5.12	119.83	110.10
1	A	201	TRP	O-C-N	5.12	130.89	122.70
1	A	239	LYS	CD-CE-NZ	5.11	123.45	111.70
1	A	80	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	A	143	GLU	CB-CA-C	-5.09	100.21	110.40
1	A	111	MET	CA-C-O	5.09	130.79	120.10
1	A	23	LEU	CA-CB-CG	-5.09	103.60	115.30
1	A	99	VAL	CA-CB-CG1	5.07	118.50	110.90
1	A	113	GLN	CG-CD-NE2	5.07	128.86	116.70
1	A	117	LEU	CB-CA-C	5.07	119.82	110.20
1	A	54	ASP	N-CA-CB	-5.05	101.51	110.60
1	A	170	LEU	O-C-N	-5.04	114.64	122.70
1	A	104	PRO	C-N-CA	-5.03	109.12	121.70
1	A	218	GLU	CG-CD-OE1	-5.03	108.24	118.30
1	A	94	LYS	CB-CG-CD	5.03	124.67	111.60
1	A	97	VAL	CA-C-N	5.03	128.26	117.20
1	A	165	PRO	N-CA-CB	-5.03	97.07	102.60
1	A	158	ALA	CB-CA-C	5.01	117.62	110.10
1	A	231	ALA	C-N-CA	-5.01	109.17	121.70
1	A	165	PRO	CA-C-O	5.01	132.22	120.20
1	A	202	SER	CB-CA-C	-5.01	100.59	110.10

There are no chirality outliers.

All (59) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	THR	Mainchain
1	A	107	TYR	Mainchain
1	A	109	ALA	Mainchain
1	A	117	LEU	Mainchain
1	A	120	GLU	Mainchain
1	A	124	ILE	Mainchain
1	A	127	VAL	Mainchain
1	A	128	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	A	139	ALA	Mainchain
1	A	140	ALA	Mainchain
1	A	141	GLU	Mainchain
1	A	142	ALA	Mainchain
1	A	159	GLU	Mainchain
1	A	169	LYS	Mainchain
1	A	173	LEU	Mainchain
1	A	179	THR	Mainchain
1	A	180	ILE	Mainchain
1	A	181	ALA	Mainchain
1	A	185	SER	Mainchain
1	A	189	THR	Mainchain
1	A	19	SER	Mainchain
1	A	199	ALA	Mainchain
1	A	201	TRP	Mainchain
1	A	202	SER	Mainchain
1	A	209	VAL	Mainchain
1	A	21	MET	Mainchain
1	A	211	TYR	Sidechain
1	A	212	LYS	Mainchain
1	A	220	ILE	Mainchain
1	A	227	ASP	Mainchain
1	A	23	LEU	Mainchain,Peptide
1	A	235	ASN	Mainchain,Peptide
1	A	236	GLY	Mainchain
1	A	24	TYR	Sidechain
1	A	245	ALA	Mainchain
1	A	250	ASP	Mainchain
1	A	28	ALA	Mainchain
1	A	32	ASP	Mainchain
1	A	36	ILE	Mainchain
1	A	41	LEU	Mainchain
1	A	45	GLN	Mainchain
1	A	46	GLN	Mainchain
1	A	49	VAL	Mainchain
1	A	55	SER	Mainchain
1	A	56	LEU	Mainchain
1	A	58	SER	Mainchain
1	A	59	GLN	Mainchain
1	A	61	LEU	Mainchain
1	A	64	LYS	Mainchain
1	A	71	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	A	72	LEU	Mainchain
1	A	87	LEU	Mainchain
1	A	92	GLU	Mainchain
1	A	94	LYS	Mainchain
1	A	96	VAL	Mainchain
1	A	98	ARG	Mainchain,Peptide

## 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	1781	0	1842	133	0
2	A	26	0	19	1	0
All	All	1807	0	1861	133	0

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 36.

All (133) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:177:LYS:O	1:A:177:LYS:HG2	1.41	1.11
1:A:177:LYS:O	1:A:177:LYS:CG	2.08	0.96
1:A:250:ASP:OD1	1:A:251:PRO:HD3	1.65	0.95
1:A:59:GLN:NE2	1:A:62:ILE:HD12	1.81	0.95
1:A:161:ARG:HG3	1:A:162:THR:H	1.34	0.90
1:A:136:ALA:O	1:A:139:ALA:HB3	1.71	0.89
1:A:50:VAL:HG11	1:A:52:TYR:CE2	2.08	0.88
1:A:161:ARG:CG	1:A:162:THR:H	1.85	0.88
1:A:41:LEU:O	1:A:45:GLN:HG3	1.77	0.84
1:A:44:LEU:HD11	1:A:52:TYR:OH	1.77	0.84
1:A:56:LEU:HD21	1:A:240:GLN:HG3	1.59	0.84
1:A:250:ASP:OD1	1:A:251:PRO:CD	2.26	0.82
1:A:159:GLU:HG3	1:A:163:PRO:HA	1.61	0.82
1:A:108:GLY:O	1:A:109:ALA:HB3	1.78	0.82
1:A:54:ASP:OD1	1:A:56:LEU:HB2	1.82	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:98:ARG:HD3	1:A:113:GLN:HE22	1.50	0.75
1:A:143:GLU:HG2	1:A:145:THR:O	1.86	0.75
1:A:231:ALA:O	1:A:235:ASN:HB2	1.85	0.75
1:A:50:VAL:HG11	1:A:52:TYR:CZ	2.23	0.73
1:A:59:GLN:HE21	1:A:62:ILE:HD12	1.54	0.72
1:A:74:THR:O	1:A:75:ALA:CB	2.37	0.72
1:A:44:LEU:CD1	1:A:52:TYR:OH	2.37	0.72
1:A:47:ALA:O	1:A:66:LYS:HE2	1.90	0.72
1:A:161:ARG:HG3	1:A:162:THR:N	2.06	0.71
1:A:168:GLU:O	1:A:173:LEU:HD11	1.91	0.70
1:A:161:ARG:CG	1:A:162:THR:N	2.56	0.69
1:A:187:THR:O	1:A:188:LEU:HD23	1.93	0.69
1:A:212:LYS:O	1:A:215:TRP:HB2	1.93	0.69
1:A:159:GLU:CG	1:A:163:PRO:HA	2.23	0.68
1:A:59:GLN:NE2	1:A:62:ILE:CD1	2.58	0.66
1:A:56:LEU:CD2	1:A:240:GLN:HG3	2.26	0.66
1:A:98:ARG:CD	1:A:113:GLN:HE22	2.08	0.66
1:A:211:TYR:CD2	1:A:212:LYS:HB2	2.31	0.65
1:A:52:TYR:CE1	1:A:99:VAL:HG21	2.31	0.65
1:A:124:ILE:N	1:A:124:ILE:HD13	2.11	0.65
1:A:82:MET:O	1:A:86:MET:HB2	1.98	0.63
1:A:50:VAL:CG1	1:A:52:TYR:CE2	2.78	0.63
1:A:78:HIS:CE1	1:A:81:GLU:HB2	2.35	0.62
1:A:184:LEU:HA	2:A:300:SAH:O3'	2.00	0.62
1:A:32:ASP:OD1	1:A:33:PRO:N	2.33	0.61
1:A:144:LEU:HB3	1:A:179:THR:HG21	1.83	0.61
1:A:46:GLN:HG3	1:A:95:MET:SD	2.41	0.60
1:A:74:THR:O	1:A:75:ALA:HB2	2.02	0.60
1:A:182:LEU:HD12	1:A:243:ILE:CG2	2.31	0.60
1:A:106:MET:O	1:A:107:TYR:C	2.41	0.59
1:A:204:ASP:O	1:A:205:THR:C	2.38	0.59
1:A:203:GLU:HG3	1:A:226:LYS:HB3	1.84	0.59
1:A:55:SER:O	1:A:56:LEU:HG	2.02	0.58
1:A:115:VAL:O	1:A:116:LEU:C	2.40	0.58
1:A:66:LYS:HB2	1:A:67:PRO:CD	2.34	0.58
1:A:55:SER:O	1:A:56:LEU:CG	2.52	0.58
1:A:84:GLY:O	1:A:85:THR:C	2.43	0.57
1:A:239:LYS:HE3	1:A:240:GLN:HE21	1.69	0.57
1:A:87:LEU:O	1:A:91:ARG:HG3	2.04	0.57
1:A:31:GLY:HA3	1:A:215:TRP:NE1	2.20	0.57
1:A:168:GLU:O	1:A:173:LEU:CD1	2.53	0.56
1:A:209:VAL:HG12	1:A:209:VAL:O	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:112:GLU:O	1:A:113:GLN:C	2.43	0.55
1:A:250:ASP:OD1	1:A:251:PRO:N	2.40	0.54
1:A:58:SER:O	1:A:62:ILE:HG13	2.06	0.54
1:A:223:THR:HG23	1:A:224:THR:N	2.23	0.54
1:A:250:ASP:CG	1:A:251:PRO:N	2.61	0.54
1:A:113:GLN:O	1:A:114:MET:C	2.45	0.54
1:A:108:GLY:O	1:A:109:ALA:CB	2.44	0.54
1:A:51:LEU:CD2	1:A:72:LEU:HD12	2.38	0.54
1:A:165:PRO:HG2	1:A:168:GLU:CD	2.29	0.53
1:A:133:VAL:HG23	1:A:183:PHE:CZ	2.44	0.53
1:A:161:ARG:O	1:A:163:PRO:HD3	2.09	0.53
1:A:147:PRO:O	1:A:148:ASP:HB2	2.09	0.53
1:A:58:SER:OG	1:A:59:GLN:N	2.40	0.52
1:A:136:ALA:O	1:A:139:ALA:CB	2.52	0.52
1:A:114:MET:O	1:A:115:VAL:C	2.48	0.52
1:A:170:LEU:O	1:A:171:THR:C	2.49	0.52
1:A:223:THR:OG1	1:A:224:THR:N	2.42	0.51
1:A:232:MET:CE	1:A:237:ILE:HG22	2.40	0.50
1:A:132:SER:O	1:A:135:ALA:HB3	2.12	0.50
1:A:20:HIS:N	1:A:20:HIS:ND1	2.58	0.50
1:A:127:VAL:O	1:A:128:PRO:C	2.48	0.50
1:A:98:ARG:HH11	1:A:113:GLN:CD	2.15	0.49
1:A:146:ILE:HB	1:A:149:LEU:HB3	1.94	0.49
1:A:209:VAL:HG22	1:A:243:ILE:HG12	1.95	0.49
1:A:211:TYR:O	1:A:212:LYS:C	2.49	0.49
1:A:250:ASP:CG	1:A:251:PRO:CD	2.82	0.48
1:A:37:THR:O	1:A:38:VAL:C	2.51	0.48
1:A:59:GLN:O	1:A:62:ILE:N	2.46	0.48
1:A:55:SER:O	1:A:56:LEU:CB	2.60	0.48
1:A:133:VAL:CG2	1:A:183:PHE:CZ	2.97	0.48
1:A:103:ASP:OD1	1:A:105:ALA:HB2	2.14	0.48
1:A:182:LEU:HD12	1:A:243:ILE:HB	1.97	0.47
1:A:110:ILE:O	1:A:114:MET:HG3	2.15	0.47
1:A:78:HIS:O	1:A:81:GLU:N	2.48	0.47
1:A:139:ALA:HB3	1:A:140:ALA:H	1.63	0.46
1:A:98:ARG:NH1	1:A:113:GLN:OE1	2.47	0.46
1:A:201:TRP:CE3	1:A:205:THR:HG21	2.50	0.46
1:A:226:LYS:HG2	1:A:227:ASP:OD1	2.14	0.46
1:A:24:TYR:N	1:A:24:TYR:CD2	2.83	0.46
1:A:133:VAL:HG23	1:A:183:PHE:HZ	1.78	0.46
1:A:52:TYR:CD1	1:A:99:VAL:HB	2.51	0.46
1:A:206:PRO:O	1:A:207:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:23:LEU:HB3	1:A:124:ILE:HD12	1.96	0.46
1:A:209:VAL:HG21	1:A:232:MET:SD	2.56	0.46
1:A:61:LEU:HA	1:A:61:LEU:HD23	1.55	0.45
1:A:203:GLU:HG3	1:A:226:LYS:CB	2.45	0.45
1:A:243:ILE:HG21	1:A:243:ILE:HD13	1.73	0.45
1:A:61:LEU:O	1:A:63:ALA:N	2.50	0.45
1:A:41:LEU:HD11	1:A:64:LYS:HD2	1.98	0.44
1:A:123:ASP:O	1:A:124:ILE:HD13	2.18	0.44
1:A:117:LEU:HD23	1:A:117:LEU:HA	1.64	0.44
1:A:78:HIS:O	1:A:79:LEU:C	2.55	0.44
1:A:222:ARG:HH11	1:A:222:ARG:HD3	1.05	0.44
1:A:28:ALA:HB1	1:A:61:LEU:CD1	2.47	0.43
1:A:249:LEU:HA	1:A:249:LEU:HD23	1.87	0.43
1:A:250:ASP:CG	1:A:251:PRO:HD3	2.35	0.43
1:A:154:ILE:HG21	1:A:154:ILE:HD13	1.71	0.42
1:A:32:ASP:O	1:A:34:ASP:N	2.51	0.42
1:A:126:ILE:HD13	1:A:126:ILE:HG21	1.71	0.42
1:A:212:LYS:HE2	1:A:240:GLN:NE2	2.34	0.42
1:A:124:ILE:HG22	1:A:125:GLU:N	2.35	0.42
1:A:74:THR:O	1:A:75:ALA:HB3	2.18	0.42
1:A:154:ILE:HB	1:A:180:ILE:HD12	2.00	0.42
1:A:18:GLY:O	1:A:21:MET:N	2.49	0.42
1:A:57:VAL:CG1	1:A:58:SER:N	2.82	0.42
1:A:26:ILE:HD13	1:A:26:ILE:HG21	1.76	0.42
1:A:82:MET:O	1:A:83:VAL:C	2.55	0.41
1:A:161:ARG:HG2	1:A:162:THR:H	1.79	0.41
1:A:124:ILE:CG2	1:A:125:GLU:N	2.83	0.41
1:A:123:ASP:C	1:A:124:ILE:HD13	2.40	0.41
1:A:232:MET:HE3	1:A:237:ILE:HG22	2.02	0.41
1:A:225:VAL:HG23	1:A:225:VAL:H	1.46	0.41
1:A:168:GLU:O	1:A:169:LYS:C	2.55	0.41
1:A:212:LYS:CE	1:A:240:GLN:NE2	2.83	0.41
1:A:197:ILE:O	1:A:198:ASN:C	2.57	0.40
1:A:183:PHE:O	1:A:184:LEU:HB2	2.21	0.40

There are no symmetry-related clashes.

## 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	232/234 (99%)	201 (87%)	23 (10%)	8 (3%)	6	32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	56	LEU
1	A	79	LEU
1	A	184	LEU
1	A	75	ALA
1	A	236	GLY
1	A	133	VAL
1	A	250	ASP

### 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	193/193 (100%)	162 (84%)	31 (16%)	3	13

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	33	PRO
1	A	44	LEU
1	A	51	LEU
1	A	55	SER
1	A	64	LYS

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Mol	Chain	Res	Type
1	A	65	SER
1	A	70	GLU
1	A	73	LYS
1	A	74	THR
1	A	86	MET
1	A	87	LEU
1	A	94	LYS
1	A	110	ILE
1	A	111	MET
1	A	131	THR
1	A	149	LEU
1	A	151	GLN
1	A	155	LEU
1	A	162	THR
1	A	173	LEU
1	A	180	ILE
1	A	183	PHE
1	A	186	SER
1	A	190	LYS
1	A	191	LYS
1	A	194	LYS
1	A	203	GLU
1	A	210	VAL
1	A	226	LYS
1	A	240	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	198	ASN
1	A	240	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 ⓘ

1 ligand is 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	SAH	A	300	-	28,28,28	2.03	8 (28%)	40,40,40	3.52	27 (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	SAH	A	300	-	-	0/15/31/31	0/1/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	SAH	C5'-SD	4.57	1.90	1.81
2	A	300	SAH	C1'-N9	-4.01	1.36	1.48
2	A	300	SAH	O3'-C3'	3.83	1.52	1.43
2	A	300	SAH	C5-C4	-3.53	1.32	1.40
2	A	300	SAH	C2'-C1'	-3.49	1.48	1.53
2	A	300	SAH	C5-N7	-3.03	1.28	1.40
2	A	300	SAH	C8-N9	-2.90	1.32	1.36
2	A	300	SAH	C8-N7	2.37	1.39	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	SAH	C8-N9-C4	-8.12	100.70	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	SAH	N3-C2-N1	-6.66	123.14	128.71
2	A	300	SAH	O4'-C1'-N9	-6.16	102.71	108.44
2	A	300	SAH	O4'-C1'-C2'	5.82	115.70	106.77
2	A	300	SAH	CG-CB-CA	5.64	122.67	113.22
2	A	300	SAH	OXT-C-CA	5.31	128.79	116.88
2	A	300	SAH	C5'-SD-CG	-5.17	86.99	102.42
2	A	300	SAH	O3'-C3'-C2'	-4.40	97.50	111.83
2	A	300	SAH	CB-CA-C	4.13	120.75	110.98
2	A	300	SAH	C-CA-N	4.11	116.16	109.36
2	A	300	SAH	N6-C6-N1	-4.00	111.52	119.36
2	A	300	SAH	O2'-C2'-C3'	-3.99	98.86	111.83
2	A	300	SAH	C2-N1-C6	-3.74	112.01	118.77
2	A	300	SAH	C4'-O4'-C1'	-3.59	105.85	109.75
2	A	300	SAH	C5-C4-N3	-3.40	118.30	125.70
2	A	300	SAH	O4'-C4'-C5'	-3.22	100.32	108.91
2	A	300	SAH	C5'-C4'-C3'	3.16	123.17	114.98
2	A	300	SAH	CB-CA-N	2.98	117.43	110.14
2	A	300	SAH	C5-C4-N9	2.97	111.45	107.16
2	A	300	SAH	C4-C5-N7	-2.92	107.02	109.52
2	A	300	SAH	C3'-C2'-C1'	-2.84	96.46	100.91
2	A	300	SAH	C4'-C5'-SD	-2.60	105.52	113.53
2	A	300	SAH	OXT-C-O	-2.48	118.45	124.07
2	A	300	SAH	CB-CG-SD	-2.44	108.86	113.57
2	A	300	SAH	C2'-C1'-N9	2.15	118.80	113.27
2	A	300	SAH	C8-N9-C1'	2.11	130.54	126.38
2	A	300	SAH	N7-C8-N9	-2.04	108.58	114.36

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	234/234 (100%)	-0.46	0 100 100	14, 32, 63, 87	0

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SAH	A	300	26/26	0.15	0.25	17,22,24,27	0

### 6.5 Other polymers

There are no such residues in this entry.