



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:16 AM UTC

PDB ID : 1UPP / pdb_00001upp
Title : SPINACH RUBISCO IN COMPLEX WITH 2-CARBOXYARABINITOL 2
BISPHOSPHATE and Calcium.
Authors : Karkehabadi, S.; Taylor, T.C.; Andersson, I.
Deposited on : 2003-10-09
Resolution : 2.30 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

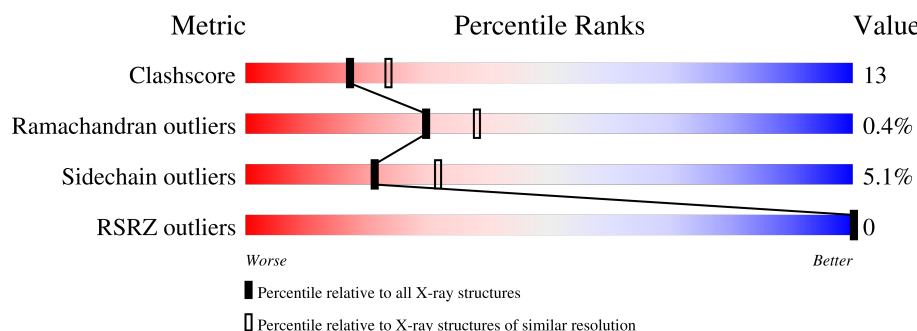
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	475	56% 33% 8% ..
1	C	475	57% 33% 8% ..
1	E	475	54% 35% 8% ..
1	G	475	57% 34% 7% .
2	I	123	60% 30% 8% .
2	J	123	60% 33% 6% .

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Mol	Chain	Length	Quality of chain
2	K	123	 57% 37% 6% •
2	L	123	 52% 36% 11% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19504 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 RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3656	2319	640	679	18			
1	C	467	Total	C	N	O	S	0	0	0
			3656	2319	640	679	18			
1	E	467	Total	C	N	O	S	0	0	0
			3656	2319	640	679	18			
1	G	467	Total	C	N	O	S	0	0	0
			3656	2319	640	679	18			

- Molecule 2 is a protein called RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	123	Total	C	N	O	S	0	0	0
			1032	673	167	185	7			
2	J	123	Total	C	N	O	S	0	0	0
			1032	673	167	185	7			
2	K	123	Total	C	N	O	S	0	0	0
			1032	673	167	185	7			
2	L	123	Total	C	N	O	S	0	0	0
			1032	673	167	185	7			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	2	GLN	LYS	conflict	UNP Q43832
I	6	ILE	THR	conflict	UNP Q43832
I	7	LEU	GLN	conflict	UNP Q43832
I	9	LEU	MET	conflict	UNP Q43832
I	11	LYS	ARG	conflict	UNP Q43832
I	109	GLU	GLN	conflict	UNP Q43832
I	113	ILE	VAL	conflict	UNP Q43832

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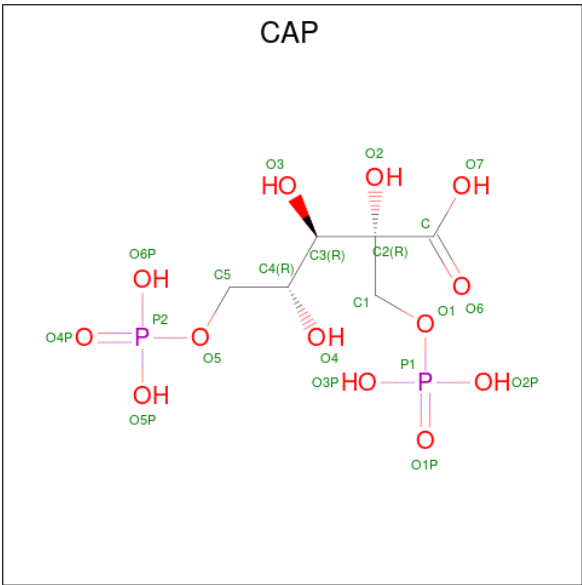
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Chain	Residue	Modelled	Actual	Comment	Reference
J	2	GLN	LYS	conflict	UNP Q43832
J	6	ILE	THR	conflict	UNP Q43832
J	7	LEU	GLN	conflict	UNP Q43832
J	9	LEU	MET	conflict	UNP Q43832
J	11	LYS	ARG	conflict	UNP Q43832
J	109	GLU	GLN	conflict	UNP Q43832
J	113	ILE	VAL	conflict	UNP Q43832
K	2	GLN	LYS	conflict	UNP Q43832
K	6	ILE	THR	conflict	UNP Q43832
K	7	LEU	GLN	conflict	UNP Q43832
K	9	LEU	MET	conflict	UNP Q43832
K	11	LYS	ARG	conflict	UNP Q43832
K	109	GLU	GLN	conflict	UNP Q43832
K	113	ILE	VAL	conflict	UNP Q43832
L	2	GLN	LYS	conflict	UNP Q43832
L	6	ILE	THR	conflict	UNP Q43832
L	7	LEU	GLN	conflict	UNP Q43832
L	9	LEU	MET	conflict	UNP Q43832
L	11	LYS	ARG	conflict	UNP Q43832
L	109	GLU	GLN	conflict	UNP Q43832
L	113	ILE	VAL	conflict	UNP Q43832

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	G	1	Total Ca 1 1	0	0

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (CCD ID: CAP) (formula: C₆H₁₄O₁₃P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			21	6	13	2		
4	C	1	Total	C	O	P	0	0
			21	6	13	2		
4	E	1	Total	C	O	P	0	0
			21	6	13	2		
4	G	1	Total	C	O	P	0	0
			21	6	13	2		

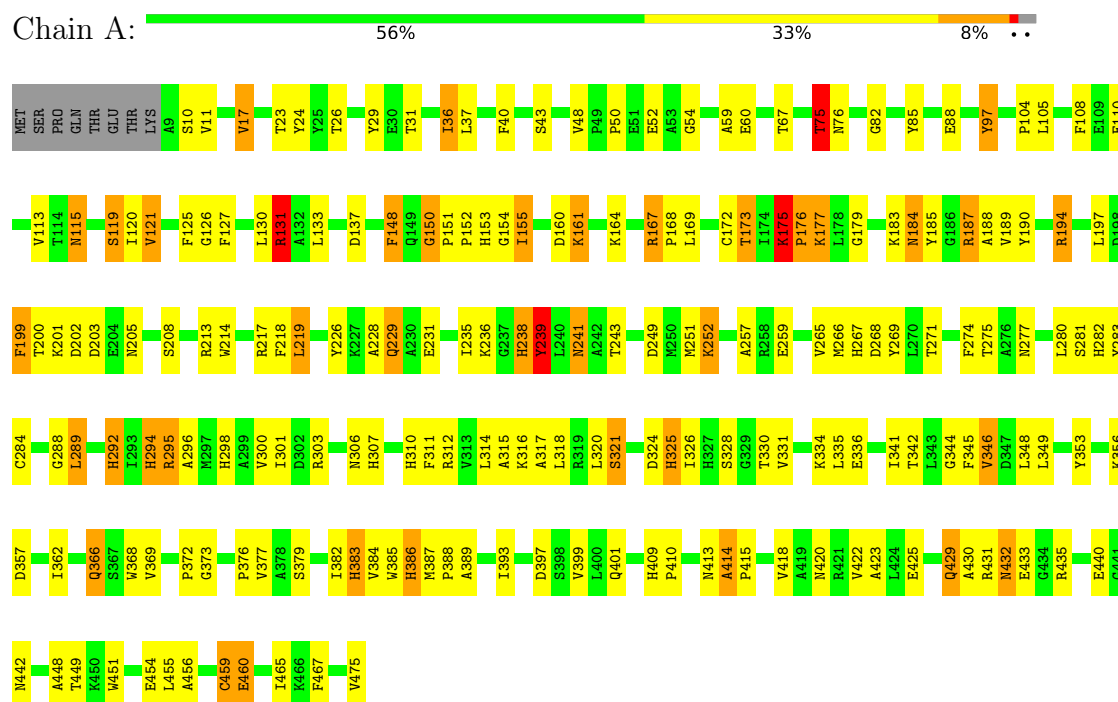
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	112	Total	O	0	0
			112	112		
5	C	121	Total	O	0	0
			121	121		
5	E	132	Total	O	0	0
			132	132		
5	G	133	Total	O	0	0
			133	133		
5	I	34	Total	O	0	0
			34	34		
5	J	44	Total	O	0	0
			44	44		
5	K	41	Total	O	0	0
			41	41		
5	L	47	Total	O	0	0
			47	47		

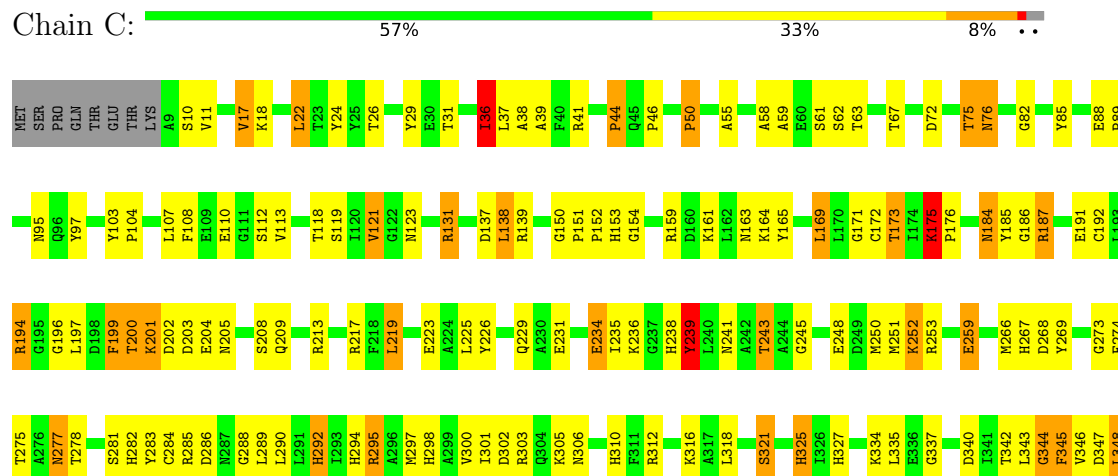
3 Residue-property plots

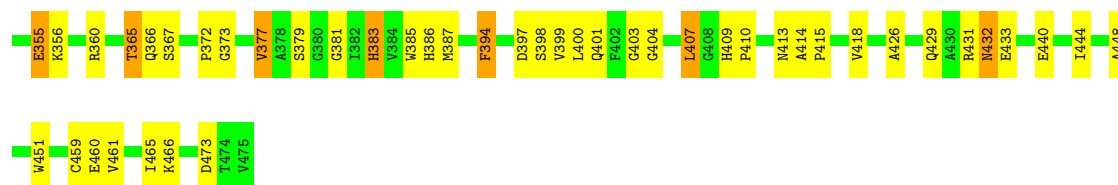
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



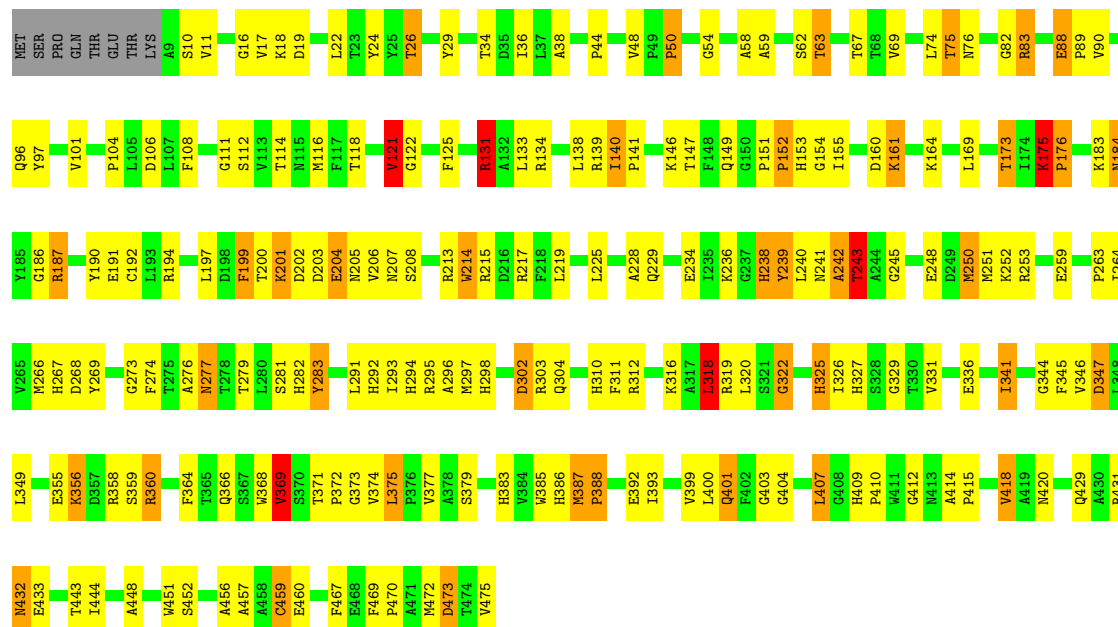
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN





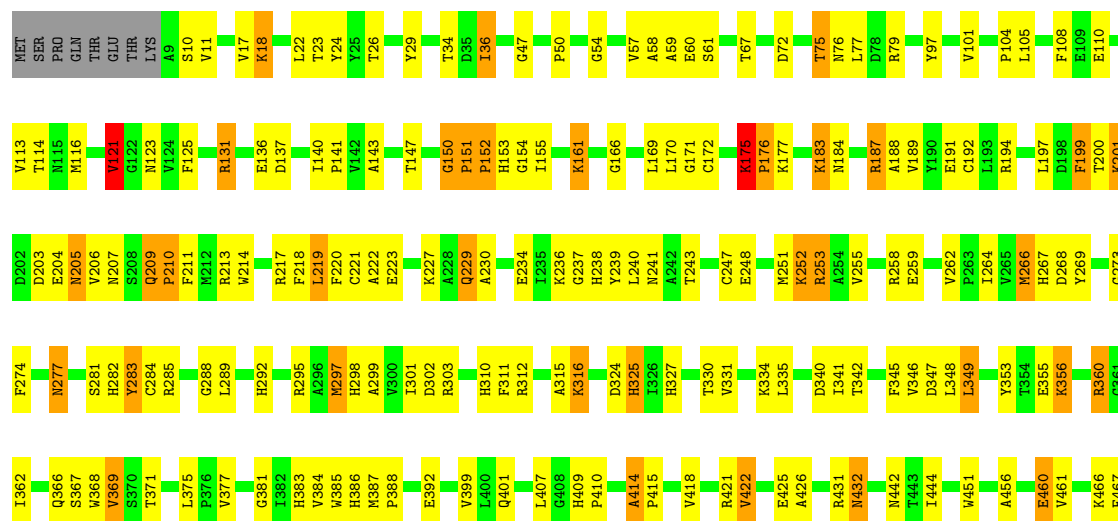
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain E: 54% 35% 8% ..



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

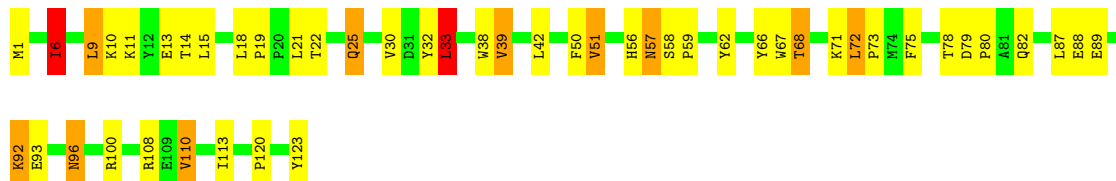
Chain G: 57% 34% 7% .





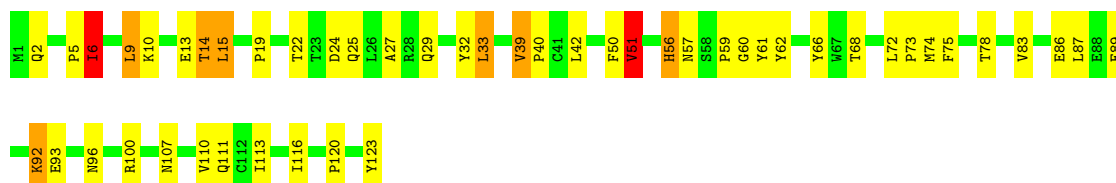
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain I: 60% 30% 8% .



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain J: 60% 33% 6% .



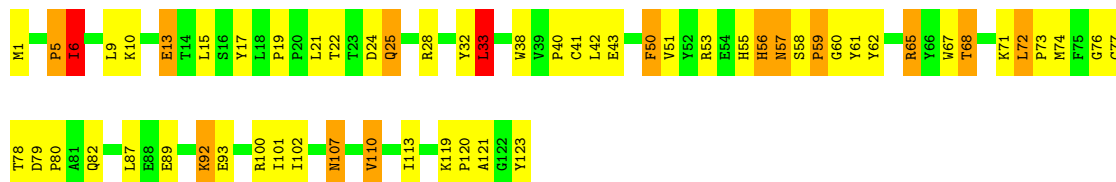
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain K: 57% 37% 6% .



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain L: 52% 36% 11% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	155.88Å 156.25Å 199.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.30 100.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	76.1 (100.00-2.30) 76.8 (100.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.256 , 0.307 0.254 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 1.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.459 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19504	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5694e-04.*

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: KCX, CA, CAP

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	1.15	1/3733 (0.0%)	2.15	149/5064 (2.9%)
1	C	1.11	4/3733 (0.1%)	2.16	152/5064 (3.0%)
1	E	1.15	5/3733 (0.1%)	2.19	164/5064 (3.2%)
1	G	1.14	2/3733 (0.1%)	2.12	155/5064 (3.1%)
2	I	0.89	0/1067	1.83	28/1453 (1.9%)
2	J	0.86	0/1067	1.83	28/1453 (1.9%)
2	K	0.82	0/1067	1.70	14/1453 (1.0%)
2	L	0.85	0/1067	1.79	29/1453 (2.0%)
All	All	1.08	12/19200 (0.1%)	2.08	719/26068 (2.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
1	E	0	2
1	G	0	3
2	I	0	1
All	All	0	9

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	176	PRO	N-CD	7.58	1.58	1.47
1	G	209	GLN	C-O	-7.04	1.18	1.24
1	A	294	HIS	CE1-NE2	7.01	1.39	1.32
1	C	294	HIS	CG-ND1	-6.27	1.31	1.38
1	E	373	GLY	N-CA	6.25	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	209	GLN	N-CA	6.18	1.50	1.46
1	C	159	ARG	C-O	-5.83	1.17	1.24
1	E	293	ILE	C-O	-5.74	1.18	1.24
1	C	209	GLN	N-CA	-5.47	1.41	1.45
1	E	238	HIS	CG-ND1	5.37	1.44	1.38
1	E	82	GLY	CA-C	5.10	1.58	1.52
1	E	213	ARG	N-CA	5.10	1.52	1.46

All (719) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	PRO	CA-N-CD	-16.10	88.96	111.50
1	C	175	LYS	O-C-N	-12.23	109.73	121.72
1	C	187	ARG	CD-NE-CZ	11.97	141.16	124.40
1	A	131	ARG	CD-NE-CZ	11.68	140.75	124.40
1	E	312	ARG	CD-NE-CZ	11.15	140.01	124.40
1	E	293	ILE	O-C-N	-10.94	110.31	123.10
1	A	177	LYS	CB-CG-CD	-10.50	87.14	111.30
1	A	154	GLY	CA-C-O	-10.48	114.24	122.52
1	E	131	ARG	CD-NE-CZ	10.31	138.83	124.40
1	C	153	HIS	CA-CB-CG	-10.28	103.52	113.80
1	G	176	PRO	N-CA-CB	10.26	114.02	103.25
1	G	176	PRO	CA-N-CD	-10.23	97.68	112.00
1	C	268	ASP	CA-CB-CG	10.16	122.76	112.60
1	C	176	PRO	N-CD-CG	-10.10	91.68	103.80
1	A	119	SER	O-C-N	-10.05	111.17	122.03
1	E	444	ILE	CA-C-O	9.97	131.74	121.17
1	E	379	SER	CA-C-O	-9.84	110.70	121.33
1	A	167	ARG	CD-NE-CZ	9.76	138.06	124.40
1	G	221	CYS	CA-C-O	-9.74	110.23	120.55
1	A	153	HIS	CA-CB-CG	-9.64	104.16	113.80
1	G	58	ALA	CA-C-O	-9.59	110.75	120.82
1	A	429	GLN	OE1-CD-NE2	-9.44	113.16	122.60
1	E	204	GLU	CA-C-O	-9.42	110.82	120.90
1	G	199	PHE	CA-CB-CG	9.34	123.14	113.80
1	G	175	LYS	CA-C-N	9.34	131.51	119.84
1	G	175	LYS	C-N-CA	9.34	131.51	119.84
1	A	119	SER	CA-C-O	9.26	130.44	120.90
1	A	176	PRO	CA-N-CD	-9.21	99.11	112.00
2	J	100	ARG	CD-NE-CZ	9.18	137.25	124.40
1	A	432	ASN	CA-CB-CG	9.04	121.64	112.60
1	E	293	ILE	CA-C-N	8.96	135.34	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	293	ILE	C-N-CA	8.96	135.34	122.09
1	C	82	GLY	N-CA-C	-8.91	99.89	112.37
2	I	30	VAL	CA-C-O	-8.89	111.71	120.95
1	C	110	GLU	O-C-N	-8.76	112.29	122.97
2	J	42	LEU	N-CA-CB	8.73	124.75	110.69
1	E	187	ARG	CD-NE-CZ	8.70	136.57	124.40
1	E	153	HIS	CA-CB-CG	-8.69	105.11	113.80
1	G	381	GLY	CA-C-N	-8.69	112.67	122.48
1	G	381	GLY	C-N-CA	-8.69	112.67	122.48
1	C	312	ARG	NE-CZ-NH1	8.62	130.12	121.50
1	E	82	GLY	N-CA-C	-8.60	100.33	112.37
1	G	187	ARG	CD-NE-CZ	8.52	136.33	124.40
1	G	131	ARG	CD-NE-CZ	8.49	136.29	124.40
1	A	294	HIS	CA-C-O	-8.49	111.31	121.66
1	G	426	ALA	O-C-N	-8.47	113.14	122.12
1	C	285	ARG	CD-NE-CZ	8.46	136.24	124.40
1	E	432	ASN	CA-CB-CG	8.42	121.02	112.60
1	E	154	GLY	CA-C-O	-8.42	112.68	122.78
1	E	44	PRO	CA-C-O	-8.39	111.82	121.56
1	E	263	PRO	N-CA-C	8.39	125.84	114.18
1	A	175	LYS	CA-C-N	8.37	130.30	119.84
1	A	175	LYS	C-N-CA	8.37	130.30	119.84
1	A	217	ARG	CG-CD-NE	8.36	130.40	112.00
1	G	324	ASP	CA-C-O	8.36	129.59	119.97
1	C	310	HIS	CA-CB-CG	-8.36	105.44	113.80
1	C	131	ARG	CD-NE-CZ	8.33	136.06	124.40
1	G	310	HIS	CA-CB-CG	-8.33	105.47	113.80
1	C	312	ARG	NE-CZ-NH2	-8.28	111.75	119.20
1	A	219	LEU	CA-C-O	-8.23	112.02	121.07
1	C	348	LEU	CA-C-O	-8.23	110.80	120.10
2	I	96	ASN	CA-CB-CG	8.22	120.82	112.60
2	I	100	ARG	CD-NE-CZ	8.22	135.91	124.40
1	G	154	GLY	CA-C-O	-8.21	116.03	122.52
1	E	175	LYS	CA-C-O	-8.21	108.92	120.16
1	A	60	GLU	CA-C-O	8.16	128.45	119.15
1	A	194	ARG	NE-CZ-NH1	-8.14	113.36	121.50
1	A	176	PRO	N-CA-CB	8.10	111.76	103.25
1	G	121	VAL	CB-CA-C	8.09	124.56	111.29
2	K	53	ARG	NE-CZ-NH1	-8.09	113.41	121.50
1	A	384	VAL	CA-C-O	-8.09	111.92	120.57
1	C	161	LYS	CA-CB-CG	8.04	130.17	114.10
1	C	164	LYS	CA-C-O	8.02	128.99	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	ALA	CA-C-O	-8.00	112.27	121.07
1	A	430	ALA	O-C-N	7.94	130.58	122.08
1	E	140	ILE	O-C-N	7.87	127.13	121.55
1	E	215	ARG	NE-CZ-NH2	7.86	126.27	119.20
2	K	100	ARG	NE-CZ-NH2	-7.86	112.13	119.20
1	C	288	GLY	CA-C-O	-7.81	109.43	119.58
1	A	197	LEU	O-C-N	-7.75	113.44	122.89
1	G	54	GLY	CA-C-N	7.74	132.43	120.82
1	G	54	GLY	C-N-CA	7.74	132.43	120.82
1	E	69	VAL	O-C-N	-7.73	115.25	123.14
1	G	175	LYS	O-C-N	7.71	130.19	121.32
1	G	67	THR	CA-C-O	-7.70	113.02	121.33
1	E	114	THR	CA-C-O	-7.67	112.34	120.63
1	C	306	ASN	OD1-CG-ND2	-7.66	114.94	122.60
1	E	325	HIS	CA-C-O	-7.60	111.92	120.66
1	A	218	PHE	CA-CB-CG	7.58	121.38	113.80
1	G	213	ARG	CA-C-N	7.55	130.40	120.28
1	G	213	ARG	C-N-CA	7.55	130.40	120.28
1	E	456	ALA	O-C-N	7.55	129.84	122.07
1	C	194	ARG	NE-CZ-NH1	-7.53	113.97	121.50
1	G	57	VAL	CA-C-O	-7.52	113.45	121.27
1	E	358	ARG	NE-CZ-NH2	-7.51	112.44	119.20
1	A	199	PHE	CA-CB-CG	7.47	121.27	113.80
1	A	187	ARG	CD-NE-CZ	7.43	134.81	124.40
1	E	245	GLY	O-C-N	-7.43	114.99	122.19
1	E	176	PRO	N-CA-CB	7.41	111.03	103.25
2	J	96	ASN	OD1-CG-ND2	-7.40	115.20	122.60
1	C	432	ASN	CA-CB-CG	7.39	119.99	112.60
1	A	303	ARG	NE-CZ-NH2	-7.38	112.56	119.20
2	L	6	ILE	N-CA-CB	-7.38	103.29	111.41
1	E	303	ARG	CD-NE-CZ	7.34	134.68	124.40
1	A	295	ARG	CA-C-N	7.33	131.53	121.05
1	A	295	ARG	C-N-CA	7.33	131.53	121.05
1	A	306	ASN	OD1-CG-ND2	-7.32	115.28	122.60
1	G	229	GLN	CA-C-O	7.28	128.47	120.82
1	A	257	ALA	O-C-N	-7.27	114.42	122.12
1	E	38	ALA	CA-C-O	-7.27	112.51	120.36
1	E	268	ASP	CA-CB-CG	7.26	119.86	112.60
1	A	17	VAL	CA-C-N	7.26	133.97	122.21
1	A	17	VAL	C-N-CA	7.26	133.97	122.21
1	C	305	LYS	CA-C-O	-7.26	112.79	120.63
1	C	348	LEU	O-C-N	7.24	130.69	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	LYS	CA-C-O	-7.23	113.17	120.90
1	G	422	VAL	N-CA-C	7.22	117.35	110.42
1	C	273	GLY	CA-C-O	-7.21	115.57	121.77
1	E	407	LEU	CA-C-O	-7.21	110.56	119.28
1	G	349	LEU	CA-C-O	-7.21	112.78	120.42
1	E	121	VAL	N-CA-CB	-7.20	99.34	111.23
1	G	460	GLU	CA-C-O	-7.18	112.94	120.55
1	A	37	LEU	CA-C-O	-7.16	112.57	120.38
1	C	321	SER	CA-C-O	7.16	128.14	120.55
1	G	108	PHE	O-C-N	-7.16	114.11	123.21
1	G	312	ARG	CD-NE-CZ	7.15	134.41	124.40
1	E	175	LYS	CA-C-N	7.14	128.77	119.84
1	E	175	LYS	C-N-CA	7.14	128.77	119.84
1	A	104	PRO	CA-C-N	7.14	130.16	120.38
1	A	104	PRO	C-N-CA	7.14	130.16	120.38
1	E	217	ARG	CD-NE-CZ	7.14	134.40	124.40
1	E	320	LEU	CA-C-N	7.14	132.54	121.19
1	E	320	LEU	C-N-CA	7.14	132.54	121.19
1	A	105	LEU	CA-C-O	-7.14	112.92	120.63
1	E	473	ASP	CA-CB-CG	7.13	119.73	112.60
1	G	432	ASN	CA-CB-CG	7.13	119.73	112.60
1	C	397	ASP	CA-C-O	7.13	130.70	120.51
1	G	421	ARG	CA-C-O	-7.12	113.00	120.55
1	G	460	GLU	N-CA-CB	7.12	120.59	110.12
1	A	148	PHE	O-C-N	-7.12	114.17	123.21
1	A	300	VAL	CA-CB-CG1	7.09	122.46	110.40
1	C	381	GLY	O-C-N	-7.08	115.47	122.41
2	J	66	TYR	O-C-N	7.07	131.72	122.95
1	A	229	GLN	CA-C-N	7.05	130.03	120.38
1	A	229	GLN	C-N-CA	7.05	130.03	120.38
1	E	282	HIS	CA-CB-CG	-7.05	106.75	113.80
1	C	50	PRO	CA-C-N	7.04	129.72	120.28
1	C	50	PRO	C-N-CA	7.04	129.72	120.28
1	E	176	PRO	CA-N-CD	-7.04	102.15	112.00
1	E	294	HIS	CA-CB-CG	-7.03	106.77	113.80
2	L	100	ARG	CD-NE-CZ	7.02	134.23	124.40
1	G	227	LYS	N-CA-C	7.01	118.92	111.28
1	E	139	ARG	NE-CZ-NH1	-6.99	114.52	121.50
1	E	139	ARG	NE-CZ-NH2	6.98	125.48	119.20
1	E	263	PRO	O-C-N	-6.97	112.69	122.38
2	I	30	VAL	O-C-N	6.96	128.62	121.87
1	C	199	PHE	CA-CB-CG	6.96	120.76	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	310	HIS	CA-CB-CG	-6.96	106.84	113.80
1	C	58	ALA	CA-C-O	-6.95	113.54	120.70
1	E	207	ASN	CA-CB-CG	6.94	119.54	112.60
1	E	67	THR	CA-C-O	-6.94	113.22	120.99
1	A	219	LEU	O-C-N	6.93	129.49	122.08
1	E	184	ASN	CA-C-O	-6.92	113.15	120.63
1	C	377	VAL	O-C-N	6.92	129.75	123.03
1	E	401	GLN	CA-C-O	-6.92	112.89	120.36
1	G	349	LEU	N-CA-C	6.91	118.89	111.36
1	C	398	SER	CA-CB-OG	-6.91	97.29	111.10
1	G	221	CYS	O-C-N	6.91	129.44	122.12
1	C	223	GLU	O-C-N	-6.90	114.86	122.03
1	G	324	ASP	O-C-N	-6.89	113.80	122.27
1	C	282	HIS	CA-CB-CG	-6.87	106.93	113.80
1	G	153	HIS	CA-CB-CG	-6.85	106.95	113.80
1	C	213	ARG	NE-CZ-NH1	-6.84	114.66	121.50
1	E	310	HIS	CA-C-O	-6.80	114.15	121.56
1	G	311	PHE	CA-CB-CG	-6.79	107.01	113.80
1	G	150	GLY	O-C-N	-6.75	115.02	121.77
1	G	137	ASP	CA-C-O	-6.75	114.00	121.23
1	A	161	LYS	CA-C-O	6.75	127.58	120.42
1	A	137	ASP	CA-CB-CG	6.74	119.34	112.60
1	G	170	LEU	CA-C-N	6.74	128.17	122.17
1	G	170	LEU	C-N-CA	6.74	128.17	122.17
1	E	341	ILE	CA-C-N	6.74	129.61	120.44
1	E	341	ILE	C-N-CA	6.74	129.61	120.44
1	E	319	ARG	NE-CZ-NH2	6.74	125.26	119.20
1	C	139	ARG	NE-CZ-NH2	6.74	125.26	119.20
1	C	113	VAL	CB-CA-C	-6.73	103.22	112.04
1	G	384	VAL	O-C-N	6.72	128.39	121.87
1	A	108	PHE	CA-CB-CG	-6.69	107.11	113.80
1	G	269	TYR	CA-CB-CG	6.69	125.94	113.90
1	C	303	ARG	NE-CZ-NH1	6.68	128.18	121.50
1	E	108	PHE	N-CA-CB	-6.66	99.53	110.52
1	E	253	ARG	CD-NE-CZ	6.66	133.72	124.40
2	L	56	HIS	CA-C-O	-6.63	114.13	121.23
1	A	282	HIS	CA-CB-CG	-6.62	107.19	113.80
1	C	325	HIS	CA-C-O	-6.61	112.66	120.60
1	A	397	ASP	OD1-CG-OD2	-6.61	107.04	122.90
1	E	134	ARG	CB-CA-C	-6.59	100.61	110.24
1	G	342	THR	N-CA-C	-6.59	103.36	111.40
1	C	121	VAL	CB-CA-C	6.58	122.08	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	96	ASN	CA-CB-CG	6.58	119.18	112.60
1	G	177	LYS	CA-C-O	-6.57	113.33	121.02
1	C	292	HIS	CA-C-N	-6.55	115.06	123.19
1	C	292	HIS	C-N-CA	-6.55	115.06	123.19
1	C	108	PHE	CA-CB-CG	-6.54	107.26	113.80
1	C	465	ILE	N-CA-C	6.54	116.89	108.12
2	I	6	ILE	N-CA-CB	-6.54	102.94	111.90
1	C	253	ARG	CA-C-O	6.54	127.54	120.55
1	E	101	VAL	CA-C-O	-6.53	113.53	120.39
1	E	452	SER	CB-CA-C	-6.50	102.95	110.17
2	L	67	TRP	CA-C-N	-6.50	112.40	122.87
2	L	67	TRP	C-N-CA	-6.50	112.40	122.87
2	I	72	LEU	O-C-N	6.49	128.78	121.32
1	C	444	ILE	CA-C-O	6.48	128.25	121.05
1	E	273	GLY	CA-C-O	-6.48	116.20	121.77
1	A	67	THR	CA-C-O	-6.48	114.34	121.33
1	E	283	TYR	CA-C-O	-6.47	113.69	120.55
1	A	459	CYS	CA-C-O	-6.47	113.69	120.55
1	A	310	HIS	CA-CB-CG	-6.46	107.34	113.80
1	G	421	ARG	O-C-N	6.46	128.97	122.12
1	G	58	ALA	O-C-N	6.46	128.72	122.07
1	A	82	GLY	N-CA-C	-6.45	103.82	112.14
1	G	219	LEU	CA-C-O	-6.45	113.98	121.07
1	C	175	LYS	CA-C-N	6.44	142.47	127.00
1	C	175	LYS	C-N-CA	6.44	142.47	127.00
1	G	331	VAL	CA-C-N	6.43	131.51	121.35
1	G	331	VAL	C-N-CA	6.43	131.51	121.35
1	G	324	ASP	N-CA-C	6.43	119.28	111.82
1	E	393	ILE	N-CA-C	-6.41	104.91	110.74
2	K	62	TYR	CA-C-O	-6.41	113.29	120.66
1	E	364	PHE	CA-C-O	-6.40	112.92	120.60
1	G	207	ASN	O-C-N	6.39	125.56	120.83
1	E	304	GLN	N-CA-C	6.39	120.07	109.46
1	C	303	ARG	NE-CZ-NH2	-6.39	113.45	119.20
1	C	67	THR	CA-C-O	-6.38	114.19	121.40
1	A	40	PHE	N-CA-C	6.37	119.63	109.24
1	A	422	VAL	CA-C-O	-6.37	114.78	121.41
1	G	473	ASP	CA-CB-CG	6.37	118.97	112.60
1	C	76	ASN	OD1-CG-ND2	6.35	128.95	122.60
1	A	325	HIS	CA-C-O	-6.35	113.36	120.66
1	C	301	ILE	CA-C-N	-6.34	112.66	122.49
1	C	301	ILE	C-N-CA	-6.34	112.66	122.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	107	ASN	CA-C-O	6.33	127.13	120.42
1	E	349	LEU	CA-C-O	-6.33	112.32	119.79
1	G	282	HIS	CA-CB-CG	-6.32	107.48	113.80
1	A	161	LYS	O-C-N	-6.32	114.95	122.15
1	C	245	GLY	CA-C-O	-6.31	113.36	120.30
1	C	383	HIS	CA-C-O	6.31	128.05	121.36
1	G	277	ASN	CA-CB-CG	-6.31	106.29	112.60
1	G	203	ASP	CA-C-O	-6.30	114.87	121.55
2	I	1	MET	CA-CB-CG	6.30	126.70	114.10
1	C	397	ASP	O-C-N	-6.29	114.23	122.59
1	C	103	TYR	O-C-N	6.28	126.98	121.39
1	A	265	VAL	CA-C-O	-6.28	115.02	121.67
1	G	137	ASP	O-C-N	6.28	130.14	123.42
1	E	291	LEU	CA-C-O	6.27	127.11	120.33
1	E	250	MET	O-C-N	6.27	128.79	122.08
1	E	274	PHE	CA-C-O	-6.27	113.91	120.55
1	C	269	TYR	CA-CB-CG	6.26	125.17	113.90
1	E	469	PHE	O-C-N	6.26	125.72	121.71
1	G	369	VAL	CA-C-N	6.26	134.30	123.91
1	G	369	VAL	C-N-CA	6.26	134.30	123.91
1	E	225	LEU	CA-C-O	-6.25	113.80	120.42
1	A	312	ARG	CA-C-O	-6.24	113.90	120.63
1	A	269	TYR	CA-CB-CG	6.23	125.12	113.90
1	C	473	ASP	CA-CB-CG	6.23	118.83	112.60
1	E	269	TYR	CA-CB-CG	6.23	125.12	113.90
2	I	25	GLN	CA-C-N	6.23	129.45	120.79
2	I	25	GLN	C-N-CA	6.23	129.45	120.79
1	C	243	THR	CA-C-O	-6.22	114.34	121.19
1	A	173	THR	CA-C-O	-6.22	113.60	120.69
1	E	253	ARG	CB-CG-CD	6.22	125.60	111.30
1	A	148	PHE	CA-C-O	6.21	127.30	120.71
1	G	104	PRO	CA-C-N	6.21	128.92	120.54
1	G	104	PRO	C-N-CA	6.21	128.92	120.54
2	I	38	TRP	CA-C-N	-6.21	116.57	123.02
2	I	38	TRP	C-N-CA	-6.21	116.57	123.02
1	E	243	THR	CA-C-O	-6.19	114.99	121.55
1	A	268	ASP	CA-CB-CG	6.19	118.79	112.60
2	I	33	LEU	CA-CB-CG	6.18	137.93	116.30
1	A	314	LEU	CA-C-N	6.18	128.84	120.44
1	A	314	LEU	C-N-CA	6.18	128.84	120.44
2	J	96	ASN	CA-CB-CG	6.17	118.77	112.60
1	C	394	PHE	N-CA-CB	-6.17	101.08	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	301	ILE	O-C-N	-6.17	114.86	122.57
1	G	355	GLU	CA-C-O	-6.17	114.84	121.56
1	G	219	LEU	O-C-N	6.16	128.67	122.08
1	G	153	HIS	O-C-N	-6.16	114.74	121.95
1	G	188	ALA	CA-C-N	6.16	128.84	120.77
1	G	188	ALA	C-N-CA	6.16	128.84	120.77
1	E	199	PHE	CA-CB-CG	6.16	119.95	113.80
1	G	312	ARG	NE-CZ-NH2	-6.15	113.67	119.20
1	A	205	ASN	O-C-N	-6.14	113.89	122.37
1	E	360	ARG	CD-NE-CZ	6.14	133.00	124.40
1	G	282	HIS	O-C-N	6.14	128.63	122.12
2	L	57	ASN	CA-CB-CG	6.14	118.74	112.60
1	E	18	LYS	CA-C-O	-6.13	114.65	121.51
1	A	203	ASP	CA-C-O	-6.12	115.06	121.55
1	G	269	TYR	CA-C-O	-6.12	114.06	120.55
1	A	281	SER	CA-C-O	6.12	126.90	120.42
1	E	318	LEU	CA-C-O	-6.11	114.07	120.55
1	E	467	PHE	CA-CB-CG	6.11	119.91	113.80
1	C	104	PRO	CA-C-N	6.09	128.45	120.28
1	C	104	PRO	C-N-CA	6.09	128.45	120.28
1	A	121	VAL	CB-CA-C	6.08	121.26	111.29
1	A	460	GLU	CB-CA-C	-6.08	101.33	110.88
2	J	51	VAL	CA-C-N	6.08	132.19	121.80
2	J	51	VAL	C-N-CA	6.08	132.19	121.80
1	A	353	TYR	CA-C-O	-6.07	112.81	120.28
1	E	401	GLN	O-C-N	6.07	130.52	123.30
1	G	325	HIS	CA-C-O	-6.06	113.69	120.66
2	L	25	GLN	OE1-CD-NE2	-6.05	116.55	122.60
2	I	30	VAL	CB-CA-C	-6.04	103.98	112.14
1	A	54	GLY	CA-C-N	6.04	128.69	120.54
1	A	54	GLY	C-N-CA	6.04	128.69	120.54
1	C	217	ARG	CD-NE-CZ	6.03	132.84	124.40
1	C	119	SER	CA-C-O	6.02	126.90	120.70
1	E	322	GLY	CA-C-N	6.01	133.20	121.41
1	E	322	GLY	C-N-CA	6.01	133.20	121.41
1	G	247	CYS	N-CA-C	6.01	117.83	111.28
1	A	346	VAL	CA-C-N	6.01	128.25	120.44
1	A	346	VAL	C-N-CA	6.01	128.25	120.44
1	A	393	ILE	CA-C-O	-6.01	113.81	120.96
1	E	104	PRO	CA-C-O	6.00	128.14	121.36
1	A	366	GLN	CG-CD-NE2	6.00	125.40	116.40
1	C	154	GLY	CA-C-O	-5.99	117.06	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	153	HIS	CA-C-O	5.99	127.04	119.61
1	A	184	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	C	355	GLU	CA-C-O	-5.99	114.23	121.05
1	G	77	LEU	CA-C-O	-5.99	113.09	119.97
1	G	131	ARG	NE-CZ-NH2	5.98	124.59	119.20
1	C	139	ARG	NE-CZ-NH1	-5.98	115.52	121.50
1	G	461	VAL	CA-C-O	-5.98	114.73	120.95
1	E	214	TRP	CA-C-O	-5.98	114.50	120.90
1	A	31	THR	N-CA-CB	5.97	118.82	110.04
1	E	329	GLY	O-C-N	-5.97	116.33	122.60
1	A	213	ARG	CA-C-N	5.97	128.28	120.28
1	A	213	ARG	C-N-CA	5.97	128.28	120.28
2	L	67	TRP	CA-C-O	-5.96	113.53	121.46
1	E	215	ARG	NH1-CZ-NH2	-5.96	111.55	119.30
1	E	240	LEU	CA-C-O	5.96	127.10	120.43
2	L	101	ILE	N-CA-CB	5.95	118.13	110.99
1	G	207	ASN	CA-C-O	-5.94	116.38	119.77
1	E	152	PRO	O-C-N	-5.94	115.46	122.17
1	E	175	LYS	O-C-N	5.94	128.15	121.32
2	I	39	VAL	O-C-N	-5.93	116.83	121.46
1	E	375	LEU	CA-C-O	5.93	123.71	119.32
1	A	110	GLU	O-C-N	-5.92	115.95	123.06
1	C	340	ASP	CA-CB-CG	5.92	118.52	112.60
1	E	118	THR	CA-CB-CG2	5.92	120.57	110.50
1	C	169	LEU	O-C-N	-5.92	116.27	122.96
1	G	266	MET	CA-C-O	-5.91	114.70	121.68
1	C	200	THR	CA-C-O	-5.91	110.76	120.80
1	A	362	ILE	N-CA-CB	-5.90	105.52	111.90
1	A	386	HIS	CA-CB-CG	5.90	119.70	113.80
1	C	72	ASP	CA-CB-CG	5.89	118.49	112.60
1	E	63	THR	O-C-N	5.89	128.82	122.34
1	E	228	ALA	CA-C-O	-5.89	114.17	120.42
1	E	118	THR	CA-C-N	-5.89	112.88	120.65
1	E	118	THR	C-N-CA	-5.89	112.88	120.65
1	C	22	LEU	O-C-N	-5.89	114.74	122.39
1	G	253	ARG	NE-CZ-NH2	-5.88	113.90	119.20
1	C	38	ALA	CA-C-O	-5.88	114.51	121.16
1	A	342	THR	CA-C-O	-5.88	114.65	120.70
1	C	426	ALA	CA-C-O	-5.87	114.33	120.55
1	G	330	THR	CB-CA-C	-5.86	99.17	109.02
1	E	444	ILE	O-C-N	-5.86	116.17	121.91
1	A	179	GLY	N-CA-C	-5.86	106.95	114.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	205	ASN	CA-C-O	-5.85	112.35	119.43
1	E	460	GLU	N-CA-CB	5.85	118.49	110.01
1	E	372	PRO	CA-C-N	-5.85	112.88	121.30
1	E	372	PRO	C-N-CA	-5.85	112.88	121.30
2	K	33	LEU	CA-CB-CG	5.85	136.77	116.30
1	A	110	GLU	CA-C-N	5.84	132.11	120.77
1	A	110	GLU	C-N-CA	5.84	132.11	120.77
1	C	365	THR	O-C-N	-5.84	115.68	122.87
1	G	356	LYS	O-C-N	-5.84	116.12	123.12
2	J	33	LEU	CA-CB-CG	5.84	136.73	116.30
1	C	131	ARG	N-CA-C	-5.82	104.36	112.45
1	A	271	THR	O-C-N	-5.82	114.66	122.23
1	C	281	SER	O-C-N	-5.82	116.08	122.07
2	J	86	GLU	CA-C-O	-5.82	114.38	120.55
1	C	138	LEU	CA-C-O	-5.81	113.62	120.60
1	E	54	GLY	CA-C-N	5.81	128.33	120.38
1	E	54	GLY	C-N-CA	5.81	128.33	120.38
1	E	418	VAL	N-CA-CB	5.80	117.33	110.55
1	C	41	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	C	460	GLU	N-CA-CB	5.80	118.42	110.01
1	C	169	LEU	CA-C-O	5.79	128.13	121.47
1	C	286	ASP	O-C-N	-5.78	114.48	122.46
1	E	320	LEU	O-C-N	-5.78	114.90	122.59
1	A	460	GLU	N-CA-CB	5.78	118.39	110.01
1	A	52	GLU	CA-C-O	5.78	126.65	120.24
1	E	420	ASN	OD1-CG-ND2	-5.77	116.83	122.60
1	C	17	VAL	CA-C-N	5.77	133.28	123.01
1	C	17	VAL	C-N-CA	5.77	133.28	123.01
1	C	196	GLY	CA-C-O	-5.77	112.73	118.96
1	E	206	VAL	O-C-N	-5.77	115.36	122.57
1	C	273	GLY	O-C-N	5.76	127.47	122.64
2	K	100	ARG	CA-C-O	5.76	128.19	121.46
1	G	362	ILE	N-CA-C	5.75	115.95	107.15
1	C	461	VAL	CA-C-O	-5.75	115.07	121.05
1	A	36	ILE	CA-C-O	-5.75	114.42	120.57
1	E	131	ARG	CG-CD-NE	5.75	124.64	112.00
1	G	237	GLY	O-C-N	-5.75	118.36	123.65
1	A	259	GLU	CB-CG-CD	5.74	122.36	112.60
1	A	75	THR	CA-CB-OG1	5.74	118.21	109.60
1	G	23	THR	N-CA-C	-5.74	106.20	113.43
1	G	268	ASP	CA-CB-CG	5.74	118.34	112.60
2	J	14	THR	N-CA-C	5.74	119.13	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	166	GLY	O-C-N	-5.73	115.25	122.41
1	A	150	GLY	O-C-N	-5.73	116.04	121.77
1	E	345	PHE	CA-CB-CG	5.73	119.53	113.80
1	E	48	VAL	CA-C-O	5.72	123.60	119.25
1	A	131	ARG	CA-C-O	5.72	126.59	120.24
1	A	238	HIS	CA-C-N	-5.72	113.43	121.72
1	A	238	HIS	C-N-CA	-5.72	113.43	121.72
1	C	61	SER	CA-C-O	-5.72	112.66	119.35
1	A	155	ILE	N-CA-C	5.71	115.91	110.42
1	C	175	LYS	C-N-CD	-5.71	108.03	120.60
1	G	161	LYS	CA-CB-CG	5.71	125.53	114.10
1	G	191	GLU	CA-C-O	-5.71	114.82	120.82
1	C	277	ASN	CA-CB-CG	-5.71	106.89	112.60
1	E	83	ARG	CB-CA-C	-5.71	101.35	110.14
1	E	114	THR	O-C-N	5.71	128.17	122.12
1	G	60	GLU	CA-C-O	5.71	126.03	119.35
2	L	60	GLY	CA-C-O	-5.71	112.17	119.13
1	E	82	GLY	CA-C-O	-5.70	115.16	121.94
1	E	460	GLU	O-C-N	5.70	127.94	122.07
2	K	86	GLU	CA-C-O	-5.70	114.51	120.55
1	A	249	ASP	N-CA-C	5.70	118.22	111.33
2	L	110	VAL	CB-CA-C	-5.69	101.58	110.69
1	E	108	PHE	CA-CB-CG	-5.69	108.11	113.80
1	G	72	ASP	O-C-N	-5.68	115.73	122.20
2	I	57	ASN	OD1-CG-ND2	5.68	128.28	122.60
2	J	116	ILE	O-C-N	-5.67	116.52	122.81
1	C	208	SER	CA-C-N	5.66	134.29	123.65
1	C	208	SER	C-N-CA	5.66	134.29	123.65
1	A	465	ILE	N-CA-C	5.66	115.70	108.12
2	J	6	ILE	CA-C-O	5.66	125.49	120.34
1	C	175	LYS	CA-C-O	-5.66	113.39	120.23
1	E	347	ASP	N-CA-C	5.66	118.17	111.33
1	G	194	ARG	NE-CZ-NH2	5.65	124.28	119.20
1	C	269	TYR	CA-C-O	-5.64	114.57	120.55
1	C	205	ASN	CA-C-N	5.64	129.53	122.48
1	C	205	ASN	C-N-CA	5.64	129.53	122.48
1	A	383	HIS	CA-C-O	5.64	126.95	121.14
1	A	366	GLN	CA-C-O	-5.63	114.27	120.24
1	E	121	VAL	CB-CA-C	5.63	120.53	111.29
1	C	107	LEU	CA-C-O	5.63	126.31	119.11
1	E	104	PRO	O-C-N	-5.63	115.75	122.89
2	I	33	LEU	CB-CA-C	5.62	119.70	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	213	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	G	353	TYR	CA-C-O	-5.61	114.21	120.66
1	E	121	VAL	CA-C-O	5.61	127.79	120.78
1	A	52	GLU	O-C-N	-5.60	114.95	122.23
2	K	98	PHE	CA-CB-CG	5.60	119.40	113.80
2	L	59	PRO	O-C-N	-5.60	115.08	122.64
1	C	248	GLU	CB-CG-CD	5.60	122.11	112.60
1	A	321	SER	CA-C-N	5.59	132.37	121.41
1	A	321	SER	C-N-CA	5.59	132.37	121.41
2	J	14	THR	O-C-N	-5.59	115.96	122.89
1	G	360	ARG	CD-NE-CZ	5.59	132.23	124.40
1	G	105	LEU	CA-C-O	-5.59	114.92	120.90
2	J	14	THR	CA-C-N	5.58	132.19	121.54
2	J	14	THR	C-N-CA	5.58	132.19	121.54
1	A	324	ASP	N-CA-C	5.57	118.28	111.82
1	A	218	PHE	CA-C-N	5.57	128.53	120.79
1	A	218	PHE	C-N-CA	5.57	128.53	120.79
1	C	185	TYR	N-CA-C	-5.56	105.12	111.07
2	I	18	LEU	O-C-N	5.56	126.28	120.99
2	J	66	TYR	N-CA-CB	5.56	118.20	109.69
1	C	82	GLY	CA-C-O	-5.56	115.33	121.94
1	G	297	MET	CB-CA-C	-5.56	104.33	109.83
1	C	290	LEU	N-CA-C	-5.55	103.20	110.53
1	E	443	THR	CA-C-O	-5.55	114.99	120.82
1	E	344	GLY	CA-C-N	-5.55	111.88	120.31
1	E	344	GLY	C-N-CA	-5.55	111.88	120.31
1	E	146	LYS	CA-C-O	-5.54	112.78	119.49
1	E	147	THR	O-C-N	-5.54	115.00	122.43
1	E	303	ARG	NE-CZ-NH2	5.54	124.19	119.20
1	G	189	VAL	CA-C-N	-5.54	113.06	120.54
1	G	189	VAL	C-N-CA	-5.54	113.06	120.54
2	L	33	LEU	CA-CB-CG	5.54	135.69	116.30
1	G	259	GLU	CB-CG-CD	5.53	122.00	112.60
1	C	184	ASN	CA-C-N	5.53	127.63	120.44
1	C	184	ASN	C-N-CA	5.53	127.63	120.44
2	J	83	VAL	CB-CA-C	-5.53	104.78	112.02
2	L	33	LEU	CB-CA-C	5.52	119.55	110.88
1	A	164	LYS	CA-C-O	5.51	126.08	120.24
1	E	279	THR	CA-CB-OG1	5.51	117.86	109.60
1	G	248	GLU	O-C-N	-5.51	115.87	122.15
2	I	9	LEU	CB-CA-C	5.50	119.97	111.28
1	C	278	THR	N-CA-C	-5.50	105.19	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	58	ALA	CA-C-O	-5.50	115.05	120.82
2	I	13	GLU	CB-CA-C	-5.50	108.63	115.89
1	C	118	THR	CA-C-O	-5.49	114.60	120.42
1	C	209	GLN	O-C-N	-5.49	117.27	121.55
1	G	258	ARG	CA-C-O	-5.49	114.60	121.02
1	A	175	LYS	CB-CA-C	5.48	120.97	110.17
2	I	33	LEU	N-CA-C	-5.48	105.20	111.07
1	A	442	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	E	412	GLY	CA-C-O	-5.48	116.82	122.25
1	C	203	ASP	CB-CG-OD2	5.48	131.00	118.40
2	L	65	ARG	O-C-N	5.47	128.79	122.17
1	E	101	VAL	O-C-N	5.47	129.17	123.26
1	C	176	PRO	N-CA-CB	5.47	108.61	102.60
1	E	111	GLY	CA-C-O	-5.47	112.25	119.25
1	G	108	PHE	CA-C-O	5.47	126.50	120.71
1	G	316	LYS	CA-C-O	5.47	126.56	120.82
1	A	161	LYS	CA-CB-CG	5.46	125.03	114.10
1	A	311	PHE	CA-CB-CG	-5.46	108.33	113.80
1	E	161	LYS	CA-CB-CG	5.46	125.03	114.10
2	J	87	LEU	O-C-N	-5.46	116.41	122.09
1	E	277	ASN	CB-CG-ND2	-5.46	108.21	116.40
2	J	56	HIS	CA-C-O	-5.46	115.39	121.23
1	G	206	VAL	O-C-N	-5.45	116.62	122.45
2	J	39	VAL	CA-C-O	5.45	122.36	119.15
2	K	52	TYR	CA-C-O	-5.44	115.61	121.38
2	L	6	ILE	N-CA-C	5.44	116.24	111.56
2	L	53	ARG	NE-CZ-NH1	-5.44	116.06	121.50
1	A	275	THR	CA-C-O	5.44	126.53	120.82
1	C	37	LEU	CA-C-O	-5.44	114.45	120.38
1	C	367	SER	CA-C-O	-5.44	115.02	121.16
1	E	374	VAL	CA-C-O	-5.44	114.52	120.72
1	C	259	GLU	CB-CG-CD	5.43	121.83	112.60
1	A	239	TYR	N-CA-C	-5.42	100.95	109.25
1	G	466	LYS	CA-C-O	-5.42	115.10	121.44
1	C	231	GLU	CA-C-O	-5.42	115.13	120.82
1	A	414	ALA	O-C-N	5.42	125.80	120.71
1	C	191	GLU	CA-C-O	-5.42	115.13	120.82
1	G	414	ALA	O-C-N	5.41	125.30	120.48
1	G	187	ARG	NH1-CZ-NH2	5.41	126.33	119.30
2	I	67	TRP	CA-C-N	-5.41	115.09	122.93
2	I	67	TRP	C-N-CA	-5.41	115.09	122.93
1	E	116	MET	N-CA-C	5.40	116.85	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ASP	CB-CG-OD2	5.40	130.83	118.40
1	A	292	HIS	O-C-N	-5.40	117.17	123.27
1	E	74	LEU	N-CA-C	-5.40	106.19	112.89
1	G	456	ALA	CA-C-O	-5.40	115.15	120.82
1	E	259	GLU	N-CA-C	5.40	117.86	111.33
1	G	191	GLU	CA-C-N	5.40	127.46	120.44
1	G	191	GLU	C-N-CA	5.40	127.46	120.44
1	A	317	ALA	N-CA-C	5.39	117.16	111.28
2	L	72	LEU	O-C-N	5.39	127.52	121.32
1	E	264	ILE	CB-CG1-CD1	5.39	125.12	113.80
2	L	43	GLU	CA-C-O	-5.39	114.81	121.06
1	C	295	ARG	NE-CZ-NH2	-5.38	114.36	119.20
2	J	116	ILE	CB-CA-C	5.38	118.15	111.15
2	K	100	ARG	NH1-CZ-NH2	5.38	126.30	119.30
1	C	294	HIS	CA-C-O	-5.37	114.84	120.80
1	G	217	ARG	CG-CD-NE	5.37	123.82	112.00
1	G	285	ARG	O-C-N	-5.37	116.51	122.09
1	A	413	ASN	CA-C-O	5.37	126.11	120.42
1	G	221	CYS	N-CA-CB	5.37	118.01	110.12
1	E	302	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	177	LYS	CB-CA-C	-5.36	102.24	110.81
1	E	191	GLU	CB-CG-CD	5.36	121.70	112.60
1	C	365	THR	CA-C-N	-5.35	115.23	122.77
1	C	365	THR	C-N-CA	-5.35	115.23	122.77
1	G	101	VAL	CA-C-O	-5.34	114.78	120.39
1	G	150	GLY	CA-C-O	5.34	129.16	121.52
2	K	43	GLU	CA-C-O	-5.34	114.20	120.60
1	G	442	ASN	OD1-CG-ND2	-5.33	117.27	122.60
2	I	30	VAL	N-CA-CB	5.33	117.79	110.54
2	J	27	ALA	CA-C-O	-5.33	115.19	120.90
1	G	456	ALA	O-C-N	5.33	127.56	122.07
2	J	9	LEU	CB-CA-C	5.33	119.70	111.28
1	E	242	ALA	CA-C-N	-5.32	112.71	120.75
1	E	242	ALA	C-N-CA	-5.32	112.71	120.75
1	E	112	SER	O-C-N	-5.32	116.46	122.84
1	G	392	GLU	O-C-N	-5.31	116.49	122.12
1	E	131	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	C	290	LEU	O-C-N	5.31	128.84	122.79
2	J	6	ILE	N-CA-CB	-5.31	104.63	111.90
1	E	327	HIS	O-C-N	5.30	129.36	122.89
1	C	108	PHE	N-CA-CB	-5.30	102.16	110.69
2	L	107	ASN	CA-C-O	5.29	126.11	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	39	ALA	CA-C-O	-5.29	114.80	120.46
1	G	367	SER	CA-C-O	-5.29	115.19	121.16
1	A	312	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	C	226	TYR	O-C-N	-5.28	116.52	122.12
2	L	13	GLU	CA-C-O	-5.28	113.63	120.71
1	A	17	VAL	CA-CB-CG2	5.28	119.37	110.40
1	C	300	VAL	CA-C-O	-5.28	115.56	121.05
1	C	460	GLU	CA-C-O	-5.28	115.28	120.82
1	G	220	PHE	CA-C-N	5.28	127.35	120.28
1	G	220	PHE	C-N-CA	5.28	127.35	120.28
1	C	152	PRO	O-C-N	-5.27	115.91	122.23
1	E	203	ASP	CB-CG-OD1	-5.27	106.28	118.40
1	E	371	THR	O-C-N	5.27	125.70	121.38
1	G	218	PHE	CA-CB-CG	5.26	119.06	113.80
1	G	371	THR	CA-C-N	5.26	125.20	119.78
1	G	371	THR	C-N-CA	5.26	125.20	119.78
2	K	67	TRP	CA-C-O	-5.26	114.92	121.55
1	G	301	ILE	N-CA-CB	-5.26	102.55	111.23
2	L	33	LEU	N-CA-C	-5.26	105.44	111.07
2	L	38	TRP	CA-C-N	-5.26	117.55	123.02
2	L	38	TRP	C-N-CA	-5.26	117.55	123.02
1	A	393	ILE	O-C-N	5.26	128.74	121.90
1	A	422	VAL	N-CA-C	5.26	115.70	110.23
1	A	88	GLU	CB-CA-C	5.25	117.08	109.20
1	C	204	GLU	CA-C-O	-5.25	114.98	120.55
1	G	207	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	G	356	LYS	CA-C-O	5.24	126.73	121.07
1	E	90	VAL	CA-C-O	5.24	126.18	120.57
1	E	203	ASP	CB-CG-OD2	5.24	130.45	118.40
1	G	143	ALA	O-C-N	-5.24	115.42	122.43
2	K	38	TRP	CA-C-O	-5.24	115.27	121.66
1	C	234	GLU	CA-CB-CG	5.23	124.55	114.10
1	E	186	GLY	CA-C-N	-5.23	113.64	120.44
1	E	186	GLY	C-N-CA	-5.23	113.64	120.44
1	C	159	ARG	N-CA-C	-5.22	105.59	111.28
1	A	281	SER	O-C-N	-5.22	116.20	122.15
1	E	48	VAL	N-CA-C	5.21	112.71	107.55
1	C	250	MET	O-C-N	5.21	127.43	122.07
1	C	112	SER	CA-C-O	-5.20	114.77	120.70
2	L	71	LYS	CA-C-O	-5.20	112.05	119.80
1	A	389	ALA	CA-C-N	5.20	127.52	120.65
1	A	389	ALA	C-N-CA	5.20	127.52	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	106	ASP	CA-C-O	-5.20	114.38	120.20
1	E	190	TYR	CA-C-O	5.20	126.06	120.55
2	I	108	ARG	CA-C-O	5.19	125.43	119.35
1	C	44	PRO	CB-CA-C	-5.19	104.18	110.98
1	G	61	SER	O-C-N	5.19	128.52	122.24
1	C	55	ALA	N-CA-C	5.19	116.94	111.28
1	E	457	ALA	O-C-N	-5.19	116.62	122.12
1	A	48	VAL	N-CA-C	5.17	113.14	107.60
1	E	214	TRP	N-CA-C	5.17	117.32	111.11
1	G	151	PRO	CA-C-O	5.17	128.06	120.56
1	E	418	VAL	O-C-N	5.17	126.98	121.91
1	G	264	ILE	CB-CG1-CD1	5.17	124.66	113.80
1	A	160	ASP	CA-CB-CG	5.17	117.77	112.60
1	C	163	ASN	CA-C-N	5.16	130.19	122.86
1	C	163	ASN	C-N-CA	5.16	130.19	122.86
1	A	301	ILE	N-CA-CB	-5.16	102.72	111.23
1	A	372	PRO	N-CA-CB	5.16	108.12	103.33
1	C	345	PHE	CA-CB-CG	5.16	118.95	113.80
2	L	33	LEU	CA-C-O	-5.16	115.41	120.82
1	G	218	PHE	O-C-N	5.15	127.58	122.12
1	A	423	ALA	N-CA-C	5.15	117.29	111.11
1	A	228	ALA	CA-C-O	5.15	126.22	120.82
1	E	312	ARG	NE-CZ-NH2	-5.15	114.57	119.20
2	I	18	LEU	N-CA-C	-5.14	104.14	110.31
1	G	114	THR	CA-C-O	-5.14	115.40	120.90
1	G	211	PHE	CA-CB-CG	-5.14	108.66	113.80
1	G	460	GLU	CB-CA-C	-5.14	102.26	110.79
2	J	107	ASN	O-C-N	-5.13	116.30	122.15
1	C	407	LEU	CA-C-O	-5.13	112.40	119.12
1	C	239	TYR	N-CA-CB	5.13	118.15	109.94
1	E	16	GLY	CA-C-O	-5.13	118.76	122.45
1	G	136	GLU	CA-C-O	5.12	125.93	120.24
1	G	220	PHE	O-C-N	-5.12	116.69	122.12
2	L	5	PRO	CA-C-N	5.12	128.26	123.08
2	L	5	PRO	C-N-CA	5.12	128.26	123.08
1	A	429	GLN	CG-CD-NE2	5.12	124.08	116.40
1	G	57	VAL	O-C-N	5.12	127.06	121.94
1	A	43	SER	CA-C-O	-5.12	115.08	120.09
1	A	108	PHE	N-CA-C	5.11	117.30	109.07
1	A	130	LEU	O-C-N	-5.11	116.72	123.21
1	G	18	LYS	CA-C-O	-5.11	115.41	121.60
1	C	110	GLU	CA-C-O	5.11	126.77	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	50	PRO	O-C-N	-5.11	116.66	122.18
1	A	199	PHE	CA-C-O	-5.11	115.62	121.40
1	E	470	PRO	CA-C-O	-5.11	115.76	121.23
1	A	188	ALA	CA-C-O	-5.11	115.46	120.82
1	G	47	GLY	CA-C-O	5.10	124.85	119.03
1	C	444	ILE	O-C-N	-5.10	116.59	121.90
1	E	248	GLU	CA-C-O	-5.10	115.46	120.82
1	G	273	GLY	O-C-N	5.10	126.92	122.64
1	G	281	SER	CA-C-N	5.10	127.11	120.28
1	G	281	SER	C-N-CA	5.10	127.11	120.28
1	A	307	HIS	O-C-N	-5.09	116.76	123.28
1	E	369	VAL	CA-C-N	5.09	132.37	123.91
1	E	369	VAL	C-N-CA	5.09	132.37	123.91
1	G	123	ASN	CB-CG-ND2	5.09	124.04	116.40
1	E	134	ARG	NE-CZ-NH1	5.09	126.59	121.50
1	C	460	GLU	CB-CA-C	-5.08	102.90	110.88
2	I	38	TRP	CA-C-O	-5.08	115.46	121.66
1	A	239	TYR	N-CA-CB	5.08	118.14	109.87
1	A	23	THR	N-CA-C	-5.07	107.16	113.55
1	C	110	GLU	CA-C-N	5.07	131.35	121.41
1	C	110	GLU	C-N-CA	5.07	131.35	121.41
1	G	229	GLN	O-C-N	-5.07	116.85	122.07
1	G	283	TYR	CA-C-N	-5.07	113.09	120.29
1	G	283	TYR	C-N-CA	-5.07	113.09	120.29
1	G	171	GLY	O-C-N	-5.07	120.05	123.95
1	E	63	THR	CA-CB-OG1	-5.07	102.00	109.60
1	E	459	CYS	CA-C-O	-5.07	115.18	120.55
1	E	206	VAL	CA-C-O	5.06	127.11	120.78
2	J	66	TYR	CA-C-O	-5.06	115.15	120.92
1	A	97	TYR	O-C-N	-5.05	117.02	123.24
1	A	115	ASN	CA-C-N	5.05	127.46	120.29
1	A	115	ASN	C-N-CA	5.05	127.46	120.29
1	C	36	ILE	CA-C-N	-5.05	116.03	123.00
1	C	36	ILE	C-N-CA	-5.05	116.03	123.00
2	L	50	PHE	CA-C-O	-5.04	115.54	121.44
1	A	289	LEU	CA-C-O	-5.04	114.85	120.54
1	E	164	LYS	CA-C-O	5.04	125.58	120.24
1	G	229	GLN	OE1-CD-NE2	5.04	127.64	122.60
1	G	316	LYS	O-C-N	-5.03	116.89	122.07
1	G	116	MET	CA-C-O	5.03	125.76	119.97
2	I	110	VAL	CB-CA-C	-5.03	102.75	110.50
1	C	154	GLY	CA-C-N	5.03	127.08	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	154	GLY	C-N-CA	5.03	127.08	120.60
2	I	88	GLU	N-CA-C	5.03	116.76	111.28
1	G	362	ILE	N-CA-CB	-5.02	105.93	111.66
1	G	421	ARG	CB-CA-C	-5.02	102.45	110.79
1	A	460	GLU	CA-C-O	-5.02	115.55	120.82
1	C	460	GLU	O-C-N	5.02	127.24	122.07
1	C	275	THR	CA-C-N	5.02	129.21	120.68
1	C	275	THR	C-N-CA	5.02	129.21	120.68
2	J	6	ILE	CB-CA-C	5.01	115.83	110.91
1	A	384	VAL	O-C-N	5.01	126.93	121.87
2	K	9	LEU	CD1-CG-CD2	-5.01	99.78	110.80
1	C	466	LYS	CA-C-N	-5.00	115.74	122.95
1	C	466	LYS	C-N-CA	-5.00	115.74	122.95
1	E	88	GLU	CB-CA-C	5.00	117.53	110.02
1	G	467	PHE	CA-CB-CG	5.00	118.80	113.80
1	E	96	GLN	OE1-CD-NE2	5.00	127.60	122.60

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	LYS	Peptide
1	A	330	THR	Mainchain
1	C	175	LYS	Mainchain
1	E	175	LYS	Peptide
1	E	243	THR	Mainchain
1	G	152	PRO	Mainchain
1	G	175	LYS	Peptide
1	G	201	KCX	Peptide
2	I	11	LYS	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3656	0	3565	100	0
1	C	3656	0	3565	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3656	0	3565	84	0
1	G	3656	0	3564	82	0
2	I	1032	0	990	36	0
2	J	1032	0	990	32	0
2	K	1032	0	990	38	0
2	L	1032	0	990	40	1
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	21	0	7	0	0
4	C	21	0	6	1	0
4	E	21	0	7	0	0
4	G	21	0	7	0	0
5	A	112	0	0	14	0
5	C	121	0	0	15	0
5	E	132	0	0	11	0
5	G	133	0	0	10	3
5	I	34	0	0	1	0
5	J	44	0	0	3	0
5	K	41	0	0	7	0
5	L	47	0	0	6	0
All	All	19504	0	18246	467	4

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 13.

All (467) 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:G:303:ARG:HG3	5:G:2084:HOH:O	1.58	1.03
2:K:22:THR:H	2:K:25:GLN:HE21	1.06	1.02
1:A:177:LYS:CD	5:A:2040:HOH:O	2.10	0.97
2:J:29:GLN:HB2	5:J:2016:HOH:O	1.67	0.95
2:J:22:THR:H	2:J:25:GLN:HE21	0.98	0.94
2:I:22:THR:H	2:I:25:GLN:HE21	1.03	0.92
2:K:42:LEU:HD22	5:K:2025:HOH:O	1.72	0.89
1:A:267:HIS:HD2	1:A:277:ASN:HD22	1.23	0.86
2:J:2:GLN:HG3	5:J:2001:HOH:O	1.75	0.86
1:A:177:LYS:HD2	5:A:2040:HOH:O	1.69	0.85
1:C:26:THR:HG22	1:C:29:TYR:HB2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:267:HIS:CD2	1:G:277:ASN:HD22	1.97	0.82
1:G:414:ALA:HB3	1:G:415:PRO:HD3	1.62	0.80
1:E:140:ILE:HB	5:E:2105:HOH:O	1.82	0.80
1:A:267:HIS:CD2	1:A:277:ASN:HD22	2.00	0.79
2:L:22:THR:H	2:L:25:GLN:HE21	1.27	0.79
1:C:267:HIS:CD2	1:C:277:ASN:HD22	2.01	0.78
1:E:383:HIS:H	1:E:386:HIS:HD2	1.32	0.78
2:J:22:THR:N	2:J:25:GLN:HE21	1.80	0.77
1:G:267:HIS:HD2	1:G:277:ASN:HD22	1.33	0.77
1:E:267:HIS:CD2	1:E:277:ASN:HD22	2.04	0.76
1:E:26:THR:HG22	1:E:29:TYR:HB2	1.66	0.76
2:I:96:ASN:HB2	5:I:2025:HOH:O	1.86	0.75
1:C:400:LEU:HD21	5:C:2106:HOH:O	1.86	0.75
1:E:241:ASN:ND2	1:E:243:THR:H	1.85	0.75
1:A:26:THR:HG22	1:A:29:TYR:HB2	1.68	0.75
2:L:40:PRO:HG2	2:L:74:MET:HB2	1.69	0.74
2:K:89:GLU:HA	5:K:2032:HOH:O	1.88	0.74
1:E:414:ALA:HB3	1:E:415:PRO:HD3	1.68	0.74
1:E:239:TYR:HE2	1:E:401:GLN:HE22	1.33	0.73
2:I:22:THR:H	2:I:25:GLN:NE2	1.84	0.73
2:I:22:THR:N	2:I:25:GLN:HE21	1.82	0.73
1:E:292:HIS:HA	1:E:325:HIS:HB2	1.70	0.72
2:J:24:ASP:HB2	5:J:2013:HOH:O	1.88	0.72
1:G:113:VAL:HG11	1:G:274:PHE:CD1	2.25	0.72
1:C:383:HIS:H	1:C:386:HIS:HD2	1.38	0.71
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.71	0.71
2:K:22:THR:N	2:K:25:GLN:HE21	1.87	0.70
2:K:99:ILE:HG23	5:K:2018:HOH:O	1.92	0.70
1:A:241:ASN:HD22	1:A:243:THR:H	1.38	0.69
1:A:383:HIS:H	1:A:386:HIS:HD2	1.36	0.69
2:J:22:THR:H	2:J:25:GLN:NE2	1.81	0.69
1:G:26:THR:HG22	1:G:29:TYR:HB2	1.74	0.69
1:A:239:TYR:HE2	1:A:401:GLN:HE22	1.40	0.69
1:C:414:ALA:HB3	1:C:415:PRO:HD3	1.76	0.68
1:A:241:ASN:ND2	1:A:243:THR:H	1.92	0.67
1:A:75:THR:HG22	1:A:76:ASN:H	1.59	0.67
1:A:177:LYS:CE	5:A:2040:HOH:O	2.40	0.67
1:C:241:ASN:ND2	1:C:243:THR:H	1.93	0.67
1:E:295:ARG:HG3	1:E:298:HIS:CD2	2.31	0.66
2:I:32:TYR:CE2	2:I:113:ILE:HD11	2.30	0.66
2:I:68:THR:HG21	2:J:6:ILE:HD11	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LYS:NZ	5:A:2040:HOH:O	2.19	0.66
1:E:267:HIS:HD2	1:E:277:ASN:HD22	1.41	0.66
1:A:328:SER:HB3	5:A:2069:HOH:O	1.95	0.66
1:G:292:HIS:HA	1:G:325:HIS:HB2	1.77	0.66
2:J:32:TYR:CE2	2:J:113:ILE:HD11	2.31	0.65
1:E:161:LYS:HE2	1:G:219:LEU:HD23	1.77	0.65
1:C:267:HIS:HD2	1:C:277:ASN:HD22	1.44	0.65
1:C:321:SER:HB2	5:C:2088:HOH:O	1.95	0.65
1:C:239:TYR:HE2	1:C:401:GLN:HE22	1.43	0.65
1:G:431:ARG:HH21	1:G:432:ASN:HD21	1.43	0.65
1:A:379:SER:HB2	1:A:401:GLN:HB2	1.77	0.65
1:C:394:PHE:HB2	5:C:2106:HOH:O	1.96	0.65
5:E:2064:HOH:O	2:K:10:LYS:HE3	1.95	0.65
2:L:92:LYS:HD2	2:L:93:GLU:N	2.12	0.65
1:G:303:ARG:HD2	5:G:2083:HOH:O	1.96	0.64
1:C:75:THR:HG22	1:C:76:ASN:H	1.62	0.64
1:G:239:TYR:HE2	1:G:401:GLN:HE22	1.44	0.64
2:L:89:GLU:HG2	2:L:92:LYS:HE2	1.78	0.63
1:C:440:GLU:HG2	5:C:2115:HOH:O	1.99	0.63
1:G:75:THR:HG22	1:G:76:ASN:H	1.62	0.63
2:K:32:TYR:CE2	2:K:113:ILE:HD11	2.32	0.63
1:C:292:HIS:HA	1:C:325:HIS:HB2	1.80	0.62
2:J:92:LYS:HD2	2:J:93:GLU:N	2.14	0.62
1:A:115:ASN:HB2	5:A:2030:HOH:O	1.99	0.62
1:A:161:LYS:HE2	1:C:219:LEU:HD23	1.81	0.62
1:C:173:THR:HB	1:C:175:LYS:HE2	1.81	0.62
2:K:92:LYS:HD2	2:K:93:GLU:N	2.14	0.62
1:E:241:ASN:HD22	1:E:243:THR:H	1.47	0.62
2:J:32:TYR:HE2	2:J:113:ILE:HD11	1.64	0.62
1:A:241:ASN:HA	1:A:266:MET:HG3	1.82	0.62
1:C:274:PHE:CD1	5:C:2088:HOH:O	2.51	0.62
2:L:32:TYR:CE2	2:L:113:ILE:HD11	2.34	0.62
2:J:89:GLU:HG2	2:J:92:LYS:HE2	1.83	0.61
2:K:42:LEU:HB3	5:K:2018:HOH:O	2.00	0.61
2:L:107:ASN:HB2	5:L:2041:HOH:O	1.98	0.61
1:E:241:ASN:HA	1:E:266:MET:HG3	1.82	0.61
1:E:385:TRP:CZ2	1:E:459:CYS:HB3	2.36	0.61
1:E:229:GLN:HE21	1:E:236:LYS:H	1.47	0.61
1:A:376:PRO:HA	5:A:2069:HOH:O	1.99	0.61
1:G:229:GLN:HE21	1:G:236:LYS:H	1.48	0.60
1:A:177:LYS:CG	5:A:2040:HOH:O	2.43	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:409:HIS:CG	1:E:410:PRO:HD2	2.36	0.60
1:E:155:ILE:HG12	1:E:375:LEU:HD13	1.84	0.60
1:E:173:THR:HB	1:E:175:LYS:HE2	1.84	0.60
1:C:123:ASN:HA	5:C:2044:HOH:O	2.00	0.60
1:G:234:GLU:HB3	2:L:13:GLU:OE2	2.02	0.60
2:I:72:LEU:HB3	2:I:73:PRO:HD2	1.84	0.60
1:E:366:GLN:NE2	5:E:2105:HOH:O	2.35	0.60
1:G:377:VAL:HG22	1:G:399:VAL:HB	1.84	0.60
2:K:86:GLU:HB3	5:K:2025:HOH:O	2.01	0.60
1:G:340:ASP:HB2	5:G:2092:HOH:O	2.01	0.59
1:E:122:GLY:HA3	5:E:2037:HOH:O	2.01	0.59
1:C:345:PHE:HA	1:C:348:LEU:HD12	1.84	0.59
1:G:230:ALA:HA	5:G:2066:HOH:O	2.02	0.59
1:G:140:ILE:H	1:G:140:ILE:HD12	1.68	0.58
1:A:251:MET:HE1	1:A:283:TYR:CD1	2.38	0.58
1:C:360:ARG:NH2	5:C:2098:HOH:O	2.35	0.58
2:I:32:TYR:HE2	2:I:113:ILE:HD11	1.65	0.58
2:L:58:SER:HB2	2:L:59:PRO:HD2	1.84	0.58
1:E:429:GLN:O	1:E:433:GLU:HG3	2.03	0.58
1:A:318:LEU:HG	1:A:326:ILE:HD12	1.85	0.58
2:K:89:GLU:HG2	2:K:92:LYS:HE2	1.84	0.58
1:A:429:GLN:O	1:A:433:GLU:HG3	2.04	0.58
2:L:32:TYR:HE2	2:L:113:ILE:HD11	1.68	0.57
2:I:92:LYS:HD2	2:I:93:GLU:N	2.19	0.57
2:K:32:TYR:HE2	2:K:113:ILE:HD11	1.70	0.57
1:E:318:LEU:HG	1:E:326:ILE:HD12	1.86	0.57
1:A:385:TRP:CZ2	1:A:459:CYS:HB3	2.40	0.56
2:K:22:THR:H	2:K:25:GLN:NE2	1.90	0.56
2:L:121:ALA:HB3	5:L:2047:HOH:O	2.04	0.56
1:E:387:MET:HB3	1:E:388:PRO:HD3	1.88	0.56
1:C:175:LYS:H	1:C:407:LEU:HD22	1.71	0.56
2:I:89:GLU:HG2	2:I:92:LYS:HE2	1.87	0.56
1:E:204:GLU:HG2	1:E:205:ASN:N	2.21	0.55
1:G:251:MET:HE1	1:G:283:TYR:CG	2.41	0.55
1:G:200:THR:OG1	1:G:238:HIS:HD2	1.90	0.55
1:G:341:ILE:HD11	1:G:475:VAL:HG23	1.88	0.55
2:K:33:LEU:HB2	2:K:113:ILE:HG13	1.89	0.55
2:K:70:TRP:CD1	5:K:2025:HOH:O	2.58	0.55
1:C:429:GLN:O	1:C:433:GLU:HG3	2.07	0.55
1:G:204:GLU:HG2	1:G:205:ASN:N	2.22	0.55
1:C:284:CYS:HB3	1:C:289:LEU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:LYS:HE2	1:C:366:GLN:HG2	1.88	0.55
1:E:194:ARG:NH1	2:K:6:ILE:HD12	2.22	0.55
2:L:22:THR:N	2:L:25:GLN:HE21	2.01	0.55
1:A:284:CYS:HB3	1:A:289:LEU:O	2.07	0.55
1:A:316:LYS:HE2	1:A:366:GLN:HG2	1.88	0.55
1:E:26:THR:CG2	1:E:29:TYR:HB2	2.37	0.54
1:C:409:HIS:CG	1:C:410:PRO:HD2	2.43	0.54
1:C:414:ALA:O	1:C:418:VAL:HG23	2.07	0.54
1:G:241:ASN:ND2	1:G:243:THR:H	2.06	0.54
1:E:208:SER:HB2	1:E:214:TRP:HB3	1.90	0.54
1:E:400:LEU:HD21	5:E:2108:HOH:O	2.06	0.54
1:A:219:LEU:HG	5:L:2026:HOH:O	2.07	0.54
1:E:24:TYR:CD2	1:E:59:ALA:HB2	2.43	0.54
1:C:62:SER:OG	1:C:63:THR:N	2.41	0.54
1:G:175:LYS:H	1:G:407:LEU:HD22	1.73	0.54
1:A:50:PRO:HG3	1:A:97:TYR:CZ	2.43	0.53
1:E:173:THR:HG23	1:E:201:KCX:HG2	1.89	0.53
1:E:202:ASP:OD1	1:E:238:HIS:HE1	1.91	0.53
1:C:373:GLY:N	5:C:2104:HOH:O	2.41	0.53
1:G:316:LYS:HE2	1:G:366:GLN:HG2	1.91	0.53
1:A:229:GLN:HE21	1:A:236:LYS:H	1.56	0.53
1:E:173:THR:HA	1:E:201:KCX:HG3	1.90	0.53
1:G:284:CYS:HB3	1:G:289:LEU:O	2.08	0.53
1:G:315:ALA:HB1	1:G:349:LEU:HD21	1.91	0.53
1:C:50:PRO:HG3	1:C:97:TYR:CZ	2.43	0.53
1:G:18:LYS:HB3	1:G:22:LEU:HD12	1.90	0.53
1:E:75:THR:HG22	1:E:76:ASN:H	1.73	0.53
1:G:267:HIS:HD2	1:G:277:ASN:ND2	2.06	0.53
1:E:473:ASP:HB3	5:E:2091:HOH:O	2.09	0.53
1:A:155:ILE:HG13	1:A:373:GLY:O	2.10	0.52
1:A:409:HIS:CG	1:A:410:PRO:HD2	2.44	0.52
2:I:33:LEU:HB2	2:I:113:ILE:HG13	1.91	0.52
2:I:58:SER:HB2	2:I:59:PRO:HD2	1.91	0.52
1:C:274:PHE:HD1	5:C:2088:HOH:O	1.90	0.52
1:E:318:LEU:CG	1:E:326:ILE:HD12	2.40	0.52
2:K:14:THR:O	2:K:15:LEU:HB2	2.09	0.52
1:A:467:PHE:HA	5:A:2106:HOH:O	2.09	0.52
1:C:431:ARG:HH21	1:C:432:ASN:HD21	1.57	0.52
2:L:120:PRO:HG2	2:L:123:TYR:CD2	2.44	0.52
1:C:241:ASN:HA	1:C:266:MET:HG3	1.91	0.52
1:A:414:ALA:O	1:A:418:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:113:VAL:HG11	1:G:274:PHE:CE1	2.44	0.52
1:G:209:GLN:HB3	1:G:210:PRO:HD2	1.92	0.52
1:G:241:ASN:HD22	1:G:243:THR:H	1.56	0.52
1:A:190:TYR:CZ	1:A:194:ARG:HD3	2.45	0.52
1:E:251:MET:HE1	1:E:283:TYR:CG	2.44	0.52
2:I:21:LEU:HA	2:I:25:GLN:NE2	2.25	0.52
1:C:337:GLY:HA2	5:C:2092:HOH:O	2.09	0.51
1:G:155:ILE:HG12	1:G:375:LEU:HD13	1.92	0.51
2:I:6:ILE:HD11	2:L:68:THR:HG21	1.92	0.51
1:A:334:LYS:HG3	1:A:335:LEU:HG	1.92	0.51
2:K:104:PHE:HB3	5:K:2034:HOH:O	2.09	0.51
1:A:382:ILE:HA	1:A:386:HIS:CD2	2.46	0.51
2:I:51:VAL:HG13	2:I:62:TYR:HB3	1.92	0.51
2:J:40:PRO:HG2	2:J:74:MET:HB2	1.92	0.51
1:E:451:TRP:CH2	2:K:19:PRO:HD3	2.46	0.51
1:A:451:TRP:CZ3	2:I:19:PRO:HD3	2.46	0.50
1:C:26:THR:CG2	1:C:29:TYR:HB2	2.37	0.50
1:C:186:GLY:HA3	2:I:66:TYR:OH	2.11	0.50
1:A:295:ARG:HG3	1:A:298:HIS:CD2	2.46	0.50
1:C:448:ALA:HA	1:C:451:TRP:NE1	2.27	0.50
2:J:10:LYS:HB3	2:J:50:PHE:CZ	2.46	0.50
1:A:24:TYR:CD2	1:A:59:ALA:HB2	2.47	0.50
1:G:295:ARG:HG3	1:G:298:HIS:CD2	2.47	0.50
1:C:137:ASP:OD1	1:C:138:LEU:N	2.43	0.50
1:C:251:MET:HE1	1:C:283:TYR:CG	2.46	0.50
2:I:39:VAL:HG11	2:I:75:PHE:CD1	2.47	0.50
1:A:251:MET:HE1	1:A:283:TYR:CG	2.47	0.49
1:E:392:GLU:HA	5:E:2109:HOH:O	2.10	0.49
2:L:22:THR:H	2:L:25:GLN:NE2	2.05	0.49
1:E:431:ARG:HH21	1:E:432:ASN:HD21	1.60	0.49
1:C:44:PRO:HD2	1:C:95:ASN:O	2.12	0.49
1:G:383:HIS:H	1:G:386:HIS:HD2	1.59	0.49
2:K:71:LYS:HD3	2:L:1:MET:HG2	1.94	0.49
1:C:241:ASN:HD22	1:C:243:THR:H	1.58	0.49
1:A:26:THR:CG2	1:A:29:TYR:HB2	2.39	0.49
1:G:451:TRP:CZ3	2:L:19:PRO:HD3	2.48	0.49
1:C:289:LEU:HD23	2:J:59:PRO:HB3	1.94	0.48
1:G:431:ARG:HE	1:G:432:ASN:ND2	2.11	0.48
1:A:357:ASP:HA	5:A:2083:HOH:O	2.12	0.48
1:A:383:HIS:CE1	1:A:385:TRP:HB2	2.48	0.48
1:G:50:PRO:HG3	1:G:97:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:TYR:O	1:A:189:VAL:HG23	2.12	0.48
2:K:42:LEU:HD21	2:K:87:LEU:HA	1.94	0.48
1:G:472:MET:CB	5:G:2084:HOH:O	2.61	0.48
1:C:225:LEU:C	1:C:225:LEU:HD12	2.39	0.48
1:G:241:ASN:HA	1:G:266:MET:HG3	1.96	0.48
1:G:303:ARG:CD	5:G:2083:HOH:O	2.59	0.48
1:A:125:PHE:CG	1:A:133:LEU:HD23	2.49	0.48
1:A:387:MET:HB3	1:A:388:PRO:HD3	1.95	0.48
1:E:62:SER:OG	1:E:63:THR:N	2.44	0.48
1:E:451:TRP:CZ3	2:K:19:PRO:HD3	2.49	0.48
1:G:327:HIS:CG	5:G:2088:HOH:O	2.67	0.48
1:A:318:LEU:CG	1:A:326:ILE:HD12	2.44	0.48
1:C:385:TRP:CZ2	1:C:459:CYS:HB3	2.49	0.48
1:G:431:ARG:HE	1:G:432:ASN:HD22	1.62	0.48
1:A:119:SER:O	1:A:120:ILE:C	2.55	0.47
1:A:208:SER:HB2	1:A:214:TRP:HB3	1.96	0.47
1:A:456:ALA:O	1:A:460:GLU:HG3	2.14	0.47
1:C:171:GLY:HA2	1:C:199:PHE:O	2.13	0.47
1:A:194:ARG:HD2	1:A:231:GLU:OE2	2.15	0.47
1:A:294:HIS:CE1	1:A:296:ALA:HB2	2.49	0.47
1:A:451:TRP:CH2	2:I:19:PRO:HD3	2.49	0.47
1:G:184:ASN:ND2	1:G:187:ARG:HH11	2.12	0.47
1:A:292:HIS:HA	1:A:325:HIS:HB2	1.97	0.47
1:A:341:ILE:HD11	1:A:475:VAL:HG23	1.95	0.47
2:L:65:ARG:NH2	5:L:2026:HOH:O	2.45	0.47
1:A:219:LEU:HD11	2:L:61:TYR:HB2	1.96	0.47
1:C:234:GLU:HB3	2:J:13:GLU:OE2	2.15	0.47
5:C:2054:HOH:O	2:J:60:GLY:HA3	2.13	0.47
1:E:281:SER:OG	1:E:322:GLY:HA3	2.15	0.47
1:G:222:ALA:O	1:G:223:GLU:C	2.57	0.47
2:I:89:GLU:HG2	2:I:92:LYS:CE	2.44	0.47
1:E:184:ASN:ND2	1:E:187:ARG:HH11	2.13	0.47
1:E:302:ASP:OD2	1:E:311:PHE:HB2	2.15	0.47
2:I:68:THR:HG21	2:J:6:ILE:CD1	2.43	0.47
2:K:10:LYS:HB3	2:K:50:PHE:CZ	2.50	0.47
2:K:51:VAL:HG13	2:K:62:TYR:HB3	1.96	0.47
1:C:31:THR:N	5:C:2015:HOH:O	2.48	0.47
1:E:160:ASP:HB3	1:G:183:LYS:HD3	1.97	0.47
1:C:297:MET:O	1:C:297:MET:HG2	2.15	0.46
1:C:451:TRP:CZ3	2:J:19:PRO:HD3	2.50	0.46
2:L:10:LYS:HB3	2:L:50:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ARG:HD2	5:A:2042:HOH:O	2.15	0.46
1:E:131:ARG:HG2	5:E:2040:HOH:O	2.15	0.46
1:E:251:MET:HE1	1:E:283:TYR:CD1	2.50	0.46
1:A:126:GLY:O	1:A:127:PHE:C	2.59	0.46
1:A:431:ARG:HE	1:A:432:ASN:ND2	2.12	0.46
1:C:26:THR:O	1:C:85:TYR:HA	2.15	0.46
1:E:377:VAL:HG22	1:E:399:VAL:HB	1.96	0.46
1:G:303:ARG:HA	5:G:2083:HOH:O	2.14	0.46
2:K:72:LEU:HB3	2:K:73:PRO:HD2	1.97	0.46
1:C:165:TYR:CD1	2:J:111:GLN:HB2	2.51	0.46
1:E:50:PRO:HG3	1:E:97:TYR:CZ	2.50	0.46
1:E:26:THR:HG22	1:E:26:THR:O	2.16	0.46
1:G:219:LEU:HD11	2:K:61:TYR:HB2	1.98	0.46
2:I:14:THR:O	2:I:15:LEU:HB2	2.15	0.46
2:K:68:THR:HG21	2:L:6:ILE:HD11	1.97	0.46
1:A:148:PHE:CD2	1:A:320:LEU:HB3	2.51	0.46
1:E:83:ARG:NH1	5:E:2024:HOH:O	2.37	0.46
1:E:316:LYS:HE2	1:E:366:GLN:HG2	1.98	0.46
1:C:184:ASN:ND2	1:C:187:ARG:HH11	2.14	0.46
1:C:431:ARG:HE	1:C:432:ASN:ND2	2.14	0.46
2:L:33:LEU:HB2	2:L:113:ILE:HG13	1.98	0.46
1:G:347:ASP:OD2	1:G:360:ARG:NH1	2.48	0.45
1:A:229:GLN:HG2	5:A:2051:HOH:O	2.15	0.45
1:C:18:LYS:HB3	1:C:22:LEU:HD12	1.98	0.45
1:C:295:ARG:HG3	1:C:298:HIS:CD2	2.51	0.45
1:E:414:ALA:O	1:E:418:VAL:HG23	2.15	0.45
1:G:169:LEU:HD13	1:G:199:PHE:CE2	2.51	0.45
1:G:251:MET:HE1	1:G:283:TYR:CD1	2.51	0.45
1:A:113:VAL:HG11	1:A:274:PHE:CD1	2.52	0.45
2:J:61:TYR:CD1	2:J:61:TYR:C	2.95	0.45
1:A:267:HIS:HD2	1:A:277:ASN:ND2	2.03	0.45
1:E:175:LYS:H	1:E:407:LEU:HD22	1.81	0.45
1:E:403:GLY:O	1:E:404:GLY:C	2.58	0.45
1:G:151:PRO:HA	1:G:152:PRO:HD3	1.91	0.45
2:J:5:PRO:HG2	2:J:9:LEU:HD11	1.98	0.45
1:G:36:ILE:HD12	1:G:36:ILE:N	2.32	0.45
2:J:51:VAL:HG13	2:J:62:TYR:HB3	1.98	0.45
1:A:454:GLU:CD	1:A:454:GLU:H	2.24	0.45
2:L:24:ASP:HB2	5:L:2010:HOH:O	2.16	0.45
1:A:169:LEU:HD13	1:A:199:PHE:CE2	2.52	0.45
1:C:229:GLN:HE21	1:C:236:LYS:H	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:SER:HB2	1:C:401:GLN:HB2	1.97	0.45
1:G:24:TYR:CD2	1:G:59:ALA:HB2	2.52	0.45
1:G:252:LYS:HE3	1:G:252:LYS:HB3	1.79	0.45
2:L:79:ASP:HB3	2:L:82:GLN:HG3	1.99	0.45
1:A:289:LEU:HD23	2:I:59:PRO:HB3	1.98	0.45
1:C:251:MET:HE1	1:C:283:TYR:CD1	2.52	0.45
1:G:150:GLY:O	1:G:151:PRO:C	2.60	0.45
1:A:345:PHE:HA	1:A:348:LEU:HD12	1.98	0.44
1:C:267:HIS:HD2	1:C:277:ASN:ND2	2.14	0.44
2:L:51:VAL:HG13	2:L:62:TYR:HB3	1.98	0.44
1:E:149:GLN:O	1:E:149:GLN:HG2	2.17	0.44
1:A:435:ARG:HD2	1:A:440:GLU:OE1	2.17	0.44
1:C:169:LEU:HD13	1:C:199:PHE:CE2	2.53	0.44
1:E:36:ILE:HD12	1:E:36:ILE:N	2.33	0.44
1:E:448:ALA:HA	1:E:451:TRP:NE1	2.32	0.44
2:L:21:LEU:HA	2:L:25:GLN:HE21	1.82	0.44
1:C:192:CYS:O	1:C:197:LEU:HD12	2.17	0.44
1:G:192:CYS:HB3	1:G:197:LEU:HD12	1.98	0.44
1:A:184:ASN:ND2	1:A:187:ARG:HH11	2.16	0.44
1:A:455:LEU:HG	1:A:459:CYS:SG	2.58	0.44
1:A:202:ASP:OD1	1:A:238:HIS:HE1	2.01	0.44
5:C:2053:HOH:O	2:J:111:GLN:HG3	2.17	0.44
1:E:267:HIS:HD2	1:E:277:ASN:ND2	2.13	0.44
2:L:5:PRO:HB2	2:L:9:LEU:CD1	2.48	0.44
1:E:368:TRP:O	1:E:369:VAL:C	2.61	0.44
1:A:431:ARG:HH21	1:A:432:ASN:HD21	1.66	0.44
1:C:194:ARG:NH1	2:J:6:ILE:HD12	2.33	0.44
1:E:138:LEU:O	1:E:316:LYS:NZ	2.48	0.43
1:G:214:TRP:CE3	1:G:253:ARG:HG2	2.53	0.43
2:I:22:THR:N	2:I:25:GLN:HB2	2.33	0.43
2:L:21:LEU:HD22	2:L:25:GLN:HB3	1.99	0.43
1:A:336:GLU:HG3	5:A:2074:HOH:O	2.18	0.43
1:A:448:ALA:HA	1:A:451:TRP:NE1	2.33	0.43
1:C:151:PRO:HG2	1:C:372:PRO:O	2.19	0.43
1:C:403:GLY:O	1:C:404:GLY:C	2.58	0.43
1:E:169:LEU:HD13	1:E:199:PHE:CE2	2.53	0.43
1:E:355:GLU:O	1:E:356:LYS:C	2.59	0.43
1:E:383:HIS:CE1	1:E:385:TRP:HB2	2.52	0.43
2:L:72:LEU:HB3	2:L:73:PRO:HD2	2.00	0.43
1:A:173:THR:HB	1:A:175:LYS:HE2	2.00	0.43
1:C:75:THR:HG22	1:C:76:ASN:N	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:LEU:HG	1:C:413:ASN:OD1	2.17	0.43
1:G:26:THR:CG2	1:G:29:TYR:HB2	2.46	0.43
1:G:387:MET:HB3	1:G:388:PRO:HD3	2.01	0.43
2:J:89:GLU:HG2	2:J:92:LYS:CE	2.47	0.43
1:A:113:VAL:HG21	1:A:321:SER:HB2	1.99	0.43
1:E:347:ASP:OD2	1:E:360:ARG:NH1	2.47	0.43
2:K:105:ASP:OD1	2:K:107:ASN:N	2.52	0.43
1:C:451:TRP:CH2	2:J:19:PRO:HD3	2.54	0.43
1:G:345:PHE:HA	1:G:348:LEU:HD12	2.01	0.43
1:A:150:GLY:O	1:A:151:PRO:C	2.61	0.43
1:A:420:ASN:HD22	1:A:420:ASN:HA	1.66	0.43
1:G:299:ALA:HA	1:G:302:ASP:OD1	2.18	0.43
2:I:89:GLU:O	2:I:92:LYS:HG3	2.17	0.43
2:K:79:ASP:HA	2:K:80:PRO:HD2	1.92	0.43
2:L:42:LEU:HD21	2:L:87:LEU:HA	2.00	0.43
1:A:26:THR:O	1:A:85:TYR:HA	2.19	0.43
1:C:327:HIS:CG	5:C:2082:HOH:O	2.71	0.43
1:E:234:GLU:HB3	2:K:13:GLU:OE2	2.18	0.43
1:G:240:LEU:HD12	1:G:262:VAL:HG21	2.01	0.43
2:K:58:SER:HB2	2:K:59:PRO:HD2	2.01	0.43
1:A:368:TRP:O	1:A:369:VAL:C	2.61	0.42
1:G:297:MET:O	1:G:297:MET:HG2	2.19	0.42
2:I:120:PRO:HG2	2:I:123:TYR:CD2	2.54	0.42
2:J:14:THR:O	2:J:15:LEU:HB2	2.18	0.42
1:A:315:ALA:HB1	1:A:349:LEU:HD21	2.01	0.42
1:C:234:GLU:OE2	2:J:13:GLU:HA	2.19	0.42
1:E:192:CYS:HB3	1:E:197:LEU:HD12	2.01	0.42
1:G:209:GLN:HB3	1:G:210:PRO:CD	2.48	0.42
1:G:414:ALA:O	1:G:418:VAL:HG23	2.20	0.42
1:G:444:ILE:HG23	5:G:2113:HOH:O	2.18	0.42
2:K:14:THR:O	2:K:15:LEU:CB	2.66	0.42
2:L:22:THR:OG1	2:L:25:GLN:HG3	2.19	0.42
1:A:294:HIS:ND1	1:A:296:ALA:HB2	2.35	0.42
1:A:376:PRO:HB3	5:A:2069:HOH:O	2.18	0.42
1:C:252:LYS:HE3	1:C:252:LYS:HB3	1.83	0.42
1:E:200:THR:OG1	1:E:238:HIS:HD2	2.02	0.42
1:C:202:ASP:OD1	1:C:238:HIS:HE1	2.02	0.42
1:C:377:VAL:HG22	1:C:399:VAL:HB	2.01	0.42
2:I:72:LEU:HD23	2:I:72:LEU:HA	1.87	0.42
1:A:377:VAL:HG22	1:A:399:VAL:HB	2.02	0.42
1:C:50:PRO:HB3	1:C:97:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:383:HIS:CE1	1:G:385:TRP:HB2	2.54	0.42
2:K:99:ILE:HB	2:K:118:TYR:HB3	2.02	0.42
1:A:229:GLN:HE21	1:A:235:ILE:HA	1.84	0.42
1:A:267:HIS:HB2	1:A:280:LEU:HD23	2.01	0.42
1:E:251:MET:HE3	1:E:251:MET:HB3	1.81	0.42
1:G:121:VAL:HG22	1:G:125:PHE:CE1	2.55	0.42
1:G:241:ASN:ND2	1:G:243:THR:OG1	2.45	0.42
1:G:284:CYS:O	1:G:288:GLY:N	2.52	0.42
2:I:14:THR:O	2:I:15:LEU:CB	2.67	0.42
2:I:71:LYS:NZ	2:I:89:GLU:OE2	2.47	0.42
2:K:120:PRO:HG2	2:K:123:TYR:CD2	2.54	0.42
1:A:219:LEU:HD23	1:G:161:LYS:HE2	2.02	0.42
1:E:88:GLU:HA	1:E:89:PRO:HD3	1.85	0.42
1:G:251:MET:O	1:G:255:VAL:HG23	2.19	0.42
2:K:105:ASP:OD1	2:K:105:ASP:C	2.63	0.42
1:G:425:GLU:OE1	2:L:17:TYR:HB2	2.19	0.42
2:L:76:GLY:O	2:L:77:CYS:C	2.63	0.42
1:A:131:ARG:HH21	1:A:131:ARG:HB3	1.84	0.42
1:C:88:GLU:HA	1:C:89:PRO:HD3	1.84	0.42
1:C:200:THR:OG1	1:C:238:HIS:HD2	2.03	0.42
1:C:235:ILE:HD11	2:J:51:VAL:HG21	2.01	0.42
1:E:341:ILE:HD11	1:E:475:VAL:HG23	2.02	0.42
1:G:418:VAL:O	1:G:422:VAL:HG23	2.19	0.42
1:A:200:THR:OG1	1:A:238:HIS:HD2	2.03	0.41
1:A:284:CYS:O	1:A:288:GLY:N	2.53	0.41
1:C:302:ASP:C	1:C:302:ASP:OD1	2.63	0.41
1:E:34:THR:O	1:E:141:PRO:HG3	2.19	0.41
1:E:151:PRO:HA	1:E:152:PRO:HD3	1.88	0.41
2:I:42:LEU:HD21	2:I:87:LEU:HA	2.02	0.41
2:I:89:GLU:HG2	2:I:92:LYS:NZ	2.35	0.41
2:J:72:LEU:HB3	2:J:73:PRO:HD2	2.01	0.41
2:K:79:ASP:HB3	2:K:82:GLN:HG3	2.02	0.41
1:C:259:GLU:HB2	5:C:2071:HOH:O	2.20	0.41
1:G:334:LYS:HG3	1:G:335:LEU:HG	2.01	0.41
2:L:5:PRO:HB2	2:L:9:LEU:HD11	2.03	0.41
1:C:342:THR:O	1:C:343:LEU:C	2.63	0.41
1:E:242:ALA:O	1:E:243:THR:C	2.62	0.41
1:G:26:THR:HG22	1:G:26:THR:O	2.20	0.41
1:G:34:THR:O	1:G:141:PRO:HG3	2.20	0.41
2:J:120:PRO:HG2	2:J:123:TYR:CD2	2.56	0.41
1:C:173:THR:HG23	1:C:201:KCX:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:TYR:HB3	2:L:55:HIS:CE1	2.56	0.41
1:A:383:HIS:HE1	1:A:385:TRP:HB2	1.85	0.41
1:A:383:HIS:N	1:A:386:HIS:HD2	2.13	0.41
1:C:150:GLY:O	1:C:151:PRO:C	2.64	0.41
1:G:386:HIS:HA	5:G:2107:HOH:O	2.20	0.41
2:L:119:LYS:HE2	5:L:2045:HOH:O	2.19	0.41
1:C:355:GLU:HA	1:C:365:THR:HG23	2.03	0.41
1:E:22:LEU:HD11	5:E:2005:HOH:O	2.19	0.41
2:L:61:TYR:CD1	2:L:61:TYR:C	2.98	0.41
1:A:167:ARG:HG3	1:A:168:PRO:O	2.21	0.41
1:E:121:VAL:HG22	1:E:125:PHE:CE1	2.55	0.41
1:E:201:KCX:HB3	1:E:201:KCX:HE3	1.87	0.41
2:L:21:LEU:HA	2:L:25:GLN:NE2	2.35	0.41
2:L:79:ASP:HA	2:L:80:PRO:HD2	1.92	0.41
1:A:455:LEU:HG	1:A:459:CYS:HG	1.85	0.41
1:C:24:TYR:CD2	1:C:59:ALA:HB2	2.56	0.41
2:I:10:LYS:HB3	2:I:50:PHE:CZ	2.56	0.41
2:I:72:LEU:HB3	2:I:73:PRO:CD	2.50	0.41
2:K:5:PRO:HG2	2:K:9:LEU:HD11	2.01	0.41
2:L:41:CYS:HB3	2:L:102:ILE:CG1	2.51	0.41
2:L:89:GLU:HG2	2:L:92:LYS:CE	2.46	0.41
1:A:194:ARG:HD2	1:A:194:ARG:HH11	1.56	0.41
1:A:425:GLU:CD	2:I:15:LEU:H	2.29	0.41
1:E:250:MET:HE1	1:E:276:ALA:O	2.21	0.41
2:J:39:VAL:HG11	2:J:75:PHE:CD1	2.56	0.41
1:A:449:THR:HG22	1:A:455:LEU:HG	2.03	0.40
1:C:344:GLY:O	1:C:347:ASP:HB2	2.21	0.40
2:K:89:GLU:HG2	2:K:92:LYS:CE	2.50	0.40
1:A:252:LYS:HB3	1:A:252:LYS:HE3	1.73	0.40
1:C:175:LYS:HE3	4:C:477:CAP:O1P	2.21	0.40
1:C:386:HIS:O	1:C:387:MET:C	2.64	0.40
1:E:336:GLU:CD	1:E:472:MET:H	2.29	0.40
1:G:110:GLU:HB3	1:G:147:THR:HB	2.03	0.40
2:I:79:ASP:HB3	2:I:82:GLN:HG3	2.03	0.40
1:A:26:THR:HG22	1:A:26:THR:O	2.20	0.40
1:C:36:ILE:HD12	1:C:36:ILE:N	2.36	0.40
2:I:79:ASP:HA	2:I:80:PRO:HD2	1.87	0.40
1:E:239:TYR:CE2	1:E:401:GLN:NE2	2.87	0.40
1:E:296:ALA:O	1:E:297:MET:HB3	2.22	0.40
1:E:359:SER:HA	5:E:2101:HOH:O	2.20	0.40
1:G:368:TRP:O	1:G:369:VAL:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:409:HIS:CG	1:G:410:PRO:HD2	2.57	0.40
1:C:26:THR:HG22	1:C:26:THR:O	2.22	0.40
1:C:334:LYS:HG3	1:C:335:LEU:HG	2.02	0.40
1:E:19:ASP:HB2	1:E:22:LEU:HG	2.04	0.40
1:E:125:PHE:CD1	1:E:133:LEU:HD23	2.56	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:2077:HOH:O	5:G:2077:HOH:O[3_555]	1.65	0.55
5:G:2081:HOH:O	5:G:2081:HOH:O[3_555]	1.89	0.31
2:L:24:ASP:OD1	2:L:28:ARG:NH2[4_555]	2.05	0.15
5:G:2086:HOH:O	5:G:2086:HOH:O[3_555]	2.12	0.08

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	464/475 (98%)	439 (95%)	22 (5%)	3 (1%)	21	27
1	C	464/475 (98%)	445 (96%)	18 (4%)	1 (0%)	43	55
1	E	464/475 (98%)	437 (94%)	24 (5%)	3 (1%)	21	27
1	G	464/475 (98%)	439 (95%)	24 (5%)	1 (0%)	43	55
2	I	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
2	J	121/123 (98%)	112 (93%)	8 (7%)	1 (1%)	16	20
2	K	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
2	L	121/123 (98%)	112 (93%)	8 (7%)	1 (1%)	16	20
All	All	2340/2392 (98%)	2209 (94%)	121 (5%)	10 (0%)	30	38

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	PRO
1	E	176	PRO
1	G	176	PRO
1	C	344	GLY
2	J	15	LEU
2	L	15	LEU
1	E	369	VAL
1	A	344	GLY
1	A	331	VAL
1	E	331	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	378/386 (98%)	363 (96%)	15 (4%)	28	42
1	C	378/386 (98%)	362 (96%)	16 (4%)	26	40
1	E	378/386 (98%)	361 (96%)	17 (4%)	24	37
1	G	378/386 (98%)	363 (96%)	15 (4%)	28	42
2	I	112/112 (100%)	102 (91%)	10 (9%)	9	12
2	J	112/112 (100%)	103 (92%)	9 (8%)	11	15
2	K	112/112 (100%)	102 (91%)	10 (9%)	9	12
2	L	112/112 (100%)	104 (93%)	8 (7%)	13	19
All	All	1960/1992 (98%)	1860 (95%)	100 (5%)	21	32

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

Mol	Chain	Res	Type
1	A	10	SER
1	A	11	VAL
1	A	17	VAL
1	A	36	ILE

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Mol	Chain	Res	Type
1	A	75	THR
1	A	121	VAL
1	A	131	ARG
1	A	152	PRO
1	A	172	CYS
1	A	183	LYS
1	A	239	TYR
1	A	241	ASN
1	A	252	LYS
1	A	346	VAL
1	A	356	LYS
1	C	10	SER
1	C	11	VAL
1	C	17	VAL
1	C	36	ILE
1	C	46	PRO
1	C	75	THR
1	C	121	VAL
1	C	131	ARG
1	C	172	CYS
1	C	173	THR
1	C	219	LEU
1	C	239	TYR
1	C	252	LYS
1	C	318	LEU
1	C	346	VAL
1	C	356	LYS
1	E	10	SER
1	E	11	VAL
1	E	17	VAL
1	E	26	THR
1	E	75	THR
1	E	121	VAL
1	E	131	ARG
1	E	173	THR
1	E	183	LYS
1	E	219	LEU
1	E	239	TYR
1	E	252	LYS
1	E	318	LEU
1	E	346	VAL
1	E	356	LYS

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Mol	Chain	Res	Type
1	E	387	MET
1	E	388	PRO
1	G	10	SER
1	G	11	VAL
1	G	17	VAL
1	G	36	ILE
1	G	75	THR
1	G	79	ARG
1	G	121	VAL
1	G	131	ARG
1	G	172	CYS
1	G	183	LYS
1	G	210	PRO
1	G	252	LYS
1	G	346	VAL
1	G	356	LYS
1	G	460	GLU
2	I	6	ILE
2	I	9	LEU
2	I	33	LEU
2	I	51	VAL
2	I	56	HIS
2	I	57	ASN
2	I	68	THR
2	I	78	THR
2	I	92	LYS
2	I	110	VAL
2	J	6	ILE
2	J	33	LEU
2	J	51	VAL
2	J	56	HIS
2	J	57	ASN
2	J	68	THR
2	J	78	THR
2	J	92	LYS
2	J	110	VAL
2	K	6	ILE
2	K	33	LEU
2	K	51	VAL
2	K	56	HIS
2	K	57	ASN
2	K	68	THR

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Mol	Chain	Res	Type
2	K	78	THR
2	K	85	ASN
2	K	92	LYS
2	K	110	VAL
2	L	6	ILE
2	L	33	LEU
2	L	56	HIS
2	L	57	ASN
2	L	68	THR
2	L	78	THR
2	L	92	LYS
2	L	110	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	184	ASN
1	A	207	ASN
1	A	229	GLN
1	A	238	HIS
1	A	241	ASN
1	A	267	HIS
1	A	277	ASN
1	A	386	HIS
1	A	420	ASN
1	A	432	ASN
1	C	184	ASN
1	C	229	GLN
1	C	238	HIS
1	C	241	ASN
1	C	267	HIS
1	C	277	ASN
1	C	386	HIS
1	C	401	GLN
1	C	432	ASN
1	E	86	HIS
1	E	149	GLN
1	E	184	ASN
1	E	229	GLN
1	E	238	HIS
1	E	241	ASN

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Mol	Chain	Res	Type
1	E	267	HIS
1	E	277	ASN
1	E	386	HIS
1	E	401	GLN
1	E	420	ASN
1	E	432	ASN
1	G	156	GLN
1	G	184	ASN
1	G	229	GLN
1	G	238	HIS
1	G	241	ASN
1	G	267	HIS
1	G	277	ASN
1	G	386	HIS
1	G	401	GLN
1	G	420	ASN
1	G	432	ASN
2	I	25	GLN
2	I	29	GLN
2	I	55	HIS
2	I	57	ASN
2	I	82	GLN
2	J	25	GLN
2	J	29	GLN
2	J	55	HIS
2	J	57	ASN
2	J	82	GLN
2	K	25	GLN
2	K	29	GLN
2	K	55	HIS
2	L	2	GLN
2	L	25	GLN
2	L	29	GLN
2	L	82	GLN
2	L	85	ASN
2	L	107	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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
1	KCX	A	201	1,3	10,11,12	1.39	1 (10%)	6,12,14	3.48	2 (33%)
1	KCX	C	201	1,3	10,11,12	1.27	1 (10%)	6,12,14	1.73	1 (16%)
1	KCX	E	201	1,3	10,11,12	1.47	1 (10%)	6,12,14	3.72	2 (33%)
1	KCX	G	201	1,3	10,11,12	1.39	1 (10%)	6,12,14	5.45	3 (50%)

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
1	KCX	A	201	1,3	-	0/9/10/12	-
1	KCX	C	201	1,3	-	1/9/10/12	-
1	KCX	E	201	1,3	-	2/9/10/12	-
1	KCX	G	201	1,3	-	1/9/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	201	KCX	OQ1-CX	3.66	1.28	1.21
1	A	201	KCX	OQ1-CX	2.72	1.26	1.21
1	G	201	KCX	OQ1-CX	2.69	1.26	1.21
1	C	201	KCX	OQ1-CX	2.27	1.25	1.21

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	201	KCX	CE-NZ-CX	11.88	142.15	121.98
1	E	201	KCX	OQ1-CX-NZ	7.32	136.05	124.92
1	A	201	KCX	CE-NZ-CX	6.27	132.61	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	KCX	OQ1-CX-NZ	5.58	133.40	124.92
1	G	201	KCX	OQ1-CX-NZ	5.37	133.08	124.92
1	E	201	KCX	CE-NZ-CX	4.65	129.87	121.98
1	C	201	KCX	CE-NZ-CX	3.57	128.04	121.98
1	G	201	KCX	CD-CG-CB	-2.04	105.92	113.62

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	201	KCX	O-C-CA-CB
1	E	201	KCX	CD-CE-NZ-CX
1	E	201	KCX	OQ1-CX-NZ-CE
1	G	201	KCX	OQ1-CX-NZ-CE

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	201	KCX	1	0
1	E	201	KCX	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
4	CAP	G	477	3	18,20,20	1.86	3 (16%)	23,31,31	2.37	9 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CAP	E	477	3	18,20,20	1.80	3 (16%)	23,31,31	2.76	11 (47%)
4	CAP	A	477	3	18,20,20	1.78	4 (22%)	23,31,31	2.96	9 (39%)
4	CAP	C	477	3	18,20,20	1.94	6 (33%)	23,31,31	2.71	11 (47%)

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
4	CAP	G	477	3	-	6/29/29/29	-
4	CAP	E	477	3	-	8/29/29/29	-
4	CAP	A	477	3	-	12/29/29/29	-
4	CAP	C	477	3	-	9/29/29/29	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	477	CAP	O4-C4	-5.43	1.32	1.43
4	C	477	CAP	O3-C3	-4.43	1.34	1.42
4	E	477	CAP	O3-C3	-4.16	1.34	1.42
4	E	477	CAP	O4-C4	-3.78	1.35	1.43
4	A	477	CAP	O4-C4	-3.74	1.35	1.43
4	C	477	CAP	O4-C4	-3.64	1.35	1.43
4	A	477	CAP	O3-C3	-3.55	1.35	1.42
4	C	477	CAP	P2-O6P	-3.15	1.43	1.54
4	G	477	CAP	O3-C3	-2.87	1.37	1.42
4	C	477	CAP	P1-O1P	-2.80	1.41	1.50
4	E	477	CAP	O7-C	-2.42	1.21	1.30
4	A	477	CAP	P2-O6P	-2.40	1.45	1.54
4	A	477	CAP	P1-O1P	-2.35	1.43	1.50
4	G	477	CAP	O7-C	-2.15	1.22	1.30
4	C	477	CAP	O7-C	-2.13	1.22	1.30
4	C	477	CAP	O2-C2	-2.07	1.38	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	477	CAP	O7-C-C2	8.54	128.37	114.06
4	C	477	CAP	O7-C-C2	6.59	125.10	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	477	CAP	O4-C4-C3	-6.13	96.53	108.78
4	E	477	CAP	O7-C-C2	5.61	123.45	114.06
4	A	477	CAP	O7-C-O6	-5.58	105.99	123.86
4	A	477	CAP	O4-C4-C3	-5.46	97.87	108.78
4	C	477	CAP	O7-C-O6	-4.99	107.90	123.86
4	G	477	CAP	O7-C-C2	4.75	122.01	114.06
4	C	477	CAP	O4-C4-C3	-4.70	99.39	108.78
4	G	477	CAP	O4-C4-C3	-4.34	100.11	108.78
4	E	477	CAP	C5-C4-C3	4.33	120.64	111.96
4	E	477	CAP	O2-C2-C	4.30	117.15	109.07
4	G	477	CAP	O2-C2-C	4.21	116.97	109.07
4	E	477	CAP	O7-C-O6	-4.18	110.48	123.86
4	E	477	CAP	O3P-P1-O1	-3.75	96.89	106.67
4	G	477	CAP	O7-C-O6	-3.58	112.42	123.86
4	C	477	CAP	O3P-P1-O1P	3.42	124.15	110.83
4	G	477	CAP	O3P-P1-O1P	3.39	124.06	110.83
4	A	477	CAP	O3P-P1-O1P	3.35	123.88	110.83
4	G	477	CAP	O3-C3-C4	-3.34	101.98	109.13
4	A	477	CAP	O2-C2-C	3.13	114.94	109.07
4	G	477	CAP	O2P-P1-O1	-3.06	98.68	106.67
4	C	477	CAP	O3P-P1-O1	-3.01	98.81	106.67
4	A	477	CAP	C5-C4-C3	2.99	117.96	111.96
4	A	477	CAP	O2-C2-C1	-2.97	101.66	108.72
4	C	477	CAP	O2-C2-C	2.95	114.60	109.07
4	E	477	CAP	O2-C2-C1	-2.93	101.77	108.72
4	C	477	CAP	C5-C4-C3	2.88	117.73	111.96
4	A	477	CAP	O2P-P1-O1	-2.82	99.33	106.67
4	C	477	CAP	O3-C3-C4	-2.56	103.64	109.13
4	C	477	CAP	O5-P2-O4P	-2.55	99.55	106.44
4	C	477	CAP	O6-C-C2	2.51	126.99	122.32
4	G	477	CAP	C5-C4-C3	2.50	116.97	111.96
4	E	477	CAP	O3P-P1-O1P	2.47	120.46	110.83
4	C	477	CAP	O5P-P2-O5	-2.43	100.34	106.67
4	G	477	CAP	O2-C2-C1	-2.28	103.31	108.72
4	E	477	CAP	O5P-P2-O5	2.20	112.41	106.67
4	E	477	CAP	O2P-P1-O1	2.20	112.41	106.67
4	A	477	CAP	O3-C3-C4	-2.03	104.78	109.13
4	E	477	CAP	O6-C-C2	2.00	126.05	122.32

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	477	CAP	O6-C-C2-O2
4	A	477	CAP	C2-C3-C4-O4
4	A	477	CAP	O3-C3-C4-O4
4	A	477	CAP	O4-C4-C5-O5
4	C	477	CAP	O1-C1-C2-C
4	C	477	CAP	O1-C1-C2-O2
4	C	477	CAP	C2-C3-C4-O4
4	C	477	CAP	O3-C3-C4-O4
4	C	477	CAP	O4-C4-C5-O5
4	E	477	CAP	C2-C3-C4-O4
4	E	477	CAP	O3-C3-C4-O4
4	E	477	CAP	O4-C4-C5-O5
4	G	477	CAP	C2-C3-C4-O4
4	G	477	CAP	O3-C3-C4-O4
4	G	477	CAP	O4-C4-C5-O5
4	A	477	CAP	C3-C4-C5-O5
4	C	477	CAP	C3-C4-C5-O5
4	E	477	CAP	C3-C4-C5-O5
4	G	477	CAP	C3-C4-C5-O5
4	A	477	CAP	O6-C-C2-C3
4	A	477	CAP	O7-C-C2-O2
4	A	477	CAP	O2-C2-C3-C4
4	C	477	CAP	O2-C2-C3-C4
4	E	477	CAP	O2-C2-C3-C4
4	G	477	CAP	O2-C2-C3-C4
4	C	477	CAP	O1-C1-C2-C3
4	A	477	CAP	O6-C-C2-C1
4	A	477	CAP	O7-C-C2-C3
4	A	477	CAP	O7-C-C2-C1
4	A	477	CAP	C1-O1-P1-O3P
4	C	477	CAP	C1-O1-P1-O3P
4	G	477	CAP	C1-O1-P1-O3P
4	E	477	CAP	O3-C3-C4-C5
4	E	477	CAP	C2-C3-C4-C5
4	E	477	CAP	O7-C-C2-O2

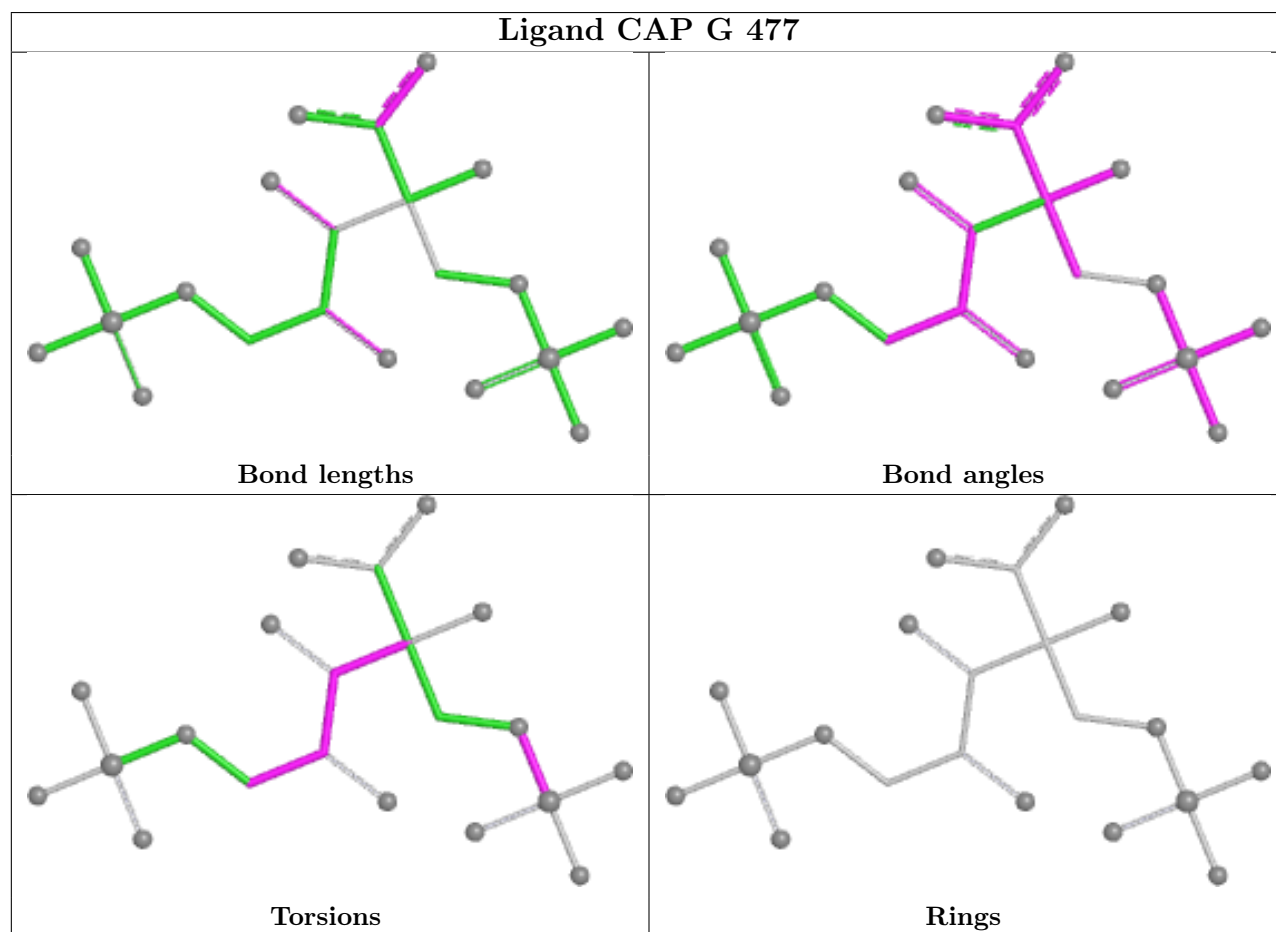
There are no ring outliers.

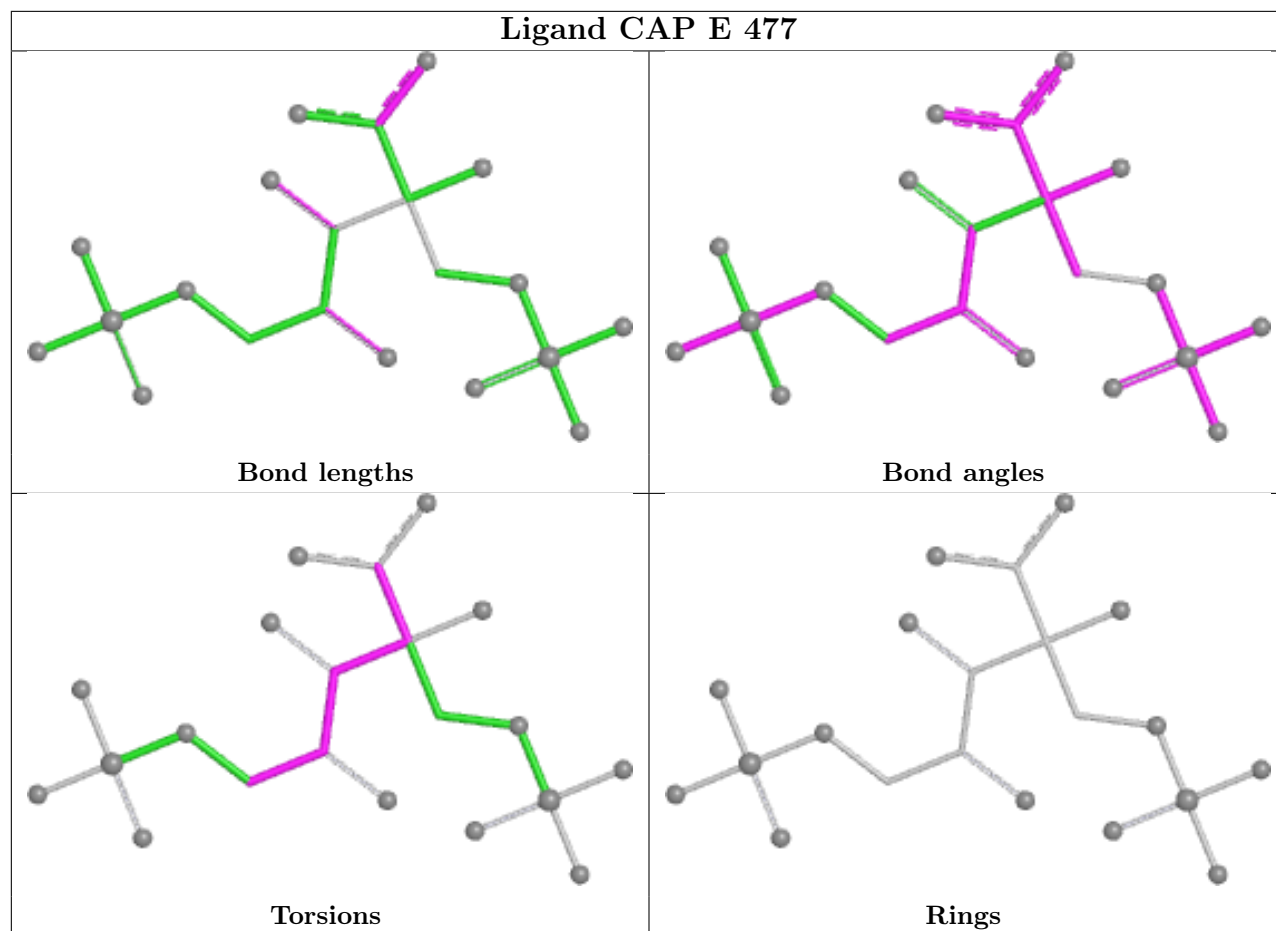
1 monomer is involved in 1 short contact:

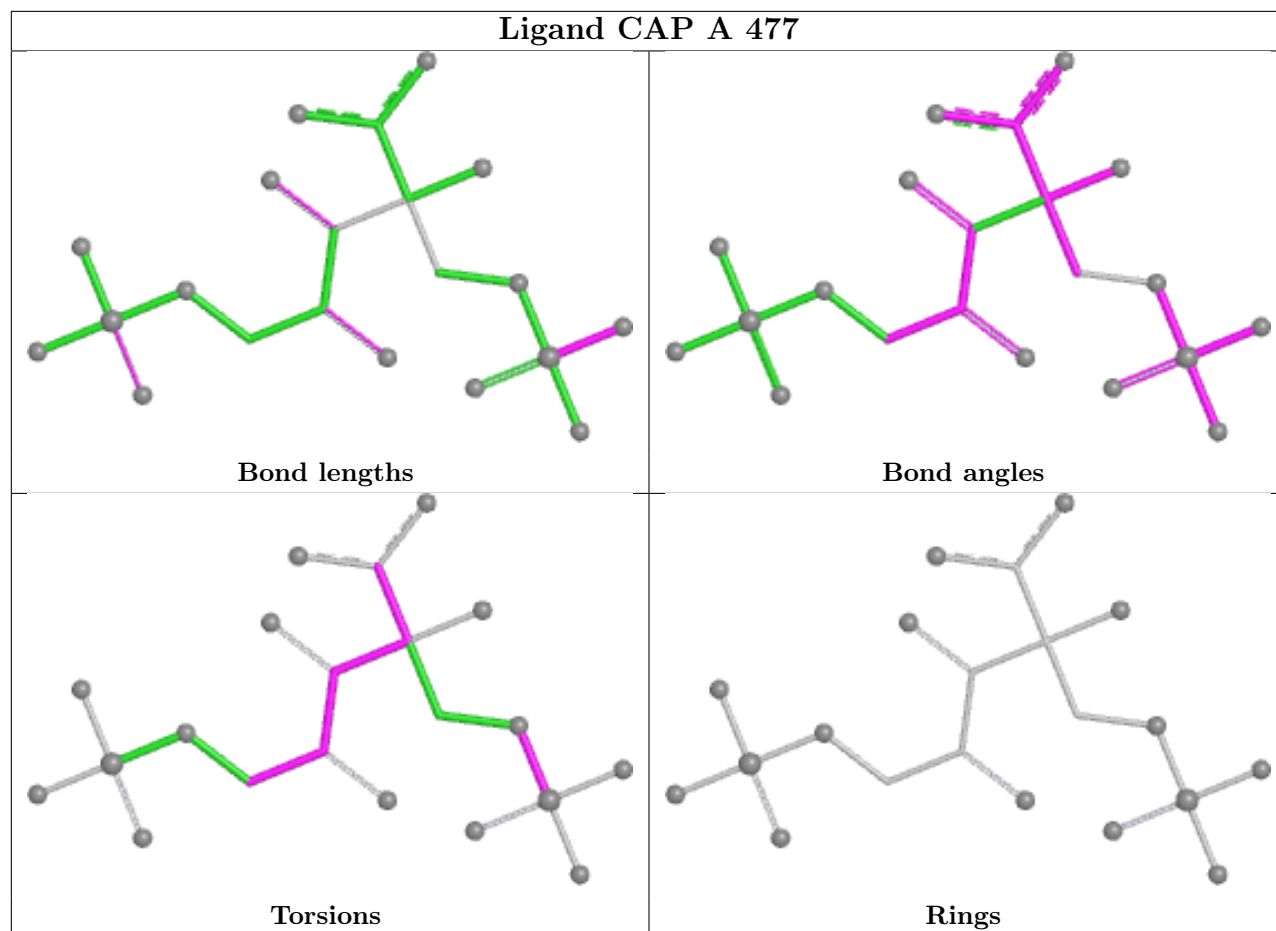
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	477	CAP	1	0

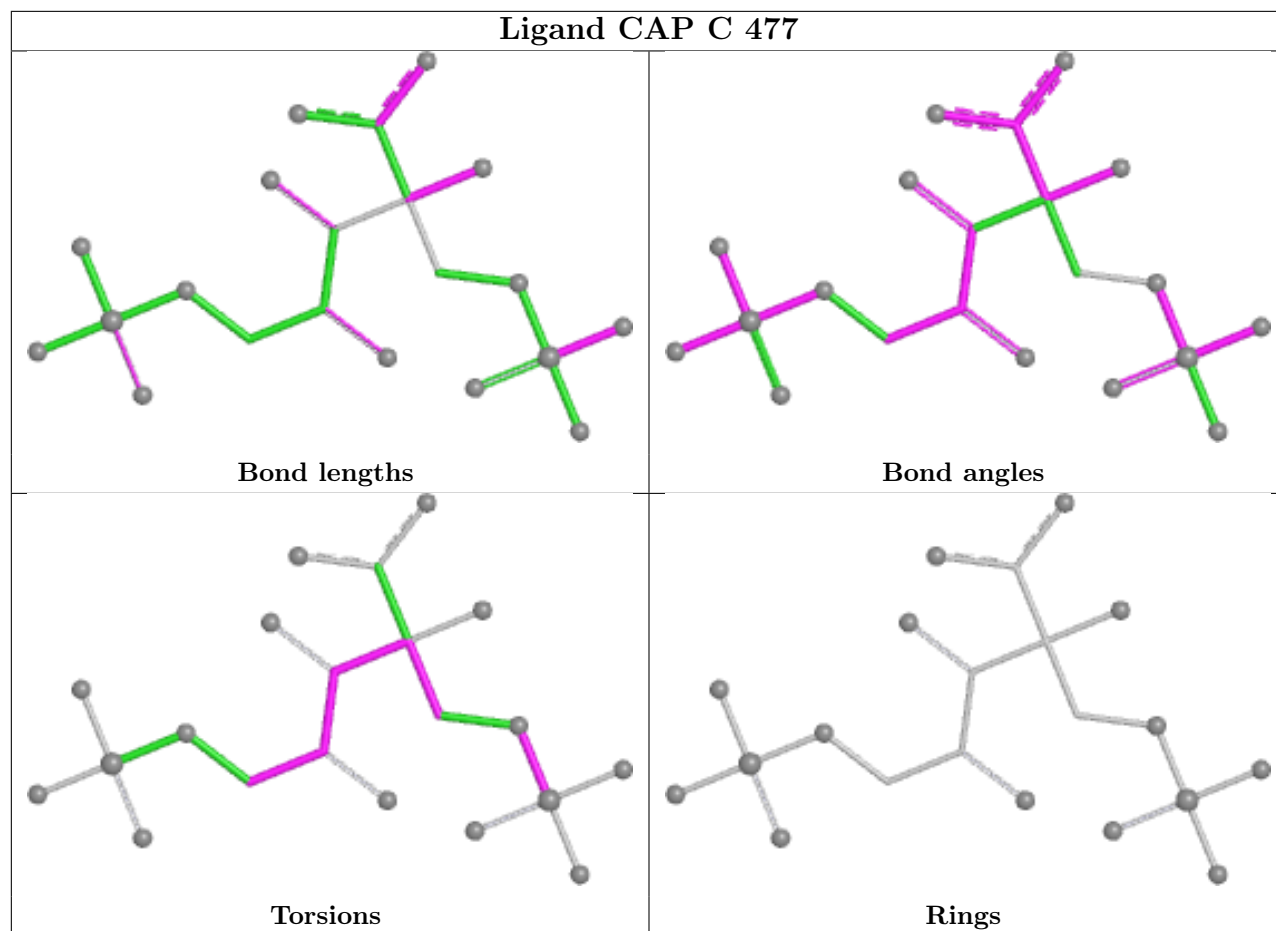
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	466/475 (98%)	-1.49	0 100 100	11, 20, 44, 85	0
1	C	466/475 (98%)	-1.47	0 100 100	11, 20, 44, 85	0
1	E	466/475 (98%)	-1.49	0 100 100	11, 20, 44, 85	0
1	G	466/475 (98%)	-1.50	0 100 100	11, 20, 45, 85	0
2	I	123/123 (100%)	-1.37	0 100 100	12, 32, 53, 67	0
2	J	123/123 (100%)	-1.37	0 100 100	12, 32, 53, 67	0
2	K	123/123 (100%)	-1.35	0 100 100	11, 32, 53, 67	0
2	L	123/123 (100%)	-1.35	0 100 100	12, 32, 53, 67	0
All	All	2356/2392 (98%)	-1.46	0 100 100	11, 21, 48, 85	0

There are no RSRZ outliers to report.

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KCX	C	201	12/13	0.99	0.03	12,15,18,18	0
1	KCX	G	201	12/13	0.99	0.03	12,14,18,18	0
1	KCX	E	201	12/13	1.00	0.02	13,14,18,19	0
1	KCX	A	201	12/13	1.00	0.02	13,14,18,18	0

6.3 Carbohydrates [i](#)

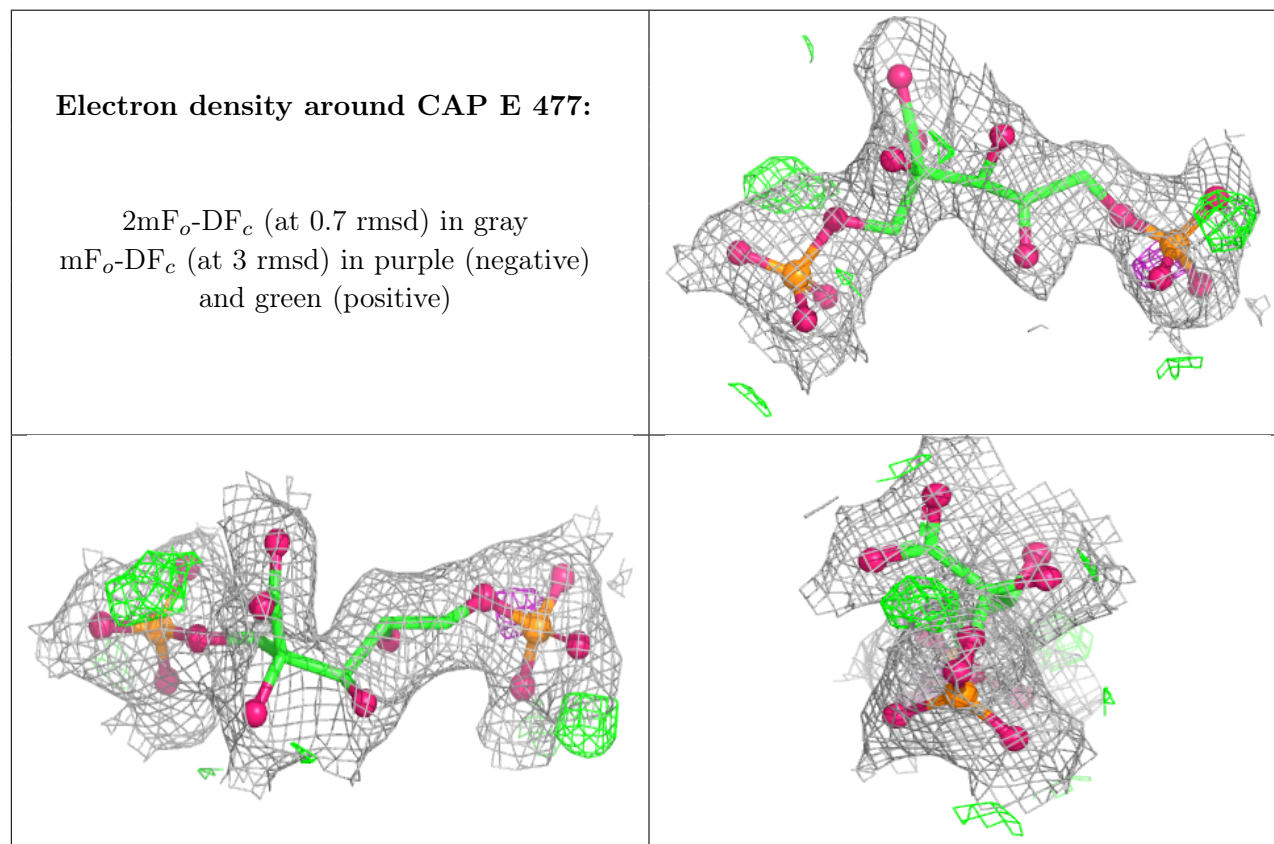
There are no oligosaccharides in this entry.

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.

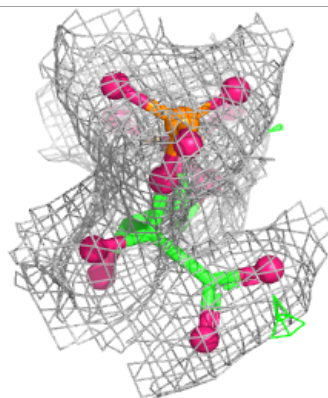
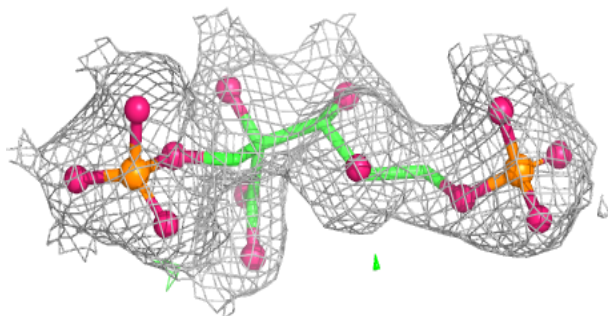
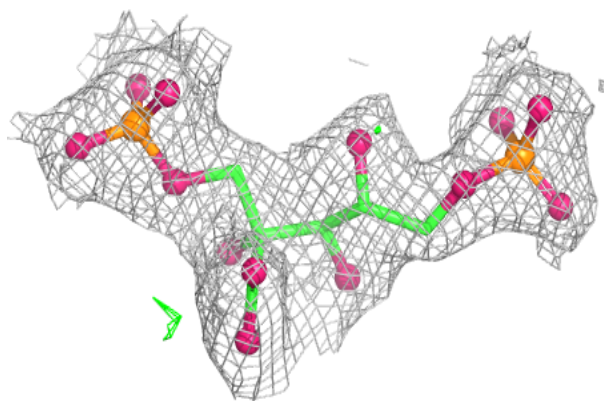
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	C	476	1/1	0.99	0.02	38,38,38,38	0
4	CAP	E	477	21/21	0.99	0.03	15,19,22,23	0
3	CA	E	476	1/1	1.00	0.04	36,36,36,36	0
3	CA	G	476	1/1	1.00	0.02	36,36,36,36	0
4	CAP	A	477	21/21	1.00	0.03	16,18,22,23	0
4	CAP	C	477	21/21	1.00	0.03	15,19,22,23	0
3	CA	A	476	1/1	1.00	0.02	38,38,38,38	0
4	CAP	G	477	21/21	1.00	0.02	15,19,23,24	0

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

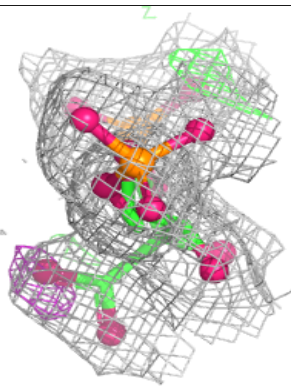
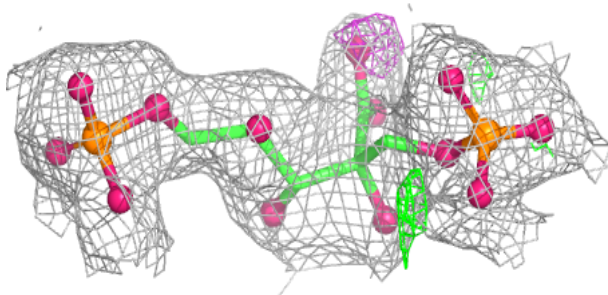
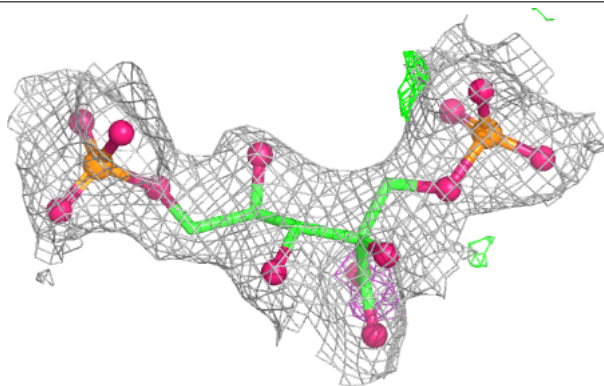


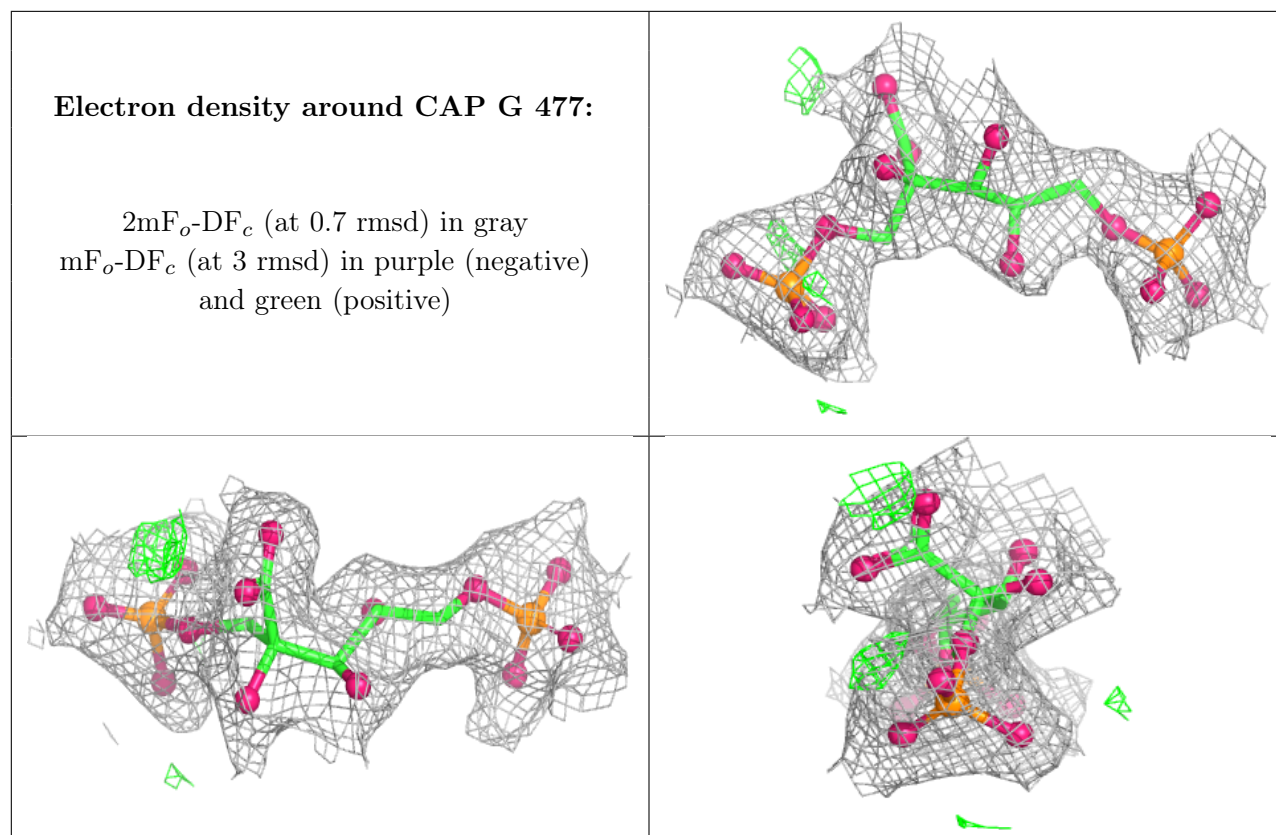
Electron density around CAP A 477:

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

**Electron density around CAP C 477:**

$2mF_o-DF_c$ (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.