



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:55 AM UTC

PDB ID : 1BHN / pdb_00001bhn
Title : NUCLEOSIDE DIPHOSPHATE KINASE ISOFORM A FROM BOVINE RETINA
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Deposited on : 1998-06-10
Resolution : 2.40 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 ⓘ](#)) 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

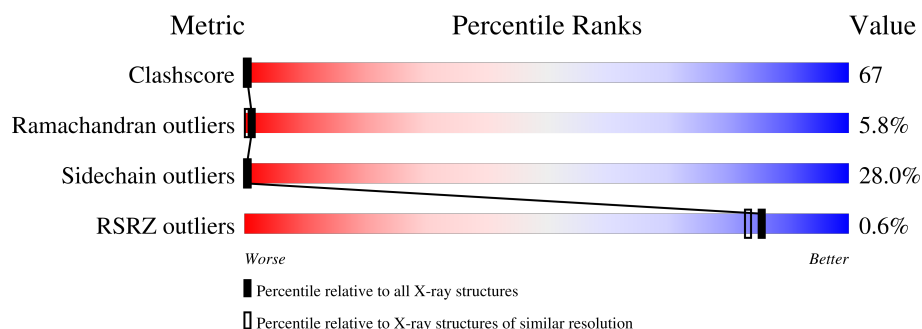
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	152	
1	B	152	
1	C	152	
1	D	152	
1	E	152	
1	F	152	

2 Entry composition [i](#)

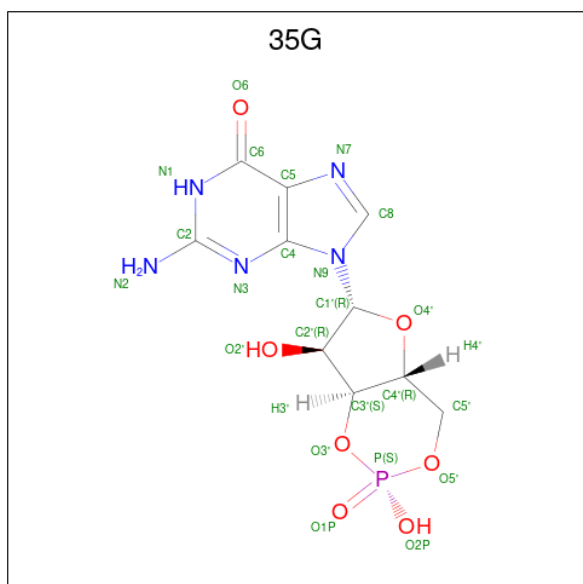
There are 4 unique types of molecules in this entry. The entry contains 7848 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NUCLEOSIDE DIPHOSPHATE TRANSFERASE.

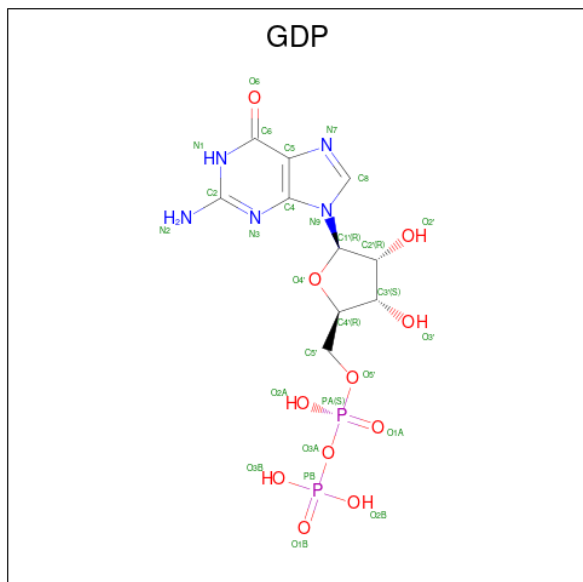
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1206	771	210	218	7			
1	B	151	Total	C	N	O	S	0	0	0
			1206	771	210	218	7			
1	C	151	Total	C	N	O	S	0	0	0
			1206	771	210	218	7			
1	D	151	Total	C	N	O	S	0	0	0
			1206	771	210	218	7			
1	E	151	Total	C	N	O	S	0	0	0
			1206	771	210	218	7			
1	F	151	Total	C	N	O	S	0	0	0
			1206	771	210	218	7			

- Molecule 2 is GUANOSINE-3',5'-MONOPHOSPHATE (CCD ID: 35G) (formula: $C_{10}H_{12}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



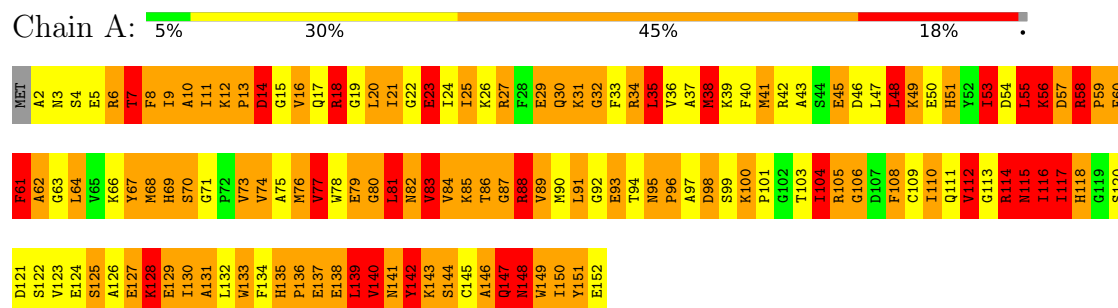
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total 49	O 49	0	0
4	B	49	Total 49	O 49	0	0
4	C	50	Total 50	O 50	0	0
4	D	40	Total 40	O 40	0	0
4	E	62	Total 62	O 62	0	0
4	F	56	Total 56	O 56	0	0

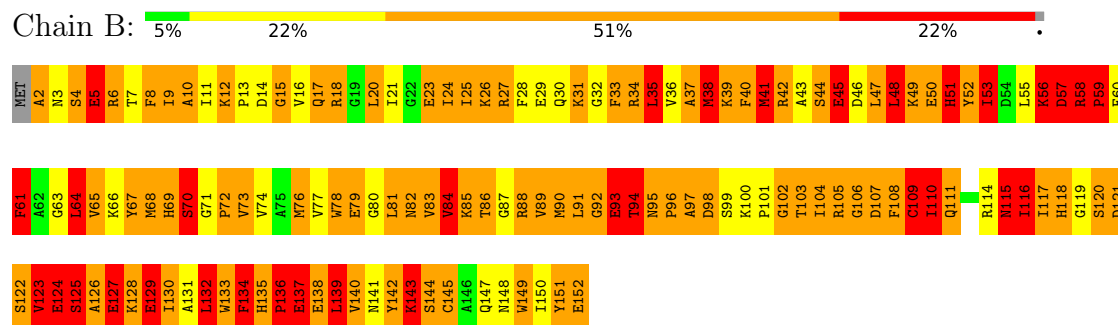
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

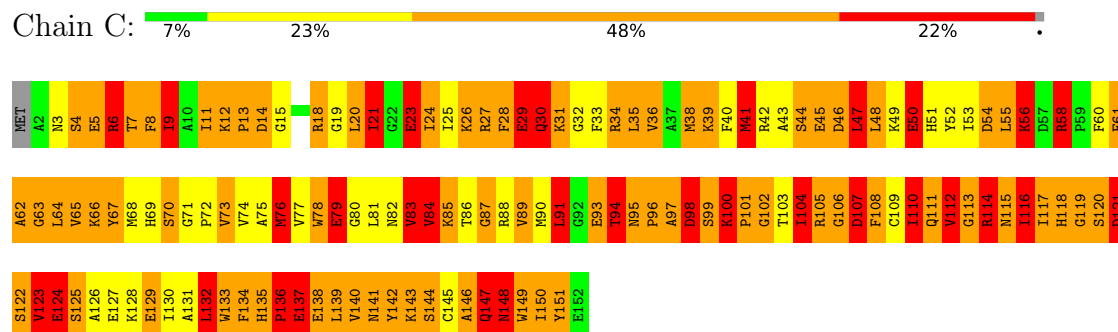
• Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE



• Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE

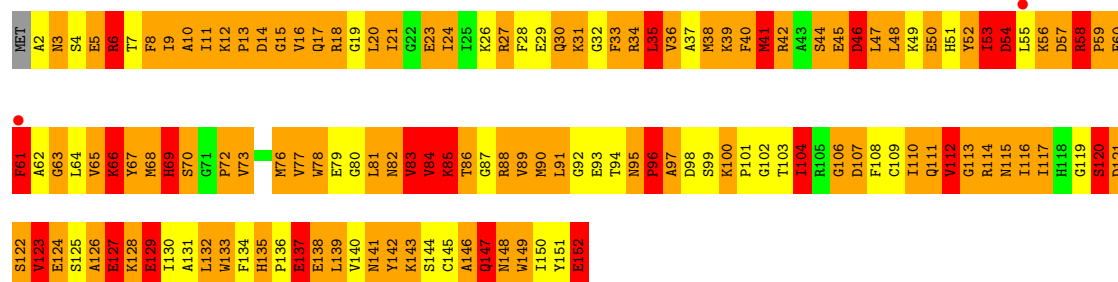


• Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE



• Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.88Å 92.11Å 131.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	79.0 (20.00-2.40) 78.7 (20.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.26Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.200 , (Not available) 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.909	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 134.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7848	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 35G

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	1.80	10/1233 (0.8%)	3.52	261/1659 (15.7%)
1	B	1.68	14/1233 (1.1%)	3.46	249/1659 (15.0%)
1	C	1.74	17/1233 (1.4%)	3.58	255/1659 (15.4%)
1	D	1.72	9/1233 (0.7%)	3.52	258/1659 (15.6%)
1	E	1.85	14/1233 (1.1%)	3.54	242/1659 (14.6%)
1	F	1.77	13/1233 (1.1%)	3.51	269/1659 (16.2%)
All	All	1.76	77/7398 (1.0%)	3.52	1534/9954 (15.4%)

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	B	3	0
1	C	0	2
1	D	2	0
1	E	0	1
All	All	5	3

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	56	LYS	C-N	-8.59	1.21	1.33
1	A	32	GLY	CA-C	7.85	1.63	1.51
1	D	91	LEU	C-O	-7.56	1.14	1.24
1	C	101	PRO	CA-C	-7.42	1.45	1.52
1	A	129	GLU	CA-C	-7.25	1.43	1.52
1	A	34	ARG	NE-CZ	7.07	1.40	1.33
1	B	45	GLU	CD-OE2	6.80	1.38	1.25
1	B	100	LYS	CA-C	-6.77	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	108	PHE	CA-C	-6.69	1.43	1.52
1	C	97	ALA	CA-C	-6.65	1.43	1.52
1	E	14	ASP	CG-OD2	6.61	1.38	1.25
1	A	35	LEU	CA-C	-6.58	1.44	1.52
1	F	20	LEU	N-CA	-6.49	1.38	1.46
1	F	92	GLY	C-O	6.49	1.29	1.23
1	F	69	HIS	N-CA	-6.45	1.40	1.46
1	F	29	GLU	CD-OE1	6.44	1.37	1.25
1	B	135	HIS	CA-C	-6.44	1.45	1.52
1	D	118	HIS	C-N	6.41	1.40	1.33
1	E	18	ARG	C-N	-6.38	1.24	1.33
1	D	79	GLU	CD-OE2	6.35	1.37	1.25
1	F	36	VAL	CA-CB	-6.35	1.46	1.54
1	F	78	TRP	CA-C	-6.35	1.45	1.52
1	C	70	SER	CA-C	-6.32	1.45	1.52
1	E	145	CYS	C-O	6.16	1.32	1.24
1	F	90	MET	CA-C	-6.10	1.44	1.52
1	E	42	ARG	NE-CZ	6.05	1.39	1.33
1	E	139	LEU	CA-C	-5.89	1.45	1.53
1	D	80	GLY	C-N	-5.88	1.25	1.33
1	F	110	ILE	CA-CB	-5.86	1.47	1.54
1	C	91	LEU	CA-C	5.84	1.60	1.52
1	C	33	PHE	CA-C	-5.83	1.45	1.52
1	C	107	ASP	CG-OD2	5.83	1.36	1.25
1	F	98	ASP	CG-OD2	5.79	1.36	1.25
1	D	64	LEU	C-N	-5.78	1.26	1.33
1	E	42	ARG	CA-C	5.72	1.60	1.52
1	E	71	GLY	C-N	-5.67	1.26	1.33
1	E	108	PHE	CA-CB	-5.65	1.45	1.53
1	D	34	ARG	NE-CZ	5.63	1.39	1.33
1	C	103	THR	C-N	-5.50	1.26	1.33
1	F	16	VAL	C-O	-5.46	1.17	1.24
1	C	108	PHE	N-CA	5.45	1.51	1.46
1	C	117	ILE	N-CA	-5.43	1.40	1.46
1	B	5	GLU	CD-OE2	5.42	1.35	1.25
1	C	21	ILE	CA-CB	-5.41	1.48	1.54
1	B	118	HIS	CG-CD2	5.38	1.41	1.35
1	E	19	GLY	CA-C	-5.35	1.44	1.51
1	D	148	ASN	CA-C	-5.35	1.46	1.52
1	E	114	ARG	CA-C	-5.34	1.47	1.53
1	B	136	PRO	N-CA	-5.34	1.40	1.47
1	B	72	PRO	N-CA	-5.32	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	121	ASP	CG-OD1	5.30	1.35	1.25
1	C	134	PHE	C-O	5.30	1.29	1.23
1	E	22	GLY	N-CA	5.29	1.52	1.45
1	F	12	LYS	C-N	5.29	1.40	1.33
1	A	29	GLU	CD-OE1	5.27	1.35	1.25
1	B	31	LYS	C-N	-5.23	1.26	1.33
1	B	6	ARG	C-O	5.23	1.30	1.23
1	C	142	TYR	CA-CB	5.20	1.62	1.53
1	C	103	THR	C-O	-5.19	1.16	1.23
1	E	121	ASP	CG-OD1	-5.17	1.15	1.25
1	B	118	HIS	ND1-CE1	5.15	1.37	1.32
1	D	129	GLU	CD-OE2	5.13	1.35	1.25
1	C	103	THR	CA-C	-5.13	1.46	1.53
1	B	116	ILE	CA-C	-5.12	1.46	1.52
1	A	91	LEU	CA-C	-5.10	1.45	1.52
1	A	64	LEU	N-CA	-5.09	1.40	1.46
1	C	9	ILE	N-CA	-5.09	1.40	1.46
1	B	23	GLU	C-N	-5.09	1.27	1.33
1	A	142	TYR	CA-CB	5.09	1.62	1.53
1	A	116	ILE	C-O	5.04	1.30	1.24
1	F	45	GLU	CD-OE2	5.04	1.34	1.25
1	A	79	GLU	CD-OE2	5.04	1.34	1.25
1	B	100	LYS	C-N	-5.03	1.27	1.33
1	C	9	ILE	C-O	-5.03	1.18	1.24
1	C	35	LEU	C-O	5.02	1.30	1.24
1	E	98	ASP	C-O	-5.02	1.17	1.23
1	F	61	PHE	CB-CG	5.01	1.62	1.50

All (1534) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	54	ASP	CA-CB-CG	-20.95	91.64	112.60
1	C	88	ARG	CD-NE-CZ	-18.80	98.08	124.40
1	A	112	VAL	CB-CA-C	-18.36	87.36	112.14
1	C	28	PHE	CA-CB-CG	-16.73	97.07	113.80
1	E	115	ASN	CA-CB-CG	-16.64	95.97	112.60
1	E	135	HIS	CA-C-O	15.02	131.97	119.66
1	D	18	ARG	NE-CZ-NH2	13.96	131.76	119.20
1	E	16	VAL	N-CA-C	-13.88	98.55	111.45
1	C	115	ASN	CA-C-N	13.70	146.64	121.97
1	C	115	ASN	C-N-CA	13.70	146.64	121.97
1	F	110	ILE	N-CA-C	13.45	122.79	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	35	LEU	CB-CA-C	-13.32	90.42	110.67
1	D	82	ASN	CA-CB-CG	13.19	125.79	112.60
1	D	125	SER	N-CA-C	-12.75	97.38	111.28
1	E	60	PHE	CA-CB-CG	12.57	126.38	113.80
1	C	146	ALA	CB-CA-C	-12.02	88.74	109.65
1	D	115	ASN	CA-CB-CG	-11.97	100.63	112.60
1	C	110	ILE	CA-C-N	-11.91	106.28	122.72
1	C	110	ILE	C-N-CA	-11.91	106.28	122.72
1	C	63	GLY	O-C-N	11.81	133.52	122.19
1	D	140	VAL	N-CA-C	11.77	124.37	108.84
1	B	108	PHE	N-CA-C	11.75	125.92	110.88
1	B	33	PHE	CA-CB-CG	-11.74	102.06	113.80
1	F	119	GLY	CA-C-O	-11.66	110.58	121.19
1	B	124	GLU	O-C-N	11.65	134.47	122.12
1	A	83	VAL	CB-CA-C	-11.57	96.89	112.04
1	A	127	GLU	N-CA-C	11.35	123.73	111.36
1	E	77	VAL	O-C-N	11.18	136.06	123.09
1	A	142	TYR	O-C-N	11.10	134.91	123.26
1	B	74	VAL	CA-CB-CG1	-11.06	91.59	110.40
1	B	110	ILE	N-CA-C	10.92	120.95	111.56
1	B	115	ASN	CA-CB-CG	-10.92	101.68	112.60
1	B	107	ASP	CA-CB-CG	-10.86	101.74	112.60
1	F	36	VAL	CA-CB-CG1	-10.85	91.96	110.40
1	B	115	ASN	CA-C-N	10.84	141.49	121.97
1	B	115	ASN	C-N-CA	10.84	141.49	121.97
1	A	63	GLY	O-C-N	10.82	132.68	122.19
1	C	70	SER	O-C-N	10.78	133.67	122.03
1	D	28	PHE	CA-CB-CG	-10.75	103.05	113.80
1	D	121	ASP	CB-CA-C	-10.70	92.22	110.09
1	D	90	MET	O-C-N	10.62	133.01	122.07
1	C	148	ASN	CA-CB-CG	-10.59	102.01	112.60
1	B	100	LYS	CB-CA-C	-10.58	93.24	109.11
1	C	127	GLU	O-C-N	10.54	134.23	122.11
1	B	151	TYR	N-CA-CB	10.51	129.11	110.83
1	E	93	GLU	CA-C-O	10.47	132.88	121.16
1	C	33	PHE	CA-C-N	-10.43	108.29	122.99
1	C	33	PHE	C-N-CA	-10.43	108.29	122.99
1	D	86	THR	N-CA-C	-10.37	99.67	110.97
1	C	91	LEU	CA-C-O	10.33	131.37	120.42
1	D	124	GLU	CA-C-O	10.33	131.67	120.82
1	A	74	VAL	CA-C-N	-10.30	107.99	122.93
1	A	74	VAL	C-N-CA	-10.30	107.99	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	ASN	N-CA-C	10.26	125.88	113.16
1	D	5	GLU	CB-CA-C	-10.23	91.53	109.64
1	E	122	SER	N-CA-CB	10.23	127.70	111.43
1	E	38	MET	CA-C-O	10.11	132.02	120.89
1	E	93	GLU	N-CA-CB	10.11	124.83	109.97
1	E	117	ILE	CA-CB-CG2	-10.10	93.33	110.50
1	A	71	GLY	CA-C-N	10.05	129.86	120.21
1	A	71	GLY	C-N-CA	10.05	129.86	120.21
1	C	33	PHE	CA-CB-CG	-10.05	103.75	113.80
1	D	100	LYS	CA-C-O	10.04	132.12	120.88
1	A	88	ARG	NE-CZ-NH2	-10.03	110.17	119.20
1	F	95	ASN	CA-C-O	10.03	125.81	119.29
1	B	98	ASP	CB-CG-OD2	-10.02	95.37	118.40
1	E	101	PRO	CB-CA-C	9.99	124.02	111.23
1	A	142	TYR	N-CA-C	-9.98	94.02	108.60
1	C	136	PRO	CB-CA-C	-9.93	95.18	111.56
1	D	46	ASP	CA-CB-CG	9.92	122.52	112.60
1	D	73	VAL	O-C-N	9.91	134.96	122.57
1	B	31	LYS	CA-C-O	9.88	131.75	119.11
1	E	42	ARG	O-C-N	-9.86	111.51	123.04
1	F	38	MET	CG-SD-CE	-9.85	79.23	100.90
1	A	108	PHE	N-CA-C	9.85	125.29	113.28
1	E	36	VAL	CA-CB-CG1	-9.85	93.66	110.40
1	E	27	ARG	NE-CZ-NH2	-9.84	110.35	119.20
1	E	95	ASN	CB-CA-C	-9.83	94.03	109.85
1	E	31	LYS	N-CA-C	-9.81	100.58	111.28
1	A	55	LEU	N-CA-CB	-9.80	97.05	110.67
1	D	80	GLY	CA-C-O	9.80	131.86	121.87
1	F	115	ASN	CA-CB-CG	-9.79	102.81	112.60
1	D	118	HIS	CA-C-N	9.77	132.28	122.80
1	D	118	HIS	C-N-CA	9.77	132.28	122.80
1	C	6	ARG	CA-CB-CG	-9.76	94.58	114.10
1	C	70	SER	CB-CA-C	-9.76	95.82	110.95
1	C	141	ASN	CA-CB-CG	-9.69	102.92	112.60
1	C	67	TYR	N-CA-CB	-9.65	95.88	110.16
1	E	115	ASN	N-CA-C	9.63	123.72	112.93
1	F	61	PHE	N-CA-CB	9.61	126.73	110.49
1	E	82	ASN	CA-CB-CG	9.60	122.20	112.60
1	B	123	VAL	N-CA-CB	9.59	121.48	110.65
1	F	31	LYS	CA-C-O	9.58	130.56	119.35
1	B	58	ARG	O-C-N	9.57	132.33	121.32
1	D	11	ILE	O-C-N	9.57	134.29	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	69	HIS	N-CA-C	-9.56	97.72	113.50
1	C	28	PHE	CA-C-O	9.53	130.72	120.90
1	A	32	GLY	O-C-N	-9.49	110.38	122.43
1	C	127	GLU	CB-CG-CD	9.48	128.71	112.60
1	B	76	MET	O-C-N	9.47	134.04	123.33
1	F	57	ASP	O-C-N	9.46	133.09	122.11
1	B	76	MET	CG-SD-CE	-9.41	80.20	100.90
1	D	83	VAL	CB-CA-C	-9.40	99.67	111.70
1	D	41	MET	CG-SD-CE	-9.40	80.22	100.90
1	B	51	HIS	CA-CB-CG	9.40	123.20	113.80
1	A	21	ILE	CA-C-O	-9.39	109.04	120.78
1	B	125	SER	CB-CA-C	9.39	125.42	110.96
1	C	26	LYS	CA-C-O	9.39	130.94	120.90
1	D	90	MET	CA-C-N	9.38	139.44	121.54
1	D	90	MET	C-N-CA	9.38	139.44	121.54
1	F	27	ARG	N-CA-CB	-9.37	95.76	110.28
1	E	118	HIS	O-C-N	9.36	134.96	123.44
1	B	59	PRO	CB-CA-C	-9.36	96.11	111.56
1	E	146	ALA	N-CA-C	9.36	125.85	113.30
1	A	115	ASN	N-CA-C	9.35	130.72	110.80
1	F	41	MET	CG-SD-CE	9.33	121.42	100.90
1	A	84	VAL	N-CA-C	9.32	120.15	110.36
1	D	33	PHE	CA-C-O	-9.31	110.57	121.46
1	F	114	ARG	CA-CB-CG	-9.29	95.52	114.10
1	E	136	PRO	CA-C-N	-9.29	106.19	122.26
1	E	136	PRO	C-N-CA	-9.29	106.19	122.26
1	B	120	SER	N-CA-CB	9.28	123.87	109.48
1	D	114	ARG	NE-CZ-NH1	9.29	130.78	121.50
1	A	114	ARG	CG-CD-NE	-9.25	91.65	112.00
1	B	28	PHE	CA-CB-CG	-9.24	104.56	113.80
1	D	141	ASN	CB-CA-C	9.18	125.47	110.78
1	B	58	ARG	CA-C-N	9.16	131.29	119.84
1	B	58	ARG	C-N-CA	9.16	131.29	119.84
1	B	135	HIS	O-C-N	9.14	129.76	121.35
1	D	51	HIS	CA-CB-CG	-9.12	104.68	113.80
1	C	87	GLY	CA-C-O	9.12	130.03	119.09
1	B	30	GLN	CA-CB-CG	-9.10	95.90	114.10
1	F	61	PHE	CA-C-N	-9.10	104.07	120.99
1	F	61	PHE	C-N-CA	-9.10	104.07	120.99
1	C	114	ARG	CA-C-N	-9.08	107.99	122.79
1	C	114	ARG	C-N-CA	-9.08	107.99	122.79
1	E	90	MET	CG-SD-CE	9.08	120.88	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	103	THR	CA-CB-CG2	9.07	125.92	110.50
1	E	92	GLY	CA-C-O	-9.05	113.29	122.25
1	D	42	ARG	CA-C-N	-9.04	105.59	120.87
1	D	42	ARG	C-N-CA	-9.04	105.59	120.87
1	E	149	TRP	N-CA-C	-9.00	102.45	113.97
1	C	95	ASN	CB-CA-C	-8.99	92.46	110.17
1	C	108	PHE	CA-C-N	-8.99	106.43	121.80
1	C	108	PHE	C-N-CA	-8.99	106.43	121.80
1	E	136	PRO	N-CA-CB	-8.94	93.86	103.25
1	B	41	MET	CA-C-O	-8.93	111.89	121.36
1	D	130	ILE	CB-CA-C	-8.93	98.32	112.16
1	B	33	PHE	N-CA-CB	-8.93	96.88	110.45
1	A	79	GLU	N-CA-C	8.92	123.06	108.52
1	B	11	ILE	CB-CA-C	-8.91	99.57	111.15
1	D	114	ARG	CD-NE-CZ	8.89	136.85	124.40
1	F	107	ASP	CA-C-N	-8.88	108.69	122.37
1	F	107	ASP	C-N-CA	-8.88	108.69	122.37
1	A	13	PRO	N-CA-CB	8.87	112.03	103.51
1	F	77	VAL	N-CA-CB	8.87	125.98	111.44
1	D	30	GLN	OE1-CD-NE2	-8.84	113.76	122.60
1	E	44	SER	CA-C-N	-8.84	107.14	121.19
1	E	44	SER	C-N-CA	-8.84	107.14	121.19
1	F	67	TYR	CB-CG-CD2	-8.83	107.55	120.80
1	D	35	LEU	CB-CA-C	-8.80	96.18	111.05
1	C	30	GLN	OE1-CD-NE2	-8.80	113.80	122.60
1	E	135	HIS	N-CA-CB	8.79	123.33	110.32
1	C	134	PHE	CA-CB-CG	8.78	122.58	113.80
1	F	90	MET	O-C-N	8.76	131.41	122.12
1	A	116	ILE	CA-C-N	-8.76	111.17	123.17
1	A	116	ILE	C-N-CA	-8.76	111.17	123.17
1	F	40	PHE	CB-CA-C	-8.75	97.38	110.67
1	D	38	MET	O-C-N	8.74	134.21	122.59
1	B	123	VAL	CB-CA-C	8.73	123.13	111.87
1	A	18	ARG	CA-CB-CG	-8.71	96.67	114.10
1	C	46	ASP	CA-CB-CG	8.69	121.29	112.60
1	A	60	PHE	CA-CB-CG	-8.68	105.12	113.80
1	C	85	LYS	CA-C-O	8.68	130.03	119.79
1	D	106	GLY	CA-C-N	8.66	132.23	120.54
1	D	106	GLY	C-N-CA	8.66	132.23	120.54
1	A	110	ILE	N-CA-C	8.65	121.61	112.96
1	C	97	ALA	CB-CA-C	-8.64	93.56	109.29
1	E	7	THR	CA-C-N	-8.64	111.28	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	7	THR	C-N-CA	-8.64	111.28	122.77
1	A	103	THR	OG1-CB-CG2	8.64	126.58	109.30
1	A	89	VAL	O-C-N	8.60	130.84	121.90
1	C	111	GLN	N-CA-CB	-8.59	96.43	110.43
1	F	137	GLU	CA-C-N	-8.58	109.19	122.49
1	F	137	GLU	C-N-CA	-8.58	109.19	122.49
1	F	126	ALA	CA-C-N	-8.57	108.78	120.44
1	F	126	ALA	C-N-CA	-8.57	108.78	120.44
1	E	78	TRP	CA-C-O	8.56	129.82	120.32
1	A	99	SER	CB-CA-C	-8.55	96.21	109.89
1	E	127	GLU	O-C-N	8.54	131.17	122.12
1	F	98	ASP	N-CA-CB	-8.51	97.30	110.92
1	D	108	PHE	N-CA-C	8.50	123.46	112.41
1	E	133	TRP	CA-C-N	-8.49	109.49	122.81
1	E	133	TRP	C-N-CA	-8.49	109.49	122.81
1	F	100	LYS	N-CA-C	8.47	121.62	109.84
1	D	88	ARG	CA-C-O	-8.47	111.44	120.42
1	B	26	LYS	O-C-N	-8.47	113.14	122.12
1	A	151	TYR	O-C-N	8.46	133.17	123.27
1	F	152	GLU	N-CA-CB	-8.46	96.11	110.50
1	C	18	ARG	N-CA-CB	-8.45	96.20	110.49
1	B	40	PHE	CB-CA-C	-8.45	96.07	109.84
1	A	57	ASP	CA-CB-CG	-8.44	104.16	112.60
1	D	108	PHE	CA-C-N	-8.44	107.37	121.80
1	D	108	PHE	C-N-CA	-8.44	107.37	121.80
1	A	74	VAL	N-CA-CB	8.44	122.09	111.46
1	A	139	LEU	O-C-N	8.41	133.78	122.59
1	E	43	ALA	CA-C-N	8.40	132.67	120.82
1	E	43	ALA	C-N-CA	8.40	132.67	120.82
1	F	104	ILE	CA-C-O	8.39	131.27	120.78
1	A	35	LEU	N-CA-C	-8.39	95.66	108.67
1	B	110	ILE	N-CA-CB	8.38	120.63	111.41
1	C	42	ARG	CB-CA-C	-8.38	96.81	111.22
1	B	84	VAL	CA-CB-CG1	-8.36	96.18	110.40
1	C	138	GLU	N-CA-C	-8.35	101.81	114.16
1	C	134	PHE	CB-CA-C	-8.33	95.07	109.65
1	A	50	GLU	N-CA-CB	-8.32	96.83	110.40
1	B	141	ASN	CB-CA-C	8.32	124.54	110.81
1	D	64	LEU	CA-C-N	-8.32	110.56	120.72
1	D	64	LEU	C-N-CA	-8.32	110.56	120.72
1	F	86	THR	CA-C-O	8.31	129.23	120.42
1	D	3	ASN	CA-CB-CG	8.31	120.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ILE	CA-CB-CG2	8.31	124.62	110.50
1	C	41	MET	CG-SD-CE	-8.30	82.63	100.90
1	C	26	LYS	O-C-N	-8.29	113.47	122.09
1	D	115	ASN	CA-C-N	8.28	136.88	121.97
1	D	115	ASN	C-N-CA	8.28	136.88	121.97
1	F	111	GLN	OE1-CD-NE2	8.28	130.88	122.60
1	C	115	ASN	CA-CB-CG	-8.27	104.33	112.60
1	F	135	HIS	ND1-CE1-NE2	8.24	116.64	108.40
1	B	81	LEU	CA-C-O	8.24	129.69	120.80
1	B	90	MET	O-C-N	8.24	131.86	122.22
1	D	133	TRP	O-C-N	8.24	132.98	122.19
1	A	136	PRO	O-C-N	-8.23	112.78	122.24
1	F	58	ARG	NE-CZ-NH2	-8.23	111.80	119.20
1	E	122	SER	CA-C-N	-8.22	107.52	121.09
1	E	122	SER	C-N-CA	-8.22	107.52	121.09
1	E	135	HIS	N-CA-C	-8.22	99.44	109.72
1	C	27	ARG	O-C-N	8.22	130.83	122.12
1	F	97	ALA	O-C-N	8.20	131.50	122.15
1	F	132	LEU	CA-C-N	-8.20	109.01	122.54
1	F	132	LEU	C-N-CA	-8.20	109.01	122.54
1	A	80	GLY	CA-C-O	8.20	129.65	121.62
1	B	124	GLU	CB-CA-C	-8.20	96.74	110.68
1	C	91	LEU	N-CA-CB	-8.20	98.03	110.16
1	D	100	LYS	O-C-N	-8.20	112.35	121.53
1	B	141	ASN	N-CA-CB	8.19	123.23	110.21
1	D	118	HIS	CA-CB-CG	-8.18	105.62	113.80
1	F	17	GLN	N-CA-C	8.18	121.30	111.82
1	F	98	ASP	CA-CB-CG	-8.18	104.42	112.60
1	A	30	GLN	OE1-CD-NE2	8.17	130.77	122.60
1	E	42	ARG	NE-CZ-NH2	8.17	126.55	119.20
1	B	55	LEU	CA-C-N	8.17	137.14	121.54
1	B	55	LEU	C-N-CA	8.17	137.14	121.54
1	C	89	VAL	CG1-CB-CG2	8.16	128.75	110.80
1	F	66	LYS	CA-C-O	8.14	129.09	120.70
1	C	65	VAL	O-C-N	-8.14	113.68	121.90
1	B	28	PHE	CA-C-O	8.13	129.32	119.97
1	F	69	HIS	CB-CA-C	8.12	127.50	110.45
1	F	78	TRP	O-C-N	8.09	132.66	123.27
1	C	88	ARG	NE-CZ-NH1	-8.09	113.41	121.50
1	B	111	GLN	N-CA-CB	-8.08	98.41	110.85
1	B	42	ARG	CA-C-N	-8.08	109.86	122.87
1	B	42	ARG	C-N-CA	-8.08	109.86	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	VAL	N-CA-C	8.08	118.86	110.62
1	B	143	LYS	CB-CA-C	-8.07	93.95	109.37
1	E	106	GLY	O-C-N	8.07	130.12	122.13
1	C	65	VAL	CA-C-N	-8.05	106.99	120.68
1	C	65	VAL	C-N-CA	-8.05	106.99	120.68
1	E	34	ARG	CA-C-N	-8.04	111.44	122.30
1	E	34	ARG	C-N-CA	-8.04	111.44	122.30
1	D	69	HIS	O-C-N	8.04	133.83	122.41
1	C	39	LYS	O-C-N	8.04	132.48	123.48
1	D	150	ILE	CB-CA-C	-8.03	101.83	111.94
1	C	39	LYS	CA-C-O	-8.01	112.08	120.89
1	D	88	ARG	NE-CZ-NH2	-8.01	111.99	119.20
1	E	111	GLN	CA-C-N	8.01	131.26	120.77
1	E	111	GLN	C-N-CA	8.01	131.26	120.77
1	D	134	PHE	N-CA-C	8.00	122.88	109.76
1	D	49	LYS	O-C-N	7.99	131.26	122.15
1	A	73	VAL	CA-C-N	-7.99	112.74	123.12
1	A	73	VAL	C-N-CA	-7.99	112.74	123.12
1	D	134	PHE	CA-CB-CG	-7.98	105.82	113.80
1	E	79	GLU	CA-C-O	7.98	129.08	120.38
1	B	35	LEU	CD1-CG-CD2	7.98	128.35	110.80
1	C	62	ALA	O-C-N	7.97	131.28	122.20
1	B	27	ARG	CA-C-O	7.96	129.42	120.90
1	B	40	PHE	O-C-N	7.95	132.35	123.04
1	C	29	GLU	N-CA-CB	7.95	121.79	109.94
1	F	45	GLU	CA-C-N	-7.92	109.66	120.28
1	F	45	GLU	C-N-CA	-7.92	109.66	120.28
1	F	122	SER	N-CA-CB	7.92	123.84	111.56
1	D	14	ASP	CA-CB-CG	7.91	120.51	112.60
1	E	34	ARG	CB-CA-C	7.91	122.59	109.53
1	B	143	LYS	CA-C-O	-7.89	112.18	120.70
1	A	85	LYS	N-CA-CB	-7.88	98.46	110.20
1	E	94	THR	CB-CA-C	7.87	123.80	110.74
1	E	144	SER	CA-C-O	-7.87	113.21	121.55
1	B	134	PHE	O-C-N	7.87	132.22	123.25
1	E	115	ASN	O-C-N	7.86	132.43	122.37
1	C	101	PRO	N-CA-CB	7.86	111.73	102.85
1	A	98	ASP	CB-CA-C	7.84	122.56	109.38
1	A	145	CYS	CA-C-O	7.84	128.98	120.20
1	C	87	GLY	CA-C-N	-7.84	107.48	122.53
1	C	87	GLY	C-N-CA	-7.84	107.48	122.53
1	D	119	GLY	O-C-N	-7.84	114.87	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	83	VAL	N-CA-CB	7.83	118.84	110.62
1	A	95	ASN	O-C-N	7.82	130.31	121.32
1	C	30	GLN	CG-CD-NE2	7.82	128.12	116.40
1	D	95	ASN	CA-C-O	7.79	126.02	119.71
1	F	4	SER	CB-CA-C	-7.79	98.59	111.13
1	D	7	THR	CA-CB-CG2	-7.79	97.26	110.50
1	E	67	TYR	CA-C-O	7.79	128.72	120.70
1	B	89	VAL	O-C-N	7.78	129.72	121.94
1	A	48	LEU	CA-C-N	-7.77	107.75	120.72
1	A	48	LEU	C-N-CA	-7.77	107.75	120.72
1	F	37	ALA	O-C-N	-7.77	113.05	123.15
1	A	142	TYR	N-CA-CB	7.76	123.40	111.46
1	A	134	PHE	N-CA-CB	-7.75	97.40	110.80
1	D	151	TYR	O-C-N	7.75	132.52	123.30
1	F	11	ILE	CB-CA-C	-7.74	100.32	110.84
1	C	135	HIS	CA-C-N	7.72	129.49	119.84
1	C	135	HIS	C-N-CA	7.72	129.49	119.84
1	B	34	ARG	CA-C-O	-7.72	112.51	120.54
1	C	44	SER	CA-C-N	-7.72	109.33	120.29
1	C	44	SER	C-N-CA	-7.72	109.33	120.29
1	A	131	ALA	CA-C-O	-7.72	109.48	120.51
1	B	7	THR	CA-CB-CG2	-7.72	97.38	110.50
1	D	4	SER	CA-C-N	7.72	132.16	120.82
1	D	4	SER	C-N-CA	7.72	132.16	120.82
1	C	47	LEU	O-C-N	7.71	130.42	122.09
1	E	88	ARG	CA-CB-CG	-7.71	98.68	114.10
1	A	34	ARG	NE-CZ-NH2	7.71	126.14	119.20
1	E	65	VAL	O-C-N	7.71	129.88	121.94
1	F	149	TRP	N-CA-C	-7.70	103.89	113.28
1	D	48	LEU	N-CA-C	7.69	119.30	111.07
1	C	66	LYS	CA-C-O	7.69	128.86	119.79
1	F	124	GLU	CB-CA-C	-7.68	95.14	110.42
1	C	120	SER	N-CA-CB	7.67	121.24	109.97
1	E	116	ILE	CA-CB-CG2	-7.66	97.48	110.50
1	A	116	ILE	N-CA-C	7.66	125.27	109.34
1	A	147	GLN	CA-C-O	7.66	129.98	121.02
1	E	130	ILE	CA-C-O	7.66	128.97	120.85
1	C	113	GLY	CA-C-O	7.66	132.74	119.34
1	C	138	GLU	O-C-N	7.66	129.73	121.85
1	F	113	GLY	CA-C-N	7.65	133.28	123.03
1	F	113	GLY	C-N-CA	7.65	133.28	123.03
1	C	58	ARG	CA-C-N	7.65	127.54	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	58	ARG	C-N-CA	7.65	127.54	119.05
1	B	64	LEU	CA-C-N	-7.65	109.75	120.53
1	B	64	LEU	C-N-CA	-7.65	109.75	120.53
1	E	85	LYS	N-CA-CB	-7.64	98.99	110.07
1	A	14	ASP	CA-CB-CG	-7.64	104.96	112.60
1	F	23	GLU	CB-CA-C	-7.63	98.17	110.84
1	B	91	LEU	CA-C-O	7.62	128.70	120.24
1	B	103	THR	CA-CB-CG2	7.62	123.45	110.50
1	A	82	ASN	CA-C-N	-7.62	109.79	120.53
1	A	82	ASN	C-N-CA	-7.62	109.79	120.53
1	A	4	SER	CB-CA-C	7.61	123.04	110.17
1	A	101	PRO	N-CA-CB	7.61	110.53	103.15
1	C	150	ILE	CA-CB-CG2	-7.61	97.57	110.50
1	E	84	VAL	O-C-N	7.60	129.36	121.91
1	A	108	PHE	CA-C-N	-7.60	108.80	121.80
1	A	108	PHE	C-N-CA	-7.60	108.80	121.80
1	F	45	GLU	CB-CG-CD	7.60	125.53	112.60
1	D	77	VAL	CA-CB-CG1	-7.60	97.48	110.40
1	F	106	GLY	CA-C-O	7.59	128.24	120.80
1	F	46	ASP	CA-CB-CG	7.59	120.19	112.60
1	F	72	PRO	CA-C-N	-7.59	111.99	122.92
1	F	72	PRO	C-N-CA	-7.59	111.99	122.92
1	B	85	LYS	CA-C-N	-7.58	110.12	120.28
1	B	85	LYS	C-N-CA	-7.58	110.12	120.28
1	D	83	VAL	N-CA-C	-7.58	102.35	110.23
1	A	98	ASP	N-CA-C	-7.58	103.59	114.12
1	E	17	GLN	CA-CB-CG	-7.58	98.95	114.10
1	E	75	ALA	CA-C-N	-7.57	110.25	122.36
1	E	75	ALA	C-N-CA	-7.57	110.25	122.36
1	F	13	PRO	CB-CA-C	7.57	122.60	111.85
1	A	25	ILE	O-C-N	7.56	129.20	121.87
1	A	103	THR	CB-CA-C	-7.56	96.78	109.48
1	C	132	LEU	N-CA-CB	-7.56	97.85	110.39
1	B	84	VAL	CA-C-O	7.55	130.22	120.78
1	D	102	GLY	O-C-N	-7.55	112.88	122.70
1	A	67	TYR	CB-CA-C	7.54	123.67	110.85
1	B	103	THR	CB-CA-C	-7.52	96.79	109.50
1	B	86	THR	CA-CB-OG1	-7.52	98.32	109.60
1	A	16	VAL	CA-CB-CG1	7.50	123.15	110.40
1	E	98	ASP	N-CA-C	-7.50	103.72	113.17
1	E	74	VAL	N-CA-C	-7.50	96.80	107.75
1	E	125	SER	CA-CB-OG	-7.49	96.12	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	30	GLN	CA-CB-CG	-7.49	99.13	114.10
1	D	117	ILE	CA-CB-CG1	7.48	123.12	110.40
1	B	132	LEU	CB-CA-C	-7.48	95.54	110.42
1	C	112	VAL	O-C-N	-7.48	113.22	122.57
1	D	112	VAL	CB-CA-C	-7.48	102.05	112.14
1	F	3	ASN	CA-CB-CG	7.48	120.08	112.60
1	B	71	GLY	O-C-N	7.47	129.25	121.77
1	C	140	VAL	N-CA-C	7.47	118.64	109.30
1	F	24	ILE	N-CA-C	7.47	118.00	110.23
1	A	83	VAL	CA-C-N	-7.46	110.97	120.60
1	A	83	VAL	C-N-CA	-7.46	110.97	120.60
1	A	73	VAL	O-C-N	7.46	131.89	122.57
1	D	90	MET	N-CA-C	7.45	119.05	111.07
1	B	26	LYS	CA-C-O	7.44	128.67	120.63
1	F	88	ARG	CD-NE-CZ	7.43	134.80	124.40
1	F	86	THR	CA-C-N	-7.42	111.60	119.99
1	F	86	THR	C-N-CA	-7.42	111.60	119.99
1	F	31	LYS	N-CA-CB	-7.41	99.52	110.49
1	C	55	LEU	N-CA-C	-7.40	102.49	112.26
1	F	110	ILE	CA-C-N	-7.40	111.07	122.62
1	F	110	ILE	C-N-CA	-7.40	111.07	122.62
1	D	85	LYS	N-CA-C	7.39	119.13	111.14
1	B	107	ASP	O-C-N	7.37	131.09	122.17
1	F	35	LEU	N-CA-CB	7.37	121.69	109.60
1	D	38	MET	CA-C-O	-7.37	109.97	120.51
1	B	131	ALA	O-C-N	7.37	132.39	122.59
1	B	100	LYS	N-CA-CB	-7.36	100.10	110.04
1	C	84	VAL	O-C-N	7.36	131.76	122.57
1	D	144	SER	CA-C-O	-7.36	113.10	121.19
1	C	124	GLU	CA-CB-CG	-7.35	99.39	114.10
1	D	130	ILE	CA-C-O	7.35	128.44	120.57
1	F	114	ARG	NE-CZ-NH2	-7.35	112.59	119.20
1	F	100	LYS	N-CA-CB	-7.34	98.94	110.03
1	E	76	MET	CG-SD-CE	-7.34	84.76	100.90
1	A	113	GLY	O-C-N	7.33	130.01	122.24
1	E	88	ARG	O-C-N	7.32	131.74	122.23
1	F	127	GLU	CA-C-O	7.32	128.23	120.70
1	B	2	ALA	CA-C-N	7.31	135.62	122.38
1	B	2	ALA	C-N-CA	7.31	135.62	122.38
1	F	61	PHE	CB-CG-CD2	7.31	133.13	120.70
1	A	133	TRP	O-C-N	7.31	132.73	122.36
1	D	134	PHE	N-CA-CB	-7.31	98.47	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	90	MET	CG-SD-CE	7.30	116.95	100.90
1	E	93	GLU	CA-C-N	-7.29	109.88	120.82
1	E	93	GLU	C-N-CA	-7.29	109.88	120.82
1	D	127	GLU	CG-CD-OE2	-7.29	101.63	118.40
1	F	81	LEU	CA-C-N	-7.29	111.64	122.07
1	F	81	LEU	C-N-CA	-7.29	111.64	122.07
1	E	55	LEU	CB-CA-C	-7.28	102.20	111.22
1	A	127	GLU	CA-CB-CG	-7.27	99.56	114.10
1	F	82	ASN	N-CA-C	7.27	121.42	111.54
1	F	44	SER	O-C-N	7.26	131.81	123.31
1	E	58	ARG	CA-C-N	7.26	128.91	119.84
1	E	58	ARG	C-N-CA	7.26	128.91	119.84
1	C	118	HIS	CA-CB-CG	-7.24	106.56	113.80
1	F	34	ARG	NE-CZ-NH2	7.24	125.71	119.20
1	E	21	ILE	CA-CB-CG2	7.23	122.79	110.50
1	B	133	TRP	CA-C-N	-7.22	109.26	121.75
1	B	133	TRP	C-N-CA	-7.22	109.26	121.75
1	C	47	LEU	N-CA-C	-7.21	103.35	111.14
1	F	58	ARG	NE-CZ-NH1	7.21	128.72	121.50
1	D	33	PHE	CA-CB-CG	-7.20	106.60	113.80
1	C	129	GLU	O-C-N	7.20	129.49	122.07
1	E	151	TYR	CA-C-N	-7.20	108.74	121.70
1	E	151	TYR	C-N-CA	-7.20	108.74	121.70
1	D	150	ILE	N-CA-C	7.20	119.21	111.58
1	B	82	ASN	CA-C-N	-7.19	110.21	120.42
1	B	82	ASN	C-N-CA	-7.19	110.21	120.42
1	C	9	ILE	N-CA-CB	-7.19	101.35	111.99
1	C	129	GLU	CB-CG-CD	7.19	124.83	112.60
1	E	43	ALA	N-CA-CB	7.19	121.88	110.23
1	A	98	ASP	N-CA-CB	7.18	120.79	110.88
1	D	97	ALA	CB-CA-C	-7.18	98.64	110.85
1	F	91	LEU	CA-C-N	-7.18	112.30	122.85
1	F	91	LEU	C-N-CA	-7.18	112.30	122.85
1	D	80	GLY	CA-C-N	-7.17	110.48	121.66
1	D	80	GLY	C-N-CA	-7.17	110.48	121.66
1	C	132	LEU	N-CA-C	-7.16	103.81	112.54
1	B	139	LEU	CD1-CG-CD2	-7.16	95.05	110.80
1	B	136	PRO	CB-CA-C	-7.16	99.75	111.56
1	B	98	ASP	CA-CB-CG	-7.15	105.45	112.60
1	B	108	PHE	CB-CA-C	-7.15	99.16	111.45
1	E	11	ILE	CB-CA-C	-7.14	101.12	110.84
1	C	98	ASP	CA-CB-CG	-7.14	105.46	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	48	LEU	N-CA-C	7.14	119.68	111.11
1	D	122	SER	CA-C-O	7.14	128.85	120.43
1	B	91	LEU	CA-C-N	-7.13	110.03	122.66
1	B	91	LEU	C-N-CA	-7.13	110.03	122.66
1	F	69	HIS	CA-C-O	7.13	126.28	118.65
1	F	102	GLY	CA-C-O	-7.13	111.85	119.55
1	B	105	ARG	NE-CZ-NH1	-7.12	114.38	121.50
1	D	54	ASP	CA-CB-CG	-7.12	105.48	112.60
1	A	87	GLY	CA-C-N	-7.12	110.19	120.29
1	A	87	GLY	C-N-CA	-7.12	110.19	120.29
1	E	18	ARG	CA-C-O	7.11	130.68	120.51
1	F	103	THR	N-CA-C	-7.11	100.28	110.59
1	B	124	GLU	CA-C-O	-7.10	112.96	120.63
1	C	122	SER	CA-C-O	7.10	129.30	121.06
1	E	126	ALA	CB-CA-C	7.09	124.54	110.42
1	C	101	PRO	O-C-N	7.09	131.79	123.21
1	A	98	ASP	CA-C-O	7.08	126.69	118.90
1	A	110	ILE	N-CA-CB	-7.08	98.59	112.75
1	F	144	SER	CA-C-N	-7.08	111.31	120.65
1	F	144	SER	C-N-CA	-7.08	111.31	120.65
1	A	150	ILE	O-C-N	7.08	131.51	121.82
1	C	78	TRP	CA-C-N	-7.07	111.71	122.81
1	C	78	TRP	C-N-CA	-7.07	111.71	122.81
1	E	78	TRP	CD2-CE2-CZ2	-7.07	115.33	122.40
1	D	15	GLY	N-CA-C	-7.06	103.74	112.77
1	A	19	GLY	N-CA-C	7.05	125.45	115.30
1	C	46	ASP	CB-CA-C	7.05	122.66	110.68
1	D	104	ILE	O-C-N	-7.05	113.83	121.80
1	E	110	ILE	CB-CA-C	-7.04	99.74	111.29
1	C	51	HIS	CA-CB-CG	-7.04	106.76	113.80
1	F	151	TYR	CA-C-O	7.04	128.13	120.32
1	C	41	MET	CA-C-N	7.03	133.54	123.14
1	C	41	MET	C-N-CA	7.03	133.54	123.14
1	F	111	GLN	CG-CD-OE1	-7.03	106.74	120.80
1	A	114	ARG	N-CA-C	7.03	121.85	113.28
1	D	2	ALA	CB-CA-C	-7.02	99.97	110.50
1	B	127	GLU	CB-CA-C	-7.02	99.58	110.81
1	F	137	GLU	CG-CD-OE2	-7.02	102.26	118.40
1	D	57	ASP	CA-CB-CG	7.02	119.62	112.60
1	F	147	GLN	N-CA-C	7.01	121.09	112.54
1	A	88	ARG	CA-C-O	7.01	127.85	120.42
1	D	148	ASN	O-C-N	7.00	129.28	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	143	LYS	CA-C-N	7.00	131.32	120.75
1	E	143	LYS	C-N-CA	7.00	131.32	120.75
1	C	95	ASN	O-C-N	7.00	129.37	121.32
1	C	118	HIS	CA-C-N	6.99	126.41	121.65
1	C	118	HIS	C-N-CA	6.99	126.41	121.65
1	D	28	PHE	O-C-N	6.99	130.22	122.11
1	D	98	ASP	CB-CG-OD2	-6.99	102.33	118.40
1	A	87	GLY	CA-C-O	6.98	127.89	119.65
1	A	57	ASP	N-CA-C	6.98	122.24	111.56
1	A	42	ARG	CA-C-N	-6.98	111.76	122.09
1	A	42	ARG	C-N-CA	-6.98	111.76	122.09
1	D	107	ASP	CA-C-N	-6.98	111.53	122.49
1	D	107	ASP	C-N-CA	-6.98	111.53	122.49
1	F	33	PHE	N-CA-C	-6.98	99.23	110.32
1	E	8	PHE	CA-C-O	6.97	127.82	120.36
1	C	100	LYS	N-CA-C	6.97	125.22	109.81
1	B	67	TYR	CB-CA-C	-6.97	99.22	110.79
1	D	145	CYS	CA-C-O	6.97	127.88	119.10
1	E	20	LEU	N-CA-CB	-6.97	99.75	111.17
1	C	24	ILE	CA-C-N	6.96	129.33	120.56
1	C	24	ILE	C-N-CA	6.96	129.33	120.56
1	B	121	ASP	O-C-N	-6.96	113.79	122.35
1	E	128	LYS	CB-CG-CD	6.95	127.28	111.30
1	A	10	ALA	CA-C-O	6.94	128.67	120.20
1	D	97	ALA	O-C-N	6.94	130.06	122.15
1	A	92	GLY	CA-C-N	6.94	130.72	120.87
1	A	92	GLY	C-N-CA	6.94	130.72	120.87
1	E	47	LEU	CA-C-O	6.93	128.46	120.00
1	F	128	LYS	O-C-N	-6.92	114.89	122.09
1	A	7	THR	CA-C-O	6.92	128.81	121.33
1	D	80	GLY	O-C-N	-6.92	115.65	123.61
1	F	150	ILE	CA-C-N	6.92	133.40	122.74
1	F	150	ILE	C-N-CA	6.92	133.40	122.74
1	B	50	GLU	O-C-N	6.92	129.45	122.12
1	A	141	ASN	CB-CA-C	6.92	120.79	110.14
1	F	144	SER	O-C-N	6.92	131.02	122.86
1	A	111	GLN	CA-C-N	-6.91	110.99	120.46
1	A	111	GLN	C-N-CA	-6.91	110.99	120.46
1	F	21	ILE	CB-CA-C	-6.91	103.12	111.97
1	B	60	PHE	O-C-N	6.91	132.17	122.36
1	C	34	ARG	NE-CZ-NH1	6.91	128.41	121.50
1	A	74	VAL	CA-C-O	-6.90	113.15	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	PRO	CB-CA-C	6.90	120.50	110.63
1	C	84	VAL	CA-C-O	-6.90	112.16	120.78
1	E	123	VAL	CA-CB-CG2	-6.90	98.67	110.40
1	F	23	GLU	CA-C-N	-6.89	111.75	120.77
1	F	23	GLU	C-N-CA	-6.89	111.75	120.77
1	A	77	VAL	CA-C-O	6.88	127.93	120.43
1	E	96	PRO	CB-CA-C	-6.87	102.09	111.85
1	F	37	ALA	CA-C-O	6.87	129.48	121.44
1	D	8	PHE	O-C-N	6.87	131.78	123.13
1	C	136	PRO	O-C-N	6.87	131.91	122.64
1	C	71	GLY	CA-C-N	6.86	126.78	119.85
1	C	71	GLY	C-N-CA	6.86	126.78	119.85
1	B	89	VAL	N-CA-CB	6.86	118.12	110.51
1	D	48	LEU	CA-C-O	6.86	128.02	120.82
1	E	25	ILE	CA-C-O	6.86	128.12	120.85
1	E	74	VAL	N-CA-CB	6.86	120.56	111.64
1	B	103	THR	CA-CB-OG1	-6.85	99.32	109.60
1	E	108	PHE	CA-C-O	-6.84	111.11	119.18
1	E	17	GLN	OE1-CD-NE2	-6.84	115.76	122.60
1	A	18	ARG	NH1-CZ-NH2	-6.83	110.42	119.30
1	F	36	VAL	N-CA-CB	-6.83	100.68	110.52
1	A	110	ILE	CB-CA-C	-6.83	105.05	111.06
1	A	48	LEU	CB-CA-C	-6.83	99.89	110.81
1	A	135	HIS	N-CA-CB	6.83	120.34	110.03
1	B	92	GLY	O-C-N	6.82	130.26	123.10
1	C	108	PHE	CA-C-O	6.82	126.10	119.08
1	E	17	GLN	N-CA-C	6.82	120.47	111.75
1	B	12	LYS	CA-C-N	6.81	127.37	119.47
1	B	12	LYS	C-N-CA	6.81	127.37	119.47
1	D	79	GLU	CA-C-N	-6.81	110.34	121.04
1	D	79	GLU	C-N-CA	-6.81	110.34	121.04
1	D	98	ASP	CA-C-N	6.81	131.10	121.02
1	D	98	ASP	C-N-CA	6.81	131.10	121.02
1	A	58	ARG	CA-CB-CG	-6.81	100.48	114.10
1	B	101	PRO	O-C-N	-6.80	114.80	123.03
1	D	102	GLY	CA-C-O	6.80	132.40	120.57
1	E	108	PHE	N-CA-C	6.80	123.80	113.61
1	B	30	GLN	N-CA-C	6.79	121.17	112.34
1	F	116	ILE	N-CA-C	6.79	123.47	109.34
1	A	2	ALA	O-C-N	6.79	133.86	123.00
1	B	98	ASP	CB-CG-OD1	6.78	133.99	118.40
1	C	35	LEU	CB-CG-CD2	6.78	131.03	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	23	GLU	CG-CD-OE1	6.77	133.98	118.40
1	B	121	ASP	CA-C-O	6.77	127.83	119.78
1	B	122	SER	N-CA-C	-6.77	98.00	108.42
1	F	132	LEU	O-C-N	-6.77	114.44	122.15
1	D	100	LYS	CA-C-N	-6.76	112.68	119.99
1	D	100	LYS	C-N-CA	-6.76	112.68	119.99
1	A	58	ARG	O-C-N	6.76	129.10	121.32
1	B	150	ILE	O-C-N	6.76	129.27	122.04
1	C	31	LYS	CA-C-O	6.76	127.78	120.55
1	D	114	ARG	CA-C-N	-6.76	113.10	123.17
1	D	114	ARG	C-N-CA	-6.76	113.10	123.17
1	C	112	VAL	CA-CB-CG1	6.76	121.89	110.40
1	D	93	GLU	CA-CB-CG	-6.76	100.58	114.10
1	F	134	PHE	CA-CB-CG	6.75	120.55	113.80
1	E	16	VAL	CG1-CB-CG2	-6.74	95.98	110.80
1	B	42	ARG	N-CA-C	-6.73	99.25	109.95
1	D	89	VAL	CA-C-O	6.73	127.74	120.47
1	D	131	ALA	O-C-N	6.73	131.54	122.59
1	F	107	ASP	N-CA-CB	-6.73	100.24	110.33
1	E	18	ARG	O-C-N	-6.73	113.64	122.59
1	F	29	GLU	CA-CB-CG	-6.72	100.65	114.10
1	F	139	LEU	CA-C-N	6.72	134.07	121.97
1	F	139	LEU	C-N-CA	6.72	134.07	121.97
1	A	24	ILE	CG1-CB-CG2	-6.72	90.54	110.70
1	E	23	GLU	CB-CG-CD	6.71	124.01	112.60
1	B	11	ILE	CA-C-N	6.71	130.88	120.68
1	B	11	ILE	C-N-CA	6.71	130.88	120.68
1	E	79	GLU	N-CA-C	6.71	119.86	109.07
1	F	34	ARG	CB-CA-C	-6.70	98.69	109.75
1	F	77	VAL	CA-CB-CG2	-6.70	99.01	110.40
1	F	115	ASN	CB-CA-C	6.70	120.45	111.14
1	E	43	ALA	O-C-N	6.69	130.93	123.16
1	A	91	LEU	CB-CA-C	-6.69	96.23	109.67
1	C	21	ILE	CG1-CB-CG2	-6.69	90.64	110.70
1	A	58	ARG	CA-C-N	6.68	128.20	119.84
1	A	58	ARG	C-N-CA	6.68	128.20	119.84
1	D	126	ALA	CA-C-O	6.68	128.01	121.00
1	A	106	GLY	CA-C-O	6.67	127.92	121.05
1	C	125	SER	N-CA-C	-6.67	104.09	111.36
1	D	77	VAL	O-C-N	6.67	130.41	123.20
1	F	28	PHE	O-C-N	6.67	130.91	122.23
1	A	122	SER	CA-C-N	-6.67	109.72	120.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	SER	C-N-CA	-6.67	109.72	120.86
1	E	100	LYS	N-CA-CB	6.67	119.04	110.04
1	A	18	ARG	N-CA-C	6.66	120.87	113.21
1	C	36	VAL	N-CA-C	6.66	118.00	111.67
1	D	70	SER	CA-CB-OG	-6.66	97.78	111.10
1	D	38	MET	CG-SD-CE	-6.66	86.26	100.90
1	A	133	TRP	N-CA-CB	6.65	120.31	110.33
1	E	85	LYS	CB-CA-C	-6.65	100.39	110.90
1	D	27	ARG	CA-C-N	6.65	131.65	120.88
1	D	27	ARG	C-N-CA	6.65	131.65	120.88
1	B	72	PRO	CA-N-CD	-6.64	102.70	112.00
1	B	109	CYS	N-CA-CB	-6.64	101.46	111.56
1	C	60	PHE	N-CA-C	6.64	121.46	113.23
1	B	82	ASN	O-C-N	-6.63	114.33	122.55
1	B	148	ASN	OD1-CG-ND2	6.63	129.23	122.60
1	E	17	GLN	CA-C-N	6.62	134.19	121.54
1	E	17	GLN	C-N-CA	6.62	134.19	121.54
1	A	148	ASN	CA-CB-CG	-6.62	105.98	112.60
1	C	97	ALA	CA-C-N	-6.62	109.74	122.06
1	C	97	ALA	C-N-CA	-6.62	109.74	122.06
1	D	90	MET	CA-CB-CG	-6.62	100.86	114.10
1	A	127	GLU	CA-C-O	6.62	127.43	120.42
1	D	140	VAL	N-CA-CB	6.61	118.16	110.82
1	F	72	PRO	CA-C-O	6.61	130.88	122.15
1	E	55	LEU	O-C-N	6.61	131.23	121.72
1	C	97	ALA	N-CA-C	-6.60	105.38	113.50
1	E	14	ASP	N-CA-CB	6.60	121.35	110.39
1	A	62	ALA	N-CA-C	6.60	120.19	111.75
1	B	70	SER	N-CA-C	6.60	120.43	112.38
1	D	56	LYS	CA-C-O	-6.59	112.82	120.20
1	F	18	ARG	NE-CZ-NH2	-6.59	113.27	119.20
1	E	61	PHE	N-CA-CB	6.58	121.62	110.49
1	F	111	GLN	O-C-N	6.58	131.33	123.24
1	A	51	HIS	N-CA-C	-6.58	103.73	111.03
1	F	135	HIS	CE1-NE2-CD2	-6.57	102.43	109.00
1	B	134	PHE	N-CA-CB	6.57	122.62	111.66
1	C	6	ARG	NE-CZ-NH2	-6.56	113.29	119.20
1	E	47	LEU	N-CA-C	-6.56	103.34	112.45
1	F	121	ASP	N-CA-C	-6.55	103.78	113.61
1	A	76	MET	N-CA-CB	-6.55	101.01	111.62
1	E	136	PRO	CB-CA-C	-6.55	100.75	111.56
1	F	52	TYR	CA-C-N	6.55	129.43	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	52	TYR	C-N-CA	6.55	129.43	120.46
1	F	33	PHE	CA-CB-CG	-6.55	107.25	113.80
1	A	64	LEU	CB-CA-C	6.54	121.16	110.88
1	B	8	PHE	CB-CA-C	6.54	121.25	110.78
1	F	76	MET	O-C-N	6.54	130.72	123.33
1	F	117	ILE	N-CA-CB	-6.53	100.46	111.23
1	F	3	ASN	CA-C-O	6.53	126.59	119.15
1	D	65	VAL	N-CA-C	6.52	116.55	110.42
1	F	115	ASN	OD1-CG-ND2	6.52	129.12	122.60
1	C	140	VAL	CG1-CB-CG2	6.52	125.14	110.80
1	A	3	ASN	CB-CA-C	-6.51	96.99	109.95
1	F	81	LEU	CB-CA-C	-6.50	100.08	109.84
1	E	23	GLU	CB-CA-C	-6.50	100.62	110.90
1	F	5	GLU	N-CA-C	-6.50	99.42	109.76
1	F	26	LYS	N-CA-C	6.50	119.19	111.71
1	A	61	PHE	CA-C-N	-6.50	110.89	120.38
1	A	61	PHE	C-N-CA	-6.50	110.89	120.38
1	A	80	GLY	O-C-N	-6.50	116.13	123.67
1	A	35	LEU	O-C-N	6.50	131.27	122.82
1	D	104	ILE	CA-C-O	6.49	127.48	120.47
1	F	148	ASN	O-C-N	6.49	130.45	122.34
1	B	126	ALA	CA-C-O	6.49	129.79	120.51
1	F	106	GLY	CA-C-N	-6.49	109.58	121.52
1	F	106	GLY	C-N-CA	-6.49	109.58	121.52
1	A	35	LEU	CA-C-O	-6.48	113.28	120.60
1	D	118	HIS	O-C-N	6.48	131.27	123.36
1	A	20	LEU	N-CA-C	6.48	121.02	113.18
1	E	55	LEU	N-CA-CB	6.48	121.72	109.93
1	F	26	LYS	CB-CG-CD	-6.48	96.40	111.30
1	A	149	TRP	N-CA-C	-6.47	105.51	113.41
1	A	115	ASN	CA-C-O	-6.47	111.26	120.51
1	D	89	VAL	CA-CB-CG2	-6.47	99.40	110.40
1	F	148	ASN	N-CA-CB	6.46	120.06	110.49
1	D	135	HIS	C-N-CD	-6.45	98.54	125.00
1	F	129	GLU	O-C-N	6.45	129.51	122.15
1	E	137	GLU	O-C-N	6.45	130.87	122.42
1	B	111	GLN	CB-CG-CD	-6.45	101.63	112.60
1	C	58	ARG	NE-CZ-NH1	6.45	127.95	121.50
1	E	139	LEU	O-C-N	6.45	130.80	122.87
1	C	48	LEU	CB-CA-C	6.45	121.12	110.81
1	A	121	ASP	CB-CA-C	-6.44	97.77	110.27
1	F	77	VAL	O-C-N	6.44	129.99	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	31	LYS	O-C-N	-6.44	114.29	122.34
1	E	22	GLY	CA-C-N	6.44	129.19	120.44
1	E	22	GLY	C-N-CA	6.44	129.19	120.44
1	A	146	ALA	CA-C-O	6.43	127.22	119.43
1	B	134	PHE	CA-CB-CG	6.43	120.23	113.80
1	D	9	ILE	N-CA-C	6.43	117.09	107.51
1	E	102	GLY	CA-C-O	6.42	126.14	119.27
1	C	38	MET	CA-C-O	-6.42	113.80	120.99
1	F	10	ALA	N-CA-CB	-6.42	99.90	110.68
1	C	93	GLU	CA-CB-CG	-6.41	101.28	114.10
1	D	35	LEU	CA-C-N	-6.41	112.35	120.56
1	D	35	LEU	C-N-CA	-6.41	112.35	120.56
1	A	5	GLU	CA-C-N	6.41	133.57	122.81
1	A	5	GLU	C-N-CA	6.41	133.57	122.81
1	C	87	GLY	O-C-N	-6.41	115.55	122.73
1	B	141	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	C	132	LEU	O-C-N	-6.40	113.85	122.43
1	C	7	THR	CA-CB-CG2	-6.39	99.63	110.50
1	D	19	GLY	CA-C-N	-6.39	112.63	122.60
1	D	19	GLY	C-N-CA	-6.39	112.63	122.60
1	D	33	PHE	CA-C-N	-6.39	113.13	122.65
1	D	33	PHE	C-N-CA	-6.39	113.13	122.65
1	F	69	HIS	CA-C-N	-6.39	109.96	121.14
1	F	69	HIS	C-N-CA	-6.39	109.96	121.14
1	D	53	ILE	CA-C-O	6.38	127.77	119.85
1	C	90	MET	CA-C-N	6.38	129.35	120.29
1	C	90	MET	C-N-CA	6.38	129.35	120.29
1	B	15	GLY	N-CA-C	-6.38	104.61	112.77
1	B	92	GLY	N-CA-C	-6.38	102.64	111.76
1	B	24	ILE	O-C-N	-6.38	115.37	121.94
1	C	47	LEU	N-CA-CB	6.38	119.31	110.07
1	D	40	PHE	O-C-N	6.38	130.49	123.22
1	B	120	SER	CA-C-N	-6.37	112.47	122.73
1	B	120	SER	C-N-CA	-6.37	112.47	122.73
1	D	62	ALA	O-C-N	6.37	131.06	122.59
1	A	51	HIS	CA-CB-CG	-6.37	107.43	113.80
1	E	108	PHE	CA-C-N	-6.37	110.91	121.80
1	E	108	PHE	C-N-CA	-6.37	110.91	121.80
1	F	97	ALA	N-CA-C	6.36	118.30	111.36
1	D	28	PHE	CE1-CZ-CE2	-6.36	108.55	120.00
1	C	138	GLU	CB-CG-CD	-6.36	101.79	112.60
1	D	91	LEU	CA-C-N	6.36	133.87	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	91	LEU	C-N-CA	6.36	133.87	121.41
1	C	50	GLU	N-CA-C	-6.35	104.36	111.28
1	B	88	ARG	NH1-CZ-NH2	6.35	127.55	119.30
1	C	23	GLU	CA-C-N	6.35	128.63	120.70
1	C	23	GLU	C-N-CA	6.35	128.63	120.70
1	E	110	ILE	N-CA-C	6.34	122.54	109.34
1	C	56	LYS	CB-CA-C	6.34	122.36	110.63
1	B	72	PRO	N-CD-CG	6.33	112.70	103.20
1	E	62	ALA	N-CA-C	6.33	121.82	111.37
1	A	128	LYS	O-C-N	6.33	128.93	122.09
1	E	92	GLY	CA-C-N	6.33	129.86	120.87
1	E	92	GLY	C-N-CA	6.33	129.86	120.87
1	F	13	PRO	CA-C-O	6.33	128.23	119.18
1	E	14	ASP	N-CA-C	-6.32	104.83	112.54
1	F	122	SER	O-C-N	6.32	130.18	123.42
1	D	120	SER	O-C-N	-6.32	115.19	122.89
1	A	11	ILE	N-CA-CB	-6.31	103.55	111.31
1	E	147	GLN	OE1-CD-NE2	-6.31	116.29	122.60
1	E	112	VAL	CB-CA-C	-6.31	103.63	111.70
1	A	134	PHE	N-CA-C	6.31	119.42	108.76
1	E	129	GLU	N-CA-C	-6.31	104.50	111.82
1	B	141	ASN	CA-C-N	6.30	132.58	121.80
1	B	141	ASN	C-N-CA	6.30	132.58	121.80
1	E	35	LEU	O-C-N	6.30	130.38	123.13
1	B	148	ASN	CB-CA-C	-6.30	97.31	110.17
1	A	112	VAL	N-CA-CB	6.30	119.10	110.54
1	E	116	ILE	CA-C-N	-6.29	110.64	121.97
1	E	116	ILE	C-N-CA	-6.29	110.64	121.97
1	D	143	LYS	CA-CB-CG	6.29	126.68	114.10
1	A	90	MET	N-CA-CB	6.29	120.08	110.14
1	E	24	ILE	CA-C-O	6.29	127.49	120.95
1	F	63	GLY	CA-C-O	6.29	127.33	120.66
1	B	46	ASP	CA-C-O	6.29	127.10	119.31
1	D	38	MET	CB-CA-C	-6.28	97.92	110.42
1	E	65	VAL	N-CA-CB	6.28	117.47	110.62
1	F	99	SER	CB-CA-C	-6.28	99.73	110.22
1	B	118	HIS	CB-CA-C	-6.28	96.57	109.94
1	C	114	ARG	CB-CG-CD	6.27	125.73	111.30
1	F	9	ILE	CB-CA-C	-6.27	101.95	110.42
1	F	10	ALA	CB-CA-C	6.27	121.19	109.71
1	F	133	TRP	N-CA-CB	6.27	119.77	110.49
1	D	98	ASP	O-C-N	6.26	131.30	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	10	ALA	CB-CA-C	-6.26	97.41	109.37
1	A	46	ASP	O-C-N	6.26	130.92	122.59
1	E	140	VAL	N-CA-CB	6.26	121.44	110.49
1	B	25	ILE	N-CA-CB	-6.26	102.65	110.47
1	C	150	ILE	CB-CA-C	-6.25	103.73	111.92
1	D	143	LYS	CB-CA-C	6.25	119.76	110.14
1	A	35	LEU	CB-CA-C	-6.25	100.34	110.77
1	D	58	ARG	N-CA-C	6.25	119.39	109.40
1	C	106	GLY	O-C-N	-6.24	114.59	122.70
1	C	24	ILE	CA-CB-CG2	-6.23	99.91	110.50
1	C	29	GLU	CA-C-N	-6.23	109.43	121.58
1	C	29	GLU	C-N-CA	-6.23	109.43	121.58
1	D	137	GLU	CB-CG-CD	6.23	123.20	112.60
1	F	137	GLU	CB-CG-CD	6.23	123.20	112.60
1	A	31	LYS	N-CA-CB	6.23	121.02	110.49
1	A	110	ILE	CA-CB-CG2	-6.23	99.91	110.50
1	D	69	HIS	CA-C-N	6.22	128.94	120.54
1	D	69	HIS	C-N-CA	6.22	128.94	120.54
1	E	93	GLU	CA-CB-CG	-6.22	101.66	114.10
1	D	25	ILE	CA-CB-CG1	6.22	120.97	110.40
1	C	139	LEU	CA-C-O	6.21	128.35	121.39
1	B	151	TYR	O-C-N	6.21	131.31	123.23
1	E	95	ASN	CA-C-N	6.21	125.90	119.56
1	E	95	ASN	C-N-CA	6.21	125.90	119.56
1	A	15	GLY	CA-C-O	6.21	127.44	121.05
1	B	88	ARG	NE-CZ-NH1	-6.21	115.29	121.50
1	D	18	ARG	NH1-CZ-NH2	-6.21	111.23	119.30
1	C	35	LEU	CB-CA-C	-6.20	99.73	109.84
1	B	17	GLN	CB-CG-CD	6.20	123.14	112.60
1	B	77	VAL	N-CA-CB	6.20	119.27	111.46
1	C	76	MET	CB-CA-C	-6.20	98.81	110.16
1	E	105	ARG	NE-CZ-NH1	6.20	127.70	121.50
1	A	142	TYR	CA-C-N	6.20	131.73	123.05
1	A	142	TYR	C-N-CA	6.20	131.73	123.05
1	A	41	MET	CB-CA-C	-6.20	99.51	111.78
1	D	64	LEU	CB-CA-C	-6.19	100.51	110.79
1	C	111	GLN	O-C-N	-6.19	116.28	123.27
1	E	115	ASN	CB-CG-OD1	-6.19	108.43	120.80
1	A	45	GLU	N-CA-CB	6.18	119.21	110.12
1	B	10	ALA	CA-C-O	-6.18	113.68	120.24
1	B	116	ILE	CA-CB-CG1	-6.18	99.89	110.40
1	F	69	HIS	CA-CB-CG	-6.18	107.61	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2	ALA	N-CA-CB	6.18	119.67	110.40
1	E	107	ASP	O-C-N	6.18	130.61	122.33
1	A	114	ARG	NE-CZ-NH2	-6.17	113.64	119.20
1	F	128	LYS	N-CA-CB	-6.17	100.74	109.94
1	D	64	LEU	CA-C-O	6.17	127.09	120.55
1	F	146	ALA	CA-C-N	-6.17	110.42	120.72
1	F	146	ALA	C-N-CA	-6.17	110.42	120.72
1	D	4	SER	N-CA-C	-6.16	103.46	113.19
1	E	143	LYS	CA-C-O	-6.16	113.93	120.40
1	A	139	LEU	CA-C-N	6.16	133.05	121.97
1	A	139	LEU	C-N-CA	6.16	133.05	121.97
1	C	146	ALA	N-CA-CB	-6.16	101.36	110.53
1	D	98	ASP	N-CA-C	6.16	120.79	113.28
1	C	91	LEU	O-C-N	-6.15	115.13	122.15
1	D	140	VAL	CA-C-N	-6.15	114.84	122.84
1	D	140	VAL	C-N-CA	-6.15	114.84	122.84
1	E	41	MET	CA-C-O	-6.15	114.23	121.06
1	F	73	VAL	CG1-CB-CG2	6.15	124.33	110.80
1	D	151	TYR	CA-C-N	6.15	132.77	121.70
1	D	151	TYR	C-N-CA	6.15	132.77	121.70
1	C	30	GLN	N-CA-C	6.15	120.62	113.18
1	D	40	PHE	CB-CA-C	-6.14	100.24	110.19
1	F	112	VAL	CB-CA-C	-6.14	101.22	111.29
1	D	116	ILE	CA-C-O	6.14	128.46	120.78
1	E	104	ILE	CA-CB-CG1	6.14	120.84	110.40
1	A	33	PHE	CA-C-N	6.14	131.64	123.05
1	A	33	PHE	C-N-CA	6.14	131.64	123.05
1	C	91	LEU	CA-C-N	6.14	130.93	121.42
1	C	91	LEU	C-N-CA	6.14	130.93	121.42
1	F	127	GLU	N-CA-C	6.13	117.76	111.14
1	F	63	GLY	CA-C-N	6.13	133.24	121.54
1	F	63	GLY	C-N-CA	6.13	133.24	121.54
1	A	6	ARG	CA-CB-CG	-6.12	101.87	114.10
1	D	47	LEU	CB-CA-C	-6.11	100.59	110.74
1	E	61	PHE	CA-CB-CG	6.11	119.91	113.80
1	C	58	ARG	NE-CZ-NH2	-6.11	113.70	119.20
1	C	132	LEU	CA-C-N	-6.11	110.28	121.52
1	C	132	LEU	C-N-CA	-6.11	110.28	121.52
1	B	152	GLU	N-CA-CB	6.11	120.88	110.50
1	C	83	VAL	CA-CB-CG2	6.10	120.78	110.40
1	C	111	GLN	N-CA-C	6.10	119.19	109.24
1	A	33	PHE	N-CA-C	6.10	118.58	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	ASN	CB-CG-ND2	6.10	125.55	116.40
1	B	48	LEU	N-CA-C	-6.09	97.82	110.80
1	E	146	ALA	CA-C-N	6.09	129.28	120.38
1	E	146	ALA	C-N-CA	6.09	129.28	120.38
1	A	29	GLU	CA-C-N	-6.09	110.94	121.66
1	A	29	GLU	C-N-CA	-6.09	110.94	121.66
1	F	103	THR	O-C-N	6.09	129.81	122.68
1	A	98	ASP	CA-C-N	-6.08	112.43	120.95
1	A	98	ASP	C-N-CA	-6.08	112.43	120.95
1	B	122	SER	O-C-N	6.08	129.48	123.46
1	D	121	ASP	N-CA-C	6.08	120.83	113.17
1	E	38	MET	O-C-N	-6.08	116.67	123.48
1	A	92	GLY	CA-C-O	-6.08	117.72	122.52
1	A	140	VAL	CA-CB-CG2	6.08	120.74	110.40
1	A	128	LYS	N-CA-C	-6.07	104.58	111.14
1	C	133	TRP	CA-C-O	6.07	126.70	119.60
1	F	67	TYR	N-CA-CB	-6.07	101.21	110.01
1	E	145	CYS	CA-C-O	6.06	126.87	119.11
1	E	29	GLU	CA-C-N	-6.06	110.54	121.14
1	E	29	GLU	C-N-CA	-6.06	110.54	121.14
1	D	127	GLU	O-C-N	6.06	130.55	122.43
1	E	11	ILE	N-CA-CB	-6.06	103.72	110.99
1	F	29	GLU	CA-C-O	6.05	129.17	120.51
1	F	104	ILE	CA-CB-CG2	-6.05	100.22	110.50
1	B	102	GLY	O-C-N	6.04	130.56	122.70
1	B	127	GLU	CA-C-N	-6.04	112.39	120.79
1	B	127	GLU	C-N-CA	-6.04	112.39	120.79
1	C	19	GLY	O-C-N	-6.04	114.85	122.70
1	F	144	SER	CB-CA-C	-6.04	98.43	109.54
1	A	18	ARG	NE-CZ-NH2	6.04	124.63	119.20
1	A	103	THR	CA-CB-OG1	6.04	118.66	109.60
1	D	27	ARG	NE-CZ-NH1	6.03	127.53	121.50
1	F	129	GLU	N-CA-C	6.03	117.94	111.36
1	A	141	ASN	CA-CB-CG	6.03	118.63	112.60
1	B	40	PHE	CA-CB-CG	-6.03	107.77	113.80
1	B	47	LEU	N-CA-CB	-6.03	101.21	110.13
1	E	41	MET	N-CA-CB	-6.02	101.52	111.69
1	F	27	ARG	CG-CD-NE	6.02	125.23	112.00
1	C	29	GLU	CG-CD-OE1	-6.01	104.57	118.40
1	E	52	TYR	N-CA-C	-6.01	105.12	112.88
1	D	78	TRP	CA-C-N	-6.01	113.37	122.81
1	D	78	TRP	C-N-CA	-6.01	113.37	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	25	ILE	CA-C-N	-6.01	111.63	120.28
1	E	25	ILE	C-N-CA	-6.01	111.63	120.28
1	D	35	LEU	N-CA-CB	6.00	118.93	110.24
1	C	98	ASP	N-CA-CB	-5.99	101.05	110.46
1	A	7	THR	CA-C-N	-5.99	114.56	123.00
1	A	7	THR	C-N-CA	-5.99	114.56	123.00
1	B	61	PHE	CA-C-O	5.99	129.07	120.51
1	F	47	LEU	CA-C-N	-5.99	111.67	121.19
1	F	47	LEU	C-N-CA	-5.99	111.67	121.19
1	B	127	GLU	N-CA-C	5.98	118.29	111.11
1	F	6	ARG	N-CA-CB	5.98	120.42	110.85
1	A	138	GLU	N-CA-C	-5.97	104.69	111.14
1	A	140	VAL	O-C-N	-5.97	115.10	122.57
1	D	6	ARG	CA-CB-CG	-5.97	102.17	114.10
1	B	93	GLU	CA-C-O	-5.96	114.20	120.58
1	E	73	VAL	CA-C-O	-5.96	115.59	121.67
1	E	134	PHE	N-CA-C	5.96	119.26	109.72
1	A	29	GLU	CB-CA-C	-5.96	99.23	110.67
1	C	79	GLU	O-C-N	5.96	130.94	123.19
1	E	118	HIS	CB-CA-C	-5.96	99.67	109.80
1	A	96	PRO	CB-CA-C	5.96	121.39	111.56
1	C	107	ASP	N-CA-C	5.96	120.55	113.28
1	E	64	LEU	O-C-N	5.96	128.21	122.07
1	D	54	ASP	O-C-N	5.96	130.68	122.46
1	F	120	SER	N-CA-CB	5.96	120.55	110.49
1	F	48	LEU	N-CA-CB	-5.95	99.60	109.72
1	A	34	ARG	NH1-CZ-NH2	-5.95	111.56	119.30
1	C	137	GLU	O-C-N	5.95	130.03	122.65
1	E	121	ASP	N-CA-C	5.95	120.27	112.89
1	D	77	VAL	CB-CA-C	-5.95	101.65	110.33
1	A	5	GLU	CB-CG-CD	-5.94	102.50	112.60
1	B	129	GLU	CB-CA-C	-5.93	98.95	110.46
1	A	49	LYS	CA-CB-CG	-5.92	102.25	114.10
1	D	81	LEU	N-CA-C	5.92	117.67	109.15
1	E	18	ARG	CD-NE-CZ	5.92	132.69	124.40
1	F	91	LEU	CD1-CG-CD2	-5.92	97.78	110.80
1	C	123	VAL	CA-C-N	-5.91	111.32	120.31
1	C	123	VAL	C-N-CA	-5.91	111.32	120.31
1	B	101	PRO	N-CA-CB	5.91	108.57	103.31
1	B	138	GLU	CA-C-O	5.91	126.43	119.28
1	E	124	GLU	N-CA-C	-5.91	104.47	111.03
1	F	85	LYS	CA-C-O	5.91	127.53	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	98	ASP	CA-C-N	5.90	130.27	122.42
1	C	98	ASP	C-N-CA	5.90	130.27	122.42
1	C	13	PRO	CA-C-O	5.89	129.05	119.86
1	A	27	ARG	NE-CZ-NH1	5.89	127.39	121.50
1	C	130	ILE	N-CA-CB	5.89	120.95	111.23
1	F	138	GLU	O-C-N	5.89	129.37	122.24
1	D	12	LYS	CA-C-N	-5.89	112.48	119.84
1	D	12	LYS	C-N-CA	-5.89	112.48	119.84
1	B	73	VAL	CA-CB-CG1	-5.89	100.39	110.40
1	F	16	VAL	N-CA-C	-5.89	104.62	110.62
1	F	108	PHE	N-CA-CB	-5.89	101.27	110.98
1	B	105	ARG	N-CA-C	-5.88	104.78	111.07
1	D	29	GLU	O-C-N	-5.88	115.08	122.20
1	E	112	VAL	N-CA-CB	5.88	116.79	110.62
1	F	101	PRO	N-CA-CB	5.88	108.80	103.33
1	B	17	GLN	CB-CA-C	-5.88	100.86	110.85
1	F	83	VAL	CB-CA-C	-5.88	104.32	112.02
1	C	6	ARG	CB-CG-CD	5.87	124.81	111.30
1	A	20	LEU	CA-C-O	5.87	126.62	119.11
1	F	100	LYS	CA-C-O	5.87	127.32	120.69
1	B	31	LYS	CA-C-N	-5.87	112.59	121.51
1	B	31	LYS	C-N-CA	-5.87	112.59	121.51
1	A	76	MET	N-CA-C	5.87	117.88	109.14
1	B	133	TRP	CD2-CE2-CZ2	-5.86	116.54	122.40
1	C	3	ASN	N-CA-CB	5.86	118.97	110.47
1	D	29	GLU	CB-CA-C	-5.86	101.11	110.84
1	F	124	GLU	CA-CB-CG	-5.86	102.38	114.10
1	C	44	SER	CA-C-O	5.86	128.66	121.87
1	F	133	TRP	CB-CA-C	-5.85	100.31	110.09
1	D	29	GLU	N-CA-CB	5.85	119.67	109.72
1	B	118	HIS	ND1-CE1-NE2	5.84	114.24	108.40
1	F	44	SER	N-CA-CB	5.84	120.90	110.80
1	C	3	ASN	CA-C-N	-5.83	111.89	122.50
1	C	3	ASN	C-N-CA	-5.83	111.89	122.50
1	D	88	ARG	CD-NE-CZ	5.83	132.56	124.40
1	A	125	SER	N-CA-C	-5.83	104.12	111.11
1	D	50	GLU	N-CA-C	-5.83	104.83	111.07
1	E	34	ARG	N-CA-C	5.82	119.74	109.96
1	A	3	ASN	O-C-N	5.82	130.93	122.43
1	D	114	ARG	NE-CZ-NH2	-5.81	113.97	119.20
1	D	95	ASN	O-C-N	5.81	126.72	120.85
1	C	84	VAL	CA-CB-CG2	-5.81	100.53	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	TRP	N-CA-C	5.80	119.97	113.01
1	C	20	LEU	CA-C-O	5.80	126.97	119.95
1	F	141	ASN	CA-C-O	5.80	126.57	120.36
1	A	26	LYS	O-C-N	5.80	128.12	122.09
1	B	135	HIS	N-CA-CB	5.80	117.83	110.23
1	B	94	THR	CA-CB-CG2	-5.80	100.64	110.50
1	F	16	VAL	CA-CB-CG1	5.80	120.25	110.40
1	E	82	ASN	N-CA-CB	5.79	120.28	110.49
1	D	117	ILE	O-C-N	5.79	129.60	123.00
1	C	118	HIS	CA-C-O	-5.79	114.34	121.11
1	B	97	ALA	O-C-N	5.79	130.24	122.49
1	C	99	SER	N-CA-C	5.79	117.72	108.41
1	C	151	TYR	CA-C-O	-5.79	114.58	120.71
1	C	73	VAL	CA-C-N	-5.78	115.23	123.10
1	C	73	VAL	C-N-CA	-5.78	115.23	123.10
1	C	34	ARG	NH1-CZ-NH2	-5.78	111.78	119.30
1	E	116	ILE	N-CA-C	5.78	121.36	109.34
1	C	101	PRO	CA-C-N	-5.77	113.51	122.86
1	C	101	PRO	C-N-CA	-5.77	113.51	122.86
1	E	10	ALA	O-C-N	-5.77	115.73	123.23
1	E	115	ASN	CB-CG-ND2	5.77	125.05	116.40
1	A	3	ASN	N-CA-CB	5.76	120.09	110.41
1	A	99	SER	CA-CB-OG	-5.76	99.57	111.10
1	B	65	VAL	O-C-N	5.76	127.53	121.89
1	A	23	GLU	CB-CA-C	-5.75	101.84	110.88
1	F	147	GLN	CA-C-N	-5.75	113.05	122.54
1	F	147	GLN	C-N-CA	-5.75	113.05	122.54
1	D	37	ALA	N-CA-C	5.75	117.82	109.07
1	C	35	LEU	O-C-N	5.75	129.76	123.04
1	C	58	ARG	CD-NE-CZ	5.75	132.44	124.40
1	C	93	GLU	CG-CD-OE2	-5.74	105.19	118.40
1	B	133	TRP	CB-CG-CD2	-5.74	118.76	126.80
1	D	47	LEU	CA-C-O	5.74	127.35	120.92
1	D	73	VAL	CA-C-O	-5.74	113.60	120.78
1	A	79	GLU	O-C-N	-5.74	116.50	123.27
1	A	38	MET	CG-SD-CE	-5.73	88.29	100.90
1	C	34	ARG	N-CA-CB	5.73	120.31	110.68
1	C	121	ASP	CA-C-O	5.73	126.31	119.60
1	C	105	ARG	O-C-N	5.73	128.22	122.03
1	A	23	GLU	O-C-N	5.72	127.97	122.07
1	A	105	ARG	CA-C-O	-5.72	114.35	120.42
1	F	110	ILE	CB-CA-C	-5.72	105.81	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	112	VAL	O-C-N	5.72	129.72	122.57
1	C	149	TRP	N-CA-C	-5.72	98.62	110.80
1	F	88	ARG	CA-CB-CG	-5.72	102.67	114.10
1	B	108	PHE	N-CA-CB	-5.71	103.05	111.51
1	B	109	CYS	CB-CA-C	5.71	120.03	110.43
1	F	5	GLU	CG-CD-OE2	-5.71	105.26	118.40
1	C	112	VAL	CB-CA-C	-5.71	101.92	111.29
1	D	64	LEU	N-CA-C	-5.71	105.05	111.28
1	D	139	LEU	CA-C-N	5.71	129.75	121.18
1	D	139	LEU	C-N-CA	5.71	129.75	121.18
1	A	53	ILE	CB-CG1-CD1	-5.71	101.81	113.80
1	B	25	ILE	CA-CB-CG2	5.71	120.20	110.50
1	C	45	GLU	CB-CG-CD	-5.71	102.90	112.60
1	A	92	GLY	N-CA-C	-5.70	105.43	112.33
1	F	132	LEU	CB-CG-CD1	-5.70	93.59	110.70
1	F	62	ALA	CB-CA-C	5.70	122.69	110.21
1	C	151	TYR	O-C-N	5.69	130.44	123.21
1	B	8	PHE	CA-C-O	5.69	126.46	120.54
1	F	47	LEU	N-CA-C	-5.69	104.99	111.14
1	F	42	ARG	NE-CZ-NH2	-5.69	114.08	119.20
1	A	14	ASP	O-C-N	5.68	128.23	122.09
1	F	93	GLU	N-CA-C	-5.68	101.22	110.20
1	D	60	PHE	N-CA-C	5.68	117.15	111.07
1	E	99	SER	N-CA-C	5.68	118.68	110.28
1	F	148	ASN	CA-CB-CG	5.68	118.28	112.60
1	B	9	ILE	CB-CA-C	-5.68	102.37	110.83
1	C	150	ILE	CA-C-N	-5.68	114.70	122.93
1	C	150	ILE	C-N-CA	-5.68	114.70	122.93
1	B	25	ILE	CB-CA-C	-5.67	104.61	112.04
1	D	27	ARG	CG-CD-NE	5.67	124.48	112.00
1	C	108	PHE	CA-CB-CG	5.67	119.47	113.80
1	F	41	MET	CA-C-N	5.67	129.94	121.72
1	F	41	MET	C-N-CA	5.67	129.94	121.72
1	D	23	GLU	CB-CG-CD	5.67	122.24	112.60
1	B	108	PHE	CB-CG-CD2	-5.67	111.07	120.70
1	D	135	HIS	ND1-CG-CD2	5.67	111.77	106.10
1	C	86	THR	CA-CB-OG1	-5.67	101.10	109.60
1	A	15	GLY	O-C-N	-5.66	116.52	122.13
1	B	40	PHE	N-CA-C	-5.66	100.75	109.76
1	D	149	TRP	CB-CG-CD2	-5.66	118.87	126.80
1	F	90	MET	CA-C-N	5.66	127.80	120.44
1	F	90	MET	C-N-CA	5.66	127.80	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	22	GLY	O-C-N	-5.66	115.34	122.70
1	E	109	CYS	CA-C-O	-5.66	115.38	121.38
1	B	57	ASP	O-C-N	5.66	130.11	122.59
1	A	140	VAL	CA-C-O	5.65	127.85	120.78
1	E	66	LYS	N-CA-CB	-5.65	101.81	110.12
1	B	8	PHE	CB-CG-CD1	-5.65	111.10	120.70
1	D	68	MET	CG-SD-CE	5.65	113.33	100.90
1	D	53	ILE	CA-C-N	-5.64	110.00	121.18
1	D	53	ILE	C-N-CA	-5.64	110.00	121.18
1	F	65	VAL	CA-C-N	-5.64	112.77	120.44
1	F	65	VAL	C-N-CA	-5.64	112.77	120.44
1	C	131	ALA	CA-C-N	-5.64	111.30	120.72
1	C	131	ALA	C-N-CA	-5.64	111.30	120.72
1	D	37	ALA	CA-C-N	-5.64	110.78	121.54
1	D	37	ALA	C-N-CA	-5.64	110.78	121.54
1	E	31	LYS	O-C-N	5.64	128.09	122.12
1	D	143	LYS	N-CA-C	5.63	117.61	108.26
1	A	50	GLU	CB-CG-CD	-5.63	103.02	112.60
1	A	122	SER	CA-CB-OG	5.63	122.37	111.10
1	A	89	VAL	CA-C-O	-5.63	114.80	121.05
1	E	150	ILE	CA-C-N	-5.63	111.89	121.85
1	E	150	ILE	C-N-CA	-5.63	111.89	121.85
1	B	145	CYS	CB-CA-C	5.62	121.04	110.63
1	F	123	VAL	CG1-CB-CG2	-5.62	98.42	110.80
1	C	52	TYR	N-CA-CB	-5.62	102.66	110.65
1	C	132	LEU	CA-C-O	5.62	126.30	119.38
1	E	89	VAL	N-CA-C	-5.62	104.89	110.62
1	B	33	PHE	CA-C-O	-5.62	115.18	121.81
1	C	114	ARG	CA-C-O	-5.62	112.11	122.62
1	A	27	ARG	CB-CG-CD	-5.61	98.39	111.30
1	F	97	ALA	CA-C-O	-5.61	114.47	120.42
1	D	88	ARG	NE-CZ-NH1	5.61	127.11	121.50
1	A	4	SER	CA-CB-OG	-5.61	99.89	111.10
1	F	152	GLU	CB-CA-C	5.61	120.75	110.10
1	E	83	VAL	N-CA-CB	5.60	120.48	111.23
1	F	137	GLU	CG-CD-OE1	5.60	131.28	118.40
1	C	103	THR	O-C-N	-5.60	116.13	122.68
1	B	140	VAL	O-C-N	5.59	129.76	122.94
1	D	129	GLU	CA-C-N	-5.59	111.64	120.47
1	D	129	GLU	C-N-CA	-5.59	111.64	120.47
1	E	112	VAL	O-C-N	5.59	128.00	121.96
1	A	27	ARG	CG-CD-NE	5.59	124.29	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	LYS	CA-CB-CG	-5.59	102.92	114.10
1	D	94	THR	CA-C-O	5.58	126.34	120.42
1	A	88	ARG	NE-CZ-NH1	5.58	127.08	121.50
1	F	20	LEU	CA-C-O	5.58	125.42	119.34
1	D	79	GLU	N-CA-CB	5.58	120.62	111.08
1	D	78	TRP	O-C-N	-5.58	116.79	123.31
1	F	73	VAL	CA-C-N	-5.58	115.63	122.93
1	F	73	VAL	C-N-CA	-5.58	115.63	122.93
1	C	26	LYS	CG-CD-CE	5.57	124.11	111.30
1	B	72	PRO	N-CA-CB	5.56	109.52	103.23
1	B	94	THR	CA-CB-OG1	5.56	117.94	109.60
1	C	55	LEU	O-C-N	5.56	129.32	122.20
1	E	124	GLU	O-C-N	5.56	128.04	122.03
1	F	57	ASP	N-CA-C	5.56	118.42	111.24
1	D	133	TRP	CE2-CD2-CE3	5.56	124.36	118.80
1	B	27	ARG	CD-NE-CZ	-5.55	116.63	124.40
1	E	91	LEU	CB-CA-C	-5.54	101.47	110.79
1	B	123	VAL	CA-CB-CG1	5.54	119.82	110.40
1	C	66	LYS	CD-CE-NZ	5.54	129.64	111.90
1	D	11	ILE	CA-CB-CG2	5.54	119.92	110.50
1	A	49	LYS	N-CA-CB	5.54	119.59	110.39
1	A	133	TRP	CE2-CD2-CE3	5.54	124.34	118.80
1	C	15	GLY	CA-C-O	5.54	126.39	120.30
1	E	6	ARG	CB-CG-CD	5.54	124.04	111.30
1	A	96	PRO	CA-N-CD	-5.54	104.25	112.00
1	B	95	ASN	CB-CG-ND2	-5.54	108.10	116.40
1	D	76	MET	O-C-N	5.54	129.59	123.33
1	E	50	GLU	N-CA-CB	-5.54	101.95	110.20
1	D	12	LYS	CA-C-O	5.53	126.94	120.69
1	E	13	PRO	CB-CA-C	-5.53	103.58	112.21
1	F	33	PHE	N-CA-CB	-5.53	101.39	110.41
1	F	41	MET	O-C-N	5.53	129.88	123.41
1	A	77	VAL	CA-CB-CG2	5.53	119.80	110.40
1	E	149	TRP	CA-CB-CG	-5.53	103.09	113.60
1	F	6	ARG	O-C-N	-5.53	116.19	123.16
1	C	63	GLY	CA-C-N	5.53	132.10	121.54
1	C	63	GLY	C-N-CA	5.53	132.10	121.54
1	A	146	ALA	N-CA-CB	-5.53	102.45	110.47
1	B	34	ARG	N-CA-CB	5.53	119.49	110.37
1	E	87	GLY	O-C-N	-5.53	116.26	122.28
1	B	150	ILE	CB-CA-C	-5.53	106.20	111.06
1	C	137	GLU	CA-CB-CG	-5.52	103.06	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	6	ARG	CD-NE-CZ	-5.52	116.67	124.40
1	F	101	PRO	CA-C-O	5.52	128.40	121.67
1	A	149	TRP	CH2-CZ2-CE2	-5.51	110.33	117.50
1	A	30	GLN	O-C-N	5.51	130.01	122.46
1	B	6	ARG	CA-C-O	5.51	127.45	121.06
1	E	84	VAL	CA-C-N	5.51	127.94	120.44
1	E	84	VAL	C-N-CA	5.51	127.94	120.44
1	F	54	ASP	CA-CB-CG	5.51	118.11	112.60
1	C	34	ARG	CG-CD-NE	5.51	124.12	112.00
1	A	114	ARG	CB-CA-C	5.50	120.29	109.72
1	B	142	TYR	O-C-N	-5.50	117.48	123.26
1	C	127	GLU	N-CA-C	5.50	120.44	111.37
1	A	40	PHE	N-CA-CB	-5.49	101.48	110.43
1	E	51	HIS	CA-C-O	5.49	126.28	119.97
1	B	17	GLN	CA-C-O	5.49	126.24	120.42
1	B	145	CYS	N-CA-C	5.49	118.02	111.71
1	D	110	ILE	O-C-N	5.49	129.43	122.57
1	A	148	ASN	CB-CA-C	5.48	120.53	110.11
1	E	39	LYS	O-C-N	5.48	129.62	123.48
1	B	114	ARG	N-CA-CB	-5.48	104.21	110.35
1	C	83	VAL	N-CA-CB	5.48	120.28	111.23
1	E	45	GLU	CA-CB-CG	-5.48	103.14	114.10
1	D	11	ILE	CB-CG1-CD1	-5.48	102.29	113.80
1	D	79	GLU	N-CA-C	5.48	118.49	109.72
1	B	23	GLU	CA-C-O	5.48	127.09	121.07
1	A	46	ASP	CA-CB-CG	-5.47	107.13	112.60
1	A	147	GLN	N-CA-CB	-5.47	100.42	109.72
1	C	27	ARG	CG-CD-NE	5.47	124.03	112.00
1	E	74	VAL	CB-CA-C	5.47	118.53	110.77
1	E	94	THR	N-CA-CB	-5.47	100.87	109.78
1	A	77	VAL	N-CA-CB	5.46	120.43	111.58
1	A	149	TRP	CE2-CD2-CE3	5.46	124.27	118.80
1	C	94	THR	O-C-N	5.46	127.91	122.12
1	D	54	ASP	CA-C-N	5.46	130.95	122.49
1	D	54	ASP	C-N-CA	5.46	130.95	122.49
1	E	62	ALA	CA-C-O	5.46	127.03	120.92
1	A	76	MET	CA-C-N	-5.45	114.84	122.75
1	A	76	MET	C-N-CA	-5.45	114.84	122.75
1	F	53	ILE	CB-CA-C	-5.45	104.78	112.14
1	E	6	ARG	CA-C-N	-5.45	113.38	122.21
1	E	6	ARG	C-N-CA	-5.45	113.38	122.21
1	F	34	ARG	NH1-CZ-NH2	-5.45	112.21	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	27	ARG	NE-CZ-NH1	-5.45	116.05	121.50
1	D	94	THR	N-CA-CB	-5.45	102.10	110.16
1	E	84	VAL	N-CA-C	5.44	115.65	110.42
1	F	84	VAL	O-C-N	-5.44	115.77	122.57
1	B	133	TRP	O-C-N	-5.44	114.95	122.46
1	A	82	ASN	CA-C-O	-5.44	114.07	120.81
1	C	11	ILE	CA-C-O	-5.43	114.30	120.66
1	B	38	MET	CA-C-N	5.43	130.38	121.58
1	B	38	MET	C-N-CA	5.43	130.38	121.58
1	E	8	PHE	CA-C-N	-5.43	116.06	123.12
1	E	8	PHE	C-N-CA	-5.43	116.06	123.12
1	D	60	PHE	CA-CB-CG	-5.43	108.37	113.80
1	E	40	PHE	CA-C-O	-5.43	114.86	121.05
1	B	147	GLN	O-C-N	5.42	127.87	122.12
1	C	89	VAL	CA-C-O	5.42	126.59	120.95
1	D	46	ASP	CA-C-O	5.42	126.70	120.90
1	E	6	ARG	O-C-N	5.42	129.43	123.25
1	A	74	VAL	CB-CA-C	-5.42	103.05	110.96
1	B	151	TYR	CB-CG-CD1	5.42	128.93	120.80
1	C	114	ARG	CD-NE-CZ	-5.42	116.82	124.40
1	B	43	ALA	CA-C-O	-5.42	115.04	121.16
1	A	42	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	B	118	HIS	O-C-N	5.41	129.44	123.33
1	E	65	VAL	CA-CB-CG2	5.41	119.60	110.40
1	F	138	GLU	CA-C-N	5.41	131.84	122.32
1	F	138	GLU	C-N-CA	5.41	131.84	122.32
1	A	34	ARG	CG-CD-NE	5.41	123.90	112.00
1	A	118	HIS	CA-CB-CG	-5.41	108.39	113.80
1	F	11	ILE	N-CA-C	-5.41	100.63	108.36
1	A	114	ARG	NH1-CZ-NH2	5.41	126.33	119.30
1	C	102	GLY	O-C-N	-5.41	116.79	122.52
1	A	103	THR	O-C-N	5.40	129.51	123.19
1	B	37	ALA	CB-CA-C	-5.40	97.57	109.56
1	C	31	LYS	N-CA-CB	-5.40	102.14	110.13
1	D	27	ARG	O-C-N	5.40	129.25	122.23
1	F	8	PHE	CA-CB-CG	-5.39	108.41	113.80
1	F	110	ILE	CA-CB-CG2	-5.39	101.34	110.50
1	C	79	GLU	CB-CG-CD	5.38	121.75	112.60
1	D	79	GLU	CA-C-O	-5.38	115.03	121.11
1	A	81	LEU	CA-C-O	5.38	128.21	120.51
1	B	33	PHE	O-C-N	5.38	128.99	122.85
1	C	94	THR	CA-C-N	5.38	134.93	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	94	THR	C-N-CA	5.38	134.93	121.80
1	A	26	LYS	CA-C-O	5.38	126.66	120.90
1	B	105	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	D	17	GLN	N-CA-C	5.38	117.58	111.02
1	F	150	ILE	O-C-N	5.38	132.12	121.91
1	B	15	GLY	CA-C-N	-5.37	113.67	120.60
1	B	15	GLY	C-N-CA	-5.37	113.67	120.60
1	B	40	PHE	CA-C-O	-5.37	114.57	120.69
1	D	29	GLU	CA-C-N	-5.37	111.20	121.94
1	D	29	GLU	C-N-CA	-5.37	111.20	121.94
1	A	14	ASP	N-CA-CB	5.36	117.85	110.07
1	E	69	HIS	O-C-N	5.36	129.81	122.46
1	F	18	ARG	CD-NE-CZ	-5.36	116.89	124.40
1	A	69	HIS	O-C-N	5.36	129.96	122.36
1	C	54	ASP	CA-C-O	5.36	125.85	119.10
1	C	104	ILE	O-C-N	5.36	127.35	121.83
1	B	64	LEU	CA-C-O	5.35	128.17	120.51
1	B	137	GLU	CG-CD-OE2	-5.35	106.09	118.40
1	B	30	GLN	O-C-N	-5.35	115.38	122.33
1	B	106	GLY	CA-C-O	5.35	129.88	120.57
1	F	11	ILE	CA-C-O	-5.35	114.85	120.57
1	C	55	LEU	CA-C-N	-5.33	112.60	120.28
1	C	55	LEU	C-N-CA	-5.33	112.60	120.28
1	E	50	GLU	CA-C-N	5.33	128.42	120.31
1	E	50	GLU	C-N-CA	5.33	128.42	120.31
1	D	22	GLY	CA-C-O	5.33	129.84	120.57
1	E	38	MET	CA-C-N	-5.33	111.40	121.63
1	E	38	MET	C-N-CA	-5.33	111.40	121.63
1	B	126	ALA	O-C-N	-5.33	115.50	122.59
1	B	107	ASP	N-CA-C	5.32	117.89	111.40
1	D	68	MET	O-C-N	5.32	129.81	122.46
1	A	60	PHE	N-CA-C	5.32	117.77	111.33
1	B	138	GLU	CA-C-N	5.32	129.50	122.42
1	B	138	GLU	C-N-CA	5.32	129.50	122.42
1	D	97	ALA	N-CA-C	-5.32	105.56	111.36
1	B	121	ASP	CB-CG-OD2	-5.32	106.17	118.40
1	D	25	ILE	N-CA-CB	5.31	116.41	110.51
1	E	46	ASP	CA-C-O	5.31	128.11	120.51
1	E	132	LEU	CB-CA-C	-5.31	102.02	110.84
1	C	148	ASN	OD1-CG-ND2	5.31	127.91	122.60
1	E	130	ILE	CA-CB-CG1	5.31	119.42	110.40
1	D	27	ARG	N-CA-CB	-5.31	102.29	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	TRP	CD2-CE3-CZ3	-5.30	111.70	118.60
1	B	53	ILE	CA-C-N	5.30	127.34	120.44
1	B	53	ILE	C-N-CA	5.30	127.34	120.44
1	D	32	GLY	CA-C-N	-5.30	113.90	122.81
1	D	32	GLY	C-N-CA	-5.30	113.90	122.81
1	E	85	LYS	CA-C-N	5.30	127.92	120.28
1	E	85	LYS	C-N-CA	5.30	127.92	120.28
1	F	100	LYS	CA-C-N	-5.30	114.49	119.85
1	F	100	LYS	C-N-CA	-5.30	114.49	119.85
1	B	68	MET	CA-C-O	5.30	125.91	119.49
1	F	41	MET	CA-CB-CG	-5.30	103.50	114.10
1	C	114	ARG	CG-CD-NE	-5.30	100.34	112.00
1	B	86	THR	CA-C-O	5.30	126.16	120.55
1	E	34	ARG	CA-CB-CG	5.30	124.69	114.10
1	B	145	CYS	N-CA-CB	-5.29	102.07	110.22
1	C	129	GLU	N-CA-C	-5.29	105.41	111.07
1	F	108	PHE	CB-CA-C	-5.29	101.53	110.64
1	B	76	MET	N-CA-CB	5.29	121.35	111.52
1	C	83	VAL	CB-CA-C	-5.29	102.62	111.29
1	A	6	ARG	N-CA-C	5.29	118.20	109.85
1	D	58	ARG	NE-CZ-NH2	-5.28	114.44	119.20
1	D	49	LYS	CA-C-N	5.28	127.31	120.44
1	D	49	LYS	C-N-CA	5.28	127.31	120.44
1	B	91	LEU	CB-CA-C	-5.28	101.04	110.70
1	C	11	ILE	O-C-N	5.28	129.79	122.88
1	E	17	GLN	CG-CD-OE1	5.27	131.35	120.80
1	A	45	GLU	O-C-N	5.27	127.70	122.12
1	A	124	GLU	O-C-N	5.27	127.72	122.03
1	D	84	VAL	CA-CB-CG2	5.27	119.35	110.40
1	D	92	GLY	N-CA-C	-5.26	100.71	113.18
1	F	65	VAL	CA-CB-CG2	-5.26	101.46	110.40
1	A	49	LYS	N-CA-C	5.26	118.95	112.54
1	D	111	GLN	N-CA-C	5.26	117.97	109.40
1	D	152	GLU	CA-C-O	-5.26	105.23	121.00
1	B	81	LEU	N-CA-CB	-5.25	100.66	109.28
1	E	152	GLU	CA-CB-CG	-5.25	103.59	114.10
1	A	133	TRP	CA-C-N	-5.25	114.65	122.74
1	A	133	TRP	C-N-CA	-5.25	114.65	122.74
1	C	80	GLY	O-C-N	5.25	129.65	123.61
1	E	68	MET	CA-CB-CG	-5.25	103.60	114.10
1	F	65	VAL	O-C-N	-5.25	116.75	121.89
1	D	115	ASN	N-CA-CB	-5.25	103.59	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	30	GLN	CA-C-N	-5.25	113.88	122.54
1	F	30	GLN	C-N-CA	-5.25	113.88	122.54
1	F	67	TYR	CB-CG-CD1	5.24	128.66	120.80
1	D	136	PRO	N-CD-CG	-5.24	95.34	103.20
1	E	67	TYR	N-CA-C	-5.24	105.48	111.14
1	F	96	PRO	CA-C-O	5.24	130.13	120.60
1	E	50	GLU	CB-CA-C	5.24	120.28	110.70
1	F	5	GLU	CA-C-O	-5.24	114.72	120.69
1	B	121	ASP	CB-CG-OD1	5.23	130.44	118.40
1	D	82	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	A	11	ILE	CA-CB-CG1	5.23	119.30	110.40
1	A	144	SER	O-C-N	-5.23	116.50	122.93
1	C	134	PHE	CA-C-O	5.23	126.72	120.28
1	A	93	GLU	CB-CG-CD	5.23	121.49	112.60
1	F	132	LEU	CB-CG-CD2	5.23	126.39	110.70
1	B	32	GLY	N-CA-C	5.22	123.05	115.32
1	A	104	ILE	CB-CA-C	5.22	119.86	111.29
1	B	48	LEU	CB-CG-CD1	5.22	126.36	110.70
1	C	5	GLU	N-CA-C	-5.22	102.55	110.28
1	F	48	LEU	CB-CA-C	5.22	119.51	110.84
1	B	122	SER	N-CA-CB	5.21	119.49	111.56
1	F	142	TYR	CA-C-O	-5.21	115.61	121.40
1	A	150	ILE	CA-C-O	-5.21	114.62	120.25
1	E	99	SER	CA-CB-OG	-5.21	100.68	111.10
1	F	12	LYS	O-C-N	5.21	128.52	121.12
1	F	108	PHE	CA-C-N	-5.21	112.73	121.75
1	F	108	PHE	C-N-CA	-5.21	112.73	121.75
1	A	68	MET	CG-SD-CE	5.21	112.36	100.90
1	F	15	GLY	N-CA-C	-5.21	100.83	113.18
1	B	8	PHE	CA-CB-CG	-5.21	108.59	113.80
1	B	37	ALA	N-CA-CB	-5.21	101.85	111.53
1	D	89	VAL	CA-CB-CG1	5.21	119.25	110.40
1	C	133	TRP	N-CA-C	5.20	119.72	112.90
1	C	151	TYR	N-CA-CB	5.20	119.07	110.69
1	D	41	MET	N-CA-C	5.20	116.98	109.07
1	E	9	ILE	CA-C-N	-5.20	115.14	122.94
1	E	9	ILE	C-N-CA	-5.20	115.14	122.94
1	C	89	VAL	O-C-N	-5.19	116.83	121.87
1	D	134	PHE	CA-C-N	5.19	128.47	121.20
1	D	134	PHE	C-N-CA	5.19	128.47	121.20
1	F	126	ALA	CB-CA-C	-5.19	102.17	110.79
1	C	19	GLY	CA-C-N	-5.19	114.34	122.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	19	GLY	C-N-CA	-5.19	114.34	122.49
1	C	101	PRO	CA-N-CD	-5.19	104.73	112.00
1	C	14	ASP	CB-CG-OD1	5.19	130.33	118.40
1	C	56	LYS	CA-C-O	5.19	125.96	120.10
1	E	35	LEU	CB-CG-CD2	5.19	126.26	110.70
1	A	149	TRP	CA-CB-CG	-5.18	103.75	113.60
1	A	14	ASP	CA-C-N	5.18	125.84	119.99
1	A	14	ASP	C-N-CA	5.18	125.84	119.99
1	F	88	ARG	O-C-N	5.18	127.47	122.09
1	B	136	PRO	N-CA-CB	-5.17	97.82	103.25
1	F	5	GLU	O-C-N	5.17	129.09	123.04
1	A	13	PRO	CA-N-CD	-5.17	104.76	112.00
1	A	78	TRP	CA-C-O	-5.17	115.06	120.80
1	B	61	PHE	N-CA-CB	5.17	119.23	110.49
1	A	111	GLN	N-CA-C	5.17	117.99	109.72
1	F	121	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	46	ASP	CA-C-N	-5.17	112.08	120.71
1	B	46	ASP	C-N-CA	-5.17	112.08	120.71
1	D	94	THR	OG1-CB-CG2	-5.16	98.97	109.30
1	C	141	ASN	O-C-N	5.16	129.36	123.27
1	C	148	ASN	N-CA-C	5.16	119.07	112.26
1	E	127	GLU	CA-C-O	-5.16	115.08	120.55
1	C	127	GLU	CG-CD-OE1	5.16	130.26	118.40
1	D	128	LYS	O-C-N	5.16	127.38	122.07
1	F	101	PRO	CA-C-N	-5.16	115.21	123.31
1	F	101	PRO	C-N-CA	-5.16	115.21	123.31
1	D	32	GLY	O-C-N	-5.15	116.00	122.70
1	F	85	LYS	CA-C-N	-5.15	112.97	120.29
1	F	85	LYS	C-N-CA	-5.15	112.97	120.29
1	A	122	SER	N-CA-CB	5.15	120.26	111.66
1	F	67	TYR	CA-CB-CG	-5.15	104.64	113.90
1	F	92	GLY	CA-C-O	5.15	126.71	122.13
1	F	54	ASP	CA-C-O	5.15	125.72	119.49
1	A	53	ILE	N-CA-C	5.14	118.27	111.17
1	B	69	HIS	CB-CA-C	5.14	119.99	109.55
1	E	97	ALA	N-CA-C	-5.14	106.51	112.89
1	F	89	VAL	CA-C-O	5.14	126.40	121.05
1	B	36	VAL	CA-CB-CG1	-5.14	101.67	110.40
1	C	18	ARG	O-C-N	-5.14	115.76	122.59
1	F	139	LEU	CA-C-O	-5.14	115.65	121.66
1	F	88	ARG	CA-C-O	5.13	126.39	120.90
1	D	127	GLU	CG-CD-OE1	5.13	130.21	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	133	TRP	CD2-CE2-CZ2	-5.13	117.27	122.40
1	D	25	ILE	CA-C-N	5.13	130.53	120.99
1	D	25	ILE	C-N-CA	5.13	130.53	120.99
1	B	134	PHE	CB-CA-C	-5.13	99.42	110.45
1	C	139	LEU	O-C-N	-5.13	116.37	122.63
1	E	129	GLU	CA-C-N	-5.13	113.14	120.42
1	E	129	GLU	C-N-CA	-5.13	113.14	120.42
1	A	86	THR	CA-CB-OG1	5.13	117.29	109.60
1	C	33	PHE	O-C-N	5.13	128.83	123.03
1	C	39	LYS	N-CA-CB	-5.13	102.41	111.39
1	E	132	LEU	N-CA-C	-5.13	102.96	111.37
1	F	129	GLU	N-CA-CB	5.12	117.75	110.16
1	F	33	PHE	O-C-N	5.12	128.80	123.06
1	B	101	PRO	CA-C-N	-5.12	111.37	121.41
1	B	101	PRO	C-N-CA	-5.12	111.37	121.41
1	C	31	LYS	CA-CB-CG	5.12	124.34	114.10
1	E	28	PHE	N-CA-CB	5.12	117.44	110.01
1	B	86	THR	N-CA-C	5.12	116.86	111.28
1	C	88	ARG	N-CA-C	-5.12	106.72	113.12
1	D	123	VAL	CA-CB-CG2	5.12	119.11	110.40
1	A	114	ARG	O-C-N	-5.12	115.15	122.41
1	F	79	GLU	CB-CA-C	5.11	119.40	109.33
1	A	9	ILE	N-CA-CB	5.11	118.20	111.25
1	D	80	GLY	N-CA-C	-5.11	103.22	110.63
1	E	140	VAL	CA-CB-CG2	-5.11	101.71	110.40
1	B	12	LYS	CA-CB-CG	-5.11	103.88	114.10
1	E	16	VAL	CA-CB-CG2	5.11	119.08	110.40
1	E	63	GLY	O-C-N	5.10	127.84	122.28
1	A	113	GLY	N-CA-C	-5.10	106.56	113.24
1	E	148	ASN	CA-CB-CG	5.10	117.70	112.60
1	F	31	LYS	N-CA-C	-5.10	106.74	113.17
1	B	78	TRP	O-C-N	-5.10	116.56	123.19
1	A	60	PHE	N-CA-CB	5.10	117.71	110.06
1	D	5	GLU	N-CA-C	-5.10	103.61	110.24
1	D	126	ALA	CB-CA-C	5.10	118.81	110.96
1	C	8	PHE	CA-CB-CG	-5.10	108.70	113.80
1	B	125	SER	N-CA-C	-5.09	105.42	110.97
1	A	68	MET	N-CA-CB	-5.09	101.48	110.39
1	B	34	ARG	N-CA-C	5.09	116.91	108.20
1	A	143	LYS	O-C-N	-5.09	117.26	123.27
1	C	105	ARG	N-CA-C	-5.09	105.38	111.03
1	E	35	LEU	CA-C-O	-5.08	114.73	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	37	ALA	CB-CA-C	-5.08	100.71	109.86
1	B	85	LYS	O-C-N	-5.08	116.83	122.07
1	C	117	ILE	CA-C-O	5.08	127.18	121.28
1	F	100	LYS	O-C-N	-5.08	115.74	121.43
1	E	35	LEU	N-CA-CB	5.08	118.70	110.17
1	B	55	LEU	N-CA-CB	-5.08	100.11	110.67
1	D	43	ALA	N-CA-CB	-5.08	103.00	110.26
1	E	131	ALA	O-C-N	5.08	127.31	122.03
1	E	88	ARG	CB-CA-C	-5.07	101.43	110.70
1	F	143	LYS	N-CA-CB	5.07	119.57	110.80
1	D	12	LYS	CA-CB-CG	-5.06	103.97	114.10
1	A	70	SER	CA-C-O	-5.06	114.38	120.10
1	F	55	LEU	N-CA-C	-5.06	100.02	110.80
1	B	63	GLY	CA-C-O	5.06	125.87	120.40
1	E	80	GLY	O-C-N	5.06	129.54	123.67
1	D	115	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	B	39	LYS	N-CA-C	5.05	116.26	107.93
1	A	95	ASN	CB-CA-C	-5.05	100.22	110.17
1	B	118	HIS	CE1-NE2-CD2	-5.05	103.95	109.00
1	B	27	ARG	CA-CB-CG	-5.05	104.01	114.10
1	C	65	VAL	N-CA-CB	-5.05	102.62	110.54
1	F	54	ASP	CA-C-N	5.04	131.17	121.54
1	F	54	ASP	C-N-CA	5.04	131.17	121.54
1	C	119	GLY	CA-C-O	-5.04	117.01	120.94
1	E	77	VAL	CA-CB-CG2	-5.04	101.84	110.40
1	B	149	TRP	CA-CB-CG	-5.04	104.03	113.60
1	A	40	PHE	CA-C-N	-5.04	113.48	122.45
1	A	40	PHE	C-N-CA	-5.04	113.48	122.45
1	A	8	PHE	O-C-N	5.03	129.10	123.27
1	B	138	GLU	CG-CD-OE2	-5.03	106.83	118.40
1	C	104	ILE	N-CA-CB	-5.03	103.03	110.58
1	F	152	GLU	CA-CB-CG	5.03	124.16	114.10
1	F	150	ILE	N-CA-C	5.03	116.91	111.58
1	C	50	GLU	CG-CD-OE1	-5.03	106.84	118.40
1	B	26	LYS	CA-C-N	-5.03	113.75	120.54
1	B	26	LYS	C-N-CA	-5.03	113.75	120.54
1	C	137	GLU	CB-CG-CD	-5.02	104.06	112.60
1	F	93	GLU	CG-CD-OE2	-5.02	106.85	118.40
1	D	88	ARG	O-C-N	5.02	127.87	122.15
1	D	103	THR	N-CA-C	5.02	117.33	110.55
1	D	149	TRP	CA-C-O	5.02	125.55	119.38
1	A	13	PRO	CB-CA-C	5.02	119.00	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	TYR	CA-C-N	-5.02	111.24	121.18
1	A	67	TYR	C-N-CA	-5.02	111.24	121.18
1	A	117	ILE	N-CA-C	5.01	115.40	108.23
1	F	131	ALA	CB-CA-C	-5.01	102.42	110.74
1	B	18	ARG	N-CA-CB	-5.01	102.30	110.42
1	D	89	VAL	N-CA-C	-5.01	104.83	111.09
1	E	76	MET	O-C-N	5.01	129.27	122.96
1	F	138	GLU	CA-C-O	5.01	125.28	119.32
1	F	36	VAL	CB-CA-C	-5.00	105.49	112.04
1	B	88	ARG	N-CA-CB	-5.00	102.04	110.49
1	E	77	VAL	N-CA-C	-5.00	101.75	108.35

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	115	ASN	CA
1	B	141	ASN	CA
1	B	151	TYR	CA
1	D	140	VAL	CA
1	D	141	ASN	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	21	ILE	Mainchain
1	C	29	GLU	Sidechain
1	E	54	ASP	Sidechain

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	1206	0	1203	168	0
1	B	1206	0	1203	179	0
1	C	1206	0	1203	161	0
1	D	1206	0	1203	177	0
1	E	1206	0	1203	188	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1206	0	1203	179	0
2	A	23	0	5	0	0
2	B	23	0	4	2	0
2	C	23	0	4	0	0
2	D	23	0	6	2	0
2	E	23	0	6	1	0
2	F	23	0	5	3	0
3	A	28	0	6	1	0
3	B	28	0	5	0	0
3	C	28	0	5	0	0
3	D	28	0	6	1	0
3	E	28	0	6	5	0
3	F	28	0	5	1	0
4	A	49	0	0	11	0
4	B	49	0	0	11	0
4	C	50	0	0	10	0
4	D	40	0	0	8	0
4	E	62	0	0	12	0
4	F	56	0	0	14	0
All	All	7848	0	7281	995	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 67.

All (995) 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:F:39:LYS:HE3	1:F:41:MET:HE2	1.27	1.08
1:C:72:PRO:HG3	1:F:140:VAL:HG11	1.31	1.06
1:C:148:ASN:H	1:C:148:ASN:ND2	1.43	1.05
1:A:147:GLN:HE22	1:A:151:TYR:HD2	1.12	0.98
1:E:16:VAL:HG13	1:E:21:ILE:HD11	1.42	0.97
1:F:58:ARG:HG2	1:F:58:ARG:HH11	1.30	0.96
1:B:39:LYS:HE3	1:B:41:MET:HE3	1.45	0.95
1:C:148:ASN:N	1:C:148:ASN:HD22	1.64	0.95
1:A:37:ALA:HB3	1:A:77:VAL:HG13	1.46	0.94
1:B:37:ALA:HB2	1:B:139:LEU:HD12	1.49	0.94
1:D:136:PRO:HD2	1:D:137:GLU:HG3	1.48	0.93
1:B:58:ARG:HG3	1:B:59:PRO:HD2	1.46	0.93
1:A:13:PRO:HD3	1:A:73:VAL:HG12	1.48	0.93
1:C:140:VAL:HG11	1:F:72:PRO:HG3	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:GLU:HA	1:D:130:ILE:HG13	1.48	0.92
1:E:21:ILE:HG23	4:E:373:HOH:O	1.68	0.92
1:C:148:ASN:H	1:C:148:ASN:HD22	0.91	0.91
1:A:148:ASN:HD22	1:A:148:ASN:H	0.98	0.91
1:D:143:LYS:NZ	1:D:143:LYS:HB2	1.84	0.91
1:A:58:ARG:HG3	1:A:58:ARG:HH11	1.36	0.90
1:C:43:ALA:HB1	1:C:47:LEU:HD13	1.53	0.89
1:B:48:LEU:HD21	1:B:68:MET:HB3	1.54	0.88
1:F:39:LYS:CE	1:F:41:MET:HE2	2.03	0.87
1:C:82:ASN:O	1:C:83:VAL:C	2.18	0.86
1:F:48:LEU:CD1	1:F:69:HIS:HB2	2.05	0.86
1:A:37:ALA:HB2	1:A:139:LEU:HD12	1.59	0.85
1:C:72:PRO:HG3	1:F:140:VAL:CG1	2.05	0.85
1:D:138:GLU:C	1:D:139:LEU:HD12	2.01	0.85
1:D:24:ILE:O	1:D:27:ARG:HB2	1.76	0.84
1:A:38:MET:HB2	1:A:76:MET:HG2	1.56	0.84
1:E:40:PHE:CE1	1:E:72:PRO:HB2	2.12	0.84
1:E:135:HIS:O	1:E:138:GLU:HB2	1.78	0.84
1:E:9:ILE:HG22	1:E:76:MET:HE3	1.59	0.84
1:E:39:LYS:HE3	1:E:41:MET:CE	2.08	0.84
1:B:49:LYS:NZ	1:B:65:VAL:HG11	1.93	0.83
1:C:58:ARG:HD3	1:C:58:ARG:N	1.93	0.83
1:E:140:VAL:HG12	1:E:141:ASN:H	1.43	0.83
1:C:100:LYS:O	1:C:106:GLY:HA3	1.79	0.82
1:E:93:GLU:O	1:E:94:THR:C	2.17	0.81
1:E:54:ASP:HA	4:E:218:HOH:O	1.79	0.81
1:F:80:GLY:O	1:F:83:VAL:HG22	1.80	0.81
1:F:86:THR:O	1:F:90:MET:HG3	1.81	0.81
1:E:46:ASP:HA	1:E:49:LYS:HG3	1.62	0.80
1:B:39:LYS:HE3	1:B:41:MET:CE	2.11	0.80
1:B:45:GLU:O	1:B:49:LYS:HB2	1.81	0.79
1:C:93:GLU:N	1:C:99:SER:HB3	1.97	0.79
1:D:110:ILE:HD13	1:E:33:PHE:CE1	2.17	0.79
1:F:8:PHE:CZ	1:F:10:ALA:HB2	2.17	0.79
1:C:93:GLU:H	1:C:99:SER:HB3	1.48	0.79
1:E:18:ARG:O	1:E:19:GLY:C	2.23	0.79
1:B:13:PRO:HD3	1:B:73:VAL:CG1	2.14	0.78
1:F:52:TYR:CE1	2:F:160:35G:H5'2	2.19	0.78
1:E:18:ARG:O	1:E:20:LEU:HG	1.83	0.78
1:B:13:PRO:HD3	1:B:73:VAL:HG12	1.64	0.78
1:B:17:GLN:HG3	1:C:149:TRP:CE2	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:VAL:HG12	1:E:141:ASN:N	1.97	0.78
1:B:61:PHE:O	1:B:65:VAL:HG23	1.82	0.78
1:D:6:ARG:HA	1:D:83:VAL:HG21	1.65	0.77
1:E:138:GLU:C	1:E:139:LEU:HD12	2.09	0.77
1:F:61:PHE:O	1:F:65:VAL:HG23	1.84	0.77
1:E:25:ILE:O	1:E:29:GLU:HG3	1.85	0.77
1:A:148:ASN:H	1:A:148:ASN:ND2	1.72	0.77
1:A:25:ILE:HG21	1:E:21:ILE:HG22	1.67	0.77
1:D:128:LYS:O	1:D:131:ALA:HB3	1.85	0.77
1:F:44:SER:O	1:F:47:LEU:N	2.18	0.77
1:A:148:ASN:HD22	1:A:148:ASN:N	1.78	0.77
1:E:44:SER:O	1:E:45:GLU:C	2.21	0.76
1:F:41:MET:HE3	1:F:133:TRP:HE3	1.49	0.76
1:F:58:ARG:HG2	1:F:58:ARG:NH1	1.96	0.76
1:D:139:LEU:HD12	1:D:139:LEU:N	2.00	0.76
1:E:143:LYS:NZ	1:E:143:LYS:HA	1.99	0.76
1:A:47:LEU:O	1:A:47:LEU:HD12	1.86	0.76
1:B:115:ASN:O	1:B:116:ILE:HG12	1.86	0.76
1:A:31:LYS:HG3	1:A:31:LYS:O	1.86	0.76
1:E:143:LYS:HE2	4:E:472:HOH:O	1.85	0.76
1:F:47:LEU:O	1:F:48:LEU:C	2.24	0.76
1:F:48:LEU:HD11	1:F:68:MET:O	1.86	0.76
1:A:43:ALA:O	1:A:69:HIS:ND1	2.17	0.76
1:B:115:ASN:C	1:B:116:ILE:HG12	2.09	0.76
1:A:31:LYS:HE3	1:C:109:CYS:O	1.85	0.75
1:A:45:GLU:O	1:A:49:LYS:HG2	1.87	0.75
1:F:88:ARG:HD2	1:F:121:ASP:HA	1.67	0.75
1:A:58:ARG:HG3	1:A:58:ARG:NH1	1.98	0.75
1:D:111:GLN:OE1	1:E:151:TYR:HA	1.87	0.75
1:A:36:VAL:HB	1:A:77:VAL:HG22	1.69	0.75
1:C:53:ILE:O	1:C:56:LYS:HB3	1.87	0.75
1:E:146:ALA:O	1:E:149:TRP:HB2	1.87	0.75
1:B:92:GLY:HA2	1:B:103:THR:HG21	1.69	0.74
1:E:39:LYS:HE3	1:E:41:MET:HE2	1.69	0.74
1:D:136:PRO:HD2	1:D:137:GLU:H	1.53	0.74
1:D:143:LYS:HE3	1:D:147:GLN:OE1	1.86	0.74
1:B:87:GLY:O	1:B:88:ARG:C	2.29	0.74
1:D:83:VAL:HG23	1:D:84:VAL:H	1.51	0.74
1:D:52:TYR:HA	4:D:445:HOH:O	1.86	0.74
1:B:136:PRO:C	1:B:137:GLU:HG3	2.12	0.74
1:B:2:ALA:O	1:B:81:LEU:HA	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLU:HG2	4:C:435:HOH:O	1.87	0.73
1:B:135:HIS:N	1:B:138:GLU:OE2	2.20	0.73
1:A:131:ALA:HA	4:A:356:HOH:O	1.88	0.73
1:E:35:LEU:HD11	1:E:38:MET:HE2	1.71	0.73
1:E:46:ASP:HB2	4:E:381:HOH:O	1.89	0.73
1:D:46:ASP:HA	1:D:49:LYS:HD3	1.71	0.73
1:D:60:PHE:O	1:D:61:PHE:C	2.31	0.73
1:F:24:ILE:HD13	1:F:117:ILE:HD12	1.71	0.73
1:A:12:LYS:O	1:A:16:VAL:HG23	1.89	0.73
1:E:143:LYS:HA	1:E:143:LYS:HZ3	1.53	0.73
1:B:25:ILE:HG21	1:D:21:ILE:HG22	1.70	0.73
1:B:57:ASP:CG	1:B:58:ARG:H	1.93	0.73
1:F:39:LYS:HE3	1:F:41:MET:CE	2.16	0.73
1:F:82:ASN:HB3	4:F:481:HOH:O	1.88	0.72
1:B:61:PHE:O	1:B:64:LEU:HB3	1.90	0.72
1:B:120:SER:OG	1:B:126:ALA:HA	1.89	0.72
1:E:80:GLY:N	1:E:83:VAL:HG22	2.05	0.72
1:B:135:HIS:O	1:B:137:GLU:N	2.23	0.72
1:B:135:HIS:O	1:B:138:GLU:HG3	1.88	0.72
1:C:78:TRP:O	1:C:83:VAL:HG11	1.90	0.72
1:F:41:MET:O	1:F:73:VAL:HG22	1.90	0.72
1:F:83:VAL:O	1:F:87:GLY:N	2.21	0.72
1:B:14:ASP:O	1:B:18:ARG:HG3	1.90	0.71
1:A:17:GLN:HG3	1:B:149:TRP:CE2	2.25	0.71
1:B:33:PHE:CE1	1:B:83:VAL:HG13	2.25	0.71
1:D:3:ASN:HB3	1:D:81:LEU:HB2	1.71	0.71
1:A:7:THR:CB	1:A:84:VAL:HG22	2.20	0.71
1:A:55:LEU:O	1:A:57:ASP:N	2.24	0.71
1:A:144:SER:O	1:A:147:GLN:HB2	1.89	0.71
1:D:121:ASP:OD1	1:D:121:ASP:N	2.20	0.71
1:A:47:LEU:HD12	1:A:47:LEU:C	2.16	0.71
1:D:46:ASP:O	1:D:50:GLU:HB2	1.90	0.71
1:E:53:ILE:O	1:E:56:LYS:HB2	1.91	0.70
1:F:48:LEU:HD11	1:F:69:HIS:HB2	1.72	0.70
1:B:45:GLU:O	1:B:49:LYS:NZ	2.23	0.70
1:C:23:GLU:O	1:C:27:ARG:HG2	1.92	0.70
1:F:94:THR:O	1:F:96:PRO:HD3	1.90	0.70
1:F:33:PHE:CD1	1:F:83:VAL:HG13	2.27	0.70
1:D:45:GLU:HG2	1:D:65:VAL:HG12	1.73	0.70
1:D:78:TRP:O	1:D:83:VAL:HG11	1.91	0.70
1:E:126:ALA:C	1:E:130:ILE:HD12	2.16	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:THR:HB	1:A:84:VAL:HG22	1.74	0.70
1:A:81:LEU:HD12	1:A:82:ASN:HD22	1.55	0.70
1:B:37:ALA:HB2	1:B:139:LEU:CD1	2.20	0.70
1:B:139:LEU:HD13	1:B:139:LEU:N	2.07	0.70
1:C:12:LYS:HD2	1:C:117:ILE:N	2.06	0.70
1:D:58:ARG:O	1:D:59:PRO:C	2.33	0.69
1:B:88:ARG:HH21	1:B:121:ASP:HB2	1.57	0.69
1:C:39:LYS:HE2	1:C:134:PHE:CE1	2.28	0.69
1:E:80:GLY:H	1:E:83:VAL:CG2	2.06	0.69
1:E:115:ASN:O	1:E:116:ILE:HG12	1.92	0.69
1:F:52:TYR:OH	2:F:160:35G:O1P	2.11	0.69
1:E:148:ASN:HD22	1:E:148:ASN:H	1.40	0.69
1:B:126:ALA:O	1:B:130:ILE:HG12	1.92	0.69
1:C:140:VAL:CG1	1:F:72:PRO:HG3	2.21	0.69
1:D:17:GLN:HG3	1:E:149:TRP:CE2	2.28	0.68
1:A:129:GLU:HA	4:A:382:HOH:O	1.93	0.68
1:C:148:ASN:ND2	1:C:148:ASN:N	2.17	0.68
1:E:39:LYS:HE3	1:E:41:MET:HE3	1.74	0.68
1:E:44:SER:HB2	4:E:456:HOH:O	1.93	0.68
1:B:94:THR:HA	1:B:105:ARG:NH1	2.08	0.68
1:F:41:MET:O	1:F:41:MET:HG3	1.94	0.68
1:D:143:LYS:HB2	1:D:143:LYS:HZ2	1.58	0.68
1:E:115:ASN:C	1:E:116:ILE:HG12	2.18	0.68
1:F:48:LEU:HD12	1:F:69:HIS:HB2	1.74	0.68
1:F:41:MET:CE	1:F:133:TRP:HE3	2.06	0.68
1:A:126:ALA:O	1:A:130:ILE:HG13	1.94	0.68
1:D:130:ILE:O	1:D:134:PHE:HB2	1.94	0.68
1:E:7:THR:OG1	1:E:120:SER:HB2	1.94	0.68
1:B:127:GLU:HA	1:B:130:ILE:HG13	1.75	0.67
1:C:143:LYS:HD3	1:C:147:GLN:OE1	1.94	0.67
1:E:61:PHE:O	1:E:64:LEU:HB3	1.94	0.67
1:E:86:THR:O	1:E:90:MET:HG3	1.93	0.67
1:C:91:LEU:HD11	1:C:117:ILE:HG12	1.76	0.67
1:C:146:ALA:O	1:C:149:TRP:HB2	1.95	0.67
1:F:84:VAL:O	1:F:85:LYS:C	2.34	0.67
1:A:135:HIS:N	1:A:138:GLU:OE2	2.27	0.67
1:B:39:LYS:CE	1:B:41:MET:HE3	2.24	0.67
1:F:53:ILE:HG23	1:F:54:ASP:N	2.10	0.67
1:A:37:ALA:O	1:A:77:VAL:N	2.25	0.67
1:E:88:ARG:HB3	4:E:263:HOH:O	1.95	0.67
1:B:143:LYS:NZ	1:B:143:LYS:HA	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ARG:O	1:B:91:LEU:HB2	1.94	0.66
1:D:52:TYR:CE1	2:D:160:35G:H5'2	2.30	0.66
1:B:34:ARG:NH2	1:B:79:GLU:OE2	2.27	0.66
1:D:95:ASN:O	1:D:98:ASP:N	2.26	0.66
1:C:95:ASN:HA	1:C:112:VAL:HG13	1.76	0.66
1:F:113:GLY:C	1:F:114:ARG:HG2	2.12	0.66
1:A:114:ARG:NH2	1:B:152:GLU:HB3	2.10	0.66
1:D:47:LEU:O	1:D:51:HIS:N	2.27	0.66
1:B:49:LYS:HB2	1:B:49:LYS:HZ3	1.59	0.66
1:E:14:ASP:OD1	1:E:67:TYR:OH	2.14	0.66
1:E:147:GLN:O	1:E:151:TYR:HB2	1.95	0.66
1:A:129:GLU:HG2	4:A:382:HOH:O	1.95	0.66
1:B:117:ILE:HG12	1:B:118:HIS:N	2.09	0.66
1:E:39:LYS:HG3	1:E:41:MET:HG2	1.77	0.66
1:A:81:LEU:CD1	1:A:82:ASN:HD22	2.09	0.66
1:C:139:LEU:N	1:C:139:LEU:HD12	2.11	0.66
1:E:27:ARG:HG3	1:E:104:ILE:CD1	2.26	0.66
1:D:151:TYR:HD1	1:F:111:GLN:HE21	1.43	0.66
1:F:30:GLN:NE2	4:F:331:HOH:O	2.29	0.66
1:B:49:LYS:HZ2	1:B:65:VAL:HG11	1.59	0.65
1:D:135:HIS:O	1:D:138:GLU:N	2.27	0.65
1:F:123:VAL:O	1:F:126:ALA:N	2.29	0.65
1:C:128:LYS:O	1:C:132:LEU:HB2	1.95	0.65
1:A:7:THR:OG1	1:A:84:VAL:HG22	1.97	0.65
1:B:57:ASP:O	1:B:61:PHE:HB3	1.96	0.65
1:F:95:ASN:O	1:F:97:ALA:N	2.29	0.65
1:C:102:GLY:N	1:C:107:ASP:OD1	2.30	0.65
1:E:18:ARG:O	1:E:20:LEU:N	2.30	0.65
1:E:80:GLY:H	1:E:83:VAL:HG22	1.62	0.65
4:A:256:HOH:O	1:E:21:ILE:HD12	1.96	0.65
1:C:122:SER:O	1:C:126:ALA:N	2.19	0.65
1:B:64:LEU:O	1:B:65:VAL:C	2.36	0.65
1:C:11:ILE:HG13	1:C:76:MET:HE1	1.78	0.65
1:E:55:LEU:H	1:E:55:LEU:HD23	1.62	0.65
1:F:34:ARG:NH1	1:F:142:TYR:CE1	2.62	0.64
1:F:115:ASN:O	1:F:117:ILE:N	2.26	0.64
1:E:50:GLU:CG	1:E:132:LEU:HD21	2.26	0.64
1:A:114:ARG:O	1:A:116:ILE:N	2.30	0.64
1:B:58:ARG:HA	4:B:409:HOH:O	1.97	0.64
1:B:95:ASN:O	1:B:97:ALA:N	2.31	0.64
1:D:17:GLN:HG3	1:E:149:TRP:CZ2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:GLY:O	1:F:90:MET:HB2	1.97	0.64
1:B:88:ARG:HH21	1:B:121:ASP:CB	2.10	0.64
1:B:86:THR:HG23	4:B:357:HOH:O	1.98	0.64
1:C:144:SER:O	1:C:147:GLN:HB3	1.98	0.64
1:F:143:LYS:HD2	1:F:147:GLN:OE1	1.98	0.64
1:F:61:PHE:O	1:F:64:LEU:HB3	1.98	0.64
1:E:55:LEU:HD22	4:E:266:HOH:O	1.97	0.64
1:F:33:PHE:CD1	1:F:80:GLY:HA3	2.33	0.64
1:A:85:LYS:O	1:A:89:VAL:HG23	1.98	0.63
1:B:125:SER:O	1:B:126:ALA:C	2.39	0.63
1:F:86:THR:O	1:F:87:GLY:C	2.36	0.63
1:C:53:ILE:HG23	1:C:54:ASP:N	2.12	0.63
1:D:123:VAL:O	1:D:126:ALA:HB3	1.98	0.63
1:A:114:ARG:CZ	1:B:152:GLU:HB3	2.29	0.63
1:B:142:TYR:HA	4:B:427:HOH:O	1.98	0.63
1:A:13:PRO:HD3	1:A:73:VAL:CG1	2.23	0.63
1:C:67:TYR:HA	1:C:70:SER:OG	1.98	0.63
1:E:118:HIS:ND1	2:E:160:35G:O1P	2.30	0.63
1:B:80:GLY:O	1:B:83:VAL:HG22	1.97	0.63
1:D:3:ASN:HA	1:D:81:LEU:HA	1.80	0.62
1:B:48:LEU:O	1:B:51:HIS:N	2.31	0.62
1:C:115:ASN:OD1	1:C:115:ASN:N	2.27	0.62
1:E:12:LYS:HE3	1:E:117:ILE:O	2.00	0.62
1:B:122:SER:OG	1:B:125:SER:HB3	1.98	0.62
1:F:14:ASP:O	1:F:18:ARG:HG3	2.00	0.62
1:A:23:GLU:O	1:A:27:ARG:HG2	1.99	0.62
1:C:43:ALA:CB	1:C:47:LEU:HD13	2.29	0.62
1:D:23:GLU:O	1:D:27:ARG:HG2	1.99	0.62
1:D:122:SER:O	1:D:126:ALA:N	2.30	0.62
1:E:10:ALA:N	1:E:118:HIS:O	2.31	0.62
1:A:34:ARG:NH1	1:A:142:TYR:CE1	2.68	0.62
1:A:147:GLN:NE2	1:A:151:TYR:HD2	1.90	0.62
1:A:11:ILE:HG13	1:A:76:MET:HE2	1.81	0.62
1:B:44:SER:OG	1:B:47:LEU:HB2	1.99	0.62
1:F:88:ARG:HD2	1:F:120:SER:O	2.00	0.62
1:E:39:LYS:NZ	1:E:133:TRP:O	2.31	0.62
1:E:113:GLY:HA3	1:F:152:GLU:OE1	1.99	0.62
1:B:139:LEU:N	1:B:139:LEU:HD22	2.14	0.62
1:C:113:GLY:O	1:C:114:ARG:HG2	1.99	0.62
1:A:36:VAL:N	1:A:77:VAL:O	2.29	0.62
1:B:51:HIS:HB2	1:B:132:LEU:CD1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:LYS:HB3	1:C:13:PRO:CD	2.30	0.62
1:C:144:SER:OG	1:C:147:GLN:HB2	1.99	0.62
1:A:135:HIS:O	1:A:138:GLU:HG3	1.99	0.61
2:B:160:35G:H5'2	4:B:503:HOH:O	2.00	0.61
1:C:111:GLN:O	1:C:114:ARG:N	2.29	0.61
1:E:127:GLU:HA	1:E:130:ILE:HD12	1.81	0.61
1:A:80:GLY:O	1:A:83:VAL:HG22	1.99	0.61
1:A:96:PRO:HG3	1:A:115:ASN:HB3	1.83	0.61
1:B:138:GLU:C	1:B:139:LEU:HD13	2.26	0.61
1:A:11:ILE:HG13	1:A:76:MET:CE	2.30	0.61
1:C:123:VAL:O	1:C:126:ALA:HB3	2.01	0.61
1:C:54:ASP:HB3	4:C:358:HOH:O	1.99	0.61
1:C:101:PRO:HG3	4:C:302:HOH:O	2.01	0.61
1:D:97:ALA:HA	4:D:239:HOH:O	2.00	0.61
1:A:64:LEU:O	1:A:68:MET:HG2	2.00	0.61
1:D:93:GLU:O	1:D:105:ARG:HD2	2.00	0.61
1:F:85:LYS:HE3	4:F:481:HOH:O	2.00	0.61
1:A:96:PRO:HB3	1:A:105:ARG:HB3	1.82	0.61
1:E:150:ILE:HG22	1:E:150:ILE:O	2.01	0.61
1:D:9:ILE:N	1:D:76:MET:O	2.33	0.61
1:D:15:GLY:N	1:D:116:ILE:HG22	2.15	0.61
1:F:123:VAL:O	1:F:124:GLU:C	2.43	0.61
1:E:50:GLU:HG2	1:E:132:LEU:HD21	1.83	0.61
1:F:91:LEU:HA	1:F:104:ILE:HG13	1.82	0.60
1:F:33:PHE:HD1	1:F:80:GLY:HA3	1.65	0.60
1:A:80:GLY:O	1:A:81:LEU:C	2.42	0.60
1:A:41:MET:HE1	1:A:133:TRP:CE3	2.36	0.60
1:B:8:PHE:CZ	1:B:10:ALA:HB2	2.36	0.60
1:A:29:GLU:OE1	1:E:19:GLY:HA2	2.00	0.60
1:B:136:PRO:O	1:B:137:GLU:HG3	2.01	0.60
1:D:11:ILE:HG22	1:D:16:VAL:HG23	1.83	0.60
1:D:46:ASP:O	1:D:47:LEU:C	2.44	0.60
1:F:5:GLU:OE2	1:F:84:VAL:HG23	2.01	0.60
1:A:38:MET:HB2	1:A:76:MET:CG	2.31	0.60
1:B:42:ARG:HA	1:B:72:PRO:HA	1.84	0.60
1:D:45:GLU:O	1:D:48:LEU:HB2	2.02	0.60
1:A:41:MET:CE	1:A:133:TRP:CZ3	2.85	0.60
1:C:41:MET:HE1	1:C:133:TRP:CE3	2.36	0.60
1:F:33:PHE:CE1	1:F:83:VAL:HG13	2.36	0.60
1:D:91:LEU:HD11	1:D:117:ILE:HD13	1.83	0.59
1:E:130:ILE:O	1:E:134:PHE:N	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:VAL:O	1:B:124:GLU:C	2.43	0.59
1:A:142:TYR:HA	4:A:389:HOH:O	2.01	0.59
1:B:41:MET:O	1:B:73:VAL:N	2.29	0.59
1:C:9:ILE:O	1:C:76:MET:HE3	2.03	0.59
1:C:34:ARG:NH1	1:C:140:VAL:O	2.34	0.59
1:C:58:ARG:HD3	1:C:58:ARG:H	1.67	0.59
1:E:80:GLY:O	1:E:83:VAL:HG22	2.02	0.59
1:F:12:LYS:O	1:F:16:VAL:HG23	2.01	0.59
1:D:7:THR:HB	1:D:84:VAL:HA	1.84	0.59
1:E:81:LEU:CD1	1:E:82:ASN:HD22	2.15	0.59
1:B:6:ARG:HA	1:B:78:TRP:O	2.02	0.59
1:E:54:ASP:C	1:E:56:LYS:H	2.09	0.59
1:B:51:HIS:C	1:B:53:ILE:H	2.10	0.59
1:B:58:ARG:O	1:B:61:PHE:N	2.32	0.59
1:E:112:VAL:HG23	1:E:113:GLY:H	1.67	0.59
1:E:125:SER:O	1:E:129:GLU:HB2	2.03	0.59
1:B:38:MET:HG3	1:B:76:MET:HB3	1.85	0.59
1:C:12:LYS:HG2	1:C:68:MET:HE1	1.85	0.59
1:D:45:GLU:HG2	1:D:65:VAL:CG1	2.32	0.59
1:B:6:ARG:HG3	1:B:79:GLU:HB2	1.84	0.58
1:B:40:PHE:CE1	1:B:72:PRO:HB2	2.38	0.58
1:B:59:PRO:HD3	4:B:409:HOH:O	2.04	0.58
1:F:129:GLU:O	1:F:133:TRP:HD1	1.86	0.58
1:C:83:VAL:O	1:C:84:VAL:C	2.45	0.58
1:A:20:LEU:O	1:A:21:ILE:C	2.39	0.58
1:D:64:LEU:HD12	1:D:64:LEU:O	2.02	0.58
1:B:58:ARG:CG	1:B:59:PRO:HD2	2.27	0.58
1:D:32:GLY:O	1:F:110:ILE:CD1	2.51	0.58
1:D:33:PHE:N	4:D:352:HOH:O	2.36	0.58
1:D:115:ASN:C	1:D:117:ILE:H	2.10	0.58
1:B:87:GLY:O	1:B:90:MET:N	2.37	0.58
1:A:97:ALA:N	4:A:249:HOH:O	2.30	0.58
1:A:152:GLU:HB3	1:C:111:GLN:CD	2.27	0.58
1:B:26:LYS:O	1:B:27:ARG:C	2.42	0.58
1:D:52:TYR:O	1:D:61:PHE:HE1	1.86	0.58
1:B:40:PHE:HB2	1:D:38:MET:HB3	1.85	0.58
1:B:143:LYS:HA	1:B:143:LYS:HZ3	1.68	0.58
1:D:35:LEU:HD21	1:D:38:MET:HB2	1.86	0.58
1:E:125:SER:O	1:E:126:ALA:C	2.46	0.58
1:B:140:VAL:HG11	1:D:72:PRO:HG3	1.86	0.58
1:C:41:MET:HE1	1:C:133:TRP:HE3	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:GLU:C	1:C:139:LEU:HD12	2.28	0.58
1:E:80:GLY:N	1:E:83:VAL:CG2	2.66	0.58
1:F:14:ASP:OD1	1:F:67:TYR:OH	2.21	0.58
1:A:87:GLY:O	1:A:91:LEU:HD13	2.03	0.58
1:A:115:ASN:O	1:A:117:ILE:N	2.31	0.57
1:D:28:PHE:CE1	1:D:90:MET:HE2	2.39	0.57
1:B:95:ASN:C	1:B:97:ALA:H	2.12	0.57
1:E:47:LEU:N	4:E:456:HOH:O	2.37	0.57
1:F:44:SER:O	1:F:47:LEU:HB3	2.03	0.57
1:B:20:LEU:O	1:B:24:ILE:HG13	2.04	0.57
1:B:89:VAL:O	1:B:103:THR:HG22	2.04	0.57
1:E:139:LEU:HD12	1:E:139:LEU:N	2.17	0.57
1:D:44:SER:OG	1:D:47:LEU:HB2	2.04	0.57
1:C:12:LYS:HD2	1:C:116:ILE:C	2.28	0.57
1:D:81:LEU:O	1:D:82:ASN:HB2	2.02	0.57
1:F:120:SER:OG	1:F:126:ALA:HA	2.05	0.57
1:D:100:LYS:O	1:D:106:GLY:HA3	2.04	0.57
1:E:55:LEU:HD13	4:E:266:HOH:O	2.03	0.57
1:F:67:TYR:C	1:F:69:HIS:H	2.13	0.57
1:C:140:VAL:HG11	1:F:72:PRO:CG	2.30	0.57
1:D:32:GLY:O	1:F:110:ILE:HD11	2.03	0.57
1:D:83:VAL:O	1:D:84:VAL:C	2.44	0.57
1:B:140:VAL:HG11	1:D:72:PRO:HB3	1.86	0.57
1:D:147:GLN:HG3	1:D:147:GLN:O	2.04	0.57
1:B:51:HIS:O	1:B:53:ILE:HG22	2.04	0.56
1:B:80:GLY:N	1:B:83:VAL:HG22	2.20	0.56
1:E:12:LYS:HB3	1:E:13:PRO:CD	2.34	0.56
1:F:8:PHE:HD2	1:F:129:GLU:OE1	1.88	0.56
1:A:43:ALA:HB3	1:A:48:LEU:HD21	1.87	0.56
1:C:113:GLY:C	1:C:114:ARG:HG2	2.30	0.56
1:D:80:GLY:HA2	4:D:446:HOH:O	2.05	0.56
1:E:20:LEU:O	1:E:24:ILE:HG13	2.05	0.56
1:E:47:LEU:HD12	1:E:47:LEU:O	2.05	0.56
1:F:3:ASN:HA	1:F:81:LEU:HA	1.87	0.56
1:C:105:ARG:HD3	1:C:115:ASN:HB2	1.87	0.56
1:D:60:PHE:O	1:D:61:PHE:O	2.22	0.56
1:F:67:TYR:O	1:F:70:SER:OG	2.19	0.56
1:F:100:LYS:HE3	4:F:364:HOH:O	2.06	0.56
1:F:126:ALA:O	1:F:130:ILE:HG13	2.05	0.56
1:D:44:SER:O	1:D:48:LEU:HD12	2.05	0.56
1:F:53:ILE:HG23	1:F:54:ASP:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:LEU:HD12	1:C:69:HIS:HB2	1.88	0.56
1:D:28:PHE:CD1	1:D:90:MET:HE2	2.41	0.56
1:D:34:ARG:NH1	1:D:142:TYR:CD1	2.72	0.56
1:E:14:ASP:HA	1:F:149:TRP:CE3	2.41	0.56
1:C:135:HIS:O	1:C:138:GLU:HB2	2.06	0.56
1:E:6:ARG:HA	1:E:78:TRP:O	2.06	0.56
1:B:92:GLY:CA	1:B:103:THR:HG21	2.35	0.55
1:F:72:PRO:HD2	4:F:233:HOH:O	2.06	0.55
1:E:60:PHE:O	1:E:61:PHE:C	2.49	0.55
1:A:86:THR:O	1:A:89:VAL:HB	2.06	0.55
1:F:135:HIS:N	1:F:138:GLU:OE2	2.37	0.55
1:C:8:PHE:HE1	1:C:75:ALA:HB1	1.70	0.55
1:C:12:LYS:HE3	1:C:117:ILE:O	2.07	0.55
1:C:25:ILE:O	1:C:28:PHE:HB2	2.07	0.55
1:E:43:ALA:HB3	1:E:48:LEU:HD21	1.89	0.55
1:E:12:LYS:HG3	1:E:117:ILE:HA	1.88	0.55
1:B:45:GLU:HG3	1:B:69:HIS:CD2	2.42	0.55
1:D:2:ALA:C	1:D:4:SER:H	2.15	0.55
1:D:2:ALA:O	1:D:4:SER:N	2.39	0.55
1:F:64:LEU:O	1:F:65:VAL:C	2.48	0.55
1:A:47:LEU:HD13	1:A:132:LEU:CD2	2.37	0.55
1:B:35:LEU:HD21	1:B:38:MET:HE2	1.88	0.55
1:D:130:ILE:O	1:D:130:ILE:HG22	2.06	0.55
1:F:88:ARG:NH1	1:F:121:ASP:HB3	2.21	0.55
1:A:79:GLU:O	1:A:79:GLU:HG2	2.04	0.55
1:B:12:LYS:HE3	1:B:117:ILE:O	2.06	0.55
1:D:94:THR:OG1	3:D:161:GDP:O2B	2.22	0.55
1:D:127:GLU:O	1:D:131:ALA:HB2	2.07	0.55
1:A:80:GLY:N	1:A:83:VAL:HG22	2.22	0.54
1:D:5:GLU:O	1:D:79:GLU:HB2	2.07	0.54
1:A:117:ILE:HG12	1:A:118:HIS:H	1.72	0.54
1:D:38:MET:HA	1:D:75:ALA:O	2.08	0.54
1:A:130:ILE:O	1:A:133:TRP:N	2.34	0.54
1:B:145:CYS:SG	1:E:146:ALA:HB2	2.47	0.54
1:D:83:VAL:HG23	1:D:84:VAL:N	2.22	0.54
1:E:24:ILE:HG21	1:E:117:ILE:HD12	1.89	0.54
1:C:29:GLU:OE2	1:F:19:GLY:HA2	2.07	0.54
1:C:95:ASN:HB3	1:C:98:ASP:HB2	1.89	0.54
1:D:132:LEU:HD23	1:D:132:LEU:O	2.07	0.54
1:F:6:ARG:HB3	1:F:77:VAL:HG12	1.88	0.54
1:E:11:ILE:HG13	1:E:76:MET:HE2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:GLN:OE1	1:F:152:GLU:HB3	2.07	0.54
1:C:67:TYR:O	1:C:70:SER:OG	2.24	0.54
1:E:88:ARG:HH22	3:E:161:GDP:PB	2.31	0.54
1:D:16:VAL:HG22	1:D:21:ILE:HD11	1.90	0.54
1:D:64:LEU:HD12	1:D:64:LEU:C	2.33	0.54
1:A:96:PRO:HD3	1:A:112:VAL:HA	1.89	0.54
1:F:143:LYS:HE3	4:F:369:HOH:O	2.08	0.54
1:A:104:ILE:HG13	4:A:306:HOH:O	2.08	0.54
1:B:117:ILE:CG1	1:B:118:HIS:N	2.70	0.54
1:C:140:VAL:HG12	1:C:142:TYR:HD1	1.73	0.54
1:A:41:MET:CE	1:A:133:TRP:HZ3	2.21	0.54
1:B:108:PHE:HE1	1:C:30:GLN:NE2	2.06	0.54
1:D:11:ILE:O	1:D:73:VAL:HB	2.08	0.53
1:D:15:GLY:CA	1:D:116:ILE:HG22	2.38	0.53
1:A:6:ARG:HG2	1:A:79:GLU:HB2	1.90	0.53
1:B:117:ILE:HG12	1:B:118:HIS:H	1.74	0.53
1:C:136:PRO:HG2	1:C:137:GLU:HG3	1.90	0.53
1:D:114:ARG:CZ	1:E:152:GLU:HB3	2.38	0.53
1:F:45:GLU:O	1:F:49:LYS:HG3	2.08	0.53
1:D:4:SER:HA	1:D:79:GLU:HG3	1.90	0.53
1:B:51:HIS:O	1:B:53:ILE:N	2.41	0.53
1:B:88:ARG:HE	1:B:121:ASP:HA	1.73	0.53
1:F:27:ARG:HG2	4:F:326:HOH:O	2.08	0.53
1:B:4:SER:O	1:B:5:GLU:C	2.52	0.53
1:B:52:TYR:OH	2:B:160:35G:O1P	2.25	0.53
1:E:81:LEU:HD11	1:E:82:ASN:HD22	1.73	0.53
1:B:108:PHE:HA	1:C:31:LYS:HA	1.91	0.53
1:B:117:ILE:CG1	1:B:118:HIS:H	2.22	0.53
1:D:3:ASN:HA	1:D:81:LEU:CA	2.38	0.53
1:D:6:ARG:CA	1:D:83:VAL:HG21	2.38	0.53
1:A:80:GLY:H	1:A:83:VAL:CG2	2.21	0.53
1:A:125:SER:O	1:A:129:GLU:HB2	2.09	0.53
1:B:33:PHE:CZ	1:B:83:VAL:HG13	2.43	0.53
1:B:79:GLU:HA	1:B:83:VAL:HG21	1.89	0.53
1:C:38:MET:HG3	1:C:76:MET:HG3	1.90	0.53
1:C:121:ASP:OD1	1:C:121:ASP:N	2.31	0.53
1:D:34:ARG:NH1	1:D:140:VAL:O	2.31	0.53
1:A:139:LEU:HD13	1:A:139:LEU:N	2.24	0.53
1:B:27:ARG:NH2	1:B:107:ASP:OD2	2.31	0.53
1:D:86:THR:O	1:D:87:GLY:C	2.51	0.53
1:D:139:LEU:N	1:D:139:LEU:CD1	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:HE	1:A:115:ASN:HB2	1.73	0.53
1:A:128:LYS:HG2	1:A:129:GLU:N	2.24	0.53
1:D:85:LYS:O	1:D:88:ARG:HB2	2.09	0.53
1:E:58:ARG:HG3	1:E:59:PRO:HD2	1.91	0.53
1:E:120:SER:OG	1:E:126:ALA:HA	2.09	0.53
1:F:34:ARG:NH1	1:F:142:TYR:CD1	2.77	0.53
1:F:35:LEU:HD21	1:F:76:MET:HG2	1.89	0.52
1:A:38:MET:HA	1:A:75:ALA:O	2.09	0.52
1:F:11:ILE:HG12	1:F:24:ILE:HD12	1.91	0.52
1:F:58:ARG:HH11	1:F:58:ARG:CG	2.14	0.52
1:F:96:PRO:HD2	1:F:112:VAL:HA	1.90	0.52
1:A:22:GLY:HA2	1:E:22:GLY:HA2	1.91	0.52
1:F:95:ASN:C	1:F:97:ALA:H	2.17	0.52
1:A:9:ILE:O	1:A:76:MET:N	2.39	0.52
1:F:88:ARG:CD	1:F:121:ASP:HA	2.38	0.52
1:B:23:GLU:O	1:B:26:LYS:HB3	2.09	0.52
1:C:12:LYS:HD2	1:C:117:ILE:CA	2.38	0.52
1:E:115:ASN:N	1:E:115:ASN:OD1	2.28	0.52
1:C:143:LYS:NZ	1:C:143:LYS:HA	2.25	0.52
1:A:100:LYS:O	1:A:106:GLY:HA3	2.10	0.52
1:A:147:GLN:NE2	1:A:151:TYR:HB2	2.25	0.52
1:D:108:PHE:HD2	1:E:30:GLN:HB2	1.75	0.52
1:D:17:GLN:HA	1:D:17:GLN:OE1	2.10	0.52
1:E:135:HIS:O	1:E:137:GLU:N	2.42	0.52
1:A:53:ILE:O	1:A:56:LYS:HB2	2.10	0.52
1:A:110:ILE:O	1:A:110:ILE:HG22	2.09	0.52
1:B:84:VAL:O	1:B:88:ARG:HG2	2.10	0.52
1:C:95:ASN:C	1:C:97:ALA:H	2.18	0.52
1:E:67:TYR:O	1:E:68:MET:C	2.49	0.52
1:F:31:LYS:O	1:F:31:LYS:HG3	2.08	0.52
1:C:53:ILE:CG2	1:C:54:ASP:N	2.73	0.51
1:C:87:GLY:O	1:C:91:LEU:HB2	2.10	0.51
1:E:34:ARG:NH1	1:E:36:VAL:HG22	2.26	0.51
1:B:51:HIS:HB2	1:B:132:LEU:HD11	1.91	0.51
1:B:85:LYS:O	1:B:89:VAL:HG23	2.10	0.51
1:C:123:VAL:CG2	1:C:124:GLU:N	2.74	0.51
1:E:117:ILE:HG12	1:E:118:HIS:N	2.25	0.51
1:E:50:GLU:HG3	1:E:132:LEU:HD21	1.90	0.51
1:F:51:HIS:O	1:F:53:ILE:HG22	2.10	0.51
1:F:122:SER:O	1:F:126:ALA:N	2.42	0.51
1:D:9:ILE:O	1:D:76:MET:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:ARG:HD3	1:D:69:HIS:CE1	2.45	0.51
1:F:61:PHE:CE1	1:F:65:VAL:HG21	2.44	0.51
1:F:127:GLU:HB3	4:F:496:HOH:O	2.11	0.51
1:C:54:ASP:C	1:C:55:LEU:HD12	2.36	0.51
1:C:104:ILE:O	1:C:108:PHE:HD2	1.94	0.51
1:E:34:ARG:HH12	1:E:36:VAL:HG22	1.75	0.51
1:A:38:MET:HA	1:A:76:MET:HA	1.92	0.51
1:B:5:GLU:HB3	1:B:80:GLY:O	2.10	0.51
1:D:150:ILE:O	1:D:150:ILE:HG22	2.10	0.51
1:E:25:ILE:HD11	4:E:373:HOH:O	2.11	0.51
1:E:140:VAL:CG1	1:E:141:ASN:H	2.18	0.51
1:F:129:GLU:O	1:F:133:TRP:N	2.43	0.51
1:C:72:PRO:CG	1:F:140:VAL:HG11	2.23	0.51
1:C:113:GLY:O	1:C:114:ARG:NE	2.39	0.51
1:D:123:VAL:HA	1:D:126:ALA:HB3	1.93	0.51
1:F:58:ARG:O	1:F:59:PRO:C	2.53	0.51
1:B:47:LEU:O	1:B:48:LEU:C	2.54	0.51
1:C:67:TYR:HA	1:C:70:SER:HG	1.76	0.51
1:D:12:LYS:HG2	1:D:68:MET:SD	2.50	0.51
1:E:11:ILE:HD12	1:E:74:VAL:HB	1.92	0.51
1:F:20:LEU:O	1:F:24:ILE:HG13	2.11	0.51
1:F:51:HIS:C	1:F:53:ILE:H	2.18	0.51
1:F:5:GLU:HG2	1:F:83:VAL:HG23	1.92	0.51
1:F:56:LYS:HD2	4:F:297:HOH:O	2.10	0.51
1:C:137:GLU:O	1:C:137:GLU:OE1	2.30	0.50
1:D:6:ARG:O	1:D:84:VAL:HG23	2.12	0.50
1:E:81:LEU:C	1:E:81:LEU:HD12	2.35	0.50
1:E:140:VAL:CG1	1:E:141:ASN:N	2.69	0.50
1:F:143:LYS:HZ3	1:F:147:GLN:CD	2.20	0.50
1:A:148:ASN:ND2	1:A:148:ASN:N	2.39	0.50
1:C:147:GLN:O	1:C:147:GLN:HG3	1.89	0.50
1:E:142:TYR:CD1	1:E:142:TYR:N	2.80	0.50
1:A:23:GLU:OE1	1:E:26:LYS:NZ	2.36	0.50
1:C:8:PHE:C	1:C:9:ILE:HG12	2.36	0.50
1:F:127:GLU:O	1:F:128:LYS:C	2.53	0.50
1:C:12:LYS:HB3	1:C:13:PRO:HD2	1.94	0.50
1:F:32:GLY:HA2	4:F:252:HOH:O	2.11	0.50
1:F:111:GLN:C	1:F:113:GLY:H	2.19	0.50
1:F:122:SER:O	1:F:125:SER:HB2	2.11	0.50
1:A:61:PHE:O	1:A:62:ALA:C	2.51	0.50
1:C:39:LYS:HE2	1:C:134:PHE:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ILE:HD13	1:E:33:PHE:CD1	2.46	0.50
1:F:6:ARG:HB3	1:F:77:VAL:CG1	2.41	0.50
1:E:88:ARG:CZ	1:E:121:ASP:HB2	2.41	0.50
1:A:130:ILE:HG22	1:A:131:ALA:N	2.26	0.50
1:B:39:LYS:HG3	1:B:41:MET:HG2	1.94	0.50
1:E:127:GLU:CA	1:E:130:ILE:HD12	2.42	0.50
1:A:139:LEU:N	1:A:139:LEU:CD1	2.74	0.50
1:A:30:GLN:NE2	4:A:325:HOH:O	2.43	0.49
1:A:129:GLU:O	1:A:130:ILE:C	2.55	0.49
1:B:48:LEU:O	1:B:49:LYS:C	2.55	0.49
1:D:12:LYS:O	1:D:13:PRO:C	2.53	0.49
1:F:135:HIS:O	1:F:138:GLU:HG3	2.10	0.49
1:B:24:ILE:O	1:B:25:ILE:C	2.52	0.49
1:B:33:PHE:CD1	1:B:83:VAL:HG13	2.47	0.49
1:A:41:MET:HE2	1:A:133:TRP:HZ3	1.76	0.49
1:C:45:GLU:HA	1:C:48:LEU:HB2	1.94	0.49
1:F:145:CYS:C	1:F:147:GLN:H	2.20	0.49
1:A:14:ASP:OD2	1:A:114:ARG:O	2.29	0.49
1:C:99:SER:O	1:C:106:GLY:HA2	2.12	0.49
1:E:60:PHE:CZ	3:E:161:GDP:C8	2.99	0.49
1:E:139:LEU:N	1:E:139:LEU:CD1	2.75	0.49
1:A:94:THR:HG23	1:A:95:ASN:N	2.25	0.49
1:A:110:ILE:HG23	4:B:399:HOH:O	2.12	0.49
1:E:33:PHE:CE1	1:E:83:VAL:HG13	2.48	0.49
1:A:22:GLY:O	1:E:22:GLY:HA3	2.12	0.49
1:A:112:VAL:HG12	1:A:112:VAL:O	2.12	0.49
1:E:50:GLU:O	1:E:53:ILE:HG22	2.12	0.49
1:E:140:VAL:HG22	4:E:375:HOH:O	2.12	0.49
1:C:129:GLU:O	1:C:133:TRP:N	2.46	0.49
1:C:143:LYS:HA	1:C:143:LYS:CE	2.42	0.49
1:E:47:LEU:HD12	1:E:47:LEU:C	2.38	0.49
1:E:60:PHE:HE2	3:E:161:GDP:O4'	1.96	0.49
1:A:85:LYS:HB2	4:A:396:HOH:O	2.12	0.49
1:C:14:ASP:O	1:C:18:ARG:HB2	2.12	0.49
1:A:47:LEU:CD1	1:A:132:LEU:HD22	2.42	0.49
1:C:139:LEU:N	1:C:139:LEU:CD1	2.74	0.49
1:D:47:LEU:HD11	1:D:132:LEU:CD2	2.43	0.49
1:F:23:GLU:O	1:F:24:ILE:C	2.53	0.49
1:F:40:PHE:CE1	1:F:72:PRO:HB2	2.47	0.49
1:C:134:PHE:HD1	1:C:138:GLU:OE1	1.96	0.49
1:B:102:GLY:N	4:B:415:HOH:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:PRO:HB2	1:F:110:ILE:O	2.13	0.48
1:A:59:PRO:O	1:A:60:PHE:C	2.56	0.48
1:B:14:ASP:OD1	1:B:67:TYR:OH	2.30	0.48
1:B:93:GLU:N	1:B:99:SER:OG	2.45	0.48
1:D:135:HIS:O	1:D:137:GLU:N	2.46	0.48
1:D:152:GLU:HG3	1:D:152:GLU:OXT	2.13	0.48
1:E:14:ASP:HA	1:F:149:TRP:HE3	1.78	0.48
1:F:41:MET:HE3	1:F:133:TRP:CE3	2.38	0.48
1:C:46:ASP:O	1:C:50:GLU:HB2	2.13	0.48
1:C:74:VAL:O	1:C:74:VAL:HG12	2.14	0.48
1:D:140:VAL:CG1	1:D:141:ASN:N	2.76	0.48
1:F:9:ILE:O	1:F:76:MET:HB2	2.13	0.48
1:D:77:VAL:HG12	1:D:78:TRP:N	2.27	0.48
1:E:43:ALA:O	1:E:69:HIS:ND1	2.29	0.48
1:F:42:ARG:HA	1:F:72:PRO:HA	1.94	0.48
1:C:96:PRO:HA	1:C:99:SER:OG	2.13	0.48
1:F:11:ILE:HD13	1:F:21:ILE:HA	1.96	0.48
1:A:136:PRO:C	1:A:138:GLU:H	2.19	0.48
1:B:48:LEU:CB	1:B:65:VAL:HG13	2.44	0.48
1:B:49:LYS:NZ	1:B:49:LYS:HB2	2.22	0.48
1:B:109:CYS:HB3	1:B:116:ILE:HD13	1.95	0.48
1:C:150:ILE:O	1:C:150:ILE:HG22	2.10	0.48
1:D:52:TYR:OH	2:D:160:35G:O1P	2.24	0.48
1:D:87:GLY:O	1:D:90:MET:HB2	2.12	0.48
1:E:81:LEU:HG	1:E:81:LEU:O	2.14	0.48
1:E:88:ARG:O	1:E:91:LEU:HB2	2.13	0.48
1:D:46:ASP:HA	1:D:49:LYS:CD	2.43	0.48
1:D:143:LYS:HB2	1:D:143:LYS:HZ3	1.74	0.48
1:A:56:LYS:HD2	1:A:57:ASP:OD1	2.13	0.48
1:C:5:GLU:O	1:C:83:VAL:HG22	2.13	0.48
1:C:7:THR:CB	1:C:84:VAL:HG22	2.44	0.48
1:D:110:ILE:CD1	1:E:33:PHE:CD1	2.96	0.48
1:D:144:SER:C	1:D:146:ALA:H	2.22	0.48
1:B:2:ALA:O	1:B:5:GLU:HB2	2.13	0.48
1:B:118:HIS:CG	1:B:119:GLY:N	2.80	0.48
1:D:42:ARG:O	1:D:43:ALA:C	2.52	0.48
1:F:45:GLU:O	1:F:46:ASP:C	2.50	0.48
1:F:87:GLY:O	1:F:91:LEU:HD13	2.14	0.48
1:B:128:LYS:HG2	1:B:129:GLU:N	2.29	0.48
1:C:6:ARG:H	1:C:6:ARG:HG3	1.22	0.48
1:E:33:PHE:CD1	1:E:83:VAL:HG13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLN:HG3	1:B:149:TRP:CZ2	2.49	0.47
1:A:34:ARG:NH2	1:A:36:VAL:HG22	2.29	0.47
1:D:27:ARG:NH1	1:D:102:GLY:O	2.46	0.47
1:E:38:MET:HA	1:E:75:ALA:O	2.14	0.47
1:E:143:LYS:HA	1:E:143:LYS:HZ2	1.77	0.47
1:A:35:LEU:O	1:A:142:TYR:OH	2.27	0.47
1:B:133:TRP:H	1:B:133:TRP:CD1	2.33	0.47
1:C:25:ILE:HD13	1:C:25:ILE:HG21	1.69	0.47
1:C:26:LYS:O	1:C:27:ARG:C	2.53	0.47
1:C:118:HIS:CG	1:C:119:GLY:N	2.82	0.47
1:C:125:SER:O	1:C:126:ALA:C	2.57	0.47
1:E:34:ARG:O	1:E:78:TRP:HA	2.13	0.47
1:A:11:ILE:HA	1:A:117:ILE:HG13	1.95	0.47
1:C:145:CYS:HB2	1:D:145:CYS:O	2.14	0.47
1:F:124:GLU:HB2	4:F:485:HOH:O	2.15	0.47
1:F:141:ASN:OD1	1:F:141:ASN:N	2.46	0.47
1:B:133:TRP:CD1	1:B:133:TRP:N	2.83	0.47
1:C:24:ILE:O	1:C:27:ARG:HB2	2.14	0.47
1:C:40:PHE:CE2	1:F:140:VAL:HB	2.49	0.47
1:C:83:VAL:HG23	1:C:84:VAL:H	1.79	0.47
1:D:51:HIS:HD2	1:D:52:TYR:CD2	2.32	0.47
1:E:135:HIS:C	1:E:137:GLU:N	2.70	0.47
1:F:67:TYR:O	1:F:69:HIS:N	2.46	0.47
1:F:123:VAL:HB	1:F:124:GLU:H	1.48	0.47
1:C:74:VAL:O	1:C:76:MET:HE2	2.13	0.47
1:E:127:GLU:N	1:E:130:ILE:HD12	2.29	0.47
1:F:143:LYS:NZ	1:F:147:GLN:OE1	2.47	0.47
1:C:111:GLN:N	4:C:209:HOH:O	2.30	0.47
1:E:129:GLU:O	1:E:133:TRP:HD1	1.98	0.47
1:A:30:GLN:C	1:A:32:GLY:H	2.23	0.47
1:A:80:GLY:H	1:A:83:VAL:HG22	1.79	0.47
1:A:82:ASN:O	1:A:83:VAL:C	2.57	0.47
1:B:59:PRO:N	4:B:365:HOH:O	2.47	0.47
1:B:110:ILE:HD11	1:C:32:GLY:C	2.39	0.47
1:E:124:GLU:O	1:E:127:GLU:N	2.48	0.47
1:A:135:HIS:HB3	1:A:137:GLU:OE2	2.15	0.47
1:B:15:GLY:O	1:B:16:VAL:C	2.57	0.47
1:B:104:ILE:O	1:B:105:ARG:C	2.57	0.47
1:B:127:GLU:O	1:B:128:LYS:C	2.51	0.47
1:B:144:SER:HB3	4:D:303:HOH:O	2.15	0.47
1:E:85:LYS:HB3	4:E:354:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:GLY:O	1:F:114:ARG:NE	2.48	0.47
1:A:118:HIS:HA	4:A:502:HOH:O	2.14	0.47
1:F:67:TYR:C	1:F:69:HIS:N	2.70	0.47
1:F:145:CYS:O	1:F:147:GLN:N	2.48	0.47
1:A:60:PHE:CD1	1:A:60:PHE:N	2.81	0.47
1:B:64:LEU:O	1:B:67:TYR:HB3	2.15	0.47
1:B:115:ASN:C	1:B:117:ILE:H	2.23	0.47
1:E:40:PHE:CZ	1:E:72:PRO:HB2	2.49	0.47
4:A:232:HOH:O	1:E:144:SER:HB3	2.13	0.46
1:B:88:ARG:HH11	1:B:88:ARG:HD2	1.54	0.46
1:C:14:ASP:OD1	1:C:67:TYR:OH	2.24	0.46
1:F:12:LYS:HB3	1:F:13:PRO:CD	2.45	0.46
1:D:114:ARG:NH2	4:D:226:HOH:O	2.48	0.46
1:E:52:TYR:O	1:E:53:ILE:C	2.56	0.46
1:F:12:LYS:NZ	2:F:160:35G:O3'	2.48	0.46
1:B:126:ALA:O	1:B:127:GLU:C	2.57	0.46
1:E:22:GLY:O	1:E:26:LYS:HB2	2.14	0.46
1:E:66:LYS:HE3	1:E:67:TYR:N	2.31	0.46
1:E:135:HIS:HB3	1:E:137:GLU:OE2	2.16	0.46
1:F:49:LYS:HA	1:F:61:PHE:HZ	1.80	0.46
1:A:41:MET:HE2	1:A:133:TRP:CZ3	2.51	0.46
1:B:48:LEU:CD2	1:B:68:MET:HB3	2.35	0.46
1:D:40:PHE:CZ	1:D:72:PRO:HG2	2.51	0.46
1:D:126:ALA:O	1:D:130:ILE:HG13	2.16	0.46
1:A:51:HIS:ND1	1:A:133:TRP:NE1	2.62	0.46
1:B:40:PHE:CZ	1:B:72:PRO:HB2	2.49	0.46
1:C:55:LEU:HD12	1:C:55:LEU:N	2.29	0.46
1:C:61:PHE:O	1:C:62:ALA:C	2.57	0.46
1:E:126:ALA:O	1:E:130:ILE:HD12	2.16	0.46
1:C:18:ARG:NH1	1:C:108:PHE:O	2.47	0.46
1:C:28:PHE:O	1:C:29:GLU:C	2.58	0.46
1:C:45:GLU:HB3	1:C:49:LYS:HE2	1.97	0.46
1:D:81:LEU:O	1:D:81:LEU:HG	2.15	0.46
1:F:36:VAL:HB	1:F:77:VAL:HB	1.96	0.46
1:F:95:ASN:C	1:F:97:ALA:N	2.73	0.46
1:A:58:ARG:NH1	1:A:58:ARG:CG	2.76	0.46
1:B:53:ILE:CG2	1:B:128:LYS:NZ	2.79	0.46
1:D:34:ARG:CG	1:D:142:TYR:CZ	2.98	0.46
1:F:65:VAL:HG23	1:F:65:VAL:H	1.40	0.46
1:C:146:ALA:C	1:C:148:ASN:N	2.74	0.46
1:D:143:LYS:HE3	1:D:147:GLN:CD	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:ILE:CG2	1:F:54:ASP:N	2.78	0.46
1:A:81:LEU:HD12	1:A:82:ASN:N	2.30	0.46
1:F:48:LEU:HD23	1:F:48:LEU:HA	1.72	0.46
1:B:128:LYS:CG	1:B:129:GLU:N	2.80	0.45
1:B:139:LEU:HD22	1:B:139:LEU:H	1.80	0.45
1:C:41:MET:O	1:C:73:VAL:HG22	2.16	0.45
1:D:56:LYS:NZ	1:D:57:ASP:OD2	2.49	0.45
1:D:108:PHE:CD2	1:E:30:GLN:HB2	2.52	0.45
1:D:134:PHE:HD1	1:D:138:GLU:OE1	1.98	0.45
1:D:135:HIS:O	1:D:136:PRO:C	2.59	0.45
1:E:109:CYS:HB3	1:E:116:ILE:HD13	1.98	0.45
1:E:134:PHE:O	1:E:136:PRO:HD3	2.16	0.45
1:F:67:TYR:C	1:F:67:TYR:CD1	2.89	0.45
1:D:67:TYR:O	1:D:70:SER:HB2	2.17	0.45
1:F:123:VAL:C	1:F:125:SER:N	2.72	0.45
1:B:86:THR:O	1:B:87:GLY:C	2.60	0.45
1:C:6:ARG:HA	1:C:83:VAL:HG21	1.97	0.45
1:D:44:SER:O	1:D:48:LEU:HB2	2.16	0.45
1:D:61:PHE:O	1:D:62:ALA:HB3	2.16	0.45
1:E:11:ILE:HG13	1:E:76:MET:CE	2.46	0.45
1:F:137:GLU:H	1:F:137:GLU:HG3	1.39	0.45
1:A:10:ALA:HA	1:A:74:VAL:O	2.17	0.45
1:B:12:LYS:HD2	4:B:404:HOH:O	2.16	0.45
1:C:26:LYS:O	1:C:30:GLN:HG2	2.16	0.45
1:E:64:LEU:O	1:E:68:MET:HG2	2.16	0.45
1:F:88:ARG:NH1	1:F:121:ASP:CB	2.79	0.45
3:F:161:GDP:O6	4:F:377:HOH:O	2.20	0.45
1:A:110:ILE:HD11	1:B:31:LYS:O	2.17	0.45
1:B:80:GLY:N	1:B:83:VAL:CG2	2.79	0.45
1:C:21:ILE:HD13	1:C:21:ILE:HG21	1.71	0.45
1:C:27:ARG:HD3	4:C:247:HOH:O	2.16	0.45
1:E:60:PHE:CE2	3:E:161:GDP:N9	2.85	0.45
1:D:41:MET:HB2	1:D:41:MET:HE2	1.25	0.45
1:F:6:ARG:HA	1:F:78:TRP:O	2.17	0.45
1:F:85:LYS:HE3	1:F:85:LYS:HB3	1.62	0.45
1:B:129:GLU:O	1:B:133:TRP:HD1	2.00	0.45
1:F:136:PRO:C	1:F:138:GLU:H	2.25	0.45
1:B:5:GLU:OE2	1:B:82:ASN:HA	2.17	0.45
1:B:35:LEU:N	1:B:78:TRP:CE3	2.85	0.45
1:D:2:ALA:C	1:D:4:SER:N	2.75	0.45
1:E:40:PHE:HD1	1:E:73:VAL:O	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:LEU:O	1:E:49:LYS:C	2.56	0.45
1:A:55:LEU:HD13	1:A:55:LEU:HA	1.37	0.45
1:B:4:SER:C	1:B:79:GLU:HG3	2.42	0.44
1:C:4:SER:HA	1:C:79:GLU:HG3	1.99	0.44
1:C:55:LEU:N	1:C:55:LEU:CD1	2.80	0.44
1:D:91:LEU:HD12	1:D:91:LEU:HA	1.71	0.44
1:D:123:VAL:C	1:D:126:ALA:HB3	2.43	0.44
1:A:55:LEU:O	1:A:56:LYS:C	2.60	0.44
1:B:12:LYS:HD3	1:B:68:MET:SD	2.57	0.44
1:B:94:THR:O	1:B:96:PRO:HD3	2.17	0.44
1:D:94:THR:HA	1:D:105:ARG:NH1	2.31	0.44
1:D:136:PRO:CD	1:D:137:GLU:H	2.26	0.44
1:E:5:GLU:OE2	1:E:84:VAL:HG23	2.17	0.44
1:E:14:ASP:OD2	1:E:116:ILE:HG22	2.18	0.44
1:D:6:ARG:NH1	4:D:294:HOH:O	2.50	0.44
1:A:84:VAL:HG13	1:A:120:SER:O	2.16	0.44
1:A:125:SER:O	1:A:126:ALA:C	2.59	0.44
1:B:95:ASN:C	1:B:97:ALA:N	2.73	0.44
1:C:91:LEU:HD11	1:C:117:ILE:CG1	2.46	0.44
1:D:28:PHE:CD1	1:D:90:MET:CE	3.01	0.44
1:D:47:LEU:O	1:D:50:GLU:HB2	2.18	0.44
1:F:5:GLU:O	1:F:83:VAL:HG21	2.18	0.44
1:F:8:PHE:CE2	1:F:10:ALA:HB2	2.52	0.44
1:A:14:ASP:O	1:A:18:ARG:HG3	2.18	0.44
1:A:47:LEU:CD1	1:A:132:LEU:CD2	2.95	0.44
1:A:129:GLU:O	1:A:133:TRP:HD1	1.99	0.44
1:B:91:LEU:O	1:B:105:ARG:HG3	2.17	0.44
1:D:45:GLU:C	1:D:49:LYS:HD2	2.42	0.44
1:F:38:MET:HB3	1:F:38:MET:HE2	1.86	0.44
1:A:38:MET:HG3	1:A:74:VAL:CG1	2.48	0.44
1:A:39:LYS:N	1:A:75:ALA:O	2.43	0.44
1:A:48:LEU:HD13	1:A:48:LEU:HA	1.53	0.44
1:A:132:LEU:HD23	1:A:132:LEU:O	2.18	0.44
1:C:8:PHE:CE1	1:C:75:ALA:HB1	2.50	0.44
1:E:8:PHE:HE1	1:E:75:ALA:HB1	1.83	0.44
1:E:30:GLN:H	1:E:30:GLN:HG2	1.49	0.44
1:E:72:PRO:C	1:E:73:VAL:HG13	2.41	0.44
1:F:47:LEU:O	1:F:48:LEU:O	2.34	0.44
1:A:31:LYS:HE2	1:C:110:ILE:HG23	2.00	0.44
1:A:140:VAL:HG12	1:A:141:ASN:H	1.82	0.44
1:E:5:GLU:C	1:E:6:ARG:HG3	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:LYS:O	1:F:106:GLY:HA3	2.17	0.44
1:A:37:ALA:HB2	1:A:139:LEU:CD1	2.40	0.44
1:C:6:ARG:HD2	4:C:380:HOH:O	2.17	0.44
1:E:44:SER:O	1:E:47:LEU:HB3	2.18	0.44
1:A:7:THR:HB	1:A:84:VAL:CG2	2.46	0.44
1:C:77:VAL:HG23	1:C:134:PHE:CE2	2.53	0.44
1:C:144:SER:O	1:C:145:CYS:C	2.60	0.44
1:D:54:ASP:OD1	1:D:54:ASP:N	2.44	0.44
1:E:48:LEU:CD1	1:E:69:HIS:HB2	2.47	0.44
1:A:83:VAL:O	1:A:84:VAL:C	2.57	0.43
1:B:29:GLU:OE2	1:D:21:ILE:HB	2.18	0.43
1:B:42:ARG:NH1	4:B:257:HOH:O	2.50	0.43
1:B:125:SER:HB3	4:B:422:HOH:O	2.18	0.43
1:B:134:PHE:HB3	1:B:138:GLU:OE2	2.18	0.43
1:C:44:SER:O	1:C:48:LEU:N	2.43	0.43
1:E:60:PHE:CE2	3:E:161:GDP:O4'	2.70	0.43
1:A:31:LYS:O	1:A:31:LYS:CG	2.62	0.43
1:C:40:PHE:HE2	1:F:140:VAL:HB	1.83	0.43
1:D:108:PHE:O	1:D:109:CYS:HB3	2.17	0.43
1:E:67:TYR:C	1:E:69:HIS:N	2.74	0.43
1:E:117:ILE:HG12	1:E:118:HIS:H	1.82	0.43
1:F:69:HIS:CD2	1:F:69:HIS:O	2.71	0.43
1:C:29:GLU:OE2	4:C:321:HOH:O	2.21	0.43
1:D:8:PHE:HB3	1:D:120:SER:OG	2.18	0.43
1:D:37:ALA:O	1:D:76:MET:HA	2.18	0.43
1:F:88:ARG:O	1:F:91:LEU:HB2	2.19	0.43
1:C:104:ILE:O	1:C:108:PHE:CD2	2.71	0.43
1:D:47:LEU:HD11	1:D:132:LEU:HD22	2.01	0.43
1:E:12:LYS:HB3	1:E:13:PRO:HD2	2.01	0.43
1:F:60:PHE:CD1	1:F:60:PHE:N	2.80	0.43
1:F:85:LYS:HB2	4:F:280:HOH:O	2.19	0.43
1:B:61:PHE:CD1	1:B:61:PHE:C	2.94	0.43
1:D:95:ASN:C	1:D:97:ALA:N	2.77	0.43
1:D:115:ASN:C	1:D:116:ILE:HG13	2.44	0.43
1:F:27:ARG:NH2	1:F:107:ASP:OD2	2.48	0.43
1:F:81:LEU:O	1:F:82:ASN:C	2.60	0.43
1:F:145:CYS:C	1:F:147:GLN:N	2.77	0.43
1:A:37:ALA:O	1:A:76:MET:HA	2.19	0.43
1:A:135:HIS:C	1:A:138:GLU:HG3	2.42	0.43
1:B:122:SER:OG	1:B:124:GLU:HG3	2.17	0.43
1:D:18:ARG:NH1	4:D:473:HOH:O	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:VAL:H	1:D:89:VAL:HG23	1.55	0.43
1:E:37:ALA:O	1:E:76:MET:HA	2.18	0.43
1:E:58:ARG:HA	1:E:59:PRO:HD3	1.78	0.43
1:A:108:PHE:O	1:A:109:CYS:HB3	2.19	0.43
1:A:117:ILE:HG12	1:A:118:HIS:N	2.33	0.43
1:B:45:GLU:HG3	1:B:69:HIS:HD2	1.82	0.43
1:B:81:LEU:O	1:B:82:ASN:C	2.59	0.43
1:B:95:ASN:O	1:B:98:ASP:N	2.40	0.43
1:B:109:CYS:CB	1:B:116:ILE:HD13	2.49	0.43
1:C:78:TRP:C	1:C:83:VAL:HG11	2.44	0.43
1:C:100:LYS:HD3	4:C:348:HOH:O	2.17	0.43
1:D:48:LEU:O	1:D:52:TYR:N	2.51	0.43
1:D:124:GLU:O	1:D:128:LYS:HB2	2.19	0.43
1:A:14:ASP:OD2	1:A:116:ILE:N	2.51	0.43
1:A:14:ASP:OD1	1:A:67:TYR:OH	2.23	0.43
1:C:61:PHE:O	1:C:63:GLY:N	2.51	0.43
1:D:149:TRP:O	1:F:114:ARG:HB3	2.18	0.43
1:E:12:LYS:HG3	1:E:117:ILE:CA	2.48	0.43
1:A:80:GLY:O	1:A:83:VAL:CG2	2.66	0.43
1:B:105:ARG:O	1:B:106:GLY:C	2.61	0.43
1:B:117:ILE:HG21	1:B:117:ILE:HD13	1.57	0.43
1:C:7:THR:HB	1:C:84:VAL:HG22	2.01	0.43
1:C:40:PHE:HD1	1:C:74:VAL:HG22	1.84	0.43
1:C:95:ASN:C	1:C:97:ALA:N	2.76	0.43
1:E:80:GLY:O	1:E:83:VAL:CG2	2.66	0.43
1:F:143:LYS:HZ3	1:F:147:GLN:NE2	2.17	0.43
1:A:12:LYS:HE3	1:A:117:ILE:O	2.19	0.43
1:A:152:GLU:HB3	1:C:111:GLN:OE1	2.19	0.43
1:F:53:ILE:O	1:F:56:LYS:HB2	2.19	0.43
1:F:152:GLU:O	1:F:152:GLU:HG2	2.18	0.43
1:A:14:ASP:OD2	1:A:116:ILE:HA	2.19	0.42
1:A:51:HIS:C	1:A:51:HIS:CD2	2.96	0.42
1:E:40:PHE:O	1:E:41:MET:HB3	2.19	0.42
1:E:95:ASN:C	1:E:97:ALA:H	2.27	0.42
1:F:2:ALA:O	1:F:81:LEU:HA	2.19	0.42
1:F:44:SER:O	1:F:48:LEU:N	2.47	0.42
1:F:143:LYS:NZ	1:F:147:GLN:CD	2.77	0.42
1:A:146:ALA:O	1:A:147:GLN:C	2.63	0.42
1:B:16:VAL:HG13	1:B:21:ILE:HD11	2.01	0.42
1:B:123:VAL:C	1:B:125:SER:N	2.75	0.42
1:C:20:LEU:O	1:C:24:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:VAL:H	1:C:65:VAL:HG23	1.62	0.42
1:D:11:ILE:HG21	1:D:11:ILE:HD13	1.46	0.42
1:D:25:ILE:HD13	1:D:25:ILE:HG21	1.80	0.42
1:E:135:HIS:C	1:E:137:GLU:H	2.27	0.42
1:F:3:ASN:HA	1:F:81:LEU:CA	2.48	0.42
1:A:9:ILE:HD12	1:A:9:ILE:HG23	1.71	0.42
1:B:93:GLU:O	1:B:99:SER:OG	2.38	0.42
1:C:18:ARG:NH1	4:C:264:HOH:O	2.28	0.42
1:E:45:GLU:O	1:E:48:LEU:HB2	2.19	0.42
1:A:30:GLN:C	1:A:32:GLY:N	2.78	0.42
1:C:118:HIS:CD2	1:C:119:GLY:N	2.88	0.42
1:D:136:PRO:HD2	1:D:137:GLU:CG	2.34	0.42
1:E:7:THR:O	1:E:77:VAL:HA	2.20	0.42
1:C:12:LYS:CB	1:C:13:PRO:CD	2.94	0.42
1:D:132:LEU:HD23	1:D:132:LEU:C	2.44	0.42
1:D:149:TRP:CE2	1:F:17:GLN:HG3	2.55	0.42
1:F:65:VAL:O	1:F:66:LYS:C	2.60	0.42
1:F:95:ASN:HA	1:F:112:VAL:HG13	2.01	0.42
1:F:111:GLN:C	1:F:113:GLY:N	2.78	0.42
1:A:136:PRO:C	1:A:138:GLU:N	2.77	0.42
1:B:135:HIS:HA	1:B:136:PRO:HD2	1.79	0.42
1:F:15:GLY:O	1:F:16:VAL:C	2.60	0.42
1:F:45:GLU:O	1:F:49:LYS:HB2	2.19	0.42
1:D:53:ILE:C	1:D:55:LEU:H	2.28	0.42
1:D:94:THR:O	1:D:96:PRO:HD3	2.19	0.42
1:E:53:ILE:HD11	1:E:56:LYS:NZ	2.35	0.42
1:A:41:MET:CE	1:A:133:TRP:CE3	3.01	0.42
1:D:31:LYS:HE2	1:F:109:CYS:O	2.19	0.42
1:D:56:LYS:NZ	1:D:56:LYS:HB3	2.34	0.42
1:D:61:PHE:C	1:D:63:GLY:H	2.26	0.42
1:D:80:GLY:O	1:D:81:LEU:C	2.59	0.42
1:D:146:ALA:O	1:D:147:GLN:C	2.62	0.42
1:E:45:GLU:O	1:E:49:LYS:HG2	2.20	0.42
1:E:135:HIS:HA	1:E:136:PRO:HD2	1.46	0.42
1:F:49:LYS:HG2	1:F:61:PHE:HZ	1.85	0.42
1:F:100:LYS:HA	1:F:100:LYS:HD3	1.95	0.42
1:B:127:GLU:HA	1:B:130:ILE:CG1	2.45	0.42
1:D:14:ASP:C	1:D:116:ILE:HG22	2.45	0.42
1:E:124:GLU:O	1:E:127:GLU:HB2	2.20	0.42
1:A:36:VAL:HG23	1:A:79:GLU:HB3	2.02	0.41
1:B:29:GLU:HG3	1:B:78:TRP:HH2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ARG:O	1:B:61:PHE:CB	2.68	0.41
1:D:15:GLY:HA2	1:D:116:ILE:HG22	2.02	0.41
1:D:51:HIS:CD2	1:D:51:HIS:C	2.96	0.41
1:D:135:HIS:O	1:D:138:GLU:HB2	2.19	0.41
1:E:128:LYS:O	1:E:131:ALA:HB3	2.19	0.41
1:C:81:LEU:HB3	1:C:151:TYR:CE1	2.55	0.41
1:C:93:GLU:H	1:C:99:SER:CB	2.25	0.41
1:E:39:LYS:CE	1:E:41:MET:HE3	2.47	0.41
1:A:80:GLY:C	1:A:83:VAL:HG22	2.45	0.41
1:B:67:TYR:C	1:B:70:SER:HG	2.28	0.41
1:C:53:ILE:HG23	1:C:54:ASP:H	1.84	0.41
1:C:118:HIS:CD2	1:C:118:HIS:C	2.96	0.41
1:D:47:LEU:HA	1:D:47:LEU:HD12	1.57	0.41
1:E:58:ARG:HG3	1:E:59:PRO:CD	2.50	0.41
1:B:129:GLU:H	1:B:129:GLU:HG2	1.53	0.41
1:C:14:ASP:OD2	1:C:116:ILE:HG23	2.21	0.41
1:C:64:LEU:HD13	1:C:64:LEU:HA	1.71	0.41
1:F:123:VAL:HG23	4:F:485:HOH:O	2.19	0.41
1:F:46:ASP:O	1:F:49:LYS:HB2	2.21	0.41
1:A:67:TYR:C	1:A:69:HIS:N	2.78	0.41
1:A:140:VAL:HG12	1:A:141:ASN:N	2.36	0.41
1:B:51:HIS:C	1:B:53:ILE:N	2.75	0.41
1:B:129:GLU:O	1:B:133:TRP:CD1	2.74	0.41
1:E:8:PHE:H	1:E:120:SER:HB2	1.85	0.41
1:E:52:TYR:OH	1:E:68:MET:HE2	2.19	0.41
1:E:132:LEU:HB3	1:E:133:TRP:CD1	2.56	0.41
1:A:100:LYS:HA	1:A:100:LYS:HD2	1.93	0.41
1:A:142:TYR:N	1:A:142:TYR:CD1	2.88	0.41
1:A:146:ALA:O	1:A:149:TRP:N	2.48	0.41
1:E:17:GLN:HG3	1:F:149:TRP:CE2	2.56	0.41
1:E:45:GLU:HB3	1:E:49:LYS:HE2	2.03	0.41
1:F:60:PHE:O	1:F:63:GLY:N	2.29	0.41
1:A:135:HIS:O	1:A:138:GLU:HB2	2.21	0.41
1:A:8:PHE:HD2	1:A:129:GLU:OE1	2.03	0.41
1:A:17:GLN:NE2	1:E:142:TYR:HD2	2.19	0.41
1:A:88:ARG:NH2	3:A:161:GDP:O1B	2.46	0.41
1:B:67:TYR:HA	1:B:70:SER:HG	1.85	0.41
1:C:140:VAL:HG12	1:C:142:TYR:CD1	2.54	0.41
1:D:24:ILE:HA	1:D:27:ARG:HG3	2.03	0.41
1:D:95:ASN:C	1:D:97:ALA:H	2.29	0.41
1:F:89:VAL:O	1:F:90:MET:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:VAL:HG12	1:A:115:ASN:ND2	2.36	0.41
1:B:111:GLN:OE1	1:C:151:TYR:HD1	2.04	0.41
1:B:140:VAL:HG11	1:D:72:PRO:CB	2.51	0.41
1:D:41:MET:O	1:D:72:PRO:HA	2.21	0.41
1:B:140:VAL:HG11	1:D:72:PRO:CG	2.50	0.40
1:C:94:THR:HG22	4:C:499:HOH:O	2.20	0.40
1:D:84:VAL:HG21	1:D:123:VAL:HA	2.01	0.40
1:E:23:GLU:O	1:E:27:ARG:HG2	2.21	0.40
1:E:26:LYS:O	1:E:26:LYS:HG2	2.19	0.40
1:E:94:THR:O	1:E:96:PRO:HD3	2.21	0.40
1:E:112:VAL:HG23	1:E:113:GLY:N	2.33	0.40
1:E:137:GLU:H	1:E:137:GLU:HG3	1.29	0.40
1:F:53:ILE:CG2	1:F:54:ASP:H	2.34	0.40
1:C:45:GLU:O	1:C:48:LEU:N	2.55	0.40
1:C:100:LYS:HA	1:C:101:PRO:HD3	1.89	0.40
1:C:149:TRP:CE3	1:C:149:TRP:HA	2.57	0.40
1:D:47:LEU:CD1	1:D:132:LEU:CD2	2.99	0.40
1:D:144:SER:C	1:D:146:ALA:N	2.79	0.40
1:E:81:LEU:HD12	1:E:82:ASN:HD22	1.85	0.40
1:A:6:ARG:HD2	1:A:36:VAL:HG21	2.03	0.40
1:A:67:TYR:C	1:A:69:HIS:H	2.29	0.40
1:A:81:LEU:O	1:A:82:ASN:C	2.62	0.40
1:A:152:GLU:N	1:C:111:GLN:OE1	2.31	0.40
1:B:49:LYS:HZ1	1:B:65:VAL:HG11	1.82	0.40
1:B:93:GLU:O	1:B:95:ASN:N	2.54	0.40
1:C:34:ARG:NH1	1:C:36:VAL:HG22	2.36	0.40
1:E:12:LYS:HB3	1:E:13:PRO:HD3	2.03	0.40
1:F:46:ASP:O	1:F:50:GLU:HB2	2.20	0.40
1:F:48:LEU:O	1:F:51:HIS:HB3	2.21	0.40
1:A:47:LEU:HD13	1:A:132:LEU:HD21	2.03	0.40
1:B:123:VAL:O	1:B:126:ALA:N	2.55	0.40
1:D:12:LYS:HB2	1:D:116:ILE:C	2.47	0.40
1:D:55:LEU:HA	1:D:55:LEU:HD23	1.48	0.40
1:E:51:HIS:ND1	1:E:133:TRP:NE1	2.63	0.40
1:E:64:LEU:O	1:E:64:LEU:HD12	2.22	0.40
1:B:9:ILE:HA	1:B:9:ILE:HD13	1.79	0.40
1:D:136:PRO:C	1:D:138:GLU:H	2.29	0.40
1:E:40:PHE:HE1	1:E:72:PRO:HB2	1.80	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	149/152 (98%)	126 (85%)	16 (11%)	7 (5%)	2	1
1	B	149/152 (98%)	118 (79%)	17 (11%)	14 (9%)	0	0
1	C	149/152 (98%)	122 (82%)	18 (12%)	9 (6%)	1	0
1	D	149/152 (98%)	119 (80%)	25 (17%)	5 (3%)	3	2
1	E	149/152 (98%)	122 (82%)	21 (14%)	6 (4%)	2	2
1	F	149/152 (98%)	117 (78%)	21 (14%)	11 (7%)	1	0
All	All	894/912 (98%)	724 (81%)	118 (13%)	52 (6%)	1	0

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	LYS
1	A	59	PRO
1	A	61	PHE
1	A	115	ASN
1	A	116	ILE
1	B	56	LYS
1	B	58	ARG
1	B	59	PRO
1	B	96	PRO
1	B	116	ILE
1	C	83	VAL
1	C	100	LYS
1	C	116	ILE
1	D	61	PHE
1	D	116	ILE
1	E	116	ILE
1	F	58	ARG
1	F	61	PHE
1	F	84	VAL
1	F	116	ILE

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Mol	Chain	Res	Type
1	A	104	ILE
1	A	130	ILE
1	B	52	TYR
1	B	53	ILE
1	B	61	PHE
1	B	94	THR
1	B	136	PRO
1	C	84	VAL
1	C	147	GLN
1	E	19	GLY
1	E	59	PRO
1	E	61	PHE
1	F	68	MET
1	B	5	GLU
1	F	59	PRO
1	F	146	ALA
1	C	112	VAL
1	E	53	ILE
1	C	61	PHE
1	C	96	PRO
1	C	136	PRO
1	F	96	PRO
1	F	120	SER
1	B	48	LEU
1	B	104	ILE
1	B	84	VAL
1	D	21	ILE
1	E	83	VAL
1	F	123	VAL
1	D	84	VAL
1	D	136	PRO
1	F	112	VAL

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	128/129 (99%)	92 (72%)	36 (28%)	0	0
1	B	128/129 (99%)	88 (69%)	40 (31%)	0	0
1	C	128/129 (99%)	88 (69%)	40 (31%)	0	0
1	D	128/129 (99%)	98 (77%)	30 (23%)	1	1
1	E	128/129 (99%)	92 (72%)	36 (28%)	0	0
1	F	128/129 (99%)	95 (74%)	33 (26%)	0	0
All	All	768/774 (99%)	553 (72%)	215 (28%)	0	0

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	14	ASP
1	A	18	ARG
1	A	23	GLU
1	A	35	LEU
1	A	38	MET
1	A	48	LEU
1	A	53	ILE
1	A	54	ASP
1	A	55	LEU
1	A	56	LYS
1	A	58	ARG
1	A	66	LYS
1	A	70	SER
1	A	77	VAL
1	A	81	LEU
1	A	83	VAL
1	A	88	ARG
1	A	93	GLU
1	A	98	ASP
1	A	100	LYS
1	A	112	VAL
1	A	114	ARG
1	A	116	ILE
1	A	117	ILE
1	A	123	VAL
1	A	127	GLU
1	A	128	LYS
1	A	137	GLU
1	A	139	LEU

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Mol	Chain	Res	Type
1	A	140	VAL
1	A	142	TYR
1	A	143	LYS
1	A	147	GLN
1	A	148	ASN
1	A	150	ILE
1	B	3	ASN
1	B	4	SER
1	B	20	LEU
1	B	35	LEU
1	B	38	MET
1	B	41	MET
1	B	44	SER
1	B	45	GLU
1	B	48	LEU
1	B	49	LYS
1	B	50	GLU
1	B	51	HIS
1	B	53	ILE
1	B	56	LYS
1	B	57	ASP
1	B	64	LEU
1	B	66	LYS
1	B	70	SER
1	B	79	GLU
1	B	83	VAL
1	B	93	GLU
1	B	109	CYS
1	B	110	ILE
1	B	115	ASN
1	B	116	ILE
1	B	117	ILE
1	B	123	VAL
1	B	124	GLU
1	B	125	SER
1	B	127	GLU
1	B	128	LYS
1	B	129	GLU
1	B	130	ILE
1	B	132	LEU
1	B	134	PHE
1	B	137	GLU

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Mol	Chain	Res	Type
1	B	139	LEU
1	B	143	LYS
1	B	144	SER
1	B	151	TYR
1	C	4	SER
1	C	6	ARG
1	C	9	ILE
1	C	12	LYS
1	C	23	GLU
1	C	30	GLN
1	C	35	LEU
1	C	41	MET
1	C	47	LEU
1	C	50	GLU
1	C	56	LYS
1	C	58	ARG
1	C	64	LEU
1	C	66	LYS
1	C	76	MET
1	C	79	GLU
1	C	83	VAL
1	C	85	LYS
1	C	89	VAL
1	C	91	LEU
1	C	94	THR
1	C	98	ASP
1	C	100	LYS
1	C	104	ILE
1	C	107	ASP
1	C	110	ILE
1	C	112	VAL
1	C	114	ARG
1	C	116	ILE
1	C	120	SER
1	C	121	ASP
1	C	123	VAL
1	C	124	GLU
1	C	132	LEU
1	C	137	GLU
1	C	141	ASN
1	C	143	LYS
1	C	144	SER

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Mol	Chain	Res	Type
1	C	147	GLN
1	C	148	ASN
1	D	4	SER
1	D	6	ARG
1	D	20	LEU
1	D	31	LYS
1	D	35	LEU
1	D	41	MET
1	D	49	LYS
1	D	50	GLU
1	D	54	ASP
1	D	56	LYS
1	D	64	LEU
1	D	66	LYS
1	D	79	GLU
1	D	83	VAL
1	D	86	THR
1	D	88	ARG
1	D	91	LEU
1	D	93	GLU
1	D	94	THR
1	D	104	ILE
1	D	112	VAL
1	D	114	ARG
1	D	121	ASP
1	D	124	GLU
1	D	130	ILE
1	D	137	GLU
1	D	140	VAL
1	D	143	LYS
1	D	144	SER
1	D	152	GLU
1	E	6	ARG
1	E	18	ARG
1	E	35	LEU
1	E	41	MET
1	E	44	SER
1	E	46	ASP
1	E	47	LEU
1	E	49	LYS
1	E	53	ILE
1	E	55	LEU

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Mol	Chain	Res	Type
1	E	58	ARG
1	E	64	LEU
1	E	65	VAL
1	E	66	LYS
1	E	76	MET
1	E	81	LEU
1	E	83	VAL
1	E	85	LYS
1	E	91	LEU
1	E	93	GLU
1	E	94	THR
1	E	100	LYS
1	E	112	VAL
1	E	116	ILE
1	E	120	SER
1	E	121	ASP
1	E	124	GLU
1	E	132	LEU
1	E	136	PRO
1	E	137	GLU
1	E	140	VAL
1	E	141	ASN
1	E	143	LYS
1	E	144	SER
1	E	147	GLN
1	E	148	ASN
1	F	6	ARG
1	F	7	THR
1	F	14	ASP
1	F	35	LEU
1	F	39	LYS
1	F	41	MET
1	F	46	ASP
1	F	50	GLU
1	F	53	ILE
1	F	54	ASP
1	F	56	LYS
1	F	57	ASP
1	F	58	ARG
1	F	60	PHE
1	F	66	LYS
1	F	69	HIS

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Mol	Chain	Res	Type
1	F	70	SER
1	F	83	VAL
1	F	84	VAL
1	F	85	LYS
1	F	96	PRO
1	F	104	ILE
1	F	112	VAL
1	F	120	SER
1	F	123	VAL
1	F	127	GLU
1	F	129	GLU
1	F	132	LEU
1	F	137	GLU
1	F	139	LEU
1	F	147	GLN
1	F	148	ASN
1	F	152	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	82	ASN
1	A	147	GLN
1	A	148	ASN
1	B	30	GLN
1	B	69	HIS
1	C	30	GLN
1	C	51	HIS
1	C	148	ASN
1	D	30	GLN
1	E	30	GLN
1	E	82	ASN
1	E	148	ASN
1	F	30	GLN
1	F	69	HIS
1	F	135	HIS

5.3.3 RNA ⓘ

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](#)

12 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	35G	D	160	-	26,26,26	1.51	2 (7%)	39,41,41	2.65	6 (15%)
3	GDP	A	161	-	29,30,30	1.10	2 (6%)	45,47,47	2.08	4 (8%)
3	GDP	B	161	-	29,30,30	1.27	2 (6%)	45,47,47	0.99	3 (6%)
2	35G	F	160	-	26,26,26	2.01	4 (15%)	39,41,41	2.12	8 (20%)
2	35G	C	160	-	26,26,26	1.77	3 (11%)	39,41,41	2.73	8 (20%)
3	GDP	D	161	-	29,30,30	0.83	1 (3%)	45,47,47	2.71	7 (15%)
3	GDP	F	161	-	29,30,30	1.21	2 (6%)	45,47,47	2.50	10 (22%)
3	GDP	C	161	-	29,30,30	1.15	2 (6%)	45,47,47	1.72	7 (15%)
2	35G	A	160	-	26,26,26	1.69	4 (15%)	39,41,41	2.87	5 (12%)
2	35G	B	160	-	26,26,26	1.58	2 (7%)	39,41,41	1.99	6 (15%)
3	GDP	E	161	-	29,30,30	0.98	2 (6%)	45,47,47	2.13	6 (13%)
2	35G	E	160	-	26,26,26	1.28	2 (7%)	39,41,41	2.33	5 (12%)

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	35G	D	160	-	-	0/4/31/31	0/4/4/4
3	GDP	A	161	-	-	2/16/32/32	0/3/3/3
3	GDP	B	161	-	-	1/16/32/32	0/3/3/3
2	35G	F	160	-	-	0/4/31/31	0/4/4/4
2	35G	C	160	-	-	0/4/31/31	0/4/4/4
3	GDP	D	161	-	-	3/16/32/32	0/3/3/3
3	GDP	F	161	-	-	3/16/32/32	0/3/3/3
3	GDP	C	161	-	-	0/16/32/32	0/3/3/3
2	35G	A	160	-	-	0/4/31/31	0/4/4/4
2	35G	B	160	-	-	0/4/31/31	0/4/4/4
3	GDP	E	161	-	-	1/16/32/32	0/3/3/3
2	35G	E	160	-	-	0/4/31/31	0/4/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	160	35G	P-O5'	-6.67	1.50	1.57
2	C	160	35G	P-O5'	-6.37	1.50	1.57
2	B	160	35G	P-O5'	-6.09	1.50	1.57
2	A	160	35G	P-O5'	-5.97	1.50	1.57
2	D	160	35G	P-O5'	-5.89	1.51	1.57
2	F	160	35G	P-O3'	-5.85	1.48	1.57
3	B	161	GDP	PA-O3A	5.33	1.65	1.59
3	F	161	GDP	PA-O3A	5.21	1.65	1.59
2	A	160	35G	P-O3'	-4.56	1.50	1.57
2	E	160	35G	P-O5'	-4.52	1.52	1.57
2	B	160	35G	P-O3'	-4.49	1.50	1.57
2	C	160	35G	P-O3'	-4.08	1.51	1.57
3	A	161	GDP	PA-O3A	3.89	1.63	1.59
2	E	160	35G	P-O3'	-3.87	1.51	1.57
3	C	161	GDP	PA-O3A	3.85	1.63	1.59
2	D	160	35G	P-O3'	-3.73	1.51	1.57
2	F	160	35G	O3'-C3'	-3.11	1.39	1.44
3	E	161	GDP	PA-O3A	3.06	1.62	1.59
3	B	161	GDP	PA-O5'	-2.75	1.48	1.59
3	C	161	GDP	PA-O5'	-2.74	1.48	1.59
2	C	160	35G	O5'-C5'	-2.67	1.42	1.46
3	F	161	GDP	PA-O5'	-2.55	1.49	1.59
3	A	161	GDP	PA-O5'	-2.51	1.49	1.59
3	D	161	GDP	PA-O5'	-2.35	1.50	1.59
2	A	160	35G	O5'-C5'	-2.27	1.42	1.46
3	E	161	GDP	PA-O5'	-2.16	1.50	1.59
2	F	160	35G	O5'-C5'	-2.11	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	160	35G	O3'-C3'	-2.10	1.41	1.44

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	160	35G	C1'-N9-C8	10.71	157.16	126.73
2	A	160	35G	C1'-N9-C8	9.99	155.10	126.73
2	D	160	35G	C1'-N9-C4	-9.86	97.36	126.49
3	F	161	GDP	O3B-PB-O2B	9.69	144.13	107.80
2	A	160	35G	C1'-N9-C4	-9.64	98.01	126.49
3	A	161	GDP	O2A-PA-O3A	9.56	133.11	107.27
3	E	161	GDP	O3B-PB-O1B	9.19	146.66	110.83
3	D	161	GDP	O3B-PB-O1B	9.05	146.09	110.83
2	C	160	35G	C1'-N9-C8	8.90	152.02	126.73
2	A	160	35G	O3'-C3'-C4'	-8.53	104.27	110.71
3	D	161	GDP	O3B-PB-O2B	-8.29	76.72	107.80
3	F	161	GDP	O2A-PA-O3A	8.27	129.63	107.27
2	E	160	35G	C1'-N9-C4	-8.22	102.21	126.49
2	F	160	35G	O5'-P-O3'	8.14	116.60	105.70
3	D	161	GDP	O2A-PA-O3A	-8.02	85.59	107.27
2	B	160	35G	O3'-C3'-C2'	7.77	123.23	115.61
2	E	160	35G	C1'-N9-C8	7.73	148.70	126.73
2	C	160	35G	C1'-N9-C4	-7.60	104.04	126.49
3	A	161	GDP	O3A-PA-O1A	-7.26	88.86	110.70
3	E	161	GDP	O3B-PB-O2B	-7.26	80.59	107.80
2	C	160	35G	O5'-P-O3'	6.43	114.31	105.70
3	F	161	GDP	O3B-PB-O1B	-6.38	85.96	110.83
3	D	161	GDP	C1'-N9-C8	6.03	143.87	126.73
2	C	160	35G	O3'-C3'-C4'	-6.03	106.16	110.71
2	E	160	35G	O5'-P-O3'	5.47	113.03	105.70
3	D	161	GDP	C1'-N9-C4	-5.40	110.54	126.49
2	F	160	35G	O3'-P-O1P	-5.34	98.95	110.39
2	A	160	35G	O5'-P-O3'	5.31	112.81	105.70
3	C	161	GDP	O3A-PA-O1A	5.28	126.60	110.70
3	F	161	GDP	O3A-PA-O1A	-5.14	95.24	110.70
2	D	160	35G	O3'-C3'-C2'	5.14	120.64	115.61
3	C	161	GDP	O2A-PA-O3A	-4.80	94.31	107.27
2	C	160	35G	N2-C2-N1	4.72	126.72	116.76
2	E	160	35G	O3'-C3'-C4'	-4.49	107.32	110.71
3	A	161	GDP	O3B-PB-O2B	4.45	124.49	107.80
2	C	160	35G	C2'-C3'-C4'	-4.26	95.77	103.24
2	B	160	35G	C1'-N9-C8	4.26	138.83	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	160	35G	O3'-C3'-C2'	-4.23	111.45	115.61
3	C	161	GDP	O3B-PB-O1B	4.18	127.14	110.83
3	E	161	GDP	O2A-PA-O3A	-4.10	96.20	107.27
2	B	160	35G	O5'-P-O3'	3.95	110.98	105.70
2	B	160	35G	C1'-N9-C4	-3.88	115.04	126.49
2	B	160	35G	O2'-C2'-C3'	3.84	121.94	111.19
3	D	161	GDP	O2B-PB-O3A	-3.49	92.94	104.64
2	F	160	35G	C1'-N9-C8	3.47	136.58	126.73
3	C	161	GDP	O4'-C1'-N9	3.40	116.07	108.36
3	C	161	GDP	C1'-N9-C8	3.38	136.34	126.73
2	D	160	35G	O2P-P-O3'	3.24	114.59	107.04
3	C	161	GDP	O3B-PB-O2B	-3.23	95.68	107.80
2	F	160	35G	O3'-C3'-C4'	-3.16	108.33	110.71
2	C	160	35G	N2-C2-N3	-3.04	113.75	119.67
3	C	161	GDP	C1'-N9-C4	-2.99	117.66	126.49
3	A	161	GDP	O3B-PB-O1B	-2.93	99.42	110.83
2	E	160	35G	O4'-C1'-N9	-2.92	101.74	108.36
3	B	161	GDP	O3B-PB-O1B	2.80	121.76	110.83
3	B	161	GDP	O2A-PA-O3A	2.79	114.82	107.27
3	F	161	GDP	C1'-N9-C8	2.69	134.37	126.73
3	D	161	GDP	O2A-PA-O1A	2.68	124.91	112.44
2	D	160	35G	O5'-P-O1P	-2.50	104.68	110.44
3	F	161	GDP	O6-C6-N1	-2.43	115.54	120.11
3	F	161	GDP	C1'-N9-C4	-2.40	119.39	126.49
2	F	160	35G	C1'-N9-C4	-2.39	119.43	126.49
2	D	160	35G	O5'-P-O3'	2.38	108.89	105.70
2	F	160	35G	O4'-C1'-N9	2.37	113.72	108.36
2	A	160	35G	O3'-C3'-C2'	2.36	117.92	115.61
2	B	160	35G	C5'-C4'-C3'	-2.23	108.37	112.56
3	E	161	GDP	O5'-C5'-C4'	2.22	116.54	108.99
2	C	160	35G	N1-C2-N3	-2.19	119.32	123.32
3	F	161	GDP	O5'-C5'-C4'	2.18	116.42	108.99
3	E	161	GDP	O2'-C2'-C3'	2.17	118.76	111.82
2	F	160	35G	O4'-C4'-C3'	-2.14	100.40	104.92
3	B	161	GDP	C1'-N9-C8	2.13	132.80	126.73
3	F	161	GDP	O4'-C1'-N9	2.08	113.06	108.36
3	F	161	GDP	C2'-C1'-N9	-2.05	107.53	113.25
3	E	161	GDP	C2'-C1'-N9	-2.01	107.66	113.25

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	161	GDP	PA-O3A-PB-O2B
3	F	161	GDP	C5'-O5'-PA-O1A
3	F	161	GDP	C5'-O5'-PA-O3A
3	D	161	GDP	PB-O3A-PA-O1A
3	E	161	GDP	PA-O3A-PB-O2B
3	A	161	GDP	PB-O3A-PA-O2A
3	F	161	GDP	C4'-C5'-O5'-PA
3	A	161	GDP	PB-O3A-PA-O1A
3	B	161	GDP	PB-O3A-PA-O2A
3	D	161	GDP	PB-O3A-PA-O2A

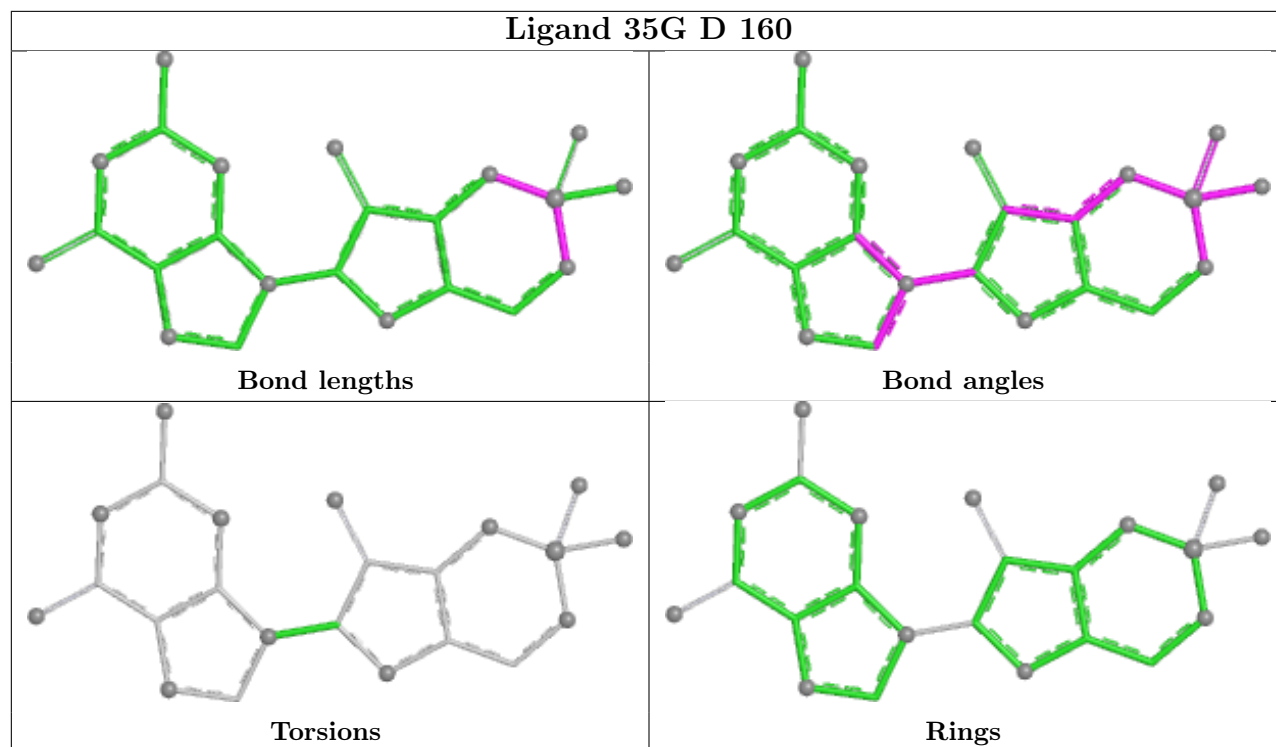
There are no ring outliers.

8 monomers are involved in 16 short contacts:

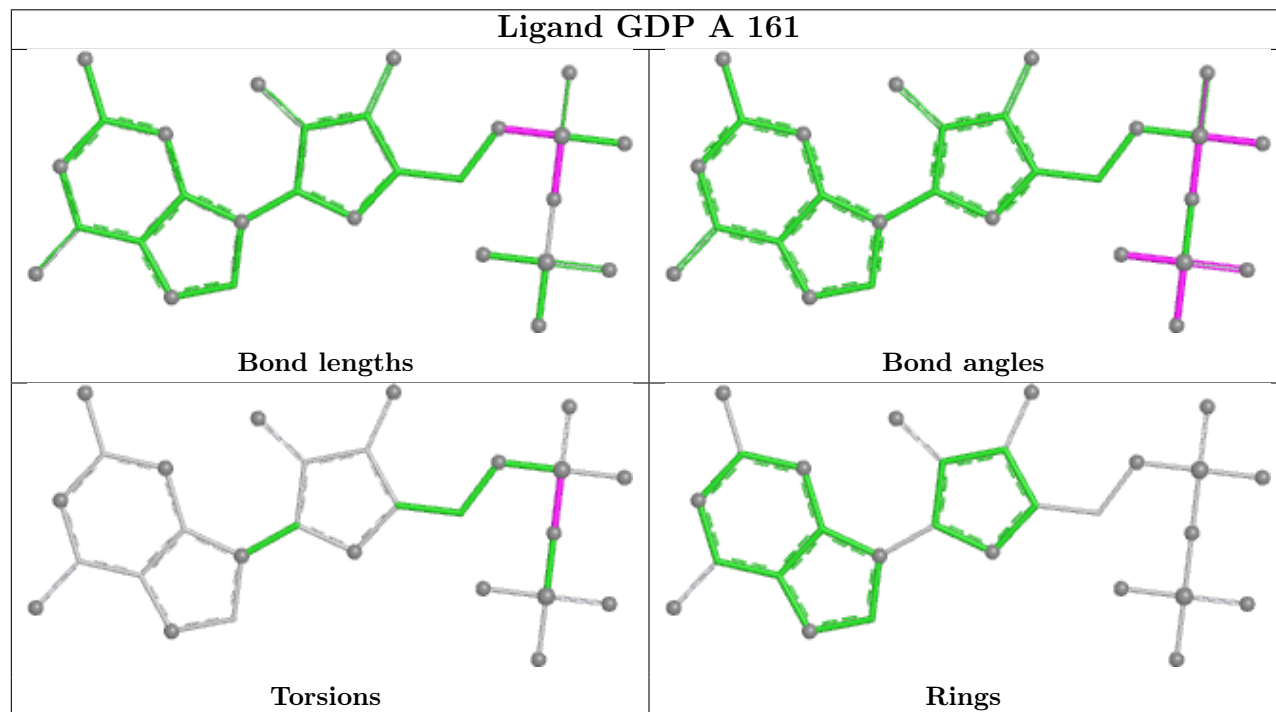
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	160	35G	2	0
3	A	161	GDP	1	0
2	F	160	35G	3	0
3	D	161	GDP	1	0
3	F	161	GDP	1	0
2	B	160	35G	2	0
3	E	161	GDP	5	0
2	E	160	35G	1	0

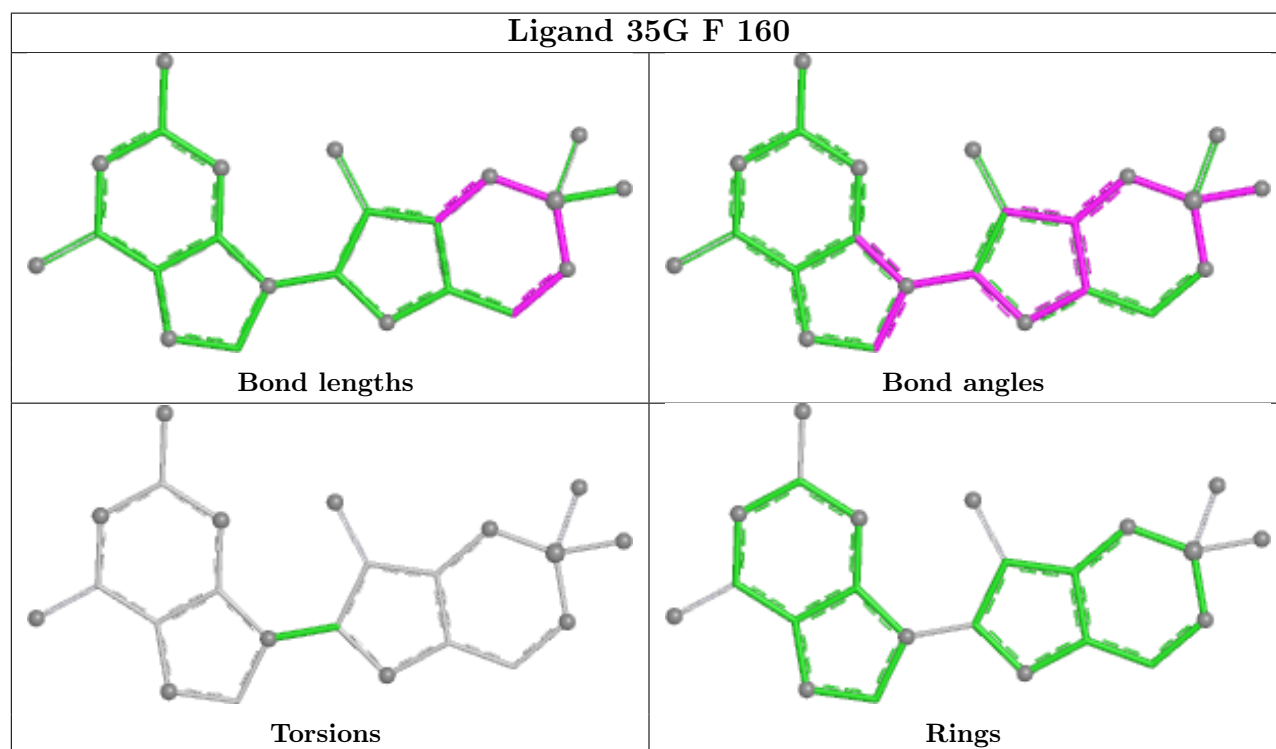
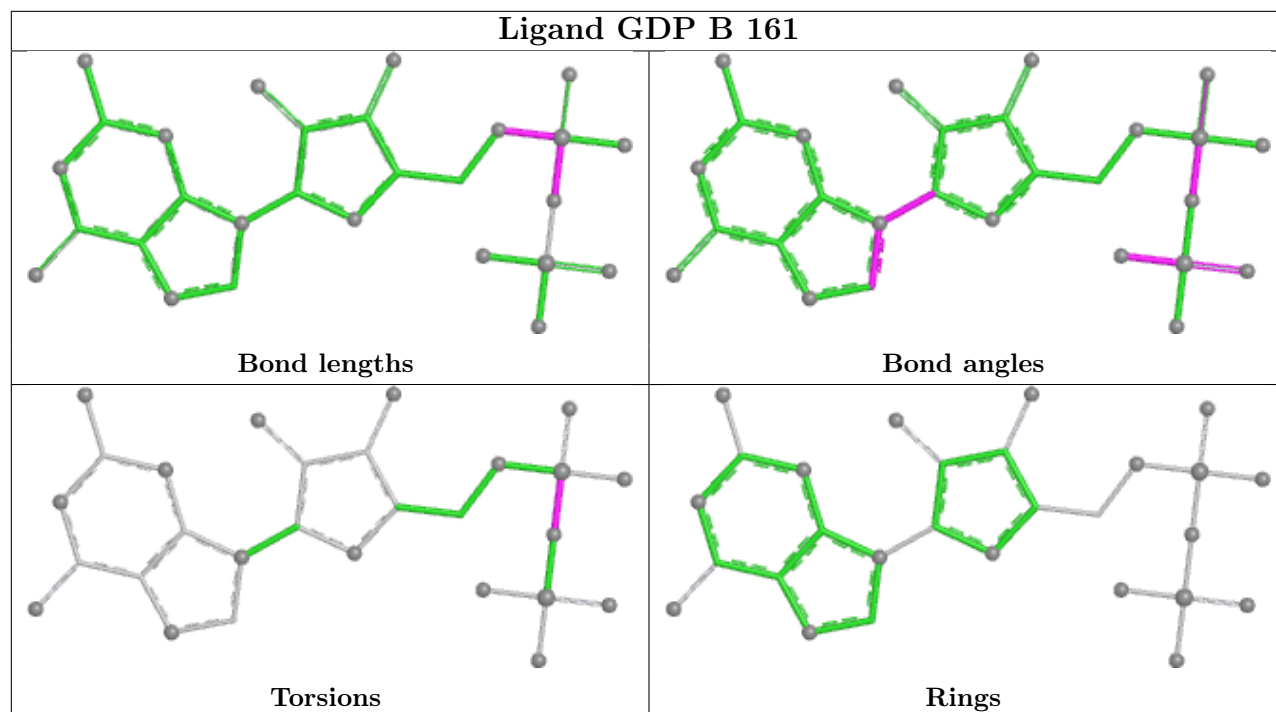
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand 35G D 160

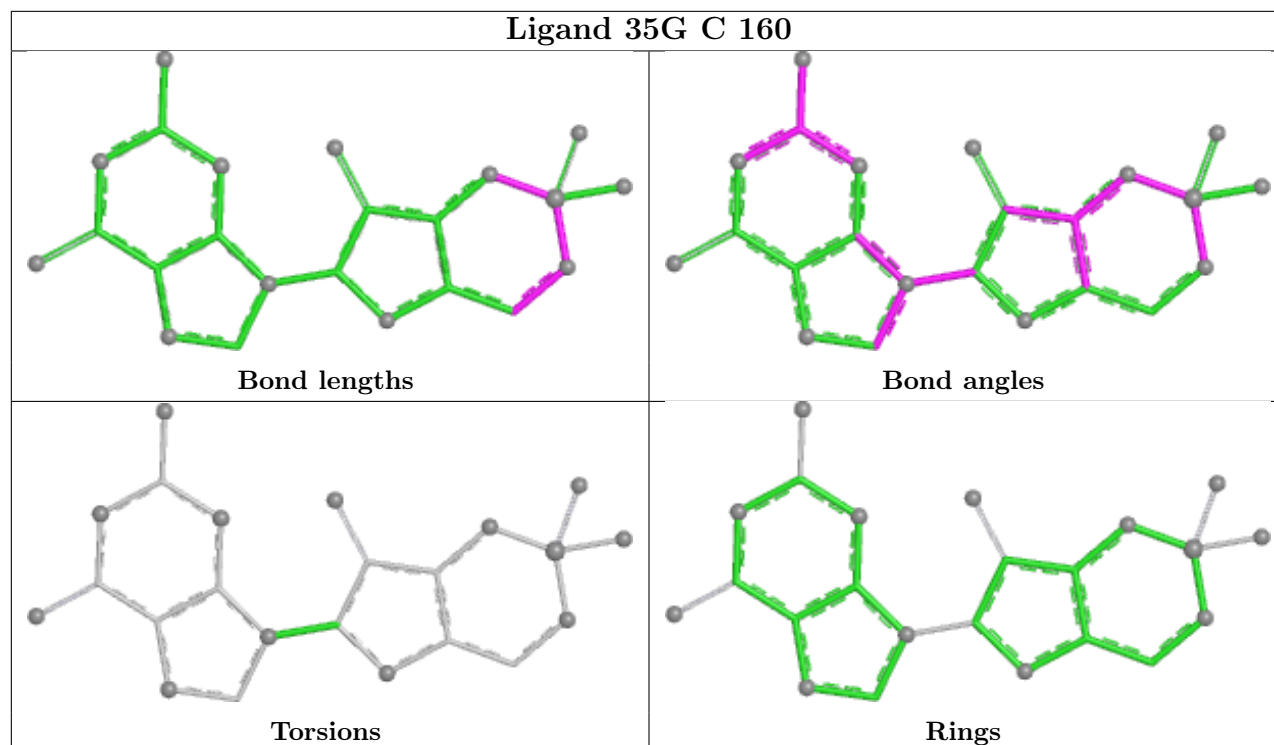


Ligand GDP A 161

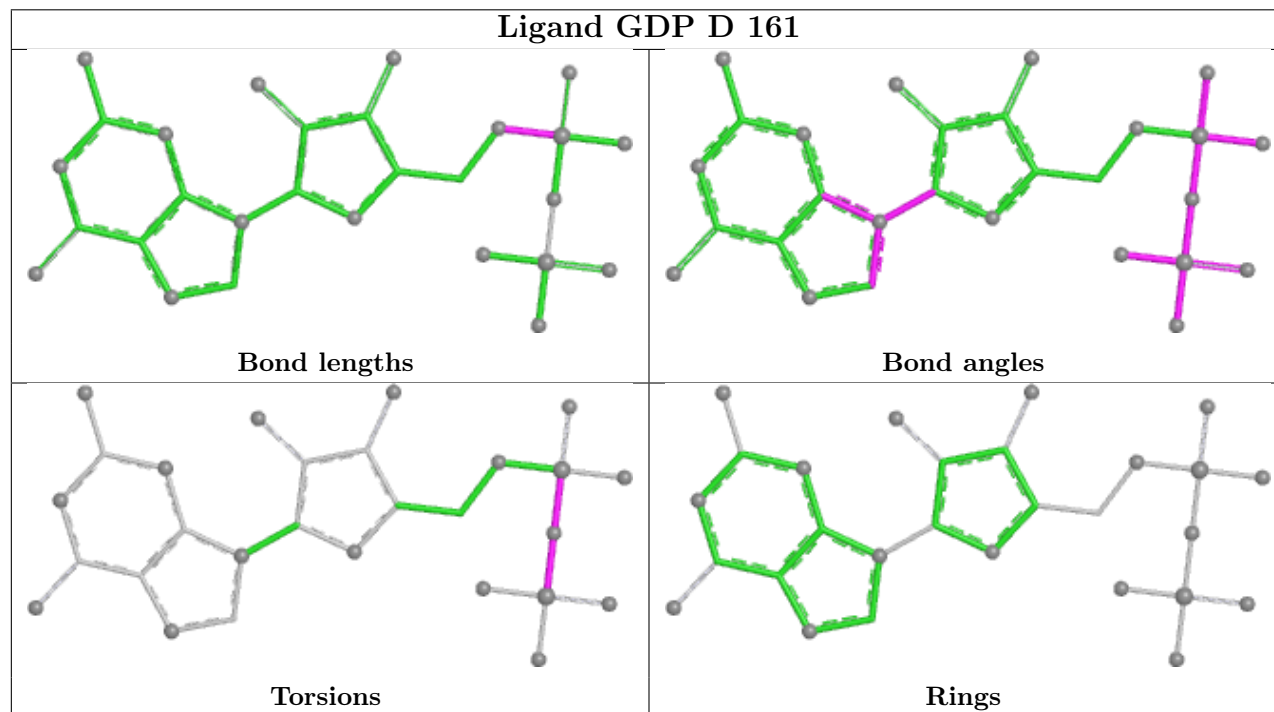


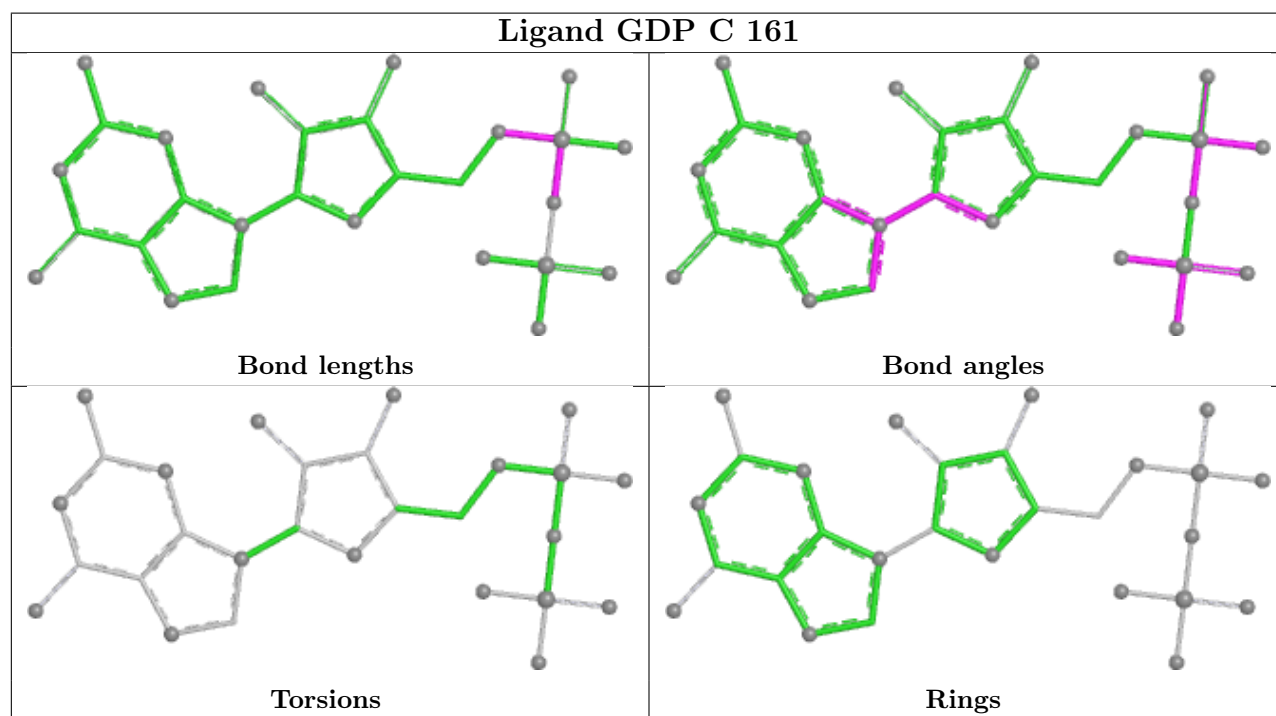
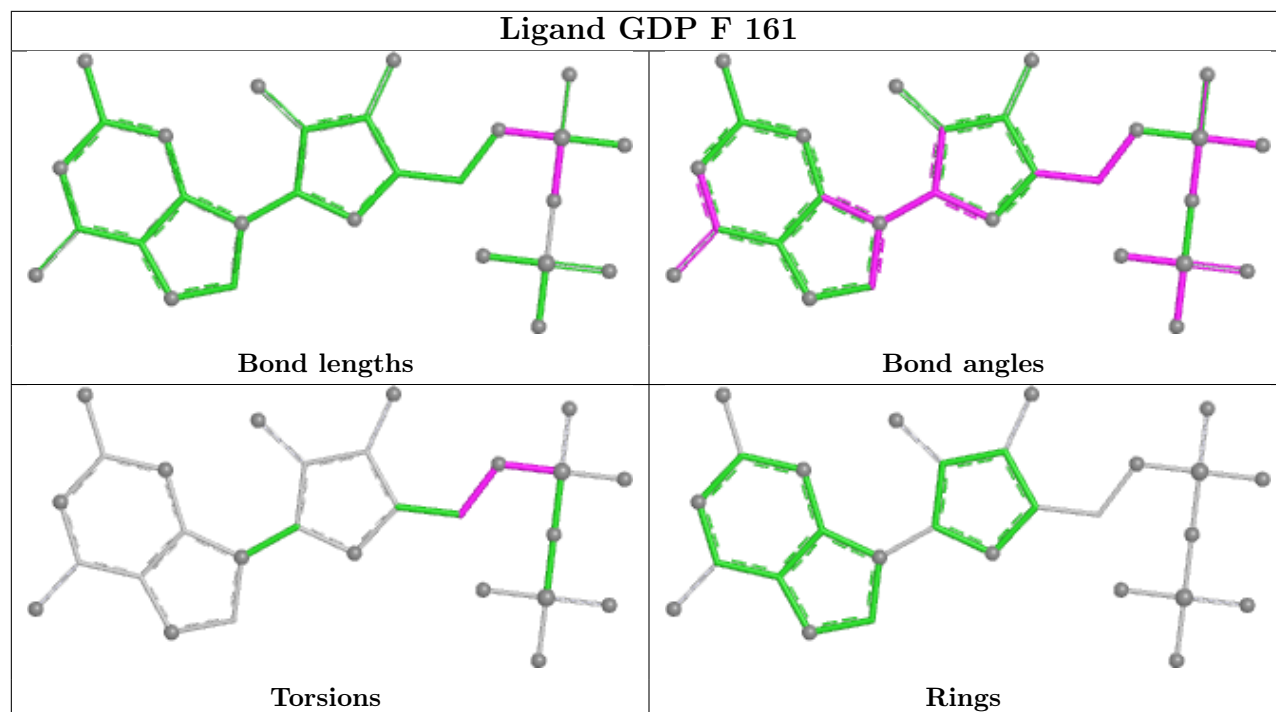


Ligand 35G C 160

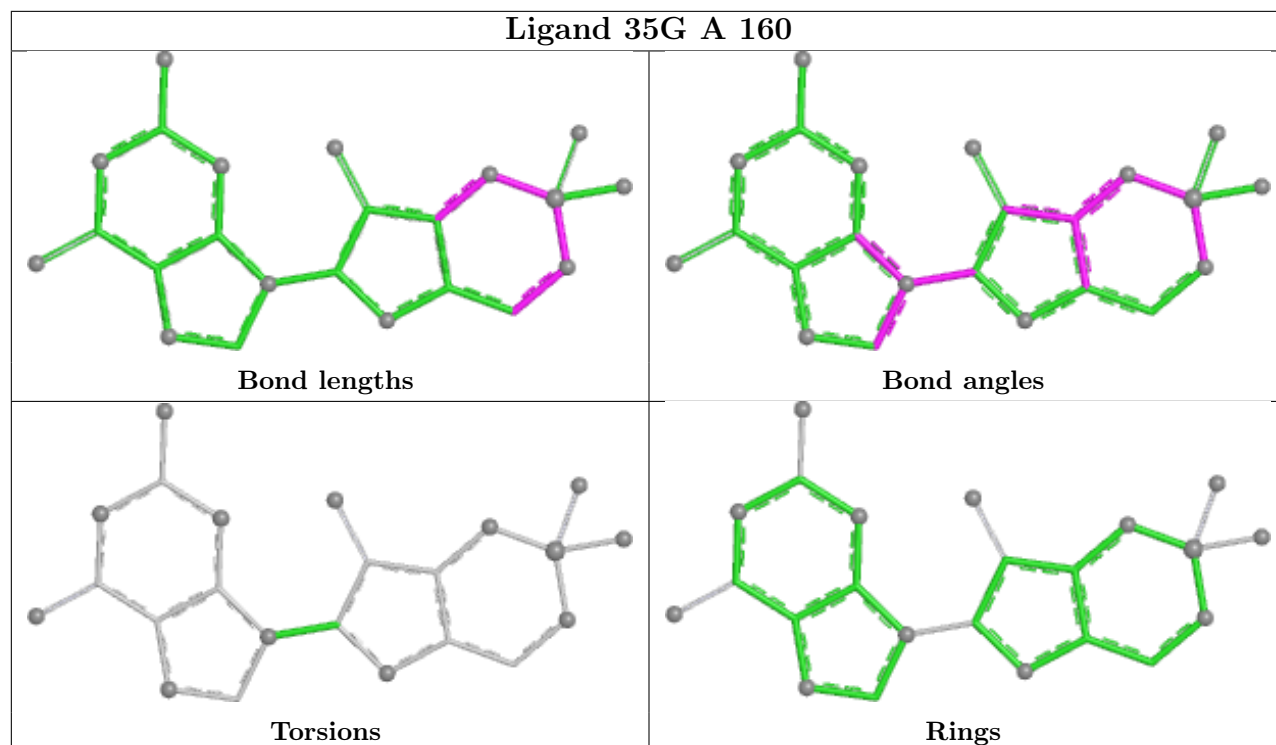


Ligand GDP D 161

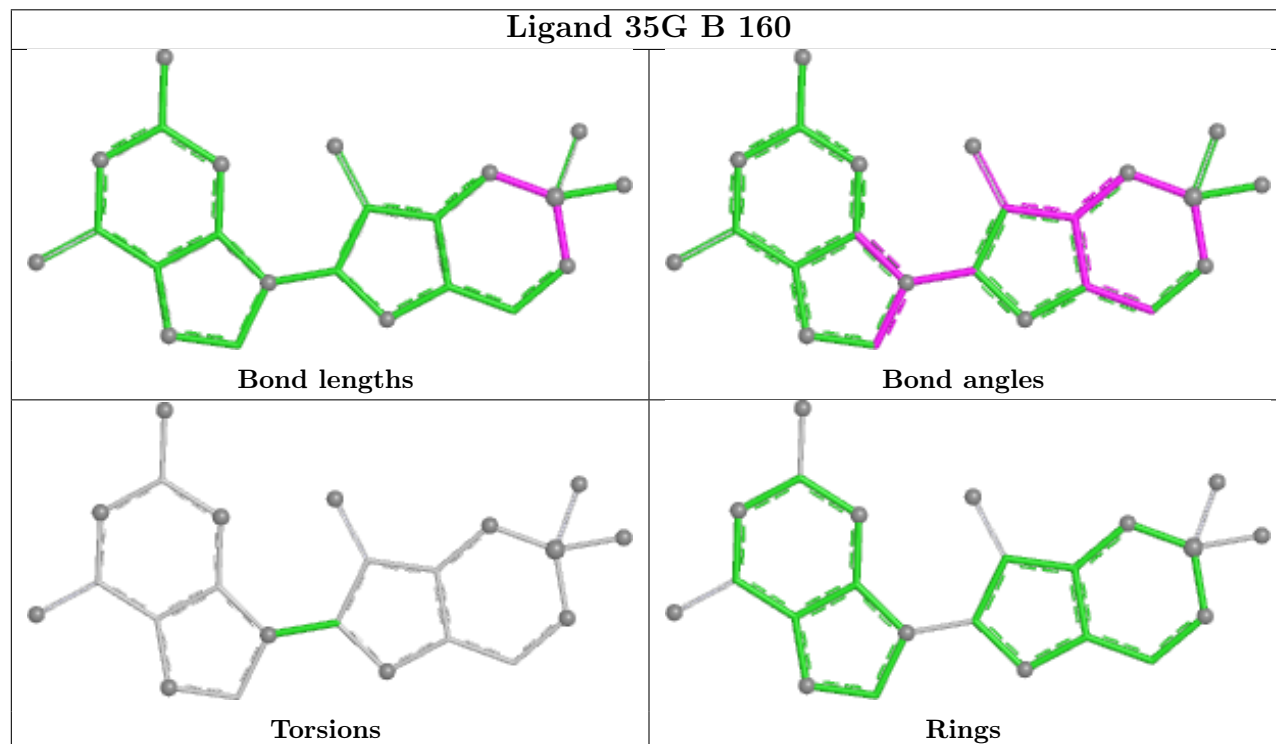


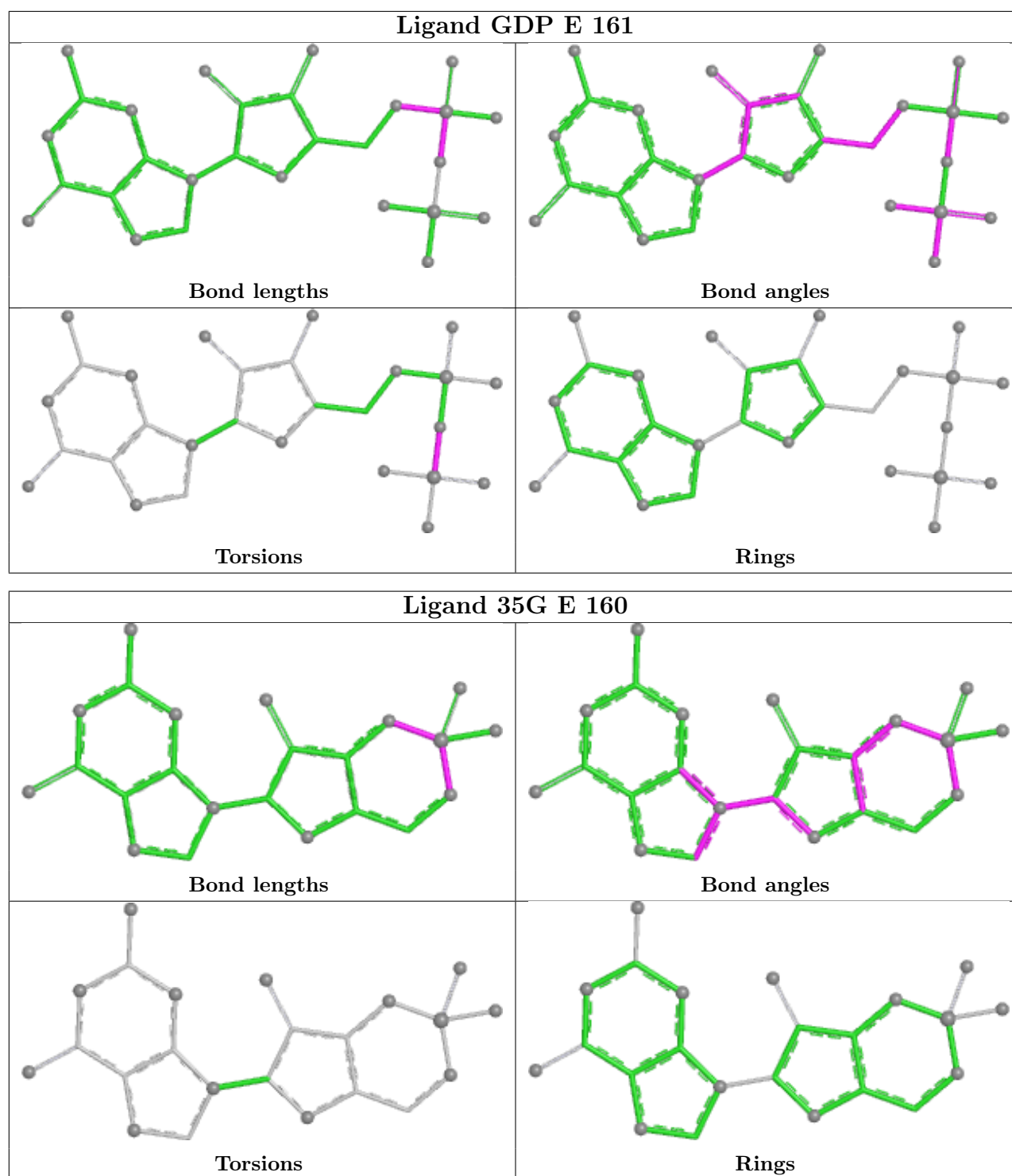


Ligand 35G A 160



Ligand 35G B 160





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	151/152 (99%)	-0.43	0	100 100	7, 25, 54, 76	0
1	B	151/152 (99%)	-0.31	0	100 100	13, 28, 67, 81	0
1	C	151/152 (99%)	-0.42	0	100 100	12, 25, 55, 71	0
1	D	151/152 (99%)	-0.36	0	100 100	7, 26, 55, 70	0
1	E	151/152 (99%)	-0.37	3 (1%)	65 60	11, 24, 58, 92	0
1	F	151/152 (99%)	-0.40	2 (1%)	75 71	10, 25, 61, 75	0
All	All	906/912 (99%)	-0.38	5 (0%)	85 83	7, 26, 60, 92	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	61	PHE	6.5
1	E	55	LEU	3.0
1	F	55	LEU	2.5
1	E	61	PHE	2.5
1	E	52	TYR	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

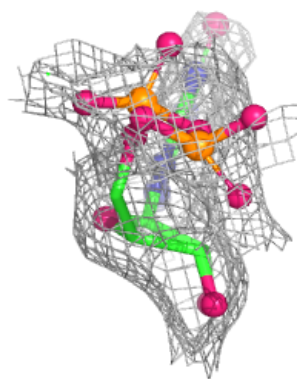
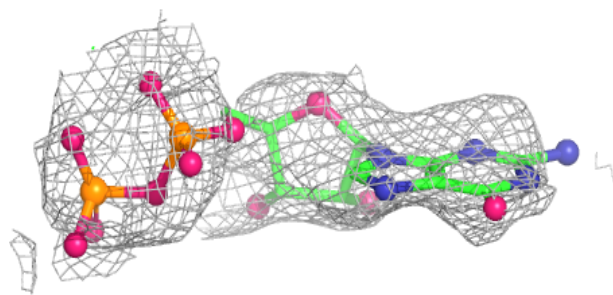
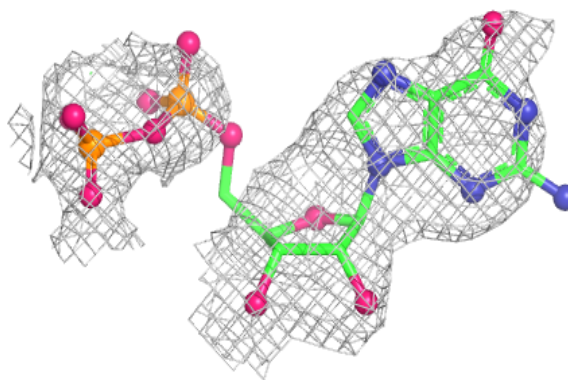
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GDP	E	161	28/28	0.84	0.15	16,79,99,99	28
3	GDP	F	161	28/28	0.84	0.15	2,99,99,99	28
3	GDP	B	161	28/28	0.89	0.16	23,99,99,99	28
2	35G	A	160	23/23	0.90	0.13	6,70,99,99	23
3	GDP	A	161	28/28	0.91	0.15	9,78,99,99	28
2	35G	B	160	23/23	0.91	0.13	13,99,99,99	23
2	35G	D	160	23/23	0.91	0.14	1,69,99,99	23
2	35G	E	160	23/23	0.91	0.12	12,53,99,99	23
3	GDP	C	161	28/28	0.93	0.11	5,32,99,99	28
2	35G	C	160	23/23	0.93	0.10	1,39,99,99	23
2	35G	F	160	23/23	0.93	0.12	11,52,99,99	23
3	GDP	D	161	28/28	0.95	0.10	4,38,99,99	28

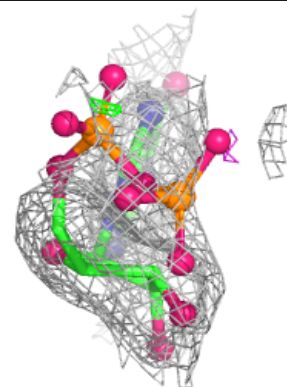
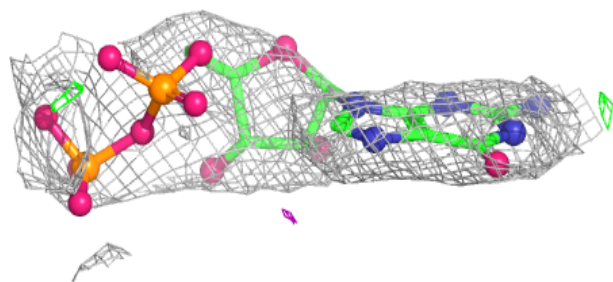
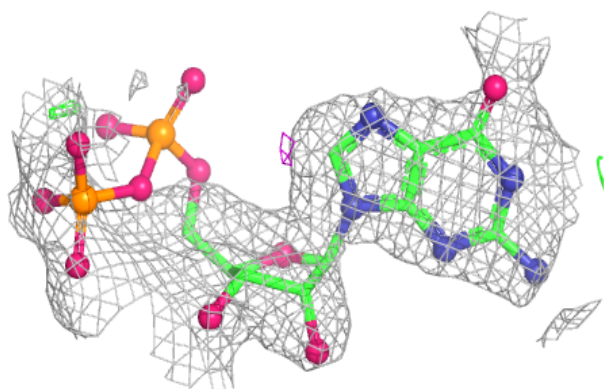
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP E 161:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

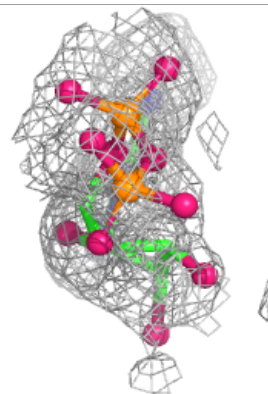
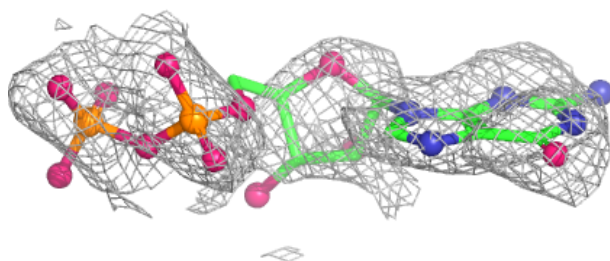
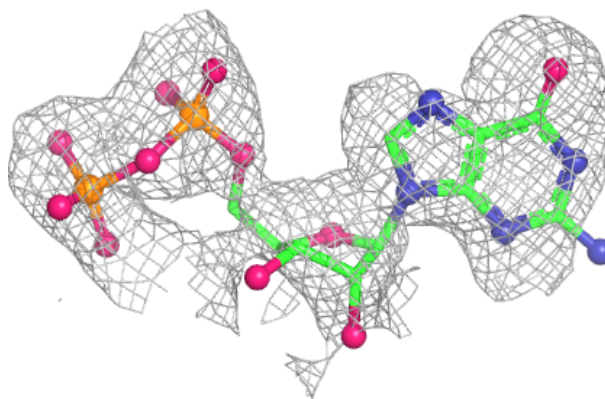
**Electron density around GDP F 161:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

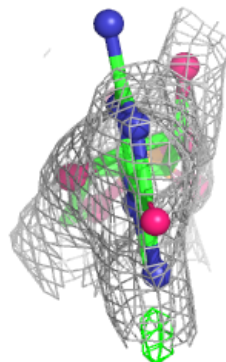
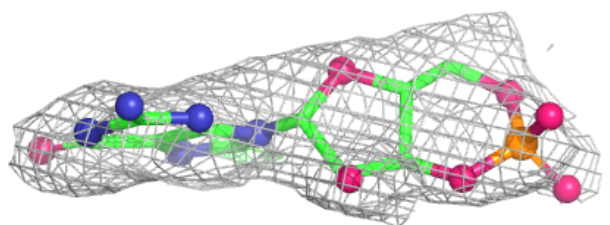
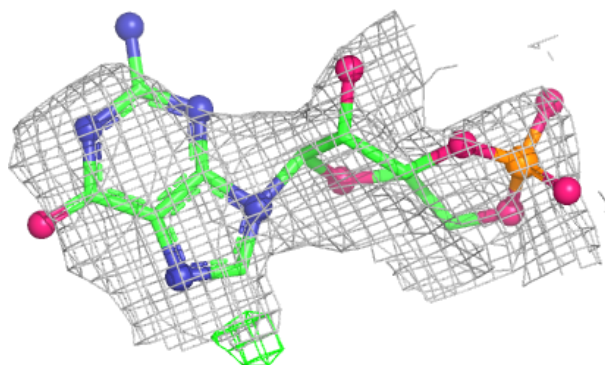


Electron density around GDP B 161:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

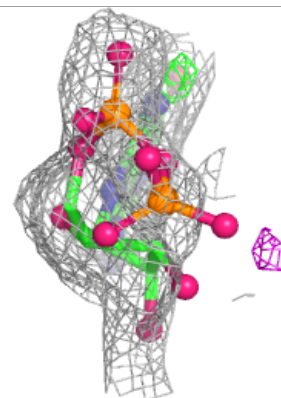
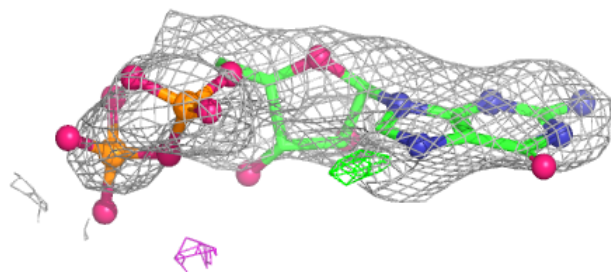
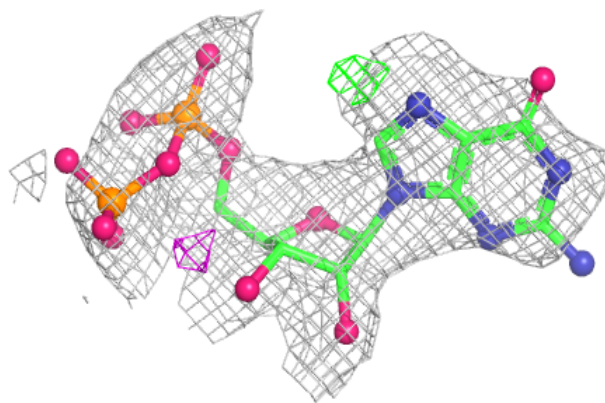
**Electron density around 35G A 160:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

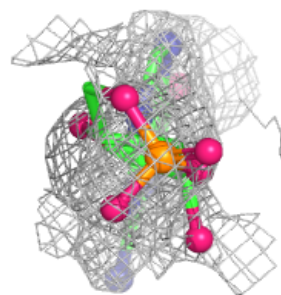
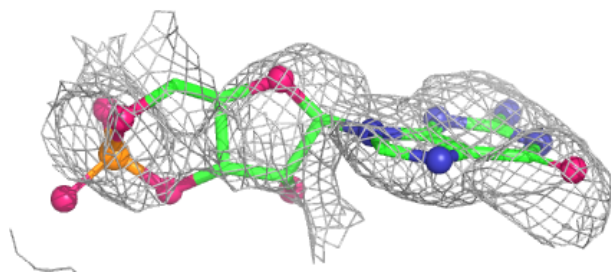
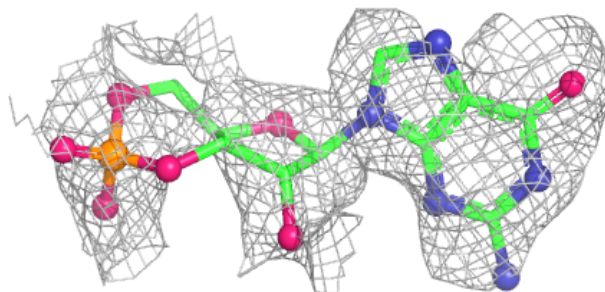


Electron density around GDP A 161:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

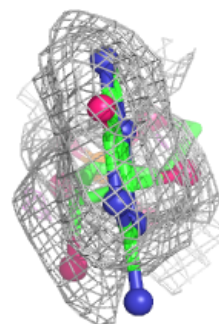
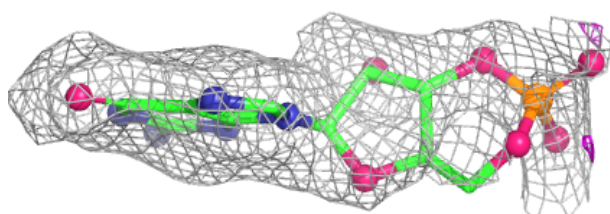
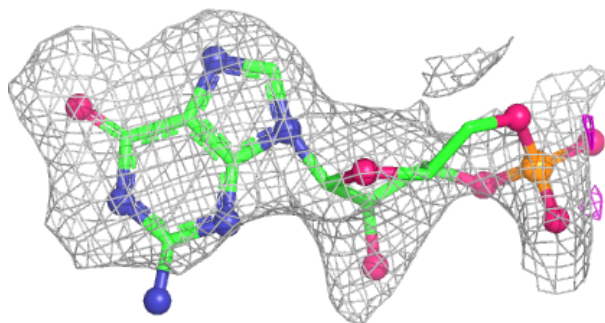
**Electron density around 35G B 160:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

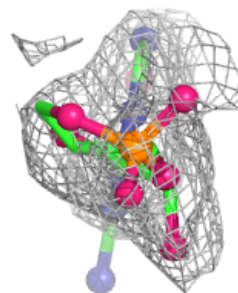
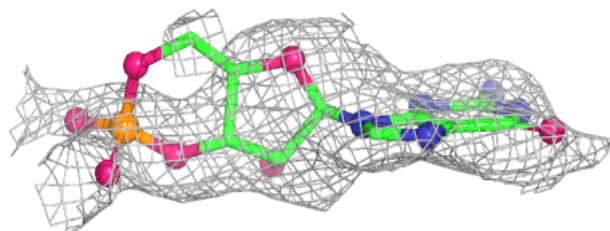
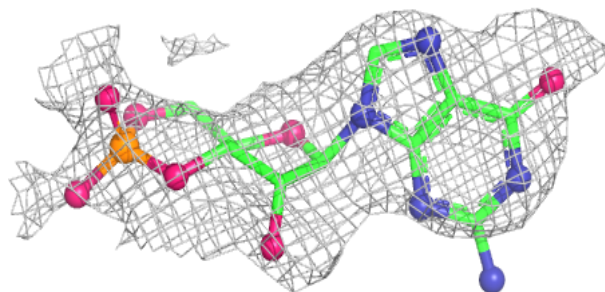


Electron density around 35G D 160:

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and green (positive)

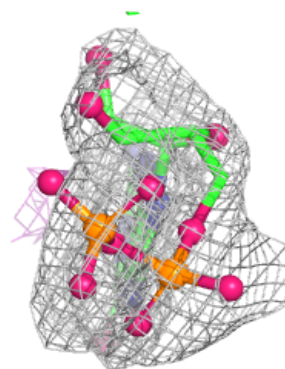
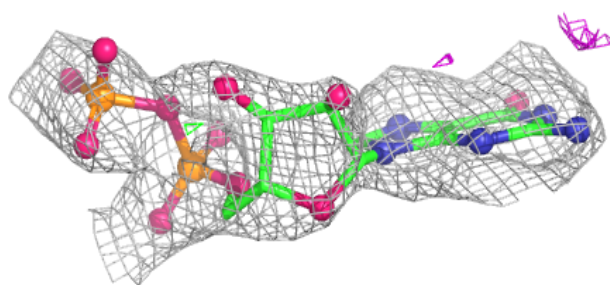
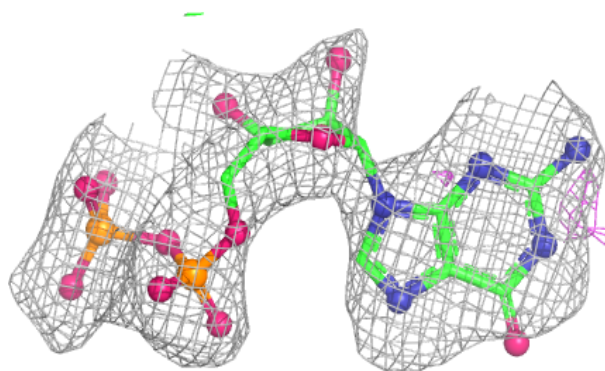
**Electron density around 35G E 160:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

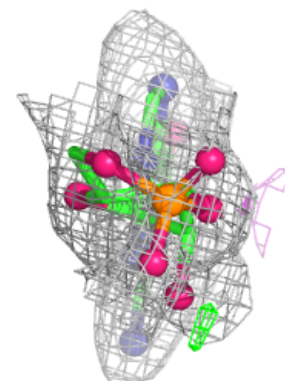
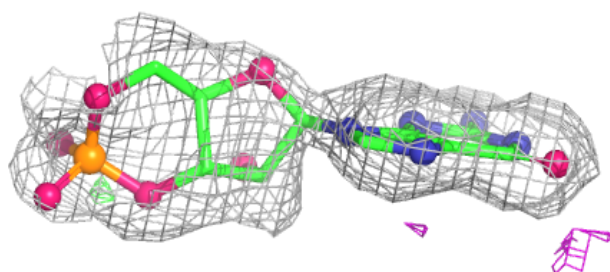
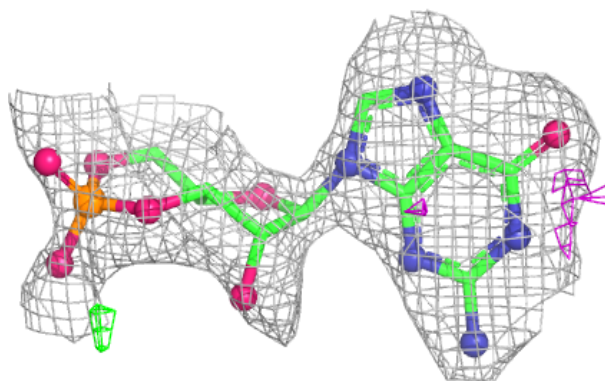


Electron density around GDP C 161:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

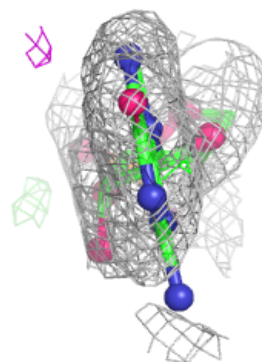
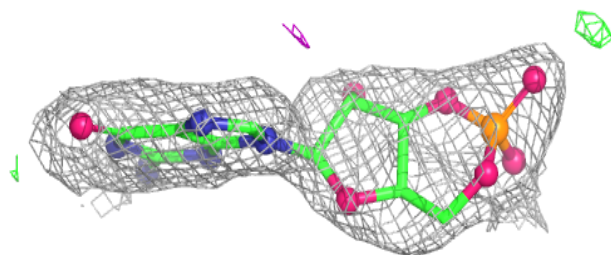
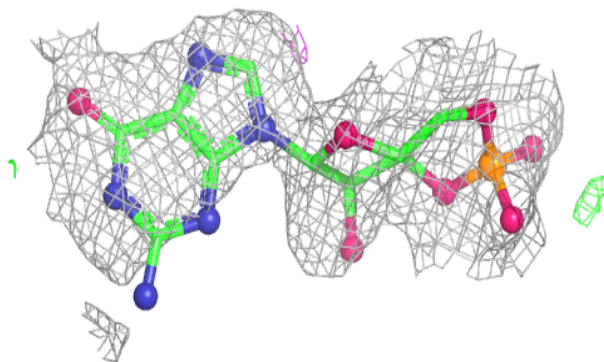
**Electron density around 35G C 160:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

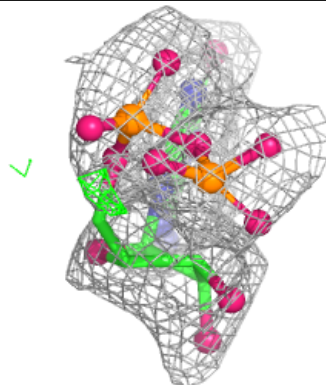
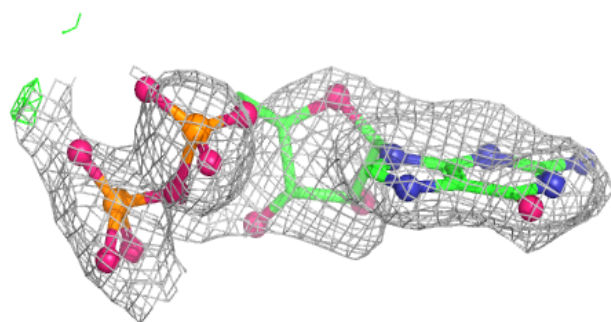
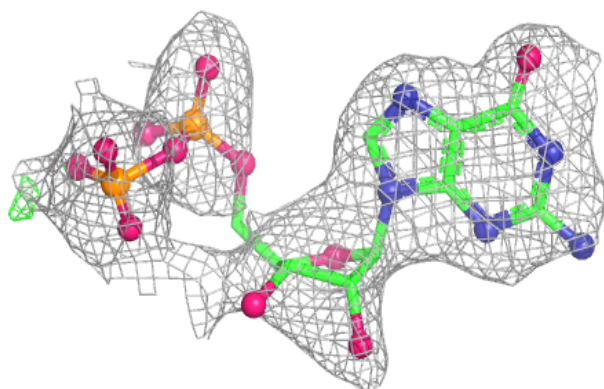


Electron density around 35G F 160:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GDP D 161:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.