



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2017 – 07:29 PM EDT

PDB ID : 1K0E  
Title : THE CRYSTAL STRUCTURE OF AMINODEOXYCHORISMATE SYNTHASE FROM FORMATE GROWN CRYSTALS  
Authors : Parsons, J.F.; Jensen, P.Y.; Pachikara, A.S.; Howard, A.J.; Eisenstein, E.; Ladner, J.E.  
Deposited on : unknown  
Resolution : 2.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

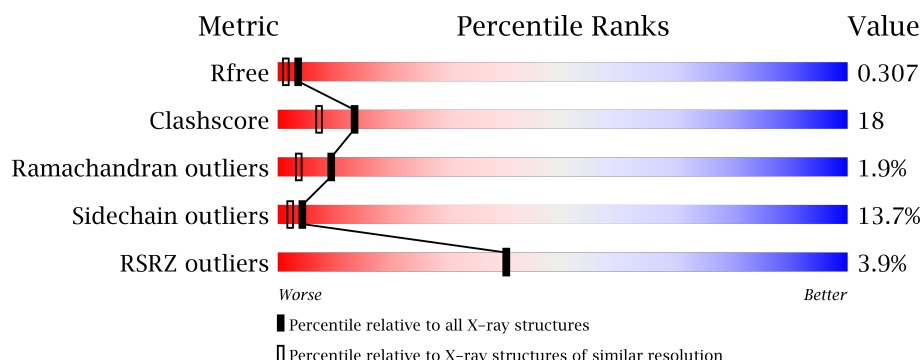
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	453	<div> <div>2%</div> <div> <div></div> <div>43%</div> <div>39%</div> <div>11%</div> <div>• •</div> </div> </div>
1	B	453	<div> <div>6%</div> <div> <div></div> <div>36%</div> <div>37%</div> <div>13%</div> <div>5%</div> <div>9%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FMT	A	1701	-	-	X	X

## 2 Entry composition [i](#)

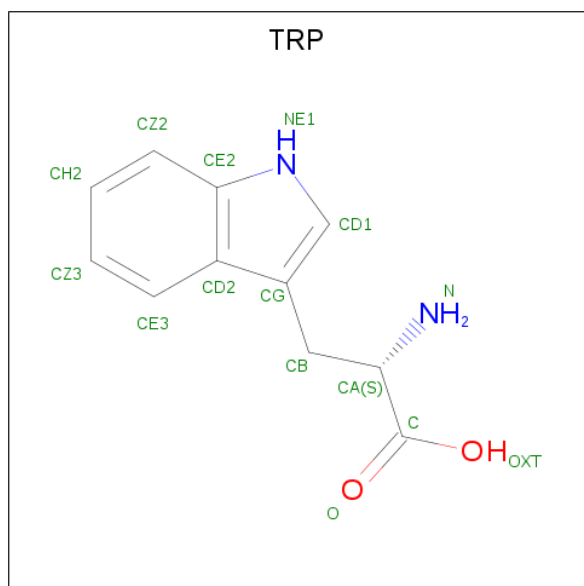
There are 4 unique types of molecules in this entry. The entry contains 7106 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called p-aminobenzoate synthase component I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3466	2186	605	662	13			
1	B	414	Total	C	N	O	S	0	0	0
			3289	2067	574	634	14			

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula:  $C_{11}H_{12}N_2O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula:  $CH_2O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		

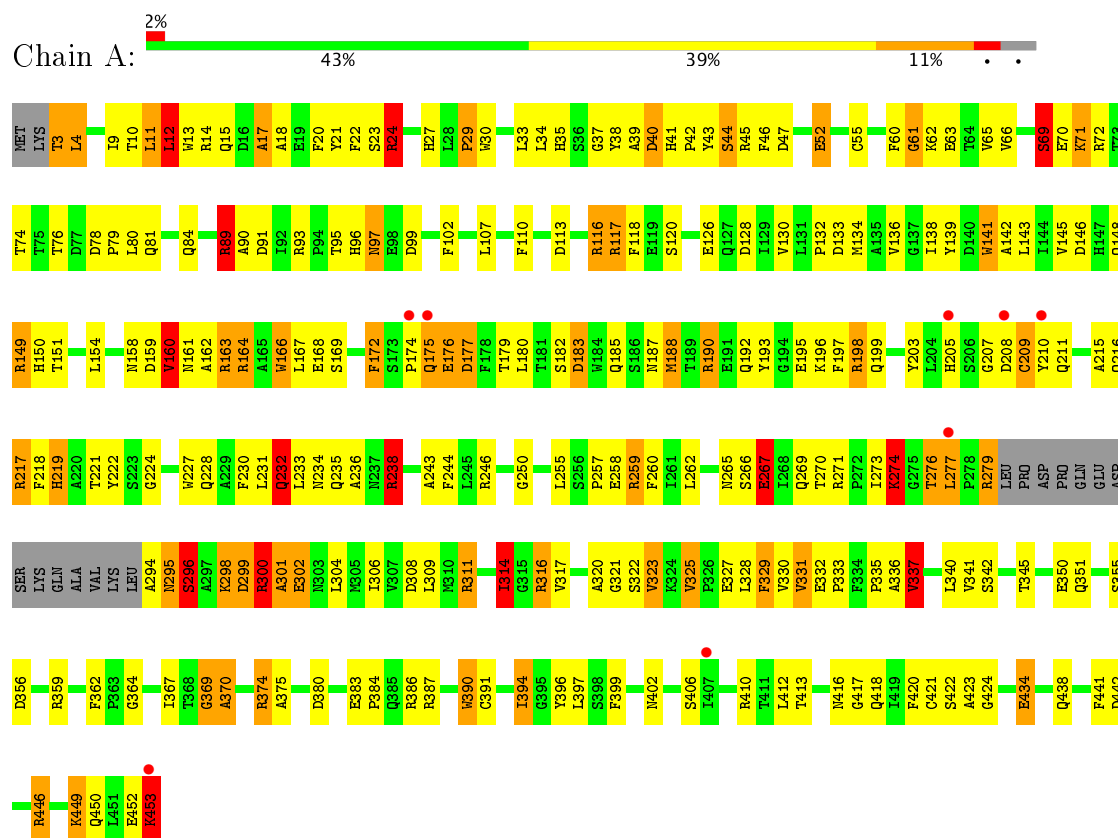
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	186	Total	O	0	0
			186	186		
4	B	132	Total	O	0	0
			132	132		

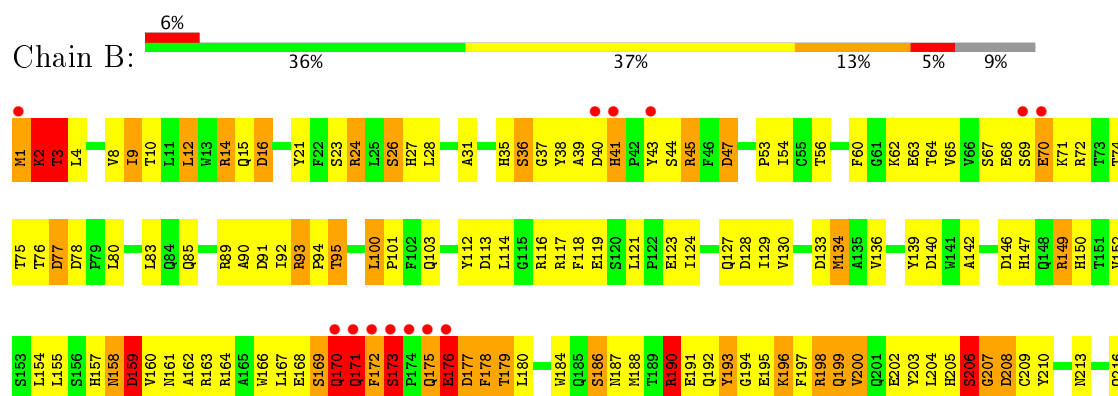
### 3 Residue-property plots

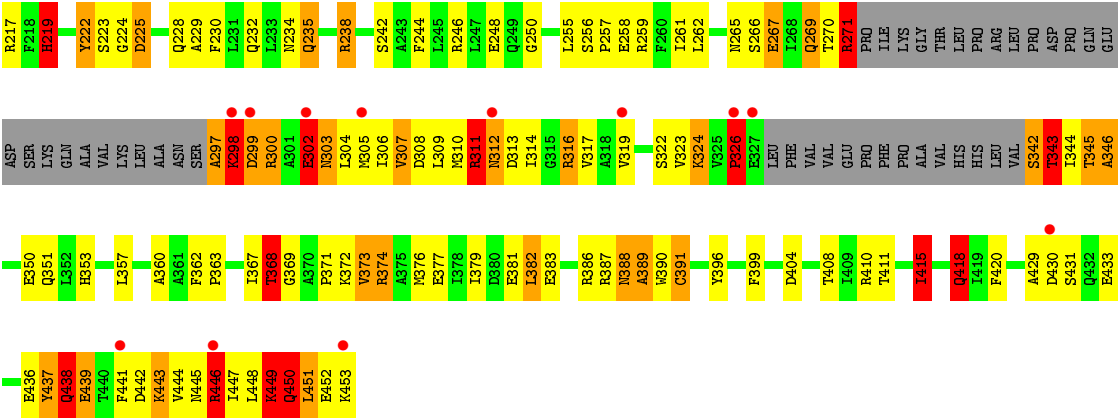
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: p-aminobenzoate synthase component I



- Molecule 1: p-aminobenzoate synthase component I





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.99 Å   185.72 Å   45.08 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	10.00 – 2.00 28.75 – 1.84	Depositor EDS
% Data completeness (in resolution range)	86.7 (10.00-2.00) 87.2 (28.75-1.84)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 1.84 Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.205   ,   0.315 0.203   ,   0.307	Depositor DCC
$R_{free}$ test set	2880 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 82.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7106	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.09	6/3543 (0.2%)	2.67	256/4813 (5.3%)
1	B	1.02	1/3357 (0.0%)	2.71	248/4552 (5.4%)
All	All	1.05	7/6900 (0.1%)	2.69	504/9365 (5.4%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	342	SER	CB-OG	6.96	1.51	1.42
1	B	186	SER	CB-OG	6.28	1.50	1.42
1	A	296	SER	CB-OG	5.84	1.49	1.42
1	A	406	SER	CB-OG	5.35	1.49	1.42
1	A	321	GLY	N-CA	5.33	1.54	1.46
1	A	250	GLY	C-O	5.08	1.31	1.23
1	A	132	PRO	N-CD	5.04	1.54	1.47

All (504) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	ARG	NE-CZ-NH2	-25.30	107.65	120.30
1	A	410	ARG	NE-CZ-NH1	25.21	132.91	120.30
1	B	89	ARG	NE-CZ-NH1	23.25	131.93	120.30
1	A	316	ARG	NE-CZ-NH2	-21.38	109.61	120.30
1	B	311	ARG	CD-NE-CZ	20.15	151.81	123.60
1	B	171	GLN	C-N-CA	19.87	171.38	121.70
1	B	163	ARG	NE-CZ-NH1	-18.64	110.98	120.30
1	B	163	ARG	NE-CZ-NH2	18.24	129.42	120.30
1	B	117	ARG	NE-CZ-NH2	-18.18	111.21	120.30
1	A	316	ARG	CA-CB-CG	16.43	149.54	113.40
1	B	446	ARG	CD-NE-CZ	16.22	146.31	123.60
1	B	190	ARG	CD-NE-CZ	15.97	145.95	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	ARG	NE-CZ-NH2	-15.84	112.38	120.30
1	B	89	ARG	CD-NE-CZ	15.61	145.45	123.60
1	A	89	ARG	CD-NE-CZ	15.40	145.16	123.60
1	A	311	ARG	CD-NE-CZ	15.36	145.10	123.60
1	B	149	ARG	NE-CZ-NH2	-14.47	113.06	120.30
1	B	198	ARG	NE-CZ-NH1	14.20	127.40	120.30
1	A	21	TYR	CB-CG-CD1	-14.12	112.53	121.00
1	A	14	ARG	NE-CZ-NH1	-14.09	113.25	120.30
1	A	116	ARG	NE-CZ-NH2	13.41	127.01	120.30
1	B	93	ARG	NE-CZ-NH2	13.37	126.98	120.30
1	A	359	ARG	NE-CZ-NH2	-13.28	113.66	120.30
1	A	246	ARG	NE-CZ-NH1	-13.04	113.78	120.30
1	B	244	PHE	CB-CG-CD1	12.97	129.88	120.80
1	A	316	ARG	NH1-CZ-NH2	12.84	133.52	119.40
1	A	320	ALA	C-N-CA	-12.75	95.53	122.30
1	A	113	ASP	CB-CG-OD2	12.71	129.74	118.30
1	B	193	TYR	CB-CG-CD1	12.70	128.62	121.00
1	B	396	TYR	CB-CG-CD1	12.65	128.59	121.00
1	A	320	ALA	O-C-N	-12.29	102.31	123.20
1	B	117	ARG	NE-CZ-NH1	12.29	126.44	120.30
1	B	222	TYR	CB-CG-CD2	12.25	128.35	121.00
1	B	116	ARG	NE-CZ-NH1	-12.08	114.26	120.30
1	A	271	ARG	CD-NE-CZ	11.71	139.99	123.60
1	A	91	ASP	CB-CG-OD1	11.57	128.71	118.30
1	B	446	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	A	175	GLN	C-N-CA	11.49	150.42	121.70
1	A	174	PRO	C-N-CA	11.43	150.28	121.70
1	A	359	ARG	NE-CZ-NH1	11.43	126.02	120.30
1	B	190	ARG	NE-CZ-NH1	-11.41	114.59	120.30
1	A	369	GLY	O-C-N	-11.40	104.45	122.70
1	A	172	PHE	CB-CG-CD1	-11.33	112.87	120.80
1	B	396	TYR	CB-CG-CD2	-11.33	114.20	121.00
1	A	387	ARG	NE-CZ-NH1	11.08	125.84	120.30
1	A	299	ASP	CB-CG-OD1	11.05	128.25	118.30
1	A	300	ARG	CD-NE-CZ	11.05	139.08	123.60
1	A	172	PHE	C-N-CA	11.03	149.27	121.70
1	B	238	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	A	38	TYR	CB-CG-CD2	10.85	127.51	121.00
1	A	386	ARG	NE-CZ-NH2	-10.81	114.90	120.30
1	A	39	ALA	O-C-N	10.74	139.89	122.70
1	B	190	ARG	NE-CZ-NH2	10.74	125.67	120.30
1	B	415	ILE	CB-CG1-CD1	10.70	143.86	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	ARG	NE-CZ-NH2	-10.48	115.06	120.30
1	A	14	ARG	NH1-CZ-NH2	10.48	130.93	119.40
1	B	230	PHE	CB-CG-CD2	10.46	128.12	120.80
1	A	271	ARG	NE-CZ-NH2	-10.29	115.16	120.30
1	B	230	PHE	CB-CG-CD1	-10.28	113.61	120.80
1	A	329	PHE	CB-CG-CD1	10.23	127.96	120.80
1	A	362	PHE	CB-CG-CD2	10.21	127.95	120.80
1	B	410	ARG	NE-CZ-NH2	10.19	125.39	120.30
1	B	387	ARG	NE-CZ-NH1	-10.19	115.21	120.30
1	A	45	ARG	NE-CZ-NH2	10.16	125.38	120.30
1	B	259	ARG	NE-CZ-NH2	10.02	125.31	120.30
1	B	205	HIS	C-N-CA	9.96	146.60	121.70
1	A	128	ASP	CB-CG-OD2	9.96	127.26	118.30
1	A	113	ASP	CB-CG-OD1	-9.90	109.39	118.30
1	B	14	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	A	311	ARG	NE-CZ-NH2	9.82	125.21	120.30
1	B	164	ARG	CD-NE-CZ	9.77	137.28	123.60
1	A	359	ARG	CD-NE-CZ	9.74	137.24	123.60
1	B	259	ARG	NE-CZ-NH1	-9.71	115.45	120.30
1	B	193	TYR	CG-CD1-CE1	9.62	128.99	121.30
1	B	112	TYR	CB-CG-CD2	9.59	126.75	121.00
1	B	311	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	B	210	TYR	CB-CG-CD1	-9.54	115.27	121.00
1	A	276	THR	CA-CB-CG2	9.30	125.42	112.40
1	A	232	GLN	CA-CB-CG	9.27	133.80	113.40
1	A	316	ARG	CD-NE-CZ	-9.12	110.83	123.60
1	A	222	TYR	CB-CG-CD2	9.06	126.44	121.00
1	B	112	TYR	CB-CG-CD1	-9.04	115.57	121.00
1	A	356	ASP	CB-CG-OD2	-9.00	110.20	118.30
1	A	14	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	B	77	ASP	CB-CG-OD2	8.94	126.34	118.30
1	A	69	SER	CA-C-N	-8.91	97.61	117.20
1	B	193	TYR	CZ-CE2-CD2	8.85	127.77	119.80
1	A	295	ASN	O-C-N	8.82	136.81	122.70
1	A	238	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	B	60	PHE	CG-CD2-CE2	-8.75	111.17	120.80
1	A	17	ALA	O-C-N	8.72	136.65	122.70
1	A	12	LEU	O-C-N	-8.71	108.77	122.70
1	B	133	ASP	CB-CG-OD2	-8.65	110.52	118.30
1	B	246	ARG	NE-CZ-NH1	-8.64	115.98	120.30
1	A	91	ASP	CA-CB-CG	8.64	132.40	113.40
1	A	38	TYR	CB-CG-CD1	-8.57	115.86	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	ARG	CD-NE-CZ	8.56	135.58	123.60
1	B	207	GLY	O-C-N	8.52	136.33	122.70
1	B	40	ASP	CB-CG-OD1	8.47	125.92	118.30
1	B	38	TYR	CB-CG-CD1	-8.46	115.92	121.00
1	B	196	LYS	CD-CE-NZ	-8.44	92.29	111.70
1	A	259	ARG	NE-CZ-NH2	8.38	124.49	120.30
1	B	184	TRP	CB-CG-CD1	8.35	137.86	127.00
1	B	206	SER	CA-C-O	8.22	137.37	120.10
1	A	13	TRP	O-C-N	-8.17	109.62	122.70
1	B	210	TYR	CG-CD2-CE2	-8.15	114.78	121.30
1	A	163	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	B	8	VAL	CA-CB-CG2	8.11	123.06	110.90
1	A	218	PHE	CB-CG-CD2	8.10	126.47	120.80
1	A	46	PHE	O-C-N	8.09	135.64	122.70
1	B	47	ASP	CB-CG-OD2	8.09	125.58	118.30
1	A	238	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	A	116	ARG	NE-CZ-NH1	-8.00	116.30	120.30
1	A	434	GLU	OE1-CD-OE2	-7.96	113.74	123.30
1	B	53	PRO	O-C-N	7.95	135.42	122.70
1	B	316	ARG	NE-CZ-NH1	-7.93	116.33	120.30
1	B	387	ARG	NH1-CZ-NH2	7.89	128.08	119.40
1	B	238	ARG	CD-NE-CZ	7.89	134.64	123.60
1	B	128	ASP	CB-CG-OD2	7.86	125.38	118.30
1	B	171	GLN	CA-C-N	7.84	134.45	117.20
1	B	90	ALA	N-CA-CB	7.83	121.07	110.10
1	B	452	GLU	CA-CB-CG	7.76	130.47	113.40
1	B	63	GLU	OE1-CD-OE2	7.76	132.61	123.30
1	B	299	ASP	CA-CB-CG	7.75	130.44	113.40
1	A	210	TYR	CA-CB-CG	7.72	128.07	113.40
1	B	133	ASP	CB-CG-OD1	7.72	125.25	118.30
1	A	452	GLU	C-N-CA	7.72	141.00	121.70
1	A	60	PHE	CB-CG-CD1	7.70	126.19	120.80
1	B	207	GLY	C-N-CA	7.68	140.91	121.70
1	A	15	GLN	CB-CG-CD	7.67	131.54	111.60
1	B	442	ASP	CB-CG-OD2	-7.66	111.40	118.30
1	A	442	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	B	198	ARG	CD-NE-CZ	7.65	134.31	123.60
1	A	374	ARG	CD-NE-CZ	-7.64	112.91	123.60
1	A	43	TYR	CZ-CE2-CD2	-7.63	112.94	119.80
1	B	386	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	B	450	GLN	O-C-N	-7.61	110.53	122.70
1	B	184	TRP	CG-CD2-CE3	-7.61	127.06	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	PRO	C-N-CA	7.60	138.27	122.30
1	A	356	ASP	CA-C-O	7.58	136.02	120.10
1	B	312	ASN	O-C-N	7.50	134.70	122.70
1	A	164	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	420	PHE	CB-CG-CD2	7.49	126.04	120.80
1	A	175	GLN	O-C-N	7.48	134.67	122.70
1	A	146	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	A	410	ARG	CG-CD-NE	-7.46	96.14	111.80
1	B	149	ARG	NH1-CZ-NH2	7.43	127.58	119.40
1	B	374	ARG	NE-CZ-NH2	7.43	124.02	120.30
1	B	38	TYR	CB-CG-CD2	7.39	125.44	121.00
1	A	78	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	207	GLY	N-CA-C	7.38	131.55	113.10
1	A	418	GLN	N-CA-CB	-7.38	97.33	110.60
1	A	418	GLN	CA-C-N	7.37	133.42	117.20
1	A	18	ALA	N-CA-CB	7.34	120.38	110.10
1	A	217	ARG	NE-CZ-NH1	-7.32	116.64	120.30
1	B	270	THR	C-N-CA	7.32	140.00	121.70
1	A	222	TYR	CB-CG-CD1	-7.31	116.62	121.00
1	A	116	ARG	CD-NE-CZ	-7.29	113.39	123.60
1	B	119	GLU	O-C-N	7.28	134.34	122.70
1	B	158	ASN	CA-CB-CG	-7.25	97.46	113.40
1	B	116	ARG	CG-CD-NE	-7.24	96.59	111.80
1	A	329	PHE	CB-CG-CD2	-7.21	115.75	120.80
1	B	438	GLN	O-C-N	-7.21	111.17	122.70
1	B	210	TYR	CD1-CE1-CZ	-7.19	113.33	119.80
1	B	139	TYR	CB-CG-CD1	-7.17	116.70	121.00
1	B	387	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	A	221	THR	CA-CB-CG2	-7.16	102.38	112.40
1	B	242	SER	O-C-N	7.12	134.10	122.70
1	A	227	TRP	CB-CG-CD2	7.12	135.86	126.60
1	A	300	ARG	O-C-N	7.11	134.07	122.70
1	A	24	ARG	CB-CA-C	-7.09	96.22	110.40
1	A	329	PHE	N-CA-CB	-7.08	97.85	110.60
1	A	230	PHE	CG-CD2-CE2	7.08	128.58	120.80
1	A	198	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	A	12	LEU	N-CA-CB	-7.04	96.33	110.40
1	B	368	THR	CA-CB-CG2	7.04	122.25	112.40
1	B	173	SER	CA-C-N	7.03	136.79	117.10
1	B	206	SER	CA-C-N	-7.03	102.13	116.20
1	A	43	TYR	CG-CD1-CE1	-7.03	115.67	121.30
1	B	197	PHE	CB-CG-CD2	7.03	125.72	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	VAL	CA-CB-CG1	-7.02	100.37	110.90
1	A	217	ARG	NE-CZ-NH2	6.97	123.79	120.30
1	B	38	TYR	CG-CD2-CE2	-6.97	115.73	121.30
1	A	279	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	A	383	GLU	OE1-CD-OE2	-6.96	114.95	123.30
1	B	36	SER	O-C-N	-6.91	111.45	123.20
1	B	95	THR	O-C-N	-6.91	111.65	122.70
1	B	225	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	B	38	TYR	CD1-CE1-CZ	-6.89	113.60	119.80
1	B	146	ASP	CB-CG-OD2	6.87	124.49	118.30
1	A	316	ARG	NE-CZ-NH1	-6.87	116.86	120.30
1	B	45	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	B	3	THR	CA-C-N	6.82	132.21	117.20
1	A	267	GLU	CB-CG-CD	6.82	132.61	114.20
1	B	213	ASN	O-C-N	-6.82	111.79	122.70
1	B	3	THR	O-C-N	-6.80	111.81	122.70
1	A	44	SER	N-CA-CB	-6.78	100.33	110.50
1	A	197	PHE	O-C-N	-6.78	111.86	122.70
1	A	327	GLU	O-C-N	6.78	133.54	122.70
1	B	130	VAL	O-C-N	-6.77	111.87	122.70
1	A	198	ARG	CD-NE-CZ	-6.75	114.14	123.60
1	A	187	ASN	O-C-N	-6.74	111.91	122.70
1	B	68	GLU	C-N-CA	-6.73	104.89	121.70
1	A	190	ARG	NE-CZ-NH2	6.71	123.65	120.30
1	A	308	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	A	61	GLY	CA-C-O	6.70	132.66	120.60
1	B	68	GLU	O-C-N	-6.69	111.99	122.70
1	A	21	TYR	CB-CG-CD2	6.69	125.01	121.00
1	B	357	LEU	CA-CB-CG	6.66	130.63	115.30
1	A	336	ALA	N-CA-CB	-6.66	100.78	110.10
1	B	217	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	B	323	VAL	O-C-N	6.66	133.35	122.70
1	A	209	CYS	CB-CA-C	-6.65	97.10	110.40
1	A	177	ASP	CB-CG-OD1	-6.64	112.32	118.30
1	B	420	PHE	CB-CG-CD2	-6.63	116.16	120.80
1	B	95	THR	N-CA-CB	-6.61	97.75	110.30
1	A	218	PHE	CA-C-O	6.60	133.97	120.10
1	A	166	TRP	CE3-CZ3-CH2	6.59	128.45	121.20
1	B	177	ASP	O-C-N	6.57	133.21	122.70
1	A	311	ARG	NH1-CZ-NH2	-6.56	112.18	119.40
1	A	179	THR	O-C-N	6.56	133.19	122.70
1	A	69	SER	CA-C-O	6.55	133.86	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	450	GLN	N-CA-CB	-6.55	98.81	110.60
1	A	197	PHE	CB-CG-CD2	6.55	125.38	120.80
1	B	67	SER	O-C-N	6.54	133.16	122.70
1	B	60	PHE	CB-CG-CD2	-6.53	116.23	120.80
1	A	394	ILE	O-C-N	-6.53	112.10	123.20
1	A	453	LYS	CA-CB-CG	6.52	127.75	113.40
1	B	437	TYR	CB-CG-CD1	6.52	124.91	121.00
1	A	188	MET	C-N-CA	-6.52	105.40	121.70
1	A	271	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	B	159	ASP	CB-CG-OD1	6.51	124.16	118.30
1	B	38	TYR	CG-CD1-CE1	6.51	126.51	121.30
1	A	302	GLU	OE1-CD-OE2	6.50	131.10	123.30
1	B	391	CYS	CA-CB-SG	-6.49	102.31	114.00
1	B	368	THR	CA-CB-OG1	-6.49	95.37	109.00
1	B	8	VAL	CG1-CB-CG2	-6.49	100.53	110.90
1	A	390	TRP	CB-CG-CD2	-6.47	118.19	126.60
1	A	29	PRO	N-CD-CG	-6.47	93.50	103.20
1	B	210	TYR	CA-CB-CG	-6.47	101.11	113.40
1	A	117	ARG	NH1-CZ-NH2	6.46	126.50	119.40
1	A	172	PHE	O-C-N	6.46	133.03	122.70
1	A	417	GLY	C-N-CA	-6.45	105.57	121.70
1	A	40	ASP	N-CA-CB	6.44	122.20	110.60
1	A	60	PHE	CG-CD2-CE2	6.44	127.89	120.80
1	B	31	ALA	N-CA-CB	6.44	119.11	110.10
1	A	139	TYR	CG-CD2-CE2	6.43	126.45	121.30
1	B	93	ARG	CD-NE-CZ	6.43	132.60	123.60
1	A	384	PRO	O-C-N	-6.43	112.42	122.70
1	A	300	ARG	C-N-CA	6.39	137.69	121.70
1	A	390	TRP	CB-CG-CD1	6.39	135.30	127.00
1	A	234	ASN	O-C-N	-6.38	112.49	122.70
1	B	171	GLN	CA-C-O	-6.37	106.73	120.10
1	B	206	SER	C-N-CA	6.36	135.65	122.30
1	A	76	THR	CA-CB-CG2	6.35	121.29	112.40
1	B	316	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	A	79	PRO	O-C-N	-6.34	112.56	122.70
1	B	388	ASN	O-C-N	-6.33	112.56	122.70
1	A	172	PHE	CB-CG-CD2	6.31	125.22	120.80
1	B	72	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	46	PHE	CB-CA-C	-6.30	97.81	110.40
1	A	30	TRP	CH2-CZ2-CE2	6.28	123.68	117.40
1	B	69	SER	C-N-CA	-6.27	106.03	121.70
1	B	70	GLU	N-CA-CB	-6.27	99.32	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	GLU	O-C-N	-6.26	112.69	122.70
1	B	246	ARG	O-C-N	6.21	132.64	122.70
1	B	311	ARG	NH1-CZ-NH2	-6.20	112.58	119.40
1	B	155	LEU	CB-CG-CD1	6.19	121.53	111.00
1	A	394	ILE	CA-C-N	6.18	128.56	116.20
1	B	154	LEU	CB-CG-CD1	-6.17	100.50	111.00
1	B	219	HIS	CA-CB-CG	-6.17	103.10	113.60
1	B	342	SER	CA-CB-OG	6.13	127.74	111.20
1	B	360	ALA	O-C-N	-6.12	112.90	122.70
1	B	2	LYS	CA-CB-CG	6.12	126.86	113.40
1	B	16	ASP	N-CA-CB	-6.11	99.60	110.60
1	A	188	MET	CB-CA-C	-6.09	98.22	110.40
1	B	176	GLU	C-N-CA	-6.09	106.48	121.70
1	A	209	CYS	C-N-CA	-6.08	106.49	121.70
1	B	307	VAL	CG1-CB-CG2	6.08	120.63	110.90
1	A	120	SER	O-C-N	-6.08	112.97	122.70
1	A	369	GLY	CA-C-N	6.08	130.58	117.20
1	A	162	ALA	CB-CA-C	-6.08	100.98	110.10
1	B	21	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	B	437	TYR	CZ-CE2-CD2	6.07	125.27	119.80
1	A	228	GLN	O-C-N	-6.07	112.99	122.70
1	A	364	GLY	C-N-CA	-6.06	109.57	122.30
1	A	387	ARG	NH1-CZ-NH2	-6.06	112.74	119.40
1	A	71	LYS	CA-CB-CG	6.04	126.68	113.40
1	B	210	TYR	CD1-CG-CD2	6.03	124.54	117.90
1	A	238	ARG	CD-NE-CZ	6.01	132.01	123.60
1	B	307	VAL	CA-CB-CG1	-6.01	101.89	110.90
1	A	369	GLY	C-N-CA	6.00	136.71	121.70
1	A	90	ALA	N-CA-CB	6.00	118.50	110.10
1	B	166	TRP	CD2-CE3-CZ3	-5.98	111.03	118.80
1	A	380	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	B	173	SER	O-C-N	-5.98	109.75	121.10
1	A	203	TYR	O-C-N	-5.97	113.14	122.70
1	A	118	PHE	C-N-CA	5.97	136.63	121.70
1	B	152	VAL	O-C-N	-5.97	113.14	122.70
1	A	166	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	A	314	ILE	C-N-CA	-5.93	109.85	122.30
1	A	342	SER	CA-CB-OG	-5.93	95.19	111.20
1	B	386	ARG	NH1-CZ-NH2	5.92	125.92	119.40
1	A	420	PHE	CZ-CE2-CD2	5.92	127.20	120.10
1	A	175	GLN	CG-CD-OE1	-5.91	109.77	121.60
1	B	12	LEU	N-CA-CB	-5.91	98.57	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	GLN	O-C-N	5.91	132.16	122.70
1	A	107	LEU	CB-CA-C	5.91	121.43	110.20
1	B	390	TRP	CH2-CZ2-CE2	-5.91	111.50	117.40
1	A	160	VAL	CA-C-O	-5.90	107.72	120.10
1	B	439	GLU	CA-CB-CG	5.89	126.36	113.40
1	A	244	PHE	CG-CD1-CE1	5.88	127.26	120.80
1	B	124	ILE	CA-C-N	5.86	130.09	117.20
1	A	126	GLU	CA-C-O	5.86	132.40	120.10
1	A	80	LEU	CA-C-O	-5.85	107.82	120.10
1	A	370	ALA	CA-C-O	5.84	132.37	120.10
1	A	420	PHE	CE1-CZ-CE2	-5.83	109.50	120.00
1	A	295	ASN	CA-C-N	-5.83	104.38	117.20
1	A	356	ASP	CA-CB-CG	-5.83	100.58	113.40
1	B	362	PHE	CD1-CE1-CZ	-5.82	113.11	120.10
1	A	11	LEU	C-N-CA	-5.82	107.16	121.70
1	A	399	PHE	CG-CD2-CE2	-5.82	114.40	120.80
1	B	257	PRO	C-N-CA	-5.81	107.17	121.70
1	A	159	ASP	CA-C-O	5.80	132.27	120.10
1	B	123	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	A	262	LEU	O-C-N	-5.79	113.44	122.70
1	B	297	ALA	O-C-N	5.76	131.92	122.70
1	A	24	ARG	N-CA-CB	5.76	120.96	110.60
1	A	387	ARG	CD-NE-CZ	-5.75	115.55	123.60
1	A	235	GLN	O-C-N	-5.75	113.51	122.70
1	B	408	THR	CA-C-O	5.75	132.17	120.10
1	B	175	GLN	CA-CB-CG	5.74	126.04	113.40
1	B	9	ILE	CA-CB-CG1	5.74	121.91	111.00
1	B	85	GLN	O-C-N	-5.74	113.51	122.70
1	A	133	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	330	VAL	C-N-CA	-5.73	107.37	121.70
1	B	127	GLN	CG-CD-OE1	-5.73	110.14	121.60
1	B	438	GLN	CA-C-O	5.73	132.13	120.10
1	A	294	ALA	CA-C-N	-5.72	104.61	117.20
1	B	140	ASP	O-C-N	5.72	131.85	122.70
1	A	3	THR	CA-C-N	-5.71	104.63	117.20
1	A	449	LYS	CB-CG-CD	5.71	126.43	111.60
1	A	441	PHE	CG-CD1-CE1	-5.70	114.53	120.80
1	A	89	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	97	ASN	CA-C-O	-5.70	108.14	120.10
1	B	146	ASP	O-C-N	5.69	131.81	122.70
1	A	72	ARG	CG-CD-NE	5.68	123.73	111.80
1	B	150	HIS	O-C-N	5.66	131.75	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	GLU	CA-C-O	5.66	131.98	120.10
1	B	437	TYR	CG-CD2-CE2	-5.64	116.78	121.30
1	A	337	VAL	N-CA-CB	-5.63	99.10	111.50
1	A	322	SER	CA-C-N	5.63	129.59	117.20
1	A	145	VAL	CA-C-O	-5.63	108.28	120.10
1	A	182	SER	O-C-N	-5.61	113.72	122.70
1	B	39	ALA	O-C-N	-5.61	113.72	122.70
1	B	184	TRP	CB-CG-CD2	-5.61	119.31	126.60
1	A	139	TYR	CB-CG-CD1	5.60	124.36	121.00
1	A	163	ARG	NH1-CZ-NH2	5.59	125.55	119.40
1	B	346	ALA	C-N-CA	-5.59	107.73	121.70
1	B	373	VAL	O-C-N	5.59	131.64	122.70
1	B	38	TYR	CA-CB-CG	-5.58	102.80	113.40
1	B	77	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	A	380	ASP	O-C-N	5.57	131.61	122.70
1	B	382	LEU	N-CA-CB	-5.56	99.28	110.40
1	B	418	GLN	CB-CG-CD	-5.56	97.15	111.60
1	A	418	GLN	CA-C-O	-5.55	108.44	120.10
1	B	213	ASN	CA-C-N	5.53	129.37	117.20
1	A	164	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	B	64	THR	O-C-N	5.52	131.53	122.70
1	B	418	GLN	OE1-CD-NE2	5.52	134.60	121.90
1	B	362	PHE	CB-CG-CD2	-5.52	116.94	120.80
1	B	194	GLY	O-C-N	-5.52	113.87	122.70
1	B	389	ALA	O-C-N	-5.51	113.88	122.70
1	B	437	TYR	O-C-N	-5.50	113.89	122.70
1	A	209	CYS	O-C-N	5.50	131.50	122.70
1	A	244	PHE	CB-CG-CD2	5.50	124.65	120.80
1	A	301	ALA	C-N-CA	-5.48	108.01	121.70
1	B	68	GLU	CA-C-N	5.48	129.25	117.20
1	A	130	VAL	CA-CB-CG2	-5.48	102.69	110.90
1	B	14	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	351	GLN	OE1-CD-NE2	-5.47	109.31	121.90
1	B	166	TRP	CE3-CZ3-CH2	5.47	127.22	121.20
1	A	102	PHE	CA-C-N	5.46	129.22	117.20
1	B	299	ASP	C-N-CA	-5.46	108.06	121.70
1	B	351	GLN	CB-CG-CD	5.46	125.79	111.60
1	B	90	ALA	O-C-N	5.45	131.42	122.70
1	B	16	ASP	CB-CG-OD1	-5.45	113.40	118.30
1	A	413	THR	C-N-CA	5.44	135.30	121.70
1	B	28	LEU	CB-CA-C	-5.44	99.86	110.20
1	B	14	ARG	O-C-N	5.44	131.40	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	319	VAL	CA-CB-CG1	5.44	119.06	110.90
1	B	27	HIS	CA-CB-CG	-5.43	104.37	113.60
1	A	166	TRP	CB-CG-CD2	5.43	133.66	126.60
1	A	45	ARG	NH1-CZ-NH2	-5.42	113.43	119.40
1	A	374	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	B	316	ARG	CA-C-O	5.42	131.49	120.10
1	A	441	PHE	CB-CG-CD2	-5.41	117.01	120.80
1	A	10	THR	O-C-N	-5.41	114.04	122.70
1	B	386	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	B	269	GLN	CB-CG-CD	-5.40	97.55	111.60
1	B	437	TYR	CG-CD1-CE1	5.39	125.61	121.30
1	B	399	PHE	CG-CD1-CE1	-5.39	114.87	120.80
1	B	127	GLN	OE1-CD-NE2	5.39	134.29	121.90
1	A	386	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	22	PHE	CD1-CE1-CZ	-5.38	113.64	120.10
1	A	141	TRP	CD1-NE1-CE2	-5.38	104.16	109.00
1	A	420	PHE	CD1-CG-CD2	-5.38	111.31	118.30
1	B	411	THR	O-C-N	-5.37	114.11	122.70
1	A	102	PHE	CB-CG-CD2	-5.36	117.05	120.80
1	A	266	SER	C-N-CA	-5.35	108.33	121.70
1	A	150	HIS	CA-CB-CG	-5.35	104.51	113.60
1	B	230	PHE	O-C-N	-5.34	114.15	122.70
1	B	430	ASP	C-N-CA	-5.34	108.35	121.70
1	A	316	ARG	C-N-CA	-5.34	108.35	121.70
1	A	47	ASP	CB-CG-OD1	5.33	123.10	118.30
1	B	404	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	63	GLU	OE1-CD-OE2	-5.33	116.91	123.30
1	A	331	VAL	CA-C-O	5.32	131.27	120.10
1	A	328	LEU	O-C-N	-5.31	114.21	122.70
1	B	300	ARG	CD-NE-CZ	5.30	131.03	123.60
1	A	320	ALA	CA-C-N	5.30	126.81	116.20
1	B	437	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	B	250	GLY	N-CA-C	-5.26	99.95	113.10
1	A	399	PHE	CZ-CE2-CD2	5.25	126.40	120.10
1	B	41	HIS	CB-CA-C	-5.25	99.90	110.40
1	A	102	PHE	CA-C-O	-5.23	109.12	120.10
1	B	142	ALA	N-CA-CB	5.22	117.41	110.10
1	B	443	LYS	C-N-CA	-5.22	108.65	121.70
1	B	222	TYR	CD1-CG-CD2	-5.22	112.16	117.90
1	A	420	PHE	CG-CD1-CE1	5.21	126.53	120.80
1	B	3	THR	C-N-CA	-5.20	108.70	121.70
1	B	54	ILE	CA-CB-CG2	-5.20	100.51	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	SER	CA-C-N	5.19	128.62	117.20
1	A	134	MET	N-CA-CB	5.19	119.94	110.60
1	B	196	LYS	O-C-N	5.19	131.00	122.70
1	B	242	SER	CA-C-N	-5.19	105.78	117.20
1	B	199	GLN	C-N-CA	-5.19	108.73	121.70
1	A	390	TRP	CH2-CZ2-CE2	5.19	122.59	117.40
1	B	166	TRP	CG-CD2-CE3	-5.18	129.23	133.90
1	A	276	THR	CA-CB-OG1	-5.18	98.12	109.00
1	B	388	ASN	CA-C-N	5.18	128.60	117.20
1	A	142	ALA	N-CA-CB	5.18	117.35	110.10
1	B	184	TRP	CD1-NE1-CE2	-5.18	104.34	109.00
1	A	234	ASN	CA-CB-CG	-5.17	102.02	113.40
1	B	191	GLU	OE1-CD-OE2	-5.17	117.09	123.30
1	B	134	MET	C-N-CA	5.16	134.61	121.70
1	B	38	TYR	CZ-CE2-CD2	5.16	124.44	119.80
1	B	60	PHE	CZ-CE2-CD2	5.16	126.29	120.10
1	A	81	GLN	CA-C-O	5.16	130.93	120.10
1	A	183	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	215	ALA	O-C-N	5.16	130.95	122.70
1	B	178	PHE	N-CA-CB	5.15	119.87	110.60
1	A	446	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	235	GLN	CA-C-O	-5.15	109.28	120.10
1	B	76	THR	O-C-N	-5.15	114.46	122.70
1	B	256	SER	CB-CA-C	-5.15	100.32	110.10
1	B	170	GLN	CA-CB-CG	-5.15	102.08	113.40
1	A	244	PHE	CZ-CE2-CD2	5.15	126.28	120.10
1	A	116	ARG	CG-CD-NE	-5.14	101.00	111.80
1	B	2	LYS	N-CA-CB	-5.14	101.35	110.60
1	A	13	TRP	CA-C-O	5.14	130.89	120.10
1	A	320	ALA	CA-C-O	5.14	130.88	120.10
1	B	166	TRP	CH2-CZ2-CE2	-5.13	112.27	117.40
1	B	67	SER	CA-C-O	-5.13	109.33	120.10
1	B	67	SER	N-CA-CB	-5.13	102.81	110.50
1	B	235	GLN	CB-CG-CD	5.12	124.92	111.60
1	A	149	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	A	228	GLN	CA-C-O	5.12	130.85	120.10
1	A	29	PRO	O-C-N	-5.12	114.51	122.70
1	A	231	LEU	CA-C-O	-5.11	109.36	120.10
1	A	323	VAL	CA-CB-CG2	-5.11	103.23	110.90
1	B	56	THR	CA-CB-CG2	5.11	119.55	112.40
1	B	353	HIS	CA-CB-CG	-5.11	104.92	113.60
1	B	297	ALA	CA-C-N	-5.10	105.98	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	ASP	CA-C-N	-5.09	106.00	117.20
1	A	34	LEU	O-C-N	-5.09	114.55	122.70
1	B	258	GLU	CB-CA-C	-5.08	100.24	110.40
1	A	66	VAL	CA-CB-CG1	-5.08	103.28	110.90
1	B	116	ARG	O-C-N	-5.08	114.57	122.70
1	B	162	ALA	N-CA-CB	-5.08	102.99	110.10
1	A	90	ALA	CB-CA-C	-5.08	102.48	110.10
1	B	179	THR	CA-C-N	-5.08	106.03	117.20
1	B	198	ARG	C-N-CA	-5.07	109.02	121.70
1	A	12	LEU	CA-C-N	5.07	128.34	117.20
1	B	172	PHE	CG-CD2-CE2	5.06	126.37	120.80
1	A	279	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	A	438	GLN	C-N-CA	-5.06	109.06	121.70
1	B	317	VAL	N-CA-CB	-5.05	100.39	111.50
1	B	208	ASP	CA-C-O	5.05	130.70	120.10
1	A	434	GLU	CB-CG-CD	5.04	127.82	114.20
1	B	179	THR	CA-C-O	5.04	130.69	120.10
1	A	43	TYR	CA-C-N	-5.04	106.11	117.20
1	A	233	LEU	CB-CG-CD1	-5.04	102.44	111.00
1	A	274	LYS	CA-C-O	-5.04	109.53	120.10
1	A	172	PHE	CA-C-N	-5.03	106.13	117.20
1	A	110	PHE	O-C-N	-5.03	114.65	123.20
1	A	416	ASN	C-N-CA	-5.03	111.74	122.30
1	A	300	ARG	CA-C-N	-5.03	106.14	117.20
1	B	351	GLN	CG-CD-OE1	5.03	131.66	121.60
1	A	12	LEU	N-CA-C	5.03	124.57	111.00
1	A	161	ASN	N-CA-CB	5.02	119.64	110.60
1	A	370	ALA	CB-CA-C	-5.02	102.57	110.10
1	B	262	LEU	CA-CB-CG	5.02	126.84	115.30
1	A	141	TRP	CE3-CZ3-CH2	-5.02	115.68	121.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3466	0	3367	109	0
1	B	3289	0	3189	131	0
2	A	15	0	9	0	0
2	B	15	0	9	1	0
3	A	3	0	2	4	0
4	A	186	0	0	10	0
4	B	132	0	0	5	0
All	All	7106	0	6576	240	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (240) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ASP:HB3	1:B:228:GLN:HG2	1.40	0.99
1:A:176:GLU:HG3	1:A:224:GLY:HA2	1.45	0.95
1:B:121:LEU:HD11	1:B:376:MET:HE3	1.51	0.93
1:B:176:GLU:HB2	1:B:225:ASP:HB2	1.56	0.84
1:A:236:ALA:HB1	1:A:446:ARG:HH22	1.40	0.84
1:B:300:ARG:HA	1:B:303:ASN:HD21	1.43	0.83
1:A:423:ALA:HA	3:A:1701:FMT:H	1.61	0.83
1:B:307:VAL:HG12	1:B:311:ARG:HH12	1.45	0.80
1:B:271:ARG:HH11	1:B:271:ARG:HG3	1.46	0.80
1:B:368:THR:HG21	1:B:372:LYS:HG3	1.63	0.80
1:B:311:ARG:HH11	1:B:311:ARG:HB2	1.48	0.78
1:B:177:ASP:O	1:B:224:GLY:HA3	1.83	0.78
1:A:40:ASP:H	1:A:238:ARG:NH2	1.84	0.76
1:A:446:ARG:HG2	1:A:449:LYS:HE3	1.67	0.76
1:B:415:ILE:HG13	1:B:415:ILE:O	1.84	0.76
1:A:208:ASP:HB3	1:A:374:ARG:HE	1.50	0.75
1:B:114:LEU:HD21	1:B:134:MET:HE3	1.69	0.74
1:A:188:MET:HE3	1:A:193:TYR:HB2	1.70	0.74
1:B:381:GLU:HG2	1:B:382:LEU:HD23	1.68	0.74
1:B:367:ILE:HD13	1:B:391:CYS:HB3	1.67	0.73
1:B:35:HIS:HD2	1:B:37:GLY:H	1.36	0.73
1:B:446:ARG:O	1:B:450:GLN:HB2	1.88	0.73
1:B:299:ASP:HA	1:B:302:GLU:HB2	1.72	0.71
1:B:300:ARG:O	1:B:304:LEU:HG	1.90	0.71
1:A:296:SER:O	1:A:300:ARG:HG2	1.89	0.71
1:A:273:ILE:HG12	1:A:341:VAL:HG22	1.72	0.71
1:B:1:MET:HG3	1:B:2:LYS:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:GLY:H	3:A:1701:FMT:H	1.57	0.70
1:B:113:ASP:HB2	4:B:1188:HOH:O	1.93	0.69
1:B:170:GLN:NE2	1:B:172:PHE:HB3	2.07	0.68
1:A:35:HIS:HD2	1:A:37:GLY:H	1.39	0.68
1:B:307:VAL:HG12	1:B:311:ARG:NH1	2.08	0.67
1:B:269:GLN:NE2	1:B:343:THR:HG21	2.09	0.67
1:B:9:ILE:HD12	1:B:160:VAL:HG22	1.77	0.67
1:B:41:HIS:HB2	1:B:44:SER:OG	1.94	0.67
1:A:23:SER:HB3	1:A:172:PHE:CD1	2.30	0.66
1:B:36:SER:HG	2:B:602:TRP:N	1.94	0.66
1:B:267:GLU:HG3	1:B:267:GLU:O	1.96	0.66
1:A:99:ASP:HB3	1:A:149:ARG:HH21	1.61	0.65
1:B:450:GLN:HG2	4:B:1280:HOH:O	1.97	0.64
1:B:303:ASN:HA	1:B:306:ILE:HG13	1.79	0.64
1:A:40:ASP:H	1:A:238:ARG:HH22	1.45	0.64
1:A:183:ASP:HB3	4:A:1097:HOH:O	1.98	0.63
1:A:41:HIS:HB3	1:A:44:SER:HB3	1.81	0.63
1:A:3:THR:HG23	1:A:4:LEU:HD12	1.81	0.62
1:B:3:THR:HG21	1:B:93:ARG:H	1.63	0.62
1:B:308:ASP:HA	1:B:311:ARG:NH1	2.15	0.62
1:B:307:VAL:HG13	1:B:344:ILE:HD11	1.82	0.62
1:B:303:ASN:O	1:B:306:ILE:HG13	2.00	0.61
1:A:208:ASP:CB	1:A:374:ARG:HE	2.14	0.60
1:B:159:ASP:OD1	1:B:161:ASN:HB2	2.01	0.60
1:B:297:ALA:O	1:B:300:ARG:HG3	2.02	0.60
1:B:4:LEU:H	1:B:4:LEU:HD23	1.66	0.60
1:B:198:ARG:O	1:B:202:GLU:HG3	2.01	0.59
1:A:89:ARG:O	1:A:89:ARG:HG2	2.02	0.59
1:A:69:SER:HB2	1:A:70:GLU:HG3	1.85	0.58
1:B:324:LYS:HG3	1:B:324:LYS:O	2.04	0.57
1:A:351:GLN:HB2	4:A:1210:HOH:O	2.03	0.57
1:A:276:THR:HB	1:A:337:VAL:HG13	1.87	0.57
1:B:271:ARG:HD3	1:B:343:THR:OG1	2.04	0.57
1:A:446:ARG:CG	1:A:449:LYS:HE3	2.35	0.57
1:A:446:ARG:HA	1:A:449:LYS:HG2	1.88	0.56
1:A:306:ILE:O	1:A:309:LEU:HB3	2.06	0.56
1:A:267:GLU:HG3	1:A:267:GLU:O	2.06	0.55
1:B:3:THR:CG2	1:B:93:ARG:H	2.18	0.55
1:A:236:ALA:HB1	1:A:446:ARG:NH2	2.16	0.55
1:B:176:GLU:CB	1:B:225:ASP:HB2	2.34	0.55
1:B:248:GLU:HG3	4:B:1140:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLU:HB2	1:A:273:ILE:HD12	1.89	0.55
1:B:373:VAL:O	1:B:377:GLU:HG3	2.07	0.55
1:A:274:LYS:HG3	1:A:306:ILE:HG13	1.88	0.55
1:A:453:LYS:HE3	4:A:1241:HOH:O	2.06	0.55
1:A:232:GLN:HG2	4:A:1192:HOH:O	2.08	0.54
1:B:103:GLN:O	1:B:157:HIS:HE1	1.91	0.54
1:B:299:ASP:CA	1:B:302:GLU:HB2	2.37	0.54
1:A:217:ARG:HG2	4:A:1044:HOH:O	2.08	0.54
1:A:446:ARG:HA	1:A:449:LYS:CD	2.37	0.54
1:A:311:ARG:O	1:A:314:ILE:HD13	2.08	0.54
1:A:33:LEU:O	1:A:243:ALA:HA	2.08	0.53
1:B:23:SER:O	1:B:26:SER:HB3	2.08	0.53
1:B:308:ASP:HA	1:B:311:ARG:CZ	2.38	0.53
1:B:35:HIS:CD2	1:B:37:GLY:H	2.22	0.53
1:A:35:HIS:HD2	1:A:37:GLY:N	2.05	0.53
1:B:24:ARG:HD2	1:B:170:GLN:HE21	1.73	0.52
1:B:179:THR:HG22	1:B:223:SER:OG	2.09	0.52
1:A:211:GLN:O	1:A:369:GLY:O	2.27	0.52
1:B:24:ARG:CB	1:B:170:GLN:HG3	2.40	0.52
1:B:306:ILE:O	1:B:309:LEU:HB3	2.10	0.52
1:A:188:MET:CE	1:A:216:GLN:HB3	2.40	0.52
1:A:325:VAL:O	1:A:325:VAL:HG12	2.09	0.52
1:A:65:VAL:HG22	1:A:74:THR:HG22	1.91	0.52
1:B:388:ASN:ND2	1:B:389:ALA:H	2.08	0.52
1:B:299:ASP:O	1:B:303:ASN:OD1	2.29	0.51
1:A:192:GLN:O	1:A:196:LYS:HG3	2.10	0.51
1:B:14:ARG:HD3	1:B:16:ASP:OD1	2.10	0.51
1:B:169:SER:O	1:B:170:GLN:O	2.28	0.51
1:A:329:PHE:HA	1:A:340:LEU:HD11	1.91	0.51
1:A:369:GLY:O	1:A:375:ALA:HB2	2.09	0.51
1:B:35:HIS:HD2	1:B:37:GLY:N	2.06	0.51
1:B:65:VAL:HG22	1:B:74:THR:HG22	1.92	0.51
1:A:446:ARG:CB	1:A:449:LYS:HE3	2.40	0.51
1:A:345:THR:HG22	4:A:1164:HOH:O	2.11	0.50
1:B:35:HIS:CD2	1:B:234:ASN:HD21	2.29	0.50
1:A:367:ILE:HD13	1:A:391:CYS:HB3	1.93	0.50
1:A:449:LYS:HG3	1:A:450:GLN:N	2.26	0.50
1:B:45:ARG:HH21	1:B:149:ARG:HG3	1.76	0.50
1:B:326:PRO:HG3	1:B:343:THR:H	1.76	0.50
1:A:300:ARG:HG3	1:A:300:ARG:O	2.11	0.50
1:B:311:ARG:NH1	1:B:311:ARG:HB2	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:THR:HG22	1:B:345:THR:HG23	1.92	0.50
1:A:295:ASN:HA	1:A:300:ARG:HD3	1.93	0.50
1:B:190:ARG:HG2	1:B:437:TYR:CE2	2.47	0.50
1:B:343:THR:HG23	1:B:344:ILE:O	2.12	0.50
1:A:396:TYR:C	1:A:397:LEU:HD12	2.32	0.49
1:B:306:ILE:HD12	1:B:307:VAL:N	2.28	0.49
1:B:190:ARG:NH1	1:B:433:GLU:OE2	2.46	0.49
1:B:168:GLU:O	1:B:170:GLN:OE1	2.30	0.49
1:A:177:ASP:HA	4:A:1320:HOH:O	2.12	0.49
1:B:269:GLN:CD	1:B:343:THR:HG21	2.32	0.49
1:B:206:SER:HB2	1:B:208:ASP:OD1	2.11	0.49
1:B:368:THR:HG22	1:B:369:GLY:O	2.13	0.49
1:B:438:GLN:NE2	1:B:441:PHE:HB2	2.27	0.49
1:B:180:LEU:HD23	1:B:222:TYR:HB3	1.94	0.49
1:B:255:LEU:N	1:B:255:LEU:HD22	2.27	0.49
1:B:322:SER:O	1:B:346:ALA:HA	2.13	0.49
1:B:100:LEU:HA	1:B:101:PRO:HD2	1.57	0.49
1:B:121:LEU:HD11	1:B:376:MET:CE	2.33	0.49
1:B:114:LEU:HD21	1:B:134:MET:CE	2.41	0.48
1:A:35:HIS:CD2	1:A:37:GLY:H	2.25	0.48
1:A:23:SER:HB3	1:A:172:PHE:CE1	2.49	0.48
1:B:114:LEU:CD2	1:B:134:MET:HE3	2.40	0.48
1:B:312:ASN:O	1:B:316:ARG:HG2	2.14	0.48
1:A:188:MET:HE2	1:A:216:GLN:HB3	1.95	0.48
1:A:295:ASN:C	1:A:300:ARG:HD3	2.34	0.48
1:B:178:PHE:CG	1:B:229:ALA:HB2	2.48	0.48
1:B:444:VAL:HA	4:B:1288:HOH:O	2.12	0.48
1:A:166:TRP:O	1:A:169:SER:OG	2.29	0.48
1:B:219:HIS:ND1	1:B:418:GLN:OE1	2.47	0.47
1:B:379:ILE:O	1:B:383:GLU:HB2	2.15	0.47
1:A:185:GLN:HB3	1:A:219:HIS:CD2	2.50	0.47
1:A:9:ILE:HD12	1:A:164:ARG:HD3	1.96	0.47
1:B:208:ASP:HB3	1:B:374:ARG:HE	1.77	0.47
1:B:92:ILE:HG22	1:B:94:PRO:HD3	1.96	0.47
1:B:16:ASP:OD1	1:B:16:ASP:N	2.48	0.47
1:A:424:GLY:H	3:A:1701:FMT:C	2.26	0.47
1:A:160:VAL:HG22	1:A:160:VAL:O	2.14	0.47
1:B:271:ARG:HG2	1:B:343:THR:OG1	2.15	0.47
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.81	0.47
1:A:276:THR:HB	1:A:337:VAL:CG1	2.44	0.47
1:A:52:GLU:HG3	1:A:166:TRP:CZ2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ARG:HB2	1:B:170:GLN:HG3	1.96	0.47
1:A:188:MET:CE	1:A:193:TYR:HB2	2.43	0.46
1:A:412:LEU:HD23	1:A:421:CYS:HB2	1.97	0.46
1:B:447:ILE:HD12	4:B:1288:HOH:O	2.15	0.46
1:A:41:HIS:CG	1:A:42:PRO:HD2	2.50	0.46
1:A:270:THR:O	1:A:270:THR:HG23	2.15	0.46
1:A:298:LYS:O	1:A:298:LYS:HD2	2.16	0.46
1:B:271:ARG:NH2	1:B:342:SER:OG	2.49	0.46
1:B:343:THR:HG22	1:B:343:THR:O	2.16	0.46
1:A:198:ARG:HD3	1:A:198:ARG:HH11	1.45	0.45
1:A:190:ARG:HE	1:A:434:GLU:CD	2.19	0.45
1:B:80:LEU:HD12	1:B:118:PHE:CZ	2.52	0.45
1:A:17:ALA:HA	1:A:20:PHE:HB3	1.97	0.45
1:B:134:MET:HG2	1:B:136:VAL:HG23	1.96	0.45
1:B:77:ASP:OD1	1:B:78:ASP:N	2.49	0.45
1:A:208:ASP:HB3	1:A:374:ARG:NE	2.27	0.45
1:B:310:MET:O	1:B:314:ILE:HG12	2.16	0.45
1:B:192:GLN:O	1:B:196:LYS:HG3	2.16	0.45
1:B:298:LYS:HG3	1:B:299:ASP:OD1	2.16	0.45
1:B:195:GLU:O	1:B:199:GLN:N	2.48	0.45
1:A:299:ASP:O	1:A:302:GLU:N	2.49	0.45
1:B:190:ARG:HG2	1:B:437:TYR:CZ	2.52	0.45
1:B:1:MET:N	1:B:94:PRO:O	2.49	0.45
1:A:9:ILE:CD1	1:A:164:ARG:HD3	2.47	0.44
1:A:332:GLU:HA	1:A:333:PRO:HD3	1.53	0.44
1:B:300:ARG:HA	1:B:303:ASN:ND2	2.23	0.44
1:A:96:HIS:NE2	1:A:265:ASN:HB2	2.32	0.44
1:A:24:ARG:H	1:A:24:ARG:HG2	1.52	0.44
1:B:303:ASN:O	1:B:306:ILE:N	2.50	0.44
1:A:12:LEU:HD13	1:A:12:LEU:HA	1.62	0.44
1:A:55:CYS:HB3	1:A:138:ILE:HB	1.98	0.44
1:B:209:CYS:HA	1:B:371:PRO:HD2	2.00	0.44
1:B:176:GLU:O	1:B:228:GLN:HG3	2.18	0.44
1:B:438:GLN:NE2	1:B:438:GLN:HA	2.33	0.44
1:B:446:ARG:HA	1:B:449:LYS:HB2	2.00	0.44
1:B:449:LYS:HD3	1:B:449:LYS:HA	1.83	0.44
1:A:195:GLU:HG2	1:A:199:GLN:HE21	1.83	0.43
1:A:97:ASN:OD1	1:A:99:ASP:N	2.46	0.43
1:B:159:ASP:OD1	1:B:161:ASN:N	2.51	0.43
1:A:446:ARG:CA	1:A:449:LYS:HG2	2.48	0.43
1:B:178:PHE:CE2	1:B:451:LEU:HG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:SER:OG	1:B:187:ASN:N	2.52	0.43
1:B:436:GLU:HA	1:B:436:GLU:OE1	2.18	0.43
1:B:444:VAL:O	1:B:448:LEU:HG	2.19	0.43
1:A:397:LEU:N	1:A:397:LEU:HD12	2.33	0.43
1:B:190:ARG:HH22	1:B:433:GLU:HG2	1.83	0.43
1:B:449:LYS:HG2	1:B:449:LYS:HZ2	1.64	0.43
1:A:394:ILE:HG21	1:A:394:ILE:HD13	1.76	0.42
1:A:446:ARG:HA	1:A:449:LYS:HD3	2.01	0.42
1:B:80:LEU:HD23	1:B:134:MET:HE2	1.99	0.42
1:B:265:ASN:O	1:B:266:SER:HB2	2.18	0.42
1:A:390:TRP:CD2	1:A:422:SER:HB2	2.54	0.42
1:B:171:GLN:CA	1:B:171:GLN:HE21	2.33	0.42
1:B:2:LYS:HB2	1:B:2:LYS:HE2	1.38	0.42
1:B:261:ILE:HD13	1:B:261:ILE:HG21	1.61	0.42
1:A:149:ARG:NH2	4:A:1261:HOH:O	2.51	0.42
1:A:424:GLY:N	3:A:1701:FMT:H	2.31	0.42
1:A:188:MET:HE1	1:A:193:TYR:HD1	1.84	0.42
1:A:84:GLN:NE2	4:A:1080:HOH:O	2.50	0.42
1:B:190:ARG:HH12	1:B:433:GLU:CG	2.32	0.42
1:A:323:VAL:HA	1:A:345:THR:O	2.19	0.42
1:B:271:ARG:HD3	1:B:343:THR:HA	2.02	0.42
1:B:310:MET:O	1:B:313:ASP:HB2	2.20	0.42
1:A:276:THR:O	1:A:277:LEU:HD13	2.19	0.41
1:A:23:SER:O	1:A:172:PHE:HD1	2.03	0.41
1:B:196:LYS:O	1:B:200:VAL:N	2.50	0.41
1:A:61:GLY:O	1:A:117:ARG:HD3	2.20	0.41
1:A:164:ARG:HH11	1:A:164:ARG:HG2	1.85	0.41
1:B:188:MET:CG	1:B:216:GLN:HG2	2.51	0.41
1:A:116:ARG:HH11	1:A:116:ARG:HD3	1.59	0.41
1:A:188:MET:HB2	1:A:188:MET:HE2	1.61	0.41
1:A:274:LYS:HG3	1:A:306:ILE:CG1	2.49	0.41
1:B:129:ILE:HD13	1:B:129:ILE:HG21	1.82	0.41
1:A:295:ASN:CA	1:A:300:ARG:HD3	2.51	0.41
1:A:4:LEU:HG	1:A:4:LEU:H	1.30	0.41
1:B:193:TYR:CE2	1:B:437:TYR:HB2	2.55	0.41
1:A:279:ARG:HD2	1:A:279:ARG:HA	1.67	0.41
1:A:190:ARG:NH2	1:A:434:GLU:OE1	2.50	0.41
1:B:297:ALA:HB3	1:B:300:ARG:HD3	2.02	0.41
1:A:141:TRP:CE2	1:A:163:ARG:HD2	2.56	0.41
1:A:259:ARG:HH11	1:A:269:GLN:NE2	2.19	0.41
1:A:260:PHE:O	1:A:270:THR:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ASN:HB3	4:A:1237:HOH:O	2.20	0.41
1:A:154:LEU:HA	1:A:154:LEU:HD12	1.93	0.41
1:A:255:LEU:HD22	1:A:255:LEU:N	2.36	0.40
1:A:329:PHE:CA	1:A:340:LEU:HD11	2.51	0.40
1:B:188:MET:HG3	1:B:216:GLN:HG2	2.03	0.40
1:B:381:GLU:HG2	1:B:382:LEU:CD2	2.45	0.40
1:A:274:LYS:HD3	1:A:274:LYS:HA	1.38	0.40
1:B:47:ASP:OD2	1:B:147:HIS:NE2	2.49	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	433/453 (96%)	401 (93%)	25 (6%)	7 (2%)	11	5
1	B	408/453 (90%)	372 (91%)	27 (7%)	9 (2%)	8	3
All	All	841/906 (93%)	773 (92%)	52 (6%)	16 (2%)	9	4

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	301	ALA
1	B	170	GLN
1	B	173	SER
1	B	298	LYS
1	B	429	ALA
1	A	296	SER
1	B	343	THR
1	A	69	SER
1	B	450	GLN

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Mol	Chain	Res	Type
1	A	176	GLU
1	A	158	ASN
1	A	370	ALA
1	B	449	LYS
1	B	207	GLY
1	B	326	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	375/390 (96%)	334 (89%)	41 (11%)	7	4
1	B	355/390 (91%)	296 (83%)	59 (17%)	2	1
All	All	730/780 (94%)	630 (86%)	100 (14%)	4	2

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	11	LEU
1	A	12	LEU
1	A	24	ARG
1	A	27	HIS
1	A	29	PRO
1	A	52	GLU
1	A	62	LYS
1	A	71	LYS
1	A	89	ARG
1	A	93	ARG
1	A	95	THR
1	A	136	VAL
1	A	143	LEU
1	A	148	GLN
1	A	151	THR
1	A	160	VAL

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Mol	Chain	Res	Type
1	A	167	LEU
1	A	168	GLU
1	A	180	LEU
1	A	205	HIS
1	A	209	CYS
1	A	219	HIS
1	A	232	GLN
1	A	238	ARG
1	A	257	PRO
1	A	267	GLU
1	A	274	LYS
1	A	277	LEU
1	A	296	SER
1	A	298	LYS
1	A	300	ARG
1	A	304	LEU
1	A	314	ILE
1	A	316	ARG
1	A	317	VAL
1	A	331	VAL
1	A	335	PRO
1	A	337	VAL
1	A	350	GLU
1	A	453	LYS
1	B	1	MET
1	B	2	LYS
1	B	3	THR
1	B	10	THR
1	B	12	LEU
1	B	15	GLN
1	B	24	ARG
1	B	26	SER
1	B	43	TYR
1	B	62	LYS
1	B	70	GLU
1	B	71	LYS
1	B	75	THR
1	B	83	LEU
1	B	91	ASP
1	B	95	THR
1	B	100	LEU
1	B	158	ASN

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Mol	Chain	Res	Type
1	B	159	ASP
1	B	167	LEU
1	B	169	SER
1	B	171	GLN
1	B	173	SER
1	B	175	GLN
1	B	176	GLU
1	B	190	ARG
1	B	200	VAL
1	B	203	TYR
1	B	204	LEU
1	B	206	SER
1	B	219	HIS
1	B	232	GLN
1	B	235	GLN
1	B	238	ARG
1	B	267	GLU
1	B	271	ARG
1	B	298	LYS
1	B	302	GLU
1	B	303	ASN
1	B	305	MET
1	B	311	ARG
1	B	324	LYS
1	B	326	PRO
1	B	343	THR
1	B	345	THR
1	B	350	GLU
1	B	368	THR
1	B	415	ILE
1	B	418	GLN
1	B	431	SER
1	B	438	GLN
1	B	439	GLU
1	B	443	LYS
1	B	445	ASN
1	B	446	ARG
1	B	449	LYS
1	B	450	GLN
1	B	451	LEU
1	B	453	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	84	GLN
1	A	127	GLN
1	A	158	ASN
1	A	199	GLN
1	A	201	GLN
1	A	211	GLN
1	A	219	HIS
1	A	237	ASN
1	A	269	GLN
1	A	339	HIS
1	A	450	GLN
1	B	35	HIS
1	B	81	GLN
1	B	84	GLN
1	B	103	GLN
1	B	157	HIS
1	B	170	GLN
1	B	171	GLN
1	B	175	GLN
1	B	211	GLN
1	B	228	GLN
1	B	303	ASN
1	B	353	HIS
1	B	388	ASN
1	B	438	GLN
1	B	445	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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

3 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	$\# Z  > 2$
3	FMT	A	1701	-	0,2,2	0.00	-	0,1,1	0.00	-
2	TRP	A	601	-	11,16,16	1.19	1 (9%)	11,22,22	1.98	5 (45%)
2	TRP	B	602	-	11,16,16	0.95	1 (9%)	11,22,22	3.71	7 (63%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMT	A	1701	-	-	0/0/0/0	0/0/0/0
2	TRP	A	601	-	-	0/3/8/8	0/2/2/2
2	TRP	B	602	-	-	0/3/8/8	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	TRP	CD1-NE1	2.14	1.41	1.36
2	A	601	TRP	CH2-CZ3	3.20	1.45	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	TRP	CH2-CZ2-CE2	-6.98	109.56	120.07
2	B	602	TRP	CZ3-CE3-CD2	-6.56	111.50	120.88
2	A	601	TRP	CZ3-CH2-CZ2	-2.64	116.68	120.45
2	B	602	TRP	CE3-CD2-CG	-2.46	129.90	134.42
2	A	601	TRP	CE3-CD2-CE2	-2.33	115.07	118.17
2	B	602	TRP	CH2-CZ3-CE3	2.04	123.36	120.45
2	A	601	TRP	CE3-CD2-CG	2.14	138.34	134.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	TRP	CZ2-CE2-CD2	2.63	125.62	121.11
2	A	601	TRP	CZ3-CE3-CD2	3.05	125.23	120.88
2	A	601	TRP	CH2-CZ2-CE2	3.33	125.09	120.07
2	B	602	TRP	CE3-CD2-CE2	3.35	122.61	118.17
2	B	602	TRP	CZ3-CH2-CZ2	4.84	127.35	120.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1701	FMT	4	0
2	B	602	TRP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	437/453 (96%)	-0.11	8 (1%) 69 68	9, 23, 51, 73	0
1	B	414/453 (91%)	0.17	25 (6%) 23 23	11, 27, 66, 144	0
All	All	851/906 (93%)	0.03	33 (3%) 40 40	9, 24, 60, 144	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	172	PHE	9.2
1	B	1	MET	8.3
1	B	173	SER	8.1
1	B	175	GLN	6.1
1	B	171	GLN	5.7
1	B	453	LYS	5.1
1	A	208	ASP	4.1
1	B	174	PRO	4.0
1	B	299	ASP	3.9
1	A	205	HIS	3.9
1	B	176	GLU	3.5
1	B	298	LYS	3.2
1	B	40	ASP	3.2
1	B	43	TYR	3.1
1	A	174	PRO	3.0
1	B	305	MET	2.7
1	B	41	HIS	2.6
1	B	326	PRO	2.6
1	B	312	ASN	2.6
1	B	319	VAL	2.5
1	B	446	ARG	2.4
1	A	453	LYS	2.4
1	A	407	ILE	2.4
1	A	277	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	69	SER	2.3
1	A	175	GLN	2.3
1	B	170	GLN	2.2
1	A	210	TYR	2.2
1	B	441	PHE	2.2
1	B	327	GLU	2.2
1	B	430	ASP	2.1
1	B	70	GLU	2.1
1	B	302	GLU	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	FMT	A	1701	3/3	0.88	0.28	3.53	22,22,25,30	0
2	TRP	B	602	15/15	0.94	0.12	-0.24	11,17,22,22	0
2	TRP	A	601	15/15	0.94	0.11	-0.40	8,15,19,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.