



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:28 PM UTC

PDB ID : 1E3K / pdb_00001e3k
Title : Human Progesteron Receptor Ligand Binding Domain in complex with the ligand metribolone (R1881)
Authors : Matias, P.M.; Donner, P.; Coelho, R.; Thomaz, M.; Peixoto, C.; Macedo, S.; Otto, N.; Joschko, S.; Scholz, P.; Wegg, A.; Basler, S.; Schafer, M.; Egner, U.; Carrondo, M.A.
Deposited on : 2000-06-19
Resolution : 2.80 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

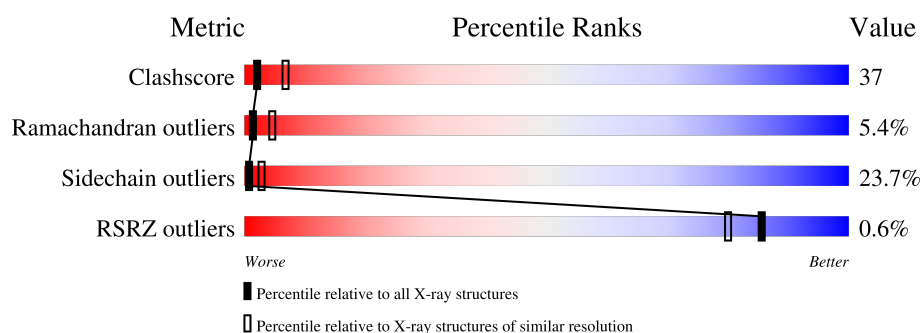
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	258	12% 34% 36% 14% .
1	B	258	9% 34% 44% 9% .

2 Entry composition [i](#)

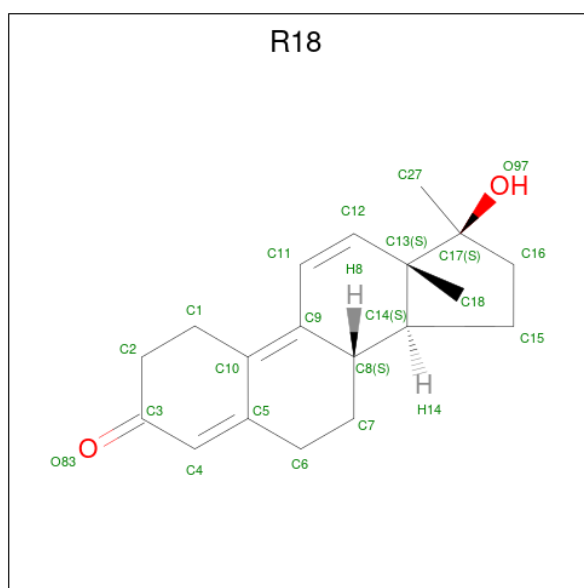
There are 3 unique types of molecules in this entry. The entry contains 4070 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROGESTERONE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			2010	1305	334	357	14			
1	B	249	Total	C	N	O	S	0	0	0
			2017	1308	334	361	14			

- Molecule 2 is (17BETA)-17-HYDROXY-17-METHYLESTRA-4,9,11-TRIEN-3-ONE (CCD ID: R18) (formula: $C_{19}H_{24}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			21	19	2		
2	B	1	Total	C	O	0	0
			21	19	2		

- Molecule 3 is water.

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.40Å 65.01Å 71.18Å 90.00° 95.65° 90.00°	Depositor
Resolution (Å)	12.50 – 2.80 12.50 – 2.80	Depositor EDS
% Data completeness (in resolution range)	67.0 (12.50-2.80) 66.3 (12.50-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.37 (at 2.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.217 , 0.343 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4070	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: R18

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	1.51	16/2053 (0.8%)	3.80	444/2778 (16.0%)
1	B	1.38	9/2060 (0.4%)	3.54	377/2786 (13.5%)
All	All	1.45	25/4113 (0.6%)	3.67	821/5564 (14.8%)

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	4
1	B	0	3
All	All	0	7

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	888	HIS	CG-ND1	8.43	1.47	1.38
1	A	759	MET	N-CA	-6.89	1.38	1.46
1	A	751	ILE	C-O	-6.35	1.17	1.24
1	B	891	CYS	C-O	6.31	1.31	1.24
1	A	735	SER	N-CA	-6.24	1.38	1.46
1	A	841	PHE	N-CA	-6.21	1.39	1.46
1	A	820	CYS	N-CA	-6.05	1.39	1.46
1	A	714	LEU	N-CA	-6.03	1.39	1.46
1	B	745	ASP	C-O	-5.84	1.17	1.24
1	A	746	ASP	N-CA	-5.71	1.39	1.46
1	B	765	TRP	C-O	-5.70	1.17	1.24
1	B	746	ASP	N-CA	-5.63	1.39	1.46
1	B	891	CYS	N-CA	-5.47	1.39	1.46
1	B	888	HIS	CE1-NE2	-5.42	1.27	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	836	ARG	C-N	-5.27	1.26	1.33
1	A	765	TRP	N-CA	-5.24	1.39	1.46
1	A	745	ASP	C-N	-5.22	1.27	1.33
1	B	909	MET	C-O	-5.21	1.18	1.24
1	A	794	PHE	N-CA	-5.18	1.39	1.46
1	A	842	GLU	CA-CB	-5.17	1.44	1.53
1	A	848	TYR	C-N	-5.14	1.27	1.33
1	A	779	ALA	N-CA	-5.10	1.40	1.46
1	B	869	ARG	CD-NE	-5.09	1.39	1.46
1	A	770	HIS	ND1-CE1	-5.09	1.27	1.32
1	A	775	MET	N-CA	-5.02	1.39	1.46

All (821) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	869	ARG	CD-NE-CZ	36.78	175.90	124.40
1	A	878	ASP	CA-CB-CG	26.32	138.92	112.60
1	A	793	SER	CA-C-N	24.09	161.19	122.65
1	A	793	SER	C-N-CA	24.09	161.19	122.65
1	A	842	GLU	CA-CB-CG	23.02	160.13	114.10
1	A	899	ARG	NE-CZ-NH2	-19.12	101.99	119.20
1	B	734	LYS	CB-CG-CD	18.79	154.53	111.30
1	B	845	ARG	CG-CD-NE	18.73	153.20	112.00
1	B	709	ASP	CA-CB-CG	18.25	130.85	112.60
1	A	758	LEU	CA-C-N	17.65	144.37	120.54
1	A	758	LEU	C-N-CA	17.65	144.37	120.54
1	B	869	ARG	NE-CZ-NH2	16.69	134.22	119.20
1	B	897	GLN	OE1-CD-NE2	16.20	138.80	122.60
1	A	747	GLN	OE1-CD-NE2	-16.05	106.55	122.60
1	A	845	ARG	CD-NE-CZ	15.81	146.53	124.40
1	B	850	ARG	CD-NE-CZ	15.20	145.69	124.40
1	B	844	MET	O-C-N	14.66	137.92	122.09
1	B	774	GLN	OE1-CD-NE2	14.40	137.00	122.60
1	A	924	MET	CA-C-N	14.23	141.15	122.51
1	A	924	MET	C-N-CA	14.23	141.15	122.51
1	A	795	TYR	N-CA-C	-14.12	95.36	111.03
1	A	879	ASN	OD1-CG-ND2	13.84	136.44	122.60
1	A	787	GLN	CB-CG-CD	13.77	136.01	112.60
1	B	886	GLN	OE1-CD-NE2	13.74	136.34	122.60
1	B	888	HIS	CA-C-O	13.54	135.21	121.00
1	A	908	MET	CA-C-N	13.41	138.64	120.54
1	A	908	MET	C-N-CA	13.41	138.64	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	899	ARG	CD-NE-CZ	13.38	143.13	124.40
1	A	770	HIS	CA-CB-CG	13.31	127.11	113.80
1	B	879	ASN	OD1-CG-ND2	13.29	135.89	122.60
1	A	751	ILE	O-C-N	-13.23	108.95	121.91
1	A	752	GLN	CG-CD-NE2	-12.51	97.63	116.40
1	A	775	MET	CA-C-O	-12.44	107.20	120.89
1	B	684	ILE	N-CA-CB	12.27	128.39	111.21
1	B	826	LEU	CA-C-O	-12.15	106.00	119.97
1	A	840	GLN	CB-CG-CD	12.13	133.23	112.60
1	A	812	GLN	CA-CB-CG	12.03	138.15	114.10
1	A	819	LEU	O-C-N	-12.02	109.38	122.12
1	B	775	MET	CA-C-O	-12.00	107.55	120.99
1	B	844	MET	CA-C-O	-11.76	108.59	120.70
1	A	732	TRP	N-CA-CB	11.75	127.06	109.91
1	B	752	GLN	CA-C-N	11.64	137.04	120.28
1	B	752	GLN	C-N-CA	11.64	137.04	120.28
1	A	787	GLN	OE1-CD-NE2	-11.63	110.97	122.60
1	B	766	ARG	NE-CZ-NH2	11.53	129.58	119.20
1	B	850	ARG	NE-CZ-NH2	-11.50	108.85	119.20
1	A	812	GLN	OE1-CD-NE2	-11.48	111.12	122.60
1	A	689	ASN	CA-CB-CG	11.47	124.07	112.60
1	B	791	GLU	CB-CG-CD	11.41	132.00	112.60
1	B	845	ARG	CD-NE-CZ	11.30	140.23	124.40
1	A	760	VAL	O-C-N	-11.29	110.15	121.90
1	B	859	ARG	CD-NE-CZ	11.28	140.19	124.40
1	B	895	PHE	CA-CB-CG	11.22	125.02	113.80
1	A	926	LYS	CA-C-O	11.21	128.78	119.36
1	A	794	PHE	N-CA-CB	-11.20	94.21	110.56
1	A	792	SER	CA-C-O	11.07	136.34	120.51
1	B	813	VAL	CA-C-O	11.04	134.58	120.78
1	A	897	GLN	CB-CG-CD	10.87	131.08	112.60
1	A	745	ASP	CA-C-N	10.71	135.06	120.38
1	A	745	ASP	C-N-CA	10.71	135.06	120.38
1	B	704	ASP	CA-CB-CG	10.65	123.25	112.60
1	A	899	ARG	NH1-CZ-NH2	10.59	133.06	119.30
1	B	768	TYR	CA-C-O	-10.57	109.22	120.42
1	A	737	PRO	O-C-N	-10.50	111.54	122.98
1	B	724	ARG	CD-NE-CZ	10.49	139.09	124.40
1	A	888	HIS	CA-C-O	10.49	131.84	120.82
1	A	751	ILE	CA-C-N	10.46	134.65	120.54
1	A	751	ILE	C-N-CA	10.46	134.65	120.54
1	A	846	SER	N-CA-C	10.44	123.64	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	824	LEU	CA-C-O	-10.43	109.36	120.63
1	A	745	ASP	CA-C-O	10.42	132.53	121.07
1	A	820	CYS	CA-C-O	-10.34	109.46	120.42
1	B	752	GLN	OE1-CD-NE2	10.30	132.90	122.60
1	A	758	LEU	N-CA-C	10.28	123.44	111.11
1	A	872	GLN	OE1-CD-NE2	10.28	132.88	122.60
1	B	809	VAL	N-CA-C	-10.12	100.50	110.72
1	B	683	LEU	CA-C-O	10.11	137.98	120.80
1	A	778	PHE	CB-CG-CD1	10.09	137.84	120.70
1	A	828	ASN	OD1-CG-ND2	-10.02	112.58	122.60
1	A	749	THR	OG1-CB-CG2	10.01	129.31	109.30
1	B	841	PHE	CA-CB-CG	-9.90	103.90	113.80
1	B	758	LEU	O-C-N	-9.87	111.52	122.08
1	B	745	ASP	N-CA-CB	-9.75	95.73	110.16
1	A	869	ARG	CD-NE-CZ	9.74	138.04	124.40
1	A	769	LYS	CA-C-O	-9.71	110.70	120.70
1	A	760	VAL	CA-C-N	9.68	135.34	120.82
1	A	760	VAL	C-N-CA	9.68	135.34	120.82
1	A	778	PHE	CA-C-N	9.68	137.75	122.26
1	A	778	PHE	C-N-CA	9.68	137.75	122.26
1	B	851	GLU	CA-C-N	9.68	134.03	120.29
1	B	851	GLU	C-N-CA	9.68	134.03	120.29
1	B	812	GLN	CA-C-N	9.67	139.38	121.97
1	B	812	GLN	C-N-CA	9.67	139.38	121.97
1	B	735	SER	CB-CA-C	-9.63	93.37	109.55
1	A	734	LYS	O-C-N	-9.62	109.53	122.43
1	A	816	GLU	N-CA-C	-9.61	100.89	111.36
1	A	911	GLU	CA-C-O	-9.54	110.34	120.55
1	B	828	ASN	CA-C-O	-9.52	106.92	119.11
1	A	904	GLU	N-CA-CB	-9.49	94.03	109.60
1	A	766	ARG	CD-NE-CZ	9.48	137.68	124.40
1	A	868	GLN	CA-C-N	9.48	132.76	120.44
1	A	868	GLN	C-N-CA	9.48	132.76	120.44
1	A	815	GLN	CB-CG-CD	-9.43	96.57	112.60
1	A	716	THR	CA-CB-OG1	-9.42	95.47	109.60
1	B	689	ASN	CB-CG-ND2	-9.42	102.28	116.40
1	B	719	ASN	CB-CG-ND2	-9.41	102.28	116.40
1	B	914	ALA	O-C-N	9.40	132.25	122.09
1	B	823	VAL	O-C-N	9.40	131.12	121.91
1	A	849	ILE	CA-C-N	9.38	133.79	120.28
1	A	849	ILE	C-N-CA	9.38	133.79	120.28
1	A	836	ARG	CD-NE-CZ	9.36	137.51	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	774	GLN	CA-C-N	9.36	139.60	121.63
1	A	774	GLN	C-N-CA	9.36	139.60	121.63
1	B	845	ARG	CA-CB-CG	9.35	132.81	114.10
1	A	869	ARG	NH1-CZ-NH2	-9.34	107.16	119.30
1	A	742	LEU	CA-C-O	9.28	131.68	121.56
1	A	788	ARG	NE-CZ-NH2	-9.27	110.85	119.20
1	A	724	ARG	NE-CZ-NH2	9.24	127.52	119.20
1	B	741	ASN	CA-CB-CG	-9.22	103.38	112.60
1	B	926	LYS	CA-C-O	9.22	126.14	119.32
1	A	819	LEU	CA-C-O	9.21	130.31	120.55
1	A	752	GLN	CA-C-O	-9.19	111.07	120.90
1	B	748	ILE	CA-C-O	-9.17	110.87	121.05
1	B	858	LEU	N-CA-CB	-9.16	96.15	110.44
1	B	909	MET	CA-C-O	-9.15	110.75	120.63
1	B	766	ARG	CD-NE-CZ	9.14	137.20	124.40
1	B	788	ARG	N-CA-CB	-9.11	95.09	110.49
1	A	688	ILE	CA-C-O	-9.09	110.84	120.57
1	A	787	GLN	CA-CB-CG	9.02	132.13	114.10
1	B	745	ASP	CA-C-N	9.00	132.68	120.44
1	B	745	ASP	C-N-CA	9.00	132.68	120.44
1	A	741	ASN	CA-CB-CG	8.98	121.58	112.60
1	A	828	ASN	N-CA-C	8.97	124.01	112.89
1	A	840	GLN	O-C-N	-8.91	112.83	122.09
1	B	880	LEU	N-CA-CB	-8.91	95.88	110.40
1	A	851	GLU	CA-C-N	8.90	132.55	120.44
1	A	851	GLU	C-N-CA	8.90	132.55	120.44
1	B	850	ARG	NE-CZ-NH1	8.86	130.36	121.50
1	A	726	LEU	N-CA-CB	-8.86	96.66	110.30
1	A	846	SER	CA-CB-OG	-8.84	93.41	111.10
1	B	769	LYS	N-CA-C	8.84	120.53	111.07
1	A	751	ILE	N-CA-CB	-8.79	100.26	110.55
1	A	752	GLN	CG-CD-OE1	8.76	138.33	120.80
1	A	869	ARG	NE-CZ-NH1	8.74	130.24	121.50
1	A	868	GLN	OE1-CD-NE2	-8.72	113.88	122.60
1	B	912	VAL	O-C-N	-8.71	113.35	121.89
1	A	757	SER	O-C-N	-8.68	112.92	122.12
1	B	828	ASN	OD1-CG-ND2	8.66	131.26	122.60
1	B	747	GLN	CA-CB-CG	8.65	131.41	114.10
1	A	794	PHE	CA-CB-CG	8.63	122.43	113.80
1	B	888	HIS	CE1-NE2-CD2	8.61	117.61	109.00
1	A	819	LEU	CA-C-N	8.60	132.51	120.29
1	A	819	LEU	C-N-CA	8.60	132.51	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	911	GLU	CA-CB-CG	8.58	131.27	114.10
1	A	752	GLN	N-CA-CB	8.57	122.71	109.94
1	B	704	ASP	N-CA-CB	8.56	122.39	109.98
1	A	856	ILE	N-CA-C	-8.53	102.03	110.30
1	B	842	GLU	CB-CG-CD	8.50	127.05	112.60
1	A	822	LYS	CB-CA-C	8.49	124.22	110.88
1	B	923	GLY	O-C-N	-8.46	112.66	122.31
1	B	775	MET	CA-CB-CG	8.45	130.99	114.10
1	A	781	ASP	CA-CB-CG	-8.44	104.16	112.60
1	A	850	ARG	CD-NE-CZ	8.43	136.21	124.40
1	B	748	ILE	CB-CG1-CD1	8.43	131.51	113.80
1	B	853	ILE	CB-CG1-CD1	-8.42	96.12	113.80
1	B	824	LEU	CA-C-O	-8.40	111.56	120.63
1	A	905	PHE	O-C-N	-8.39	109.38	121.54
1	A	882	ASP	CA-CB-CG	-8.38	104.22	112.60
1	B	916	GLN	OE1-CD-NE2	8.37	130.97	122.60
1	A	850	ARG	CA-CB-CG	8.35	130.81	114.10
1	A	732	TRP	CA-CB-CG	8.35	129.46	113.60
1	A	723	GLU	O-C-N	-8.34	112.11	122.20
1	A	742	LEU	O-C-N	-8.34	113.02	122.86
1	A	842	GLU	CB-CA-C	8.34	126.68	110.67
1	A	721	LEU	CA-C-N	8.33	137.75	121.41
1	A	721	LEU	C-N-CA	8.33	137.75	121.41
1	B	849	ILE	O-C-N	-8.33	113.75	121.91
1	A	808	PHE	CA-C-N	8.32	131.05	120.56
1	A	808	PHE	C-N-CA	8.32	131.05	120.56
1	B	747	GLN	OE1-CD-NE2	-8.32	114.28	122.60
1	B	743	HIS	CA-CB-CG	-8.32	105.48	113.80
1	A	804	ILE	N-CA-CB	8.28	122.80	111.21
1	B	828	ASN	N-CA-C	8.23	123.14	113.18
1	A	792	SER	O-C-N	-8.22	111.66	122.59
1	B	890	TYR	O-C-N	8.22	130.83	122.12
1	A	905	PHE	CA-C-O	8.21	126.39	119.66
1	B	900	ALA	N-CA-C	-8.20	101.39	111.40
1	A	745	ASP	O-C-N	-8.17	113.34	122.08
1	A	816	GLU	CA-C-O	-8.16	111.77	120.42
1	A	840	GLN	OE1-CD-NE2	-8.14	114.46	122.60
1	B	685	PRO	CB-CA-C	-8.13	101.00	110.92
1	B	879	ASN	CB-CG-OD1	-8.13	104.55	120.80
1	A	736	LEU	CB-CA-C	8.11	119.29	109.31
1	A	801	MET	O-C-N	-8.12	113.65	122.09
1	B	783	ILE	O-C-N	-8.10	114.68	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	753	TYR	O-C-N	-8.10	112.75	122.22
1	B	746	ASP	O-C-N	-8.09	113.35	122.09
1	A	800	THR	CA-CB-OG1	-8.07	97.50	109.60
1	A	854	LYS	N-CA-C	8.07	120.79	111.11
1	B	758	LEU	CA-C-N	8.07	131.43	120.38
1	B	758	LEU	C-N-CA	8.07	131.43	120.38
1	B	892	LEU	CA-CB-CG	8.06	144.52	116.30
1	B	849	ILE	CA-C-N	8.06	136.93	121.54
1	B	849	ILE	C-N-CA	8.06	136.93	121.54
1	A	758	LEU	O-C-N	-8.06	113.71	122.09
1	A	829	THR	CA-C-O	-8.05	110.38	120.28
1	B	754	SER	CA-C-O	-8.03	110.12	119.59
1	A	864	VAL	N-CA-CB	-8.02	101.59	110.65
1	B	737	PRO	CB-CA-C	7.99	124.74	111.56
1	B	748	ILE	N-CA-CB	7.98	120.78	110.57
1	B	780	PRO	CA-N-CD	-7.97	100.84	112.00
1	A	721	LEU	O-C-N	-7.95	113.70	122.12
1	A	904	GLU	OE1-CD-OE2	7.94	141.97	122.90
1	A	916	GLN	CB-CA-C	7.94	122.29	109.27
1	A	737	PRO	CB-CA-C	7.93	122.02	111.71
1	A	760	VAL	CA-C-O	7.93	129.85	121.05
1	B	766	ARG	NE-CZ-NH1	-7.91	113.59	121.50
1	B	856	ILE	N-CA-CB	7.90	119.28	110.51
1	B	836	ARG	O-C-N	-7.89	113.57	122.09
1	A	860	GLN	N-CA-CB	7.87	121.92	110.58
1	B	826	LEU	O-C-N	7.87	131.95	122.27
1	A	823	VAL	CB-CA-C	-7.87	101.52	112.14
1	B	689	ASN	OD1-CG-ND2	7.86	130.46	122.60
1	A	753	TYR	CG-CD1-CE1	-7.85	109.42	121.20
1	B	743	HIS	CA-C-O	-7.85	112.59	121.07
1	A	746	ASP	N-CA-CB	-7.85	98.29	110.06
1	A	783	ILE	CA-C-O	-7.85	111.48	120.66
1	B	916	GLN	CG-CD-NE2	-7.84	104.65	116.40
1	B	799	LEU	CA-C-O	-7.82	112.27	120.55
1	A	764	GLY	O-C-N	-7.80	112.56	122.70
1	A	856	ILE	CB-CG1-CD1	7.79	130.17	113.80
1	A	912	VAL	CA-CB-CG2	7.79	123.65	110.40
1	A	924	MET	CB-CA-C	7.79	121.44	111.40
1	B	690	LEU	CA-C-N	-7.74	110.38	120.44
1	B	690	LEU	C-N-CA	-7.74	110.38	120.44
1	B	865	SER	CA-C-O	7.71	129.10	121.00
1	A	874	THR	CA-C-O	-7.67	112.34	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	887	LEU	CA-C-N	7.66	130.40	120.44
1	A	887	LEU	C-N-CA	7.66	130.40	120.44
1	B	782	LEU	CB-CA-C	-7.66	101.26	111.82
1	B	869	ARG	NH1-CZ-NH2	-7.65	109.35	119.30
1	B	912	VAL	CA-C-N	7.65	130.20	120.56
1	B	912	VAL	C-N-CA	7.65	130.20	120.56
1	A	906	PRO	CA-C-O	7.64	131.86	122.08
1	A	774	GLN	O-C-N	-7.58	113.23	122.25
1	B	815	GLN	CG-CD-NE2	-7.57	105.04	116.40
1	B	698	VAL	CB-CA-C	7.54	123.95	111.51
1	B	812	GLN	O-C-N	-7.54	113.14	122.57
1	B	790	LYS	CB-CG-CD	7.54	128.64	111.30
1	A	931	HIS	N-CA-C	7.53	121.22	110.14
1	A	804	ILE	CA-CB-CG1	7.53	123.20	110.40
1	A	868	GLN	CB-CG-CD	7.52	125.38	112.60
1	B	899	ARG	CD-NE-CZ	7.51	134.91	124.40
1	A	689	ASN	OD1-CG-ND2	7.50	130.10	122.60
1	B	810	LYS	CB-CA-C	7.50	123.59	110.85
1	B	761	PHE	CA-CB-CG	-7.49	106.31	113.80
1	B	917	LEU	CA-C-O	7.48	130.41	120.16
1	A	766	ARG	CA-CB-CG	7.47	129.04	114.10
1	A	887	LEU	O-C-N	-7.46	114.33	122.09
1	A	785	ASN	CB-CG-ND2	-7.45	105.22	116.40
1	B	888	HIS	N-CA-C	7.45	119.09	110.97
1	A	732	TRP	CA-C-O	-7.44	113.19	121.00
1	A	817	GLU	N-CA-CB	7.43	120.85	110.07
1	A	882	ASP	CA-C-O	-7.43	112.95	120.90
1	A	932	LYS	CA-CB-CG	7.43	128.96	114.10
1	A	882	ASP	O-C-N	7.42	129.81	122.09
1	B	769	LYS	CB-CA-C	-7.40	99.25	110.88
1	A	691	LEU	O-C-N	-7.39	113.26	122.20
1	B	845	ARG	NH1-CZ-NH2	-7.38	109.71	119.30
1	A	724	ARG	CG-CD-NE	7.37	128.21	112.00
1	B	822	LYS	CB-CA-C	7.35	122.42	110.88
1	A	815	GLN	OE1-CD-NE2	7.35	129.95	122.60
1	A	923	GLY	CA-C-O	7.35	128.85	120.03
1	A	888	HIS	CA-CB-CG	7.33	121.12	113.80
1	A	789	MET	N-CA-CB	7.31	121.59	110.70
1	B	770	HIS	N-CA-C	7.29	122.27	113.23
1	A	786	GLU	CA-C-O	7.28	128.13	120.42
1	B	791	GLU	CA-C-O	-7.27	110.11	120.51
1	B	899	ARG	CA-CB-CG	7.27	128.65	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	700	TYR	O-C-N	-7.26	114.57	122.85
1	B	683	LEU	O-C-N	-7.26	111.38	123.00
1	A	911	GLU	O-C-N	7.25	130.94	122.17
1	B	740	ARG	NE-CZ-NH2	-7.24	112.68	119.20
1	B	897	GLN	CB-CG-CD	-7.24	100.29	112.60
1	B	782	LEU	CA-C-O	-7.24	109.16	120.81
1	A	857	GLY	O-C-N	-7.21	113.32	122.70
1	B	773	GLY	N-CA-C	-7.21	105.10	115.27
1	A	813	VAL	CA-C-O	7.21	129.07	120.85
1	B	769	LYS	CA-C-O	-7.20	113.26	120.82
1	B	825	LEU	N-CA-C	7.20	119.12	111.28
1	B	888	HIS	CG-CD2-NE2	-7.19	100.01	107.20
1	B	914	ALA	CA-C-O	-7.19	113.30	120.70
1	A	692	MET	N-CA-CB	7.18	122.63	110.49
1	B	910	SER	CA-C-N	7.18	130.40	120.63
1	B	910	SER	C-N-CA	7.18	130.40	120.63
1	A	741	ASN	OD1-CG-ND2	-7.18	115.42	122.60
1	A	845	ARG	N-CA-CB	7.16	120.37	109.91
1	B	691	LEU	CA-C-O	-7.16	113.30	120.82
1	B	838	GLN	CB-CA-C	7.16	122.72	110.84
1	A	750	LEU	CA-C-N	-7.15	111.55	120.56
1	A	750	LEU	C-N-CA	-7.15	111.55	120.56
1	A	888	HIS	CA-C-N	7.15	129.86	120.28
1	A	888	HIS	C-N-CA	7.15	129.86	120.28
1	B	727	LEU	O-C-N	-7.14	114.67	122.09
1	B	911	GLU	OE1-CD-OE2	-7.13	105.80	122.90
1	B	906	PRO	CA-C-O	-7.11	112.78	121.31
1	A	683	LEU	CA-C-O	-7.11	111.32	119.14
1	B	925	VAL	O-C-N	-7.09	115.17	123.04
1	A	716	THR	CA-CB-CG2	7.08	122.54	110.50
1	B	873	LEU	N-CA-C	-7.08	103.62	112.90
1	B	809	VAL	CA-CB-CG2	7.08	122.43	110.40
1	B	803	GLN	CG-CD-NE2	-7.07	105.79	116.40
1	B	739	PHE	O-C-N	-7.05	114.17	122.20
1	B	753	TYR	CA-C-O	-7.04	112.15	120.10
1	B	895	PHE	O-C-N	-7.03	113.25	122.59
1	B	830	ILE	CA-CB-CG2	-7.00	98.60	110.50
1	A	912	VAL	CG1-CB-CG2	-6.99	95.42	110.80
1	A	897	GLN	CG-CD-NE2	6.98	126.87	116.40
1	B	907	GLU	N-CA-C	6.97	125.65	110.80
1	B	889	LEU	O-C-N	-6.97	114.09	122.11
1	B	878	ASP	CA-C-O	6.96	128.13	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	854	LYS	O-C-N	-6.96	114.85	122.09
1	A	880	LEU	N-CA-CB	6.96	122.11	110.41
1	A	815	GLN	N-CA-C	6.95	119.75	111.33
1	A	753	TYR	CB-CG-CD2	-6.95	110.37	120.80
1	B	741	ASN	CB-CG-ND2	6.94	126.82	116.40
1	A	808	PHE	CA-CB-CG	6.94	120.74	113.80
1	A	779	ALA	CA-C-O	6.94	126.85	120.26
1	A	789	MET	CA-CB-CG	6.94	127.97	114.10
1	A	771	VAL	N-CA-CB	6.93	122.66	111.23
1	A	893	ASN	CA-C-O	-6.92	112.01	119.97
1	A	817	GLU	CA-CB-CG	6.92	127.93	114.10
1	B	848	TYR	O-C-N	-6.92	113.06	122.33
1	B	873	LEU	CA-C-O	-6.91	111.51	119.60
1	B	902	SER	CA-C-N	-6.90	114.23	122.93
1	B	902	SER	C-N-CA	-6.90	114.23	122.93
1	A	909	MET	N-CA-CB	-6.90	99.66	109.94
1	A	744	ILE	CA-C-N	6.88	130.36	120.79
1	A	744	ILE	C-N-CA	6.88	130.36	120.79
1	B	686	PRO	CA-C-N	6.88	129.50	120.28
1	B	686	PRO	C-N-CA	6.88	129.50	120.28
1	B	765	TRP	N-CA-C	-6.87	103.72	111.14
1	A	799	LEU	N-CA-CB	6.87	120.17	109.94
1	A	744	ILE	N-CA-CB	6.86	122.55	111.23
1	A	904	GLU	CB-CA-C	6.85	121.09	110.67
1	A	816	GLU	CG-CD-OE1	6.85	134.16	118.40
1	A	752	GLN	O-C-N	6.83	129.20	122.09
1	A	783	ILE	N-CA-C	6.83	117.48	107.37
1	A	690	LEU	CB-CA-C	6.83	121.68	110.90
1	A	763	LEU	N-CA-C	-6.82	103.54	110.97
1	A	760	VAL	N-CA-C	6.81	116.93	110.53
1	A	855	ALA	CA-C-N	6.81	129.21	120.70
1	A	855	ALA	C-N-CA	6.81	129.21	120.70
1	B	842	GLU	CA-CB-CG	6.79	127.68	114.10
1	B	905	PHE	CA-CB-CG	-6.79	107.01	113.80
1	A	911	GLU	CA-CB-CG	6.77	127.64	114.10
1	A	833	GLU	CA-CB-CG	6.77	127.64	114.10
1	B	727	LEU	N-CA-CB	-6.76	99.87	109.94
1	A	859	ARG	CD-NE-CZ	-6.75	114.95	124.40
1	A	720	GLN	N-CA-C	-6.74	103.86	111.07
1	B	836	ARG	NE-CZ-NH1	-6.74	114.76	121.50
1	A	719	ASN	N-CA-CB	-6.73	100.16	110.13
1	A	750	LEU	CA-C-O	-6.73	113.42	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	916	GLN	CB-CG-CD	6.73	124.04	112.60
1	B	920	ILE	CA-C-O	-6.73	113.95	120.95
1	B	823	VAL	N-CA-CB	6.72	118.42	110.55
1	B	921	LEU	N-CA-CB	6.72	120.70	110.28
1	B	693	SER	N-CA-C	6.72	120.35	111.75
1	A	755	TRP	N-CA-C	-6.72	103.20	111.40
1	B	766	ARG	CG-CD-NE	6.72	126.78	112.00
1	B	814	SER	N-CA-CB	-6.71	99.47	110.41
1	B	726	LEU	CB-CA-C	-6.71	99.52	110.79
1	A	748	ILE	CB-CG1-CD1	-6.71	99.72	113.80
1	A	794	PHE	N-CA-C	6.70	121.17	112.92
1	A	843	GLU	N-CA-CB	6.70	119.72	110.01
1	B	774	GLN	CG-CD-NE2	-6.69	106.36	116.40
1	A	800	THR	N-CA-C	6.69	118.65	111.36
1	A	797	LEU	CA-C-O	-6.69	113.39	120.55
1	B	856	ILE	CB-CA-C	-6.67	103.35	111.88
1	B	724	ARG	NE-CZ-NH2	-6.66	113.21	119.20
1	B	931	HIS	CA-C-O	6.66	132.12	120.80
1	A	837	SER	CA-CB-OG	6.65	124.41	111.10
1	B	808	PHE	CA-C-O	6.65	128.11	120.00
1	A	810	LYS	CA-CB-CG	6.65	127.39	114.10
1	A	848	TYR	CA-C-O	-6.65	111.95	119.79
1	B	925	VAL	N-CA-C	6.63	119.90	108.95
1	A	783	ILE	CB-CA-C	-6.63	101.97	111.19
1	B	909	MET	CA-C-N	6.63	130.06	120.38
1	B	909	MET	C-N-CA	6.63	130.06	120.38
1	B	803	GLN	CA-C-O	6.62	127.57	120.55
1	B	919	LYS	CB-CG-CD	6.61	126.50	111.30
1	B	891	CYS	CA-C-O	-6.59	113.91	120.70
1	B	806	GLN	OE1-CD-NE2	-6.59	116.01	122.60
1	B	729	VAL	CA-CB-CG2	-6.58	99.20	110.40
1	A	774	GLN	N-CA-CB	-6.58	100.52	110.73
1	A	816	GLU	CB-CG-CD	6.58	123.79	112.60
1	A	879	ASN	N-CA-C	6.57	119.44	111.82
1	B	724	ARG	NE-CZ-NH1	6.57	128.07	121.50
1	B	753	TYR	N-CA-CB	6.57	120.33	110.22
1	A	928	LEU	CA-C-N	-6.56	113.66	122.72
1	A	928	LEU	C-N-CA	-6.56	113.66	122.72
1	A	721	LEU	CB-CA-C	6.56	121.68	110.79
1	B	691	LEU	CB-CA-C	6.56	121.17	110.88
1	A	869	ARG	O-C-N	6.55	128.82	122.07
1	A	767	SER	CA-CB-OG	-6.55	98.00	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	898	SER	CA-C-O	-6.55	112.70	120.10
1	A	838	GLN	O-C-N	-6.55	113.88	122.59
1	A	688	ILE	N-CA-C	-6.54	102.88	111.05
1	B	801	MET	CA-C-O	6.53	127.68	120.82
1	B	683	LEU	CA-C-N	6.53	134.21	122.13
1	B	683	LEU	C-N-CA	6.53	134.21	122.13
1	B	735	SER	N-CA-C	6.53	122.21	113.72
1	B	815	GLN	CG-CD-OE1	6.52	133.85	120.80
1	A	758	LEU	CA-C-O	-6.51	113.93	120.90
1	A	860	GLN	CB-CG-CD	6.51	123.67	112.60
1	B	917	LEU	N-CA-CB	-6.51	98.78	110.37
1	A	774	GLN	CB-CA-C	6.49	121.69	110.72
1	B	821	MET	N-CA-C	-6.49	105.19	113.23
1	B	914	ALA	N-CA-C	-6.49	104.14	111.14
1	A	746	ASP	CA-CB-CG	-6.48	106.12	112.60
1	A	685	PRO	CB-CA-C	6.48	118.82	110.92
1	B	785	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	A	793	SER	O-C-N	-6.47	113.98	122.59
1	A	746	ASP	CA-C-N	6.47	129.48	120.29
1	A	746	ASP	C-N-CA	6.47	129.48	120.29
1	A	812	GLN	CB-CG-CD	6.46	123.58	112.60
1	A	687	LEU	CD1-CG-CD2	6.45	124.99	110.80
1	B	731	LYS	CG-CD-CE	6.45	126.13	111.30
1	A	850	ARG	NE-CZ-NH2	-6.43	113.41	119.20
1	B	801	MET	O-C-N	-6.43	115.45	122.07
1	A	786	GLU	CB-CA-C	-6.42	99.93	110.85
1	A	802	TRP	CA-CB-CG	-6.42	101.40	113.60
1	A	725	GLN	CA-C-O	-6.39	112.12	119.60
1	A	856	ILE	O-C-N	6.39	128.52	121.94
1	A	915	ALA	CA-C-N	-6.39	112.21	121.98
1	A	915	ALA	C-N-CA	-6.39	112.21	121.98
1	B	837	SER	CB-CA-C	-6.38	103.37	111.22
1	B	788	ARG	CA-CB-CG	-6.38	101.35	114.10
1	B	904	GLU	CB-CG-CD	6.38	123.44	112.60
1	B	901	LEU	CD1-CG-CD2	6.37	124.82	110.80
1	A	791	GLU	CA-C-O	-6.36	111.42	120.51
1	B	803	GLN	N-CA-CB	-6.34	100.80	110.12
1	B	819	LEU	O-C-N	-6.34	114.16	122.59
1	B	716	THR	CA-C-N	6.33	131.41	120.58
1	B	716	THR	C-N-CA	6.33	131.41	120.58
1	B	745	ASP	CA-CB-CG	-6.32	106.28	112.60
1	A	724	ARG	NE-CZ-NH1	-6.32	115.18	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	757	SER	CA-CB-OG	6.31	123.72	111.10
1	B	877	LEU	CA-C-N	6.31	128.64	120.44
1	B	877	LEU	C-N-CA	6.31	128.64	120.44
1	B	776	LEU	N-CA-CB	6.30	120.03	109.94
1	A	759	MET	CA-CB-CG	6.30	126.71	114.10
1	B	821	MET	N-CA-CB	6.30	120.27	110.44
1	A	770	HIS	N-CA-CB	6.29	119.89	110.65
1	A	849	ILE	O-C-N	-6.29	115.65	121.94
1	A	752	GLN	N-CA-C	-6.28	103.57	111.11
1	A	804	ILE	CA-C-O	-6.28	111.54	119.95
1	A	891	CYS	CA-C-N	-6.28	111.38	120.29
1	A	891	CYS	C-N-CA	-6.28	111.38	120.29
1	A	815	GLN	O-C-N	-6.28	115.47	122.12
1	A	757	SER	CA-C-N	6.27	129.00	120.54
1	A	757	SER	C-N-CA	6.27	129.00	120.54
1	A	684	ILE	N-CA-CB	6.26	119.98	111.21
1	A	826	LEU	N-CA-C	-6.26	104.55	111.82
1	B	769	LYS	CG-CD-CE	6.26	125.69	111.30
1	B	829	THR	CA-C-O	-6.23	111.57	120.11
1	B	689	ASN	O-C-N	6.23	129.93	122.27
1	B	836	ARG	CA-C-N	6.21	134.66	122.61
1	B	836	ARG	C-N-CA	6.21	134.66	122.61
1	A	746	ASP	O-C-N	-6.21	115.54	122.12
1	A	802	TRP	N-CA-C	6.21	120.41	112.34
1	A	896	ILE	CA-C-O	-6.21	113.02	120.78
1	A	686	PRO	CA-C-N	6.20	128.91	120.54
1	A	686	PRO	C-N-CA	6.20	128.91	120.54
1	A	857	GLY	N-CA-C	6.20	127.86	113.18
1	B	827	LEU	CD1-CG-CD2	-6.19	97.17	110.80
1	A	749	THR	CA-C-O	-6.19	114.26	121.07
1	A	812	GLN	CA-C-N	6.18	130.19	121.66
1	A	812	GLN	C-N-CA	6.18	130.19	121.66
1	A	713	SER	CA-C-N	6.18	128.47	120.44
1	A	713	SER	C-N-CA	6.18	128.47	120.44
1	A	733	SER	CA-C-O	-6.18	113.96	120.63
1	A	842	GLU	N-CA-CB	-6.17	100.71	110.28
1	A	757	SER	CB-CA-C	6.17	121.04	110.79
1	B	765	TRP	CA-C-N	6.17	129.17	120.28
1	B	765	TRP	C-N-CA	6.17	129.17	120.28
1	A	795	TYR	N-CA-CB	6.17	118.92	109.98
1	B	794	PHE	CA-CB-CG	6.17	119.97	113.80
1	B	809	VAL	N-CA-CB	6.17	119.83	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	ILE	CB-CG1-CD1	6.16	126.75	113.80
1	B	733	SER	O-C-N	6.16	129.43	122.22
1	B	886	GLN	CG-CD-NE2	-6.16	107.17	116.40
1	A	908	MET	CA-C-O	6.15	127.04	120.70
1	A	719	ASN	CA-CB-CG	-6.15	106.45	112.60
1	A	805	PRO	CA-C-N	6.14	129.01	120.29
1	A	805	PRO	C-N-CA	6.14	129.01	120.29
1	A	841	PHE	CD1-CE1-CZ	-6.14	108.94	120.00
1	A	779	ALA	N-CA-C	6.14	113.75	108.22
1	A	805	PRO	N-CA-CB	6.14	109.41	103.51
1	A	823	VAL	N-CA-CB	6.13	118.88	110.54
1	A	841	PHE	CE1-CZ-CE2	6.13	131.04	120.00
1	B	719	ASN	OD1-CG-ND2	6.13	128.73	122.60
1	B	820	CYS	N-CA-CB	-6.13	100.13	110.49
1	A	846	SER	CA-C-O	6.11	127.44	120.90
1	B	911	GLU	CG-CD-OE2	6.11	132.45	118.40
1	B	930	PHE	N-CA-C	6.10	117.93	111.28
1	B	915	ALA	CA-C-O	-6.10	114.37	120.90
1	B	831	PRO	CA-N-CD	-6.09	103.47	112.00
1	A	866	SER	CA-C-N	6.09	128.76	120.54
1	A	866	SER	C-N-CA	6.09	128.76	120.54
1	A	868	GLN	N-CA-C	-6.09	104.76	111.82
1	A	926	LYS	CD-CE-NZ	6.08	131.37	111.90
1	B	919	LYS	CA-CB-CG	6.08	126.27	114.10
1	B	885	LYS	CA-C-O	6.08	126.85	119.38
1	A	690	LEU	N-CA-C	-6.07	104.58	111.14
1	A	888	HIS	CB-CG-CD2	-6.07	123.31	131.20
1	B	816	GLU	O-C-N	6.06	129.06	122.15
1	B	844	MET	CB-CA-C	-6.06	101.32	110.90
1	B	688	ILE	CB-CA-C	6.06	120.32	112.14
1	B	775	MET	CA-C-N	6.06	131.01	121.99
1	B	775	MET	C-N-CA	6.06	131.01	121.99
1	A	904	GLU	N-CA-C	6.04	117.85	109.15
1	A	810	LYS	CG-CD-CE	6.04	125.19	111.30
1	A	758	LEU	N-CA-CB	-6.04	100.94	109.94
1	B	767	SER	CA-CB-OG	-6.02	99.05	111.10
1	A	731	LYS	CG-CD-CE	6.02	125.14	111.30
1	B	913	ILE	O-C-N	-6.02	116.02	121.91
1	A	704	ASP	CA-C-N	6.01	133.03	121.54
1	A	704	ASP	C-N-CA	6.01	133.03	121.54
1	A	878	ASP	OD1-CG-OD2	-6.00	108.49	122.90
1	B	886	GLN	N-CA-C	6.00	117.69	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	856	ILE	N-CA-CB	6.00	117.16	110.62
1	B	716	THR	O-C-N	-6.00	114.59	122.39
1	A	888	HIS	O-C-N	-5.99	115.90	122.07
1	B	747	GLN	CB-CG-CD	5.99	122.78	112.60
1	B	872	GLN	OE1-CD-NE2	5.96	128.56	122.60
1	A	872	GLN	CG-CD-NE2	-5.96	107.47	116.40
1	B	794	PHE	CA-C-O	5.96	129.03	120.51
1	A	845	ARG	CA-C-O	-5.96	114.75	121.00
1	B	913	ILE	N-CA-CB	-5.95	103.59	110.55
1	B	917	LEU	CB-CA-C	5.95	121.89	110.17
1	B	810	LYS	N-CA-C	-5.94	104.88	111.36
1	B	688	ILE	CA-C-O	-5.94	114.77	120.95
1	B	726	LEU	CA-CB-CG	5.94	137.09	116.30
1	A	800	THR	CA-C-N	5.93	128.55	120.54
1	A	800	THR	C-N-CA	5.93	128.55	120.54
1	B	772	SER	CA-C-O	5.92	127.92	118.92
1	A	697	ASP	N-CA-C	5.92	118.55	110.55
1	B	741	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	B	903	VAL	CA-C-O	5.92	126.91	120.57
1	B	914	ALA	N-CA-CB	5.92	118.65	110.07
1	B	911	GLU	CB-CG-CD	5.92	122.66	112.60
1	A	732	TRP	NE1-CE2-CD2	-5.91	99.72	107.40
1	A	778	PHE	CD1-CG-CD2	-5.91	109.74	118.60
1	B	845	ARG	CB-CG-CD	5.89	124.86	111.30
1	A	744	ILE	CA-CB-CG2	5.89	120.52	110.50
1	A	883	LEU	CA-C-N	5.88	128.81	120.53
1	A	883	LEU	C-N-CA	5.88	128.81	120.53
1	A	783	ILE	N-CA-CB	5.88	119.07	111.67
1	A	837	SER	CB-CA-C	-5.87	103.92	111.50
1	B	812	GLN	CA-CB-CG	5.87	125.85	114.10
1	A	732	TRP	O-C-N	5.87	128.14	122.03
1	A	736	LEU	CA-C-O	5.87	126.19	119.61
1	A	860	GLN	CA-CB-CG	5.87	125.84	114.10
1	A	872	GLN	N-CA-C	5.87	117.76	111.36
1	B	704	ASP	CA-C-O	-5.85	114.88	120.90
1	B	787	GLN	N-CA-CB	-5.84	100.62	110.49
1	B	888	HIS	O-C-N	-5.83	115.97	122.03
1	A	930	PHE	N-CA-C	5.83	118.11	111.11
1	A	821	MET	N-CA-CB	5.83	119.27	110.30
1	A	912	VAL	N-CA-CB	5.83	118.46	110.54
1	B	928	LEU	CB-CA-C	5.82	119.94	110.22
1	A	911	GLU	CB-CA-C	5.82	120.56	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	781	ASP	N-CA-C	5.82	120.07	113.15
1	B	858	LEU	CA-C-O	5.82	126.07	119.27
1	A	907	GLU	OE1-CD-OE2	-5.80	108.98	122.90
1	B	790	LYS	CA-CB-CG	5.80	125.70	114.10
1	B	801	MET	CA-C-N	5.80	129.96	120.63
1	B	801	MET	C-N-CA	5.80	129.96	120.63
1	A	755	TRP	CA-CB-CG	-5.79	102.60	113.60
1	B	881	HIS	CA-CB-CG	-5.79	108.01	113.80
1	A	788	ARG	O-C-N	-5.78	114.91	122.59
1	A	788	ARG	N-CA-C	5.76	123.07	110.80
1	A	822	LYS	CA-C-O	-5.76	114.77	120.82
1	A	723	GLU	CA-C-N	5.76	130.34	120.72
1	A	723	GLU	C-N-CA	5.76	130.34	120.72
1	A	809	VAL	N-CA-C	-5.76	104.89	110.42
1	B	756	MET	N-CA-CB	5.76	119.51	109.72
1	A	738	GLY	CA-C-O	-5.76	110.55	120.57
1	A	904	GLU	CB-CG-CD	-5.76	102.81	112.60
1	B	687	LEU	CA-CB-CG	5.75	136.41	116.30
1	B	750	LEU	CA-C-N	-5.74	113.72	120.72
1	B	750	LEU	C-N-CA	-5.74	113.72	120.72
1	B	904	GLU	CA-C-O	-5.74	114.00	120.43
1	A	684	ILE	O-C-N	5.74	127.64	121.10
1	A	718	LEU	CB-CA-C	5.73	121.83	110.42
1	B	794	PHE	O-C-N	-5.73	114.97	122.59
1	B	889	LEU	CA-C-N	5.73	128.23	120.38
1	B	889	LEU	C-N-CA	5.73	128.23	120.38
1	A	875	LYS	CA-CB-CG	5.72	125.54	114.10
1	A	877	LEU	CA-C-N	5.72	127.94	120.28
1	A	877	LEU	C-N-CA	5.72	127.94	120.28
1	B	748	ILE	CB-CA-C	-5.71	104.54	112.02
1	B	913	ILE	CA-CB-CG1	-5.71	100.69	110.40
1	A	845	ARG	NE-CZ-NH1	5.71	127.21	121.50
1	B	869	ARG	N-CA-C	5.71	117.96	111.11
1	A	886	GLN	CB-CG-CD	-5.71	102.90	112.60
1	B	868	GLN	OE1-CD-NE2	-5.70	116.90	122.60
1	A	929	LEU	CA-C-O	-5.70	114.22	120.43
1	B	889	LEU	N-CA-CB	-5.70	100.49	109.78
1	B	744	ILE	CA-C-N	5.70	128.38	120.29
1	B	744	ILE	C-N-CA	5.70	128.38	120.29
1	A	821	MET	N-CA-C	-5.69	105.06	112.23
1	B	702	GLY	N-CA-C	5.69	122.69	114.10
1	A	840	GLN	CA-C-O	5.69	126.99	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	851	GLU	CG-CD-OE2	5.68	131.47	118.40
1	A	744	ILE	CB-CA-C	-5.68	101.97	111.29
1	B	692	MET	N-CA-CB	5.68	120.09	110.49
1	B	843	GLU	CA-C-N	5.68	128.16	120.44
1	B	843	GLU	C-N-CA	5.68	128.16	120.44
1	A	693	SER	CA-C-O	-5.68	113.69	120.10
1	B	874	THR	CA-C-O	-5.68	114.40	120.42
1	A	748	ILE	CA-C-O	-5.67	115.16	121.17
1	B	731	LYS	N-CA-C	-5.67	105.24	111.82
1	B	723	GLU	CB-CG-CD	-5.67	102.97	112.60
1	A	794	PHE	CA-C-O	5.66	126.18	119.56
1	B	839	THR	CA-CB-CG2	5.66	120.12	110.50
1	A	767	SER	O-C-N	5.66	128.20	122.09
1	A	740	ARG	CB-CA-C	-5.66	99.90	110.36
1	A	874	THR	O-C-N	-5.65	115.33	122.17
1	A	764	GLY	CA-C-N	5.64	132.32	121.54
1	A	764	GLY	C-N-CA	5.64	132.32	121.54
1	B	687	LEU	CA-C-O	5.64	126.53	120.55
1	B	829	THR	O-C-N	-5.64	115.61	123.34
1	B	723	GLU	CG-CD-OE2	5.63	131.35	118.40
1	B	845	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	B	806	GLN	CB-CA-C	5.62	121.84	110.38
1	B	729	VAL	N-CA-C	5.62	116.35	110.62
1	A	815	GLN	CA-C-N	5.61	128.26	120.29
1	A	815	GLN	C-N-CA	5.61	128.26	120.29
1	A	768	TYR	CA-C-O	-5.61	114.93	120.82
1	B	801	MET	CA-CB-CG	-5.61	102.88	114.10
1	A	809	VAL	CA-CB-CG1	5.60	119.93	110.40
1	A	729	VAL	CA-C-N	-5.60	113.39	120.56
1	A	729	VAL	C-N-CA	-5.60	113.39	120.56
1	B	782	LEU	CA-C-N	-5.59	116.25	123.19
1	B	782	LEU	C-N-CA	-5.59	116.25	123.19
1	A	798	CYS	CA-CB-SG	5.58	127.25	114.40
1	A	878	ASP	N-CA-CB	5.58	118.33	110.12
1	B	720	GLN	CG-CD-NE2	5.58	124.77	116.40
1	B	842	GLU	N-CA-CB	5.57	118.15	110.07
1	A	689	ASN	CB-CG-ND2	-5.57	108.05	116.40
1	A	741	ASN	N-CA-C	-5.57	105.84	113.30
1	B	891	CYS	CB-CA-C	5.56	119.69	110.90
1	A	695	GLU	O-C-N	5.56	127.71	121.32
1	A	732	TRP	CD1-NE1-CE2	5.55	118.89	108.90
1	B	728	SER	N-CA-C	5.55	118.04	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	818	PHE	N-CA-CB	5.54	118.25	109.82
1	B	824	LEU	CD1-CG-CD2	5.54	122.99	110.80
1	B	823	VAL	CA-C-O	-5.53	115.31	121.17
1	A	839	THR	CA-C-O	-5.53	112.61	120.51
1	B	860	GLN	N-CA-CB	5.52	119.82	110.49
1	A	714	LEU	CA-C-N	5.52	127.99	120.54
1	A	714	LEU	C-N-CA	5.52	127.99	120.54
1	A	716	THR	O-C-N	-5.52	116.27	122.12
1	A	889	LEU	CA-C-O	-5.52	114.70	120.55
1	B	711	SER	CA-C-O	5.51	126.36	120.24
1	B	702	GLY	O-C-N	-5.51	117.01	122.41
1	B	726	LEU	N-CA-C	-5.51	104.68	111.40
1	A	755	TRP	CB-CA-C	5.50	120.02	110.79
1	B	905	PHE	CB-CA-C	-5.49	101.47	109.38
1	A	897	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	B	892	LEU	N-CA-CB	5.49	118.19	110.12
1	B	794	PHE	CB-CA-C	5.49	121.34	110.42
1	A	924	MET	O-C-N	-5.48	113.39	121.89
1	B	928	LEU	CA-C-N	-5.48	115.16	122.72
1	B	928	LEU	C-N-CA	-5.48	115.16	122.72
1	B	896	ILE	CA-C-O	-5.48	113.93	120.78
1	B	854	LYS	O-C-N	-5.48	115.81	122.22
1	A	806	GLN	N-CA-CB	5.47	118.26	110.16
1	A	838	GLN	N-CA-CB	5.46	119.72	110.49
1	A	911	GLU	OE1-CD-OE2	-5.46	109.81	122.90
1	A	788	ARG	NH1-CZ-NH2	5.45	126.39	119.30
1	A	720	GLN	CA-CB-CG	5.45	124.99	114.10
1	A	760	VAL	CA-CB-CG2	-5.44	101.16	110.40
1	A	778	PHE	O-C-N	-5.44	115.36	122.59
1	B	891	CYS	O-C-N	5.44	127.96	122.09
1	A	836	ARG	CA-C-O	-5.44	115.10	120.70
1	A	815	GLN	N-CA-CB	-5.42	101.92	110.06
1	B	724	ARG	CG-CD-NE	5.42	123.93	112.00
1	A	763	LEU	O-C-N	-5.42	116.39	122.03
1	A	819	LEU	CB-CA-C	5.41	119.77	110.79
1	A	731	LYS	CB-CG-CD	5.41	123.73	111.30
1	A	797	LEU	CD1-CG-CD2	5.39	122.66	110.80
1	A	740	ARG	CD-NE-CZ	-5.38	116.86	124.40
1	A	753	TYR	CD1-CG-CD2	5.38	126.18	118.10
1	A	756	MET	CA-CB-CG	-5.38	103.33	114.10
1	B	820	CYS	CA-C-N	-5.38	112.19	121.66
1	B	820	CYS	C-N-CA	-5.38	112.19	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	852	LEU	CA-C-N	5.37	127.82	120.46
1	A	852	LEU	C-N-CA	5.37	127.82	120.46
1	A	879	ASN	CA-CB-CG	-5.37	107.23	112.60
1	B	886	GLN	CA-C-O	-5.37	115.37	120.90
1	A	760	VAL	CA-CB-CG1	5.36	119.52	110.40
1	B	782	LEU	N-CA-CB	5.36	121.19	111.11
1	A	785	ASN	CB-CG-OD1	5.36	131.51	120.80
1	A	846	SER	CB-CA-C	-5.35	102.24	110.81
1	A	791	GLU	N-CA-CB	5.35	119.53	110.49
1	A	848	TYR	N-CA-C	5.35	118.97	112.23
1	B	820	CYS	CA-C-O	-5.35	112.86	120.51
1	A	887	LEU	CB-CG-CD1	5.34	126.74	110.70
1	A	897	GLN	N-CA-C	5.34	118.63	112.97
1	A	800	THR	O-C-N	-5.34	116.06	122.15
1	B	697	ASP	CA-C-N	5.33	127.84	120.49
1	B	697	ASP	C-N-CA	5.33	127.84	120.49
1	B	751	ILE	CB-CA-C	5.33	118.74	111.87
1	B	821	MET	CA-CB-CG	5.33	124.76	114.10
1	A	697	ASP	O-C-N	-5.33	116.78	122.85
1	B	749	THR	CA-CB-OG1	-5.33	101.61	109.60
1	B	786	GLU	CA-CB-CG	-5.32	103.45	114.10
1	A	817	GLU	CA-C-N	5.32	128.80	120.82
1	A	817	GLU	C-N-CA	5.32	128.80	120.82
1	A	817	GLU	N-CA-C	-5.32	105.39	111.14
1	B	791	GLU	O-C-N	5.31	129.66	122.59
1	A	789	MET	N-CA-C	-5.31	106.67	112.72
1	A	847	SER	CA-CB-OG	5.31	121.72	111.10
1	B	830	ILE	CA-CB-CG1	5.30	119.42	110.40
1	B	792	SER	CA-C-N	5.30	131.67	121.54
1	B	792	SER	C-N-CA	5.30	131.67	121.54
1	B	914	ALA	CB-CA-C	-5.30	102.53	110.90
1	A	753	TYR	N-CA-C	5.29	119.36	113.01
1	B	913	ILE	CA-CB-CG2	5.29	119.50	110.50
1	B	747	GLN	CA-C-O	-5.28	114.13	120.10
1	A	686	PRO	N-CA-C	5.28	120.87	113.53
1	A	807	GLU	CA-C-N	5.27	129.60	120.58
1	A	807	GLU	C-N-CA	5.27	129.60	120.58
1	A	733	SER	N-CA-C	5.27	117.70	111.33
1	A	703	HIS	N-CA-CB	-5.27	101.84	110.43
1	A	908	MET	O-C-N	-5.26	116.41	122.09
1	A	760	VAL	CB-CA-C	5.26	118.91	112.02
1	A	713	SER	N-CA-C	5.26	117.09	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	770	HIS	ND1-CE1-NE2	-5.25	103.15	108.40
1	B	776	LEU	CB-CA-C	-5.25	102.01	110.77
1	A	748	ILE	CB-CA-C	-5.24	105.26	111.97
1	B	863	VAL	CA-C-O	5.24	127.32	120.78
1	B	705	ASN	CA-C-O	-5.23	113.03	120.51
1	A	737	PRO	N-CA-CB	-5.23	98.51	103.17
1	A	770	HIS	CE1-NE2-CD2	5.23	114.23	109.00
1	A	749	THR	CA-CB-OG1	-5.22	101.77	109.60
1	A	769	LYS	CB-CA-C	-5.22	102.65	110.90
1	B	813	VAL	CB-CA-C	-5.22	102.72	111.29
1	B	754	SER	O-C-N	5.22	128.46	122.25
1	B	769	LYS	CB-CG-CD	5.22	123.30	111.30
1	B	751	ILE	O-C-N	-5.21	116.36	121.94
1	B	917	LEU	O-C-N	-5.21	115.33	121.32
1	B	836	ARG	N-CA-CB	5.21	117.62	110.07
1	B	916	GLN	CA-C-O	-5.20	113.15	119.03
1	B	905	PHE	N-CA-CB	5.20	117.04	110.23
1	B	771	VAL	CA-CB-CG2	5.20	119.24	110.40
1	A	904	GLU	CG-CD-OE1	-5.20	106.44	118.40
1	A	906	PRO	N-CA-C	5.20	119.20	111.41
1	B	800	THR	CA-C-O	5.19	126.05	120.55
1	B	919	LYS	CA-C-O	-5.19	113.09	120.51
1	B	740	ARG	CA-CB-CG	-5.19	103.72	114.10
1	A	732	TRP	N-CA-C	-5.17	105.33	110.97
1	B	869	ARG	CA-C-O	-5.17	115.37	120.90
1	A	877	LEU	CB-CG-CD1	-5.15	95.24	110.70
1	A	753	TYR	O-C-N	-5.15	115.36	122.46
1	B	814	SER	CB-CA-C	5.15	118.31	109.51
1	B	818	PHE	O-C-N	5.15	127.59	122.08
1	A	732	TRP	NE1-CE2-CZ2	5.14	137.81	130.10
1	A	733	SER	CA-C-N	5.14	129.31	120.72
1	A	733	SER	C-N-CA	5.14	129.31	120.72
1	A	869	ARG	CA-CB-CG	5.14	124.38	114.10
1	A	707	LYS	CA-C-O	5.14	125.92	120.63
1	A	931	HIS	CA-CB-CG	-5.13	108.67	113.80
1	B	845	ARG	N-CA-CB	5.13	117.76	110.06
1	B	903	VAL	CA-CB-CG2	5.13	119.12	110.40
1	B	869	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	B	761	PHE	N-CA-C	5.12	121.71	110.80
1	B	876	LEU	N-CA-C	5.12	117.25	111.11
1	B	789	MET	CA-C-N	5.11	131.30	121.54
1	B	789	MET	C-N-CA	5.11	131.30	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	908	MET	N-CA-CB	5.11	117.48	110.07
1	B	911	GLU	N-CA-CB	5.10	117.38	109.98
1	B	894	THR	N-CA-C	-5.10	105.80	112.23
1	A	793	SER	CA-CB-OG	-5.10	100.90	111.10
1	B	722	GLY	N-CA-C	5.10	118.81	112.64
1	A	693	SER	N-CA-CB	5.09	118.07	110.22
1	A	847	SER	CA-C-O	-5.09	114.11	119.97
1	B	790	LYS	CG-CD-CE	5.09	123.02	111.30
1	A	802	TRP	CA-C-O	5.09	125.62	119.61
1	A	925	VAL	CB-CA-C	-5.09	101.32	110.48
1	B	772	SER	N-CA-CB	-5.09	106.51	114.45
1	A	711	SER	CA-C-N	5.08	127.51	120.29
1	A	711	SER	C-N-CA	5.08	127.51	120.29
1	B	819	LEU	CB-CG-CD2	5.08	125.95	110.70
1	A	778	PHE	CB-CG-CD2	-5.07	112.08	120.70
1	B	723	GLU	CB-CA-C	5.07	118.92	110.81
1	B	819	LEU	CA-C-O	-5.06	113.27	120.51
1	B	806	GLN	N-CA-C	-5.06	105.85	112.23
1	B	753	TYR	CG-CD2-CE2	5.06	128.79	121.20
1	A	723	GLU	CA-CB-CG	5.06	124.22	114.10
1	B	799	LEU	CB-CA-C	5.06	119.19	110.79
1	A	845	ARG	NH1-CZ-NH2	-5.06	112.73	119.30
1	A	854	LYS	CA-C-O	5.05	126.31	120.90
1	B	904	GLU	O-C-N	5.05	128.94	123.13
1	B	923	GLY	CA-C-O	5.05	126.10	119.69
1	B	828	ASN	CA-CB-CG	-5.04	107.56	112.60
1	A	695	GLU	CA-C-N	5.04	125.03	119.89
1	A	695	GLU	C-N-CA	5.04	125.03	119.89
1	A	764	GLY	CA-C-O	5.04	129.34	120.57
1	B	849	ILE	CB-CA-C	5.03	118.41	111.97
1	A	712	SER	N-CA-C	5.03	116.84	111.36
1	B	907	GLU	CG-CD-OE2	-5.03	106.84	118.40
1	A	782	LEU	CD1-CG-CD2	5.02	121.85	110.80
1	B	814	SER	CA-CB-OG	5.02	121.14	111.10
1	B	833	GLU	CB-CA-C	-5.02	100.98	110.01
1	B	751	ILE	CA-CB-CG1	-5.01	101.88	110.40
1	A	780	PRO	O-C-N	-5.01	116.77	122.18
1	A	698	VAL	CA-C-O	-5.00	115.88	121.23

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	687	LEU	Mainchain
1	A	792	SER	Peptide
1	A	861	LYS	Peptide
1	A	929	LEU	Peptide
1	B	739	PHE	Mainchain
1	B	861	LYS	Peptide
1	B	915	ALA	Mainchain

5.2 Too-close contacts [i](#)

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	2010	0	2054	139	0
1	B	2017	0	2078	173	0
2	A	21	0	24	6	0
2	B	21	0	24	1	0
3	A	1	0	0	0	0
All	All	4070	0	4180	309	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 37.

All (309) 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:727:LEU:HG	1:B:908:MET:HE1	1.31	1.09
1:A:720:GLN:HE21	1:A:724:ARG:NE	1.56	1.03
1:B:784:LEU:HD22	1:B:788:ARG:HD3	1.40	1.01
1:B:721:LEU:HD11	1:B:725:GLN:HE21	1.22	0.98
1:A:825:LEU:HD23	1:A:828:ASN:HD22	1.23	0.98
1:A:720:GLN:HE21	1:A:724:ARG:HE	1.06	0.96
1:A:692:MET:HE3	1:A:692:MET:HA	1.52	0.90
1:A:752:GLN:HG2	1:A:912:VAL:HG12	1.51	0.90
1:B:800:THR:HA	1:B:803:GLN:NE2	1.93	0.83
1:B:692:MET:SD	1:B:815:GLN:NE2	2.51	0.83
1:B:690:LEU:HD23	1:B:737:PRO:HG3	1.62	0.82
1:A:720:GLN:NE2	1:A:724:ARG:HE	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:LEU:HD22	1:B:788:ARG:CD	2.09	0.81
1:A:726:LEU:O	1:A:730:VAL:HG23	1.81	0.80
1:B:855:ALA:HA	1:B:858:LEU:HD12	1.63	0.78
1:B:830:ILE:HG22	1:B:831:PRO:HD3	1.66	0.77
1:B:753:TYR:HE1	1:B:916:GLN:NE2	1.83	0.77
1:B:844:MET:HE3	1:B:848:TYR:HE2	1.52	0.75
1:A:868:GLN:O	1:A:872:GLN:HG3	1.86	0.74
1:B:685:PRO:HG2	1:B:688:ILE:HD12	1.67	0.74
1:A:701:ALA:HB2	1:A:721:LEU:HD13	1.68	0.74
1:B:790:LYS:HG3	1:B:791:GLU:HG3	1.69	0.74
1:A:771:VAL:HG21	1:A:775:MET:HB2	1.69	0.74
1:B:721:LEU:HD11	1:B:725:GLN:NE2	2.01	0.73
1:B:814:SER:HB2	1:B:859:ARG:NH1	2.03	0.73
1:A:811:LEU:O	1:A:869:ARG:NH1	2.20	0.73
1:B:690:LEU:CD2	1:B:737:PRO:HG3	2.18	0.73
1:A:825:LEU:HD23	1:A:828:ASN:ND2	2.02	0.73
1:B:917:LEU:N	1:B:918:PRO:HD2	2.04	0.73
1:A:718:LEU:O	2:A:1000:R18:H11	1.88	0.73
1:A:720:GLN:HG3	1:A:724:ARG:HE	1.53	0.73
1:A:892:LEU:HD21	1:B:892:LEU:HD11	1.69	0.72
1:B:744:ILE:O	1:B:748:ILE:HD12	1.90	0.72
1:B:797:LEU:HD23	1:B:801:MET:HE2	1.71	0.72
1:B:814:SER:HB2	1:B:859:ARG:HH11	1.53	0.72
1:A:792:SER:O	1:A:794:PHE:HB3	1.90	0.72
1:A:685:PRO:HG2	1:A:688:ILE:HD12	1.72	0.71
1:A:752:GLN:CG	1:A:912:VAL:HG12	2.20	0.71
1:B:733:SER:HB2	1:B:739:PHE:CD2	2.25	0.71
1:A:720:GLN:O	1:A:724:ARG:HD2	1.91	0.70
1:B:714:LEU:HD23	1:B:794:PHE:CE2	2.27	0.70
1:A:806:GLN:OE1	1:A:806:GLN:HA	1.91	0.69
1:A:913:ILE:HA	1:A:917:LEU:HG	1.74	0.69
1:B:855:ALA:O	1:B:858:LEU:HB2	1.93	0.69
1:B:917:LEU:N	1:B:918:PRO:CD	2.56	0.68
1:B:684:ILE:CG2	1:B:688:ILE:HB	2.22	0.68
1:B:925:VAL:O	1:B:927:PRO:HD3	1.91	0.68
1:A:837:SER:HB3	1:A:840:GLN:OE1	1.93	0.68
1:B:855:ALA:HA	1:B:858:LEU:CD1	2.23	0.68
1:B:757:SER:OG	1:B:825:LEU:HD13	1.93	0.68
1:B:864:VAL:O	1:B:868:GLN:HG3	1.94	0.68
1:A:790:LYS:O	1:A:791:GLU:C	2.37	0.67
1:A:760:VAL:HG21	1:A:887:LEU:HD11	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:LYS:CB	1:A:708:PRO:HD2	2.24	0.67
1:A:789:MET:HG2	1:A:798:CYS:SG	2.36	0.66
1:A:851:GLU:OE1	1:A:851:GLU:HA	1.94	0.66
1:B:821:MET:HB3	1:B:877:LEU:HD11	1.75	0.66
1:B:876:LEU:O	1:B:876:LEU:HD23	1.95	0.66
1:B:727:LEU:CG	1:B:908:MET:HE1	2.19	0.66
1:A:830:ILE:HB	1:A:831:PRO:HD2	1.77	0.66
1:A:893:ASN:OD1	1:B:918:PRO:HG2	1.95	0.66
1:B:685:PRO:HB2	1:B:688:ILE:HG13	1.79	0.65
1:B:883:LEU:O	1:B:886:GLN:HB2	1.97	0.65
1:A:765:TRP:HB2	1:A:818:PHE:CE1	2.32	0.65
1:B:880:LEU:O	1:B:884:VAL:HG23	1.96	0.65
1:B:759:MET:HG2	2:B:1000:R18:H21	1.79	0.63
1:B:889:LEU:H	1:B:921:LEU:HD21	1.63	0.63
1:A:826:LEU:O	1:A:826:LEU:HD12	1.98	0.63
1:A:896:ILE:HD11	1:B:892:LEU:CD1	2.28	0.63
1:A:901:LEU:O	1:A:902:SER:HB2	1.97	0.63
1:B:870:PHE:O	1:B:874:THR:HG23	1.98	0.63
1:B:725:GLN:O	1:B:729:VAL:HG23	1.99	0.63
1:B:787:GLN:CD	1:B:790:LYS:HE2	2.24	0.63
1:B:897:GLN:O	1:B:901:LEU:HG	1.99	0.62
1:B:830:ILE:CG2	1:B:831:PRO:HD3	2.29	0.62
1:A:691:LEU:O	1:A:692:MET:C	2.43	0.62
1:B:767:SER:OG	1:B:777:TYR:N	2.29	0.62
1:A:892:LEU:HD23	1:B:918:PRO:HB3	1.81	0.62
1:A:698:VAL:HG21	1:A:780:PRO:HG3	1.82	0.61
1:B:838:GLN:HA	1:B:838:GLN:NE2	2.16	0.61
1:A:860:GLN:HE21	1:A:860:GLN:HA	1.65	0.61
1:A:917:LEU:N	1:A:918:PRO:CD	2.63	0.61
1:B:854:LYS:O	1:B:858:LEU:HG	2.00	0.60
1:A:755:TRP:CD1	1:A:755:TRP:H	2.18	0.60
1:A:847:SER:HB2	1:A:850:ARG:NH2	2.16	0.60
1:A:746:ASP:OD2	1:A:835:LEU:HB3	2.02	0.60
1:A:768:TYR:HD1	1:A:809:VAL:HG23	1.66	0.60
1:B:746:ASP:CG	1:B:835:LEU:HD22	2.26	0.60
1:B:845:ARG:O	1:B:849:ILE:HG13	2.01	0.60
1:B:837:SER:O	1:B:840:GLN:HB2	2.01	0.60
1:B:849:ILE:O	1:B:852:LEU:HB3	2.02	0.60
1:B:733:SER:HB2	1:B:739:PHE:HD2	1.67	0.59
1:B:763:LEU:O	1:B:764:GLY:C	2.45	0.59
1:B:821:MET:HE3	1:B:873:LEU:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:714:LEU:HD23	1:B:794:PHE:CZ	2.37	0.59
1:B:830:ILE:HG21	1:B:835:LEU:CD1	2.33	0.59
1:B:787:GLN:O	1:B:790:LYS:HG2	2.02	0.59
1:B:797:LEU:HD23	1:B:801:MET:CE	2.31	0.59
1:A:743:HIS:ND1	1:A:836:ARG:HD3	2.17	0.58
1:B:746:ASP:CB	1:B:835:LEU:HD22	2.33	0.58
1:B:875:LYS:HD3	1:B:931:HIS:HD2	1.67	0.58
1:B:889:LEU:N	1:B:921:LEU:HD21	2.19	0.58
1:A:860:GLN:CG	1:A:869:ARG:HG2	2.34	0.58
1:A:852:LEU:O	1:A:856:ILE:HG13	2.04	0.58
1:B:868:GLN:O	1:B:872:GLN:HG3	2.03	0.58
1:B:753:TYR:HE1	1:B:916:GLN:HE21	1.49	0.58
1:B:826:LEU:O	1:B:826:LEU:HG	2.04	0.58
1:A:755:TRP:HE3	1:A:759:MET:HE3	1.69	0.57
1:B:844:MET:HE3	1:B:848:TYR:CE2	2.38	0.57
1:B:692:MET:SD	1:B:815:GLN:CD	2.88	0.57
1:B:765:TRP:HB2	1:B:818:PHE:CE1	2.40	0.57
1:B:837:SER:O	1:B:838:GLN:C	2.47	0.57
1:A:684:ILE:HB	1:A:689:ASN:HD21	1.68	0.57
1:B:804:ILE:HB	1:B:805:PRO:HD3	1.87	0.57
1:A:755:TRP:CH2	1:A:909:MET:HE2	2.39	0.56
1:B:892:LEU:HD12	1:B:896:ILE:HD11	1.86	0.56
1:B:917:LEU:H	1:B:918:PRO:HD2	1.68	0.56
1:B:750:LEU:HD21	1:B:830:ILE:HG23	1.87	0.56
1:B:852:LEU:O	1:B:856:ILE:HG13	2.06	0.56
1:B:684:ILE:HG22	1:B:688:ILE:HB	1.87	0.56
1:B:691:LEU:HD23	1:B:694:ILE:HD11	1.87	0.56
1:B:830:ILE:CB	1:B:831:PRO:CD	2.84	0.56
1:A:763:LEU:O	1:A:764:GLY:C	2.48	0.55
1:B:830:ILE:HG21	1:B:835:LEU:HD11	1.87	0.55
1:B:830:ILE:HB	1:B:831:PRO:CD	2.37	0.55
1:B:721:LEU:CD1	1:B:725:GLN:HE21	2.08	0.55
1:B:787:GLN:OE1	1:B:790:LYS:HE2	2.07	0.55
1:A:704:ASP:O	1:A:706:THR:N	2.40	0.55
1:A:860:GLN:HG3	1:A:869:ARG:HG2	1.88	0.55
1:B:779:ALA:HB1	1:B:780:PRO:CD	2.37	0.55
1:A:752:GLN:HG2	1:A:912:VAL:CG1	2.32	0.55
1:A:707:LYS:CB	1:A:708:PRO:CD	2.86	0.54
1:B:703:HIS:HD2	1:B:717:SER:OG	1.90	0.54
1:B:767:SER:HG	1:B:777:TYR:N	2.04	0.54
1:B:835:LEU:HB2	1:B:838:GLN:NE2	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:GLU:OE1	1:A:873:LEU:HD11	2.08	0.54
1:B:892:LEU:HD23	1:B:921:LEU:HD12	1.89	0.54
1:B:841:PHE:CZ	1:B:845:ARG:HG3	2.43	0.54
1:B:830:ILE:HD11	1:B:928:LEU:HD11	1.88	0.54
1:B:700:TYR:CE2	1:B:780:PRO:HG2	2.43	0.54
1:A:723:GLU:CD	1:A:908:MET:HB2	2.34	0.53
1:B:742:LEU:O	1:B:747:GLN:NE2	2.31	0.53
1:A:869:ARG:O	1:A:872:GLN:HB2	2.08	0.53
1:A:917:LEU:HB2	1:A:918:PRO:HD3	1.89	0.53
1:A:701:ALA:CB	1:A:721:LEU:HD13	2.39	0.52
1:B:776:LEU:HD12	1:B:789:MET:HE2	1.90	0.52
1:A:897:GLN:HB2	1:A:901:LEU:HD12	1.91	0.52
1:B:755:TRP:CZ3	1:B:909:MET:HE3	2.45	0.52
1:B:763:LEU:HD22	1:B:778:PHE:CE1	2.45	0.52
1:A:909:MET:HE1	2:A:1000:R18:H181	1.92	0.52
1:A:740:ARG:HG3	1:A:741:ASN:ND2	2.25	0.51
1:A:757:SER:HB2	1:A:884:VAL:HG21	1.92	0.51
1:A:690:LEU:HD13	1:A:737:PRO:HG2	1.92	0.51
1:A:800:THR:HG21	1:A:886:GLN:OE1	2.10	0.51
1:B:888:HIS:HB3	1:B:921:LEU:HD21	1.92	0.51
1:A:751:ILE:O	1:A:752:GLN:C	2.54	0.51
1:A:795:TYR:CZ	1:A:799:LEU:HD21	2.45	0.51
1:B:892:LEU:HD23	1:B:921:LEU:CD1	2.40	0.51
1:B:815:GLN:O	1:B:815:GLN:HG3	2.08	0.51
1:B:837:SER:HB3	1:B:840:GLN:HB2	1.92	0.51
1:B:766:ARG:HD2	1:B:777:TYR:CD1	2.46	0.50
1:B:830:ILE:CB	1:B:831:PRO:HD3	2.41	0.50
1:B:736:LEU:HD12	1:B:737:PRO:HD2	1.93	0.50
1:B:892:LEU:CD2	1:B:921:LEU:HD12	2.42	0.50
1:B:742:LEU:HB2	1:B:747:GLN:HG3	1.92	0.50
1:B:814:SER:OG	1:B:817:GLU:HG3	2.11	0.50
1:B:719:ASN:HD22	1:B:905:PHE:HA	1.76	0.50
1:A:705:ASN:O	1:A:706:THR:C	2.53	0.50
1:A:838:GLN:O	1:A:841:PHE:HB3	2.12	0.50
1:A:717:SER:O	1:A:718:LEU:C	2.54	0.50
1:B:795:TYR:OH	1:B:799:LEU:HD21	2.12	0.50
1:A:740:ARG:HG3	1:A:741:ASN:HD22	1.77	0.50
1:B:766:ARG:HD2	1:B:777:TYR:HD1	1.76	0.49
1:A:917:LEU:N	1:A:918:PRO:HD2	2.27	0.49
1:B:755:TRP:O	1:B:756:MET:C	2.56	0.49
1:A:746:ASP:OD2	1:A:836:ARG:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:830:ILE:HG21	1:B:835:LEU:HG	1.93	0.49
1:A:720:GLN:HG3	1:A:724:ARG:NE	2.26	0.49
1:B:830:ILE:CD1	1:B:928:LEU:HD11	2.43	0.49
1:B:683:LEU:O	1:B:684:ILE:HG12	2.13	0.49
1:B:719:ASN:O	1:B:722:GLY:N	2.45	0.49
1:A:752:GLN:O	1:A:755:TRP:HD1	1.94	0.49
1:B:830:ILE:HG21	1:B:835:LEU:CG	2.43	0.48
1:A:868:GLN:O	1:A:871:TYR:HB3	2.13	0.48
1:A:827:LEU:HD11	1:A:844:MET:HE2	1.95	0.48
1:B:685:PRO:HG2	1:B:688:ILE:CD1	2.39	0.48
1:A:804:ILE:HD11	1:A:880:LEU:HD22	1.96	0.48
1:B:841:PHE:CD1	1:B:841:PHE:C	2.91	0.48
1:B:719:ASN:O	1:B:720:GLN:C	2.56	0.48
1:A:895:PHE:O	1:A:898:SER:HB3	2.14	0.47
1:B:716:THR:OG1	1:B:903:VAL:HG13	2.14	0.47
1:A:837:SER:O	1:A:838:GLN:C	2.57	0.47
1:A:721:LEU:HD23	2:A:1000:R18:H11A	1.96	0.47
1:B:790:LYS:CG	1:B:791:GLU:N	2.77	0.47
1:A:781:ASP:OD1	1:A:781:ASP:N	2.45	0.47
1:A:897:GLN:HB2	1:A:901:LEU:CD1	2.44	0.47
1:B:776:LEU:CD1	1:B:789:MET:HE2	2.45	0.47
1:A:700:TYR:CD1	1:A:700:TYR:N	2.83	0.47
1:A:786:GLU:OE2	1:A:802:TRP:CH2	2.67	0.47
1:A:804:ILE:HG12	1:A:880:LEU:CD2	2.44	0.47
1:B:706:THR:O	1:B:707:LYS:C	2.58	0.47
1:B:835:LEU:HB2	1:B:838:GLN:HE21	1.80	0.47
1:B:800:THR:HA	1:B:803:GLN:HE21	1.76	0.47
1:B:767:SER:HG	1:B:777:TYR:H	1.52	0.47
1:B:880:LEU:HD23	1:B:883:LEU:HD13	1.96	0.47
2:A:1000:R18:H182	2:A:1000:R18:H8	1.69	0.46
1:B:691:LEU:O	1:B:692:MET:C	2.56	0.46
1:B:855:ALA:CA	1:B:858:LEU:HD12	2.40	0.46
1:B:743:HIS:ND1	1:B:745:ASP:HB2	2.30	0.46
1:A:804:ILE:HD13	1:A:804:ILE:HG21	1.76	0.46
1:A:886:GLN:O	1:A:887:LEU:C	2.57	0.46
1:B:850:ARG:O	1:B:854:LYS:HG3	2.16	0.46
1:A:692:MET:HA	1:A:692:MET:CE	2.35	0.46
1:A:746:ASP:O	1:A:750:LEU:HG	2.15	0.46
1:A:778:PHE:HZ	1:A:801:MET:HE1	1.80	0.46
1:A:901:LEU:O	1:A:902:SER:CB	2.61	0.46
1:B:892:LEU:CD1	1:B:896:ILE:HD11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:746:ASP:HB3	1:B:835:LEU:HD22	1.95	0.45
1:B:798:CYS:HA	1:B:801:MET:HE3	1.97	0.45
1:B:690:LEU:HD23	1:B:737:PRO:CG	2.40	0.45
1:A:743:HIS:O	1:A:744:ILE:C	2.59	0.45
1:B:795:TYR:CE2	1:B:799:LEU:HD11	2.52	0.45
1:B:687:LEU:O	1:B:688:ILE:C	2.57	0.45
1:B:780:PRO:HD2	1:B:781:ASP:H	1.82	0.45
1:B:917:LEU:H	1:B:918:PRO:CD	2.24	0.45
1:A:860:GLN:HE21	1:A:860:GLN:CA	2.28	0.45
1:B:739:PHE:CZ	1:B:747:GLN:HA	2.52	0.45
1:A:708:PRO:O	1:A:709:ASP:C	2.59	0.45
1:A:752:GLN:HE21	1:A:912:VAL:HG12	1.82	0.45
1:B:703:HIS:CG	1:B:704:ASP:N	2.85	0.45
1:B:837:SER:OG	1:B:840:GLN:NE2	2.49	0.45
1:A:687:LEU:HD12	1:A:687:LEU:HA	1.76	0.45
1:B:779:ALA:HB1	1:B:780:PRO:HD3	1.99	0.45
1:A:765:TRP:CB	1:A:818:PHE:CE1	2.99	0.45
1:A:919:LYS:HD2	1:A:924:MET:O	2.16	0.45
1:B:859:ARG:O	1:B:861:LYS:N	2.47	0.45
1:B:746:ASP:OD1	1:B:835:LEU:HD22	2.16	0.44
1:B:788:ARG:O	1:B:792:SER:HB3	2.17	0.44
1:A:790:LYS:O	1:A:792:SER:N	2.51	0.44
1:A:755:TRP:O	1:A:756:MET:C	2.56	0.44
1:A:755:TRP:CD1	1:A:755:TRP:N	2.85	0.44
1:A:897:GLN:O	1:A:901:LEU:HG	2.17	0.44
1:B:739:PHE:CE2	1:B:747:GLN:HB3	2.53	0.44
1:B:817:GLU:OE2	1:B:856:ILE:HA	2.17	0.44
1:B:828:ASN:HD22	1:B:828:ASN:HA	1.34	0.44
1:A:709:ASP:CG	1:A:788:ARG:HH21	2.26	0.44
1:A:860:GLN:HG2	1:A:869:ARG:HG2	1.99	0.44
1:B:827:LEU:HD11	1:B:844:MET:HG2	2.00	0.44
1:A:690:LEU:HD23	1:A:694:ILE:HG12	1.99	0.43
1:A:723:GLU:OE1	1:A:909:MET:HB2	2.17	0.43
1:A:743:HIS:O	1:A:746:ASP:HB2	2.18	0.43
1:B:844:MET:CE	1:B:848:TYR:HE2	2.28	0.43
1:B:723:GLU:OE2	1:B:908:MET:HB2	2.17	0.43
1:B:850:ARG:HA	1:B:853:ILE:HD12	2.00	0.43
1:A:778:PHE:HZ	1:A:801:MET:CE	2.30	0.43
1:A:905:PHE:N	1:A:905:PHE:CD1	2.86	0.43
1:B:720:GLN:HG2	1:B:724:ARG:HH21	1.82	0.43
1:A:889:LEU:O	1:A:889:LEU:HD12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:752:GLN:O	1:B:755:TRP:CD1	2.71	0.43
1:B:860:GLN:HB3	1:B:865:SER:OG	2.19	0.43
1:A:720:GLN:CG	1:A:724:ARG:HE	2.25	0.43
1:A:755:TRP:HH2	1:A:909:MET:HE2	1.82	0.43
1:B:760:VAL:HG21	1:B:887:LEU:HD11	2.00	0.43
1:B:794:PHE:O	1:B:795:TYR:C	2.62	0.43
1:B:913:ILE:HG12	1:B:917:LEU:HD22	2.01	0.43
1:A:743:HIS:CG	1:A:836:ARG:HD3	2.54	0.42
1:B:719:ASN:ND2	1:B:905:PHE:HA	2.34	0.42
1:B:848:TYR:O	1:B:849:ILE:C	2.56	0.42
1:A:736:LEU:HA	1:A:737:PRO:HD3	1.78	0.42
1:A:888:HIS:HB3	1:A:921:LEU:HD21	2.00	0.42
1:A:888:HIS:C	1:A:921:LEU:HD11	2.44	0.42
1:B:871:TYR:CD1	1:B:931:HIS:NE2	2.87	0.42
1:A:870:PHE:O	1:A:871:TYR:C	2.63	0.42
1:B:771:VAL:HB	1:B:775:MET:HE3	2.02	0.42
1:B:838:GLN:O	1:B:839:THR:C	2.62	0.42
1:A:743:HIS:CE1	1:A:836:ARG:HD3	2.55	0.42
1:B:747:GLN:O	1:B:751:ILE:HD12	2.19	0.42
1:B:917:LEU:HD12	1:B:917:LEU:HA	1.69	0.41
1:A:817:GLU:CD	1:A:873:LEU:HD11	2.45	0.41
1:A:714:LEU:HD12	1:A:714:LEU:HA	1.80	0.41
1:A:799:LEU:O	1:A:802:TRP:CB	2.68	0.41
1:B:800:THR:O	1:B:803:GLN:HB2	2.20	0.41
1:A:744:ILE:HD13	1:A:744:ILE:HA	1.69	0.41
1:B:743:HIS:NE2	1:B:836:ARG:NH1	2.68	0.41
1:A:688:ILE:HG21	1:A:816:GLU:HG3	2.03	0.41
1:A:721:LEU:HD23	2:A:1000:R18:C1	2.51	0.41
1:A:703:HIS:HD2	1:A:717:SER:OG	2.03	0.41
1:A:871:TYR:C	1:A:871:TYR:CD1	2.98	0.41
1:A:701:ALA:CA	1:A:721:LEU:HD13	2.50	0.41
1:B:777:TYR:OH	1:B:780:PRO:HA	2.20	0.41
1:A:761:PHE:CD2	1:A:822:LYS:HB2	2.55	0.41
1:A:891:CYS:HB2	2:A:1000:R18:H161	2.01	0.41
1:B:750:LEU:HD21	1:B:830:ILE:CG2	2.50	0.41
1:B:752:GLN:O	1:B:755:TRP:HD1	2.03	0.41
1:B:811:LEU:HD23	1:B:811:LEU:HA	1.89	0.41
1:B:869:ARG:HA	1:B:872:GLN:OE1	2.21	0.41
1:A:762:GLY:HA2	1:A:765:TRP:HB3	2.03	0.41
1:B:723:GLU:HB2	1:B:906:PRO:HG2	2.03	0.40
1:A:899:ARG:HD2	1:A:899:ARG:HA	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:GLU:HA	1:B:696:PRO:HD3	1.90	0.40
1:A:748:ILE:HG22	1:A:752:GLN:OE1	2.21	0.40
1:A:690:LEU:O	1:A:691:LEU:C	2.63	0.40
1:A:698:VAL:HG22	1:A:700:TYR:CE1	2.56	0.40
1:A:700:TYR:HD1	1:A:700:TYR:H	1.69	0.40
1:A:750:LEU:HG	1:A:750:LEU:H	1.76	0.40
1:A:752:GLN:O	1:A:755:TRP:CD1	2.73	0.40
1:A:785:ASN:O	1:A:789:MET:HE3	2.20	0.40
1:A:880:LEU:O	1:A:881:HIS:C	2.65	0.40
1:B:789:MET:O	1:B:791:GLU:N	2.54	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	249/258 (96%)	205 (82%)	30 (12%)	14 (6%)	1	4
1	B	247/258 (96%)	197 (80%)	37 (15%)	13 (5%)	1	5
All	All	496/516 (96%)	402 (81%)	67 (14%)	27 (5%)	1	4

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	706	THR
1	A	787	GLN
1	A	788	ARG
1	A	793	SER
1	B	787	GLN
1	B	789	MET
1	B	790	LYS
1	B	907	GLU

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Mol	Chain	Res	Type
1	A	792	SER
1	A	895	PHE
1	B	788	ARG
1	A	705	ASN
1	B	793	SER
1	A	857	GLY
1	A	896	ILE
1	B	705	ASN
1	B	860	GLN
1	A	764	GLY
1	B	684	ILE
1	B	720	GLN
1	A	863	VAL
1	A	881	HIS
1	B	863	VAL
1	B	882	ASP
1	A	744	ILE
1	B	918	PRO
1	A	918	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	227/240 (95%)	165 (73%)	62 (27%)	0	1
1	B	232/240 (97%)	185 (80%)	47 (20%)	1	4
All	All	459/480 (96%)	350 (76%)	109 (24%)	1	3

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	683	LEU
1	A	690	LEU
1	A	694	ILE
1	A	698	VAL

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Mol	Chain	Res	Type
1	A	700	TYR
1	A	710	THR
1	A	713	SER
1	A	714	LEU
1	A	715	LEU
1	A	717	SER
1	A	728	SER
1	A	730	VAL
1	A	731	LYS
1	A	733	SER
1	A	734	LYS
1	A	736	LEU
1	A	737	PRO
1	A	741	ASN
1	A	742	LEU
1	A	744	ILE
1	A	749	THR
1	A	750	LEU
1	A	759	MET
1	A	760	VAL
1	A	763	LEU
1	A	770	HIS
1	A	771	VAL
1	A	774	GLN
1	A	786	GLU
1	A	787	GLN
1	A	789	MET
1	A	799	LEU
1	A	802	TRP
1	A	809	VAL
1	A	810	LYS
1	A	821	MET
1	A	822	LYS
1	A	833	GLU
1	A	837	SER
1	A	840	GLN
1	A	844	MET
1	A	846	SER
1	A	847	SER
1	A	851	GLU
1	A	854	LYS
1	A	860	GLN

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Mol	Chain	Res	Type
1	A	863	VAL
1	A	864	VAL
1	A	867	SER
1	A	869	ARG
1	A	880	LEU
1	A	883	LEU
1	A	897	GLN
1	A	898	SER
1	A	902	SER
1	A	904	GLU
1	A	905	PHE
1	A	909	MET
1	A	917	LEU
1	A	924	MET
1	A	926	LYS
1	A	932	LYS
1	B	686	PRO
1	B	697	ASP
1	B	698	VAL
1	B	707	LYS
1	B	713	SER
1	B	726	LEU
1	B	728	SER
1	B	731	LYS
1	B	734	LYS
1	B	744	ILE
1	B	750	LEU
1	B	757	SER
1	B	759	MET
1	B	760	VAL
1	B	766	ARG
1	B	769	LYS
1	B	772	SER
1	B	784	LEU
1	B	787	GLN
1	B	788	ARG
1	B	790	LYS
1	B	804	ILE
1	B	813	VAL
1	B	821	MET
1	B	828	ASN
1	B	830	ILE

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Mol	Chain	Res	Type
1	B	832	LEU
1	B	833	GLU
1	B	839	THR
1	B	840	GLN
1	B	845	ARG
1	B	864	VAL
1	B	880	LEU
1	B	883	LEU
1	B	887	LEU
1	B	889	LEU
1	B	892	LEU
1	B	893	ASN
1	B	897	GLN
1	B	899	ARG
1	B	901	LEU
1	B	908	MET
1	B	909	MET
1	B	910	SER
1	B	911	GLU
1	B	912	VAL
1	B	919	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	689	ASN
1	A	703	HIS
1	A	720	GLN
1	A	741	ASN
1	A	747	GLN
1	A	752	GLN
1	A	828	ASN
1	A	838	GLN
1	A	860	GLN
1	A	888	HIS
1	B	703	HIS
1	B	725	GLN
1	B	752	GLN
1	B	803	GLN
1	B	812	GLN
1	B	815	GLN
1	B	828	ASN

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Mol	Chain	Res	Type
1	B	838	GLN
1	B	840	GLN
1	B	888	HIS
1	B	893	ASN
1	B	916	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	R18	B	1000	-	23,24,24	1.37	3 (13%)	30,39,39	3.04	17 (56%)
2	R18	A	1000	-	23,24,24	1.82	5 (21%)	30,39,39	3.13	17 (56%)

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	R18	B	1000	-	-	-	0/4/4/4
2	R18	A	1000	-	-	-	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	R18	C11-C9	4.66	1.55	1.45
2	A	1000	R18	C17-C13	3.71	1.64	1.55
2	A	1000	R18	C27-C17	3.44	1.57	1.52
2	B	1000	R18	C27-C17	3.39	1.57	1.52
2	B	1000	R18	O83-C3	-2.73	1.18	1.23
2	A	1000	R18	C18-C13	2.25	1.57	1.53
2	B	1000	R18	C10-C9	-2.24	1.34	1.36
2	A	1000	R18	O97-C17	-2.13	1.41	1.44

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	R18	C11-C9-C10	9.18	129.32	122.46
2	A	1000	R18	C8-C9-C10	-7.10	114.94	120.83
2	B	1000	R18	C14-C8-C9	-5.36	100.84	108.59
2	B	1000	R18	O97-C17-C16	5.31	122.28	109.51
2	B	1000	R18	O83-C3-C4	-5.15	112.38	121.65
2	B	1000	R18	O97-C17-C27	-4.95	97.71	107.72
2	A	1000	R18	C7-C6-C5	-4.79	101.20	111.28
2	A	1000	R18	C6-C7-C8	-4.40	102.66	111.45
2	B	1000	R18	C27-C17-C13	4.31	120.55	112.66
2	B	1000	R18	C7-C6-C5	-4.25	102.34	111.28
2	A	1000	R18	C27-C17-C16	4.07	118.56	112.13
2	B	1000	R18	O83-C3-C2	4.04	129.62	121.59
2	B	1000	R18	C8-C9-C10	-3.67	117.79	120.83
2	B	1000	R18	O97-C17-C13	-3.58	102.92	111.13
2	A	1000	R18	O97-C17-C13	3.42	118.98	111.13
2	B	1000	R18	C8-C9-C11	3.36	119.95	116.49
2	B	1000	R18	C13-C12-C11	-3.26	115.93	122.57
2	B	1000	R18	C1-C2-C3	-3.25	107.14	113.26
2	A	1000	R18	C4-C5-C10	-3.11	118.71	121.83
2	B	1000	R18	C15-C16-C17	-3.07	104.16	107.19
2	B	1000	R18	C7-C8-C14	-3.05	106.80	111.66
2	A	1000	R18	C12-C11-C9	-2.96	117.37	123.87
2	B	1000	R18	C5-C10-C9	2.95	123.45	121.50
2	A	1000	R18	C5-C10-C9	2.81	123.35	121.50
2	A	1000	R18	C2-C3-C4	-2.70	112.64	116.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	R18	C4-C5-C10	-2.69	119.13	121.83
2	A	1000	R18	C27-C17-C13	-2.67	107.78	112.66
2	A	1000	R18	C2-C1-C10	-2.59	107.15	112.70
2	B	1000	R18	C14-C13-C12	2.48	109.78	108.14
2	A	1000	R18	C1-C2-C3	-2.33	108.87	113.26
2	A	1000	R18	C7-C8-C14	-2.28	108.03	111.66
2	A	1000	R18	O97-C17-C27	-2.14	103.38	107.72
2	A	1000	R18	O83-C3-C2	2.12	125.81	121.59
2	A	1000	R18	C3-C4-C5	-2.10	121.11	122.92

There are no chirality outliers.

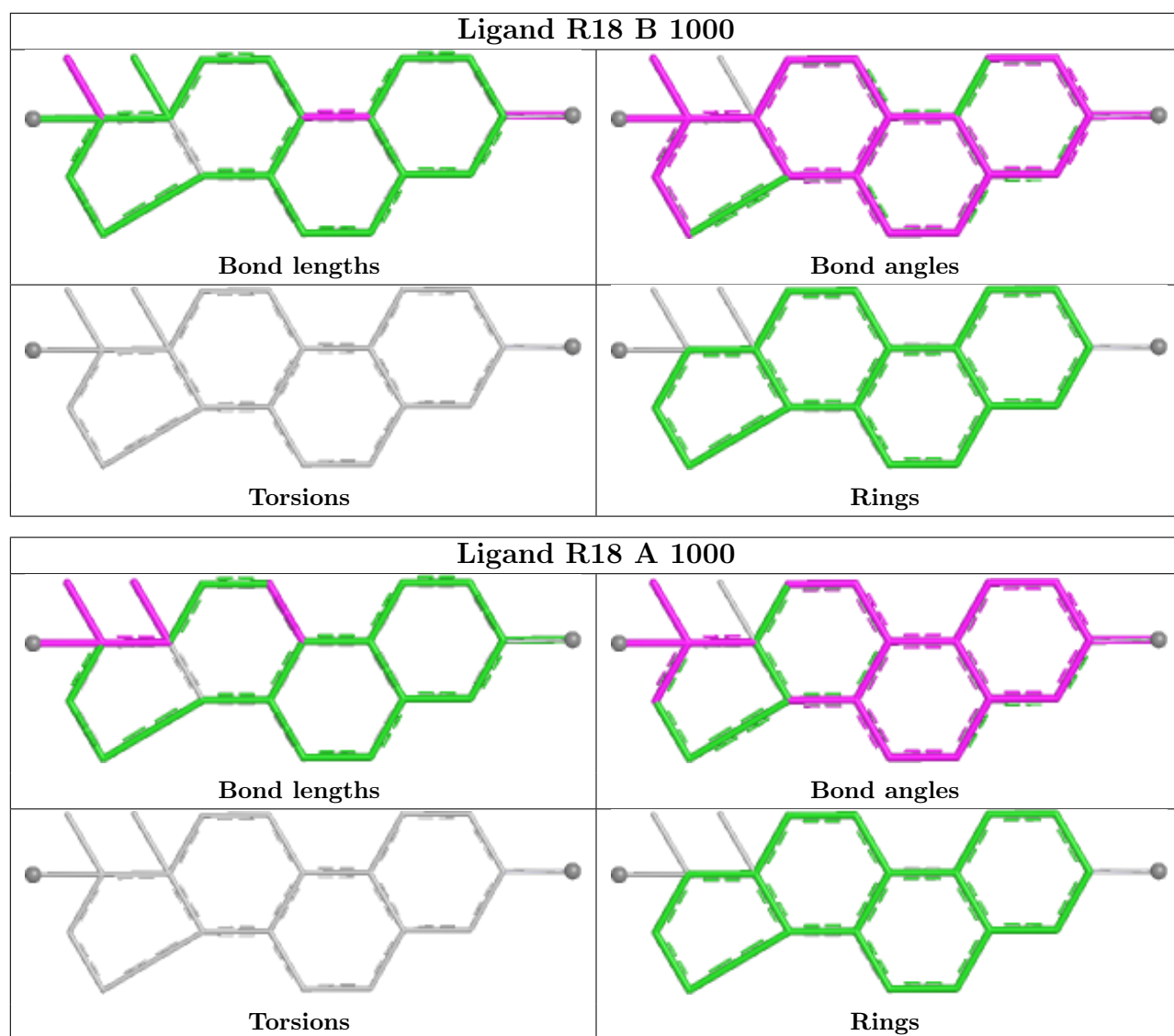
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1000	R18	1	0
2	A	1000	R18	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	251/258 (97%)	-0.31	2 (0%) 82 75	6, 29, 68, 85	0
1	B	249/258 (96%)	-0.41	1 (0%) 88 84	6, 29, 68, 86	0
All	All	500/516 (96%)	-0.36	3 (0%) 85 80	6, 29, 70, 86	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	705	ASN	3.3
1	B	705	ASN	2.2
1	A	866	SER	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](#)

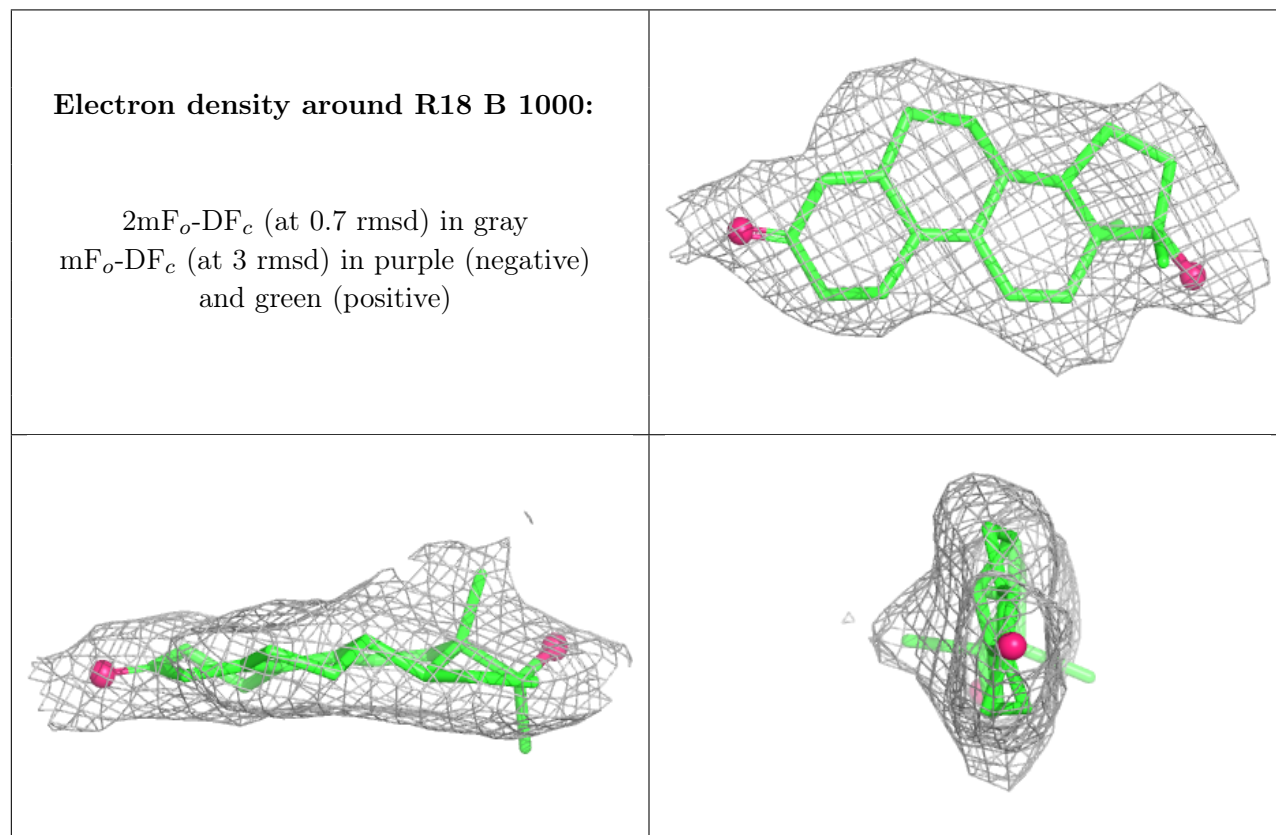
There are no oligosaccharides in this entry.

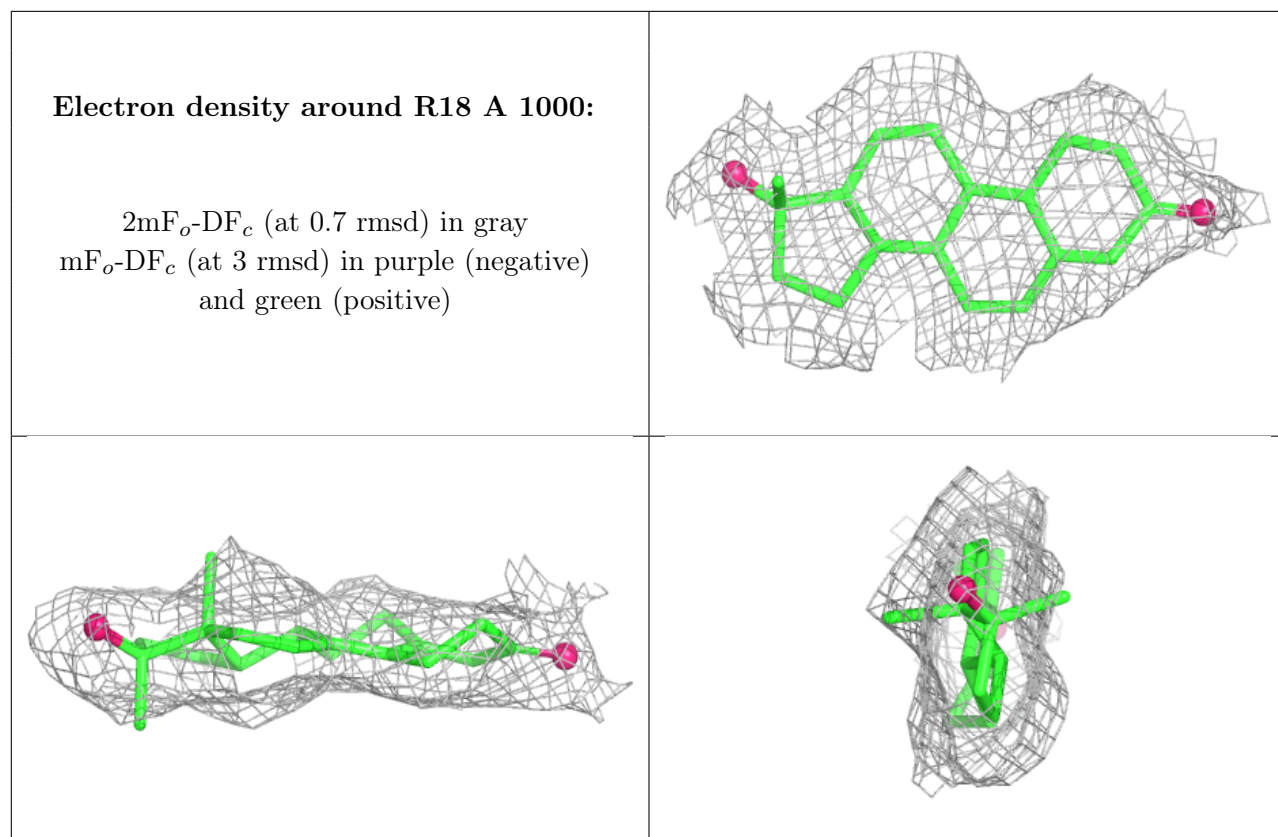
6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	R18	B	1000	21/21	0.95	0.07	2,13,19,21	0
2	R18	A	1000	21/21	0.96	0.06	2,5,9,10	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.