



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 03:58 AM UTC

PDB ID : 6UQE / pdb_00006uqe
EMDB ID : EMD-20845
Title : ClpA/ClpP Disengaged State bound to RepA-GFP
Authors : Lopez, K.L.; Rizo, A.R.; Southworth, D.R.
Deposited on : 2019-10-18
Resolution : 3.00 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

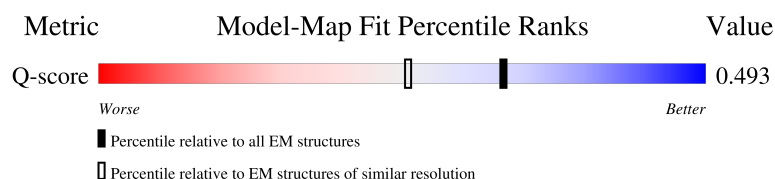
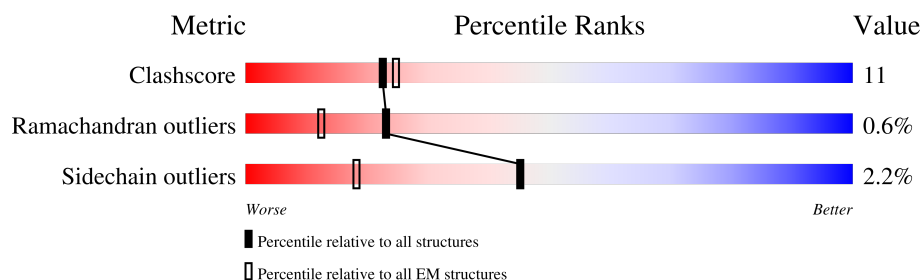
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	578	37% 81% 14% ...
1	B	578	14% 77% 18% ..
1	C	578	5% 86% 12% .
1	D	578	10% 84% 12% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	578	
1	F	578	
2	G	192	
2	H	192	
2	I	192	
2	J	192	
2	K	192	
2	L	192	
2	M	192	
2	N	192	
2	O	192	
2	P	192	
2	Q	192	
2	R	192	
2	S	192	
2	T	192	
3	X	10	
4	Y	11	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ADP	A	801	X	-	-	-
5	ADP	A	802	X	-	-	-
5	ADP	E	801	X	-	-	-
5	ADP	E	802	X	-	X	-
5	ADP	F	801	X	-	-	-
6	AGS	B	801	X	-	-	-
6	AGS	B	802	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	AGS	C	801	X	-	-	-
6	AGS	C	802	X	-	-	-
6	AGS	D	801	X	-	-	-
6	AGS	D	802	X	-	-	-
6	AGS	E	803	X	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 48402 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ATP-dependent Clp protease ATP-binding subunit ClpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	562	Total	C	N	O	S	0	0
			4377	2760	778	825	14		
1	B	578	Total	C	N	O	S	0	0
			4511	2841	805	851	14		
1	C	578	Total	C	N	O	S	0	0
			4511	2841	805	851	14		
1	D	578	Total	C	N	O	S	0	0
			4510	2841	805	850	14		
1	E	578	Total	C	N	O	S	0	0
			4511	2841	805	851	14		
1	F	578	Total	C	N	O	S	0	0
			4511	2841	805	851	14		

- Molecule 2 is a protein called ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	H	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	I	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	J	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	K	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	L	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	M	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	N	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		
2	O	192	Total	C	N	O	S	0	0
			1501	946	260	283	12		

Continued on next page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	192	Total 1501	C 946	N 260	O 283	S 12	0	0
2	Q	192	Total 1501	C 946	N 260	O 283	S 12	0	0
2	R	192	Total 1501	C 946	N 260	O 283	S 12	0	0
2	S	192	Total 1501	C 946	N 260	O 283	S 12	0	0
2	T	192	Total 1501	C 946	N 260	O 283	S 12	0	0

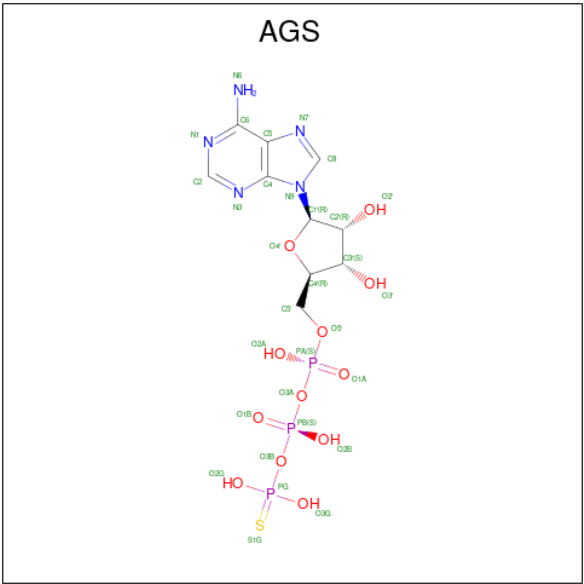
- | Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 3 | X | 10 | Total | C | N | O | 0 | 0 |
| | | | 50 | 30 | 10 | 10 | | |

- | Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 4 | Y | 11 | Total | C | N | O | 0 | 0 |
| | | | 55 | 33 | 11 | 11 | | |

- # ADP

Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 6 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



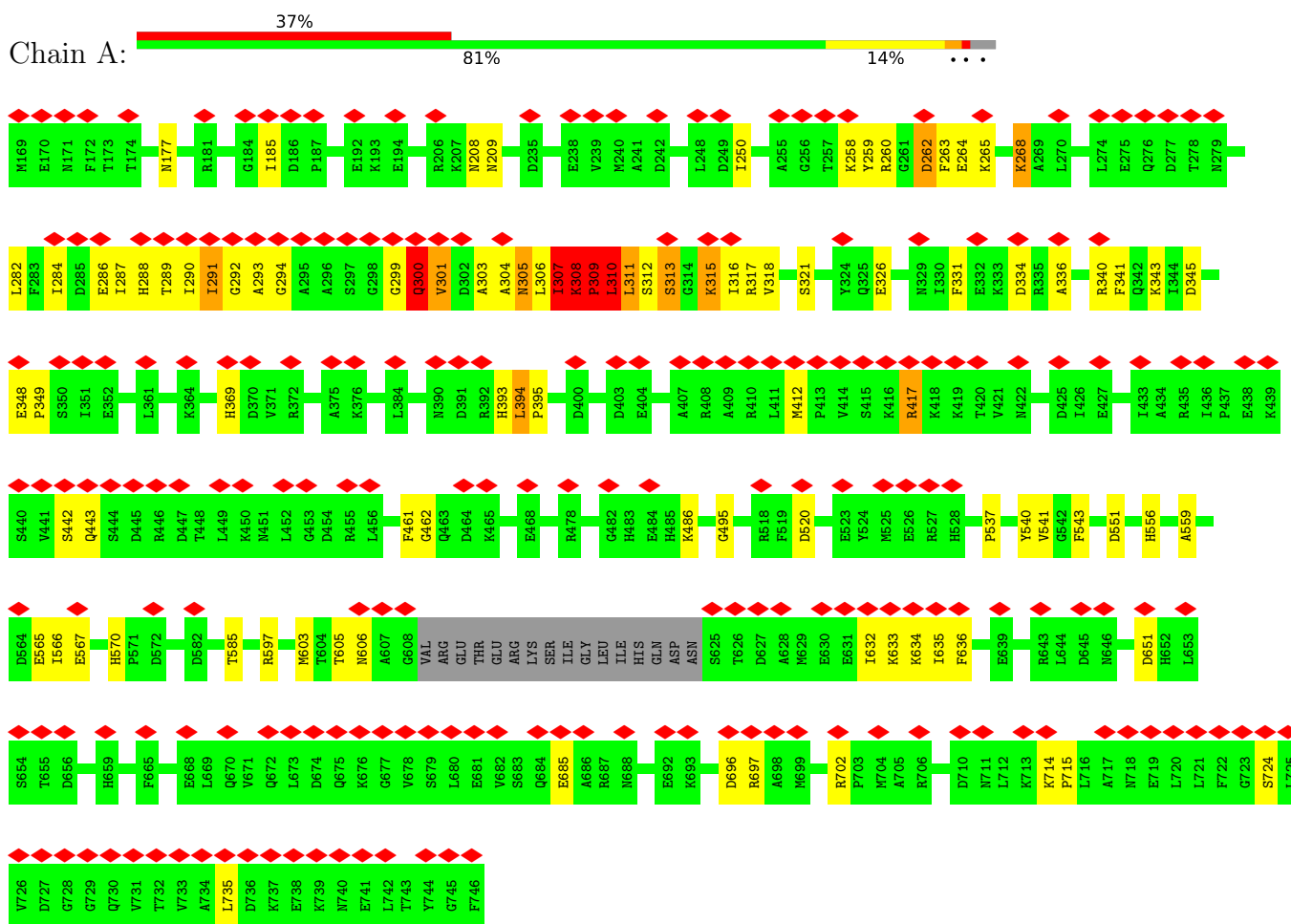
Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
6	E	1	31	10	5	12	3	1	0

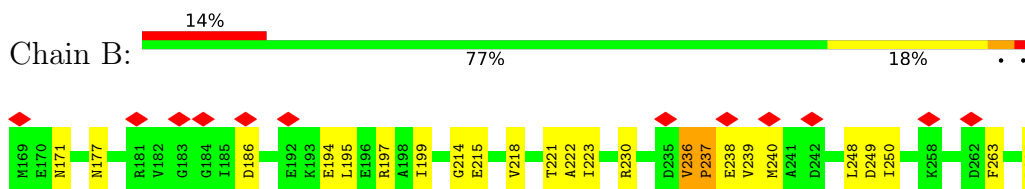
3 Residue-property plots

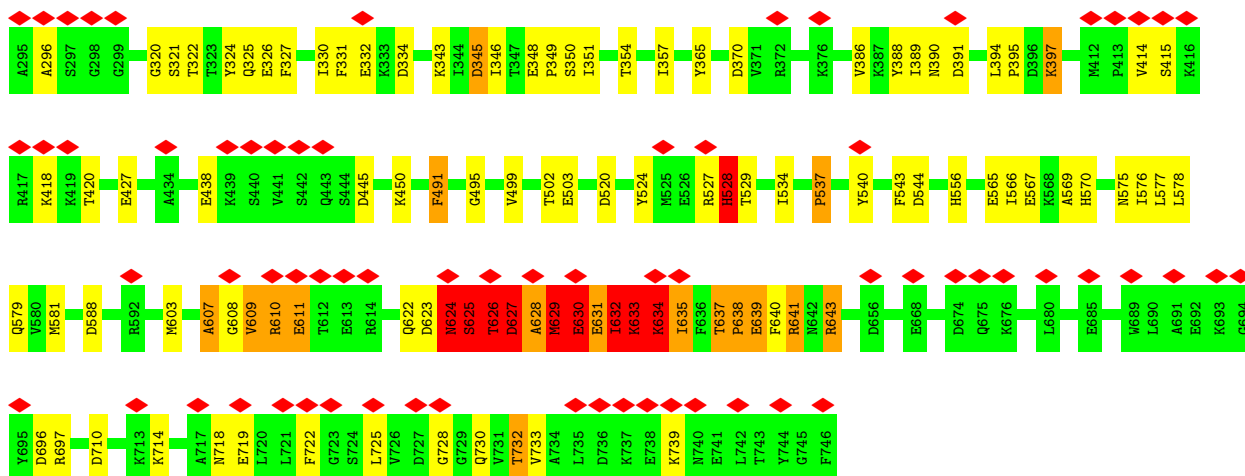
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: ATP-dependent Clp protease ATP-binding subunit ClpA

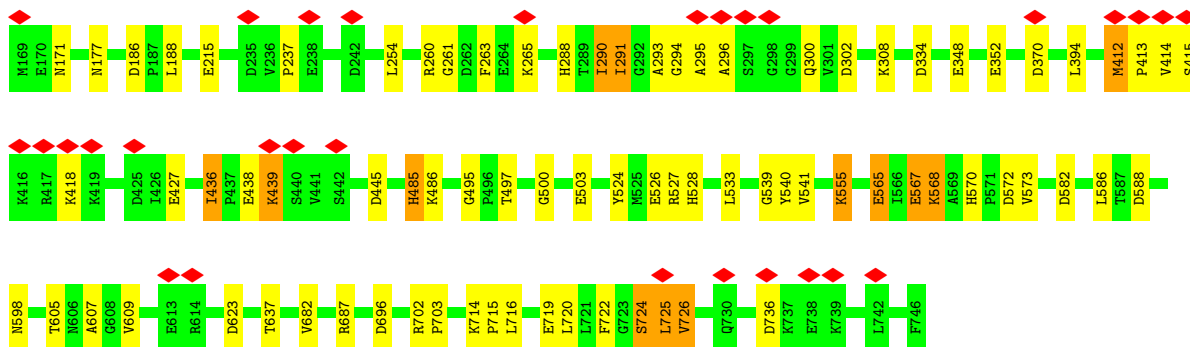
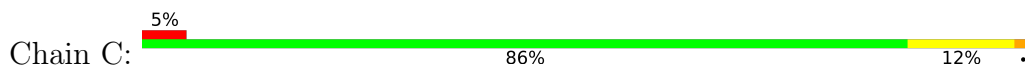


• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

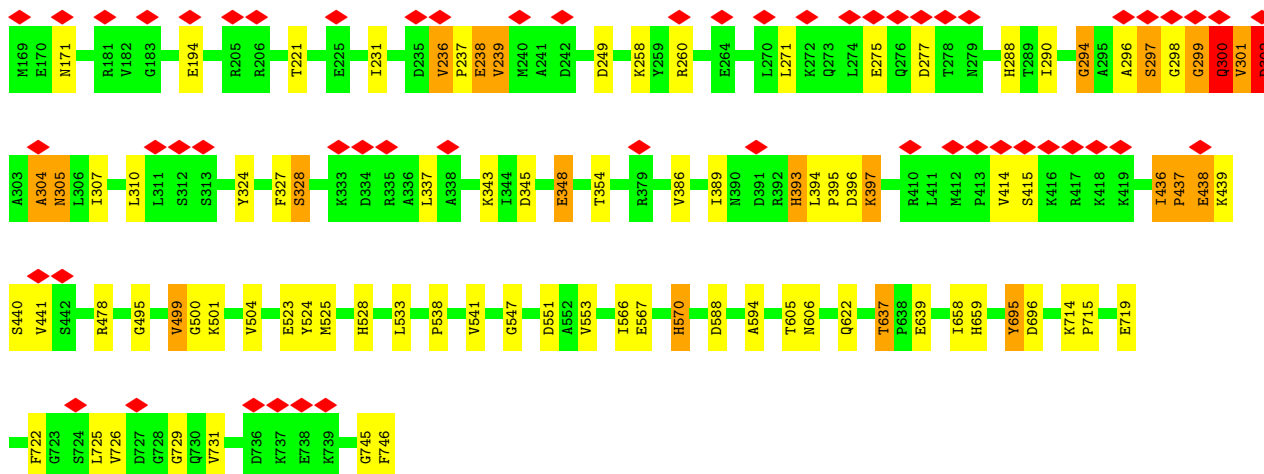
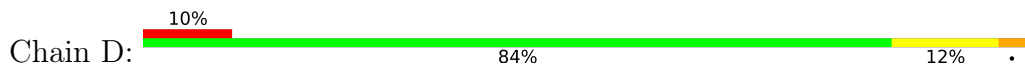




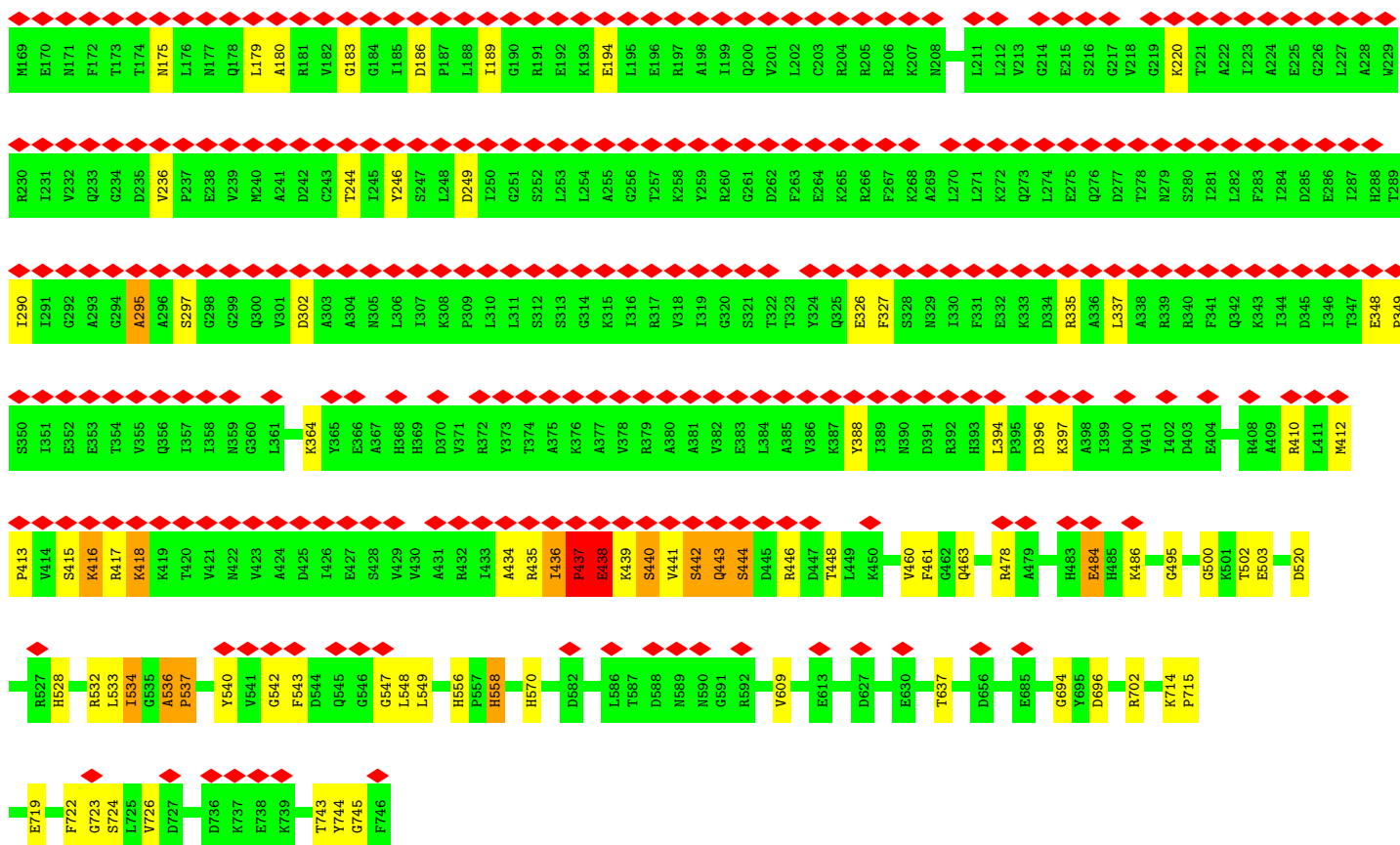
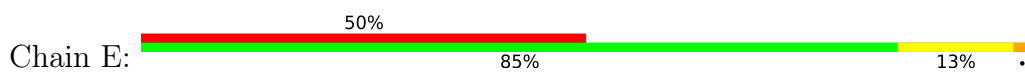
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA



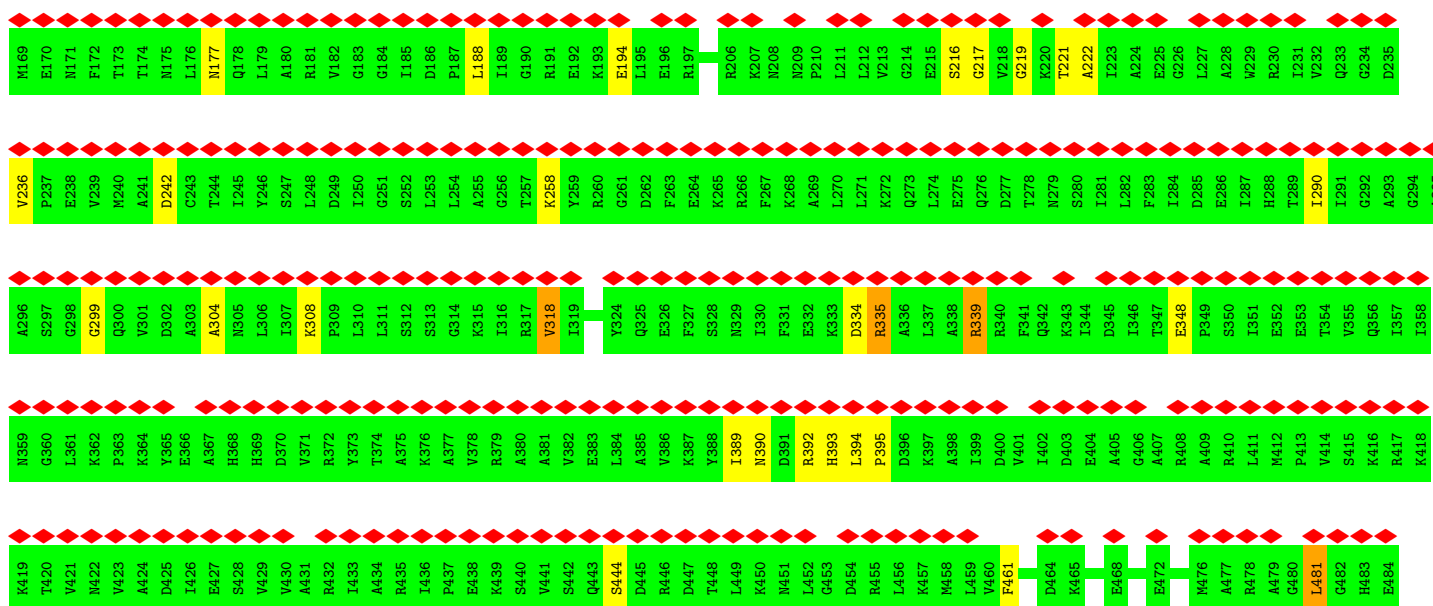
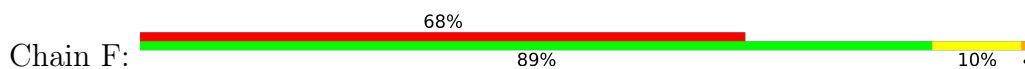
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

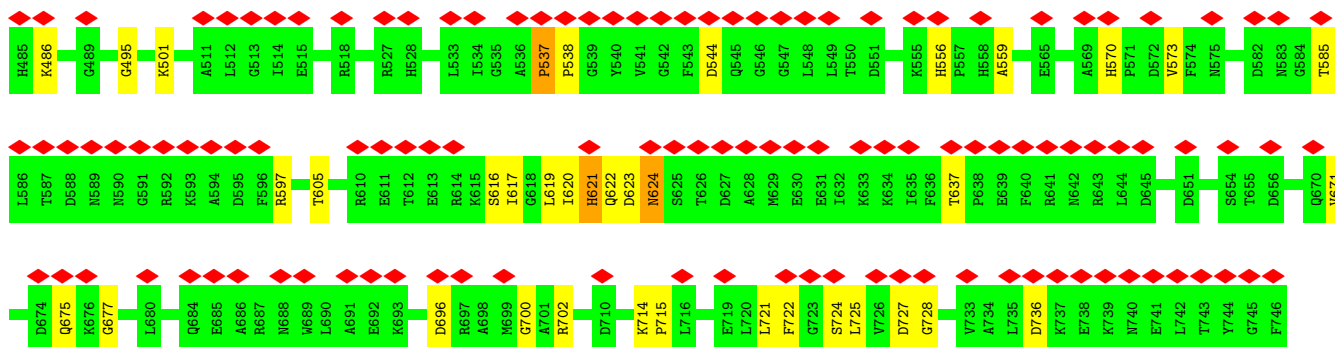


- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

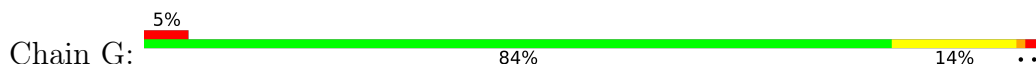


• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA





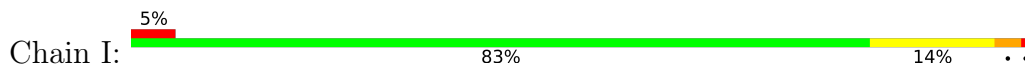
- Molecule 2: ATP-dependent Clp protease proteolytic subunit



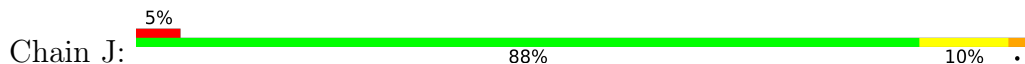
- Molecule 2: ATP-dependent Clp protease proteolytic subunit



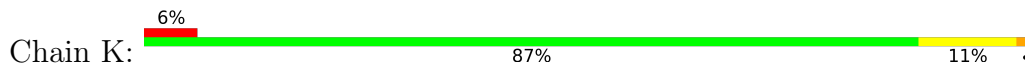
- Molecule 2: ATP-dependent Clp protease proteolytic subunit

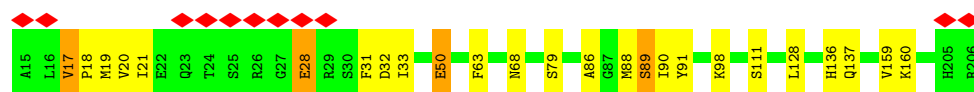


- Molecule 2: ATP-dependent Clp protease proteolytic subunit

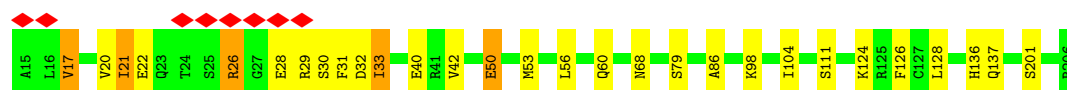
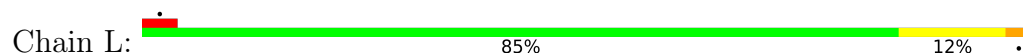


- Molecule 2: ATP-dependent Clp protease proteolytic subunit





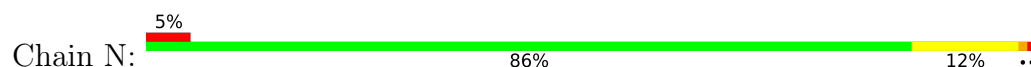
- Molecule 2: ATP-dependent Clp protease proteolytic subunit



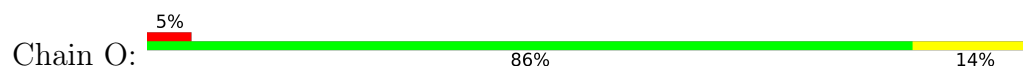
- Molecule 2: ATP-dependent Clp protease proteolytic subunit



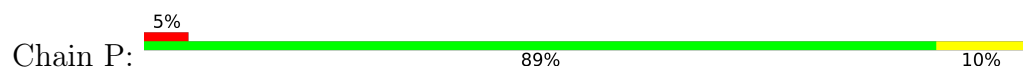
- Molecule 2: ATP-dependent Clp protease proteolytic subunit



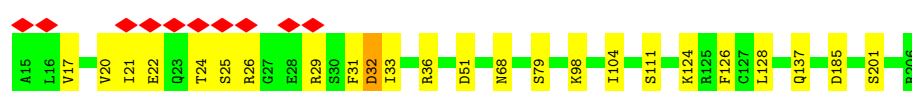
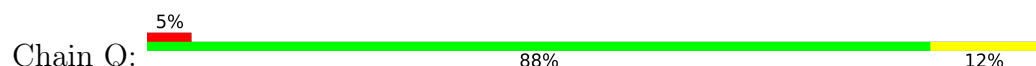
- Molecule 2: ATP-dependent Clp protease proteolytic subunit



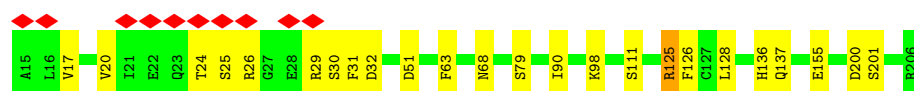
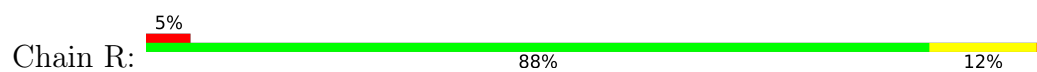
- Molecule 2: ATP-dependent Clp protease proteolytic subunit



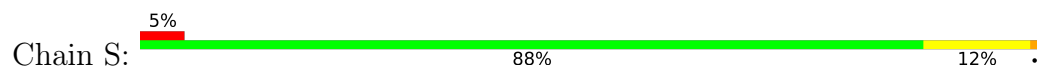
- Molecule 2: ATP-dependent Clp protease proteolytic subunit



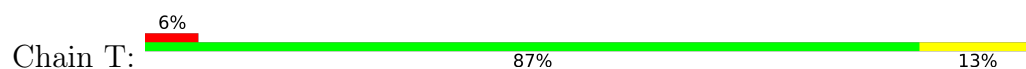
- Molecule 2: ATP-dependent Clp protease proteolytic subunit



- Molecule 2: ATP-dependent Clp protease proteolytic subunit



- Molecule 2: ATP-dependent Clp protease proteolytic subunit



- Molecule 3: RepA-GFP



- Molecule 4: RepA-GFP



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	169000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	69	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	58616	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.117	Depositor
Minimum map value	-1.677	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.77	Depositor
Map size (Å)	511.8, 511.8, 511.8	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.853, 0.853, 0.853	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.19	12/4441 (0.3%)	1.30	44/5991 (0.7%)
1	B	1.18	1/4577 (0.0%)	1.32	50/6175 (0.8%)
1	C	1.29	5/4577 (0.1%)	1.23	22/6175 (0.4%)
1	D	1.28	5/4576 (0.1%)	1.25	26/6175 (0.4%)
1	E	1.19	4/4577 (0.1%)	1.33	35/6175 (0.6%)
1	F	1.05	3/4576 (0.1%)	1.25	34/6172 (0.6%)
2	G	1.45	3/1525 (0.2%)	1.26	12/2054 (0.6%)
2	H	1.66	24/1525 (1.6%)	1.49	24/2054 (1.2%)
2	I	1.27	0/1525	1.24	10/2054 (0.5%)
2	J	1.37	1/1525 (0.1%)	1.25	12/2054 (0.6%)
2	K	1.38	1/1525 (0.1%)	1.27	14/2054 (0.7%)
2	L	1.37	1/1525 (0.1%)	1.26	12/2054 (0.6%)
2	M	1.41	1/1525 (0.1%)	1.24	14/2054 (0.7%)
2	N	1.34	2/1525 (0.1%)	1.26	15/2054 (0.7%)
2	O	1.32	1/1525 (0.1%)	1.26	14/2054 (0.7%)
2	P	1.39	1/1525 (0.1%)	1.24	13/2054 (0.6%)
2	Q	1.43	0/1525	1.26	14/2054 (0.7%)
2	R	1.42	1/1525 (0.1%)	1.25	16/2054 (0.8%)
2	S	1.42	2/1525 (0.1%)	1.33	17/2054 (0.8%)
2	T	1.39	1/1525 (0.1%)	1.26	13/2054 (0.6%)
All	All	1.29	69/48674 (0.1%)	1.28	411/65619 (0.6%)

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	3
1	B	1	1
1	E	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	3
2	H	0	3
All	All	1	11

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	536	ALA	C-N	19.52	1.50	1.33
1	D	437	PRO	N-CA	18.11	1.70	1.47
2	G	104	ILE	C-O	-10.91	1.12	1.24
1	D	436	ILE	C-N	10.86	1.45	1.33
2	H	77	ILE	C-O	-10.64	1.12	1.24
2	H	90	ILE	C-O	-10.51	1.11	1.24
2	H	84	ILE	C-O	-10.41	1.12	1.24
2	H	92	ASP	C-O	-10.01	1.11	1.24
2	H	79	SER	C-O	-9.49	1.12	1.24
2	H	83	VAL	C-O	-9.26	1.14	1.24
2	H	96	PHE	C-O	-9.05	1.13	1.24
2	G	105	CYS	C-O	-8.89	1.14	1.24
1	E	558	HIS	CB-CG	-8.71	1.38	1.50
1	A	308	LYS	C-O	-8.55	1.13	1.24
2	H	103	THR	C-O	-8.18	1.13	1.23
1	A	310	LEU	C-O	-8.01	1.13	1.24
2	H	91	TYR	C-O	-7.84	1.14	1.24
2	H	87	GLY	C-O	-7.57	1.13	1.23
2	G	106	MET	C-O	-7.37	1.14	1.24
1	A	310	LEU	CA-C	-7.34	1.43	1.52
2	H	80	PRO	C-O	-7.22	1.14	1.24
2	H	89	SER	C-O	-7.21	1.14	1.24
2	H	102	SER	CA-CB	-6.98	1.44	1.53
2	H	98	LYS	C-O	-6.85	1.18	1.24
1	A	300	GLN	C-N	6.83	1.43	1.33
2	S	32	ASP	CB-CG	-6.73	1.35	1.52
1	A	303	ALA	C-O	-6.68	1.15	1.23
2	H	94	MET	C-O	-6.66	1.16	1.24
2	H	81	GLY	C-O	-6.62	1.16	1.23
2	H	88	MET	C-O	-6.57	1.14	1.23
2	H	102	SER	C-O	-6.52	1.16	1.24
2	H	101	VAL	C-O	-6.51	1.17	1.24
2	T	136	HIS	CB-CG	-6.38	1.41	1.50
2	J	136	HIS	CB-CG	-6.36	1.41	1.50
2	H	93	THR	C-O	-6.32	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	136	HIS	CB-CG	-6.27	1.41	1.50
1	E	528	HIS	CB-CG	-6.09	1.41	1.50
2	K	136	HIS	CB-CG	-6.08	1.41	1.50
2	H	82	GLY	C-O	-6.06	1.15	1.23
2	R	136	HIS	CB-CG	-6.01	1.41	1.50
1	A	310	LEU	N-CA	-6.00	1.38	1.46
1	D	528	HIS	CB-CG	-5.97	1.41	1.50
2	H	78	ASN	C-O	-5.94	1.15	1.23
1	A	308	LYS	CA-C	-5.83	1.45	1.52
1	B	556	HIS	CB-CG	-5.80	1.42	1.50
1	C	288	HIS	CB-CG	-5.69	1.42	1.50
2	L	136	HIS	CB-CG	-5.61	1.42	1.50
1	D	288	HIS	CB-CG	-5.57	1.42	1.50
1	A	597	ARG	CD-NE	-5.55	1.38	1.46
1	C	485	HIS	CB-CG	-5.52	1.42	1.50
2	H	85	THR	C-O	-5.51	1.14	1.23
1	D	570	HIS	CB-CG	-5.49	1.42	1.50
2	P	136	HIS	CB-CG	-5.48	1.42	1.50
1	A	307	ILE	C-O	-5.45	1.17	1.23
1	C	188	LEU	CB-CG	-5.43	1.42	1.53
2	N	53	MET	SD-CE	-5.42	1.66	1.79
2	N	136	HIS	CB-CG	-5.38	1.42	1.50
2	H	79	SER	CA-CB	-5.37	1.44	1.53
1	A	307	ILE	CA-C	-5.31	1.45	1.52
1	A	369	HIS	CB-CG	-5.31	1.42	1.50
1	C	290	ILE	C-O	-5.28	1.17	1.24
1	F	597	ARG	CD-NE	-5.25	1.39	1.46
1	F	597	ARG	CG-CD	-5.24	1.36	1.52
1	C	565	GLU	CG-CD	-5.17	1.39	1.52
2	M	136	HIS	CB-CG	-5.17	1.43	1.50
2	O	53	MET	SD-CE	-5.17	1.66	1.79
1	E	556	HIS	CB-CG	-5.16	1.43	1.50
1	A	556	HIS	CB-CG	-5.12	1.43	1.50
1	F	537	PRO	CA-C	5.05	1.56	1.52

All (411) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	536	ALA	CA-C-N	25.10	137.98	119.66
1	E	536	ALA	C-N-CA	25.10	137.98	119.66
1	D	436	ILE	CA-C-N	16.87	139.55	119.98
1	D	436	ILE	C-N-CA	16.87	139.55	119.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	31	PHE	CB-CA-C	-15.00	83.66	110.36
1	D	414	VAL	N-CA-C	-14.86	98.97	113.53
2	K	89	SER	N-CA-C	-13.15	93.57	110.53
2	H	93	THR	CA-CB-OG1	-12.25	91.23	109.60
1	C	445	ASP	N-CA-C	-11.93	98.83	113.50
1	B	414	VAL	N-CA-C	-11.77	102.00	113.53
1	B	631	GLU	CA-C-N	11.49	137.87	121.55
1	B	631	GLU	C-N-CA	11.49	137.87	121.55
1	A	307	ILE	CB-CA-C	-11.48	97.48	111.94
1	C	412	MET	CA-C-N	10.20	129.81	119.82
1	C	412	MET	C-N-CA	10.20	129.81	119.82
1	B	633	LYS	CB-CA-C	-10.19	89.31	110.40
1	B	445	ASP	N-CA-C	-10.17	101.19	114.31
1	E	448	THR	N-CA-C	-9.95	101.65	113.88
1	A	636	PHE	CA-CB-CG	9.52	123.32	113.80
1	E	436	ILE	C-N-CD	-8.90	88.51	125.00
1	D	437	PRO	CA-N-CD	-8.50	100.09	112.00
1	A	495	GLY	CA-C-N	8.50	129.02	119.92
1	A	495	GLY	C-N-CA	8.50	129.02	119.92
1	D	722	PHE	N-CA-C	-8.46	97.95	109.54
2	G	79	SER	CA-C-N	8.36	128.56	119.87
2	G	79	SER	C-N-CA	8.36	128.56	119.87
1	B	495	GLY	CA-C-N	8.32	128.20	120.21
1	B	495	GLY	C-N-CA	8.32	128.20	120.21
2	Q	79	SER	CA-C-N	8.14	128.34	119.87
2	Q	79	SER	C-N-CA	8.14	128.34	119.87
2	L	79	SER	CA-C-N	8.14	127.78	119.56
2	L	79	SER	C-N-CA	8.14	127.78	119.56
1	A	303	ALA	N-CA-C	8.06	122.71	109.24
2	K	79	SER	CA-C-N	8.05	128.24	119.87
2	K	79	SER	C-N-CA	8.05	128.24	119.87
2	N	79	SER	CA-C-N	8.03	128.22	119.87
2	N	79	SER	C-N-CA	8.03	128.22	119.87
1	C	495	GLY	CA-C-N	8.02	127.97	120.03
1	C	495	GLY	C-N-CA	8.02	127.97	120.03
1	B	628	ALA	CA-C-N	8.01	135.03	122.93
1	B	628	ALA	C-N-CA	8.01	135.03	122.93
2	J	79	SER	CA-C-N	7.99	128.18	119.87
2	J	79	SER	C-N-CA	7.99	128.18	119.87
1	B	609	VAL	N-CA-C	7.96	118.01	110.53
2	I	79	SER	CA-C-N	7.93	128.11	119.87
2	I	79	SER	C-N-CA	7.93	128.11	119.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	79	SER	CA-C-N	7.91	128.10	119.87
2	S	79	SER	C-N-CA	7.91	128.10	119.87
2	O	79	SER	CA-C-N	7.91	128.10	119.87
2	O	79	SER	C-N-CA	7.91	128.10	119.87
2	R	79	SER	CA-C-N	7.91	128.10	119.87
2	R	79	SER	C-N-CA	7.91	128.10	119.87
2	S	90	ILE	N-CA-C	-7.83	103.28	111.58
2	H	28	GLU	CA-C-N	7.80	136.44	121.54
2	H	28	GLU	C-N-CA	7.80	136.44	121.54
2	O	90	ILE	N-CA-C	-7.79	103.32	111.58
1	E	537	PRO	CA-C-N	7.77	129.55	119.84
1	E	537	PRO	C-N-CA	7.77	129.55	119.84
1	F	318	VAL	CA-C-O	-7.76	112.24	120.39
2	H	90	ILE	N-CA-C	-7.76	101.60	113.16
2	M	17	VAL	CA-C-N	7.68	127.64	120.03
2	M	17	VAL	C-N-CA	7.68	127.64	120.03
1	A	300	GLN	CA-C-O	-7.58	111.94	120.43
1	F	486	LYS	CA-C-N	7.57	128.02	119.92
1	F	486	LYS	C-N-CA	7.57	128.02	119.92
1	B	390	ASN	N-CA-C	7.54	122.67	113.17
2	T	90	ILE	N-CA-C	-7.47	103.66	111.58
1	F	495	GLY	CA-C-N	7.45	127.38	119.85
1	F	495	GLY	C-N-CA	7.45	127.38	119.85
1	F	624	ASN	N-CA-C	7.43	118.41	108.38
1	E	745	GLY	N-CA-C	-7.40	101.90	112.55
1	F	461	PHE	CA-CB-CG	-7.36	106.44	113.80
1	B	629	MET	N-CA-C	7.34	119.50	110.91
1	D	297	SER	CA-C-N	7.33	134.89	121.70
1	D	297	SER	C-N-CA	7.33	134.89	121.70
1	E	556	HIS	CA-C-N	7.24	126.91	119.82
1	E	556	HIS	C-N-CA	7.24	126.91	119.82
2	M	79	SER	CA-C-N	7.19	127.80	120.04
2	M	79	SER	C-N-CA	7.19	127.80	120.04
1	A	394	LEU	N-CA-C	7.13	122.52	113.25
1	A	331	PHE	N-CA-C	-7.13	101.34	110.53
2	L	137	GLN	CA-C-N	7.08	127.07	119.78
2	L	137	GLN	C-N-CA	7.08	127.07	119.78
1	A	300	GLN	CA-C-N	-7.07	108.97	121.70
1	A	300	GLN	C-N-CA	-7.07	108.97	121.70
2	H	17	VAL	CA-C-N	7.07	127.03	120.03
2	H	17	VAL	C-N-CA	7.07	127.03	120.03
1	B	630	GLU	N-CA-C	-7.07	104.13	112.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	79	SER	CA-C-N	7.06	127.67	120.04
2	P	79	SER	C-N-CA	7.06	127.67	120.04
2	O	51	ASP	N-CA-C	7.04	119.04	111.36
2	G	106	MET	CA-C-O	-6.99	113.15	120.70
2	H	88	MET	CB-CG-SD	-6.99	91.73	112.70
1	E	744	TYR	N-CA-C	6.99	119.75	110.53
2	P	98	LYS	N-CA-C	6.98	121.70	112.35
2	O	128	LEU	CA-C-N	6.96	127.55	119.47
2	O	128	LEU	C-N-CA	6.96	127.55	119.47
2	Q	68	ASN	CA-C-N	6.95	126.63	119.82
2	Q	68	ASN	C-N-CA	6.95	126.63	119.82
2	G	68	ASN	CA-C-N	6.93	126.62	119.82
2	G	68	ASN	C-N-CA	6.93	126.62	119.82
1	A	393	HIS	CA-CB-CG	-6.93	106.87	113.80
2	I	17	VAL	CA-C-N	6.92	126.88	120.03
2	I	17	VAL	C-N-CA	6.92	126.88	120.03
2	P	128	LEU	CA-C-N	6.91	127.48	119.47
2	P	128	LEU	C-N-CA	6.91	127.48	119.47
2	H	103	THR	CA-C-O	-6.89	113.75	120.92
2	K	17	VAL	CA-C-N	6.89	126.85	120.03
2	K	17	VAL	C-N-CA	6.89	126.85	120.03
2	M	68	ASN	CA-C-N	6.88	126.56	119.82
2	M	68	ASN	C-N-CA	6.88	126.56	119.82
1	D	495	GLY	CA-C-N	6.85	126.79	120.21
1	D	495	GLY	C-N-CA	6.85	126.79	120.21
2	N	51	ASP	N-CA-C	6.85	118.83	111.36
2	J	51	ASP	N-CA-C	6.84	118.82	111.36
1	B	628	ALA	N-CA-C	-6.84	103.42	112.72
1	E	290	ILE	N-CA-C	-6.84	104.33	111.58
1	E	444	SER	N-CA-C	-6.82	102.15	111.56
2	S	51	ASP	N-CA-C	6.80	118.70	111.28
2	G	17	VAL	CA-C-N	6.80	126.76	120.03
2	G	17	VAL	C-N-CA	6.80	126.76	120.03
2	S	17	VAL	CA-C-N	6.80	126.76	120.03
2	S	17	VAL	C-N-CA	6.80	126.76	120.03
1	E	542	GLY	N-CA-C	-6.79	101.32	110.56
1	E	495	GLY	CA-C-N	6.77	127.16	119.92
1	E	495	GLY	C-N-CA	6.77	127.16	119.92
2	J	17	VAL	CA-C-N	6.76	126.73	120.03
2	J	17	VAL	C-N-CA	6.76	126.73	120.03
2	R	90	ILE	N-CA-C	-6.71	103.69	111.00
2	S	68	ASN	CA-C-N	6.70	126.39	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	68	ASN	C-N-CA	6.70	126.39	119.56
1	F	556	HIS	CA-C-N	6.69	126.32	119.56
1	F	556	HIS	C-N-CA	6.69	126.32	119.56
2	R	17	VAL	CA-C-N	6.67	126.65	119.78
2	R	17	VAL	C-N-CA	6.67	126.65	119.78
2	Q	17	VAL	CA-C-N	6.63	126.61	119.78
2	Q	17	VAL	C-N-CA	6.63	126.61	119.78
2	T	17	VAL	CA-C-N	6.63	126.59	120.03
2	T	17	VAL	C-N-CA	6.63	126.59	120.03
1	E	437	PRO	N-CA-C	6.62	126.11	112.47
2	H	100	ASP	CB-CA-C	-6.62	98.27	109.72
2	N	128	LEU	CA-C-N	6.61	127.14	119.47
2	N	128	LEU	C-N-CA	6.61	127.14	119.47
2	M	128	LEU	CA-C-N	6.60	127.12	119.47
2	M	128	LEU	C-N-CA	6.60	127.12	119.47
2	Q	128	LEU	CA-C-N	6.59	126.29	119.56
2	Q	128	LEU	C-N-CA	6.59	126.29	119.56
1	F	348	GLU	CA-C-N	6.58	127.04	120.52
1	F	348	GLU	C-N-CA	6.58	127.04	120.52
2	L	68	ASN	CA-C-N	6.58	126.27	119.82
2	L	68	ASN	C-N-CA	6.58	126.27	119.82
2	O	137	GLN	CA-C-N	6.57	126.49	119.85
2	O	137	GLN	C-N-CA	6.57	126.49	119.85
2	S	31	PHE	CA-C-N	6.57	130.19	120.87
2	S	31	PHE	C-N-CA	6.57	130.19	120.87
1	A	300	GLN	N-CA-C	6.55	119.37	108.96
2	H	128	LEU	CA-C-N	6.54	126.23	119.56
2	H	128	LEU	C-N-CA	6.54	126.23	119.56
2	K	68	ASN	CA-C-N	6.54	126.23	119.82
2	K	68	ASN	C-N-CA	6.54	126.23	119.82
1	B	348	GLU	CA-C-N	6.53	126.50	120.03
1	B	348	GLU	C-N-CA	6.53	126.50	120.03
2	H	87	GLY	CA-C-N	6.52	134.26	123.25
2	H	87	GLY	C-N-CA	6.52	134.26	123.25
2	G	98	LYS	N-CA-C	6.51	121.60	112.75
1	A	308	LYS	CA-C-N	-6.50	111.71	119.84
1	A	308	LYS	C-N-CA	-6.50	111.71	119.84
1	D	302	ASP	CB-CA-C	-6.50	97.69	113.15
1	E	609	VAL	N-CA-C	6.48	117.23	110.62
2	N	68	ASN	CA-C-N	6.47	126.17	119.82
2	N	68	ASN	C-N-CA	6.47	126.17	119.82
2	O	68	ASN	CA-C-N	6.47	126.16	119.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	68	ASN	C-N-CA	6.47	126.16	119.82
2	M	51	ASP	N-CA-C	6.43	118.28	111.28
2	Q	51	ASP	N-CA-C	6.42	118.28	111.28
1	B	633	LYS	CB-CG-CD	6.42	126.06	111.30
1	B	634	LYS	N-CA-C	-6.42	105.87	113.38
1	E	388	TYR	N-CA-C	6.41	122.17	113.97
1	A	702	ARG	CA-C-N	6.40	126.09	119.82
1	A	702	ARG	C-N-CA	6.40	126.09	119.82
2	T	68	ASN	CA-C-N	6.40	126.09	119.82
2	T	68	ASN	C-N-CA	6.40	126.09	119.82
2	R	68	ASN	CA-C-N	6.37	126.06	119.56
2	R	68	ASN	C-N-CA	6.37	126.06	119.56
2	N	17	VAL	CA-C-N	6.37	126.33	120.03
2	N	17	VAL	C-N-CA	6.37	126.33	120.03
2	L	128	LEU	CA-C-N	6.36	126.05	119.56
2	L	128	LEU	C-N-CA	6.36	126.05	119.56
1	A	309	PRO	CA-N-CD	-6.35	103.11	112.00
2	P	137	GLN	CA-C-N	6.34	126.26	119.85
2	P	137	GLN	C-N-CA	6.34	126.26	119.85
2	R	128	LEU	CA-C-N	6.34	126.03	119.56
2	R	128	LEU	C-N-CA	6.34	126.03	119.56
1	A	417	ARG	CA-C-O	-6.33	114.16	121.82
2	J	98	LYS	N-CA-C	6.33	120.84	112.35
2	J	128	LEU	CA-C-N	6.33	126.01	119.56
2	J	128	LEU	C-N-CA	6.33	126.01	119.56
2	T	128	LEU	CA-C-N	6.31	125.99	119.56
2	T	128	LEU	C-N-CA	6.31	125.99	119.56
1	B	248	LEU	N-CA-C	6.30	119.51	109.24
2	R	98	LYS	N-CA-C	6.30	121.32	112.75
2	L	17	VAL	CA-C-N	6.28	126.25	120.03
2	L	17	VAL	C-N-CA	6.28	126.25	120.03
1	F	702	ARG	CA-C-N	6.28	125.97	119.82
1	F	702	ARG	C-N-CA	6.28	125.97	119.82
1	E	236	VAL	CA-C-N	6.27	126.24	119.78
1	E	236	VAL	C-N-CA	6.27	126.24	119.78
2	S	31	PHE	CA-CB-CG	6.27	120.07	113.80
2	H	79	SER	CA-C-O	-6.26	112.86	119.50
1	B	186	ASP	CA-C-N	6.24	126.15	119.85
1	B	186	ASP	C-N-CA	6.24	126.15	119.85
1	E	694	GLY	CA-C-N	-6.23	112.12	122.21
1	E	694	GLY	C-N-CA	-6.23	112.12	122.21
1	F	299	GLY	CA-C-N	6.22	132.91	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	299	GLY	C-N-CA	6.22	132.91	121.70
2	J	68	ASN	CA-C-N	6.22	125.92	119.82
2	J	68	ASN	C-N-CA	6.22	125.92	119.82
1	B	739	LYS	N-CA-C	-6.22	106.29	114.31
2	M	98	LYS	N-CA-C	6.20	121.18	112.75
2	H	89	SER	CA-C-O	-6.20	111.65	120.51
2	K	128	LEU	CA-C-N	6.19	125.87	119.56
2	K	128	LEU	C-N-CA	6.19	125.87	119.56
2	S	98	LYS	N-CA-C	6.17	121.15	112.75
2	I	68	ASN	CA-C-N	6.16	125.86	119.82
2	I	68	ASN	C-N-CA	6.16	125.86	119.82
2	G	137	GLN	CA-C-N	6.16	126.12	119.78
2	G	137	GLN	C-N-CA	6.16	126.12	119.78
2	N	90	ILE	N-CA-C	-6.14	104.31	111.00
2	S	137	GLN	CA-C-N	6.13	126.04	119.85
2	S	137	GLN	C-N-CA	6.13	126.04	119.85
2	P	17	VAL	CA-C-N	6.13	126.09	120.03
2	P	17	VAL	C-N-CA	6.13	126.09	120.03
2	S	128	LEU	CA-C-N	6.12	125.80	119.56
2	S	128	LEU	C-N-CA	6.12	125.80	119.56
1	C	605	THR	N-CA-C	6.10	118.12	108.79
2	L	98	LYS	N-CA-C	6.08	120.50	112.35
1	A	651	ASP	N-CA-C	6.08	119.07	110.50
2	M	137	GLN	CA-C-N	6.08	125.99	119.85
2	M	137	GLN	C-N-CA	6.08	125.99	119.85
1	D	299	GLY	N-CA-C	-6.07	106.88	115.43
2	H	137	GLN	CA-C-N	6.05	125.97	119.85
2	H	137	GLN	C-N-CA	6.05	125.97	119.85
1	B	633	LYS	N-CA-C	-6.02	102.76	110.53
2	T	98	LYS	N-CA-C	6.01	120.93	112.75
1	B	624	ASN	CA-CB-CG	6.01	118.61	112.60
2	I	128	LEU	CA-C-N	6.00	125.68	119.56
2	I	128	LEU	C-N-CA	6.00	125.68	119.56
1	A	632	ILE	CA-C-N	5.99	128.59	120.38
1	A	632	ILE	C-N-CA	5.99	128.59	120.38
2	G	111	SER	CB-CA-C	-5.99	109.09	117.23
1	B	388	TYR	N-CA-C	5.98	121.63	113.97
2	T	51	ASP	N-CA-C	5.96	119.02	111.69
1	F	236	VAL	CA-C-N	5.96	125.92	119.78
1	F	236	VAL	C-N-CA	5.96	125.92	119.78
2	P	68	ASN	CA-C-N	5.95	125.62	119.56
2	P	68	ASN	C-N-CA	5.95	125.62	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	585	THR	N-CA-C	5.94	118.31	108.99
2	O	17	VAL	CA-C-N	5.91	125.88	120.03
2	O	17	VAL	C-N-CA	5.91	125.88	120.03
2	K	28	GLU	N-CA-C	5.90	118.11	108.55
2	H	91	TYR	N-CA-C	-5.89	103.64	111.24
2	H	98	LYS	CA-C-O	-5.87	113.15	118.79
2	R	137	GLN	CA-C-N	5.87	125.78	119.85
2	R	137	GLN	C-N-CA	5.87	125.78	119.85
1	F	537	PRO	CB-CA-C	5.87	118.08	110.92
2	Q	98	LYS	N-CA-C	5.86	120.72	112.75
2	T	137	GLN	CA-C-N	5.86	125.77	119.85
2	T	137	GLN	C-N-CA	5.86	125.77	119.85
1	A	570	HIS	CA-C-N	5.85	126.25	119.47
1	A	570	HIS	C-N-CA	5.85	126.25	119.47
1	B	624	ASN	CB-CA-C	5.84	120.02	111.73
1	B	499	VAL	N-CA-C	5.82	118.05	111.88
2	Q	137	GLN	CA-C-N	5.81	125.72	119.85
2	Q	137	GLN	C-N-CA	5.81	125.72	119.85
2	Q	32	ASP	N-CA-C	-5.80	102.32	110.50
1	C	607	ALA	N-CA-C	5.80	117.60	111.28
1	F	637	THR	CA-C-N	5.78	126.18	119.47
1	F	637	THR	C-N-CA	5.78	126.18	119.47
1	B	222	ALA	N-CA-C	-5.77	104.99	111.28
2	P	51	ASP	N-CA-C	5.76	117.64	111.36
1	C	609	VAL	N-CA-C	5.75	116.40	110.82
1	F	573	VAL	N-CA-C	-5.75	104.91	110.72
2	K	98	LYS	N-CA-C	5.74	120.05	112.35
2	H	88	MET	N-CA-C	-5.74	103.09	111.30
1	E	570	HIS	CA-C-N	5.73	126.12	119.47
1	E	570	HIS	C-N-CA	5.73	126.12	119.47
1	B	543	PHE	N-CA-C	5.72	118.25	111.33
1	D	294	GLY	N-CA-C	-5.71	102.31	112.54
1	A	308	LYS	N-CA-C	5.71	122.43	109.81
1	C	294	GLY	N-CA-C	-5.70	101.67	112.51
1	E	743	THR	CA-C-N	5.70	131.35	120.97
1	E	743	THR	C-N-CA	5.70	131.35	120.97
1	A	412	MET	CA-C-N	5.70	126.97	119.84
1	A	412	MET	C-N-CA	5.70	126.97	119.84
1	A	306	LEU	CA-C-N	-5.70	112.11	121.34
1	A	306	LEU	C-N-CA	-5.70	112.11	121.34
2	H	111	SER	CB-CA-C	-5.69	109.49	117.23
2	K	137	GLN	CA-C-N	5.67	125.57	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	137	GLN	C-N-CA	5.67	125.57	119.85
2	N	137	GLN	CA-C-N	5.66	125.57	119.85
2	N	137	GLN	C-N-CA	5.66	125.57	119.85
1	B	607	ALA	N-CA-C	5.66	117.45	111.28
1	B	576	ILE	N-CA-C	-5.66	105.59	111.58
1	A	556	HIS	CA-C-N	5.65	125.33	119.56
1	A	556	HIS	C-N-CA	5.65	125.33	119.56
1	D	415	SER	N-CA-C	-5.63	105.72	112.59
1	B	534	ILE	N-CA-C	5.63	119.16	113.47
1	F	722	PHE	CA-CB-CG	-5.63	108.17	113.80
2	M	16	LEU	N-CA-C	-5.62	105.23	111.36
1	B	634	LYS	CA-C-O	-5.60	113.79	119.78
2	O	111	SER	CB-CA-C	-5.60	109.62	117.23
1	F	481	LEU	CA-C-O	-5.60	112.93	120.15
2	M	111	SER	CB-CA-C	-5.59	109.62	117.23
1	B	634	LYS	CB-CA-C	5.56	120.29	111.23
2	H	94	MET	N-CA-C	-5.56	104.86	111.69
2	Q	111	SER	CB-CA-C	-5.55	109.68	117.23
1	F	724	SER	N-CA-C	-5.53	105.33	111.36
2	H	103	THR	OG1-CB-CG2	-5.50	98.30	109.30
2	O	98	LYS	N-CA-C	5.50	120.22	112.75
1	A	303	ALA	CA-C-O	5.49	126.97	120.66
1	B	223	ILE	CB-CA-C	-5.48	104.84	112.02
1	B	728	GLY	N-CA-C	-5.47	107.66	115.64
2	J	137	GLN	CA-C-N	5.47	125.37	119.85
2	J	137	GLN	C-N-CA	5.47	125.37	119.85
1	B	626	THR	N-CA-C	-5.46	105.22	111.07
1	C	237	PRO	N-CA-C	-5.46	102.61	111.19
1	D	637	THR	CA-C-N	5.44	125.52	119.32
1	D	637	THR	C-N-CA	5.44	125.52	119.32
1	D	541	VAL	N-CA-C	5.44	117.84	111.05
1	A	341	PHE	CA-CB-CG	5.43	119.23	113.80
1	D	305	ASN	N-CA-C	-5.43	99.23	110.80
1	A	307	ILE	CA-C-O	5.42	126.48	120.46
1	D	277	ASP	CA-CB-CG	5.42	118.02	112.60
1	C	308	LYS	CA-C-N	5.41	125.08	119.56
1	C	308	LYS	C-N-CA	5.41	125.08	119.56
1	E	637	THR	CA-C-N	5.41	125.49	119.32
1	E	637	THR	C-N-CA	5.41	125.49	119.32
1	D	249	ASP	CA-CB-CG	-5.41	107.19	112.60
2	R	51	ASP	N-CA-C	5.41	118.34	111.69
1	B	177	ASN	N-CA-C	-5.40	105.43	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	570	HIS	CA-C-N	5.39	125.72	119.47
1	F	570	HIS	C-N-CA	5.39	125.72	119.47
1	D	722	PHE	CA-CB-CG	-5.38	108.42	113.80
1	E	702	ARG	CA-C-N	5.37	125.04	119.56
1	E	702	ARG	C-N-CA	5.37	125.04	119.56
1	A	559	ALA	N-CA-C	5.37	117.62	110.53
1	C	215	GLU	N-CA-C	-5.37	103.30	110.55
2	P	111	SER	CB-CA-C	-5.36	109.94	117.23
1	D	221	THR	N-CA-C	-5.36	105.10	111.69
2	N	98	LYS	N-CA-C	5.36	120.03	112.75
1	E	486	LYS	CA-C-N	5.30	125.59	119.92
1	E	486	LYS	C-N-CA	5.30	125.59	119.92
1	C	177	ASN	N-CA-C	-5.30	105.55	112.23
2	G	31	PHE	CA-CB-CG	5.30	119.10	113.80
2	I	111	SER	CB-CA-C	-5.29	110.03	117.23
1	F	444	SER	N-CA-C	5.29	117.22	108.13
1	F	559	ALA	N-CA-C	5.28	117.50	110.53
1	B	420	THR	N-CA-C	-5.28	102.64	110.46
1	D	348	GLU	CA-C-N	5.27	125.25	120.03
1	D	348	GLU	C-N-CA	5.27	125.25	120.03
1	B	415	SER	CA-C-N	5.27	129.62	122.19
1	B	415	SER	C-N-CA	5.27	129.62	122.19
1	C	541	VAL	N-CA-C	5.26	117.63	111.05
1	F	389	ILE	N-CA-C	5.26	115.67	107.99
1	F	290	ILE	N-CA-C	-5.25	107.30	111.81
1	C	186	ASP	CA-C-N	5.24	125.15	119.85
1	C	186	ASP	C-N-CA	5.24	125.15	119.85
2	I	98	LYS	N-CA-C	5.24	119.88	112.75
2	T	16	LEU	N-CA-C	-5.24	105.57	111.28
1	B	625	SER	N-CA-C	-5.23	107.92	114.56
1	F	177	ASN	N-CA-C	-5.22	105.26	111.69
1	A	177	ASN	N-CA-C	-5.22	105.65	112.23
1	B	632	ILE	N-CA-C	-5.22	105.72	113.39
1	E	484	GLU	CA-C-O	-5.21	112.27	119.05
2	R	111	SER	CB-CA-C	-5.21	110.14	117.23
1	A	309	PRO	N-CA-C	-5.21	101.73	112.47
1	E	337	LEU	N-CA-C	-5.21	106.61	113.12
1	A	635	ILE	N-CA-C	-5.20	107.33	111.81
1	B	345	ASP	CA-CB-CG	5.18	117.78	112.60
2	N	16	LEU	N-CA-C	-5.18	105.71	111.36
1	F	725	LEU	N-CA-C	-5.16	101.75	109.95
1	B	365	TYR	N-CA-C	-5.15	105.36	111.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	633	LYS	N-CA-CB	5.14	117.79	110.44
1	B	537	PRO	CA-C-N	5.14	125.43	119.93
1	B	537	PRO	C-N-CA	5.14	125.43	119.93
2	L	111	SER	CB-CA-C	-5.13	110.25	117.23
1	B	221	THR	N-CA-C	-5.12	107.20	113.50
2	N	111	SER	CB-CA-C	-5.12	110.26	117.23
1	B	415	SER	N-CA-C	-5.12	105.76	112.41
1	C	497	THR	N-CA-C	5.11	117.71	110.50
1	A	724	SER	N-CA-C	-5.11	105.79	112.23
2	H	77	ILE	CB-CA-C	-5.11	104.65	110.73
1	F	585	THR	N-CA-C	5.10	117.38	108.76
2	T	111	SER	CB-CA-C	-5.10	110.29	117.23
1	E	189	ILE	N-CA-C	5.09	115.18	107.80
1	F	392	ARG	N-CA-C	-5.08	100.81	108.52
1	D	695	TYR	N-CA-C	5.07	117.66	110.10
2	K	111	SER	CB-CA-C	-5.07	110.34	117.23
1	A	262	ASP	N-CA-C	5.05	119.52	112.90
1	C	415	SER	N-CA-C	-5.04	106.44	112.59
1	C	637	THR	CA-C-N	5.04	125.06	119.32
1	C	637	THR	C-N-CA	5.04	125.06	119.32
1	D	304	ALA	CA-C-N	5.04	131.16	121.54
1	D	304	ALA	C-N-CA	5.04	131.16	121.54
2	R	30	SER	CA-C-N	-5.02	114.93	122.81
2	R	30	SER	C-N-CA	-5.02	114.93	122.81
1	A	462	GLY	N-CA-C	-5.02	103.69	112.77
1	A	185	ILE	N-CA-C	5.00	115.29	107.99
1	A	486	LYS	CA-C-N	5.00	125.27	119.92
1	A	486	LYS	C-N-CA	5.00	125.27	119.92
1	C	736	ASP	CA-CB-CG	5.00	117.60	112.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	629	MET	CA

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	300	GLN	Peptide
1	A	313	SER	Peptide
1	A	417	ARG	Mainchain
1	B	627	ASP	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	E	484	GLU	Mainchain
1	F	318	VAL	Mainchain
1	F	481	LEU	Mainchain
1	F	620	ILE	Peptide
2	H	27	GLY	Peptide
2	H	79	SER	Mainchain
2	H	89	SER	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4377	0	4468	135	0
1	B	4511	0	4609	196	0
1	C	4511	0	4609	116	0
1	D	4510	0	4609	100	0
1	E	4511	0	4609	132	0
1	F	4511	0	4608	58	0
2	G	1501	0	1512	37	0
2	H	1501	0	1512	92	0
2	I	1501	0	1512	84	0
2	J	1501	0	1512	42	0
2	K	1501	0	1512	38	0
2	L	1501	0	1512	30	0
2	M	1501	0	1512	34	0
2	N	1501	0	1512	34	0
2	O	1501	0	1512	26	0
2	P	1501	0	1512	28	0
2	Q	1501	0	1512	20	0
2	R	1501	0	1512	16	0
2	S	1501	0	1512	17	0
2	T	1501	0	1512	15	0
3	X	50	0	13	19	0
4	Y	55	0	15	7	0
5	A	54	0	23	1	0
5	E	54	0	22	19	0
5	F	27	0	11	1	0
6	B	62	0	24	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	62	0	22	1	0
6	D	62	0	22	1	0
6	E	31	0	11	9	0
All	All	48402	0	48843	1094	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 11.

All (1094) 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)
2:I:29:ARG:HD3	2:I:31:PHE:CE1	1.15	1.66
2:J:31:PHE:CZ	2:K:21:ILE:HD11	1.43	1.50
2:J:31:PHE:CE2	2:K:21:ILE:HD11	1.47	1.48
1:A:259:TYR:CD2	3:X:2:UNK:O	1.69	1.45
1:C:263:PHE:CZ	1:C:293:ALA:CB	2.04	1.39
1:E:441:VAL:HG11	1:F:721:LEU:CD2	1.52	1.38
1:B:540:TYR:OH	1:C:528:HIS:CB	1.71	1.38
2:J:31:PHE:CZ	2:K:21:ILE:CD1	2.04	1.38
2:I:29:ARG:HD3	2:I:31:PHE:CZ	1.58	1.37
2:I:29:ARG:CD	2:I:31:PHE:CE1	2.08	1.36
1:D:437:PRO:N	1:D:437:PRO:CA	1.70	1.36
1:B:540:TYR:CZ	1:C:528:HIS:CD2	2.16	1.32
2:N:17:VAL:CG1	2:N:33:ILE:HG22	1.59	1.31
1:A:307:ILE:HD12	1:A:340:ARG:NH1	1.44	1.30
1:B:287:ILE:CD1	1:B:320:GLY:HA3	1.61	1.29
2:M:17:VAL:CG1	2:M:33:ILE:HG22	1.64	1.26
5:E:801:ADP:O4'	5:E:801:ADP:C1'	1.64	1.23
1:E:438:GLU:O	1:E:439:LYS:HG2	1.36	1.23
1:C:539:GLY:O	4:Y:7:UNK:CB	1.87	1.22
5:F:801:ADP:O4'	5:F:801:ADP:C1'	1.64	1.21
1:C:263:PHE:CZ	1:C:293:ALA:HB1	1.71	1.20
1:A:259:TYR:CE2	3:X:2:UNK:O	1.93	1.20
2:J:31:PHE:HZ	2:K:21:ILE:CD1	1.47	1.20
1:B:540:TYR:OH	1:C:528:HIS:CG	1.93	1.20
2:I:32:ASP:OD2	2:I:35:SER:CB	1.90	1.18
1:A:537:PRO:CD	1:B:528:HIS:NE2	2.05	1.18
2:N:17:VAL:HG13	2:N:33:ILE:CG2	1.70	1.18
1:C:263:PHE:CE2	1:C:293:ALA:CB	2.27	1.18
1:E:437:PRO:O	1:E:438:GLU:CB	1.83	1.17
1:E:335:ARG:NH2	5:E:802:ADP:O3B	1.76	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:441:VAL:CG1	1:F:721:LEU:CD2	2.22	1.16
2:H:17:VAL:CG1	2:H:33:ILE:HG22	1.74	1.16
1:C:527:ARG:N	1:C:570:HIS:CD2	2.15	1.15
2:I:29:ARG:CD	2:I:31:PHE:HE1	1.53	1.15
2:K:17:VAL:CG1	2:K:33:ILE:HG22	1.77	1.15
2:J:29:ARG:NE	2:K:28:GLU:OE1	1.79	1.15
2:N:18:PRO:HG2	2:N:33:ILE:HD13	1.24	1.14
1:E:442:SER:OG	1:E:446:ARG:HD3	1.33	1.13
1:B:287:ILE:HD12	1:B:320:GLY:CA	1.78	1.12
2:M:17:VAL:HG13	2:M:33:ILE:CG2	1.79	1.11
2:N:33:ILE:HG21	2:O:56:LEU:HD11	1.30	1.11
2:H:61:MET:HE3	2:H:93:THR:HG21	1.29	1.10
2:I:29:ARG:CD	2:I:31:PHE:CZ	2.31	1.10
1:A:250:ILE:HD13	1:A:290:ILE:HG21	1.32	1.10
1:B:540:TYR:OH	1:C:528:HIS:HB2	1.39	1.10
1:D:525:MET:O	1:D:570:HIS:HB2	1.51	1.09
2:K:17:VAL:HG13	2:K:33:ILE:HG22	1.17	1.09
2:H:18:PRO:HG2	2:H:33:ILE:HD13	1.18	1.09
2:I:17:VAL:CG1	2:I:33:ILE:HG22	1.82	1.09
1:B:386:VAL:HG22	1:B:394:LEU:HD11	1.36	1.08
2:H:32:ASP:OD2	2:I:15:ALA:HB2	1.50	1.08
1:E:719:GLU:HA	1:E:723:GLY:HA3	1.26	1.08
1:A:537:PRO:HG3	1:B:528:HIS:CE1	1.87	1.07
1:E:244:THR:HG21	1:E:246:TYR:CZ	1.87	1.07
1:B:287:ILE:HD13	1:B:320:GLY:HA3	1.32	1.07
2:I:50:GLU:O	2:I:86:ALA:HB1	1.52	1.07
1:E:441:VAL:CG1	1:F:721:LEU:HD23	1.83	1.07
2:J:31:PHE:CZ	2:K:21:ILE:CG1	2.37	1.07
1:A:250:ILE:HD13	1:A:290:ILE:CG2	1.83	1.07
1:E:244:THR:CG2	1:E:246:TYR:CE1	2.37	1.07
2:I:50:GLU:O	2:I:86:ALA:CB	2.03	1.06
2:I:137:GLN:NE2	2:P:145:GLN:OE1	1.88	1.06
1:D:236:VAL:HG12	1:D:237:PRO:HD2	1.37	1.06
1:E:179:LEU:O	1:E:183:GLY:O	1.73	1.05
1:E:348:GLU:OE2	1:E:394:LEU:N	1.90	1.05
1:A:250:ILE:HG21	1:A:290:ILE:CG2	1.86	1.05
1:A:537:PRO:HD3	1:B:528:HIS:CE1	1.91	1.05
2:M:18:PRO:HG2	2:M:33:ILE:HD13	1.36	1.05
1:D:348:GLU:OE2	1:D:393:HIS:HB3	1.56	1.05
1:A:307:ILE:CD1	1:A:340:ARG:HH12	1.68	1.04
2:M:17:VAL:HG13	2:M:33:ILE:HG22	1.13	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:719:GLU:CA	1:E:723:GLY:HA3	1.88	1.04
1:B:296:ALA:CB	3:X:1:UNK:O	2.06	1.03
1:C:263:PHE:CZ	1:C:293:ALA:HB2	1.88	1.03
2:I:32:ASP:OD2	2:I:35:SER:HB2	1.52	1.03
1:B:540:TYR:CE1	1:C:528:HIS:HD2	1.77	1.03
1:A:537:PRO:CD	1:B:528:HIS:CE1	2.42	1.02
1:A:259:TYR:HD2	3:X:2:UNK:O	1.18	1.02
1:B:637:THR:HB	1:B:638:PRO:HD3	1.39	1.02
1:E:441:VAL:HG11	1:F:721:LEU:HD23	1.34	1.02
1:B:287:ILE:CD1	1:B:320:GLY:CA	2.37	1.02
1:B:296:ALA:HB3	3:X:1:UNK:O	1.60	1.02
2:H:17:VAL:HG13	2:H:33:ILE:CG2	1.87	1.02
1:B:263:PHE:CZ	1:B:293:ALA:CB	2.43	1.01
1:B:578:LEU:HD11	1:B:643:ARG:HH11	1.25	1.01
1:D:296:ALA:O	1:D:297:SER:OG	1.77	1.01
2:I:31:PHE:HE2	2:J:21:ILE:HD11	1.24	1.01
1:E:441:VAL:HG11	1:F:721:LEU:HD21	1.37	1.01
2:G:128:LEU:HD22	2:G:129:PRO:HD2	1.42	1.01
1:B:354:THR:HG23	1:B:395:PRO:HB3	1.40	1.01
1:E:244:THR:HG21	1:E:246:TYR:CE1	1.95	1.01
1:B:354:THR:HG23	1:B:395:PRO:CB	1.91	1.00
1:D:538:PRO:HB2	1:E:536:ALA:HB2	1.40	1.00
2:N:17:VAL:HG13	2:N:33:ILE:HG22	1.03	1.00
1:B:578:LEU:HD12	1:B:643:ARG:HD2	1.42	1.00
1:A:282:LEU:HB3	1:A:318:VAL:HG22	1.43	1.00
1:C:527:ARG:HB2	1:C:570:HIS:NE2	1.77	0.99
2:H:31:PHE:HZ	2:I:21:ILE:CG1	1.76	0.99
1:E:442:SER:OG	1:E:446:ARG:CD	1.88	0.99
1:B:578:LEU:HD11	1:B:643:ARG:NH1	1.77	0.99
1:C:263:PHE:CE2	1:C:293:ALA:HB3	1.95	0.98
1:B:263:PHE:CZ	1:B:293:ALA:HB1	1.98	0.98
1:B:296:ALA:HB2	3:X:1:UNK:CA	1.92	0.98
2:H:61:MET:HE3	2:H:93:THR:CG2	1.93	0.98
2:N:17:VAL:CG1	2:N:32:ASP:OD1	2.11	0.98
1:B:386:VAL:CG2	1:B:394:LEU:HD11	1.93	0.98
2:N:18:PRO:CG	2:N:33:ILE:HD13	1.92	0.98
2:H:31:PHE:HZ	2:I:21:ILE:HG13	1.25	0.97
2:M:17:VAL:HG11	2:M:32:ASP:OD1	1.64	0.97
1:A:537:PRO:CG	1:B:528:HIS:NE2	2.28	0.97
5:E:802:ADP:O2A	1:F:221:THR:OG1	1.83	0.97
2:K:17:VAL:HG13	2:K:33:ILE:CG2	1.93	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:PRO:CG	1:B:528:HIS:CE1	2.49	0.96
1:B:719:GLU:O	1:B:725:LEU:HB3	1.66	0.96
2:J:31:PHE:CZ	2:K:21:ILE:HG13	2.00	0.95
2:H:17:VAL:HG13	2:H:33:ILE:HG22	1.44	0.95
1:E:441:VAL:O	1:E:443:GLN:N	2.00	0.95
1:F:617:ILE:HG21	2:I:40:GLU:HG3	1.46	0.95
1:C:263:PHE:CE1	1:C:293:ALA:HB1	2.00	0.95
1:E:441:VAL:HG21	1:E:478:ARG:O	1.67	0.95
1:B:287:ILE:HD12	1:B:320:GLY:HA2	1.47	0.95
1:C:348:GLU:OE2	1:C:394:LEU:N	2.00	0.94
1:A:307:ILE:HD12	1:A:340:ARG:HH12	0.78	0.94
2:H:29:ARG:HH21	2:H:39:LYS:NZ	1.64	0.94
2:H:18:PRO:CG	2:H:33:ILE:HD13	1.97	0.94
1:C:439:LYS:HE2	1:C:439:LYS:H	1.31	0.94
2:N:17:VAL:HG11	2:N:32:ASP:OD1	1.66	0.94
2:M:18:PRO:CG	2:M:33:ILE:HD13	1.97	0.94
1:E:719:GLU:HA	1:E:723:GLY:CA	1.96	0.93
2:I:17:VAL:HG13	2:I:33:ILE:CG2	1.98	0.93
1:E:502:THR:OG1	6:E:803:AGS:O1A	1.86	0.93
1:D:719:GLU:HB3	1:D:725:LEU:CD1	1.98	0.93
2:I:32:ASP:OD2	2:I:35:SER:N	2.00	0.93
1:B:578:LEU:CD1	1:B:643:ARG:HH11	1.81	0.92
1:B:349:PRO:HG3	1:B:395:PRO:HD3	1.51	0.92
1:B:633:LYS:HG2	1:B:641:ARG:HH12	1.34	0.92
1:A:288:HIS:CA	1:A:291:ILE:HD11	1.99	0.92
2:G:105:CYS:O	2:G:105:CYS:SG	2.25	0.92
1:B:296:ALA:HB2	3:X:1:UNK:C	1.99	0.92
2:I:137:GLN:NE2	2:P:145:GLN:CD	2.28	0.92
1:D:260:ARG:NH2	1:D:298:GLY:O	2.02	0.92
1:A:250:ILE:CD1	1:A:290:ILE:HG21	2.00	0.91
1:A:537:PRO:HD2	1:B:528:HIS:NE2	1.83	0.91
1:A:348:GLU:OE2	1:A:394:LEU:N	2.02	0.90
2:G:106:MET:HA	2:G:128:LEU:HD12	1.53	0.90
1:A:287:ILE:N	1:A:321:SER:O	2.04	0.90
2:N:18:PRO:HG2	2:N:33:ILE:CD1	2.01	0.90
1:B:540:TYR:CZ	1:C:528:HIS:CG	2.55	0.90
1:E:719:GLU:OE1	1:E:723:GLY:CA	2.19	0.90
2:G:106:MET:CA	2:G:128:LEU:HD12	2.01	0.90
1:B:540:TYR:CE1	1:C:528:HIS:CD2	2.57	0.90
2:I:29:ARG:HG3	2:I:29:ARG:HH11	1.38	0.89
1:B:624:ASN:O	1:B:624:ASN:ND2	2.06	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:ARG:HB2	1:C:570:HIS:CE1	2.08	0.89
1:B:296:ALA:HB2	3:X:1:UNK:CB	2.01	0.89
1:A:250:ILE:CG2	1:A:290:ILE:HG21	2.03	0.89
2:N:33:ILE:HG21	2:O:56:LEU:CD1	2.01	0.88
1:B:633:LYS:HG3	1:B:641:ARG:NH1	1.88	0.88
1:B:296:ALA:CB	3:X:1:UNK:C	2.52	0.88
1:C:263:PHE:CE2	1:C:293:ALA:HB1	1.99	0.88
1:E:244:THR:HG22	1:E:246:TYR:CE1	2.08	0.87
2:I:17:VAL:CG1	2:I:33:ILE:CG2	2.52	0.87
1:A:250:ILE:HG21	1:A:290:ILE:HG21	1.54	0.87
1:B:633:LYS:CG	1:B:641:ARG:NH1	2.37	0.87
2:J:31:PHE:CE2	2:K:21:ILE:CD1	2.43	0.87
1:B:263:PHE:CZ	1:B:293:ALA:HB3	2.09	0.87
1:E:440:SER:CB	1:E:443:GLN:HA	2.05	0.87
1:C:524:TYR:CZ	1:C:533:LEU:HD21	2.09	0.87
2:K:50:GLU:O	2:K:86:ALA:HB1	1.74	0.86
2:L:50:GLU:O	2:L:86:ALA:CB	2.23	0.86
1:A:308:LYS:NZ	1:A:336:ALA:HB1	1.90	0.86
2:G:50:GLU:O	2:G:86:ALA:CB	2.24	0.85
1:A:209:ASN:OD1	1:A:317:ARG:HA	1.77	0.85
1:B:540:TYR:HH	1:C:528:HIS:HB2	1.41	0.85
2:I:17:VAL:HG12	2:I:33:ILE:HG22	1.59	0.85
1:B:236:VAL:HB	1:B:237:PRO:HD2	1.57	0.84
2:S:124:LYS:HA	2:S:126:PHE:CE1	2.12	0.84
1:D:348:GLU:CD	1:D:393:HIS:HB3	2.03	0.84
1:D:547:GLY:O	1:D:551:ASP:HB3	1.77	0.84
1:D:567:GLU:CD	1:D:606:ASN:H	1.86	0.84
1:E:438:GLU:O	1:E:439:LYS:CG	2.22	0.84
2:I:31:PHE:CE2	2:J:21:ILE:HD11	2.13	0.83
1:A:250:ILE:CG2	1:A:290:ILE:CG2	2.56	0.83
1:B:637:THR:CB	1:B:638:PRO:HD3	2.09	0.83
1:D:547:GLY:O	1:D:551:ASP:CB	2.27	0.83
1:F:677:GLY:O	1:F:728:GLY:HA2	1.76	0.83
1:D:299:GLY:HA2	1:E:297:SER:OG	1.77	0.83
1:F:619:LEU:O	2:H:96:PHE:HZ	1.62	0.82
2:K:50:GLU:O	2:K:86:ALA:CB	2.26	0.82
2:I:111:SER:OG	2:I:136:HIS:HE1	1.61	0.82
2:L:17:VAL:CG1	2:L:32:ASP:OD1	2.27	0.82
2:M:17:VAL:CG1	2:M:32:ASP:OD1	2.27	0.82
2:L:50:GLU:O	2:L:86:ALA:HB1	1.80	0.82
1:E:440:SER:OG	1:E:443:GLN:HA	1.79	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:29:ARG:HB3	2:O:31:PHE:HE1	1.45	0.82
1:C:586:LEU:HD12	1:D:523:GLU:OE2	1.78	0.82
1:D:499:VAL:CG1	1:D:501:LYS:HG3	2.11	0.81
2:J:29:ARG:HG2	2:K:28:GLU:CD	2.05	0.81
1:B:625:SER:O	1:B:628:ALA:HB2	1.79	0.81
1:C:527:ARG:CA	1:C:570:HIS:CD2	2.62	0.81
2:H:105:CYS:HB3	2:H:127:CYS:HA	1.62	0.81
1:D:567:GLU:OE2	1:D:606:ASN:HB2	1.81	0.81
5:E:802:ADP:O2A	1:F:221:THR:CB	2.29	0.81
1:A:258:LYS:O	1:A:299:GLY:N	2.14	0.81
2:N:124:LYS:HA	2:N:126:PHE:CZ	2.16	0.80
2:I:18:PRO:HG2	2:I:33:ILE:HD13	1.62	0.80
1:A:311:LEU:HD12	1:A:311:LEU:N	1.96	0.80
2:H:18:PRO:HG2	2:H:33:ILE:CD1	2.05	0.80
2:J:31:PHE:HE2	2:K:21:ILE:HD11	1.35	0.80
1:E:348:GLU:CD	1:E:394:LEU:H	1.90	0.80
2:M:18:PRO:HG2	2:M:33:ILE:CD1	2.11	0.80
1:E:719:GLU:OE1	1:E:723:GLY:HA3	1.78	0.80
1:A:208:ASN:ND2	1:A:317:ARG:HD2	1.97	0.80
2:J:31:PHE:HZ	2:K:21:ILE:HD12	1.45	0.80
1:E:438:GLU:C	1:E:439:LYS:HG2	2.07	0.79
2:H:17:VAL:CG1	2:H:33:ILE:CG2	2.51	0.79
1:B:389:ILE:CG2	1:B:397:LYS:HD3	2.12	0.79
1:B:626:THR:O	1:B:628:ALA:N	2.15	0.79
1:F:617:ILE:CG2	2:I:40:GLU:HG3	2.12	0.79
2:N:124:LYS:HA	2:N:126:PHE:CE1	2.18	0.79
1:B:540:TYR:CZ	1:C:528:HIS:HD2	1.78	0.79
2:G:125:ARG:O	2:G:199:VAL:HB	1.83	0.79
1:D:236:VAL:HG12	1:D:237:PRO:CD	2.12	0.79
1:E:437:PRO:O	1:E:438:GLU:HB2	0.90	0.78
2:I:31:PHE:HE2	2:J:21:ILE:CD1	1.95	0.78
1:B:540:TYR:OH	1:C:528:HIS:HB3	1.79	0.78
1:B:637:THR:CB	1:B:638:PRO:CD	2.61	0.78
1:B:633:LYS:CG	1:B:641:ARG:HH12	1.95	0.78
2:L:124:LYS:HA	2:L:126:PHE:CE1	2.19	0.78
2:I:111:SER:OG	2:I:136:HIS:CE1	2.37	0.78
2:L:17:VAL:CG1	2:L:33:ILE:HG22	2.14	0.78
1:C:439:LYS:H	1:C:439:LYS:CE	1.96	0.78
1:B:296:ALA:HB2	3:X:1:UNK:O	1.80	0.78
1:B:237:PRO:HD2	1:B:240:MET:HB2	1.65	0.78
2:H:31:PHE:CZ	2:I:21:ILE:CG1	2.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:THR:CG2	1:B:395:PRO:HB3	2.13	0.77
1:A:311:LEU:HD12	1:A:311:LEU:H	1.48	0.77
1:B:578:LEU:CD1	1:B:643:ARG:NH1	2.43	0.77
1:C:720:LEU:O	1:C:726:VAL:HG23	1.85	0.77
2:L:56:LEU:HD11	2:M:33:ILE:HG21	1.67	0.77
2:P:22:GLU:OE2	2:P:31:PHE:HZ	1.68	0.77
1:E:440:SER:HB2	1:E:443:GLN:N	1.98	0.77
2:J:29:ARG:HG2	2:K:28:GLU:OE2	1.85	0.77
2:G:128:LEU:CD2	2:G:129:PRO:HD2	2.15	0.77
1:B:195:LEU:O	1:B:199:ILE:HG12	1.85	0.76
1:B:630:GLU:C	1:B:632:ILE:H	1.92	0.76
2:N:20:VAL:HB	2:O:63:PHE:CZ	2.20	0.76
2:O:29:ARG:HB3	2:O:31:PHE:CE1	2.21	0.76
1:E:438:GLU:C	1:E:439:LYS:CG	2.58	0.76
1:E:441:VAL:HG21	1:E:478:ARG:C	2.11	0.76
2:L:17:VAL:HG11	2:L:32:ASP:OD1	1.83	0.76
1:A:208:ASN:ND2	1:A:317:ARG:CD	2.49	0.76
2:I:32:ASP:OD2	2:I:35:SER:OG	2.02	0.76
1:B:215:GLU:OE2	1:C:555:LYS:HE2	1.85	0.75
2:L:17:VAL:HG13	2:L:33:ILE:HG22	1.68	0.75
2:J:124:LYS:HA	2:J:126:PHE:CE1	2.21	0.75
1:A:308:LYS:CE	1:A:336:ALA:HB1	2.15	0.75
1:E:440:SER:N	1:E:441:VAL:HA	2.02	0.75
1:B:389:ILE:HG22	1:B:397:LYS:HD3	1.67	0.75
1:E:440:SER:HB2	1:E:443:GLN:CA	2.17	0.75
2:N:21:ILE:HD11	2:O:31:PHE:HE2	1.51	0.75
1:D:538:PRO:CB	1:E:536:ALA:HB2	2.16	0.75
1:E:442:SER:O	1:E:443:GLN:C	2.30	0.75
1:D:499:VAL:HG12	1:D:501:LYS:HG3	1.69	0.75
2:O:22:GLU:OE2	2:O:39:LYS:NZ	2.20	0.75
1:B:349:PRO:CG	1:B:395:PRO:HD3	2.18	0.74
2:I:29:ARG:CG	2:I:31:PHE:CZ	2.71	0.74
2:K:19:MET:HE3	2:K:31:PHE:O	1.86	0.74
1:A:315:LYS:HD2	1:A:315:LYS:N	2.02	0.74
1:B:637:THR:HB	1:B:638:PRO:CD	2.17	0.74
1:D:354:THR:HG23	1:D:395:PRO:HB3	1.68	0.74
2:H:17:VAL:HG12	2:H:33:ILE:HG22	1.67	0.74
2:P:22:GLU:OE2	2:P:31:PHE:CZ	2.40	0.74
1:A:260:ARG:HB3	3:X:1:UNK:CB	2.18	0.74
1:B:540:TYR:CE2	1:C:528:HIS:CD2	2.75	0.74
1:D:719:GLU:HB3	1:D:725:LEU:HD12	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:33:ILE:HD11	2:O:60:GLN:HG2	1.70	0.73
2:H:29:ARG:HH21	2:H:39:LYS:HZ2	1.33	0.73
1:A:250:ILE:HG21	1:A:290:ILE:HG22	1.69	0.73
1:A:284:ILE:CD1	1:A:318:VAL:HG11	2.18	0.73
2:H:26:ARG:NE	2:H:26:ARG:H	1.87	0.73
2:H:61:MET:CE	2:H:93:THR:CG2	2.65	0.73
3:X:7:UNK:C	3:X:8:UNK:O	2.19	0.73
1:D:296:ALA:C	1:D:297:SER:HG	1.89	0.73
1:E:440:SER:HB2	1:E:443:GLN:HA	1.68	0.73
1:B:389:ILE:HB	1:B:397:LYS:CD	2.20	0.72
1:E:436:ILE:HG22	1:E:437:PRO:N	2.04	0.72
1:E:441:VAL:CG2	1:E:478:ARG:O	2.37	0.72
2:H:17:VAL:HG13	2:H:33:ILE:HG21	1.69	0.72
1:A:287:ILE:HG22	1:A:321:SER:H	1.55	0.72
1:A:307:ILE:HD12	1:A:340:ARG:CZ	2.17	0.72
1:B:263:PHE:CE1	1:B:293:ALA:HB1	2.23	0.72
1:C:524:TYR:CE2	1:C:533:LEU:HD21	2.25	0.72
2:I:32:ASP:CG	2:I:35:SER:H	1.97	0.72
1:A:288:HIS:HA	1:A:291:ILE:HD11	1.70	0.72
1:A:304:ALA:O	1:A:307:ILE:HG13	1.88	0.72
2:N:17:VAL:HG12	2:N:32:ASP:OD1	1.87	0.72
2:N:124:LYS:C	2:N:126:PHE:CE1	2.67	0.72
1:D:302:ASP:OD1	1:D:302:ASP:N	2.14	0.72
2:G:50:GLU:O	2:G:86:ALA:HB1	1.88	0.72
1:A:250:ILE:CD1	1:A:290:ILE:HG12	2.19	0.72
2:P:17:VAL:HG11	2:P:32:ASP:OD1	1.90	0.72
1:C:527:ARG:H	1:C:570:HIS:CD2	2.08	0.72
2:I:32:ASP:OD2	2:I:35:SER:CA	2.37	0.72
2:I:29:ARG:HH11	2:I:29:ARG:CG	2.03	0.71
2:T:124:LYS:HA	2:T:126:PHE:CE1	2.24	0.71
1:F:619:LEU:O	2:H:96:PHE:CZ	2.44	0.71
1:A:250:ILE:CG1	1:A:290:ILE:HG21	2.19	0.71
1:B:236:VAL:HB	1:B:237:PRO:CD	2.19	0.71
1:E:335:ARG:HH22	5:E:802:ADP:PB	2.13	0.71
1:A:537:PRO:HG3	1:B:528:HIS:NE2	1.98	0.71
1:C:439:LYS:HE2	1:C:439:LYS:N	2.05	0.71
1:D:538:PRO:HB2	1:E:536:ALA:CB	2.19	0.71
5:E:802:ADP:O2B	1:F:217:GLY:N	2.23	0.71
1:A:537:PRO:HG2	1:A:540:TYR:CD1	2.25	0.71
1:E:441:VAL:HG13	1:E:442:SER:N	2.06	0.71
2:J:31:PHE:CE1	2:K:21:ILE:HG13	2.25	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:56:LEU:HD11	2:K:33:ILE:HG21	1.73	0.71
1:E:443:GLN:HG3	1:E:444:SER:N	2.06	0.71
1:B:540:TYR:HH	1:C:528:HIS:CB	1.96	0.70
2:I:29:ARG:CG	2:I:31:PHE:CE1	2.74	0.70
1:A:262:ASP:OD1	1:A:265:LYS:HE2	1.91	0.70
2:Q:124:LYS:HA	2:Q:126:PHE:CE1	2.26	0.70
1:A:308:LYS:HZ2	1:A:336:ALA:HB1	1.56	0.70
2:H:103:THR:HG23	2:H:120:GLY:HA3	1.73	0.70
1:A:288:HIS:N	1:A:291:ILE:HD11	2.07	0.70
1:F:616:SER:HB2	1:F:621:HIS:HB2	1.74	0.70
1:C:436:ILE:HD11	1:C:598:ASN:CG	2.17	0.70
1:E:440:SER:CB	1:E:443:GLN:CA	2.70	0.70
1:C:527:ARG:HA	1:C:570:HIS:CG	2.27	0.69
1:F:619:LEU:HD21	2:H:62:LEU:HD21	1.72	0.69
2:O:124:LYS:HA	2:O:126:PHE:CE1	2.26	0.69
1:A:208:ASN:HD21	1:A:317:ARG:HD3	1.57	0.69
1:C:527:ARG:N	1:C:570:HIS:HD2	1.87	0.69
1:C:570:HIS:HB3	1:C:573:VAL:HG23	1.75	0.69
1:D:260:ARG:CZ	1:D:298:GLY:O	2.40	0.69
2:H:31:PHE:CZ	2:I:21:ILE:HG13	2.17	0.69
1:C:439:LYS:NZ	1:C:439:LYS:HB3	2.06	0.69
2:I:17:VAL:HG13	2:I:33:ILE:HG21	1.73	0.69
2:J:17:VAL:CG1	2:J:33:ILE:HG22	2.23	0.69
1:B:357:ILE:HD11	1:B:395:PRO:CG	2.23	0.69
1:E:719:GLU:O	1:E:723:GLY:N	2.26	0.69
2:I:29:ARG:HG3	2:I:29:ARG:NH1	2.07	0.69
1:B:540:TYR:CZ	1:C:528:HIS:HB2	2.27	0.68
1:A:307:ILE:O	1:A:309:PRO:N	2.26	0.68
2:H:85:THR:O	2:H:85:THR:OG1	2.10	0.68
1:B:354:THR:HG23	1:B:395:PRO:HB2	1.73	0.68
1:D:231:ILE:HA	1:D:236:VAL:HG21	1.75	0.68
1:B:632:ILE:O	1:B:635:ILE:HB	1.94	0.68
2:S:22:GLU:OE1	2:S:31:PHE:CE2	2.47	0.68
1:E:441:VAL:CG1	1:F:721:LEU:HD22	2.22	0.67
1:A:311:LEU:HD11	1:A:340:ARG:HH11	1.59	0.67
1:C:439:LYS:O	1:C:439:LYS:HG2	1.93	0.67
2:M:17:VAL:HG12	2:M:33:ILE:HG22	1.74	0.67
1:A:250:ILE:HD13	1:A:290:ILE:HG23	1.76	0.67
5:E:802:ADP:H5'1	1:F:219:GLY:HA2	1.75	0.67
1:E:540:TYR:O	4:Y:11:UNK:HA	1.94	0.67
1:B:288:HIS:CE1	1:B:326:GLU:CD	2.72	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:ALA:HB3	1:B:632:ILE:HD11	1.76	0.67
1:D:500:GLY:O	1:D:504:VAL:N	2.27	0.67
1:E:244:THR:CG2	1:E:246:TYR:CZ	2.66	0.67
1:E:540:TYR:HA	4:Y:11:UNK:HA	1.77	0.67
1:B:389:ILE:HB	1:B:397:LYS:HD2	1.77	0.67
1:A:208:ASN:HD21	1:A:317:ARG:CD	2.06	0.66
1:A:288:HIS:HB2	1:A:326:GLU:HB3	1.77	0.66
1:E:440:SER:HB2	1:E:441:VAL:O	1.94	0.66
2:N:21:ILE:HD11	2:O:31:PHE:CE2	2.30	0.66
1:D:354:THR:HG23	1:D:395:PRO:CB	2.24	0.66
2:P:17:VAL:CG1	2:P:32:ASP:OD1	2.43	0.66
1:B:296:ALA:HB2	3:X:1:UNK:N	2.11	0.66
2:G:106:MET:CB	2:G:128:LEU:HD12	2.26	0.65
2:I:29:ARG:CD	2:I:31:PHE:HZ	2.00	0.65
1:E:441:VAL:HG13	1:E:442:SER:H	1.60	0.65
1:F:617:ILE:HD11	2:H:63:PHE:HA	1.78	0.65
1:B:287:ILE:HG22	1:B:322:THR:HB	1.76	0.65
1:D:499:VAL:HG13	1:D:500:GLY:N	2.11	0.65
1:E:534:ILE:O	1:E:547:GLY:HA3	1.96	0.65
1:B:218:VAL:HG22	1:B:346:ILE:HG22	1.79	0.65
1:A:567:GLU:OE1	1:A:605:THR:HA	1.97	0.65
1:B:581:MET:HE3	1:B:643:ARG:HD3	1.78	0.65
1:D:231:ILE:HA	1:D:236:VAL:CG2	2.26	0.65
1:C:527:ARG:HA	1:C:570:HIS:CD2	2.31	0.65
1:E:244:THR:HG21	1:E:246:TYR:OH	1.97	0.65
2:I:21:ILE:HD13	2:I:30:SER:HB2	1.79	0.65
2:J:76:TYR:CD2	2:J:106:MET:CE	2.80	0.65
5:E:802:ADP:O2'	1:F:222:ALA:HB2	1.97	0.65
1:A:250:ILE:HD11	1:A:290:ILE:HG12	1.78	0.65
2:I:21:ILE:HD13	2:I:30:SER:CB	2.27	0.65
1:E:719:GLU:CB	1:E:723:GLY:HA3	2.27	0.64
1:C:524:TYR:CE2	1:C:533:LEU:CD2	2.80	0.64
2:Q:20:VAL:HB	2:R:63:PHE:CZ	2.32	0.64
1:C:567:GLU:HG2	1:C:567:GLU:O	1.97	0.64
2:R:29:ARG:HB3	2:R:31:PHE:HE1	1.60	0.64
2:J:29:ARG:CG	2:K:28:GLU:OE1	2.45	0.64
1:A:259:TYR:HE2	3:X:2:UNK:O	1.70	0.64
1:D:301:VAL:CG2	1:E:295:ALA:HB1	2.28	0.64
2:L:17:VAL:HG12	2:L:32:ASP:OD1	1.96	0.64
2:P:17:VAL:CG1	2:P:32:ASP:OD2	2.46	0.64
1:C:719:GLU:HB3	1:C:725:LEU:HB2	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:ILE:O	1:D:397:LYS:HD3	1.97	0.64
1:D:566:ILE:O	1:D:566:ILE:HG13	1.98	0.64
2:J:29:ARG:HG2	2:K:28:GLU:OE1	1.97	0.64
2:J:29:ARG:CD	2:K:28:GLU:OE1	2.45	0.64
1:C:527:ARG:CB	1:C:570:HIS:NE2	2.58	0.63
1:A:537:PRO:HG3	1:B:528:HIS:CD2	2.34	0.63
1:C:254:LEU:CD2	1:C:263:PHE:CE1	2.82	0.63
2:G:128:LEU:HD22	2:G:129:PRO:CD	2.24	0.63
1:D:389:ILE:O	1:D:397:LYS:CD	2.47	0.63
1:A:537:PRO:CG	1:B:528:HIS:CD2	2.82	0.63
1:B:630:GLU:HB3	1:B:633:LYS:HE3	1.80	0.62
1:D:236:VAL:CG1	1:D:237:PRO:HD2	2.23	0.62
1:E:436:ILE:CG2	1:E:437:PRO:N	2.61	0.62
2:J:17:VAL:HG13	2:J:33:ILE:HG22	1.82	0.62
2:N:124:LYS:CA	2:N:126:PHE:CE1	2.81	0.62
1:E:441:VAL:HG21	1:E:478:ARG:HB3	1.82	0.62
2:H:115:PHE:CZ	2:H:163:MET:HE1	2.34	0.62
1:B:218:VAL:HG21	1:B:346:ILE:O	2.00	0.62
2:K:17:VAL:HG12	2:K:33:ILE:HG22	1.78	0.62
1:B:263:PHE:HZ	1:B:293:ALA:HB3	1.64	0.62
1:B:610:ARG:O	1:B:610:ARG:HG2	1.99	0.62
1:C:526:GLU:C	1:C:570:HIS:CD2	2.78	0.62
2:G:129:PRO:HD2	2:M:92:ASP:OD2	2.00	0.62
1:D:567:GLU:OE1	1:D:605:THR:HA	1.99	0.62
1:B:626:THR:C	1:B:628:ALA:N	2.55	0.62
1:E:348:GLU:HG2	1:E:349:PRO:HD2	1.82	0.62
1:B:629:MET:SD	1:B:631:GLU:HB2	2.40	0.62
2:J:124:LYS:HA	2:J:126:PHE:CZ	2.35	0.62
1:A:308:LYS:NZ	1:A:336:ALA:CB	2.62	0.61
1:C:261:GLY:O	1:C:265:LYS:HG3	2.00	0.61
1:B:581:MET:HE3	1:B:643:ARG:CD	2.30	0.61
1:B:732:THR:HG22	1:B:732:THR:O	2.00	0.61
1:D:499:VAL:HG13	1:D:501:LYS:H	1.64	0.61
5:E:802:ADP:C8	1:F:395:PRO:HG2	2.34	0.61
2:R:29:ARG:HB3	2:R:31:PHE:CE1	2.35	0.61
1:D:271:LEU:O	1:D:275:GLU:HG3	2.00	0.61
1:F:622:GLN:O	1:F:624:ASN:N	2.33	0.61
1:A:260:ARG:HA	1:A:299:GLY:HA2	1.82	0.61
1:C:254:LEU:HD21	1:C:263:PHE:CE1	2.34	0.61
1:C:719:GLU:HB3	1:C:724:SER:OG	2.00	0.61
1:A:287:ILE:HG22	1:A:321:SER:O	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LEU:HD23	1:A:315:LYS:HD3	1.82	0.61
1:D:238:GLU:CD	1:D:238:GLU:H	2.08	0.61
1:D:553:VAL:HG11	1:D:594:ALA:HB1	1.82	0.61
1:D:294:GLY:HA3	1:D:302:ASP:HA	1.82	0.61
2:H:61:MET:CE	2:H:93:THR:HG22	2.30	0.61
2:I:137:GLN:CD	2:P:145:GLN:CD	2.68	0.61
2:L:56:LEU:CD1	2:M:33:ILE:HG21	2.30	0.61
2:H:26:ARG:O	2:H:26:ARG:HG2	1.99	0.61
2:P:124:LYS:HA	2:P:126:PHE:CE1	2.36	0.61
1:D:547:GLY:O	1:D:551:ASP:HB2	2.01	0.61
2:H:115:PHE:CE2	2:H:163:MET:HE1	2.35	0.61
1:A:311:LEU:HD13	1:A:311:LEU:C	2.26	0.60
1:A:348:GLU:OE2	1:A:394:LEU:CB	2.48	0.60
1:E:441:VAL:HG12	1:F:721:LEU:HD23	1.79	0.60
2:T:29:ARG:HB3	2:T:31:PHE:HE1	1.65	0.60
1:C:290:ILE:HD12	1:C:290:ILE:O	2.01	0.60
1:F:617:ILE:CG2	2:I:40:GLU:CG	2.80	0.60
1:E:440:SER:CB	1:E:443:GLN:N	2.64	0.60
2:J:29:ARG:HH21	2:K:28:GLU:HB2	1.67	0.60
6:E:803:AGS:O2A	6:E:803:AGS:H4'	2.01	0.60
1:F:621:HIS:HD2	2:I:206:ARG:NH1	2.00	0.60
2:G:28:GLU:OE2	2:M:26:ARG:NE	2.35	0.60
1:B:626:THR:C	1:B:628:ALA:H	2.10	0.59
2:L:124:LYS:HA	2:L:126:PHE:CZ	2.36	0.59
2:S:21:ILE:CD1	2:S:30:SER:HB2	2.31	0.59
1:A:311:LEU:HD11	1:A:340:ARG:HD2	1.83	0.59
1:B:357:ILE:HD11	1:B:395:PRO:HG2	1.82	0.59
1:C:291:ILE:HG22	1:C:291:ILE:O	2.00	0.59
2:N:17:VAL:HG13	2:N:33:ILE:HG21	1.76	0.59
1:A:264:GLU:OE2	1:A:300:GLN:O	2.20	0.59
2:G:106:MET:CB	2:G:128:LEU:CD1	2.80	0.59
2:H:26:ARG:H	2:H:26:ARG:HE	1.49	0.59
2:H:90:ILE:HG22	2:H:90:ILE:O	2.03	0.59
2:P:17:VAL:CG1	2:P:32:ASP:CG	2.75	0.59
1:B:296:ALA:CB	3:X:1:UNK:N	2.65	0.59
2:S:21:ILE:HD11	2:T:31:PHE:HE2	1.67	0.59
2:H:105:CYS:HB3	2:H:127:CYS:CB	2.33	0.59
1:B:579:GLN:O	1:B:579:GLN:HG2	2.01	0.59
2:J:104:ILE:HA	2:J:126:PHE:O	2.02	0.59
1:A:551:ASP:OD1	1:A:551:ASP:N	2.34	0.58
1:B:503:GLU:OE1	1:B:503:GLU:HA	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:617:ILE:HG23	1:F:617:ILE:O	2.02	0.58
1:B:349:PRO:HD2	1:B:394:LEU:O	2.04	0.58
2:H:105:CYS:HB3	2:H:127:CYS:CA	2.30	0.58
2:K:19:MET:CE	2:K:31:PHE:O	2.52	0.58
1:C:439:LYS:HB3	1:C:439:LYS:HZ3	1.66	0.58
1:C:719:GLU:CB	1:C:724:SER:OG	2.51	0.58
2:L:26:ARG:HB2	2:L:26:ARG:NH1	2.19	0.58
1:E:175:ASN:HB2	1:E:246:TYR:CE2	2.38	0.58
1:D:719:GLU:O	1:D:725:LEU:HD12	2.04	0.58
2:H:63:PHE:CZ	2:I:20:VAL:HB	2.39	0.58
2:H:29:ARG:HH21	2:H:39:LYS:HZ1	1.47	0.58
1:A:537:PRO:HG3	1:B:528:HIS:ND1	2.16	0.58
2:G:128:LEU:CD2	2:G:129:PRO:CD	2.81	0.58
2:J:76:TYR:CD2	2:J:106:MET:HE3	2.38	0.58
1:E:534:ILE:O	1:E:547:GLY:CA	2.52	0.58
2:H:47:GLY:O	2:H:79:SER:HB2	2.04	0.58
1:F:621:HIS:HD2	2:I:206:ARG:CZ	2.15	0.58
2:H:32:ASP:OD2	2:I:15:ALA:CB	2.41	0.58
2:I:29:ARG:HD3	2:I:31:PHE:HE1	0.80	0.58
1:A:349:PRO:HD2	1:A:395:PRO:HD3	1.87	0.57
1:C:524:TYR:CZ	1:C:533:LEU:CD2	2.86	0.57
1:C:540:TYR:HA	4:Y:7:UNK:HA	1.85	0.57
1:C:524:TYR:CE2	1:C:533:LEU:HG	2.39	0.57
1:D:348:GLU:OE2	1:D:393:HIS:CB	2.44	0.57
2:L:17:VAL:HG13	2:L:33:ILE:CG2	2.34	0.57
2:L:124:LYS:C	2:L:126:PHE:CE1	2.82	0.57
2:S:124:LYS:CA	2:S:126:PHE:CE1	2.87	0.57
1:D:297:SER:HB2	1:D:298:GLY:HA2	1.86	0.57
2:N:17:VAL:CG1	2:N:33:ILE:CG2	2.48	0.57
1:F:617:ILE:HG21	2:I:40:GLU:CG	2.30	0.57
1:B:578:LEU:CD1	1:B:643:ARG:HD2	2.26	0.57
2:N:33:ILE:CG2	2:O:56:LEU:CD1	2.81	0.57
1:A:287:ILE:HG22	1:A:321:SER:C	2.30	0.57
1:B:296:ALA:CB	3:X:1:UNK:CA	2.77	0.57
1:B:629:MET:HG3	1:B:631:GLU:HB2	1.87	0.57
2:H:115:PHE:CE1	2:H:163:MET:CE	2.88	0.57
1:E:723:GLY:O	1:E:726:VAL:HG13	2.05	0.56
2:H:51:ASP:OD1	2:H:86:ALA:CB	2.52	0.56
1:B:566:ILE:HG13	1:B:566:ILE:O	2.05	0.56
1:E:540:TYR:O	4:Y:10:UNK:O	2.21	0.56
2:I:29:ARG:HG2	2:I:31:PHE:CZ	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:124:LYS:HA	2:Q:126:PHE:CZ	2.41	0.56
1:B:263:PHE:HZ	1:B:293:ALA:CB	2.11	0.56
2:G:28:GLU:OE2	2:M:26:ARG:CD	2.54	0.56
2:I:137:GLN:HE22	2:O:184:ARG:HH22	1.54	0.56
2:R:155:GLU:HA	2:R:155:GLU:OE1	2.06	0.56
2:S:124:LYS:HA	2:S:126:PHE:CZ	2.41	0.56
2:T:29:ARG:HB3	2:T:31:PHE:CE1	2.41	0.56
2:T:91:TYR:OH	2:T:166:LEU:HD22	2.05	0.56
1:B:238:GLU:OE2	1:C:414:VAL:HG12	2.06	0.56
1:C:719:GLU:CB	1:C:725:LEU:HB2	2.36	0.56
2:I:137:GLN:NE2	2:I:183:GLU:O	2.38	0.56
2:M:18:PRO:HG2	2:M:33:ILE:HB	1.86	0.56
2:S:21:ILE:HD11	2:T:31:PHE:CE2	2.40	0.56
2:L:40:GLU:O	2:L:42:VAL:HG23	2.05	0.56
1:E:186:ASP:OD2	1:E:364:LYS:NZ	2.39	0.56
2:H:105:CYS:O	2:H:128:LEU:HG	2.06	0.56
1:A:264:GLU:CD	1:A:300:GLN:O	2.48	0.56
1:B:288:HIS:CE1	1:B:326:GLU:OE1	2.58	0.56
1:D:345:ASP:OD2	1:E:435:ARG:CZ	2.53	0.56
2:H:29:ARG:NH2	2:H:39:LYS:HZ2	2.03	0.56
2:L:124:LYS:CA	2:L:126:PHE:CE1	2.89	0.56
1:E:244:THR:HG22	1:E:246:TYR:CD1	2.41	0.56
2:M:17:VAL:HG13	2:M:33:ILE:HG21	1.83	0.55
1:A:307:ILE:O	1:A:308:LYS:C	2.46	0.55
2:L:60:GLN:HG2	2:M:33:ILE:HD11	1.88	0.55
1:A:288:HIS:HA	1:A:291:ILE:CD1	2.34	0.55
2:H:51:ASP:OD1	2:H:86:ALA:HB1	2.07	0.55
2:N:124:LYS:O	2:N:126:PHE:CE1	2.60	0.55
1:B:357:ILE:CD1	1:B:395:PRO:HG3	2.37	0.55
1:D:499:VAL:HG22	1:D:500:GLY:H	1.71	0.55
1:B:627:ASP:C	1:B:629:MET:H	2.13	0.55
1:C:263:PHE:HZ	1:C:293:ALA:HB2	1.61	0.55
2:H:88:MET:O	2:H:88:MET:HG3	2.06	0.55
2:J:124:LYS:C	2:J:126:PHE:CE1	2.85	0.55
2:P:21:ILE:CD1	2:P:30:SER:HB2	2.36	0.55
2:P:185:ASP:OD1	2:P:185:ASP:N	2.38	0.55
1:A:250:ILE:HD13	1:A:290:ILE:HG12	1.88	0.55
1:A:287:ILE:CG2	1:A:321:SER:H	2.20	0.55
1:D:725:LEU:HD23	1:D:746:PHE:CE1	2.42	0.55
1:E:719:GLU:OE1	1:E:723:GLY:HA2	2.05	0.55
2:H:29:ARG:NH2	2:H:39:LYS:NZ	2.46	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:105:CYS:HB3	2:H:127:CYS:HB2	1.89	0.55
1:B:194:GLU:N	1:B:194:GLU:OE1	2.40	0.54
1:B:629:MET:CG	1:B:631:GLU:HB2	2.36	0.54
1:C:260:ARG:HH12	1:D:300:GLN:HG2	1.71	0.54
1:D:236:VAL:CG1	1:D:237:PRO:CD	2.84	0.54
1:E:719:GLU:HA	1:E:723:GLY:N	2.22	0.54
2:H:103:THR:CG2	2:H:120:GLY:HA3	2.36	0.54
1:B:195:LEU:CD1	1:B:230:ARG:HE	2.21	0.54
1:D:297:SER:HA	1:D:299:GLY:H	1.72	0.54
2:I:50:GLU:O	2:I:86:ALA:HB2	1.99	0.54
1:C:527:ARG:CB	1:C:570:HIS:CE1	2.87	0.54
2:R:29:ARG:HD2	2:R:31:PHE:CZ	2.42	0.54
1:A:287:ILE:HG22	1:A:321:SER:N	2.22	0.54
1:A:311:LEU:N	1:A:311:LEU:CD1	2.70	0.54
1:A:290:ILE:HD12	1:A:290:ILE:O	2.08	0.54
1:B:195:LEU:HD11	1:B:230:ARG:HE	1.72	0.54
1:E:179:LEU:C	1:E:183:GLY:O	2.48	0.54
2:R:20:VAL:HB	2:S:63:PHE:CZ	2.43	0.54
1:B:450:LYS:HB2	1:C:722:PHE:HE2	1.71	0.54
2:O:29:ARG:HD2	2:O:31:PHE:CZ	2.42	0.54
1:A:259:TYR:O	1:A:299:GLY:HA2	2.09	0.53
1:A:250:ILE:CG2	1:A:290:ILE:HG22	2.33	0.53
1:E:335:ARG:CZ	5:E:802:ADP:O3B	2.52	0.53
2:H:18:PRO:HD2	2:H:33:ILE:HG21	1.90	0.53
2:H:26:ARG:HG2	2:H:26:ARG:HH11	1.72	0.53
2:H:95:GLN:NE2	2:H:95:GLN:N	2.56	0.53
2:J:76:TYR:HD2	2:J:106:MET:HE3	1.72	0.53
1:D:622:GLN:NE2	2:G:74:TYR:CE1	2.76	0.53
5:E:802:ADP:C8	1:F:395:PRO:CG	2.90	0.53
2:T:25:SER:OG	2:T:26:ARG:N	2.42	0.53
1:A:288:HIS:C	1:A:291:ILE:HD11	2.33	0.53
1:C:427:GLU:HB3	1:C:439:LYS:HZ2	1.74	0.53
1:D:345:ASP:OD2	1:E:435:ARG:NE	2.42	0.53
1:E:442:SER:O	1:E:443:GLN:O	2.27	0.53
1:D:389:ILE:HB	1:D:397:LYS:HD2	1.91	0.53
2:K:20:VAL:HG22	2:K:32:ASP:O	2.08	0.53
2:M:18:PRO:HG3	2:M:33:ILE:HD13	1.85	0.53
2:T:104:ILE:HA	2:T:126:PHE:O	2.09	0.53
1:B:633:LYS:C	1:B:635:ILE:N	2.65	0.53
1:E:719:GLU:OE1	1:E:724:SER:N	2.42	0.53
2:G:128:LEU:HD22	2:M:92:ASP:OD2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:GLY:HA2	1:B:324:TYR:CE1	2.44	0.53
2:I:29:ARG:HG2	2:I:31:PHE:CE1	2.44	0.53
2:M:32:ASP:C	2:M:34:TYR:H	2.17	0.53
1:B:608:GLY:HA3	1:B:629:MET:HB3	1.89	0.53
2:J:124:LYS:CA	2:J:126:PHE:CE1	2.91	0.53
1:A:208:ASN:O	1:A:317:ARG:HB3	2.08	0.52
1:B:710:ASP:OD1	1:B:714:LYS:NZ	2.42	0.52
1:E:348:GLU:HG2	1:E:394:LEU:HB2	1.91	0.52
1:A:259:TYR:O	1:A:299:GLY:CA	2.57	0.52
1:E:440:SER:H	1:E:441:VAL:HA	1.71	0.52
1:A:284:ILE:HD12	1:A:318:VAL:HG11	1.88	0.52
1:D:499:VAL:CG1	1:D:501:LYS:CG	2.86	0.52
1:E:441:VAL:C	1:E:443:GLN:N	2.67	0.52
1:E:719:GLU:O	1:E:723:GLY:CA	2.57	0.52
2:S:124:LYS:C	2:S:126:PHE:CE1	2.87	0.52
2:G:106:MET:HA	2:G:128:LEU:CD1	2.33	0.52
2:J:17:VAL:HG13	2:J:33:ILE:CG2	2.39	0.52
2:P:17:VAL:HG12	2:P:32:ASP:CG	2.35	0.52
1:A:287:ILE:HG12	1:A:291:ILE:HG12	1.92	0.52
1:C:439:LYS:N	1:C:439:LYS:HZ3	2.07	0.52
2:J:76:TYR:CD2	2:J:106:MET:HE1	2.45	0.52
2:S:22:GLU:CD	2:S:31:PHE:HE2	2.18	0.52
1:D:290:ILE:HD12	1:D:304:ALA:HB2	1.92	0.52
1:E:302:ASP:OD2	1:F:258:LYS:NZ	2.43	0.52
5:E:802:ADP:N1	1:F:188:LEU:HD12	2.24	0.52
2:O:124:LYS:C	2:O:126:PHE:CE1	2.88	0.52
1:C:726:VAL:HG12	1:C:726:VAL:O	2.10	0.52
1:D:275:GLU:OE2	1:D:310:LEU:HD22	2.10	0.52
1:F:671:VAL:O	1:F:675:GLN:HG3	2.09	0.52
2:G:128:LEU:HD22	2:M:92:ASP:CB	2.40	0.52
2:Q:25:SER:OG	2:Q:26:ARG:N	2.43	0.52
2:Q:104:ILE:HA	2:Q:126:PHE:O	2.09	0.52
1:B:637:THR:OG1	1:B:638:PRO:CD	2.57	0.52
1:E:441:VAL:CG2	1:E:478:ARG:HB3	2.39	0.52
1:F:619:LEU:CD2	2:H:62:LEU:HD21	2.40	0.52
1:F:621:HIS:CD2	2:I:206:ARG:NH1	2.77	0.52
1:A:537:PRO:HG3	1:B:528:HIS:CG	2.44	0.52
1:E:220:LYS:NZ	5:E:801:ADP:O3B	2.35	0.52
6:E:803:AGS:O2A	6:E:803:AGS:O3'	2.28	0.52
2:O:124:LYS:HA	2:O:126:PHE:CZ	2.44	0.52
1:A:288:HIS:CG	1:A:326:GLU:HG3	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:ARG:HG2	1:D:300:GLN:OE1	2.09	0.52
1:D:343:LYS:NZ	1:D:345:ASP:OD1	2.40	0.52
1:F:617:ILE:HG22	2:I:40:GLU:HB3	1.92	0.52
2:N:33:ILE:CG2	2:O:56:LEU:HD11	2.22	0.52
2:H:77:ILE:HG22	2:H:77:ILE:O	2.07	0.51
1:B:330:ILE:HG22	1:B:330:ILE:O	2.10	0.51
1:E:503:GLU:HA	1:E:503:GLU:OE1	2.10	0.51
1:A:264:GLU:OE1	1:A:300:GLN:O	2.28	0.51
1:B:610:ARG:HG3	1:B:610:ARG:HH11	1.76	0.51
1:D:438:GLU:OE1	1:D:438:GLU:HA	2.10	0.51
2:O:104:ILE:HA	2:O:126:PHE:O	2.10	0.51
2:S:22:GLU:OE1	2:S:31:PHE:HE2	1.92	0.51
2:T:124:LYS:C	2:T:126:PHE:CE1	2.88	0.51
1:A:311:LEU:CD1	1:A:340:ARG:HD2	2.40	0.51
1:B:389:ILE:HB	1:B:397:LYS:HD3	1.91	0.51
1:F:617:ILE:CG2	2:I:40:GLU:CB	2.89	0.51
2:H:31:PHE:CE2	2:I:21:ILE:HD11	2.45	0.51
2:Q:185:ASP:N	2:Q:185:ASP:OD1	2.41	0.51
1:A:537:PRO:HD3	1:B:528:HIS:NE2	1.98	0.51
1:E:719:GLU:CD	1:E:723:GLY:HA3	2.36	0.51
2:H:112:MET:CE	2:H:115:PHE:CD2	2.93	0.51
2:I:21:ILE:CD1	2:I:30:SER:CB	2.88	0.51
2:L:104:ILE:HA	2:L:126:PHE:O	2.11	0.51
1:B:389:ILE:CB	1:B:397:LYS:HD3	2.40	0.51
1:E:719:GLU:CA	1:E:723:GLY:CA	2.70	0.51
1:C:719:GLU:CA	1:C:724:SER:OG	2.58	0.51
1:D:301:VAL:HG23	1:E:295:ALA:HB1	1.93	0.51
2:P:17:VAL:HG11	2:P:32:ASP:CG	2.34	0.51
1:B:544:ASP:OD1	1:B:544:ASP:N	2.37	0.51
2:I:137:GLN:NE2	2:P:145:GLN:NE2	2.59	0.51
2:P:31:PHE:CD1	2:P:31:PHE:N	2.77	0.51
1:B:215:GLU:OE2	1:C:555:LYS:CE	2.56	0.51
1:B:491:PHE:N	1:B:491:PHE:CD1	2.79	0.51
1:C:524:TYR:HE2	1:C:533:LEU:HG	1.76	0.51
2:P:104:ILE:HA	2:P:126:PHE:O	2.10	0.51
2:S:104:ILE:HA	2:S:126:PHE:O	2.11	0.51
1:A:537:PRO:HD3	1:B:528:HIS:HE1	1.63	0.50
2:H:50:GLU:CD	2:H:53:MET:H	2.20	0.50
2:L:29:ARG:HB3	2:L:31:PHE:CE1	2.46	0.50
1:B:285:ASP:OD1	1:B:285:ASP:N	2.43	0.50
1:E:461:PHE:N	6:E:803:AGS:HN62	2.09	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:89:SER:O	2:H:89:SER:OG	2.27	0.50
2:N:25:SER:OG	2:N:26:ARG:N	2.44	0.50
1:E:179:LEU:O	1:E:183:GLY:C	2.52	0.50
1:E:441:VAL:CG1	1:E:442:SER:N	2.74	0.50
2:G:128:LEU:CD2	2:M:92:ASP:HB3	2.42	0.50
1:A:311:LEU:C	1:A:311:LEU:CD1	2.83	0.50
1:B:357:ILE:CD1	1:B:395:PRO:CG	2.89	0.50
1:D:296:ALA:O	1:D:297:SER:CB	2.57	0.50
2:N:33:ILE:CD1	2:O:60:GLN:HG2	2.40	0.50
1:B:287:ILE:HG22	1:B:321:SER:O	2.12	0.50
1:C:436:ILE:HG12	1:C:598:ASN:ND2	2.27	0.50
1:E:437:PRO:CD	1:E:558:HIS:CE1	2.94	0.50
2:I:25:SER:OG	2:I:26:ARG:N	2.42	0.50
2:L:26:ARG:HB2	2:L:26:ARG:CZ	2.42	0.50
1:B:643:ARG:O	1:B:643:ARG:HG3	2.12	0.50
2:K:88:MET:C	2:K:89:SER:O	2.48	0.50
2:H:73:ILE:O	2:H:101:VAL:HA	2.11	0.50
2:I:31:PHE:CE2	2:J:21:ILE:CD1	2.86	0.50
1:C:565:GLU:C	1:C:567:GLU:H	2.19	0.50
1:F:621:HIS:CD2	1:F:621:HIS:H	2.29	0.50
2:T:124:LYS:HA	2:T:126:PHE:CZ	2.46	0.50
2:H:79:SER:O	2:H:79:SER:OG	2.22	0.50
2:O:124:LYS:CA	2:O:126:PHE:CE1	2.95	0.50
1:A:262:ASP:OD1	1:A:265:LYS:CE	2.60	0.49
1:B:631:GLU:N	1:B:631:GLU:CD	2.69	0.49
1:D:231:ILE:CA	1:D:236:VAL:HG21	2.40	0.49
1:E:441:VAL:CG1	1:E:442:SER:H	2.25	0.49
2:O:22:GLU:OE1	2:O:36:ARG:NE	2.45	0.49
1:B:296:ALA:HB3	3:X:1:UNK:C	2.31	0.49
1:B:427:GLU:OE2	1:B:438:GLU:N	2.44	0.49
1:E:440:SER:CB	1:E:441:VAL:C	2.85	0.49
1:B:195:LEU:CD1	1:B:230:ARG:NE	2.75	0.49
1:C:439:LYS:H	1:C:439:LYS:NZ	2.10	0.49
1:A:287:ILE:HG23	1:A:287:ILE:O	2.12	0.49
1:A:343:LYS:NZ	1:A:345:ASP:OD1	2.45	0.49
2:H:124:LYS:HA	2:H:126:PHE:CE1	2.47	0.49
2:I:21:ILE:CD1	2:I:30:SER:HB3	2.42	0.49
2:T:22:GLU:OE2	2:T:39:LYS:NZ	2.46	0.49
1:A:305:ASN:HB3	1:B:286:GLU:OE1	2.12	0.49
1:B:502:THR:OG1	6:B:802:AGS:PB	2.70	0.49
2:H:26:ARG:HG2	2:H:26:ARG:NH1	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:682:VAL:O	1:C:687:ARG:NH1	2.45	0.49
1:E:441:VAL:HG21	1:E:478:ARG:CA	2.43	0.49
2:Q:21:ILE:CG1	2:R:31:PHE:HE2	2.25	0.49
2:R:25:SER:OG	2:R:26:ARG:N	2.43	0.49
1:A:284:ILE:HD11	1:A:318:VAL:HG11	1.93	0.49
1:A:288:HIS:CD2	1:A:289:THR:HG23	2.48	0.49
5:E:802:ADP:O2A	1:F:221:THR:HB	2.11	0.49
2:G:25:SER:OG	2:G:26:ARG:N	2.45	0.49
2:H:115:PHE:CE1	2:H:163:MET:HE1	2.47	0.49
2:S:22:GLU:CD	2:S:31:PHE:CE2	2.91	0.49
1:A:287:ILE:CG1	1:A:291:ILE:HG12	2.43	0.49
1:B:632:ILE:HA	1:B:635:ILE:HG13	1.95	0.49
1:D:436:ILE:HB	1:D:437:PRO:HD2	1.95	0.49
1:E:520:ASP:C	1:E:520:ASP:OD1	2.54	0.49
1:A:685:GLU:O	1:A:735:LEU:HD11	2.13	0.49
1:E:415:SER:O	1:E:417:ARG:N	2.46	0.49
2:H:40:GLU:O	2:H:42:VAL:HG23	2.13	0.49
2:H:72:ASP:OD1	2:H:100:ASP:HB2	2.13	0.49
2:J:25:SER:OG	2:J:26:ARG:N	2.45	0.49
1:C:719:GLU:HA	1:C:724:SER:OG	2.13	0.48
1:F:696:ASP:O	1:F:700:GLY:N	2.46	0.48
1:C:348:GLU:HG3	1:C:394:LEU:O	2.14	0.48
2:H:95:GLN:NE2	2:H:95:GLN:CA	2.75	0.48
1:A:258:LYS:C	1:A:299:GLY:H	2.19	0.48
1:C:570:HIS:C	1:C:572:ASP:H	2.21	0.48
1:E:441:VAL:HG13	1:F:721:LEU:HD22	1.93	0.48
2:T:124:LYS:CA	2:T:126:PHE:CE1	2.96	0.48
1:A:442:SER:OG	1:A:443:GLN:N	2.46	0.48
1:B:325:GLN:O	1:B:325:GLN:HG2	2.13	0.48
1:E:418:LYS:HA	1:E:418:LYS:CE	2.44	0.48
2:H:31:PHE:CZ	2:I:21:ILE:HG12	2.48	0.48
1:A:308:LYS:HZ2	1:A:336:ALA:CB	2.23	0.48
1:C:486:LYS:NZ	1:C:582:ASP:OD1	2.47	0.48
1:C:524:TYR:CE2	1:C:533:LEU:CG	2.97	0.48
1:C:526:GLU:C	1:C:570:HIS:HD2	2.19	0.48
1:C:588:ASP:OD1	1:C:588:ASP:C	2.57	0.48
1:E:175:ASN:HB2	1:E:246:TYR:HE2	1.77	0.48
1:B:334:ASP:C	1:B:334:ASP:OD1	2.56	0.48
2:G:51:ASP:OD1	2:G:86:ALA:HB2	2.12	0.48
2:M:127:CYS:SG	2:M:190:ALA:HB1	2.54	0.48
1:A:292:GLY:HA2	1:A:293:ALA:HA	1.56	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:65:GLU:HG3	2:H:97:ILE:HB	1.95	0.48
1:B:450:LYS:HB2	1:C:722:PHE:CE2	2.49	0.48
1:B:633:LYS:C	1:B:635:ILE:H	2.20	0.48
1:C:716:LEU:HD23	1:C:725:LEU:CD2	2.44	0.48
2:P:21:ILE:HD13	2:P:30:SER:HB2	1.95	0.48
2:H:103:THR:O	2:H:103:THR:OG1	2.08	0.48
2:N:126:PHE:HD2	2:N:201:SER:OG	1.97	0.48
2:R:126:PHE:HD2	2:R:201:SER:OG	1.95	0.48
2:M:26:ARG:HB2	2:M:26:ARG:CZ	2.42	0.47
1:B:322:THR:HG21	1:B:327:PHE:HB2	1.95	0.47
2:I:137:GLN:OE1	2:P:145:GLN:HB3	2.13	0.47
2:K:63:PHE:CZ	2:L:20:VAL:CG1	2.97	0.47
1:E:440:SER:N	1:E:441:VAL:CA	2.72	0.47
2:G:128:LEU:HD22	2:M:92:ASP:HB3	1.95	0.47
1:B:171:ASN:OD1	1:B:171:ASN:N	2.45	0.47
1:D:567:GLU:OE2	1:D:606:ASN:CB	2.59	0.47
2:L:126:PHE:CD2	2:L:201:SER:OG	2.68	0.47
2:M:18:PRO:HD2	2:M:33:ILE:HG21	1.96	0.47
1:F:621:HIS:CD2	2:I:206:ARG:CZ	2.97	0.47
2:N:29:ARG:HD2	2:N:31:PHE:CE1	2.49	0.47
2:H:115:PHE:CD1	2:H:163:MET:HE3	2.49	0.47
2:P:25:SER:OG	2:P:26:ARG:N	2.47	0.47
1:A:565:GLU:C	1:A:567:GLU:H	2.21	0.47
1:B:696:ASP:OD1	1:B:697:ARG:N	2.48	0.47
1:D:290:ILE:CD1	1:D:304:ALA:HB2	2.45	0.47
1:D:745:GLY:O	1:D:746:PHE:C	2.57	0.47
2:H:115:PHE:CE1	2:H:163:MET:HE3	2.50	0.47
2:I:40:GLU:O	2:I:42:VAL:HG23	2.14	0.47
2:L:126:PHE:HD2	2:L:201:SER:OG	1.98	0.47
1:E:719:GLU:C	1:E:723:GLY:H	2.22	0.47
1:C:171:ASN:OD1	1:C:171:ASN:N	2.44	0.47
6:D:802:AGS:O1A	6:D:802:AGS:H8	2.15	0.47
2:G:126:PHE:HD2	2:G:201:SER:OG	1.98	0.47
1:A:293:ALA:HA	1:A:294:GLY:HA3	1.70	0.46
1:B:630:GLU:CB	1:B:633:LYS:HE3	2.44	0.46
1:C:527:ARG:NH1	1:C:572:ASP:OD2	2.48	0.46
1:D:393:HIS:ND1	1:D:393:HIS:N	2.62	0.46
2:K:33:ILE:O	2:K:33:ILE:HG13	2.15	0.46
1:B:528:HIS:ND1	1:B:528:HIS:C	2.73	0.46
1:B:637:THR:OG1	1:B:638:PRO:HD2	2.16	0.46
2:R:125:ARG:O	2:R:200:ASP:N	2.39	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:ASP:C	1:C:302:ASP:OD1	2.58	0.46
1:E:460:VAL:HG13	6:E:803:AGS:N6	2.29	0.46
5:E:802:ADP:O3B	1:F:216:SER:HB2	2.15	0.46
1:F:393:HIS:CG	1:F:394:LEU:H	2.34	0.46
2:H:96:PHE:C	2:H:96:PHE:CD2	2.92	0.46
2:S:25:SER:OG	2:S:26:ARG:N	2.43	0.46
2:T:29:ARG:HD2	2:T:31:PHE:CZ	2.51	0.46
1:B:237:PRO:HG2	1:B:239:VAL:HG22	1.98	0.46
1:B:238:GLU:OE2	1:C:414:VAL:CG1	2.64	0.46
1:C:254:LEU:HD23	1:C:263:PHE:CE1	2.50	0.46
2:H:115:PHE:CD1	2:H:163:MET:CE	2.98	0.46
2:P:30:SER:O	2:P:30:SER:OG	2.33	0.46
1:A:259:TYR:C	1:A:299:GLY:HA2	2.41	0.46
2:I:30:SER:O	2:I:30:SER:OG	2.31	0.46
1:A:714:LYS:HB3	1:A:715:PRO:HD3	1.96	0.46
1:B:249:ASP:OD1	1:B:250:ILE:N	2.49	0.46
1:C:334:ASP:OD1	1:C:334:ASP:C	2.59	0.46
1:D:304:ALA:HB1	1:D:337:LEU:HD11	1.97	0.46
1:D:637:THR:HG23	1:D:639:GLU:HG2	1.98	0.46
2:H:84:ILE:HD11	2:H:138:PRO:HB3	1.98	0.46
2:I:18:PRO:CG	2:I:33:ILE:HD13	2.41	0.46
2:G:128:LEU:HD22	2:M:92:ASP:CG	2.41	0.46
2:H:31:PHE:CZ	2:I:21:ILE:HD11	2.51	0.46
2:P:17:VAL:HG12	2:P:32:ASP:OD2	2.13	0.46
1:A:268:LYS:HD3	1:A:268:LYS:HA	1.61	0.46
1:B:634:LYS:HE3	1:B:634:LYS:HB2	1.46	0.46
1:D:725:LEU:HD23	1:D:746:PHE:CZ	2.51	0.46
2:H:115:PHE:CD2	2:H:163:MET:HE1	2.50	0.46
1:A:567:GLU:CD	1:A:606:ASN:H	2.23	0.46
1:B:215:GLU:O	1:B:218:VAL:HG12	2.16	0.46
1:C:524:TYR:OH	1:C:533:LEU:CD2	2.63	0.46
1:E:437:PRO:HD2	1:E:558:HIS:CE1	2.51	0.46
1:B:354:THR:CG2	1:B:395:PRO:CB	2.77	0.46
2:O:22:GLU:OE1	2:O:36:ARG:CD	2.64	0.46
1:D:275:GLU:OE2	1:D:310:LEU:CD2	2.64	0.45
1:D:389:ILE:O	1:D:397:LYS:HD2	2.16	0.45
1:E:412:MET:HB3	1:E:413:PRO:HD3	1.98	0.45
2:H:32:ASP:OD1	2:H:33:ILE:N	2.50	0.45
2:P:124:LYS:HA	2:P:126:PHE:CZ	2.51	0.45
1:D:567:GLU:OE2	1:D:606:ASN:N	2.47	0.45
2:G:106:MET:O	2:G:106:MET:HG3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:THR:HG1	6:B:802:AGS:PB	2.39	0.45
2:H:17:VAL:CG1	2:H:32:ASP:OD1	2.64	0.45
1:B:588:ASP:OD1	1:B:588:ASP:C	2.59	0.45
1:B:718:ASN:O	1:B:722:PHE:CG	2.70	0.45
1:D:298:GLY:N	1:D:300:GLN:OE1	2.45	0.45
1:E:533:LEU:HD22	1:E:549:LEU:HB2	1.99	0.45
2:H:26:ARG:NE	2:H:26:ARG:N	2.62	0.45
2:Q:20:VAL:CG1	2:R:63:PHE:CZ	3.00	0.45
1:B:350:SER:OG	1:B:351:ILE:N	2.49	0.45
1:F:304:ALA:O	1:F:308:LYS:NZ	2.49	0.45
1:F:537:PRO:HB2	1:F:538:PRO:HD3	1.99	0.45
2:H:63:PHE:CZ	2:I:20:VAL:CG1	3.00	0.45
1:B:370:ASP:O	1:B:418:LYS:NZ	2.49	0.45
2:J:29:ARG:NE	2:K:28:GLU:CD	2.68	0.45
2:N:18:PRO:HG3	2:N:33:ILE:HD13	1.90	0.45
1:A:263:PHE:HB3	1:A:301:VAL:N	2.32	0.45
1:B:386:VAL:HG22	1:B:394:LEU:CD1	2.26	0.45
1:B:581:MET:CE	1:B:640:PHE:CE1	3.00	0.45
1:C:412:MET:N	1:C:413:PRO:CD	2.80	0.45
1:E:434:ALA:HB3	1:E:436:ILE:HD12	1.99	0.45
1:F:696:ASP:OD1	1:F:696:ASP:C	2.59	0.45
2:M:17:VAL:CG1	2:M:33:ILE:CG2	2.53	0.45
2:T:126:PHE:HD2	2:T:201:SER:OG	2.00	0.45
1:B:577:LEU:C	1:B:579:GLN:H	2.23	0.45
1:B:581:MET:HE3	1:B:643:ARG:HG3	1.98	0.45
1:D:588:ASP:OD1	1:D:588:ASP:C	2.60	0.45
1:E:437:PRO:HD2	1:E:558:HIS:HE1	1.82	0.45
2:Q:22:GLU:OE1	2:Q:36:ARG:CD	2.65	0.45
1:A:263:PHE:CB	1:A:301:VAL:H	2.29	0.45
1:A:461:PHE:H	5:A:802:ADP:N6	2.15	0.45
1:B:632:ILE:HA	1:B:632:ILE:HD12	1.42	0.45
1:D:327:PHE:O	1:D:327:PHE:CG	2.70	0.45
2:G:56:LEU:HD11	2:H:33:ILE:HG21	1.99	0.45
1:B:609:VAL:C	1:B:611:GLU:H	2.25	0.45
1:C:263:PHE:CD1	1:C:293:ALA:HB1	2.48	0.45
1:F:617:ILE:HG22	2:I:40:GLU:CB	2.47	0.45
2:I:137:GLN:HE21	2:P:145:GLN:NE2	2.15	0.45
2:K:90:ILE:O	2:K:91:TYR:C	2.59	0.45
1:E:461:PHE:H	6:E:803:AGS:HN62	1.63	0.44
2:K:63:PHE:CZ	2:L:20:VAL:HB	2.52	0.44
2:N:20:VAL:CB	2:O:63:PHE:CZ	2.96	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:21:ILE:HD11	2:Q:31:PHE:HE2	1.82	0.44
1:B:357:ILE:HD13	1:B:395:PRO:HG3	1.99	0.44
1:B:391:ASP:N	1:B:391:ASP:OD1	2.42	0.44
1:C:296:ALA:HA	3:X:4:UNK:HA	1.99	0.44
1:D:440:SER:HB3	1:D:478:ARG:NH2	2.32	0.44
1:C:714:LYS:HB2	1:C:715:PRO:HD3	1.99	0.44
5:E:802:ADP:C6	1:F:188:LEU:HD12	2.52	0.44
2:R:24:THR:OG1	2:R:25:SER:N	2.49	0.44
1:C:527:ARG:CA	1:C:570:HIS:NE2	2.81	0.44
1:D:696:ASP:OD1	1:D:696:ASP:C	2.57	0.44
2:I:60:GLN:HA	2:J:33:ILE:HD11	1.99	0.44
1:E:503:GLU:HB2	6:E:803:AGS:O3'	2.17	0.44
1:E:714:LYS:HB2	1:E:715:PRO:HD3	1.99	0.44
1:C:263:PHE:CD2	1:C:293:ALA:HB1	2.48	0.44
1:E:503:GLU:HB2	6:E:803:AGS:O2A	2.17	0.44
1:F:544:ASP:OD1	1:F:544:ASP:N	2.51	0.44
2:H:17:VAL:HG11	2:H:32:ASP:OD1	2.17	0.44
2:I:56:LEU:HD11	2:J:33:ILE:HG21	2.00	0.44
2:L:21:ILE:HD13	2:L:21:ILE:HA	1.81	0.44
1:D:258:LYS:O	3:X:8:UNK:N	2.51	0.44
1:E:175:ASN:HA	1:E:246:TYR:CD2	2.52	0.44
1:A:288:HIS:CD2	1:A:326:GLU:HG3	2.53	0.44
1:A:520:ASP:OD1	1:A:520:ASP:C	2.60	0.44
1:D:714:LYS:HB2	1:D:715:PRO:HD3	1.99	0.44
1:D:729:GLY:O	1:D:746:PHE:CD2	2.70	0.44
1:F:617:ILE:HG22	2:I:40:GLU:CG	2.45	0.44
1:A:305:ASN:OD1	1:A:305:ASN:N	2.50	0.44
1:B:287:ILE:CG2	1:B:322:THR:HB	2.48	0.44
1:D:327:PHE:O	1:D:327:PHE:CD2	2.71	0.44
1:E:348:GLU:CG	1:E:349:PRO:HD2	2.47	0.44
2:H:26:ARG:C	2:H:26:ARG:CZ	2.91	0.44
1:B:288:HIS:CD2	1:B:288:HIS:O	2.70	0.43
1:E:326:GLU:O	1:E:327:PHE:C	2.61	0.43
1:E:534:ILE:C	1:E:547:GLY:HA3	2.43	0.43
2:I:60:GLN:HG2	2:J:33:ILE:HD13	2.00	0.43
1:D:194:GLU:N	1:D:194:GLU:OE1	2.51	0.43
1:D:304:ALA:HA	1:D:307:ILE:HG22	2.00	0.43
1:D:441:VAL:HG12	1:D:441:VAL:O	2.18	0.43
1:F:194:GLU:OE1	1:F:194:GLU:N	2.50	0.43
2:H:185:ASP:OD1	2:H:185:ASP:N	2.50	0.43
2:O:29:ARG:HD2	2:O:31:PHE:HZ	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ASP:OD1	1:A:334:ASP:C	2.61	0.43
1:B:575:ASN:OD1	1:C:568:LYS:HE3	2.18	0.43
1:B:625:SER:O	1:B:628:ALA:CB	2.59	0.43
1:E:500:GLY:N	6:E:803:AGS:O2B	2.46	0.43
2:G:65:GLU:HG3	2:G:99:PRO:CD	2.49	0.43
1:A:315:LYS:HD2	1:A:315:LYS:H	1.80	0.43
1:D:239:VAL:CG1	1:E:410:ARG:NH1	2.82	0.43
1:E:335:ARG:NH1	5:E:802:ADP:O3B	2.51	0.43
2:N:104:ILE:HA	2:N:126:PHE:O	2.18	0.43
1:A:696:ASP:OD1	1:A:696:ASP:C	2.62	0.43
1:B:520:ASP:C	1:B:520:ASP:OD1	2.62	0.43
1:B:565:GLU:C	1:B:567:GLU:H	2.26	0.43
2:G:106:MET:H	2:G:106:MET:HG2	1.59	0.43
2:I:21:ILE:CD1	2:I:30:SER:HB2	2.48	0.43
1:A:307:ILE:O	1:A:309:PRO:CD	2.66	0.43
1:B:327:PHE:O	1:B:327:PHE:CD2	2.72	0.43
1:B:343:LYS:NZ	1:B:345:ASP:OD1	2.50	0.43
1:B:537:PRO:O	1:B:540:TYR:HB2	2.19	0.43
2:N:19:MET:HA	2:N:31:PHE:O	2.18	0.43
2:O:25:SER:OG	2:O:26:ARG:N	2.50	0.43
2:Q:29:ARG:HD2	2:Q:31:PHE:CZ	2.54	0.43
1:A:263:PHE:HB3	1:A:300:GLN:C	2.43	0.43
1:C:696:ASP:OD1	1:C:696:ASP:C	2.58	0.43
2:J:56:LEU:CD1	2:K:33:ILE:HG21	2.47	0.43
2:M:28:GLU:N	2:M:28:GLU:CD	2.77	0.43
1:A:209:ASN:OD1	1:A:317:ARG:CA	2.56	0.43
1:A:308:LYS:CD	1:A:336:ALA:HB1	2.49	0.43
1:B:502:THR:OG1	6:B:802:AGS:O3A	2.37	0.43
1:F:736:ASP:OD1	1:F:736:ASP:C	2.62	0.43
2:I:65:GLU:HG3	2:I:99:PRO:HD2	2.01	0.43
1:B:569:ALA:O	1:B:570:HIS:C	2.61	0.42
1:B:630:GLU:OE1	1:B:630:GLU:HA	2.19	0.42
1:C:352:GLU:H	1:C:352:GLU:CD	2.26	0.42
1:E:302:ASP:OD1	1:E:302:ASP:N	2.46	0.42
1:E:696:ASP:C	1:E:696:ASP:OD1	2.59	0.42
2:Q:124:LYS:C	2:Q:126:PHE:CE1	2.97	0.42
2:Q:124:LYS:CA	2:Q:126:PHE:CE1	3.00	0.42
1:B:287:ILE:HB	1:B:321:SER:H	1.83	0.42
1:B:581:MET:HE3	1:B:643:ARG:CG	2.48	0.42
1:C:485:HIS:O	1:C:485:HIS:ND1	2.50	0.42
1:F:335:ARG:O	1:F:339:ARG:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:29:ARG:NE	2:I:31:PHE:HZ	2.17	0.42
2:L:26:ARG:NH2	2:M:28:GLU:OE1	2.52	0.42
2:Q:20:VAL:CB	2:R:63:PHE:CZ	3.02	0.42
1:C:254:LEU:HD23	1:C:263:PHE:CD1	2.54	0.42
1:D:637:THR:OG1	1:D:639:GLU:CD	2.62	0.42
1:D:725:LEU:HD22	1:D:729:GLY:HA2	2.01	0.42
1:E:441:VAL:HG21	1:E:478:ARG:CB	2.47	0.42
1:F:501:LYS:NZ	1:F:605:THR:O	2.53	0.42
2:G:128:LEU:HB2	2:G:131:SER:HB3	2.01	0.42
2:H:32:ASP:C	2:H:34:TYR:N	2.76	0.42
1:A:259:TYR:O	1:A:299:GLY:HA3	2.19	0.42
1:A:348:GLU:OE2	1:A:394:LEU:HB3	2.19	0.42
1:B:327:PHE:HA	1:B:331:PHE:CB	2.50	0.42
1:B:639:GLU:H	1:B:639:GLU:HG2	1.36	0.42
1:C:439:LYS:H	1:C:439:LYS:HZ3	1.67	0.42
1:D:231:ILE:HA	1:D:236:VAL:HG23	2.02	0.42
2:H:31:PHE:CZ	2:I:21:ILE:CD1	3.03	0.42
2:Q:21:ILE:CG1	2:R:31:PHE:CE2	3.02	0.42
1:D:324:TYR:O	1:D:328:SER:HB2	2.20	0.42
1:E:443:GLN:CG	1:E:444:SER:N	2.75	0.42
5:E:802:ADP:H8	1:F:395:PRO:HG2	1.83	0.42
2:H:25:SER:OG	2:H:26:ARG:N	2.52	0.42
2:I:29:ARG:NE	2:I:31:PHE:CZ	2.86	0.42
2:I:137:GLN:CD	2:P:145:GLN:HB3	2.45	0.42
2:I:150:GLU:HB2	2:P:157:LEU:HD11	2.01	0.42
2:M:184:ARG:O	2:M:185:ASP:C	2.62	0.42
2:Q:24:THR:OG1	2:Q:25:SER:N	2.51	0.42
2:Q:32:ASP:O	2:Q:33:ILE:C	2.61	0.42
1:A:291:ILE:HD12	1:A:291:ILE:H	1.85	0.42
1:C:348:GLU:CD	1:C:394:LEU:H	2.09	0.42
1:C:702:ARG:N	1:C:703:PRO:CD	2.82	0.42
1:E:194:GLU:OE1	1:E:194:GLU:N	2.48	0.42
2:K:18:PRO:HD2	2:K:33:ILE:HG21	2.01	0.42
1:D:171:ASN:N	1:D:171:ASN:OD1	2.53	0.42
2:H:112:MET:HE3	2:H:115:PHE:HD2	1.85	0.42
2:Q:29:ARG:HB3	2:Q:31:PHE:HE1	1.84	0.42
2:R:20:VAL:CG1	2:S:63:PHE:CZ	3.01	0.42
1:E:532:ARG:O	1:E:548:LEU:HG	2.20	0.42
5:E:802:ADP:C5'	1:F:219:GLY:HA2	2.48	0.42
1:F:242:ASP:OD1	1:F:242:ASP:N	2.44	0.42
1:D:294:GLY:H	1:D:302:ASP:CB	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:PRO:N	1:D:437:PRO:C	2.66	0.42
2:H:51:ASP:OD1	2:H:86:ALA:HB2	2.19	0.42
1:B:322:THR:CG2	1:B:327:PHE:HB2	2.49	0.41
1:C:570:HIS:C	1:C:572:ASP:N	2.77	0.41
2:O:126:PHE:HD2	2:O:201:SER:OG	2.03	0.41
1:A:633:LYS:O	1:A:634:LYS:C	2.61	0.41
1:B:566:ILE:HG21	1:B:603:MET:HB3	2.02	0.41
1:C:300:GLN:N	1:C:300:GLN:OE1	2.53	0.41
1:E:249:ASP:OD1	1:E:249:ASP:C	2.62	0.41
2:G:185:ASP:N	2:G:185:ASP:OD1	2.47	0.41
2:P:124:LYS:C	2:P:126:PHE:CE1	2.98	0.41
1:B:631:GLU:OE2	1:B:631:GLU:HA	2.20	0.41
1:C:370:ASP:OD2	1:C:418:LYS:NZ	2.53	0.41
1:C:586:LEU:CD1	1:D:523:GLU:OE2	2.61	0.41
1:F:714:LYS:HB2	1:F:715:PRO:HD3	2.02	0.41
2:J:28:GLU:HB3	2:J:29:ARG:H	1.61	0.41
1:C:436:ILE:HD11	1:C:598:ASN:CB	2.50	0.41
1:D:524:TYR:CZ	1:D:533:LEU:HD21	2.55	0.41
2:S:184:ARG:O	2:S:185:ASP:C	2.60	0.41
1:A:541:VAL:HA	4:Y:4:UNK:CB	2.51	0.41
1:B:581:MET:HE2	1:B:640:PHE:CE1	2.55	0.41
1:C:290:ILE:O	1:C:290:ILE:CG1	2.67	0.41
1:C:500:GLY:HA2	1:C:503:GLU:HB2	2.02	0.41
1:E:180:ALA:HA	1:E:183:GLY:O	2.21	0.41
2:H:22:GLU:OE1	2:H:36:ARG:NE	2.54	0.41
2:J:184:ARG:O	2:J:185:ASP:C	2.63	0.41
1:D:658:ILE:HG13	1:D:695:TYR:CD1	2.56	0.41
1:E:440:SER:HB2	1:E:441:VAL:C	2.46	0.41
2:G:60:GLN:HG2	2:H:33:ILE:HD11	2.03	0.41
1:C:503:GLU:HG2	6:C:802:AGS:H4'	2.02	0.41
1:D:386:VAL:CG2	1:D:394:LEU:HD21	2.51	0.41
2:G:125:ARG:HE	2:G:125:ARG:HB2	1.57	0.41
2:H:32:ASP:C	2:H:34:TYR:H	2.27	0.41
2:Q:126:PHE:HD2	2:Q:201:SER:OG	2.04	0.41
1:A:307:ILE:HD12	1:A:340:ARG:NH2	2.35	0.41
1:B:195:LEU:HD23	1:B:195:LEU:HA	1.82	0.41
1:C:524:TYR:OH	1:C:533:LEU:HD21	2.17	0.41
1:E:536:ALA:HA	1:E:537:PRO:HD3	1.66	0.41
1:E:540:TYR:C	4:Y:11:UNK:HA	2.46	0.41
2:G:65:GLU:HG3	2:G:99:PRO:HD2	2.02	0.41
2:K:89:SER:O	2:K:90:ILE:HB	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:159:VAL:O	2:K:160:LYS:C	2.64	0.41
2:N:46:THR:HG21	2:O:55:ASN:OD1	2.21	0.41
1:A:696:ASP:OD1	1:A:697:ARG:N	2.54	0.41
1:B:578:LEU:HD12	1:B:643:ARG:HH11	1.76	0.41
1:C:720:LEU:HD23	1:C:725:LEU:HB3	2.02	0.41
1:D:658:ILE:O	1:D:659:HIS:C	2.62	0.41
2:H:112:MET:HE3	2:H:115:PHE:CD2	2.55	0.41
2:L:21:ILE:HD13	2:L:30:SER:HA	2.02	0.41
2:L:50:GLU:CD	2:L:53:MET:H	2.28	0.41
2:M:17:VAL:HG12	2:M:32:ASP:OD1	2.14	0.41
2:T:184:ARG:O	2:T:185:ASP:C	2.63	0.41
1:B:730:GLN:C	1:B:730:GLN:CD	2.89	0.40
1:C:623:ASP:O	2:M:71:LYS:NZ	2.53	0.40
1:E:348:GLU:HG3	1:E:394:LEU:O	2.21	0.40
1:E:396:ASP:O	1:E:397:LYS:C	2.61	0.40
2:G:189:SER:O	2:G:190:ALA:C	2.63	0.40
1:A:348:GLU:OE2	1:A:394:LEU:HB2	2.22	0.40
1:A:685:GLU:O	1:A:735:LEU:CD1	2.70	0.40
1:F:334:ASP:C	1:F:334:ASP:OD1	2.63	0.40
2:S:84:ILE:O	2:S:85:THR:C	2.64	0.40
1:A:537:PRO:HG3	1:B:528:HIS:O	2.21	0.40
1:B:631:GLU:OE2	1:B:631:GLU:CA	2.70	0.40
2:N:126:PHE:CD1	2:N:126:PHE:N	2.90	0.40
1:B:236:VAL:CB	1:B:237:PRO:CD	2.90	0.40
1:B:502:THR:CG2	6:B:802:AGS:O1B	2.70	0.40
1:C:716:LEU:CD2	1:C:725:LEU:CD2	3.00	0.40
1:D:231:ILE:CG1	1:D:236:VAL:HG21	2.51	0.40
2:G:104:ILE:HA	2:G:126:PHE:O	2.21	0.40
2:L:26:ARG:NH1	2:L:26:ARG:CB	2.84	0.40
2:M:26:ARG:H	2:M:26:ARG:HG3	1.65	0.40
2:Q:21:ILE:HG13	2:R:31:PHE:CZ	2.57	0.40
1:A:250:ILE:CB	1:A:290:ILE:HG21	2.51	0.40
1:A:566:ILE:HG21	1:A:603:MET:HB3	2.04	0.40
1:B:524:TYR:HA	1:B:529:THR:HG21	2.04	0.40
1:B:629:MET:HG3	1:B:631:GLU:CB	2.51	0.40
1:B:718:ASN:O	1:B:722:PHE:CD2	2.74	0.40
2:G:65:GLU:O	2:G:65:GLU:HG2	2.20	0.40
2:K:89:SER:O	2:K:91:TYR:N	2.54	0.40
2:L:124:LYS:O	2:L:126:PHE:CE1	2.75	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 PDB entries followed by that with respect to all EM entries.

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	558/578 (96%)	537 (96%)	18 (3%)	3 (0%)	24	60
1	B	576/578 (100%)	545 (95%)	24 (4%)	7 (1%)	10	40
1	C	576/578 (100%)	553 (96%)	21 (4%)	2 (0%)	36	70
1	D	576/578 (100%)	555 (96%)	17 (3%)	4 (1%)	18	53
1	E	576/578 (100%)	554 (96%)	15 (3%)	7 (1%)	10	40
1	F	574/578 (99%)	559 (97%)	12 (2%)	3 (0%)	24	60
2	G	190/192 (99%)	177 (93%)	13 (7%)	0	100	100
2	H	190/192 (99%)	171 (90%)	15 (8%)	4 (2%)	5	27
2	I	190/192 (99%)	180 (95%)	8 (4%)	2 (1%)	11	43
2	J	190/192 (99%)	184 (97%)	6 (3%)	0	100	100
2	K	190/192 (99%)	180 (95%)	10 (5%)	0	100	100
2	L	190/192 (99%)	181 (95%)	9 (5%)	0	100	100
2	M	190/192 (99%)	180 (95%)	9 (5%)	1 (0%)	24	60
2	N	190/192 (99%)	182 (96%)	7 (4%)	1 (0%)	24	60
2	O	190/192 (99%)	184 (97%)	6 (3%)	0	100	100
2	P	190/192 (99%)	183 (96%)	7 (4%)	0	100	100
2	Q	190/192 (99%)	184 (97%)	6 (3%)	0	100	100
2	R	190/192 (99%)	183 (96%)	7 (4%)	0	100	100
2	S	190/192 (99%)	184 (97%)	6 (3%)	0	100	100
2	T	190/192 (99%)	183 (96%)	7 (4%)	0	100	100
All	All	6096/6156 (99%)	5839 (96%)	223 (4%)	34 (1%)	23	56

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	293	ALA
1	B	637	THR
1	E	438	GLU
1	E	442	SER
1	E	443	GLN
1	F	623	ASP
1	C	295	ALA
1	D	300	GLN
1	D	305	ASN
1	E	295	ALA
1	E	416	LYS
1	F	727	ASP
2	H	28	GLU
2	H	29	ARG
2	H	86	ALA
1	B	528	HIS
1	C	724	SER
2	I	29	ARG
1	D	439	LYS
1	E	543	PHE
1	A	309	PRO
1	B	610	ARG
1	B	638	PRO
1	F	390	ASN
2	H	89	SER
1	B	237	PRO
1	E	437	PRO
2	I	28	GLU
2	M	33	ILE
1	B	290	ILE
1	D	499	VAL
1	A	301	VAL
2	N	33	ILE

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 PDB entries followed by that with respect to all EM entries.

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	469/485 (97%)	457 (97%)	12 (3%)	40	72
1	B	485/485 (100%)	460 (95%)	25 (5%)	21	55
1	C	485/485 (100%)	476 (98%)	9 (2%)	50	76
1	D	485/485 (100%)	472 (97%)	13 (3%)	39	71
1	E	485/485 (100%)	478 (99%)	7 (1%)	59	80
1	F	485/485 (100%)	482 (99%)	3 (1%)	78	88
2	G	162/162 (100%)	157 (97%)	5 (3%)	35	68
2	H	162/162 (100%)	147 (91%)	15 (9%)	8	32
2	I	162/162 (100%)	158 (98%)	4 (2%)	42	72
2	J	162/162 (100%)	160 (99%)	2 (1%)	63	82
2	K	162/162 (100%)	161 (99%)	1 (1%)	78	88
2	L	162/162 (100%)	156 (96%)	6 (4%)	30	64
2	M	162/162 (100%)	157 (97%)	5 (3%)	35	68
2	N	162/162 (100%)	160 (99%)	2 (1%)	63	82
2	O	162/162 (100%)	162 (100%)	0	100	100
2	P	162/162 (100%)	161 (99%)	1 (1%)	78	88
2	Q	162/162 (100%)	162 (100%)	0	100	100
2	R	162/162 (100%)	160 (99%)	2 (1%)	63	82
2	S	162/162 (100%)	162 (100%)	0	100	100
2	T	162/162 (100%)	161 (99%)	1 (1%)	78	88
All	All	5162/5178 (100%)	5049 (98%)	113 (2%)	45	74

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	LYS
1	A	286	GLU
1	A	291	ILE
1	A	305	ASN
1	A	307	ILE
1	A	310	LEU
1	A	311	LEU
1	A	312	SER
1	A	313	SER
1	A	315	LYS
1	A	316	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	543	PHE
1	B	197	ARG
1	B	236	VAL
1	B	332	GLU
1	B	397	LYS
1	B	491	PHE
1	B	527	ARG
1	B	528	HIS
1	B	611	GLU
1	B	622	GLN
1	B	623	ASP
1	B	624	ASN
1	B	625	SER
1	B	626	THR
1	B	627	ASP
1	B	629	MET
1	B	630	GLU
1	B	632	ILE
1	B	633	LYS
1	B	634	LYS
1	B	635	ILE
1	B	639	GLU
1	B	641	ARG
1	B	643	ARG
1	B	732	THR
1	B	733	VAL
1	C	291	ILE
1	C	436	ILE
1	C	438	GLU
1	C	439	LYS
1	C	555	LYS
1	C	567	GLU
1	C	568	LYS
1	C	725	LEU
1	C	726	VAL
1	D	236	VAL
1	D	238	GLU
1	D	239	VAL
1	D	300	GLN
1	D	301	VAL
1	D	302	ASP
1	D	328	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	393	HIS
1	D	396	ASP
1	D	397	LYS
1	D	438	GLU
1	D	726	VAL
1	D	731	VAL
1	E	416	LYS
1	E	418	LYS
1	E	438	GLU
1	E	440	SER
1	E	463	GLN
1	E	534	ILE
1	E	722	PHE
1	F	335	ARG
1	F	339	ARG
1	F	621	HIS
2	G	50	GLU
2	G	104	ILE
2	G	105	CYS
2	G	106	MET
2	G	125	ARG
2	H	21	ILE
2	H	26	ARG
2	H	28	GLU
2	H	29	ARG
2	H	33	ILE
2	H	50	GLU
2	H	67	GLU
2	H	83	VAL
2	H	85	THR
2	H	89	SER
2	H	93	THR
2	H	95	GLN
2	H	101	VAL
2	H	104	ILE
2	H	106	MET
2	I	29	ARG
2	I	33	ILE
2	I	50	GLU
2	I	136	HIS
2	J	28	GLU
2	J	33	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	50	GLU
2	L	21	ILE
2	L	22	GLU
2	L	26	ARG
2	L	28	GLU
2	L	33	ILE
2	L	50	GLU
2	M	26	ARG
2	M	28	GLU
2	M	29	ARG
2	M	33	ILE
2	M	127	CYS
2	N	33	ILE
2	N	126	PHE
2	P	31	PHE
2	R	32	ASP
2	R	125	ARG
2	T	32	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	273	GLN
1	A	288	HIS
1	A	325	GLN
1	A	545	GLN
1	A	556	HIS
1	A	652	HIS
1	A	659	HIS
1	B	288	HIS
1	B	556	HIS
1	B	684	GLN
1	C	483	HIS
1	C	528	HIS
1	C	556	HIS
1	C	570	HIS
1	C	598	ASN
1	C	660	GLN
1	C	672	GLN
1	D	483	HIS
1	D	579	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	590	ASN
1	E	177	ASN
1	E	646	ASN
1	F	621	HIS
2	H	95	GLN
2	I	55	ASN
2	I	136	HIS
2	I	137	GLN
2	J	55	ASN
2	K	55	ASN
2	L	23	GLN
2	M	55	ASN
2	Q	55	ASN
2	R	55	ASN
2	S	55	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
6	AGS	B	801	-	32,33,33	2.98	13 (40%)	45,52,52	2.41	16 (35%)
6	AGS	C	802	-	32,33,33	3.00	15 (46%)	45,52,52	2.25	13 (28%)
6	AGS	B	802	-	32,33,33	2.89	16 (50%)	45,52,52	2.08	12 (26%)
6	AGS	D	802	-	32,33,33	3.21	17 (53%)	45,52,52	2.19	15 (33%)
5	ADP	A	802	-	28,29,29	2.92	12 (42%)	43,45,45	2.39	14 (32%)
5	ADP	E	801	-	28,29,29	3.04	10 (35%)	43,45,45	2.29	11 (25%)
6	AGS	C	801	-	32,33,33	2.95	14 (43%)	45,52,52	2.16	14 (31%)
6	AGS	E	803	-	32,33,33	3.22	13 (40%)	45,52,52	2.03	13 (28%)
5	ADP	E	802	-	28,29,29	3.27	8 (28%)	43,45,45	2.18	11 (25%)
5	ADP	A	801	-	28,29,29	2.93	11 (39%)	43,45,45	2.35	12 (27%)
5	ADP	F	801	-	28,29,29	3.11	12 (42%)	43,45,45	2.31	15 (34%)
6	AGS	D	801	-	32,33,33	2.57	14 (43%)	45,52,52	1.99	14 (31%)

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
6	AGS	B	801	-	2/2/7/7	5/21/38/38	0/3/3/3
6	AGS	C	802	-	2/2/7/7	6/21/38/38	0/3/3/3
6	AGS	B	802	-	3/3/7/7	1/21/38/38	0/3/3/3
6	AGS	D	802	-	3/3/7/7	4/21/38/38	0/3/3/3
5	ADP	A	802	-	1/1/6/6	3/16/32/32	0/3/3/3
5	ADP	E	801	-	2/2/6/6	4/16/32/32	0/3/3/3
6	AGS	C	801	-	2/2/7/7	4/21/38/38	0/3/3/3
6	AGS	E	803	-	2/2/7/7	1/21/38/38	0/3/3/3
5	ADP	E	802	-	2/2/6/6	7/16/32/32	0/3/3/3
5	ADP	A	801	-	2/2/6/6	4/16/32/32	0/3/3/3
5	ADP	F	801	-	2/2/6/6	0/16/32/32	0/3/3/3
6	AGS	D	801	-	2/2/7/7	6/21/38/38	0/3/3/3

All (155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	801	ADP	O4'-C1'	9.89	1.64	1.42
5	E	801	ADP	O4'-C1'	9.64	1.64	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	802	ADP	PA-O3A	9.30	1.69	1.59
5	A	802	ADP	O4'-C1'	9.28	1.63	1.42
5	A	801	ADP	O4'-C1'	8.99	1.62	1.42
5	E	802	ADP	O4'-C1'	8.68	1.62	1.42
6	E	803	AGS	PA-O3A	8.18	1.68	1.59
6	C	802	AGS	PB-O3B	-7.78	1.51	1.59
6	B	801	AGS	PB-O3B	-7.77	1.51	1.59
6	D	802	AGS	PB-O3B	-7.51	1.51	1.59
6	E	803	AGS	C3'-C4'	-7.28	1.34	1.53
6	D	802	AGS	C3'-C4'	-6.88	1.35	1.53
5	A	802	ADP	O4'-C4'	-6.69	1.30	1.45
6	B	802	AGS	PB-O3B	-6.50	1.52	1.59
6	C	802	AGS	C3'-C4'	-6.49	1.36	1.53
6	D	802	AGS	O4'-C1'	6.42	1.56	1.42
6	C	802	AGS	O4'-C1'	6.37	1.56	1.42
6	C	801	AGS	O4'-C1'	6.37	1.56	1.42
6	C	801	AGS	C3'-C4'	-6.34	1.36	1.53
5	E	802	ADP	O4'-C4'	-6.34	1.30	1.45
6	E	803	AGS	PB-O3A	6.27	1.66	1.59
6	E	803	AGS	O4'-C1'	6.21	1.56	1.42
6	D	801	AGS	C3'-C4'	-6.19	1.37	1.53
6	E	803	AGS	C2'-C1'	-6.08	1.34	1.53
5	E	802	ADP	C2'-C1'	-6.05	1.34	1.53
6	B	802	AGS	O4'-C1'	6.01	1.55	1.42
6	C	801	AGS	PB-O3B	-5.93	1.53	1.59
5	F	801	ADP	PA-O3A	5.85	1.65	1.59
5	F	801	ADP	O4'-C4'	-5.83	1.32	1.45
6	C	801	AGS	C2'-C1'	-5.74	1.35	1.53
6	C	801	AGS	O4'-C4'	5.68	1.57	1.45
6	B	801	AGS	C3'-C4'	-5.68	1.38	1.53
6	B	802	AGS	C3'-C4'	-5.63	1.38	1.53
6	B	801	AGS	O4'-C1'	5.60	1.54	1.42
6	D	801	AGS	O4'-C1'	5.59	1.54	1.42
5	E	801	ADP	C2'-C1'	-5.56	1.36	1.53
6	B	801	AGS	C2'-C1'	-5.50	1.36	1.53
6	B	802	AGS	O4'-C4'	5.35	1.56	1.45
6	B	802	AGS	C2'-C1'	-5.31	1.36	1.53
6	D	801	AGS	C2'-C1'	-5.24	1.37	1.53
5	A	801	ADP	C2'-C1'	-5.21	1.37	1.53
5	E	801	ADP	PA-O3A	5.20	1.65	1.59
5	A	801	ADP	O4'-C4'	-5.16	1.33	1.45
6	B	801	AGS	O4'-C4'	5.15	1.56	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	802	ADP	C6-N6	5.14	1.47	1.34
6	D	802	AGS	C2'-C1'	-5.10	1.37	1.53
6	C	802	AGS	C2'-C1'	-4.94	1.38	1.53
5	E	801	ADP	O4'-C4'	-4.90	1.34	1.45
5	A	801	ADP	PA-O3A	4.90	1.64	1.59
5	F	801	ADP	C2'-C1'	-4.86	1.38	1.53
6	D	802	AGS	O4'-C4'	4.83	1.55	1.45
6	E	803	AGS	O4'-C4'	4.80	1.55	1.45
5	A	802	ADP	PA-O3A	4.65	1.64	1.59
5	A	802	ADP	C2'-C1'	-4.55	1.39	1.53
6	B	801	AGS	C2'-C3'	4.51	1.65	1.53
6	D	801	AGS	O4'-C4'	4.48	1.54	1.45
6	C	802	AGS	C2'-C3'	4.31	1.65	1.53
6	D	802	AGS	C5'-C4'	4.31	1.64	1.51
6	D	801	AGS	C2'-C3'	4.19	1.64	1.53
6	C	802	AGS	O4'-C4'	4.18	1.54	1.45
6	B	801	AGS	C5'-C4'	4.13	1.64	1.51
6	D	802	AGS	PG-S1G	-4.10	1.81	1.90
6	B	802	AGS	C5'-C4'	4.08	1.63	1.51
6	E	803	AGS	C6-N6	3.97	1.44	1.34
6	B	802	AGS	C2'-C3'	3.92	1.64	1.53
6	D	802	AGS	C2'-C3'	3.87	1.63	1.53
6	C	801	AGS	C2'-C3'	3.87	1.63	1.53
5	E	801	ADP	C5-N7	-3.71	1.32	1.39
5	F	801	ADP	C5-N7	-3.50	1.32	1.39
6	C	802	AGS	C5-N7	-3.48	1.32	1.39
5	A	801	ADP	C6-N6	3.43	1.43	1.34
5	E	801	ADP	C6-N6	3.40	1.42	1.34
6	C	801	AGS	C5'-C4'	3.37	1.61	1.51
6	E	803	AGS	C2'-C3'	3.33	1.62	1.53
6	D	802	AGS	PA-O3A	3.33	1.63	1.59
5	E	801	ADP	C2-N1	3.28	1.39	1.33
5	F	801	ADP	C2-N1	3.26	1.39	1.33
5	E	801	ADP	C3'-C4'	3.20	1.61	1.53
5	F	801	ADP	C4-N3	3.17	1.40	1.34
5	F	801	ADP	C6-N6	3.16	1.42	1.34
5	A	801	ADP	C5-N7	-3.15	1.33	1.39
5	A	801	ADP	C1'-N9	3.15	1.55	1.46
6	D	802	AGS	C4-N3	3.13	1.40	1.34
5	E	801	ADP	C1'-N9	3.12	1.55	1.46
5	A	802	ADP	C6-N6	3.07	1.42	1.34
5	A	801	ADP	C3'-C4'	3.05	1.60	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	802	AGS	C5'-C4'	3.04	1.60	1.51
6	D	802	AGS	O3'-C3'	-3.03	1.35	1.43
6	E	803	AGS	PG-O2G	3.01	1.64	1.54
6	C	802	AGS	C4-N3	2.99	1.40	1.34
6	C	801	AGS	O3'-C3'	-2.96	1.35	1.43
6	C	801	AGS	C4-N3	2.96	1.39	1.34
6	D	802	AGS	C5-N7	-2.94	1.33	1.39
5	E	801	ADP	C4-N3	2.94	1.39	1.34
5	A	802	ADP	C5-N7	-2.86	1.33	1.39
5	A	801	ADP	C2-N1	2.86	1.39	1.33
6	D	801	AGS	C5'-C4'	2.86	1.60	1.51
6	C	802	AGS	PG-S1G	-2.83	1.84	1.90
6	D	801	AGS	C4-N3	2.81	1.39	1.34
5	A	802	ADP	C5'-C4'	2.80	1.60	1.51
5	F	801	ADP	C5'-C4'	2.78	1.59	1.51
6	B	802	AGS	C5-N7	-2.77	1.34	1.39
6	C	802	AGS	O3'-C3'	-2.75	1.36	1.43
6	B	801	AGS	C5-N7	-2.74	1.34	1.39
6	D	801	AGS	C5-N7	-2.74	1.34	1.39
6	C	801	AGS	C8-N9	-2.73	1.32	1.37
6	C	801	AGS	C5-N7	-2.73	1.34	1.39
5	A	801	ADP	C4-N3	2.72	1.39	1.34
6	B	802	AGS	C4-N3	2.72	1.39	1.34
6	E	803	AGS	O3'-C3'	-2.72	1.36	1.43
6	B	801	AGS	PG-S1G	-2.71	1.84	1.90
6	E	803	AGS	C5'-C4'	2.71	1.59	1.51
6	D	802	AGS	PB-O2B	-2.70	1.42	1.55
6	C	802	AGS	C8-N9	-2.68	1.33	1.37
5	E	802	ADP	C8-N9	-2.67	1.33	1.37
6	D	801	AGS	O3'-C3'	-2.66	1.36	1.43
6	D	802	AGS	C8-N9	-2.65	1.33	1.37
6	D	801	AGS	PB-O3B	-2.64	1.56	1.59
6	D	801	AGS	PG-O2G	2.62	1.63	1.54
6	E	803	AGS	PG-O3G	2.57	1.63	1.54
5	F	801	ADP	C3'-C4'	2.56	1.59	1.53
6	C	801	AGS	C2-N3	2.55	1.38	1.33
6	B	801	AGS	C4-N3	2.54	1.39	1.34
6	B	802	AGS	C6-N6	2.50	1.40	1.34
5	A	802	ADP	C4-N3	2.49	1.39	1.34
6	B	802	AGS	C1'-N9	2.49	1.53	1.46
5	A	801	ADP	C5'-C4'	2.48	1.59	1.51
6	B	801	AGS	O3'-C3'	-2.45	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	801	AGS	C8-N9	-2.45	1.33	1.37
5	E	802	ADP	C5-N7	-2.45	1.34	1.39
6	C	801	AGS	PG-O2G	2.44	1.62	1.54
6	E	803	AGS	C8-N9	-2.44	1.33	1.37
6	B	802	AGS	PG-O3G	2.41	1.62	1.54
5	A	802	ADP	C1'-N9	2.38	1.52	1.46
5	A	802	ADP	C3'-C4'	2.33	1.58	1.53
5	F	801	ADP	C8-N9	-2.32	1.33	1.37
6	C	802	AGS	C6-N6	2.25	1.40	1.34
6	D	801	AGS	PG-O3G	2.21	1.61	1.54
5	F	801	ADP	C1'-N9	2.18	1.52	1.46
6	C	801	AGS	PG-O3G	2.18	1.61	1.54
6	D	802	AGS	PG-O3G	2.16	1.61	1.54
6	B	802	AGS	PA-O3A	2.16	1.61	1.59
6	B	802	AGS	C8-N9	-2.13	1.33	1.37
6	D	802	AGS	C6-N6	2.13	1.39	1.34
5	A	802	ADP	C8-N9	-2.12	1.33	1.37
6	B	801	AGS	PG-O2G	2.12	1.61	1.54
6	D	801	AGS	C2-N3	2.11	1.37	1.33
6	B	802	AGS	O3'-C3'	-2.11	1.37	1.43
6	C	802	AGS	C2-N3	2.10	1.37	1.33
6	B	802	AGS	PG-O2G	2.08	1.61	1.54
5	A	802	ADP	C2-N1	2.08	1.37	1.33
6	C	802	AGS	PG-O2G	2.08	1.61	1.54
6	D	802	AGS	PB-O3A	-2.06	1.57	1.59
5	E	802	ADP	C3'-C4'	2.04	1.58	1.53
6	D	801	AGS	C8-N9	-2.00	1.34	1.37

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	801	ADP	C2'-C1'-N9	7.17	131.13	113.30
5	A	802	ADP	C2'-C1'-N9	6.95	130.57	113.30
5	A	801	ADP	C2'-C1'-N9	6.86	130.35	113.30
5	E	801	ADP	C5-C4-N3	-6.16	118.23	126.72
5	A	801	ADP	C5-C4-N3	-6.14	118.27	126.72
5	E	802	ADP	C5-C4-N3	-6.03	118.41	126.72
5	A	802	ADP	C5-C4-N3	-5.88	118.61	126.72
6	E	803	AGS	C5-C4-N3	-5.87	118.64	126.72
5	F	801	ADP	C5-C4-N3	-5.83	118.68	126.72
6	C	801	AGS	C5-C4-N3	-5.78	118.77	126.72
6	B	802	AGS	C5-C4-N3	-5.75	118.80	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	801	ADP	C2'-C1'-N9	5.61	127.25	113.30
6	C	802	AGS	C5-C4-N3	-5.60	119.00	126.72
6	D	802	AGS	C5-C4-N3	-5.43	119.24	126.72
6	B	801	AGS	C5-C4-N3	-5.13	119.65	126.72
6	C	802	AGS	N3-C2-N1	-5.10	120.87	128.58
6	D	801	AGS	C5-C4-N3	-5.07	119.73	126.72
5	F	801	ADP	N3-C2-N1	-5.06	120.92	128.58
5	E	802	ADP	O4'-C1'-N9	-5.00	98.48	108.09
6	D	801	AGS	N3-C2-N1	-4.97	121.06	128.58
6	C	801	AGS	N3-C2-N1	-4.94	121.11	128.58
6	B	801	AGS	O4'-C1'-N9	4.92	117.54	108.09
5	E	801	ADP	N3-C2-N1	-4.91	121.14	128.58
5	A	801	ADP	N3-C2-N1	-4.89	121.19	128.58
6	B	801	AGS	N3-C2-N1	-4.80	121.31	128.58
6	C	801	AGS	PB-O3B-PG	-4.72	115.90	133.17
5	E	801	ADP	N3-C4-N9	4.69	135.14	127.17
6	D	802	AGS	N3-C2-N1	-4.65	121.54	128.58
5	E	802	ADP	C2'-C1'-N9	4.64	124.84	113.30
5	A	802	ADP	N3-C2-N1	-4.63	121.58	128.58
6	C	801	AGS	N3-C4-N9	4.58	134.95	127.17
6	B	802	AGS	N3-C2-N1	-4.55	121.69	128.58
6	D	802	AGS	PB-O3B-PG	-4.55	116.52	133.17
6	B	801	AGS	N3-C4-N9	4.53	134.87	127.17
6	B	801	AGS	C4'-O4'-C1'	-4.52	99.48	109.47
5	F	801	ADP	N3-C4-N9	4.49	134.80	127.17
6	C	802	AGS	PB-O3B-PG	-4.44	116.91	133.17
6	C	802	AGS	N3-C4-N9	4.41	134.67	127.17
6	E	803	AGS	N3-C2-N1	-4.39	121.93	128.58
5	E	802	ADP	N3-C2-N1	-4.35	122.00	128.58
6	D	801	AGS	N3-C4-N9	4.26	134.41	127.17
5	A	802	ADP	O4'-C4'-C3'	-4.18	96.85	105.15
5	A	801	ADP	N3-C4-N9	4.17	134.26	127.17
6	B	802	AGS	C4-C5-N7	-4.14	105.85	110.58
6	B	801	AGS	O2B-PB-O3B	4.07	118.28	107.27
5	F	801	ADP	O4'-C4'-C3'	-4.04	97.13	105.15
5	A	802	ADP	N3-C4-N9	4.02	134.00	127.17
5	E	802	ADP	C4-C5-N7	-4.00	106.00	110.58
6	D	802	AGS	O2G-PG-O3B	4.00	118.00	104.64
5	E	802	ADP	N3-C4-N9	4.00	133.96	127.17
5	A	801	ADP	C4-C5-N7	-4.00	106.01	110.58
5	A	801	ADP	C2-N3-C4	3.94	121.46	111.83
5	A	802	ADP	C2-N3-C4	3.94	121.45	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	803	AGS	C4-C5-N7	-3.92	106.10	110.58
6	B	801	AGS	PB-O3B-PG	-3.89	118.93	133.17
6	D	802	AGS	N3-C4-N9	3.89	133.78	127.17
6	D	802	AGS	C4-C5-N7	-3.89	106.14	110.58
6	E	803	AGS	N3-C4-N9	3.86	133.74	127.17
5	A	802	ADP	C4-C5-N7	-3.86	106.17	110.58
5	A	802	ADP	O4'-C1'-N9	-3.84	100.71	108.09
6	C	802	AGS	C5-N7-C8	3.83	109.47	103.45
5	E	801	ADP	C2-N3-C4	3.80	121.12	111.83
5	E	802	ADP	C2-N3-C4	3.77	121.03	111.83
6	B	802	AGS	N3-C4-N9	3.75	133.55	127.17
5	A	801	ADP	C5-N7-C8	3.74	109.32	103.45
6	C	802	AGS	O4'-C4'-C3'	-3.72	97.77	105.15
6	B	802	AGS	PB-O3B-PG	-3.72	119.56	133.17
5	A	801	ADP	O4'-C1'-C2'	-3.70	98.70	106.62
6	E	803	AGS	C2-N3-C4	3.69	120.85	111.83
6	D	802	AGS	O2A-PA-O3A	3.68	117.23	107.27
6	B	802	AGS	C2-N3-C4	3.68	120.81	111.83
5	F	801	ADP	C5-N7-C8	3.65	109.19	103.45
5	F	801	ADP	C2-N3-C4	3.62	120.68	111.83
6	B	802	AGS	C5-N7-C8	3.62	109.14	103.45
6	B	802	AGS	O2B-PB-O3B	3.57	116.92	107.27
6	C	802	AGS	C4-C5-N7	-3.56	106.52	110.58
6	D	801	AGS	PB-O3B-PG	-3.56	120.16	133.17
6	C	801	AGS	C2-N3-C4	3.53	120.45	111.83
5	E	802	ADP	C5-N7-C8	3.49	108.93	103.45
5	F	801	ADP	C4-C5-N7	-3.48	106.61	110.58
6	C	802	AGS	C2-N3-C4	3.46	120.29	111.83
6	D	802	AGS	C5-N7-C8	3.46	108.88	103.45
5	A	802	ADP	C5-N7-C8	3.44	108.85	103.45
6	E	803	AGS	C3'-C2'-C1'	3.43	107.95	101.46
6	E	803	AGS	C5-N7-C8	3.40	108.79	103.45
6	B	801	AGS	C2-N3-C4	3.39	120.11	111.83
6	B	801	AGS	C5-N7-C8	3.38	108.77	103.45
6	C	801	AGS	C5-N7-C8	3.34	108.69	103.45
5	E	801	ADP	C5-N7-C8	3.33	108.69	103.45
6	B	801	AGS	C4-N9-C8	3.32	109.23	105.74
6	D	801	AGS	C2-N3-C4	3.32	119.94	111.83
6	C	801	AGS	C4-C5-N7	-3.31	106.79	110.58
5	E	801	ADP	O4'-C1'-N9	-3.31	101.73	108.09
6	D	802	AGS	C2-N3-C4	3.29	119.86	111.83
6	B	802	AGS	O2G-PG-O3B	3.25	115.50	104.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	801	AGS	O2G-PG-O3B	3.17	115.22	104.64
6	B	801	AGS	N9-C8-N7	-3.14	109.48	113.94
5	E	801	ADP	O4'-C1'-C2'	-3.14	99.90	106.62
6	C	801	AGS	O2G-PG-O3B	3.12	115.06	104.64
6	B	801	AGS	C4-C5-N7	-3.11	107.03	110.58
6	E	803	AGS	N9-C8-N7	-3.09	109.55	113.94
5	E	802	ADP	N9-C8-N7	-3.08	109.57	113.94
5	A	801	ADP	O4'-C1'-N9	-3.01	102.30	108.09
5	E	801	ADP	C4-C5-N7	-2.96	107.19	110.58
6	C	802	AGS	O2A-PA-O3A	2.96	115.26	107.27
6	C	802	AGS	O2G-PG-O3B	2.95	114.48	104.64
6	D	801	AGS	C2'-C1'-N9	2.90	120.50	113.30
6	D	801	AGS	C5-N7-C8	2.89	107.99	103.45
6	D	802	AGS	O5'-C5'-C4'	2.88	118.79	108.99
6	B	801	AGS	O4'-C1'-C2'	-2.85	100.52	106.62
6	E	803	AGS	C2'-C3'-C4'	2.85	108.11	102.61
5	F	801	ADP	O4'-C1'-N9	-2.75	102.80	108.09
6	E	803	AGS	PB-O3B-PG	-2.70	123.28	133.17
6	C	802	AGS	N9-C8-N7	-2.65	110.17	113.94
6	B	801	AGS	C2'-C1'-N9	2.63	119.83	113.30
6	D	802	AGS	O4'-C4'-C3'	-2.61	99.97	105.15
6	C	802	AGS	C4'-O4'-C1'	-2.60	103.73	109.47
6	D	801	AGS	O4'-C1'-C2'	-2.59	101.08	106.62
6	B	801	AGS	C5-C6-N6	-2.59	116.88	123.29
6	C	801	AGS	O4'-C1'-N9	2.57	113.03	108.09
6	D	801	AGS	C4-C5-N7	-2.55	107.67	110.58
5	F	801	ADP	O2B-PB-O3A	2.55	113.18	104.64
6	E	803	AGS	C4'-O4'-C1'	-2.54	103.87	109.47
6	B	802	AGS	N9-C8-N7	-2.53	110.34	113.94
6	C	802	AGS	O2B-PB-O3A	2.51	114.06	107.27
5	F	801	ADP	N9-C8-N7	-2.50	110.39	113.94
5	A	802	ADP	N9-C8-N7	-2.48	110.42	113.94
5	E	801	ADP	O2B-PB-O3A	2.46	112.89	104.64
6	D	801	AGS	N9-C8-N7	-2.45	110.46	113.94
6	C	801	AGS	O4'-C1'-C2'	-2.43	101.42	106.62
5	A	801	ADP	C3'-C2'-C1'	2.42	106.05	101.46
5	A	802	ADP	O2A-PA-O3A	2.42	113.81	107.27
6	B	802	AGS	O4'-C1'-C2'	-2.41	101.46	106.62
5	E	801	ADP	C5-C6-N6	-2.36	117.45	123.29
5	F	801	ADP	C5-C6-N6	-2.36	117.45	123.29
5	F	801	ADP	O3B-PB-O3A	2.31	112.37	104.64
6	D	802	AGS	N9-C8-N7	-2.31	110.66	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	801	AGS	N9-C8-N7	-2.30	110.67	113.94
5	E	802	ADP	C3'-C2'-C1'	2.27	105.75	101.46
6	D	801	AGS	C5-C6-N6	-2.26	117.68	123.29
6	E	803	AGS	O4'-C1'-N9	2.25	112.41	108.09
6	D	801	AGS	O2B-PB-O3A	2.24	113.33	107.27
5	A	801	ADP	N9-C8-N7	-2.23	110.77	113.94
5	A	802	ADP	C6-C5-N7	2.22	136.38	132.09
5	F	801	ADP	O2A-PA-O3A	2.21	113.25	107.27
6	D	801	AGS	C4-N9-C8	2.18	108.03	105.74
6	D	801	AGS	O3G-PG-O3B	2.18	111.91	104.64
6	D	802	AGS	O3G-PG-O3B	2.16	111.86	104.64
6	C	801	AGS	O2B-PB-O1B	-2.14	102.49	112.44
5	A	802	ADP	O4'-C1'-C2'	-2.14	102.03	106.62
6	B	802	AGS	O4'-C1'-N9	2.12	112.17	108.09
5	A	802	ADP	C3'-C2'-C1'	2.12	105.48	101.46
6	E	803	AGS	C4-N9-C8	2.09	107.93	105.74
5	F	801	ADP	C3'-C2'-C1'	2.08	105.39	101.46
6	C	801	AGS	C2'-C1'-N9	2.04	118.38	113.30
5	E	802	ADP	C4-N9-C8	2.04	107.88	105.74
6	C	801	AGS	C1'-N9-C8	-2.04	122.58	127.09
5	A	801	ADP	O2B-PB-O3A	2.03	111.43	104.64
6	D	802	AGS	O4'-C4'-C5'	2.00	115.75	109.33
6	D	802	AGS	C2'-C1'-N9	2.00	118.28	113.30

All (25) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	801	ADP	C3'
5	A	801	ADP	C1'
5	A	802	ADP	C1'
5	E	801	ADP	C3'
5	E	801	ADP	C1'
5	E	802	ADP	C2'
5	E	802	ADP	C3'
5	F	801	ADP	C3'
5	F	801	ADP	C1'
6	B	801	AGS	C3'
6	B	801	AGS	C4'
6	B	802	AGS	C1'
6	B	802	AGS	C3'
6	B	802	AGS	C4'
6	C	801	AGS	C3'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
6	C	801	AGS	C4'
6	C	802	AGS	C3'
6	C	802	AGS	C4'
6	D	801	AGS	C3'
6	D	801	AGS	C4'
6	D	802	AGS	C1'
6	D	802	AGS	C3'
6	D	802	AGS	C4'
6	E	803	AGS	C3'
6	E	803	AGS	C4'

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	801	ADP	C5'-O5'-PA-O2A
5	A	801	ADP	C5'-O5'-PA-O3A
5	A	801	ADP	C4'-C5'-O5'-PA
5	A	802	ADP	C5'-O5'-PA-O1A
5	E	801	ADP	C5'-O5'-PA-O2A
5	E	801	ADP	C5'-O5'-PA-O3A
6	B	801	AGS	C5'-O5'-PA-O1A
6	B	801	AGS	C5'-O5'-PA-O3A
6	B	801	AGS	O4'-C1'-N9-C8
6	B	801	AGS	O4'-C1'-N9-C4
6	C	801	AGS	C4'-C5'-O5'-PA
6	C	802	AGS	C5'-O5'-PA-O1A
6	C	802	AGS	C5'-O5'-PA-O3A
6	C	802	AGS	C4'-C5'-O5'-PA
6	D	801	AGS	C5'-O5'-PA-O1A
6	D	801	AGS	C5'-O5'-PA-O2A
6	D	801	AGS	C5'-O5'-PA-O3A
6	E	803	AGS	C4'-C5'-O5'-PA
6	C	802	AGS	C3'-C4'-C5'-O5'
6	D	802	AGS	C4'-C5'-O5'-PA
6	C	802	AGS	O4'-C4'-C5'-O5'
6	D	801	AGS	C4'-C5'-O5'-PA
5	A	802	ADP	O4'-C1'-N9-C4
6	C	801	AGS	C2'-C1'-N9-C4
6	C	801	AGS	C2'-C1'-N9-C8
6	B	802	AGS	C4'-C5'-O5'-PA
5	A	802	ADP	O4'-C1'-N9-C8
6	D	801	AGS	C2'-C1'-N9-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	801	ADP	PB-O3A-PA-O5'
5	E	801	ADP	PB-O3A-PA-O5'
5	E	802	ADP	PB-O3A-PA-O5'
5	E	802	ADP	C2'-C1'-N9-C4
6	D	801	AGS	C2'-C1'-N9-C8
6	C	802	AGS	C5'-O5'-PA-O2A
6	D	802	AGS	C5'-O5'-PA-O1A
5	E	802	ADP	PA-O3A-PB-O1B
5	E	802	ADP	C2'-C1'-N9-C8
6	D	802	AGS	PB-O3A-PA-O1A
5	E	801	ADP	C4'-C5'-O5'-PA
6	B	801	AGS	PB-O3B-PG-O2G
5	E	802	ADP	PA-O3A-PB-O2B
5	E	802	ADP	PA-O3A-PB-O3B
6	C	801	AGS	PB-O3A-PA-O1A
6	D	802	AGS	PB-O3A-PA-O2A
5	E	802	ADP	O4'-C4'-C5'-O5'

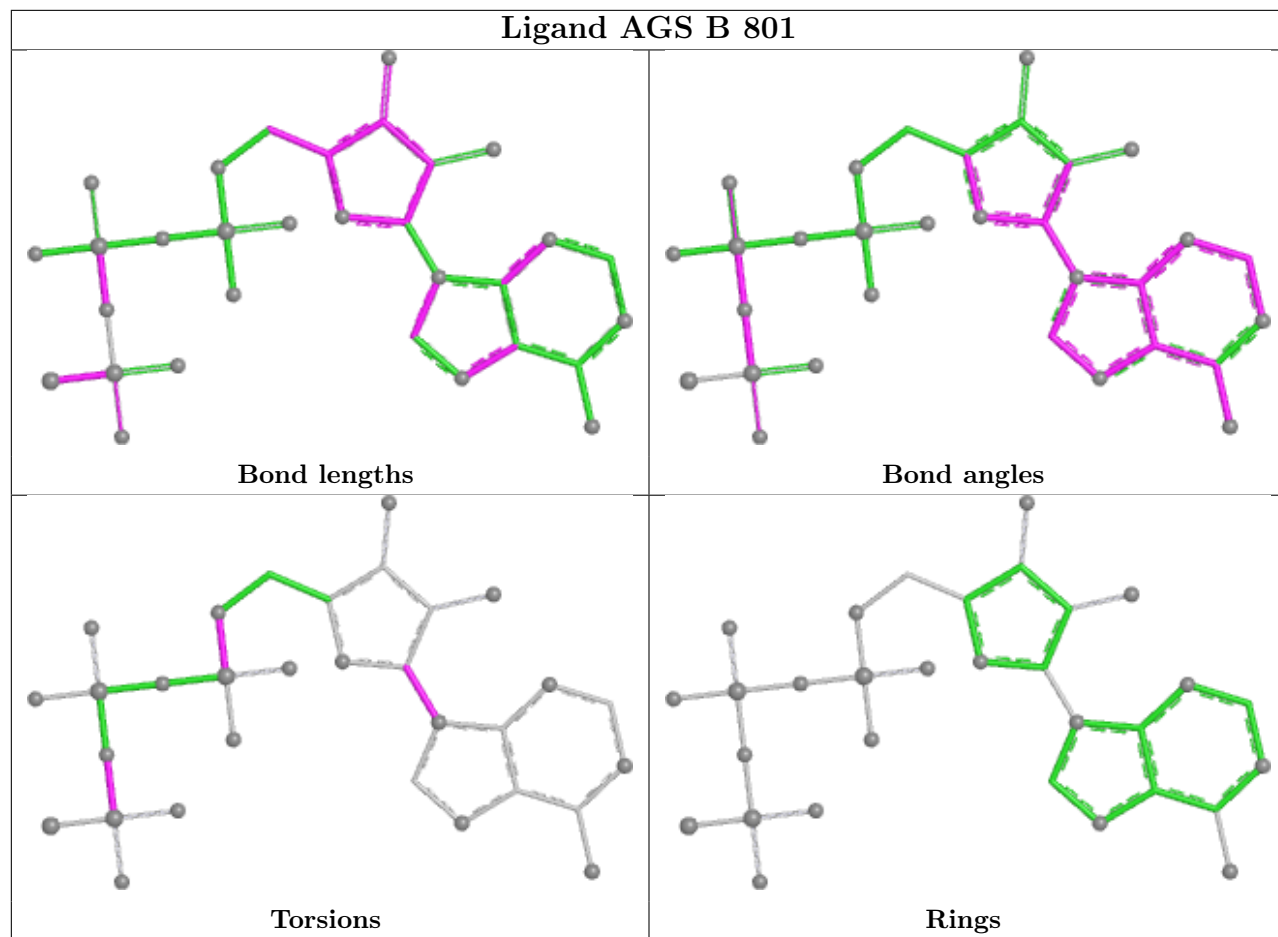
There are no ring outliers.

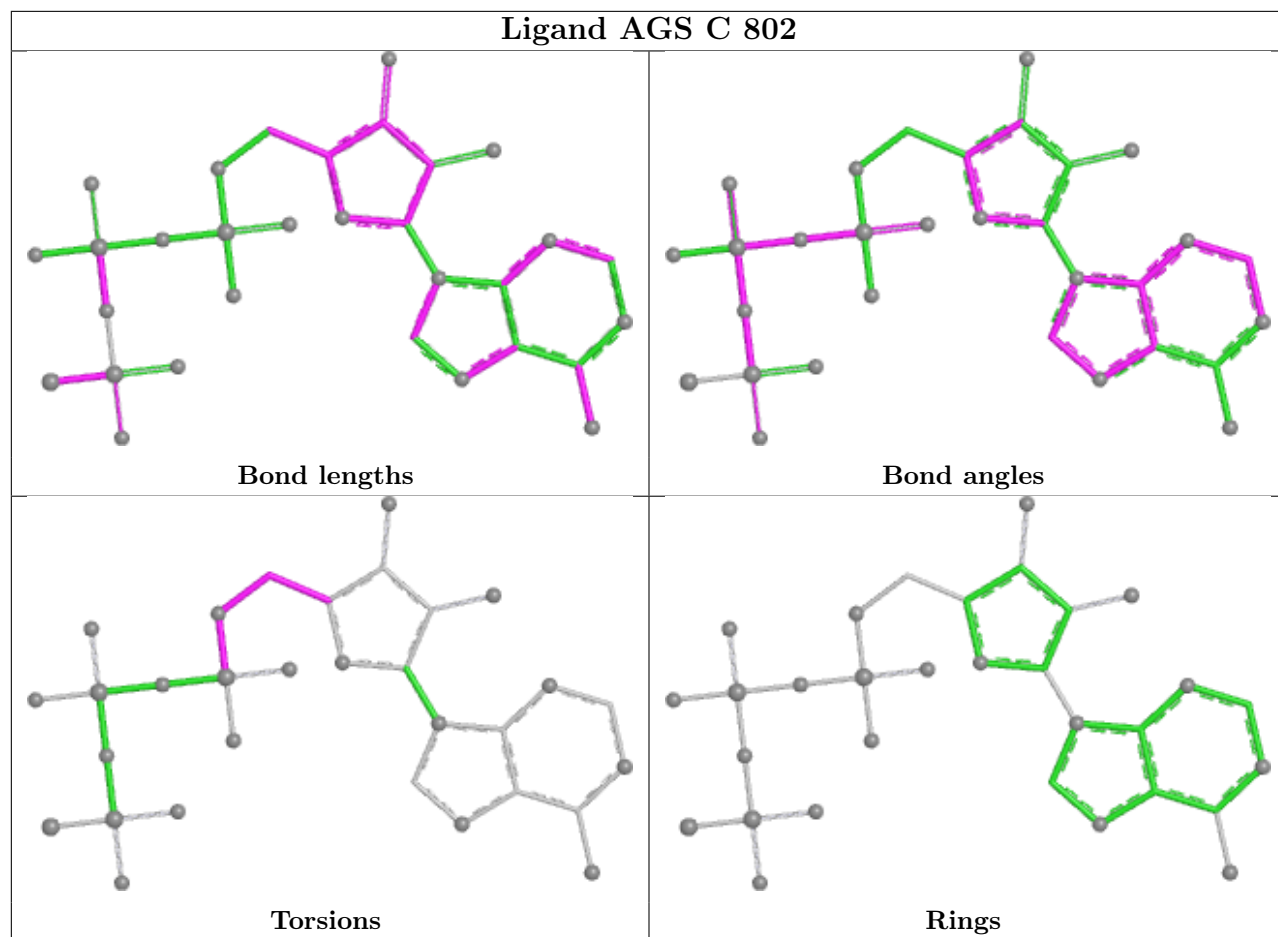
8 monomers are involved in 36 short contacts:

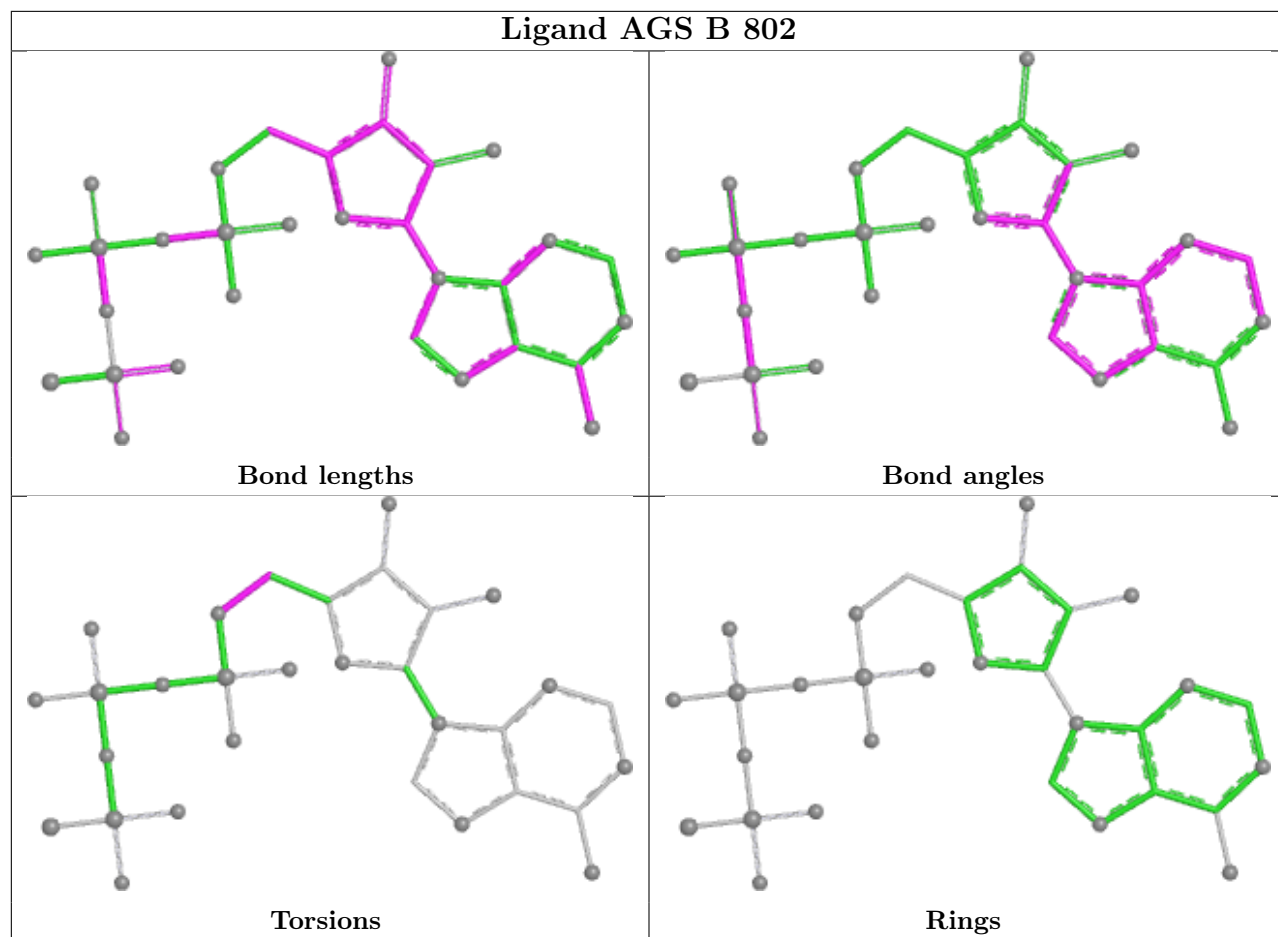
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	802	AGS	1	0
6	B	802	AGS	4	0
6	D	802	AGS	1	0
5	A	802	ADP	1	0
5	E	801	ADP	2	0
6	E	803	AGS	9	0
5	E	802	ADP	17	0
5	F	801	ADP	1	0

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

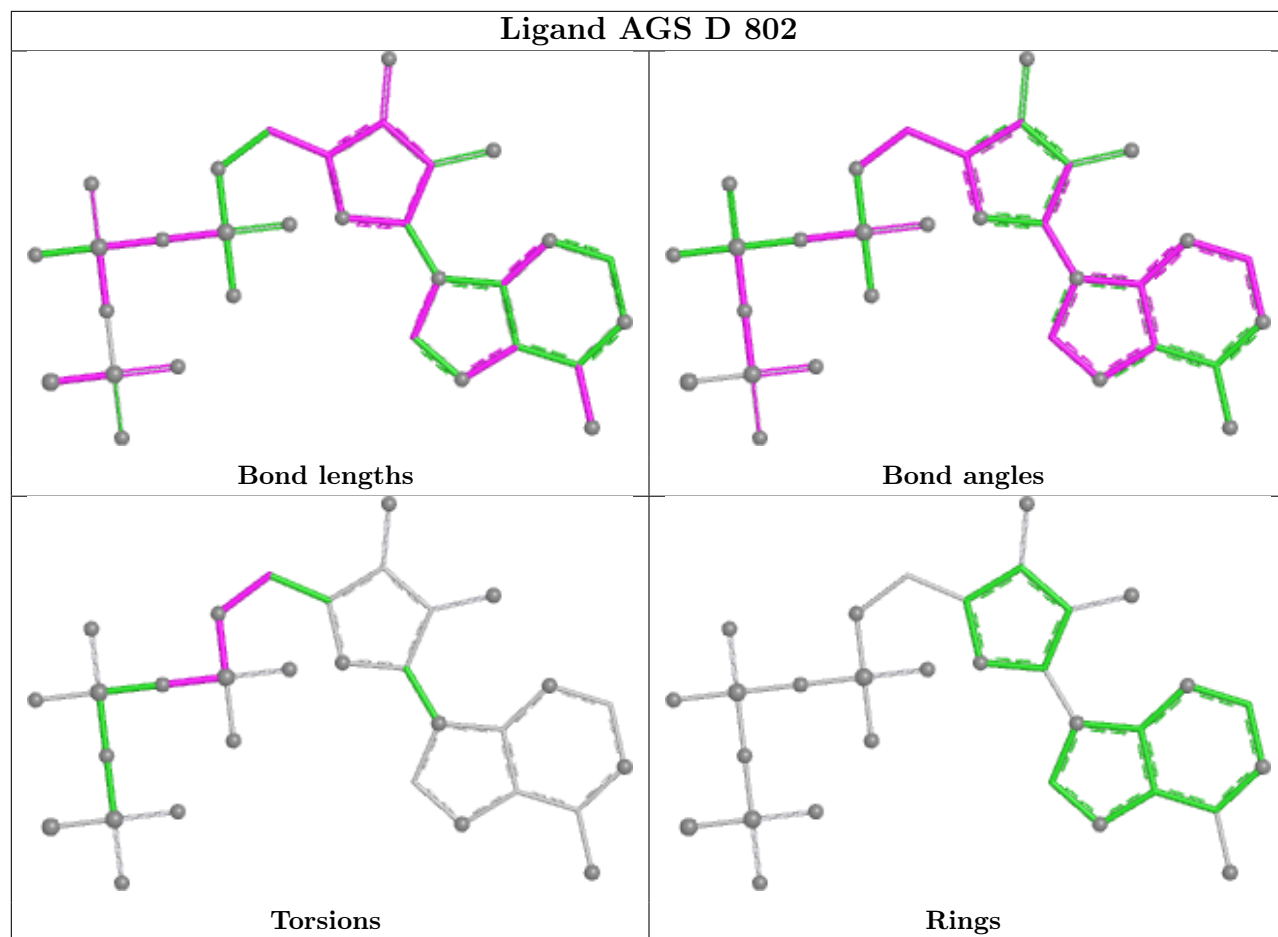
equivalents in the CSD to analyse the geometry.



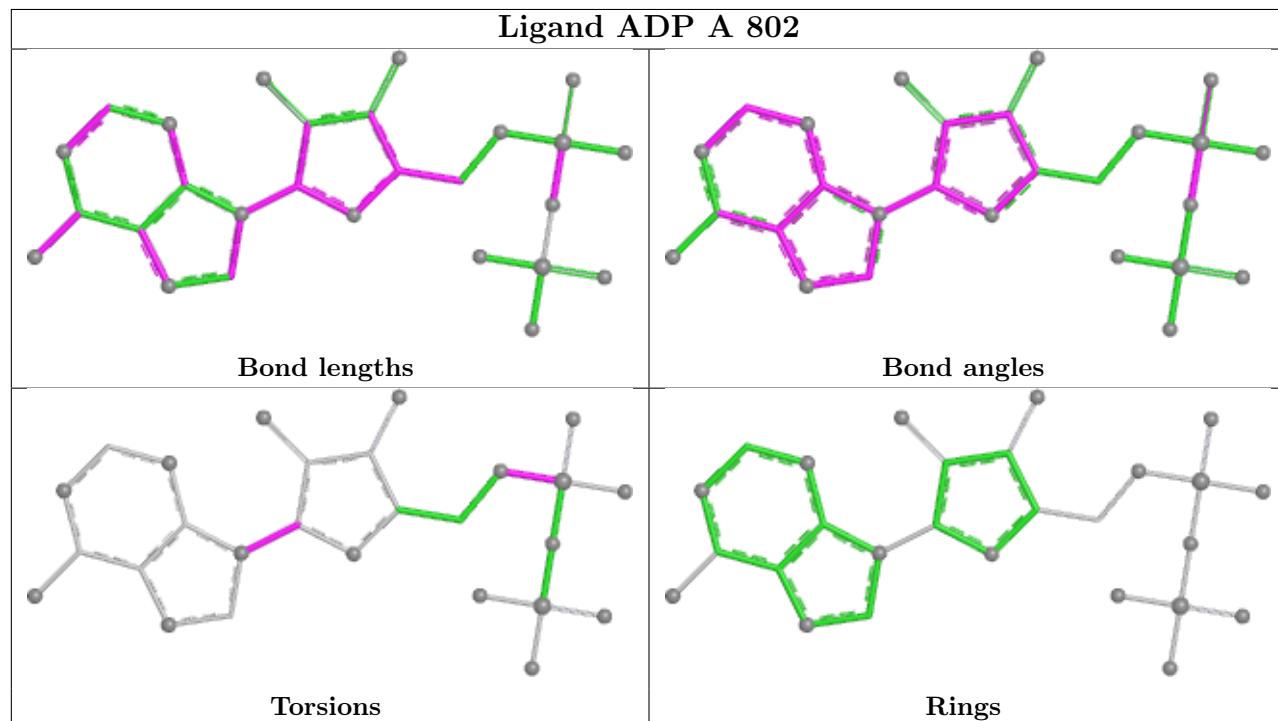


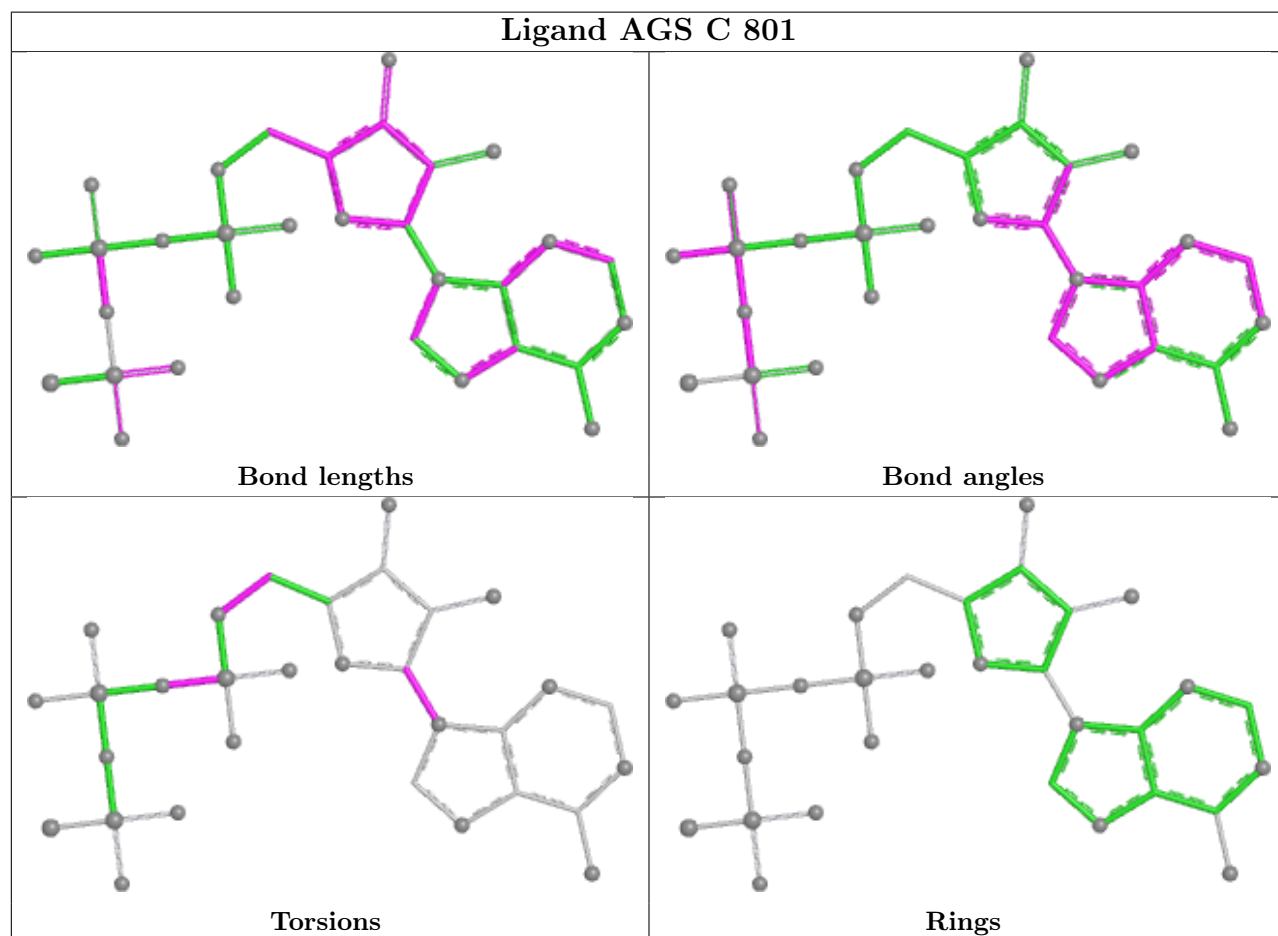
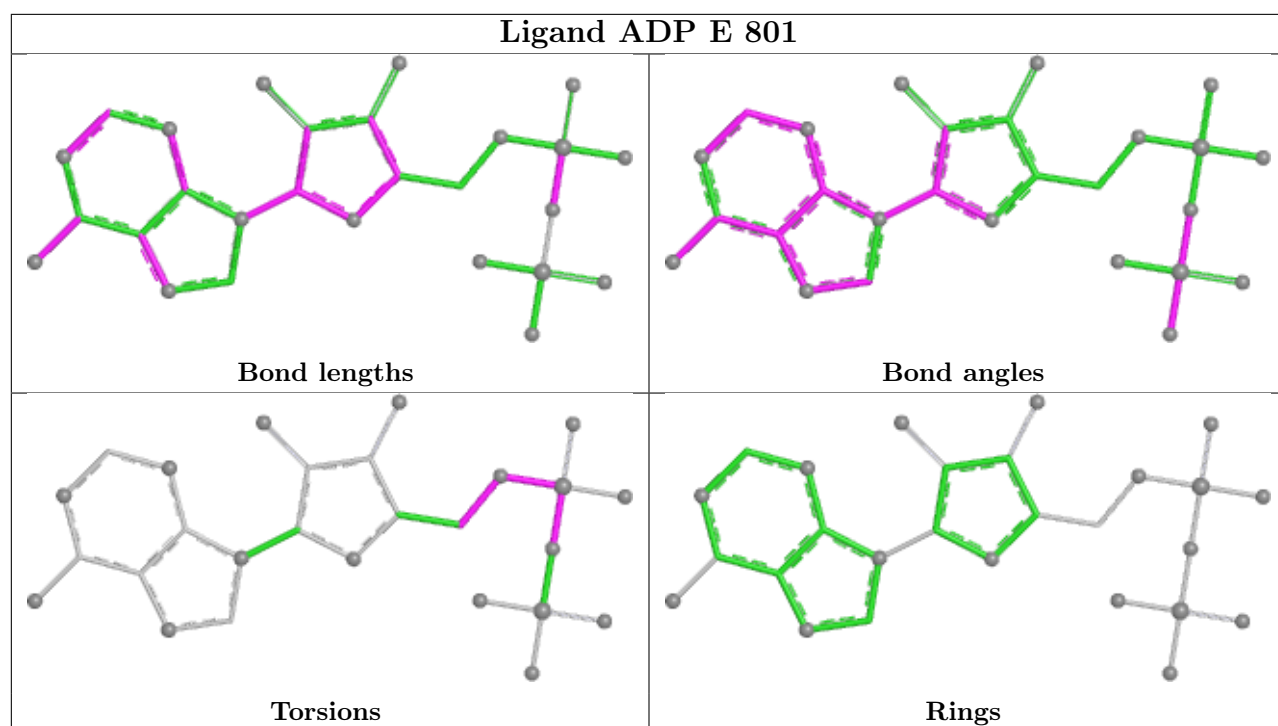


Ligand AGS D 802

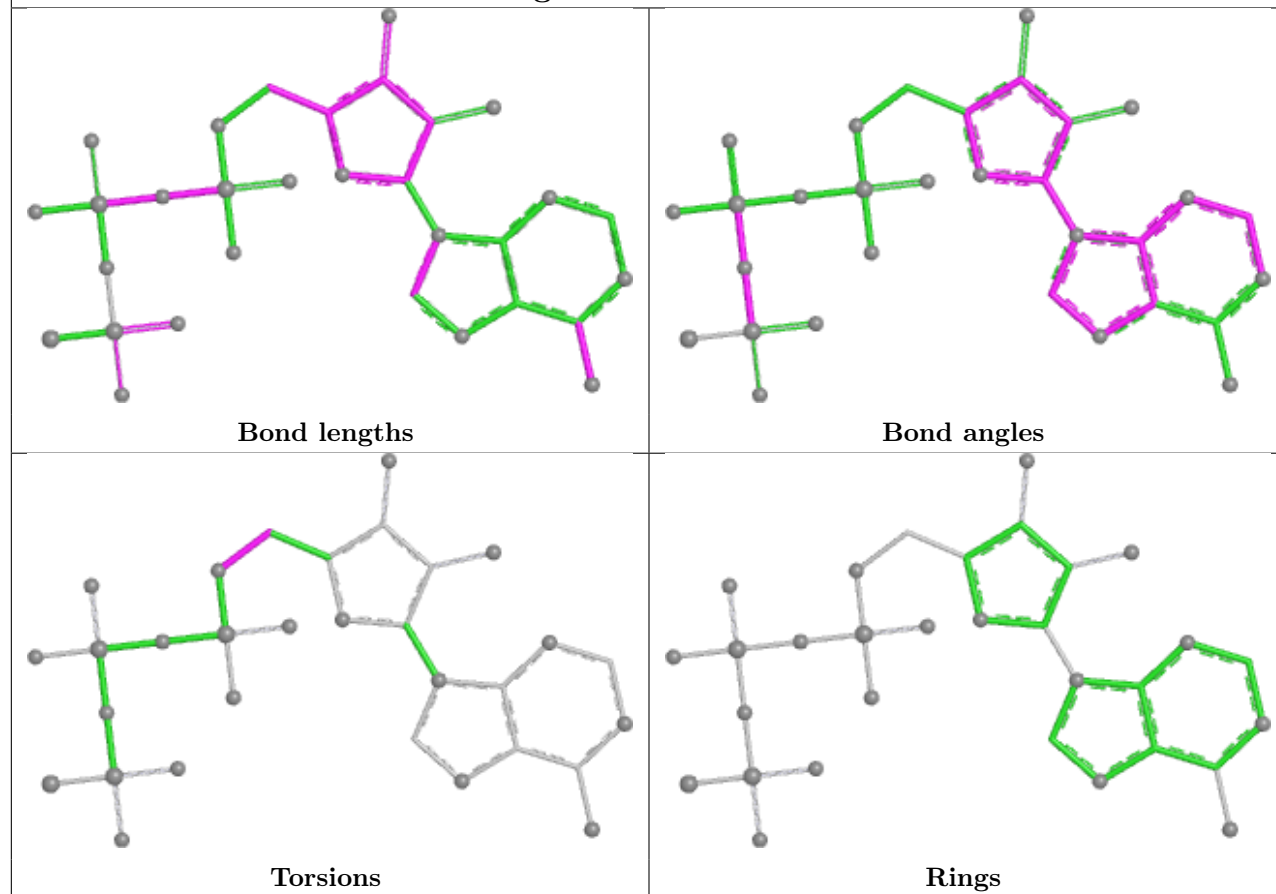


Ligand ADP A 802

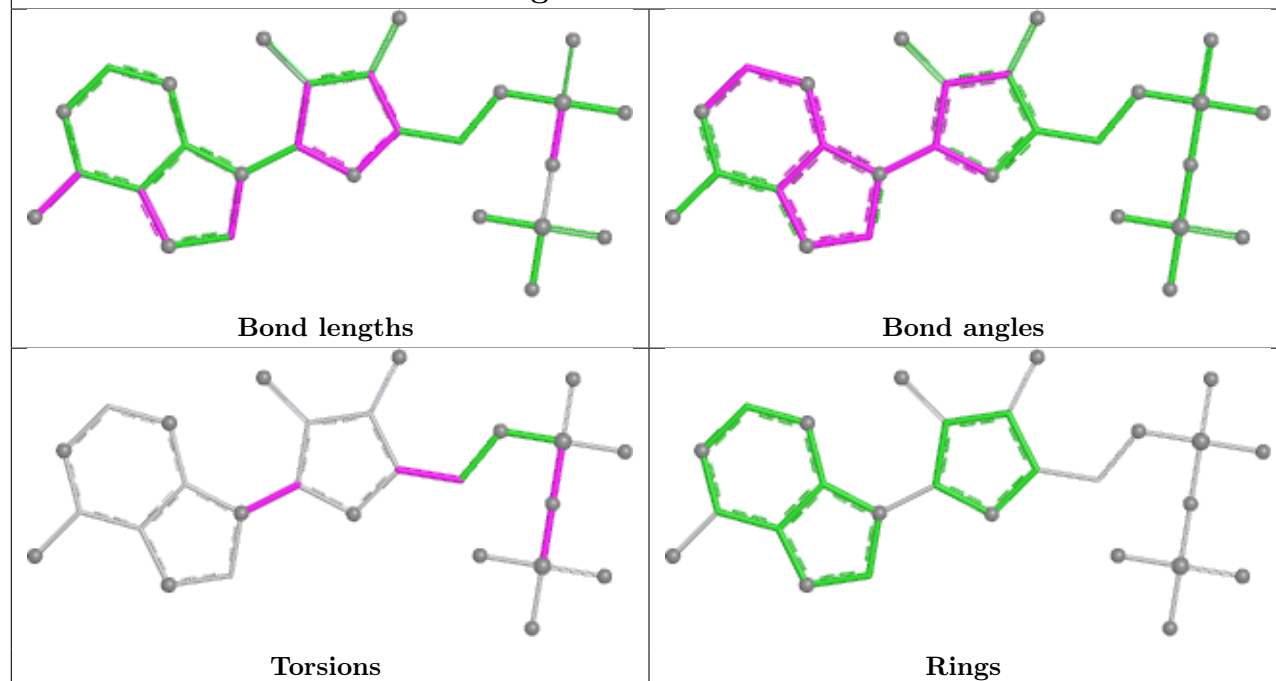


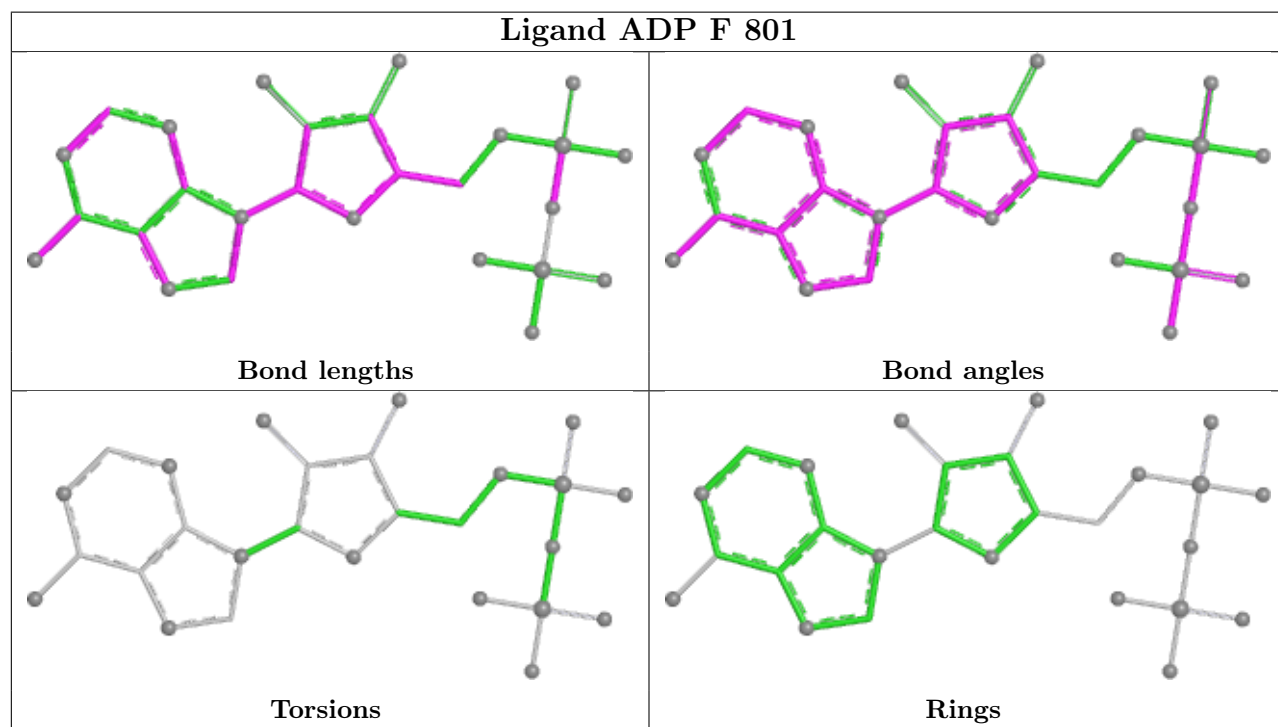
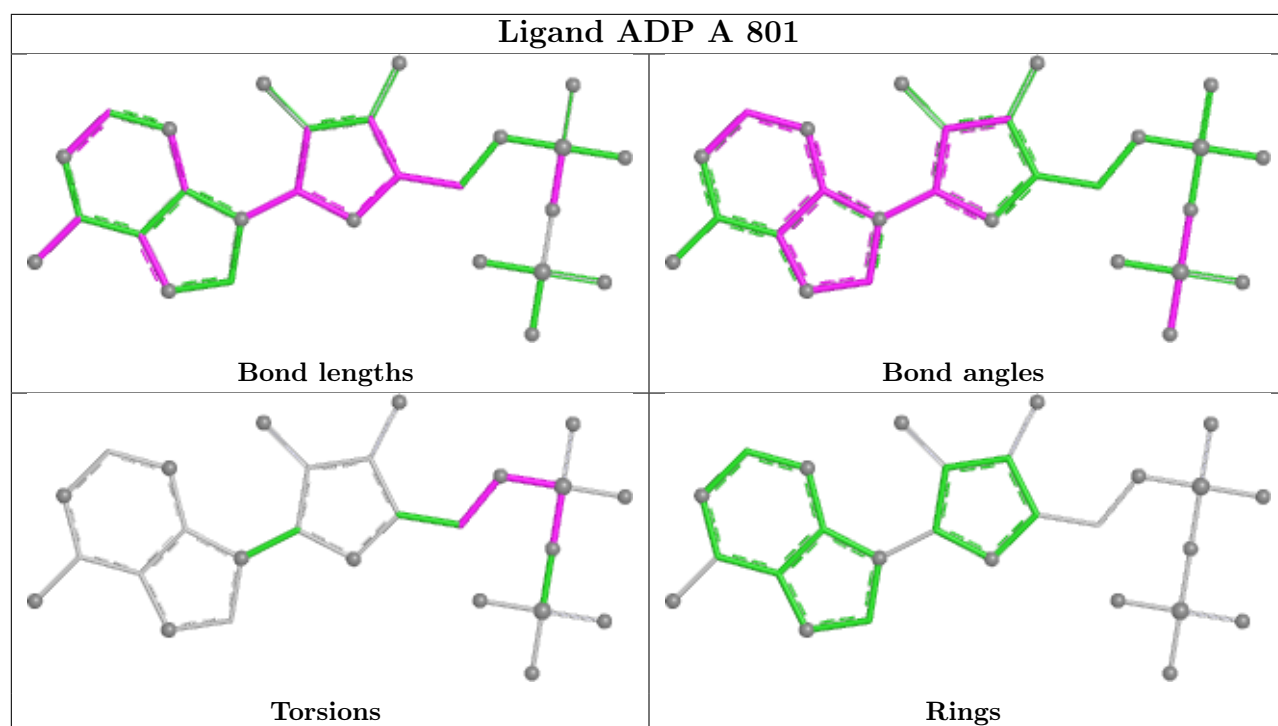


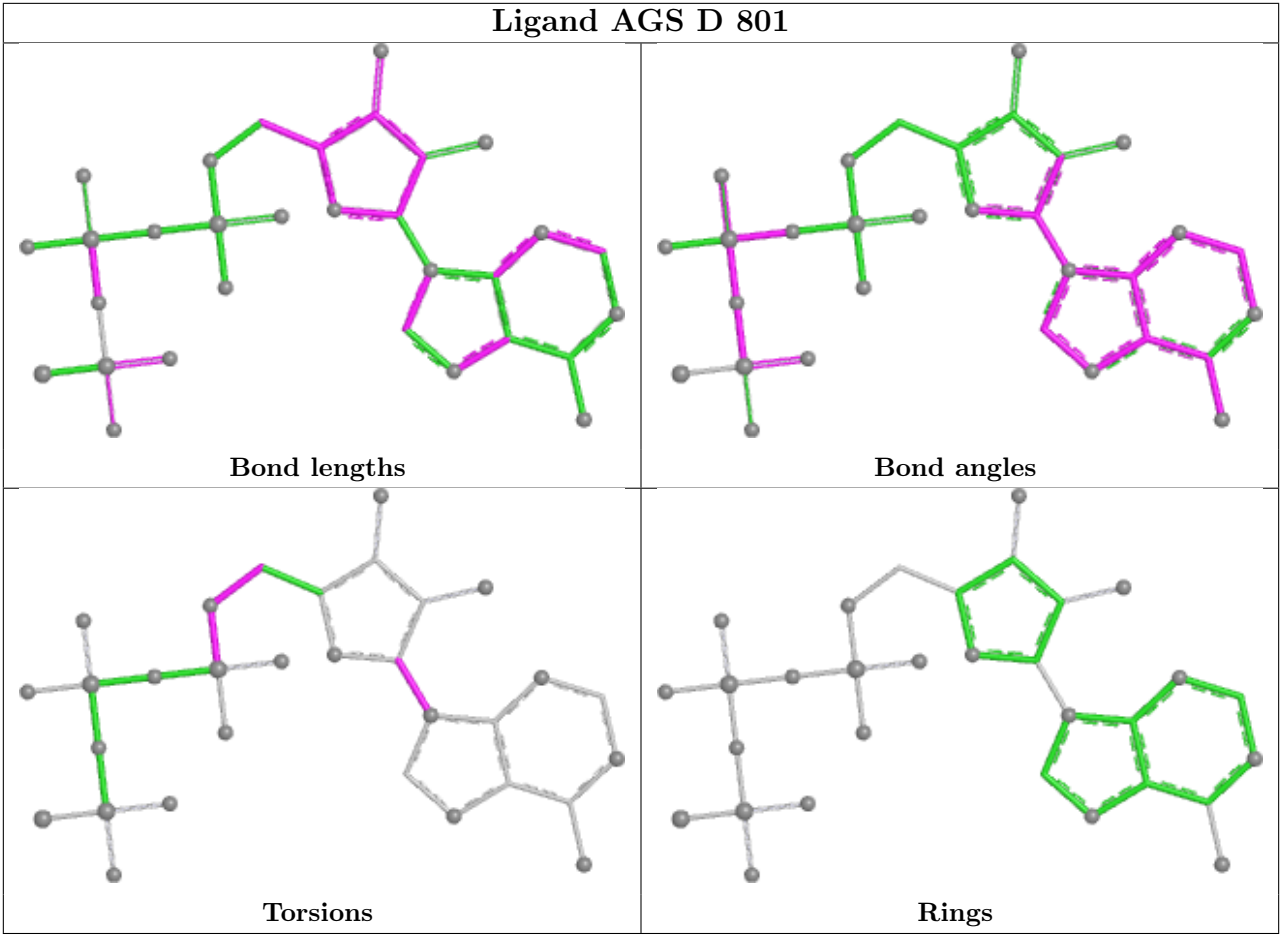
Ligand AGS E 803



Ligand ADP E 802







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	214:GLY	C	215:GLU	N	3.06

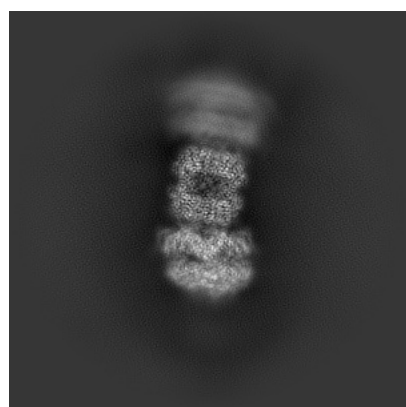
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20845. These allow visual inspection of the internal detail of the map and identification of artifacts.

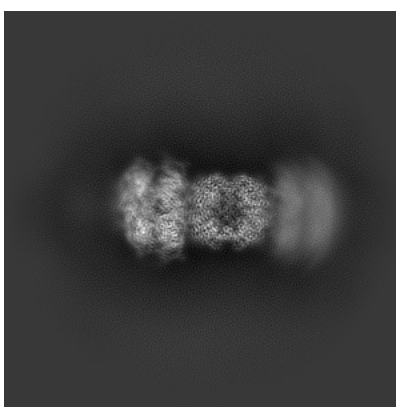
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

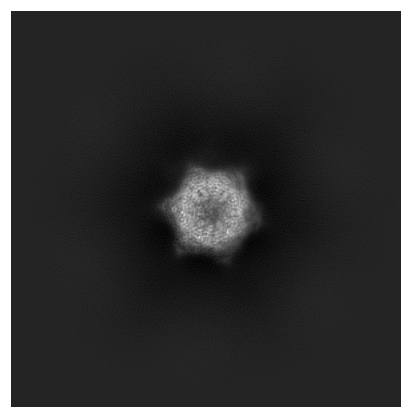
6.1.1 Primary map



X



Y

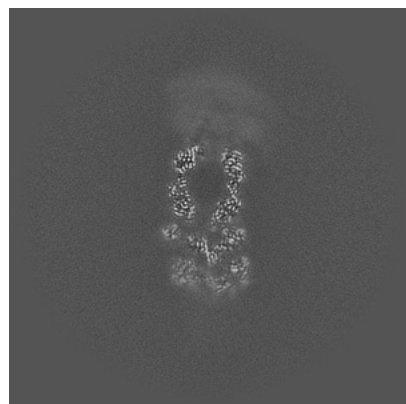


Z

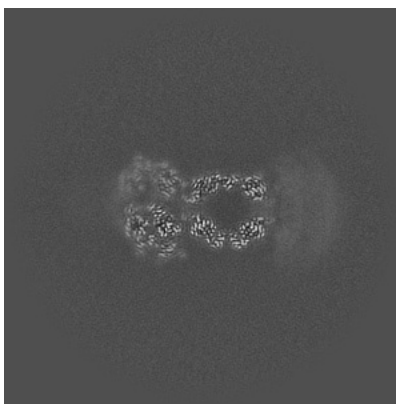
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

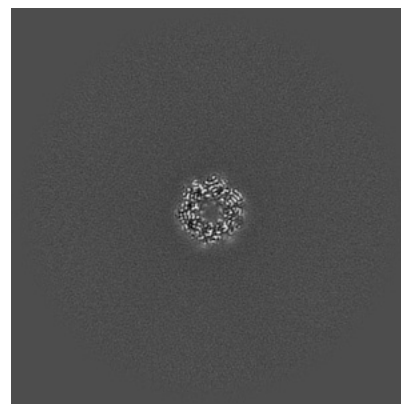
6.2.1 Primary map



X Index: 300



Y Index: 300

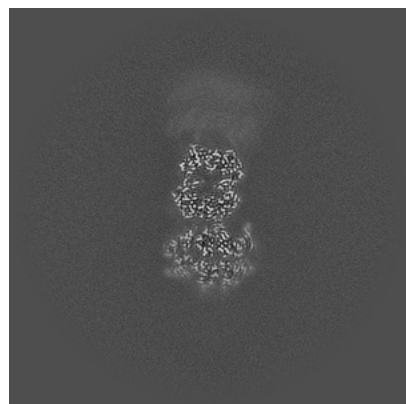


Z Index: 300

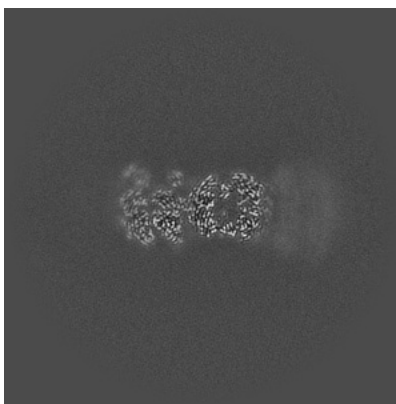
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

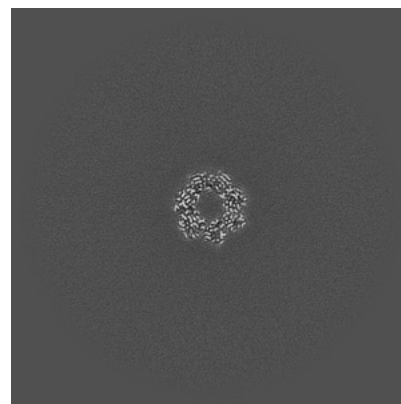
6.3.1 Primary map



X Index: 273



Y Index: 324

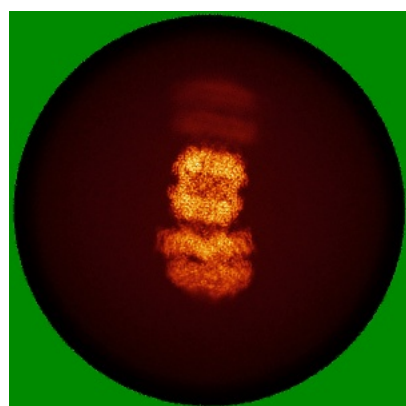


Z Index: 363

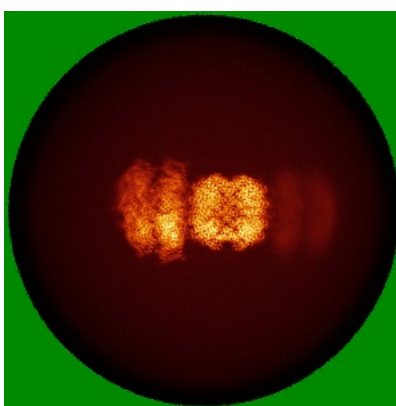
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

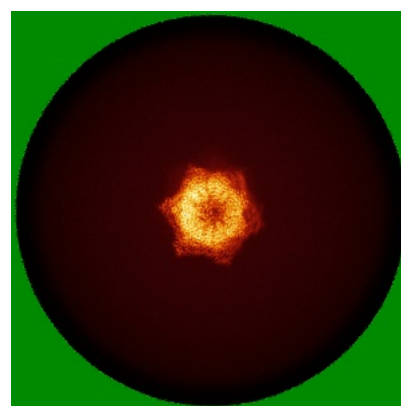
6.4.1 Primary map



X



Y

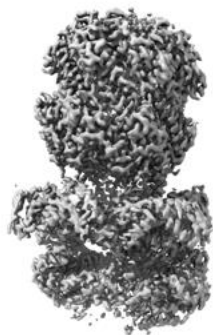


Z

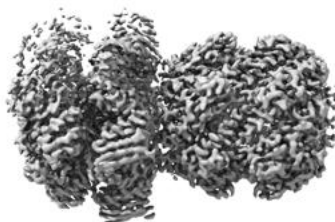
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

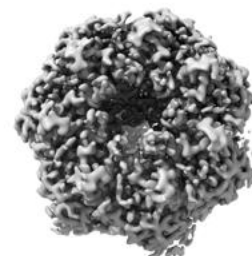
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.77. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

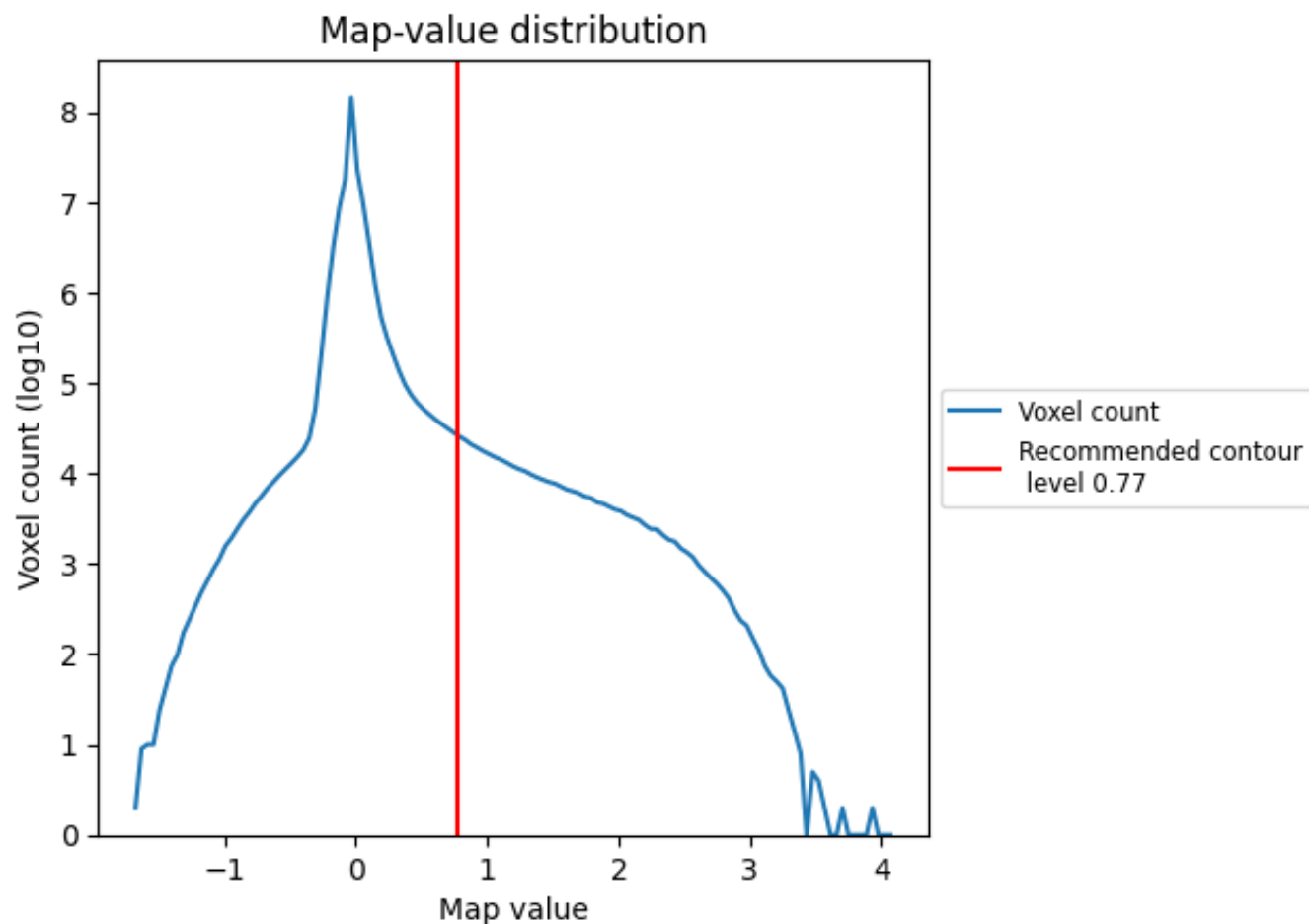
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

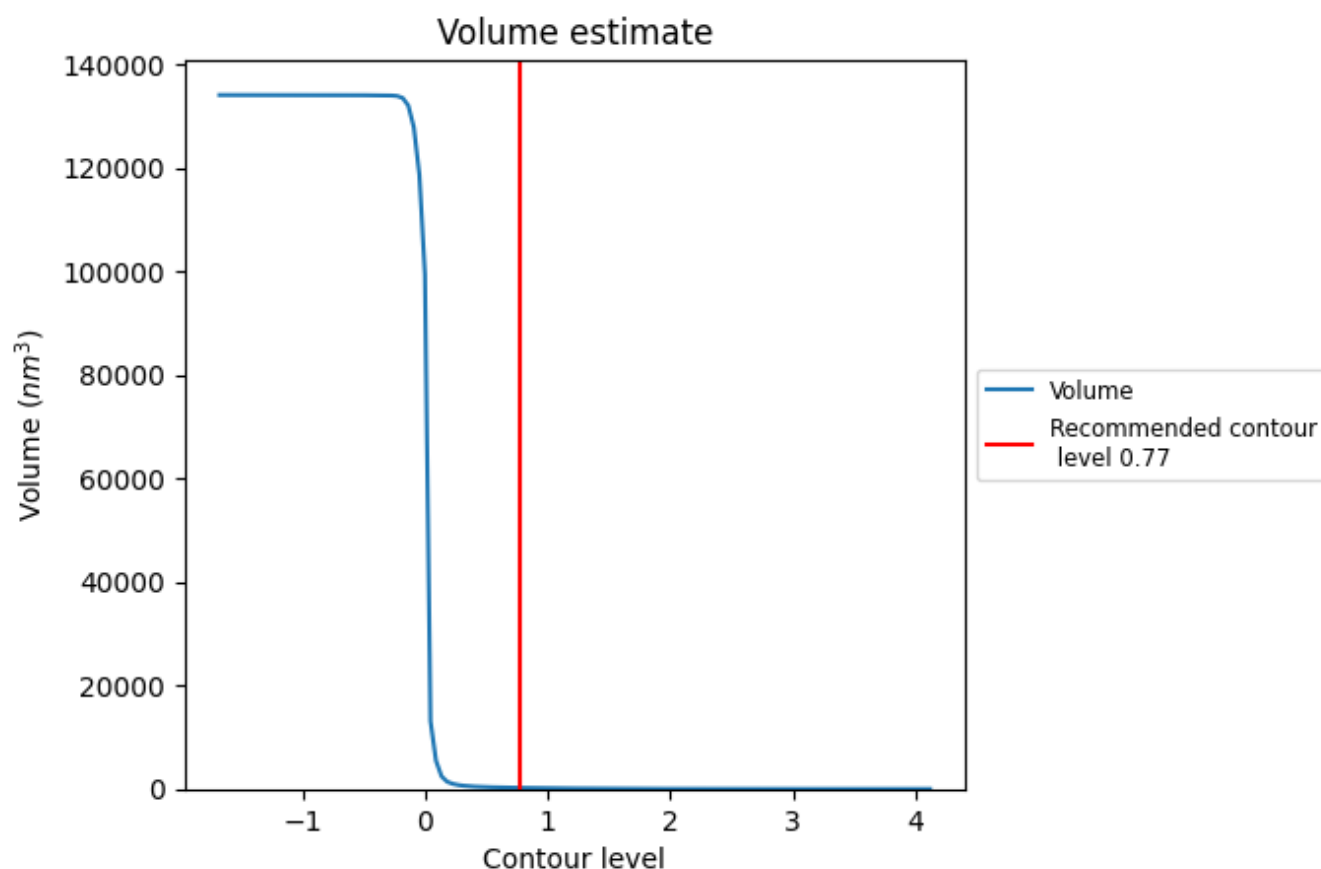
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

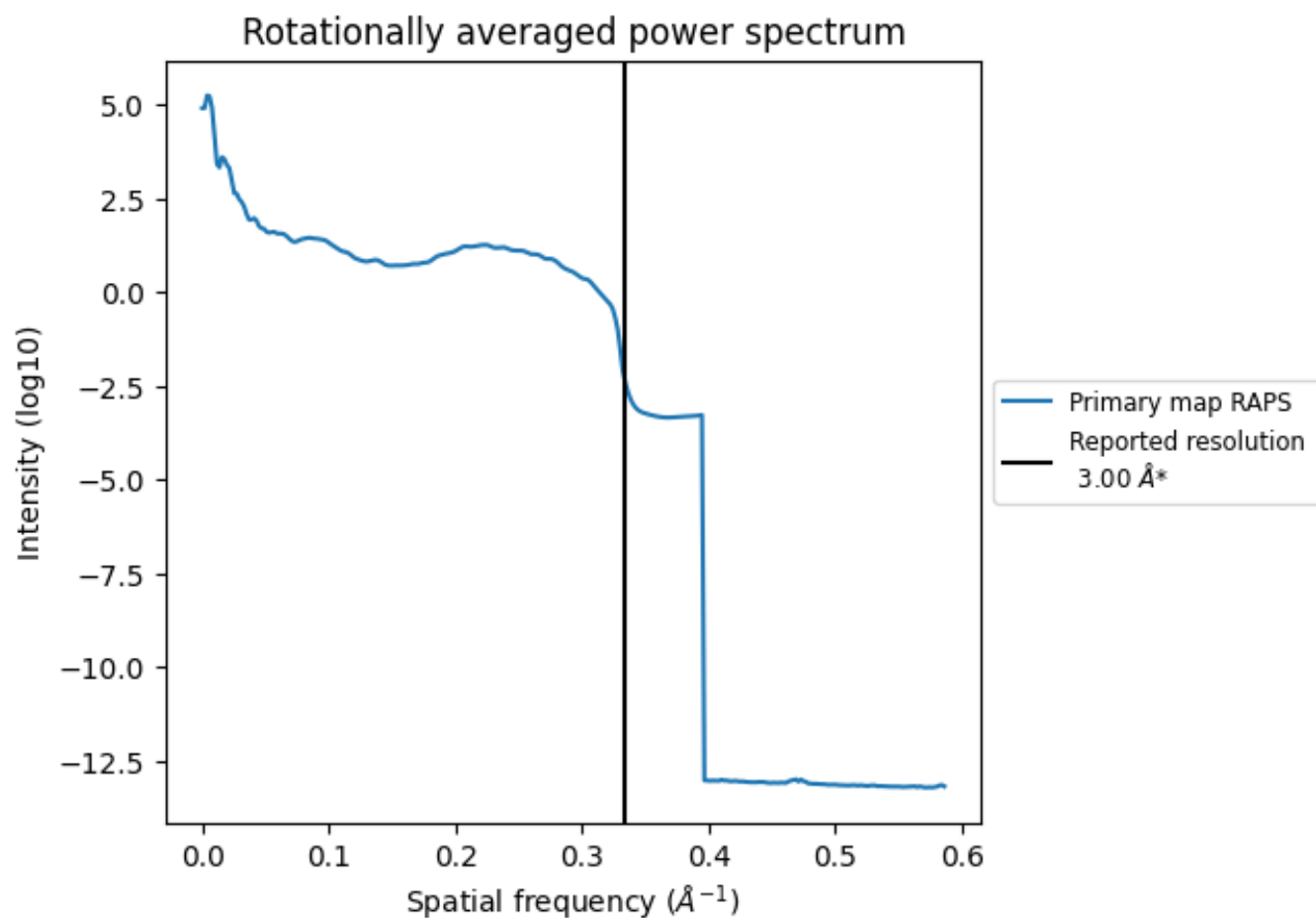
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 214 nm³; this corresponds to an approximate mass of 193 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

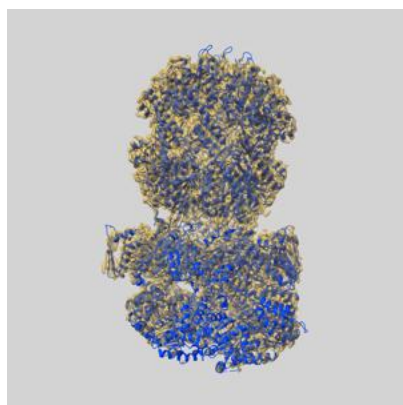
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

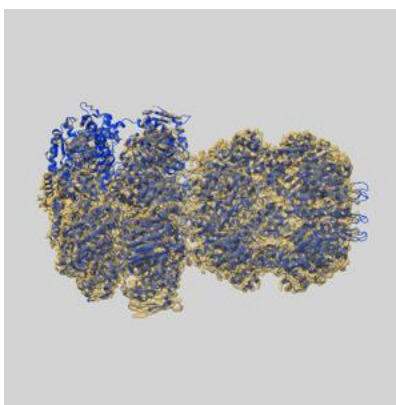
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20845 and PDB model 6UQE. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

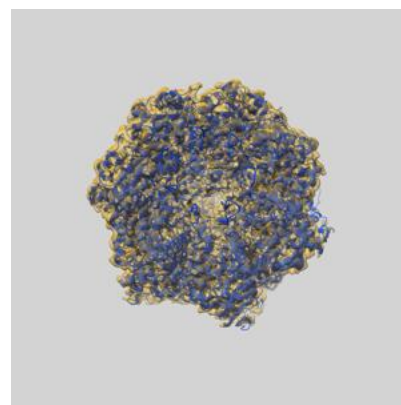
9.1 Map-model overlay [i](#)



X



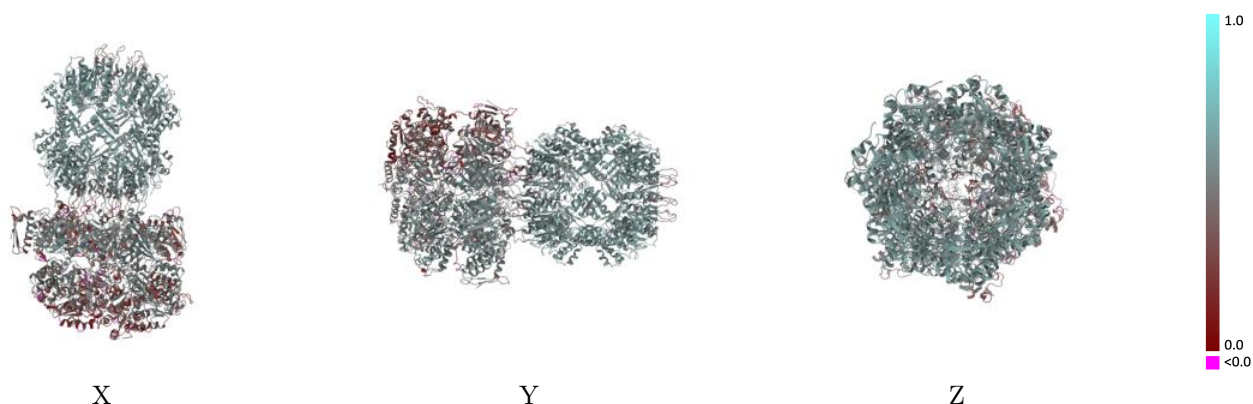
Y



Z

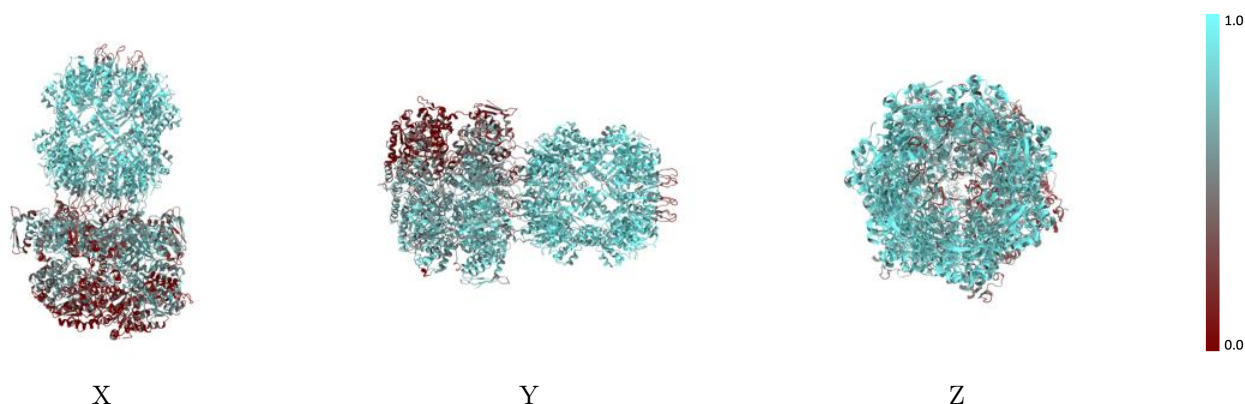
The images above show the 3D surface view of the map at the recommended contour level 0.77 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



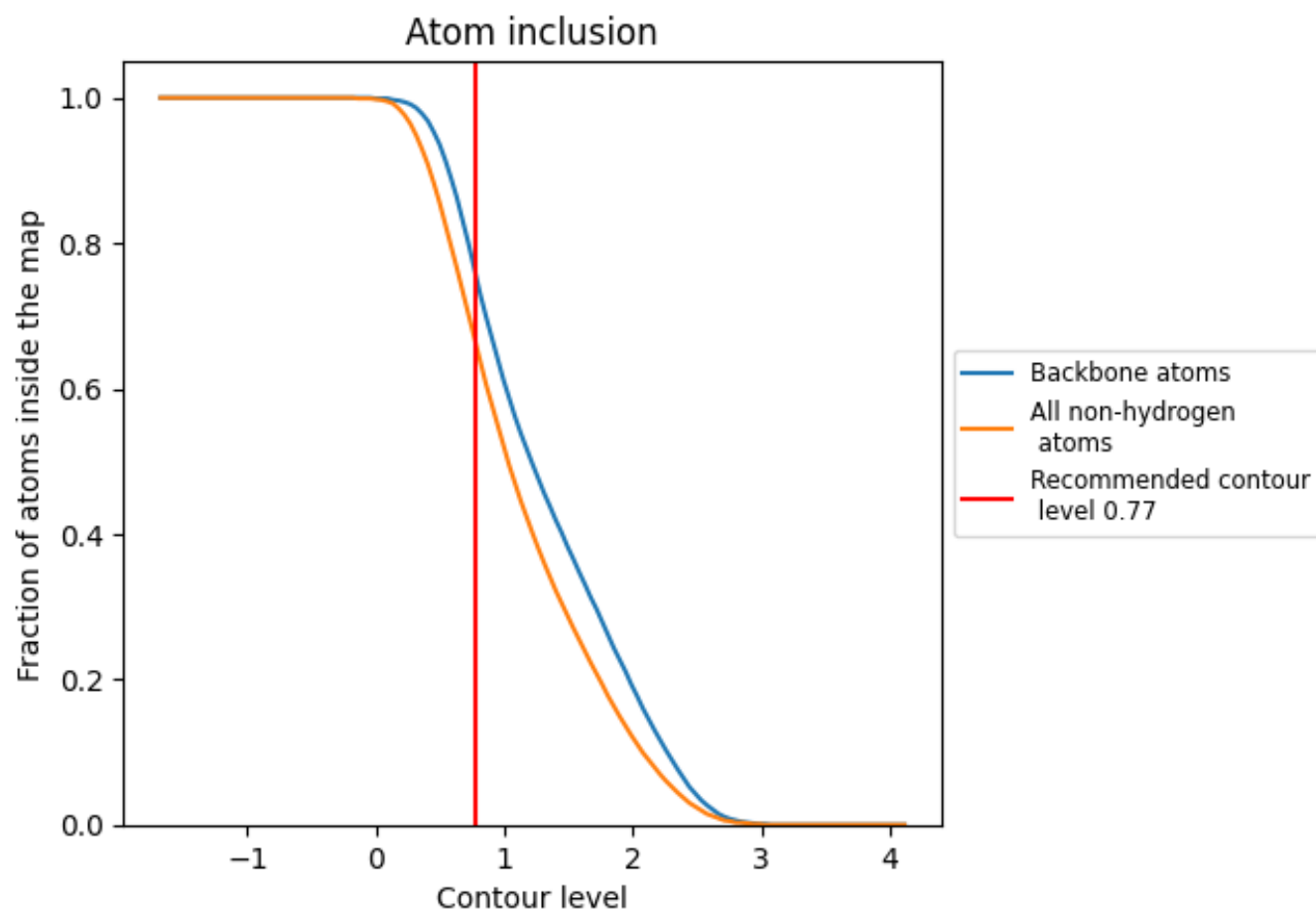
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.77).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.77) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6670	 0.4930
A	 0.4780	 0.4220
B	 0.6560	 0.4860
C	 0.7390	 0.5160
D	 0.6950	 0.5000
E	 0.4250	 0.4090
F	 0.2750	 0.3550
G	 0.8390	 0.5490
H	 0.8220	 0.5400
I	 0.8100	 0.5420
J	 0.8200	 0.5460
K	 0.8170	 0.5510
L	 0.8330	 0.5540
M	 0.8450	 0.5590
N	 0.8060	 0.5420
O	 0.8100	 0.5500
P	 0.8320	 0.5560
Q	 0.8300	 0.5600
R	 0.8320	 0.5540
S	 0.8400	 0.5600
T	 0.8150	 0.5520
X	 0.3200	 0.3930
Y	 0.7640	 0.5010

