



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:12 AM UTC

PDB ID : 1BCP / pdb_00001bcp
Title : BINARY COMPLEX OF PERTUSSIS TOXIN AND ATP
Authors : Hazes, B.; Read, R.J.
Deposited on : 1995-11-21
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

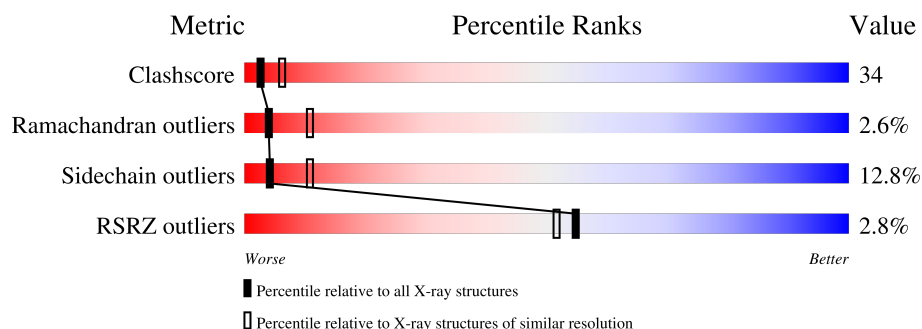
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



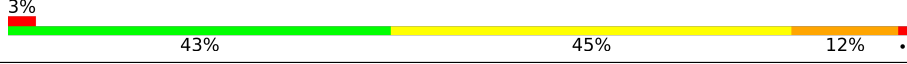
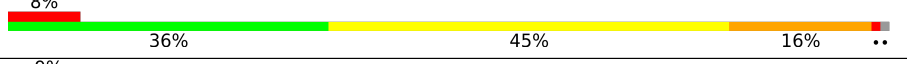
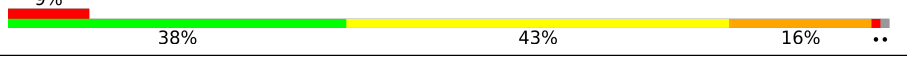
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	235	% 47% 38% 10% 5%
1	G	235	5% 45% 40% 10% 5%
2	B	199	% 44% 44% 11% .
2	H	199	% 45% 46% 8% .
3	C	199	3% 40% 44% 12% .
3	I	199	2% 41% 42% 15% .
4	D	110	44% 51% 5% .

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Mol	Chain	Length	Quality of chain
4	E	110	
4	J	110	
4	K	110	
5	F	99	
5	L	99	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14621 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PERTUSSIS TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1769	1095	318	350	6			
1	G	224	Total	C	N	O	S	0	0	0
			1769	1095	318	350	6			

- Molecule 2 is a protein called PERTUSSIS TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	197	Total	C	N	O	S	0	0	0
			1529	966	261	293	9			
2	H	197	Total	C	N	O	S	0	0	0
			1529	966	261	293	9			

- Molecule 3 is a protein called PERTUSSIS TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	196	Total	C	N	O	S	0	0	0
			1521	969	258	285	9			
3	I	196	Total	C	N	O	S	0	0	0
			1521	969	258	285	9			

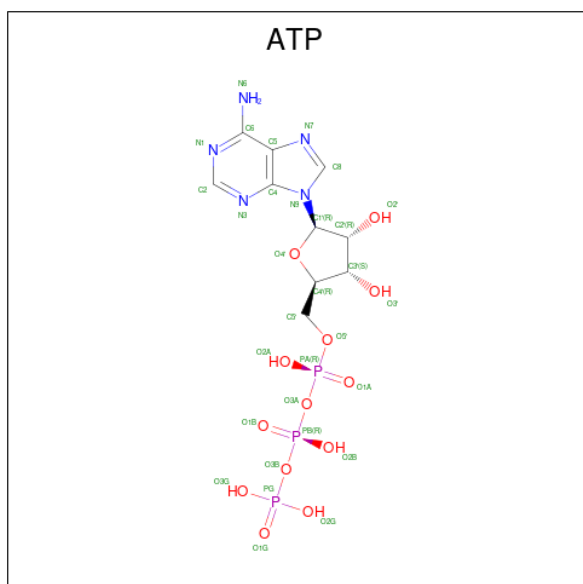
- Molecule 4 is a protein called PERTUSSIS TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	110	Total	C	N	O	S	0	0	0
			838	536	143	147	12			
4	E	110	Total	C	N	O	S	0	0	0
			838	536	143	147	12			
4	J	110	Total	C	N	O	S	0	0	0
			838	536	143	147	12			
4	K	110	Total	C	N	O	S	0	0	0
			838	536	143	147	12			

- Molecule 5 is a protein called PERTUSSIS TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	98	Total	C	N	O	S	0	0	0
			764	489	125	144	6			
5	L	98	Total	C	N	O	S	0	0	0
			764	489	125	144	6			

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	10	Total	O	0	0
			10	10		
7	B	4	Total	O	0	0
			4	4		
7	C	6	Total	O	0	0
			6	6		
7	E	5	Total	O	0	0
			5	5		
7	G	1	Total	O	0	0
			1	1		

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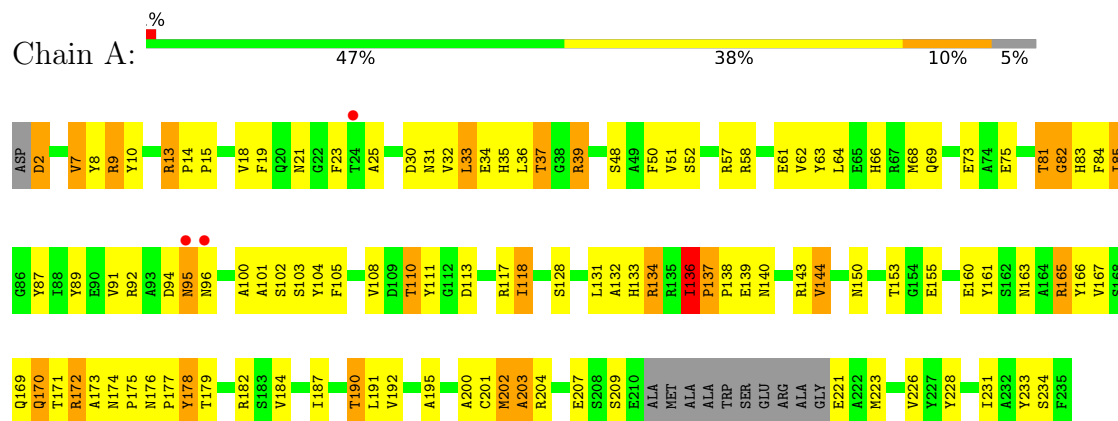
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	3	Total 3	O 3	0	0
7	I	4	Total 4	O 4	0	0
7	J	3	Total 3	O 3	0	0
7	K	4	Total 4	O 4	0	0
7	L	1	Total 1	O 1	0	0

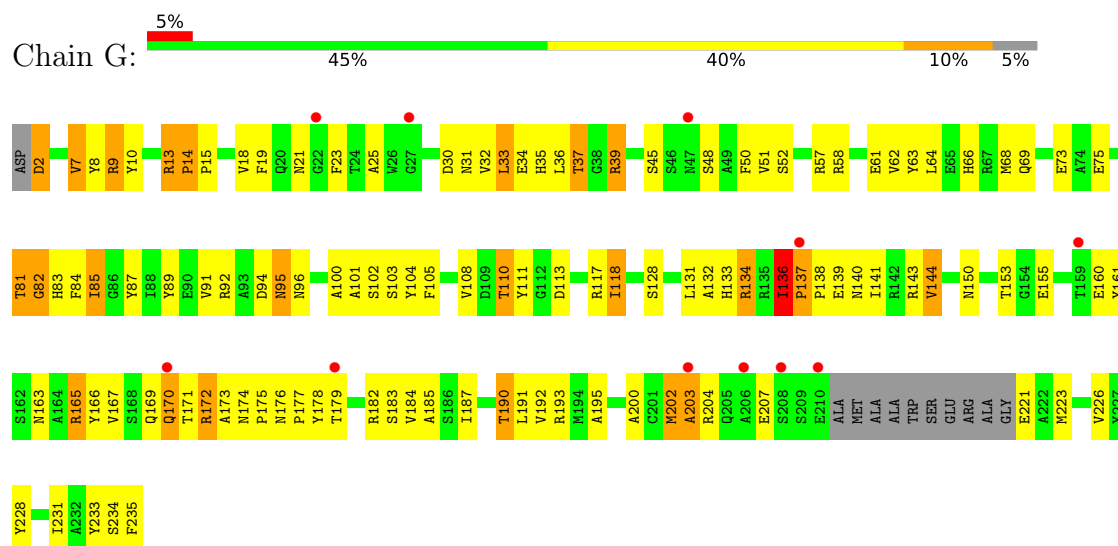
3 Residue-property plots [i](#)

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

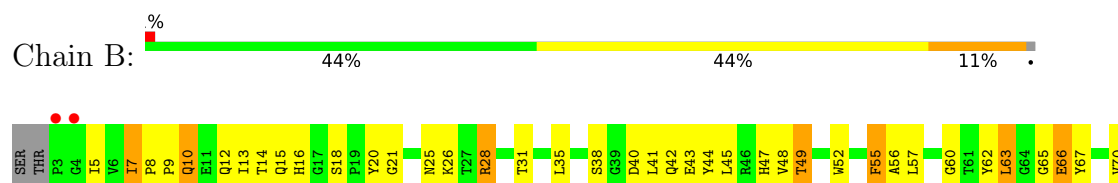
• Molecule 1: PERTUSSIS TOXIN

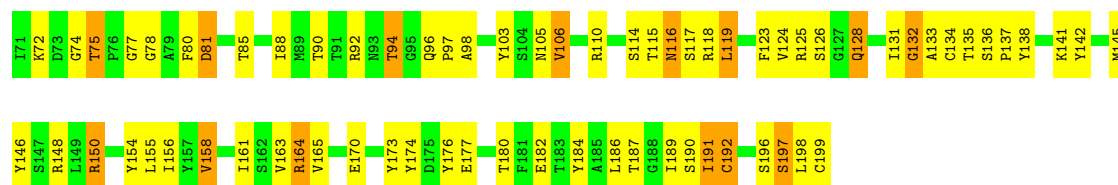


• Molecule 1: PERTUSSIS TOXIN

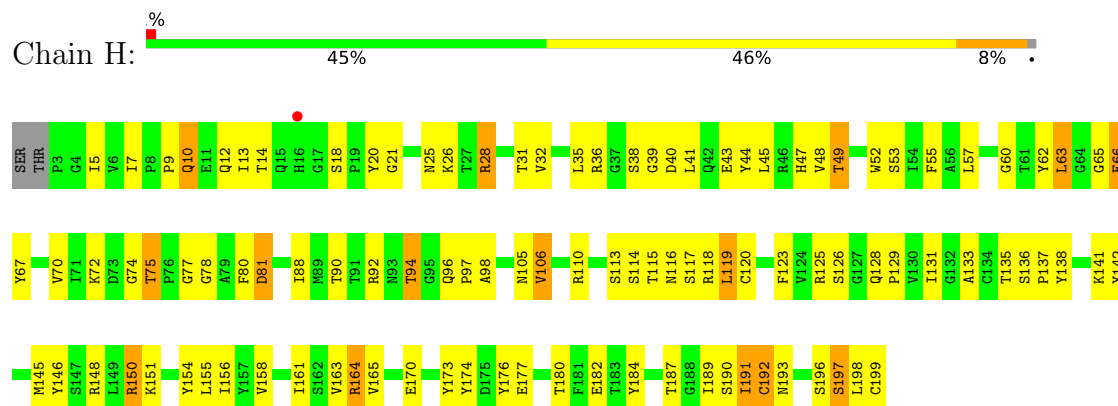


• Molecule 2: PERTUSSIS TOXIN

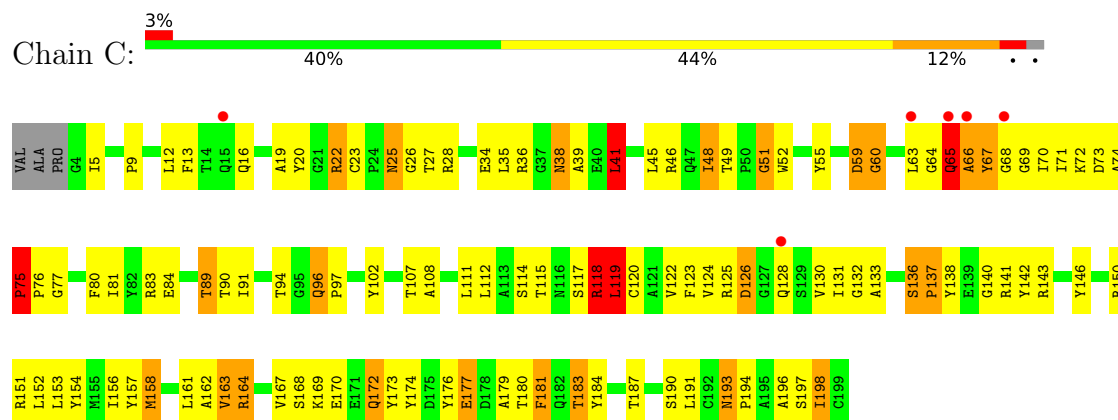




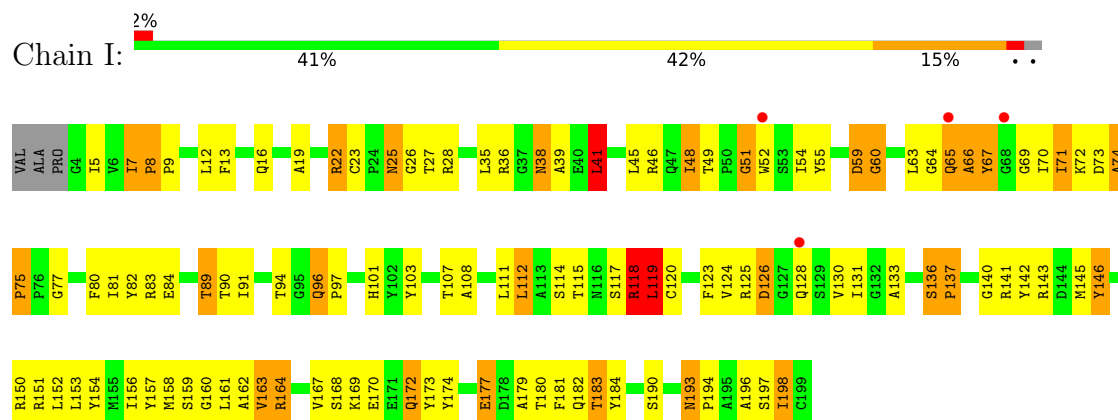
- Molecule 2: PERTUSSIS TOXIN



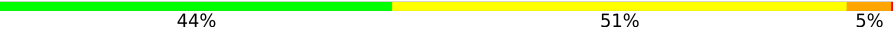
- Molecule 3: PERTUSSIS TOXIN

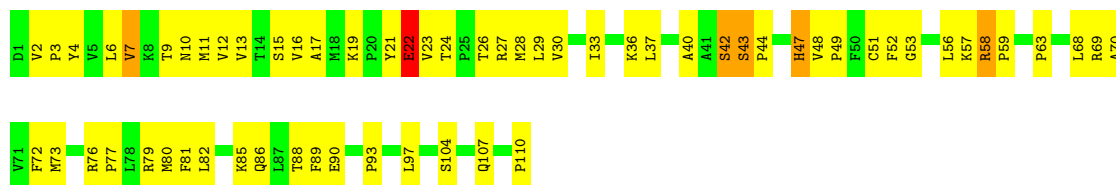


- Molecule 3: PERTUSSIS TOXIN



- Molecule 4: PERTUSSIS TOXIN

Chain D:  44% 51% 5% •



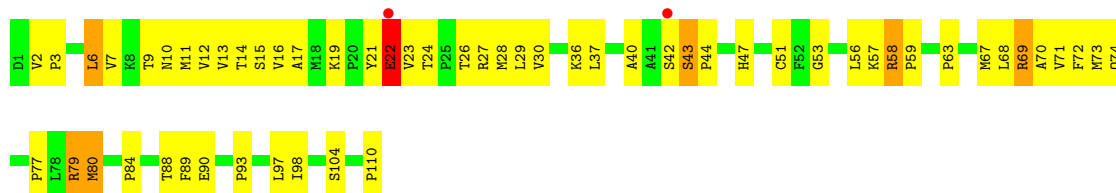
• Molecule 4: PERTUSSIS TOXIN

Chain E:  3% 51% 35% 13% •



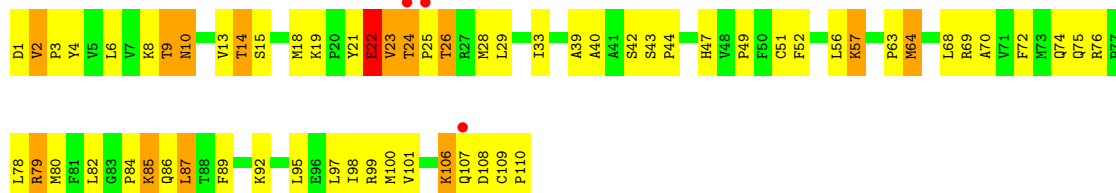
• Molecule 4: PERTUSSIS TOXIN

Chain J:  2% 48% 45% 5% •



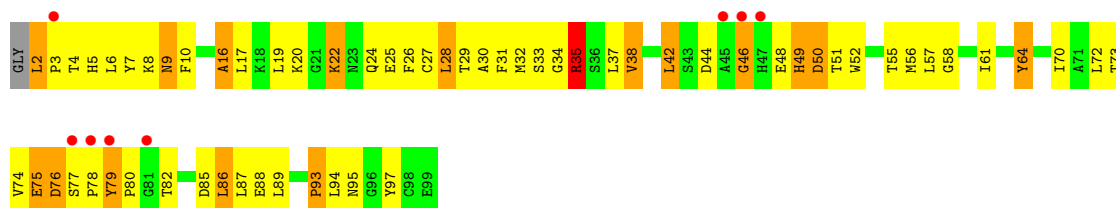
• Molecule 4: PERTUSSIS TOXIN

Chain K:  3% 43% 45% 12% •

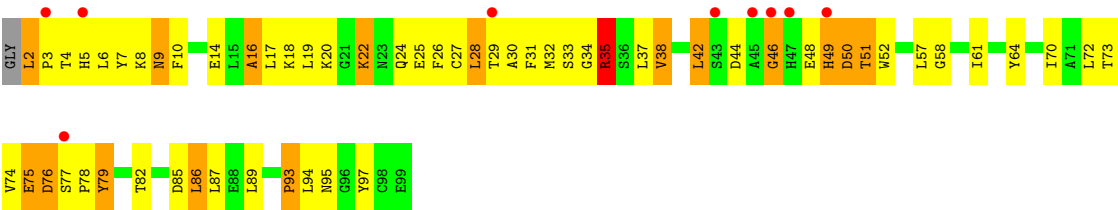


• Molecule 5: PERTUSSIS TOXIN

Chain F:  8% 36% 45% 16% ••



● Molecule 5: PERTUSSIS TOXIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	163.80Å 98.20Å 194.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.70 8.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.70) 63.4 (8.00-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.51Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.232 , (Not available) 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.935	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14621	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.85	0/1809	1.19	14/2457 (0.6%)
1	G	0.75	0/1809	1.17	12/2457 (0.5%)
2	B	1.01	0/1566	1.25	12/2126 (0.6%)
2	H	0.95	0/1566	1.26	11/2126 (0.5%)
3	C	1.08	1/1557 (0.1%)	1.37	18/2115 (0.9%)
3	I	0.95	0/1557	1.35	20/2115 (0.9%)
4	D	1.10	1/856 (0.1%)	1.38	10/1155 (0.9%)
4	E	1.25	1/856 (0.1%)	1.35	9/1155 (0.8%)
4	J	1.09	1/856 (0.1%)	1.38	9/1155 (0.8%)
4	K	0.99	0/856	1.27	7/1155 (0.6%)
5	F	0.85	0/782	1.22	9/1059 (0.8%)
5	L	0.77	0/782	1.22	9/1059 (0.8%)
All	All	0.96	4/14852 (0.0%)	1.28	140/20134 (0.7%)

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	1
1	G	0	1
3	I	0	1
5	F	0	1
5	L	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	187	THR	CA-CB	-6.47	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	80	MET	SD-CE	-5.64	1.65	1.79
4	E	67	MET	SD-CE	-5.52	1.65	1.79
4	D	52	PHE	C-O	-5.07	1.17	1.23

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	138	TYR	N-CA-C	9.92	122.17	111.36
4	K	26	THR	N-CA-C	-9.85	100.92	113.72
2	B	138	TYR	N-CA-C	9.80	122.04	111.36
2	H	192	CYS	N-CA-C	9.67	125.33	109.95
2	B	192	CYS	N-CA-C	9.58	125.19	109.95
4	E	26	THR	N-CA-C	-9.52	101.35	113.72
3	C	67	TYR	N-CA-C	-9.45	101.74	113.18
3	C	89	THR	N-CA-C	-9.35	96.64	110.48
5	F	35	ARG	N-CA-C	8.96	122.71	110.35
4	J	58	ARG	CA-C-N	8.86	130.92	119.84
4	J	58	ARG	C-N-CA	8.86	130.92	119.84
5	L	35	ARG	N-CA-C	8.81	122.51	110.35
2	H	18	SER	CA-C-N	8.77	128.90	120.31
2	H	18	SER	C-N-CA	8.77	128.90	120.31
3	I	67	TYR	N-CA-C	-8.57	102.81	113.18
5	L	46	GLY	N-CA-C	-8.45	101.89	114.90
2	B	18	SER	CA-C-N	8.38	128.53	120.31
2	B	18	SER	C-N-CA	8.38	128.53	120.31
5	F	46	GLY	N-CA-C	-8.38	101.99	114.90
4	D	58	ARG	CA-C-N	8.32	130.24	119.84
4	D	58	ARG	C-N-CA	8.32	130.24	119.84
2	H	191	ILE	N-CA-C	-8.20	95.73	107.37
1	A	136	ILE	CA-C-N	8.16	128.79	120.38
1	A	136	ILE	C-N-CA	8.16	128.79	120.38
3	I	89	THR	N-CA-C	-8.15	97.32	110.20
4	E	76	ARG	CA-C-N	8.13	128.62	119.83
4	E	76	ARG	C-N-CA	8.13	128.62	119.83
1	G	136	ILE	CA-C-N	8.05	128.67	120.38
1	G	136	ILE	C-N-CA	8.05	128.67	120.38
3	C	124	VAL	N-CA-C	8.01	119.32	108.11
3	I	38	ASN	N-CA-C	7.94	120.91	109.71
2	B	191	ILE	N-CA-C	-7.81	96.28	107.37
3	C	118	ARG	N-CA-C	7.66	122.23	110.36
4	E	24	THR	CA-C-N	7.64	129.39	119.84
4	E	24	THR	C-N-CA	7.64	129.39	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	VAL	N-CA-C	-7.63	104.02	112.80
1	G	184	VAL	N-CA-C	-7.51	104.16	112.80
2	H	57	LEU	N-CA-C	-7.49	99.13	110.14
3	C	38	ASN	N-CA-C	7.47	120.24	109.71
1	A	176	ASN	CA-C-N	7.46	127.50	119.90
1	A	176	ASN	C-N-CA	7.46	127.50	119.90
3	I	164	ARG	N-CA-C	-7.45	96.26	108.41
4	K	76	ARG	CA-C-N	7.44	127.86	119.83
4	K	76	ARG	C-N-CA	7.44	127.86	119.83
3	I	124	VAL	N-CA-C	7.33	118.37	108.11
5	L	38	VAL	N-CA-C	-7.33	97.73	108.87
5	F	38	VAL	N-CA-C	-7.23	97.87	108.87
5	F	51	THR	N-CA-C	-7.18	104.39	113.01
1	G	176	ASN	CA-C-N	7.13	127.17	119.90
1	G	176	ASN	C-N-CA	7.13	127.17	119.90
4	K	24	THR	CA-C-N	7.07	128.68	119.84
4	K	24	THR	C-N-CA	7.07	128.68	119.84
1	G	13	ARG	CA-C-N	7.06	127.65	120.38
1	G	13	ARG	C-N-CA	7.06	127.65	120.38
5	L	51	THR	N-CA-C	-7.01	104.59	113.01
3	I	90	THR	N-CA-C	6.95	121.76	113.28
4	K	79	ARG	N-CA-C	-6.92	95.57	107.61
4	J	79	ARG	N-CA-C	-6.91	95.93	108.02
2	B	57	LEU	N-CA-C	-6.89	100.00	110.14
1	A	13	ARG	CA-C-N	6.89	127.48	120.38
1	A	13	ARG	C-N-CA	6.89	127.48	120.38
4	D	79	ARG	N-CA-C	-6.79	96.13	108.02
3	I	118	ARG	N-CA-C	6.76	120.83	110.36
1	A	14	PRO	CA-C-N	6.74	127.00	119.32
1	A	14	PRO	C-N-CA	6.74	127.00	119.32
3	C	119	LEU	N-CA-C	-6.72	97.95	108.90
4	J	43	SER	CA-C-N	6.66	126.44	119.05
4	J	43	SER	C-N-CA	6.66	126.44	119.05
3	C	164	ARG	N-CA-C	-6.59	97.67	108.41
3	C	90	THR	N-CA-C	6.58	121.31	113.28
3	C	153	LEU	N-CA-C	-6.52	104.10	111.14
1	G	14	PRO	CA-C-N	6.49	126.72	119.32
1	G	14	PRO	C-N-CA	6.49	126.72	119.32
4	E	79	ARG	N-CA-C	-6.48	96.34	107.61
4	D	30	VAL	N-CA-C	-6.33	97.22	107.28
3	I	153	LEU	N-CA-C	-6.28	104.35	111.07
3	C	66	ALA	N-CA-C	-6.26	104.54	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	SER	N-CA-C	6.19	119.85	108.58
3	I	119	LEU	N-CA-C	-6.18	98.31	108.76
3	C	26	GLY	N-CA-C	-6.17	106.57	113.79
3	C	137	PRO	N-CA-C	-6.13	107.63	114.92
3	I	137	PRO	N-CA-C	-6.10	107.66	114.92
3	C	75	PRO	CA-C-N	6.02	126.96	119.98
3	C	75	PRO	C-N-CA	6.02	126.96	119.98
1	A	172	ARG	N-CA-C	-6.01	99.83	108.60
4	E	10	ASN	N-CA-C	5.96	119.77	111.90
3	I	75	PRO	CA-C-N	5.95	126.88	119.98
3	I	75	PRO	C-N-CA	5.95	126.88	119.98
1	G	172	ARG	N-CA-C	-5.90	99.99	108.60
4	D	43	SER	CA-C-N	5.84	125.54	119.05
4	D	43	SER	C-N-CA	5.84	125.54	119.05
5	L	86	LEU	N-CA-C	-5.84	100.31	109.25
5	F	42	LEU	N-CA-C	-5.83	99.14	109.06
1	A	179	THR	N-CA-C	5.82	118.60	108.76
4	J	30	VAL	N-CA-C	-5.81	98.04	107.28
3	I	7	ILE	N-CA-C	5.80	113.30	107.55
4	K	10	ASN	N-CA-C	5.79	119.54	111.90
3	I	23	CYS	N-CA-C	-5.77	101.02	109.50
2	B	106	VAL	N-CA-C	5.76	116.33	110.05
3	I	41	LEU	N-CA-C	-5.76	105.00	111.28
5	F	86	LEU	N-CA-C	-5.75	100.46	109.25
2	H	32	VAL	N-CA-C	-5.74	105.14	110.53
1	G	179	THR	N-CA-C	5.73	118.44	108.76
5	L	42	LEU	N-CA-C	-5.72	99.33	109.06
4	J	15	SER	N-CA-C	-5.71	100.06	108.79
1	A	137	PRO	N-CA-C	5.68	117.63	110.70
1	G	137	PRO	N-CA-C	5.66	117.60	110.70
5	F	9	ASN	N-CA-C	5.66	119.38	111.74
4	D	7	VAL	N-CA-C	-5.64	100.28	108.17
5	L	31	PHE	N-CA-C	5.62	118.61	109.06
5	L	9	ASN	N-CA-C	5.60	119.30	111.74
5	F	31	PHE	N-CA-C	5.56	118.53	109.24
2	H	106	VAL	N-CA-C	5.50	116.43	110.21
5	L	16	ALA	N-CA-C	5.48	117.55	108.13
5	F	16	ALA	N-CA-C	5.45	117.51	108.13
2	B	49	THR	N-CA-C	5.41	117.56	107.99
3	I	8	PRO	CA-C-N	-5.37	114.45	120.14
3	I	8	PRO	C-N-CA	-5.37	114.45	120.14
4	D	70	ALA	N-CA-C	5.37	116.81	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	70	ALA	N-CA-C	5.35	116.80	111.07
2	H	49	THR	N-CA-C	5.33	117.42	107.99
3	I	66	ALA	N-CA-C	-5.32	105.15	111.69
3	C	23	CYS	N-CA-C	-5.29	101.72	109.50
3	C	41	LEU	N-CA-C	-5.24	105.57	111.28
2	H	197	SER	N-CA-C	-5.24	106.58	112.87
4	J	7	VAL	N-CA-C	-5.16	100.94	108.17
3	I	26	GLY	N-CA-C	-5.16	107.75	113.79
4	D	15	SER	N-CA-C	-5.15	101.24	109.07
2	B	197	SER	N-CA-C	-5.15	106.69	112.87
3	C	181	PHE	N-CA-C	-5.14	101.47	109.24
1	A	178	TYR	N-CA-C	-5.13	103.27	110.50
2	B	128	GLN	N-CA-C	5.12	121.12	109.81
3	C	138	TYR	N-CA-C	5.12	119.52	113.12
4	E	30	VAL	N-CA-C	-5.11	99.59	106.85
3	I	71	ILE	N-CA-C	-5.11	99.76	107.73
4	D	33	ILE	N-CA-C	-5.09	98.75	109.34
2	B	132	GLY	N-CA-C	-5.08	102.30	111.19
2	B	35	LEU	N-CA-C	-5.05	105.66	111.07
4	E	14	THR	N-CA-C	5.04	119.70	113.50
2	H	53	SER	N-CA-C	5.01	118.38	109.96

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	63	TYR	Sidechain
5	F	64	TYR	Sidechain
1	G	63	TYR	Sidechain
3	I	146	TYR	Sidechain
5	L	64	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1769	0	1655	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1769	0	1655	115	0
2	B	1529	0	1481	109	0
2	H	1529	0	1481	107	0
3	C	1521	0	1484	113	0
3	I	1521	0	1484	112	0
4	D	838	0	874	54	0
4	E	838	0	874	61	0
4	J	838	0	874	63	0
4	K	838	0	874	68	0
5	F	764	0	747	73	0
5	L	764	0	747	68	0
6	E	31	0	12	5	0
6	K	31	0	12	5	0
7	A	10	0	0	2	0
7	B	4	0	0	0	0
7	C	6	0	0	1	0
7	E	5	0	0	0	0
7	G	1	0	0	0	0
7	H	3	0	0	0	0
7	I	4	0	0	2	0
7	J	3	0	0	2	0
7	K	4	0	0	1	0
7	L	1	0	0	1	0
All	All	14621	0	14254	971	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 34.

All (971) 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:H:163:VAL:HG21	2:H:189:ILE:HG22	1.31	1.10
2:B:163:VAL:HG21	2:B:189:ILE:HG22	1.35	1.05
5:F:7:TYR:HB3	5:F:10:PHE:CE2	1.96	1.00
3:C:63:LEU:HD12	3:C:70:ILE:HB	1.38	0.99
5:L:7:TYR:HB3	5:L:10:PHE:CE2	1.97	0.99
6:E:111:ATP:O1A	5:F:58:GLY:HA3	1.65	0.95
3:I:46:ARG:HH21	3:I:65:GLN:HB2	1.33	0.94
2:H:163:VAL:HG22	2:H:164:ARG:H	1.31	0.93
3:I:63:LEU:HD12	3:I:70:ILE:HB	1.51	0.92
3:C:46:ARG:HH21	3:C:65:GLN:HB2	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:THR:HG22	2:B:116:ASN:HD22	1.36	0.90
2:B:115:THR:HG22	2:B:116:ASN:ND2	1.86	0.90
2:H:63:LEU:HD13	2:H:70:VAL:HB	1.54	0.90
2:B:163:VAL:HG22	2:B:164:ARG:H	1.33	0.89
5:L:70:ILE:HD12	5:L:89:LEU:HD11	1.54	0.88
1:A:51:VAL:HB	1:A:132:ALA:HB3	1.55	0.88
2:H:115:THR:HG22	2:H:116:ASN:ND2	1.88	0.88
1:G:51:VAL:HB	1:G:132:ALA:HB3	1.55	0.88
5:F:70:ILE:HD12	5:F:89:LEU:HD11	1.55	0.88
1:A:170:GLN:HA	1:A:170:GLN:HE21	1.40	0.87
1:G:170:GLN:HE21	1:G:170:GLN:HA	1.39	0.87
4:K:106:LYS:HE2	4:K:110:PRO:HA	1.57	0.86
2:H:115:THR:HG22	2:H:116:ASN:HD22	1.40	0.86
2:B:63:LEU:H	2:B:63:LEU:HD12	1.41	0.86
1:G:32:VAL:HG11	1:G:103:SER:HB3	1.57	0.86
3:I:28:ARG:NH1	3:I:177:GLU:HA	1.91	0.85
1:A:32:VAL:HG11	1:A:103:SER:HB3	1.59	0.85
6:K:111:ATP:O1A	5:L:58:GLY:HA3	1.78	0.84
2:H:63:LEU:HD12	2:H:63:LEU:H	1.42	0.83
3:C:28:ARG:NH1	3:C:177:GLU:HA	1.92	0.83
6:K:111:ATP:O5'	6:K:111:ATP:H2'	1.79	0.83
3:I:96:GLN:HG2	3:I:97:PRO:HD2	1.61	0.83
6:E:111:ATP:H2'	6:E:111:ATP:O5'	1.78	0.83
4:D:11:MET:SD	4:D:36:LYS:HB2	2.19	0.82
2:B:63:LEU:HD13	2:B:70:VAL:HB	1.59	0.82
2:B:94:THR:HG22	2:B:96:GLN:H	1.44	0.82
3:C:96:GLN:HG2	3:C:97:PRO:HD2	1.62	0.81
2:H:163:VAL:HG21	2:H:189:ILE:CG2	2.08	0.81
3:I:13:PHE:CD2	3:I:41:LEU:HD21	2.15	0.81
4:J:80:MET:HE2	4:J:97:LEU:HD13	1.63	0.81
5:F:7:TYR:HB3	5:F:10:PHE:HE2	1.45	0.80
1:G:134:ARG:HH11	1:G:134:ARG:HB2	1.47	0.80
1:A:52:SER:OG	1:A:202:MET:HE3	1.82	0.80
3:C:13:PHE:CD2	3:C:41:LEU:HD21	2.18	0.79
4:K:84:PRO:HG2	4:K:85:LYS:HD3	1.62	0.79
3:I:38:ASN:OD1	3:I:41:LEU:HB2	1.82	0.79
4:E:106:LYS:HE2	4:E:110:PRO:HA	1.65	0.79
1:G:52:SER:OG	1:G:202:MET:HE3	1.82	0.79
2:B:163:VAL:HG21	2:B:189:ILE:CG2	2.10	0.79
1:A:134:ARG:HH11	1:A:134:ARG:HB2	1.48	0.78
1:G:75:GLU:HB2	1:G:82:GLY:H	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:10:ASN:O	4:J:37:LEU:HD12	1.83	0.78
1:A:39:ARG:HH11	1:A:39:ARG:HB2	1.49	0.78
4:E:84:PRO:HG2	4:E:85:LYS:HD3	1.65	0.78
2:B:52:TRP:CG	4:J:93:PRO:HB3	2.19	0.77
2:B:150:ARG:HG2	2:B:150:ARG:HH11	1.48	0.77
2:B:148:ARG:HB3	5:F:17:LEU:HD21	1.65	0.77
4:E:1:ASP:HA	4:E:86:GLN:HG3	1.65	0.77
2:H:94:THR:HG22	2:H:96:GLN:H	1.50	0.77
4:K:106:LYS:CE	4:K:110:PRO:HA	2.15	0.77
1:G:19:PHE:CD1	1:G:163:ASN:HB2	2.20	0.77
2:H:92:ARG:HG3	2:H:174:TYR:HE2	1.48	0.76
1:A:19:PHE:CD1	1:A:163:ASN:HB2	2.20	0.76
2:H:150:ARG:HG2	2:H:150:ARG:HH11	1.51	0.75
2:H:63:LEU:HD11	2:H:72:LYS:HD2	1.68	0.75
3:C:63:LEU:HD12	3:C:70:ILE:CB	2.16	0.75
1:A:75:GLU:HB2	1:A:82:GLY:H	1.49	0.75
2:B:63:LEU:HD11	2:B:72:LYS:HD2	1.68	0.75
5:L:7:TYR:HB3	5:L:10:PHE:HE2	1.45	0.75
1:G:39:ARG:HH11	1:G:39:ARG:HB2	1.50	0.75
1:A:170:GLN:HA	1:A:170:GLN:NE2	2.02	0.74
4:K:14:THR:HG23	5:L:93:PRO:HG3	1.69	0.74
5:L:29:THR:HG21	5:L:37:LEU:HD13	1.70	0.74
4:J:11:MET:SD	4:J:36:LYS:HB2	2.28	0.74
3:C:38:ASN:OD1	3:C:41:LEU:HB2	1.87	0.73
1:A:201:CYS:HB2	7:A:242:HOH:O	1.86	0.73
4:D:80:MET:HE2	4:D:97:LEU:HD13	1.68	0.73
5:F:22:LYS:HE2	5:F:22:LYS:HA	1.70	0.73
4:E:14:THR:HG23	5:F:93:PRO:HG3	1.70	0.73
2:H:28:ARG:HH21	2:H:177:GLU:HA	1.53	0.73
4:K:1:ASP:HA	4:K:86:GLN:HG3	1.70	0.73
2:B:155:LEU:HD22	5:F:61:ILE:HG23	1.69	0.73
4:D:28:MET:SD	4:D:56:LEU:HD21	2.28	0.73
1:G:91:VAL:HG21	1:G:136:ILE:HD11	1.71	0.73
3:C:125:ARG:O	3:C:128:GLN:HG2	1.88	0.73
5:F:29:THR:HG21	5:F:37:LEU:HD13	1.70	0.72
4:J:28:MET:SD	4:J:56:LEU:HD21	2.29	0.72
5:L:22:LYS:HE2	5:L:22:LYS:HA	1.70	0.72
3:C:63:LEU:CD1	3:C:70:ILE:HB	2.19	0.71
2:B:92:ARG:HG3	2:B:174:TYR:HE2	1.54	0.71
2:H:145:MET:HG2	5:L:24:GLN:CD	2.15	0.71
2:H:145:MET:HG2	5:L:24:GLN:NE2	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:19:LYS:HG2	4:K:29:LEU:HB2	1.72	0.71
1:G:170:GLN:HA	1:G:170:GLN:NE2	2.02	0.71
4:E:19:LYS:HG2	4:E:29:LEU:HB2	1.72	0.71
1:A:91:VAL:HG21	1:A:136:ILE:HD11	1.72	0.71
2:B:145:MET:HG2	5:F:24:GLN:CD	2.16	0.70
2:H:163:VAL:HG22	2:H:164:ARG:N	2.06	0.70
3:C:28:ARG:HH12	3:C:177:GLU:HA	1.55	0.70
4:E:57:LYS:HD3	5:F:49:HIS:CD2	2.26	0.70
1:A:33:LEU:O	1:A:37:THR:HB	1.91	0.70
4:E:9:THR:HG21	4:E:110:PRO:HD2	1.72	0.70
3:I:28:ARG:HH12	3:I:177:GLU:HA	1.54	0.70
4:J:3:PRO:HD2	7:J:113:HOH:O	1.92	0.70
4:D:10:ASN:O	4:D:37:LEU:HD12	1.92	0.70
3:C:193:ASN:HD22	3:C:196:ALA:H	1.40	0.69
3:I:193:ASN:HD22	3:I:196:ALA:H	1.41	0.69
5:F:75:GLU:HB2	5:F:87:LEU:HD11	1.74	0.69
1:G:33:LEU:O	1:G:37:THR:HB	1.92	0.69
1:G:58:ARG:O	1:G:62:VAL:HG23	1.92	0.69
3:I:167:VAL:HG22	3:I:184:TYR:HB2	1.73	0.69
1:A:96:ASN:OD1	1:A:133:HIS:HB3	1.92	0.69
3:C:167:VAL:CG2	3:C:184:TYR:HB2	2.23	0.69
4:D:21:TYR:HE2	4:D:27:ARG:HH21	1.41	0.69
2:B:163:VAL:HG22	2:B:164:ARG:N	2.07	0.69
5:L:75:GLU:HB2	5:L:87:LEU:HD11	1.73	0.69
1:G:96:ASN:OD1	1:G:133:HIS:HB3	1.93	0.69
2:H:155:LEU:HD22	5:L:61:ILE:HG23	1.74	0.69
4:D:26:THR:HG23	4:D:57:LYS:HG3	1.75	0.68
1:A:58:ARG:O	1:A:62:VAL:HG23	1.93	0.68
2:H:28:ARG:NH2	2:H:177:GLU:HA	2.08	0.68
3:I:52:TRP:HE3	3:I:67:TYR:CZ	2.11	0.68
3:I:167:VAL:CG2	3:I:184:TYR:HB2	2.24	0.67
4:E:106:LYS:CE	4:E:110:PRO:HA	2.23	0.67
4:J:26:THR:HG23	4:J:57:LYS:HG3	1.77	0.67
3:C:167:VAL:HG22	3:C:184:TYR:HB2	1.76	0.67
3:C:168:SER:C	3:C:170:GLU:H	2.01	0.67
5:L:48:GLU:OE1	5:L:48:GLU:HA	1.94	0.67
5:F:6:LEU:HD21	5:F:8:LYS:HG3	1.77	0.66
5:L:6:LEU:HD21	5:L:8:LYS:HG3	1.77	0.66
5:F:48:GLU:OE1	5:F:48:GLU:HA	1.95	0.66
2:H:98:ALA:HB2	2:H:170:GLU:CD	2.21	0.66
4:K:57:LYS:HD3	5:L:49:HIS:CD2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:198:LEU:HD22	5:L:27:CYS:HB2	1.78	0.66
2:H:137:PRO:HB3	2:H:146:TYR:CD2	2.31	0.66
4:K:9:THR:HG21	4:K:110:PRO:HD2	1.78	0.66
1:A:111:TYR:CD1	1:A:182:ARG:HB2	2.30	0.65
6:K:111:ATP:O5'	6:K:111:ATP:C2'	2.44	0.65
6:E:111:ATP:O5'	6:E:111:ATP:C2'	2.44	0.65
5:F:22:LYS:HA	5:F:22:LYS:CE	2.24	0.65
3:I:27:THR:HG22	3:I:89:THR:HA	1.76	0.65
2:H:106:VAL:HB	2:H:123:PHE:HB3	1.79	0.65
5:L:22:LYS:HA	5:L:22:LYS:CE	2.25	0.65
1:G:111:TYR:CD1	1:G:182:ARG:HB2	2.32	0.65
3:I:101:HIS:HE1	7:I:201:HOH:O	1.80	0.65
2:B:106:VAL:HB	2:B:123:PHE:HB3	1.78	0.65
5:F:48:GLU:O	5:F:49:HIS:HB3	1.97	0.64
4:K:106:LYS:NZ	4:K:110:PRO:HA	2.11	0.64
1:A:204:ARG:HA	1:A:223:MET:HE1	1.78	0.64
3:C:137:PRO:HB3	3:C:146:TYR:CD2	2.32	0.64
1:G:204:ARG:HA	1:G:223:MET:HE1	1.78	0.64
2:B:98:ALA:HB2	2:B:170:GLU:CD	2.22	0.64
2:B:21:GLY:HA3	2:B:80:PHE:CD2	2.32	0.64
2:H:28:ARG:HH21	2:H:177:GLU:HG3	1.63	0.64
2:B:110:ARG:NH1	2:B:176:TYR:HD2	1.96	0.64
2:B:28:ARG:HH21	2:B:177:GLU:HA	1.63	0.64
3:C:49:THR:HG22	3:C:55:TYR:CE2	2.34	0.63
4:E:79:ARG:HG3	4:E:109:CYS:SG	2.39	0.63
3:I:168:SER:C	3:I:170:GLU:H	2.03	0.63
2:B:77:GLY:HA2	2:B:80:PHE:CE1	2.33	0.63
3:I:182:GLN:HA	7:I:203:HOH:O	1.99	0.63
5:L:48:GLU:O	5:L:49:HIS:HB3	1.97	0.63
1:A:143:ARG:NH1	1:A:143:ARG:HB2	2.14	0.63
3:I:46:ARG:NH2	3:I:65:GLN:HB2	2.11	0.63
3:I:49:THR:HG22	3:I:55:TYR:CE2	2.32	0.62
4:K:106:LYS:HA	4:K:109:CYS:O	1.98	0.62
2:B:28:ARG:NH2	2:B:177:GLU:HA	2.14	0.62
5:L:29:THR:CG2	5:L:37:LEU:HD13	2.29	0.62
5:L:7:TYR:HB3	5:L:10:PHE:CD2	2.34	0.62
2:B:12:GLN:NE2	2:B:92:ARG:HG2	2.15	0.62
4:E:21:TYR:CD1	4:E:22:GLU:HG2	2.34	0.62
1:G:143:ARG:HB2	1:G:143:ARG:NH1	2.15	0.62
3:I:96:GLN:CG	3:I:97:PRO:HD2	2.29	0.62
3:C:52:TRP:CE2	3:C:66:ALA:HB1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:77:GLY:HA2	2:H:80:PHE:CE1	2.34	0.62
2:H:154:TYR:O	2:H:158:VAL:HG22	2.00	0.62
3:I:125:ARG:O	3:I:128:GLN:HG2	2.00	0.62
5:F:7:TYR:HB3	5:F:10:PHE:CD2	2.35	0.62
5:F:29:THR:CG2	5:F:37:LEU:HD13	2.29	0.61
2:B:154:TYR:O	2:B:158:VAL:HG22	2.00	0.61
1:G:195:ALA:HB1	4:K:75:GLN:CG	2.31	0.61
5:L:6:LEU:HD21	5:L:8:LYS:HD2	1.82	0.61
2:B:28:ARG:HH21	2:B:177:GLU:HG3	1.65	0.61
3:C:96:GLN:CG	3:C:97:PRO:HD2	2.30	0.61
4:E:106:LYS:HA	4:E:109:CYS:O	2.00	0.61
2:H:148:ARG:HB3	5:L:17:LEU:HD21	1.83	0.61
1:G:137:PRO:HG2	1:G:140:ASN:OD1	2.00	0.61
4:E:1:ASP:CG	4:E:85:LYS:HA	2.26	0.61
3:I:60:GLY:HA3	3:I:72:LYS:O	2.01	0.61
3:C:27:THR:HG22	3:C:89:THR:HA	1.82	0.60
1:G:200:ALA:O	1:G:204:ARG:HB2	2.00	0.60
4:J:21:TYR:HE2	4:J:27:ARG:HH21	1.48	0.60
2:B:148:ARG:HG2	2:B:148:ARG:HH11	1.66	0.60
2:H:75:THR:HG22	2:H:78:GLY:HA3	1.82	0.60
1:G:195:ALA:HB1	4:K:75:GLN:HG3	1.83	0.60
2:H:21:GLY:HA3	2:H:80:PHE:CD2	2.36	0.60
2:H:193:ASN:HB2	5:L:14:GLU:OE1	2.02	0.60
3:C:194:PRO:O	3:C:197:SER:N	2.34	0.60
1:G:13:ARG:HG3	1:G:13:ARG:HH11	1.67	0.60
1:G:50:PHE:HZ	1:G:178:TYR:CE2	2.20	0.60
3:I:118:ARG:HA	3:I:136:SER:HB2	1.82	0.60
1:A:200:ALA:O	1:A:204:ARG:HB2	2.01	0.60
5:F:6:LEU:HD21	5:F:8:LYS:HD2	1.83	0.60
4:J:40:ALA:O	4:J:43:SER:N	2.34	0.60
1:A:137:PRO:HG2	1:A:140:ASN:OD1	2.01	0.60
2:B:75:THR:HG22	2:B:78:GLY:HA3	1.83	0.59
3:I:63:LEU:HD12	3:I:70:ILE:CB	2.30	0.59
4:K:21:TYR:CD1	4:K:22:GLU:HG2	2.38	0.59
4:K:26:THR:HA	5:L:49:HIS:HE1	1.67	0.59
1:A:13:ARG:HH11	1:A:13:ARG:HG3	1.68	0.59
1:A:50:PHE:HZ	1:A:178:TYR:CE2	2.20	0.59
4:D:9:THR:HG21	4:D:110:PRO:HD2	1.84	0.59
3:I:19:ALA:HA	3:I:83:ARG:O	2.02	0.59
3:I:114:SER:HB3	3:I:117:SER:HB3	1.85	0.59
2:B:150:ARG:HG2	2:B:150:ARG:NH1	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ARG:NH2	3:C:65:GLN:HB2	2.13	0.59
4:E:106:LYS:NZ	4:E:110:PRO:HA	2.18	0.59
2:B:118:ARG:HA	2:B:136:SER:HB2	1.83	0.59
4:E:64:MET:HE3	4:E:64:MET:HA	1.84	0.58
3:I:94:THR:CG2	3:I:96:GLN:HB2	2.33	0.58
1:A:75:GLU:HB2	1:A:82:GLY:N	2.18	0.58
1:A:195:ALA:HB1	4:E:75:GLN:HG3	1.85	0.58
2:B:52:TRP:CD1	4:J:93:PRO:HB3	2.37	0.58
2:H:110:ARG:NH1	2:H:176:TYR:HD2	2.02	0.58
4:D:21:TYR:CE1	4:D:23:VAL:HG12	2.38	0.58
3:I:137:PRO:HB3	3:I:146:TYR:CD2	2.38	0.58
1:A:15:PRO:HD3	1:A:87:TYR:CE2	2.39	0.58
1:G:15:PRO:HD3	1:G:87:TYR:CE2	2.38	0.58
1:G:169:GLN:HA	1:G:169:GLN:OE1	2.03	0.58
1:G:31:ASN:HD22	1:G:34:GLU:H	1.51	0.58
3:I:63:LEU:CD1	3:I:70:ILE:HB	2.31	0.58
1:A:139:GLU:H	1:A:139:GLU:CD	2.12	0.58
1:A:195:ALA:HB1	4:E:75:GLN:CG	2.34	0.58
3:C:52:TRP:HE3	3:C:67:TYR:CZ	2.21	0.58
3:C:131:ILE:HD11	3:C:184:TYR:CD2	2.39	0.58
1:A:31:ASN:HD22	1:A:34:GLU:H	1.51	0.57
1:A:169:GLN:OE1	1:A:169:GLN:HA	2.03	0.57
2:B:52:TRP:CE3	2:B:66:GLU:HB3	2.39	0.57
4:K:74:GLN:OE1	4:K:74:GLN:HA	2.04	0.57
3:C:94:THR:CG2	3:C:96:GLN:HB2	2.34	0.57
1:G:165:ARG:HH11	1:G:165:ARG:HB3	1.69	0.57
3:I:141:ARG:C	3:I:143:ARG:H	2.12	0.57
1:G:134:ARG:HB2	1:G:134:ARG:NH1	2.18	0.57
3:C:63:LEU:HD12	3:C:70:ILE:HD13	1.87	0.57
3:C:63:LEU:O	3:C:69:GLY:HA2	2.05	0.57
4:K:64:MET:HE1	4:K:100:MET:HG2	1.87	0.57
2:B:145:MET:HG2	5:F:24:GLN:OE1	2.04	0.57
1:G:15:PRO:HB3	1:G:19:PHE:CE2	2.40	0.57
2:B:52:TRP:C	2:B:67:TYR:HE1	2.12	0.57
2:H:52:TRP:CE3	2:H:66:GLU:HB3	2.39	0.57
2:H:94:THR:CG2	2:H:96:GLN:HG3	2.34	0.57
2:B:148:ARG:HG2	2:B:148:ARG:NH1	2.20	0.57
1:G:75:GLU:HB2	1:G:82:GLY:N	2.17	0.57
4:J:80:MET:HE2	4:J:97:LEU:CD1	2.34	0.57
1:A:163:ASN:OD1	1:A:165:ARG:N	2.38	0.57
1:G:104:TYR:HD2	1:G:105:PHE:CD1	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:94:THR:HG23	2:H:96:GLN:HG3	1.86	0.57
2:H:148:ARG:HH11	2:H:148:ARG:HG2	1.69	0.56
4:K:1:ASP:CG	4:K:85:LYS:HA	2.30	0.56
4:K:51:CYS:HB2	4:K:87:LEU:HD23	1.86	0.56
1:A:32:VAL:O	1:A:36:LEU:HD13	2.04	0.56
3:C:150:ARG:HG3	3:C:151:ARG:N	2.18	0.56
2:H:13:ILE:HA	2:H:88:ILE:HD12	1.87	0.56
1:G:139:GLU:CD	1:G:139:GLU:H	2.12	0.56
1:G:150:ASN:ND2	1:G:153:THR:HG23	2.21	0.56
2:H:52:TRP:C	2:H:67:TYR:HE1	2.14	0.56
4:J:21:TYR:CE1	4:J:23:VAL:HG12	2.41	0.56
2:B:49:THR:O	2:B:65:GLY:HA2	2.06	0.56
4:E:3:PRO:HG2	4:E:4:TYR:CD1	2.40	0.56
1:G:163:ASN:OD1	1:G:165:ARG:N	2.38	0.56
3:I:177:GLU:CD	4:K:79:ARG:HH22	2.13	0.56
2:B:96:GLN:HB3	2:B:97:PRO:HD2	1.88	0.56
4:K:3:PRO:HG2	4:K:4:TYR:CD1	2.40	0.56
4:D:40:ALA:O	4:D:43:SER:N	2.38	0.56
4:E:51:CYS:HB2	4:E:87:LEU:HD23	1.88	0.56
1:A:150:ASN:ND2	1:A:153:THR:HG23	2.21	0.56
2:H:49:THR:O	2:H:65:GLY:HA2	2.06	0.56
2:H:96:GLN:HB3	2:H:97:PRO:HD2	1.87	0.56
1:A:104:TYR:HD2	1:A:105:PHE:CD1	2.23	0.56
1:A:134:ARG:HB2	1:A:134:ARG:NH1	2.19	0.56
2:B:55:PHE:CD1	2:B:55:PHE:N	2.74	0.56
2:H:150:ARG:HG2	2:H:150:ARG:NH1	2.17	0.56
2:B:137:PRO:HB3	2:B:146:TYR:CD2	2.40	0.55
3:C:142:TYR:CD1	3:C:142:TYR:N	2.73	0.55
2:H:92:ARG:HD3	2:H:174:TYR:OH	2.07	0.55
2:H:196:SER:OG	2:H:198:LEU:HB2	2.05	0.55
3:C:141:ARG:C	3:C:143:ARG:H	2.14	0.55
4:J:13:VAL:HG11	4:J:68:LEU:HD11	1.89	0.55
1:A:15:PRO:HB3	1:A:19:PHE:CE2	2.41	0.55
1:G:32:VAL:O	1:G:36:LEU:HD13	2.06	0.55
1:A:165:ARG:HB3	1:A:165:ARG:HH11	1.69	0.55
2:H:12:GLN:NE2	2:H:92:ARG:HG2	2.21	0.55
5:L:10:PHE:CD1	5:L:32:MET:HB2	2.42	0.55
5:F:5:HIS:O	5:F:73:THR:HG23	2.07	0.55
5:F:10:PHE:CD1	5:F:32:MET:HB2	2.42	0.55
2:B:90:THR:O	2:B:173:TYR:HA	2.07	0.55
2:H:148:ARG:HG2	2:H:148:ARG:NH1	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:198:ILE:HG23	4:J:90:GLU:HG3	1.89	0.55
1:A:111:TYR:HB3	1:A:182:ARG:NH2	2.22	0.55
4:J:10:ASN:HB3	4:J:37:LEU:CD1	2.37	0.55
4:E:74:GLN:OE1	4:E:74:GLN:HA	2.06	0.55
4:K:79:ARG:HG3	4:K:109:CYS:SG	2.48	0.54
5:L:4:THR:HG22	5:L:5:HIS:N	2.22	0.54
5:L:5:HIS:O	5:L:73:THR:HG23	2.07	0.54
5:F:3:PRO:HG2	5:F:76:ASP:HB2	1.89	0.54
5:F:78:PRO:HG2	5:F:79:TYR:CE1	2.43	0.54
1:G:19:PHE:CE1	1:G:163:ASN:HB2	2.42	0.54
3:I:51:GLY:CA	3:I:66:ALA:HB2	2.36	0.54
3:I:142:TYR:N	3:I:142:TYR:CD1	2.74	0.54
4:K:64:MET:HE3	4:K:64:MET:HA	1.89	0.54
1:A:19:PHE:CE1	1:A:163:ASN:HB2	2.42	0.54
2:B:119:LEU:HB2	4:D:63:PRO:HB3	1.90	0.54
4:E:9:THR:HG21	4:E:110:PRO:CD	2.37	0.54
2:H:90:THR:O	2:H:173:TYR:HA	2.08	0.54
5:F:9:ASN:OD1	5:F:97:TYR:HB3	2.07	0.54
1:A:35:HIS:CD2	1:A:131:LEU:HD21	2.43	0.54
3:C:141:ARG:HB3	3:C:142:TYR:CD1	2.42	0.54
2:H:141:LYS:HG3	2:H:142:TYR:CE1	2.43	0.54
4:K:78:LEU:HD13	4:K:100:MET:HE3	1.90	0.54
2:B:12:GLN:HB3	2:B:88:ILE:HG13	1.89	0.54
4:D:13:VAL:HG11	4:D:68:LEU:HD11	1.88	0.54
2:H:12:GLN:HB3	2:H:88:ILE:HG13	1.90	0.54
2:B:94:THR:CG2	2:B:96:GLN:HG3	2.37	0.54
5:F:4:THR:HG22	5:F:5:HIS:N	2.22	0.54
3:I:28:ARG:NH1	3:I:177:GLU:CA	2.69	0.54
1:A:9:ARG:HD2	1:A:10:TYR:O	2.08	0.54
4:J:16:VAL:O	4:J:17:ALA:HB2	2.07	0.54
5:L:9:ASN:OD1	5:L:97:TYR:HB3	2.08	0.54
1:A:31:ASN:ND2	1:A:34:GLU:H	2.06	0.54
1:G:35:HIS:CD2	1:G:131:LEU:HD21	2.43	0.54
2:B:191:ILE:HG21	5:F:64:TYR:CZ	2.43	0.53
3:C:51:GLY:CA	3:C:66:ALA:HB2	2.38	0.53
3:C:67:TYR:HB2	3:C:70:ILE:CD1	2.39	0.53
4:J:10:ASN:HB3	4:J:37:LEU:HD12	1.89	0.53
1:G:143:ARG:HB2	1:G:143:ARG:HH11	1.74	0.53
1:G:9:ARG:HD2	1:G:10:TYR:O	2.07	0.53
3:I:52:TRP:HA	3:I:67:TYR:CE1	2.43	0.53
5:L:3:PRO:HG2	5:L:76:ASP:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:78:PRO:HG2	5:L:79:TYR:CE1	2.43	0.53
4:E:57:LYS:HD3	5:F:49:HIS:NE2	2.22	0.53
2:H:106:VAL:HG21	2:H:165:VAL:HG12	1.91	0.53
2:H:199:CYS:OXT	5:L:18:LYS:NZ	2.39	0.53
1:A:228:TYR:HD1	1:A:231:ILE:HD11	1.73	0.53
3:C:168:SER:O	3:C:170:GLU:N	2.42	0.53
4:D:11:MET:SD	4:D:36:LYS:CB	2.96	0.53
2:B:10:GLN:OE1	2:B:40:ASP:HB3	2.08	0.53
2:B:63:LEU:HD12	2:B:63:LEU:N	2.19	0.53
3:C:36:ARG:HG2	3:C:71:ILE:HD13	1.89	0.53
4:J:21:TYR:O	4:J:23:VAL:N	2.42	0.53
5:L:3:PRO:HG2	5:L:76:ASP:CB	2.38	0.53
1:A:111:TYR:CE1	1:A:182:ARG:HB2	2.43	0.53
1:A:113:ASP:HB3	4:D:12:VAL:HG11	1.89	0.53
2:B:92:ARG:HD3	2:B:174:TYR:OH	2.07	0.53
3:I:63:LEU:HD12	3:I:70:ILE:HD13	1.90	0.53
1:A:23:PHE:HB2	1:A:136:ILE:HG23	1.91	0.53
3:C:19:ALA:HA	3:C:83:ARG:O	2.08	0.53
4:D:16:VAL:O	4:D:17:ALA:HB2	2.08	0.53
4:J:28:MET:HG2	4:J:56:LEU:HD21	1.90	0.53
1:G:111:TYR:CE1	1:G:182:ARG:HB2	2.44	0.53
3:I:112:LEU:HG	4:K:101:VAL:HG22	1.91	0.53
3:C:123:PHE:HE2	3:C:133:ALA:HB3	1.74	0.53
5:F:3:PRO:HG2	5:F:76:ASP:CB	2.38	0.53
5:F:44:ASP:C	5:F:46:GLY:H	2.17	0.53
2:H:118:ARG:HA	2:H:136:SER:HB2	1.91	0.53
1:G:111:TYR:HB3	1:G:182:ARG:NH2	2.23	0.52
1:G:228:TYR:HD1	1:G:231:ILE:HD11	1.74	0.52
2:H:92:ARG:HG3	2:H:174:TYR:CE2	2.37	0.52
2:B:118:ARG:CB	2:B:136:SER:HB2	2.40	0.52
2:B:164:ARG:CZ	2:B:199:CYS:HB3	2.40	0.52
3:C:22:ARG:HG3	4:E:85:LYS:HZ1	1.75	0.52
3:I:118:ARG:HG3	3:I:120:CYS:SG	2.49	0.52
2:B:13:ILE:HA	2:B:88:ILE:HD12	1.91	0.52
2:H:114:SER:OG	2:H:117:SER:HB3	2.09	0.52
3:C:114:SER:HB3	3:C:117:SER:HB3	1.92	0.52
3:C:118:ARG:HA	3:C:136:SER:HB2	1.91	0.52
5:F:57:LEU:O	5:F:61:ILE:HG13	2.09	0.52
1:G:31:ASN:ND2	1:G:34:GLU:H	2.07	0.52
1:A:143:ARG:HB2	1:A:143:ARG:HH11	1.73	0.52
1:A:233:TYR:CD2	4:D:73:MET:HE3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:THR:HG23	2:B:96:GLN:HG3	1.92	0.52
2:H:55:PHE:CD1	2:H:55:PHE:N	2.78	0.52
4:J:51:CYS:SG	4:J:89:PHE:HB2	2.49	0.52
4:D:21:TYR:O	4:D:23:VAL:N	2.43	0.52
2:H:92:ARG:CG	2:H:174:TYR:HE2	2.20	0.52
5:L:6:LEU:HD21	5:L:8:LYS:CG	2.40	0.52
3:I:157:TYR:CE2	4:K:70:ALA:HB1	2.45	0.52
2:B:52:TRP:CD2	4:J:93:PRO:HB3	2.45	0.52
1:G:2:ASP:HB3	1:G:172:ARG:NH1	2.25	0.52
5:L:35:ARG:N	5:L:35:ARG:HD3	2.26	0.51
5:L:57:LEU:O	5:L:61:ILE:HG13	2.09	0.51
1:G:235:PHE:OXT	2:H:151:LYS:HE2	2.11	0.51
2:H:60:GLY:HA2	2:H:74:GLY:HA3	1.92	0.51
3:I:52:TRP:CE3	3:I:67:TYR:CZ	2.95	0.51
3:I:52:TRP:CE2	3:I:66:ALA:HB1	2.45	0.51
3:C:16:GLN:HA	3:C:16:GLN:OE1	2.10	0.51
3:C:152:LEU:O	3:C:156:ILE:HG12	2.10	0.51
4:E:15:SER:HB2	5:F:93:PRO:HD3	1.91	0.51
1:G:23:PHE:HB2	1:G:136:ILE:HG23	1.91	0.51
1:G:62:VAL:O	1:G:66:HIS:HD2	1.94	0.51
5:L:6:LEU:HD21	5:L:8:LYS:CD	2.40	0.51
3:C:151:ARG:NH2	6:E:111:ATP:O3G	2.43	0.51
1:G:83:HIS:CD2	1:G:150:ASN:HA	2.45	0.51
3:I:16:GLN:OE1	3:I:16:GLN:HA	2.11	0.51
1:A:83:HIS:CD2	1:A:150:ASN:HA	2.46	0.51
3:I:154:TYR:CE1	3:I:158:MET:HG3	2.44	0.51
3:C:5:ILE:HA	3:C:179:ALA:O	2.10	0.51
5:F:78:PRO:HG2	5:F:79:TYR:CZ	2.45	0.51
3:I:112:LEU:C	3:I:112:LEU:HD23	2.36	0.51
5:L:94:LEU:O	5:L:95:ASN:HB2	2.11	0.51
1:A:2:ASP:HB3	1:A:172:ARG:NH1	2.25	0.51
2:B:155:LEU:HD22	5:F:61:ILE:CG2	2.40	0.51
3:I:5:ILE:HA	3:I:179:ALA:O	2.11	0.51
5:L:78:PRO:HG2	5:L:79:TYR:CZ	2.46	0.51
1:A:165:ARG:HH11	1:A:165:ARG:CG	2.24	0.51
3:C:49:THR:O	3:C:65:GLN:HG3	2.11	0.51
5:F:6:LEU:HD21	5:F:8:LYS:CG	2.40	0.51
5:F:94:LEU:O	5:F:95:ASN:HB2	2.11	0.51
1:G:69:GLN:O	1:G:73:GLU:HG3	2.11	0.51
3:I:35:LEU:CD1	3:I:41:LEU:HD13	2.41	0.51
4:J:21:TYR:HD1	4:J:23:VAL:H	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:27:ARG:NH1	4:J:53:GLY:HA3	2.27	0.51
2:B:196:SER:OG	2:B:198:LEU:HB2	2.10	0.50
3:C:118:ARG:HG3	3:C:120:CYS:SG	2.52	0.50
1:G:165:ARG:HH11	1:G:165:ARG:CG	2.24	0.50
2:H:193:ASN:HD22	5:L:14:GLU:CD	2.19	0.50
3:I:49:THR:O	3:I:65:GLN:HG3	2.11	0.50
3:I:131:ILE:HD11	3:I:184:TYR:CD2	2.47	0.50
5:L:44:ASP:C	5:L:46:GLY:H	2.18	0.50
3:I:111:LEU:HD11	3:I:157:TYR:CD2	2.47	0.50
2:B:45:LEU:HB3	2:B:62:TYR:CE2	2.47	0.50
2:B:148:ARG:HB3	5:F:17:LEU:CD2	2.38	0.50
2:B:163:VAL:HG23	2:B:190:SER:O	2.11	0.50
3:C:154:TYR:CE1	3:C:158:MET:HG3	2.46	0.50
3:C:172:GLN:HG2	3:C:174:TYR:CZ	2.47	0.50
1:G:87:TYR:CD1	1:G:87:TYR:N	2.79	0.50
1:G:113:ASP:HB3	4:J:12:VAL:HG11	1.94	0.50
2:H:105:ASN:O	2:H:105:ASN:ND2	2.44	0.50
3:I:9:PRO:HD2	3:I:12:LEU:CD1	2.42	0.50
1:A:94:ASP:O	1:A:173:ALA:HA	2.11	0.50
2:B:105:ASN:ND2	2:B:105:ASN:O	2.44	0.50
3:C:168:SER:C	3:C:170:GLU:N	2.67	0.50
5:F:4:THR:CG2	5:F:5:HIS:N	2.75	0.50
5:F:6:LEU:HD21	5:F:8:LYS:CD	2.41	0.50
3:I:35:LEU:HD13	3:I:41:LEU:HD13	1.93	0.50
3:I:193:ASN:ND2	3:I:196:ALA:H	2.07	0.50
1:A:100:ALA:HA	1:A:131:LEU:HD11	1.94	0.50
1:A:228:TYR:CD1	1:A:231:ILE:HD11	2.46	0.50
1:G:110:THR:HG22	1:G:111:TYR:CZ	2.47	0.50
1:G:228:TYR:CD1	1:G:231:ILE:HD11	2.47	0.50
2:H:25:ASN:O	2:H:26:LYS:HB2	2.12	0.50
4:J:16:VAL:HG12	4:J:17:ALA:H	1.77	0.50
1:A:62:VAL:O	1:A:66:HIS:HD2	1.94	0.50
2:B:92:ARG:HG3	2:B:174:TYR:CE2	2.41	0.50
2:B:106:VAL:HG21	2:B:165:VAL:HG12	1.92	0.50
4:K:68:LEU:O	4:K:72:PHE:HB3	2.10	0.50
1:A:69:GLN:O	1:A:73:GLU:HG3	2.11	0.50
4:E:68:LEU:O	4:E:72:PHE:HB3	2.11	0.50
3:I:107:THR:HG22	3:I:108:ALA:N	2.26	0.50
3:I:150:ARG:HG3	3:I:151:ARG:N	2.27	0.50
3:I:194:PRO:O	3:I:197:SER:N	2.41	0.50
4:J:9:THR:HG21	4:J:110:PRO:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:69:ARG:HG3	6:K:111:ATP:C4	2.47	0.50
1:A:87:TYR:CD1	1:A:87:TYR:N	2.80	0.49
2:B:141:LYS:HG3	2:B:142:TYR:CE1	2.47	0.49
3:C:112:LEU:C	3:C:112:LEU:HD23	2.37	0.49
3:C:193:ASN:ND2	3:C:196:ALA:H	2.07	0.49
4:E:80:MET:HE3	4:E:97:LEU:HD13	1.94	0.49
2:H:63:LEU:HD12	2:H:63:LEU:N	2.20	0.49
5:L:4:THR:CG2	5:L:5:HIS:N	2.75	0.49
2:B:60:GLY:HA2	2:B:74:GLY:HA3	1.94	0.49
3:C:9:PRO:HD2	3:C:12:LEU:CD1	2.42	0.49
3:C:168:SER:OG	3:C:170:GLU:HB2	2.12	0.49
5:F:35:ARG:HD3	5:F:35:ARG:N	2.27	0.49
3:I:63:LEU:O	3:I:69:GLY:HA2	2.12	0.49
1:G:68:MET:HB2	1:G:84:PHE:CD2	2.48	0.49
1:G:95:ASN:O	1:G:174:ASN:HB2	2.13	0.49
1:G:139:GLU:HB3	1:G:167:VAL:HB	1.95	0.49
4:K:33:ILE:HD11	4:K:89:PHE:HE2	1.77	0.49
3:C:96:GLN:HG2	3:C:97:PRO:CD	2.40	0.49
4:E:64:MET:HE1	4:E:100:MET:HG2	1.94	0.49
3:I:94:THR:HG22	3:I:96:GLN:HB2	1.94	0.49
3:I:168:SER:O	3:I:170:GLU:N	2.44	0.49
4:J:11:MET:SD	4:J:36:LYS:CB	2.99	0.49
1:A:110:THR:HG22	1:A:111:TYR:CZ	2.47	0.49
4:D:51:CYS:SG	4:D:89:PHE:HB2	2.53	0.49
4:E:13:VAL:HG11	4:E:68:LEU:HD11	1.94	0.49
4:E:43:SER:OG	4:E:44:PRO:HD2	2.12	0.49
3:I:140:GLY:O	3:I:143:ARG:HB2	2.13	0.49
3:I:41:LEU:O	3:I:41:LEU:HD22	2.12	0.49
3:I:73:ASP:O	3:I:74:ALA:HB2	2.11	0.49
4:D:21:TYR:HE2	4:D:27:ARG:NH2	2.09	0.49
1:G:100:ALA:HA	1:G:131:LEU:HD11	1.94	0.49
2:H:118:ARG:CB	2:H:136:SER:HB2	2.43	0.49
3:C:60:GLY:HA3	3:C:72:LYS:O	2.13	0.48
1:G:165:ARG:HH11	1:G:165:ARG:CB	2.25	0.48
1:A:104:TYR:O	1:A:108:VAL:HG23	2.14	0.48
1:A:139:GLU:HB3	1:A:167:VAL:HB	1.94	0.48
1:A:165:ARG:HH11	1:A:165:ARG:CB	2.26	0.48
3:C:63:LEU:HB2	3:C:70:ILE:CD1	2.43	0.48
2:H:163:VAL:HG23	2:H:190:SER:O	2.13	0.48
4:K:13:VAL:HG11	4:K:68:LEU:HD11	1.95	0.48
2:B:81:ASP:OD1	2:B:81:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:52:TRP:CZ3	2:H:66:GLU:HB3	2.48	0.48
3:C:181:PHE:C	3:C:181:PHE:CD1	2.92	0.48
4:D:3:PRO:HB2	4:D:4:TYR:HD1	1.79	0.48
2:H:164:ARG:CZ	2:H:199:CYS:HB3	2.43	0.48
3:I:13:PHE:CE2	3:I:41:LEU:HD21	2.48	0.48
3:I:123:PHE:HE2	3:I:133:ALA:HB3	1.78	0.48
4:K:52:PHE:CE1	4:K:68:LEU:HD22	2.48	0.48
4:K:52:PHE:HE1	4:K:68:LEU:HD22	1.78	0.48
1:A:68:MET:HB2	1:A:84:PHE:CD2	2.48	0.48
2:B:118:ARG:HG3	2:B:134:CYS:HB3	1.95	0.48
2:H:141:LYS:HG3	2:H:142:TYR:CD1	2.48	0.48
4:D:26:THR:HG22	4:D:26:THR:O	2.13	0.48
4:D:80:MET:HB3	4:D:97:LEU:HD11	1.94	0.48
2:H:63:LEU:HD13	2:H:70:VAL:CB	2.34	0.48
4:J:84:PRO:HD2	7:J:111:HOH:O	2.13	0.48
3:C:25:ASN:OD1	3:C:25:ASN:N	2.46	0.48
1:G:94:ASP:O	1:G:173:ALA:HA	2.12	0.48
3:I:168:SER:C	3:I:170:GLU:N	2.69	0.48
3:C:28:ARG:NH1	3:C:177:GLU:CA	2.71	0.48
3:C:70:ILE:N	3:C:70:ILE:HD12	2.28	0.48
2:B:63:LEU:HD13	2:B:70:VAL:CB	2.39	0.48
2:B:163:VAL:HG23	2:B:190:SER:C	2.38	0.48
4:D:40:ALA:HB1	4:D:42:SER:OG	2.14	0.48
4:E:21:TYR:O	4:E:23:VAL:N	2.47	0.48
1:G:37:THR:HG21	1:G:187:ILE:HG12	1.96	0.48
1:G:104:TYR:O	1:G:108:VAL:HG23	2.14	0.48
3:I:12:LEU:HD11	3:I:174:TYR:CE2	2.48	0.48
3:I:190:SER:HA	4:J:17:ALA:HB2	1.94	0.48
1:A:95:ASN:O	1:A:174:ASN:HB2	2.13	0.48
3:C:94:THR:HG22	3:C:96:GLN:HB2	1.95	0.48
2:B:118:ARG:CA	2:B:136:SER:HB2	2.43	0.47
4:E:18:MET:O	5:F:88:GLU:HB2	2.13	0.47
3:I:36:ARG:HG2	3:I:71:ILE:HD13	1.96	0.47
2:B:198:LEU:HD22	5:F:27:CYS:HB2	1.96	0.47
4:D:47:HIS:O	4:D:49:PRO:HD3	2.15	0.47
1:G:15:PRO:HB3	1:G:19:PHE:CD2	2.49	0.47
3:I:168:SER:OG	3:I:170:GLU:HB2	2.13	0.47
4:K:47:HIS:O	4:K:49:PRO:HD3	2.14	0.47
1:A:15:PRO:HB3	1:A:19:PHE:CD2	2.50	0.47
1:A:153:THR:HB	1:A:155:GLU:HG3	1.96	0.47
4:D:21:TYR:HD1	4:D:23:VAL:H	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:GLU:OE1	1:G:39:ARG:HD3	2.14	0.47
2:H:9:PRO:HG2	2:H:92:ARG:HD2	1.96	0.47
2:H:145:MET:HE3	5:L:24:GLN:OE1	2.14	0.47
3:I:12:LEU:HD11	3:I:174:TYR:CD2	2.49	0.47
1:A:34:GLU:OE1	1:A:39:ARG:HD3	2.13	0.47
3:C:177:GLU:CD	4:E:79:ARG:HH22	2.22	0.47
2:H:10:GLN:OE1	2:H:40:ASP:HB3	2.13	0.47
3:I:152:LEU:O	3:I:156:ILE:HG12	2.14	0.47
5:L:74:VAL:HA	5:L:85:ASP:O	2.14	0.47
5:F:74:VAL:HA	5:F:85:ASP:O	2.14	0.47
1:G:118:ILE:HG13	4:J:72:PHE:CE1	2.50	0.47
3:I:108:ALA:HB2	3:I:123:PHE:CE1	2.48	0.47
4:J:28:MET:CG	4:J:56:LEU:HD21	2.44	0.47
4:K:43:SER:OG	4:K:44:PRO:HD2	2.15	0.47
3:C:9:PRO:HD2	3:C:12:LEU:HD12	1.97	0.47
3:C:52:TRP:HA	3:C:67:TYR:CE1	2.50	0.47
2:H:81:ASP:OD1	2:H:81:ASP:N	2.46	0.47
2:H:193:ASN:ND2	5:L:14:GLU:CD	2.72	0.47
3:I:67:TYR:CD1	3:I:67:TYR:N	2.81	0.47
4:J:11:MET:O	4:J:77:PRO:HA	2.15	0.47
2:B:105:ASN:HD22	2:B:125:ARG:HG3	1.80	0.47
3:C:119:LEU:HB2	4:E:63:PRO:HB3	1.95	0.47
4:E:74:GLN:O	4:E:75:GLN:HB2	2.14	0.47
1:G:160:GLU:C	1:G:161:TYR:CD1	2.93	0.47
2:H:196:SER:HG	2:H:198:LEU:HB2	1.77	0.47
3:I:125:ARG:O	3:I:126:ASP:C	2.57	0.47
4:K:26:THR:HA	5:L:49:HIS:CE1	2.49	0.47
3:C:41:LEU:HD22	3:C:41:LEU:O	2.14	0.47
4:D:93:PRO:HB3	2:H:52:TRP:CG	2.49	0.47
5:F:26:PHE:CE1	5:F:42:LEU:HB3	2.50	0.47
2:H:110:ARG:NE	4:J:104:SER:HB3	2.29	0.47
1:A:37:THR:HG21	1:A:187:ILE:HG12	1.97	0.47
4:E:24:THR:HA	4:E:25:PRO:HD3	1.56	0.47
1:G:13:ARG:HG3	1:G:13:ARG:NH1	2.30	0.47
1:G:153:THR:HB	1:G:155:GLU:HG3	1.97	0.47
1:A:160:GLU:C	1:A:161:TYR:CD1	2.93	0.46
4:E:18:MET:HB3	4:E:28:MET:HE1	1.96	0.46
2:H:156:ILE:HD13	2:H:189:ILE:HG21	1.97	0.46
4:J:21:TYR:HE2	4:J:27:ARG:NH2	2.13	0.46
1:A:13:ARG:HG3	1:A:13:ARG:NH1	2.30	0.46
3:C:167:VAL:HG21	3:C:184:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:9:PRO:HD2	3:I:12:LEU:HD12	1.97	0.46
3:I:114:SER:O	4:K:64:MET:HG2	2.15	0.46
4:E:84:PRO:HD2	4:E:85:LYS:HZ2	1.81	0.46
3:I:25:ASN:OD1	3:I:25:ASN:N	2.48	0.46
3:I:181:PHE:CD1	3:I:181:PHE:C	2.93	0.46
5:F:4:THR:O	5:F:5:HIS:CG	2.69	0.46
3:I:67:TYR:HB2	3:I:70:ILE:CD1	2.45	0.46
4:E:19:LYS:CG	4:E:29:LEU:HB2	2.44	0.46
3:I:91:ILE:HG23	3:I:91:ILE:O	2.16	0.46
4:J:80:MET:HB3	4:J:97:LEU:HD11	1.98	0.46
5:L:4:THR:O	5:L:5:HIS:CG	2.69	0.46
5:L:26:PHE:CE1	5:L:42:LEU:HB3	2.50	0.46
2:B:12:GLN:HE22	2:B:92:ARG:HG2	1.81	0.46
2:B:43:GLU:O	2:B:44:TYR:C	2.58	0.46
2:B:191:ILE:HG21	5:F:64:TYR:OH	2.16	0.46
3:C:107:THR:HG22	3:C:108:ALA:N	2.29	0.46
4:E:84:PRO:HD2	4:E:85:LYS:NZ	2.30	0.46
5:F:20:LYS:HE2	5:F:20:LYS:HB3	1.83	0.46
5:F:32:MET:O	5:F:34:GLY:N	2.48	0.46
1:G:113:ASP:OD2	4:J:14:THR:HG21	2.16	0.46
3:I:52:TRP:H	3:I:66:ALA:HB3	1.79	0.46
4:J:16:VAL:HG12	4:J:17:ALA:N	2.31	0.46
4:K:4:TYR:O	4:K:6:LEU:HD23	2.16	0.46
4:K:19:LYS:CG	4:K:29:LEU:HB2	2.43	0.46
5:L:77:SER:OG	5:L:82:THR:HB	2.16	0.46
4:D:80:MET:HB3	4:D:97:LEU:CD1	2.46	0.46
4:K:80:MET:HE3	4:K:97:LEU:HD13	1.97	0.46
3:C:52:TRP:CZ2	3:C:66:ALA:HB1	2.51	0.46
4:E:76:ARG:HA	4:E:77:PRO:HD3	1.63	0.46
4:K:18:MET:HB3	4:K:28:MET:HE1	1.97	0.46
2:B:52:TRP:CZ3	2:B:66:GLU:HB3	2.50	0.46
3:C:13:PHE:CE2	3:C:41:LEU:HD21	2.50	0.46
1:A:202:MET:O	1:A:204:ARG:N	2.48	0.46
2:B:92:ARG:CG	2:B:174:TYR:HE2	2.24	0.46
4:D:21:TYR:C	4:D:23:VAL:H	2.24	0.46
2:H:63:LEU:HD21	2:H:72:LYS:HE3	1.96	0.46
4:K:23:VAL:HG12	4:K:24:THR:N	2.30	0.46
3:C:12:LEU:HD11	3:C:174:TYR:CD2	2.50	0.45
4:K:3:PRO:HG2	4:K:4:TYR:HD1	1.80	0.45
2:B:63:LEU:HD21	2:B:72:LYS:HE3	1.98	0.45
3:C:126:ASP:OD1	3:C:128:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:190:SER:HA	4:D:17:ALA:HB2	1.98	0.45
4:D:28:MET:HG2	4:D:56:LEU:HD21	1.98	0.45
2:H:198:LEU:HA	7:L:100:HOH:O	2.15	0.45
5:L:32:MET:O	5:L:34:GLY:N	2.49	0.45
1:A:207:GLU:HG3	1:A:223:MET:HE2	1.98	0.45
4:D:21:TYR:C	4:D:21:TYR:CD1	2.94	0.45
3:I:60:GLY:CA	3:I:72:LYS:O	2.65	0.45
3:C:45:LEU:HA	3:C:45:LEU:HD23	1.66	0.45
3:C:52:TRP:H	3:C:66:ALA:HB3	1.80	0.45
3:C:73:ASP:O	3:C:74:ALA:HB2	2.17	0.45
1:G:18:VAL:HG21	1:G:89:TYR:CZ	2.52	0.45
1:G:85:ILE:HG22	1:G:87:TYR:CE1	2.52	0.45
5:L:30:ALA:HB3	5:L:38:VAL:HB	1.99	0.45
3:C:63:LEU:CD1	3:C:70:ILE:HD13	2.46	0.45
1:G:7:VAL:HG22	1:G:91:VAL:HB	1.99	0.45
1:G:207:GLU:HG3	1:G:223:MET:HE2	1.98	0.45
4:J:58:ARG:HA	4:J:59:PRO:HD2	1.57	0.45
4:K:8:LYS:HG3	4:K:82:LEU:HD12	1.97	0.45
4:K:9:THR:HG21	4:K:110:PRO:CD	2.45	0.45
4:K:57:LYS:HE3	4:K:57:LYS:HB2	1.73	0.45
4:K:107:GLN:HG2	4:K:108:ASP:H	1.82	0.45
1:A:18:VAL:HG21	1:A:89:TYR:CZ	2.51	0.45
5:F:77:SER:OG	5:F:82:THR:HB	2.17	0.45
1:G:233:TYR:CD2	4:J:73:MET:HE3	2.51	0.45
3:I:52:TRP:H	3:I:66:ALA:CB	2.29	0.45
4:K:84:PRO:HD2	4:K:85:LYS:NZ	2.31	0.45
2:B:52:TRP:CZ2	4:J:93:PRO:HD3	2.52	0.45
4:D:16:VAL:HG12	4:D:17:ALA:N	2.30	0.45
4:E:107:GLN:HG2	4:E:108:ASP:N	2.32	0.45
5:F:29:THR:HG23	5:F:37:LEU:HB3	1.99	0.45
3:I:119:LEU:HB2	4:K:63:PRO:HB3	1.98	0.45
5:L:16:ALA:O	5:L:26:PHE:HA	2.17	0.45
2:B:25:ASN:O	2:B:26:LYS:HB2	2.16	0.45
2:B:114:SER:OG	2:B:117:SER:HB3	2.16	0.45
3:C:131:ILE:HD11	3:C:184:TYR:CE2	2.52	0.45
5:L:75:GLU:CB	5:L:87:LEU:HD11	2.44	0.45
1:A:118:ILE:N	7:A:241:HOH:O	2.49	0.45
3:C:12:LEU:HD11	3:C:174:TYR:CE2	2.52	0.45
3:C:20:TYR:OH	3:C:83:ARG:HB2	2.17	0.45
5:F:30:ALA:HB3	5:F:38:VAL:HB	1.99	0.45
5:F:73:THR:HG22	5:F:87:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:ALA:HA	1:G:131:LEU:CD1	2.47	0.45
1:G:233:TYR:CE1	4:J:69:ARG:HD2	2.52	0.45
3:I:190:SER:HA	4:J:17:ALA:CB	2.47	0.45
1:A:7:VAL:HG22	1:A:91:VAL:HB	1.99	0.45
1:A:10:TYR:CD2	1:A:64:LEU:HB2	2.52	0.45
7:C:203:HOH:O	4:E:63:PRO:HD2	2.16	0.45
4:D:11:MET:O	4:D:77:PRO:HA	2.17	0.45
2:H:133:ALA:HA	2:H:184:TYR:O	2.17	0.45
2:B:12:GLN:NE2	2:B:92:ARG:CG	2.80	0.44
5:F:16:ALA:O	5:F:26:PHE:HA	2.16	0.44
5:F:75:GLU:CB	5:F:87:LEU:HD11	2.43	0.44
2:H:163:VAL:HG23	2:H:190:SER:C	2.42	0.44
5:L:73:THR:HG22	5:L:87:LEU:HD12	1.99	0.44
5:F:2:LEU:O	5:F:4:THR:N	2.51	0.44
3:I:163:VAL:HG13	3:I:164:ARG:N	2.32	0.44
4:K:64:MET:HE1	4:K:100:MET:SD	2.57	0.44
1:A:85:ILE:HG22	1:A:87:TYR:CE1	2.52	0.44
1:A:100:ALA:HA	1:A:131:LEU:CD1	2.47	0.44
5:F:35:ARG:HG3	5:F:35:ARG:HH11	1.83	0.44
3:I:145:MET:HE2	3:I:145:MET:HB3	1.89	0.44
1:A:233:TYR:CE2	4:D:73:MET:HE3	2.52	0.44
2:B:38:SER:HB3	2:B:41:LEU:HD12	2.00	0.44
3:I:7:ILE:O	3:I:8:PRO:C	2.58	0.44
4:K:2:VAL:HG22	4:K:3:PRO:HD2	2.00	0.44
1:A:94:ASP:HA	1:A:171:THR:HB	2.00	0.44
1:A:191:LEU:HD23	1:A:191:LEU:HA	1.82	0.44
2:B:47:HIS:CG	2:B:47:HIS:O	2.70	0.44
1:G:143:ARG:HD3	1:G:160:GLU:OE1	2.16	0.44
2:H:118:ARG:CZ	2:H:173:TYR:CD1	3.01	0.44
3:I:51:GLY:HA3	3:I:66:ALA:HB2	2.00	0.44
3:C:55:TYR:HD1	3:C:84:GLU:HB2	1.83	0.44
1:G:52:SER:HG	1:G:202:MET:HE3	1.79	0.44
1:G:202:MET:O	1:G:203:ALA:C	2.60	0.44
5:L:70:ILE:HD12	5:L:89:LEU:CD1	2.38	0.44
1:A:202:MET:O	1:A:203:ALA:C	2.59	0.44
3:C:52:TRP:H	3:C:66:ALA:CB	2.30	0.44
2:H:45:LEU:HB3	2:H:62:TYR:CE2	2.52	0.44
2:H:137:PRO:HB3	2:H:146:TYR:HD2	1.80	0.44
2:H:137:PRO:HD3	2:H:146:TYR:CD2	2.53	0.44
4:K:40:ALA:O	4:K:43:SER:N	2.51	0.44
1:A:113:ASP:CB	4:D:12:VAL:HG11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:10:ASN:HB3	4:D:37:LEU:CD1	2.47	0.44
4:E:23:VAL:HG12	4:E:24:THR:N	2.33	0.44
1:G:195:ALA:HB1	4:K:75:GLN:HG2	1.99	0.44
3:I:141:ARG:HD3	3:I:142:TYR:CE1	2.53	0.44
4:J:16:VAL:HG21	4:J:72:PHE:CD2	2.53	0.44
4:K:106:LYS:HZ1	4:K:110:PRO:HB3	1.83	0.44
1:A:37:THR:HA	1:A:190:THR:HG23	2.00	0.44
1:A:228:TYR:HD1	1:A:231:ILE:CD1	2.31	0.44
2:B:148:ARG:N	2:B:148:ARG:CD	2.81	0.44
5:F:77:SER:HB3	5:F:82:THR:O	2.18	0.44
2:H:26:LYS:HE2	2:H:116:ASN:O	2.17	0.44
2:H:63:LEU:H	2:H:63:LEU:CD1	2.22	0.44
1:A:31:ASN:ND2	1:A:33:LEU:H	2.15	0.43
1:A:144:VAL:HG13	1:A:144:VAL:O	2.18	0.43
3:C:35:LEU:HD13	3:C:41:LEU:HD13	2.00	0.43
3:C:141:ARG:HG2	3:C:142:TYR:CE1	2.52	0.43
3:C:154:TYR:CD1	3:C:154:TYR:C	2.96	0.43
4:D:76:ARG:HA	4:D:77:PRO:HD2	1.89	0.43
4:E:3:PRO:HG2	4:E:4:TYR:HD1	1.80	0.43
1:G:48:SER:OG	1:G:50:PHE:HB2	2.18	0.43
2:H:47:HIS:CG	2:H:47:HIS:O	2.71	0.43
2:B:110:ARG:NE	4:D:104:SER:HB3	2.32	0.43
4:D:21:TYR:HD2	4:D:27:ARG:HB2	1.82	0.43
4:D:58:ARG:HA	4:D:59:PRO:HD2	1.61	0.43
1:G:10:TYR:CD2	1:G:64:LEU:HB2	2.53	0.43
2:H:119:LEU:HB2	4:J:63:PRO:HB3	2.00	0.43
4:J:43:SER:HA	4:J:44:PRO:HD3	1.70	0.43
4:K:24:THR:HA	4:K:25:PRO:HD3	1.57	0.43
1:A:48:SER:OG	1:A:50:PHE:HB2	2.17	0.43
1:G:138:PRO:HG2	1:G:139:GLU:OE2	2.18	0.43
1:A:30:ASP:OD2	1:A:178:TYR:HE2	2.00	0.43
2:B:156:ILE:HD13	2:B:189:ILE:HG21	2.00	0.43
4:D:10:ASN:HB3	4:D:37:LEU:HD12	2.00	0.43
5:F:56:MET:HE3	5:F:56:MET:HB3	1.81	0.43
1:G:202:MET:O	1:G:204:ARG:N	2.51	0.43
3:I:154:TYR:CD1	3:I:154:TYR:C	2.96	0.43
5:L:29:THR:HG23	5:L:37:LEU:HB3	1.99	0.43
5:L:50:ASP:C	5:L:52:TRP:N	2.76	0.43
1:A:143:ARG:HD3	1:A:160:GLU:OE1	2.18	0.43
4:D:16:VAL:HG12	4:D:17:ALA:H	1.84	0.43
4:D:43:SER:HA	4:D:44:PRO:HD3	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:50:ASP:C	5:F:52:TRP:N	2.76	0.43
1:G:14:PRO:HA	1:G:15:PRO:HD3	1.84	0.43
1:G:94:ASP:HA	1:G:171:THR:HB	2.00	0.43
1:G:143:ARG:HG2	1:G:144:VAL:H	1.84	0.43
1:G:31:ASN:ND2	1:G:33:LEU:H	2.16	0.43
1:G:233:TYR:CE2	4:J:69:ARG:HG3	2.53	0.43
4:E:78:LEU:HD13	4:E:100:MET:HE3	2.00	0.43
3:I:70:ILE:HD12	3:I:70:ILE:N	2.33	0.43
3:I:96:GLN:HG2	3:I:97:PRO:CD	2.40	0.43
4:J:80:MET:HB3	4:J:97:LEU:CD1	2.49	0.43
3:C:52:TRP:CE3	3:C:67:TYR:CZ	3.06	0.43
3:C:164:ARG:NH2	3:C:198:ILE:O	2.51	0.43
4:E:57:LYS:HE3	4:E:57:LYS:HB2	1.82	0.43
4:E:67:MET:SD	4:E:100:MET:HG3	2.59	0.43
3:I:55:TYR:HD1	3:I:84:GLU:HB2	1.84	0.43
5:L:10:PHE:CE1	5:L:32:MET:HB2	2.53	0.43
1:A:143:ARG:HG2	1:A:144:VAL:H	1.84	0.43
3:C:51:GLY:HA3	3:C:66:ALA:HB2	2.01	0.43
3:C:111:LEU:HD11	3:C:157:TYR:CD2	2.54	0.43
3:I:159:SER:O	3:I:160:GLY:C	2.62	0.43
4:E:97:LEU:HD21	4:E:100:MET:SD	2.59	0.43
3:I:60:GLY:HA2	3:I:74:ALA:HB3	2.00	0.43
5:L:73:THR:O	5:L:87:LEU:HD12	2.19	0.43
1:A:48:SER:C	1:A:50:PHE:H	2.27	0.42
1:A:138:PRO:HG2	1:A:139:GLU:OE2	2.18	0.42
3:C:63:LEU:HB2	3:C:70:ILE:HD13	2.00	0.42
3:C:122:VAL:HG23	3:C:176:TYR:CZ	2.54	0.42
5:F:50:ASP:C	5:F:52:TRP:H	2.27	0.42
1:G:30:ASP:OD2	1:G:178:TYR:HE2	2.02	0.42
2:H:47:HIS:O	2:H:47:HIS:ND1	2.51	0.42
3:I:141:ARG:HG2	3:I:142:TYR:CE1	2.54	0.42
1:A:81:THR:O	1:A:83:HIS:N	2.53	0.42
2:B:77:GLY:HA2	2:B:80:PHE:CD1	2.53	0.42
2:B:145:MET:HE2	2:B:145:MET:HB3	1.68	0.42
3:C:162:ALA:O	3:C:163:VAL:HG23	2.20	0.42
4:E:81:PHE:N	4:E:81:PHE:CD1	2.88	0.42
1:G:92:ARG:HD2	1:G:169:GLN:HB2	2.01	0.42
3:I:59:ASP:HB2	3:I:60:GLY:H	1.57	0.42
4:J:6:LEU:N	4:J:6:LEU:HD22	2.34	0.42
4:J:21:TYR:HD2	4:J:27:ARG:HB2	1.83	0.42
5:L:2:LEU:O	5:L:4:THR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:2:VAL:HG12	4:E:84:PRO:HA	2.01	0.42
4:E:107:GLN:HG2	4:E:108:ASP:H	1.84	0.42
4:K:107:GLN:HG2	4:K:108:ASP:N	2.33	0.42
1:A:32:VAL:O	1:A:32:VAL:HG12	2.19	0.42
1:A:92:ARG:HD2	1:A:169:GLN:HB2	2.01	0.42
1:A:174:ASN:OD1	1:A:175:PRO:HD2	2.20	0.42
2:B:56:ALA:O	2:B:85:THR:HA	2.20	0.42
4:E:57:LYS:CD	5:F:49:HIS:NE2	2.82	0.42
4:E:106:LYS:NZ	4:E:106:LYS:HB3	2.34	0.42
2:H:118:ARG:CA	2:H:136:SER:HB2	2.48	0.42
3:C:112:LEU:HG	4:E:101:VAL:HG22	2.01	0.42
3:C:125:ARG:O	3:C:128:GLN:CG	2.65	0.42
4:D:27:ARG:NH1	4:D:53:GLY:HA3	2.35	0.42
1:G:81:THR:O	1:G:83:HIS:N	2.52	0.42
2:H:39:GLY:O	2:H:40:ASP:C	2.62	0.42
3:I:45:LEU:HA	3:I:48:ILE:HG22	2.01	0.42
4:K:21:TYR:O	4:K:23:VAL:N	2.52	0.42
1:A:8:TYR:CD2	1:A:57:ARG:HG3	2.54	0.42
1:A:15:PRO:O	1:A:19:PHE:HB2	2.20	0.42
3:C:157:TYR:CE2	4:E:70:ALA:HB1	2.55	0.42
3:C:198:ILE:HG23	4:D:90:GLU:HG3	2.02	0.42
4:D:21:TYR:HD1	4:D:21:TYR:C	2.27	0.42
4:E:57:LYS:HA	5:F:49:HIS:CD2	2.54	0.42
5:F:10:PHE:CE1	5:F:32:MET:HB2	2.53	0.42
1:G:48:SER:C	1:G:50:PHE:H	2.27	0.42
1:G:118:ILE:HD13	1:G:118:ILE:O	2.20	0.42
1:G:228:TYR:HD1	1:G:231:ILE:CD1	2.32	0.42
2:H:148:ARG:CD	2:H:148:ARG:N	2.83	0.42
3:I:125:ARG:HB2	3:I:130:VAL:HG21	2.02	0.42
4:K:69:ARG:CZ	6:K:111:ATP:C8	3.03	0.42
2:B:141:LYS:HG3	2:B:142:TYR:CD1	2.54	0.42
3:C:125:ARG:HB2	3:C:130:VAL:HG21	2.02	0.42
4:D:19:LYS:NZ	4:D:22:GLU:HG3	2.35	0.42
2:H:196:SER:C	2:H:198:LEU:N	2.76	0.42
3:I:54:ILE:HD13	3:I:82:TYR:CZ	2.54	0.42
3:I:77:GLY:HA2	3:I:80:PHE:CD2	2.54	0.42
2:B:133:ALA:HA	2:B:184:TYR:O	2.19	0.42
3:C:140:GLY:O	3:C:143:ARG:HB2	2.20	0.42
4:D:21:TYR:C	4:D:23:VAL:N	2.77	0.42
1:G:193:ARG:HH11	1:G:223:MET:HG3	1.85	0.42
2:H:118:ARG:HG3	2:H:120:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:161:ILE:HG21	2:H:191:ILE:HG12	2.02	0.42
4:K:98:ILE:O	4:K:99:ARG:HB2	2.19	0.42
2:B:8:PRO:HA	2:B:9:PRO:HD3	1.92	0.42
3:C:28:ARG:NH2	3:C:34:GLU:OE1	2.53	0.42
4:D:7:VAL:HG22	4:D:81:PHE:CD2	2.55	0.42
4:D:36:LYS:O	4:D:37:LEU:C	2.63	0.42
1:G:15:PRO:O	1:G:19:PHE:HB2	2.19	0.42
1:A:101:ALA:O	1:A:104:TYR:HB3	2.20	0.42
1:A:117:ARG:HG2	1:A:117:ARG:HH11	1.85	0.42
2:B:9:PRO:HG2	2:B:92:ARG:HD2	2.01	0.42
2:B:118:ARG:CZ	2:B:173:TYR:CD1	3.03	0.42
5:F:79:TYR:HA	5:F:80:PRO:HD3	1.85	0.42
1:G:139:GLU:CD	1:G:139:GLU:N	2.78	0.42
1:G:207:GLU:H	1:G:207:GLU:HG2	1.72	0.42
2:H:158:VAL:HG12	4:J:74:GLN:HG2	2.01	0.42
2:H:163:VAL:CG2	2:H:190:SER:H	2.33	0.42
4:J:26:THR:HG22	4:J:26:THR:O	2.19	0.42
5:L:35:ARG:HH11	5:L:35:ARG:HG3	1.84	0.42
1:A:139:GLU:CD	1:A:139:GLU:N	2.78	0.41
1:A:207:GLU:H	1:A:207:GLU:HG2	1.71	0.41
2:B:131:ILE:HD11	2:B:184:TYR:CD2	2.55	0.41
2:B:133:ALA:HB1	2:B:186:LEU:HB2	2.02	0.41
4:E:21:TYR:H	4:E:28:MET:HA	1.85	0.41
5:F:28:LEU:HD21	5:F:86:LEU:HD22	2.02	0.41
2:H:105:ASN:HD22	2:H:125:ARG:HG3	1.85	0.41
2:H:110:ARG:HE	4:J:104:SER:HB3	1.85	0.41
3:I:67:TYR:O	3:I:70:ILE:HD11	2.20	0.41
3:I:118:ARG:CA	3:I:136:SER:HB2	2.48	0.41
4:K:74:GLN:O	4:K:75:GLN:HB2	2.19	0.41
2:B:52:TRP:CH2	4:J:93:PRO:HD3	2.55	0.41
4:D:16:VAL:HG21	4:D:72:PHE:CD2	2.55	0.41
4:E:40:ALA:O	4:E:43:SER:N	2.52	0.41
5:F:26:PHE:HE1	5:F:42:LEU:HD23	1.84	0.41
1:G:113:ASP:CB	4:J:12:VAL:HG11	2.50	0.41
1:G:144:VAL:HG13	1:G:144:VAL:O	2.19	0.41
2:H:63:LEU:HD21	2:H:72:LYS:CE	2.51	0.41
4:K:6:LEU:HA	7:K:113:HOH:O	2.19	0.41
1:A:30:ASP:OD2	1:A:178:TYR:CE2	2.74	0.41
1:A:102:SER:O	1:A:103:SER:C	2.62	0.41
2:B:45:LEU:HB3	2:B:62:TYR:HE2	1.85	0.41
3:C:75:PRO:HA	3:C:76:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:85:LYS:HG2	4:D:86:GLN:N	2.34	0.41
1:G:174:ASN:OD1	1:G:175:PRO:HD2	2.21	0.41
2:H:35:LEU:O	2:H:36:ARG:C	2.63	0.41
4:J:9:THR:HG22	4:J:79:ARG:HG3	2.02	0.41
3:C:91:ILE:HG23	3:C:91:ILE:O	2.20	0.41
5:F:73:THR:O	5:F:87:LEU:HD12	2.19	0.41
1:G:37:THR:HA	1:G:190:THR:HG23	2.01	0.41
1:G:101:ALA:O	1:G:104:TYR:HB3	2.19	0.41
1:G:8:TYR:CD2	1:G:57:ARG:HG3	2.56	0.41
2:H:52:TRP:O	2:H:67:TYR:HE1	2.01	0.41
2:H:145:MET:HB3	2:H:145:MET:HE2	1.69	0.41
2:H:148:ARG:HH11	2:H:148:ARG:CG	2.32	0.41
4:J:19:LYS:NZ	4:J:22:GLU:HG3	2.36	0.41
4:K:18:MET:SD	4:K:28:MET:HE1	2.61	0.41
5:L:77:SER:HB3	5:L:82:THR:O	2.21	0.41
2:B:63:LEU:HD21	2:B:72:LYS:HD2	2.02	0.41
3:C:131:ILE:HG12	3:C:132:GLY:N	2.34	0.41
4:D:85:LYS:HE2	4:D:85:LYS:HB3	1.72	0.41
4:E:2:VAL:HG13	4:E:4:TYR:H	1.84	0.41
5:F:19:LEU:HD12	5:F:20:LYS:H	1.86	0.41
5:F:30:ALA:HB2	5:F:72:LEU:HD21	2.02	0.41
5:F:70:ILE:HD12	5:F:89:LEU:CD1	2.38	0.41
3:I:63:LEU:HB2	3:I:70:ILE:CD1	2.51	0.41
4:J:21:TYR:C	4:J:23:VAL:N	2.78	0.41
4:K:42:SER:O	4:K:43:SER:C	2.64	0.41
5:L:28:LEU:HD21	5:L:86:LEU:HD22	2.02	0.41
5:L:30:ALA:HB2	5:L:72:LEU:HD21	2.02	0.41
1:A:36:LEU:N	1:A:36:LEU:HD12	2.36	0.41
3:C:65:GLN:C	3:C:68:GLY:H	2.29	0.41
4:D:48:VAL:HG11	4:D:82:LEU:HD13	2.03	0.41
6:E:111:ATP:H4'	5:F:55:THR:HG23	2.03	0.41
5:F:86:LEU:HD12	5:F:86:LEU:HA	1.92	0.41
1:G:102:SER:O	1:G:103:SER:C	2.63	0.41
2:H:43:GLU:O	2:H:44:TYR:C	2.63	0.41
2:H:131:ILE:HD11	2:H:184:TYR:CD2	2.56	0.41
4:J:6:LEU:HD22	4:J:6:LEU:H	1.84	0.41
4:K:86:GLN:HG2	4:K:95:LEU:HD13	2.02	0.41
3:C:65:GLN:HA	3:C:68:GLY:C	2.46	0.41
3:C:173:TYR:HB2	3:C:183:THR:OG1	2.21	0.41
3:I:172:GLN:HG2	3:I:174:TYR:CZ	2.56	0.41
4:J:21:TYR:C	4:J:21:TYR:CD1	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:26:PHE:HE1	5:L:42:LEU:HD23	1.85	0.41
2:B:15:GLN:HG3	2:B:16:HIS:ND1	2.36	0.41
2:B:145:MET:HG2	5:F:24:GLN:NE2	2.36	0.41
2:B:161:ILE:O	2:B:161:ILE:HG22	2.21	0.41
2:B:163:VAL:CG2	2:B:190:SER:H	2.33	0.41
3:C:35:LEU:CD1	3:C:41:LEU:HD13	2.50	0.41
3:C:59:ASP:HB2	3:C:60:GLY:H	1.53	0.41
3:C:125:ARG:O	3:C:126:ASP:C	2.63	0.41
3:C:190:SER:O	3:C:191:LEU:C	2.63	0.41
4:E:52:PHE:HE1	4:E:68:LEU:HD22	1.85	0.41
1:G:91:VAL:HG11	1:G:136:ILE:HD11	2.03	0.41
1:G:117:ARG:HH11	1:G:117:ARG:HG2	1.86	0.41
3:I:162:ALA:O	3:I:163:VAL:HG23	2.21	0.41
4:K:15:SER:HB2	5:L:93:PRO:HD3	2.03	0.41
5:L:50:ASP:C	5:L:52:TRP:H	2.27	0.41
1:A:165:ARG:O	1:A:166:TYR:C	2.64	0.41
2:B:7:ILE:HA	2:B:8:PRO:HD3	1.89	0.41
2:B:103:TYR:CD1	2:B:103:TYR:N	2.89	0.41
2:B:131:ILE:HG13	2:B:132:GLY:N	2.36	0.41
3:C:77:GLY:HA2	3:C:80:PHE:CD2	2.56	0.41
1:G:191:LEU:HD23	1:G:191:LEU:HA	1.83	0.41
2:H:145:MET:HG2	5:L:24:GLN:OE1	2.21	0.41
3:I:141:ARG:HB3	3:I:142:TYR:CD1	2.56	0.41
3:C:94:THR:HG21	3:C:96:GLN:HB2	2.04	0.40
2:H:196:SER:C	2:H:198:LEU:H	2.29	0.40
4:J:21:TYR:C	4:J:23:VAL:H	2.29	0.40
4:J:67:MET:O	4:J:71:VAL:HG22	2.21	0.40
5:L:19:LEU:HD12	5:L:20:LYS:H	1.87	0.40
2:B:26:LYS:HE2	2:B:116:ASN:O	2.21	0.40
2:B:52:TRP:CE2	4:J:93:PRO:HD3	2.56	0.40
1:G:183:SER:OG	1:G:185:ALA:HB3	2.21	0.40
3:I:52:TRP:CZ2	3:I:66:ALA:HB1	2.56	0.40
3:I:103:TYR:HE1	3:I:167:VAL:CG1	2.34	0.40
4:J:98:ILE:HD13	4:J:98:ILE:HG21	1.87	0.40
4:K:2:VAL:HG13	4:K:4:TYR:H	1.86	0.40
2:B:47:HIS:O	2:B:47:HIS:ND1	2.55	0.40
3:C:45:LEU:HA	3:C:48:ILE:HG22	2.02	0.40
1:G:30:ASP:OD2	1:G:178:TYR:CE2	2.75	0.40
1:G:36:LEU:N	1:G:36:LEU:HD12	2.37	0.40
1:G:91:VAL:CG2	1:G:136:ILE:HD11	2.46	0.40
2:H:38:SER:HB3	2:H:41:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:77:GLY:O	3:I:80:PHE:HB2	2.21	0.40
2:B:110:ARG:NH1	2:B:176:TYR:CD2	2.83	0.40
1:G:91:VAL:HG11	1:G:136:ILE:CD1	2.51	0.40
1:G:141:ILE:O	1:G:166:TYR:HB2	2.21	0.40
3:I:167:VAL:HG21	3:I:184:TYR:HB2	2.01	0.40
4:K:2:VAL:HG12	4:K:84:PRO:HA	2.02	0.40
2:B:52:TRP:O	2:B:67:TYR:HE1	2.05	0.40
3:C:36:ARG:HG3	3:C:71:ILE:HG21	2.02	0.40
3:C:102:TYR:CE2	3:C:164:ARG:CZ	3.04	0.40
4:D:40:ALA:C	4:D:42:SER:N	2.79	0.40
4:E:1:ASP:OD1	4:E:85:LYS:HA	2.21	0.40
4:E:2:VAL:HG13	4:E:3:PRO:N	2.36	0.40
1:G:32:VAL:O	1:G:32:VAL:HG12	2.21	0.40
2:H:52:TRP:C	2:H:67:TYR:CE1	2.98	0.40
3:I:22:ARG:HG3	4:K:85:LYS:HZ1	1.87	0.40
3:I:173:TYR:HB2	3:I:183:THR:OG1	2.22	0.40
4:K:56:LEU:HD22	5:L:51:THR:HB	2.03	0.40
4:K:64:MET:HE1	4:K:100:MET:CG	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	220/235 (94%)	190 (86%)	24 (11%)	6 (3%)	4	10
1	G	220/235 (94%)	190 (86%)	23 (10%)	7 (3%)	3	7
2	B	195/199 (98%)	165 (85%)	29 (15%)	1 (0%)	24	48
2	H	195/199 (98%)	165 (85%)	29 (15%)	1 (0%)	24	48
3	C	194/199 (98%)	166 (86%)	20 (10%)	8 (4%)	2	5
3	I	194/199 (98%)	166 (86%)	20 (10%)	8 (4%)	2	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	108/110 (98%)	98 (91%)	8 (7%)	2 (2%)	6	17
4	E	108/110 (98%)	94 (87%)	11 (10%)	3 (3%)	4	9
4	J	108/110 (98%)	99 (92%)	8 (7%)	1 (1%)	14	35
4	K	108/110 (98%)	94 (87%)	11 (10%)	3 (3%)	4	9
5	F	96/99 (97%)	88 (92%)	4 (4%)	4 (4%)	2	4
5	L	96/99 (97%)	88 (92%)	4 (4%)	4 (4%)	2	4
All	All	1842/1904 (97%)	1603 (87%)	191 (10%)	48 (3%)	4	11

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	ALA
1	A	144	VAL
3	C	39	ALA
3	C	161	LEU
4	E	22	GLU
4	E	23	VAL
4	E	39	ALA
5	F	76	ASP
1	G	25	ALA
1	G	144	VAL
3	I	39	ALA
3	I	161	LEU
4	K	22	GLU
4	K	23	VAL
4	K	39	ALA
5	L	76	ASP
1	A	110	THR
2	B	10	GLN
3	C	60	GLY
4	D	22	GLU
5	F	33	SER
5	F	50	ASP
1	G	110	THR
2	H	10	GLN
3	I	51	GLY
3	I	60	GLY
4	J	22	GLU
5	L	33	SER
5	L	50	ASP

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Mol	Chain	Res	Type
1	A	203	ALA
1	A	234	SER
3	C	51	GLY
3	C	64	GLY
3	C	169	LYS
5	F	49	HIS
1	G	203	ALA
1	G	234	SER
3	I	64	GLY
3	I	126	ASP
3	I	169	LYS
5	L	49	HIS
1	A	82	GLY
3	C	126	ASP
1	G	82	GLY
3	C	65	GLN
4	D	107	GLN
1	G	45	SER
3	I	74	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/191 (97%)	162 (88%)	23 (12%)	4	11
1	G	185/191 (97%)	162 (88%)	23 (12%)	4	11
2	B	164/166 (99%)	136 (83%)	28 (17%)	2	6
2	H	164/166 (99%)	139 (85%)	25 (15%)	3	7
3	C	155/157 (99%)	134 (86%)	21 (14%)	4	9
3	I	155/157 (99%)	134 (86%)	21 (14%)	4	9
4	D	94/94 (100%)	85 (90%)	9 (10%)	8	20
4	E	94/94 (100%)	82 (87%)	12 (13%)	4	11
4	J	94/94 (100%)	85 (90%)	9 (10%)	8	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	K	94/94 (100%)	83 (88%)	11 (12%)	5	13
5	F	83/83 (100%)	75 (90%)	8 (10%)	8	20
5	L	83/83 (100%)	75 (90%)	8 (10%)	8	20
All	All	1550/1570 (99%)	1352 (87%)	198 (13%)	4	11

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	7	VAL
1	A	9	ARG
1	A	21	ASN
1	A	33	LEU
1	A	37	THR
1	A	39	ARG
1	A	61	GLU
1	A	81	THR
1	A	85	ILE
1	A	95	ASN
1	A	118	ILE
1	A	128	SER
1	A	134	ARG
1	A	136	ILE
1	A	165	ARG
1	A	170	GLN
1	A	177	PRO
1	A	190	THR
1	A	192	VAL
1	A	202	MET
1	A	221	GLU
1	A	226	VAL
2	B	5	ILE
2	B	7	ILE
2	B	14	THR
2	B	20	TYR
2	B	28	ARG
2	B	31	THR
2	B	42	GLN
2	B	48	VAL
2	B	55	PHE
2	B	63	LEU

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Mol	Chain	Res	Type
2	B	66	GLU
2	B	75	THR
2	B	81	ASP
2	B	94	THR
2	B	116	ASN
2	B	119	LEU
2	B	124	VAL
2	B	126	SER
2	B	128	GLN
2	B	135	THR
2	B	150	ARG
2	B	158	VAL
2	B	164	ARG
2	B	180	THR
2	B	182	GLU
2	B	187	THR
2	B	192	CYS
2	B	197	SER
3	C	22	ARG
3	C	25	ASN
3	C	41	LEU
3	C	48	ILE
3	C	59	ASP
3	C	65	GLN
3	C	75	PRO
3	C	81	ILE
3	C	96	GLN
3	C	115	THR
3	C	118	ARG
3	C	119	LEU
3	C	136	SER
3	C	158	MET
3	C	163	VAL
3	C	172	GLN
3	C	177	GLU
3	C	180	THR
3	C	183	THR
3	C	193	ASN
3	C	198	ILE
4	D	2	VAL
4	D	6	LEU
4	D	22	GLU

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Mol	Chain	Res	Type
4	D	24	THR
4	D	29	LEU
4	D	42	SER
4	D	47	HIS
4	D	69	ARG
4	D	88	THR
4	E	1	ASP
4	E	2	VAL
4	E	9	THR
4	E	10	ASN
4	E	14	THR
4	E	22	GLU
4	E	57	LYS
4	E	64	MET
4	E	85	LYS
4	E	87	LEU
4	E	92	LYS
4	E	106	LYS
5	F	2	LEU
5	F	22	LYS
5	F	25	GLU
5	F	28	LEU
5	F	35	ARG
5	F	75	GLU
5	F	79	TYR
5	F	93	PRO
1	G	2	ASP
1	G	7	VAL
1	G	9	ARG
1	G	21	ASN
1	G	33	LEU
1	G	37	THR
1	G	39	ARG
1	G	61	GLU
1	G	81	THR
1	G	85	ILE
1	G	95	ASN
1	G	118	ILE
1	G	128	SER
1	G	134	ARG
1	G	136	ILE
1	G	165	ARG

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Mol	Chain	Res	Type
1	G	170	GLN
1	G	177	PRO
1	G	190	THR
1	G	192	VAL
1	G	202	MET
1	G	221	GLU
1	G	226	VAL
2	H	5	ILE
2	H	7	ILE
2	H	14	THR
2	H	20	TYR
2	H	28	ARG
2	H	31	THR
2	H	48	VAL
2	H	63	LEU
2	H	66	GLU
2	H	75	THR
2	H	81	ASP
2	H	94	THR
2	H	113	SER
2	H	119	LEU
2	H	126	SER
2	H	128	GLN
2	H	129	PRO
2	H	135	THR
2	H	150	ARG
2	H	164	ARG
2	H	180	THR
2	H	182	GLU
2	H	187	THR
2	H	192	CYS
2	H	197	SER
3	I	22	ARG
3	I	25	ASN
3	I	41	LEU
3	I	48	ILE
3	I	59	ASP
3	I	65	GLN
3	I	75	PRO
3	I	81	ILE
3	I	96	GLN
3	I	112	LEU

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Mol	Chain	Res	Type
3	I	115	THR
3	I	118	ARG
3	I	119	LEU
3	I	136	SER
3	I	163	VAL
3	I	172	GLN
3	I	177	GLU
3	I	180	THR
3	I	183	THR
3	I	193	ASN
3	I	198	ILE
4	J	2	VAL
4	J	6	LEU
4	J	22	GLU
4	J	24	THR
4	J	29	LEU
4	J	42	SER
4	J	47	HIS
4	J	69	ARG
4	J	88	THR
4	K	2	VAL
4	K	9	THR
4	K	10	ASN
4	K	14	THR
4	K	22	GLU
4	K	57	LYS
4	K	64	MET
4	K	85	LYS
4	K	87	LEU
4	K	92	LYS
4	K	106	LYS
5	L	2	LEU
5	L	22	LYS
5	L	25	GLU
5	L	28	LEU
5	L	35	ARG
5	L	75	GLU
5	L	79	TYR
5	L	93	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	42	GLN
1	A	66	HIS
1	A	170	GLN
1	A	176	ASN
2	B	12	GLN
2	B	42	GLN
2	B	105	ASN
2	B	116	ASN
3	C	172	GLN
3	C	193	ASN
1	G	31	ASN
1	G	42	GLN
1	G	66	HIS
1	G	170	GLN
1	G	176	ASN
2	H	12	GLN
2	H	42	GLN
2	H	96	GLN
2	H	105	ASN
2	H	116	ASN
2	H	193	ASN
3	I	101	HIS
3	I	172	GLN
3	I	193	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	ATP	E	111	-	32,33,33	1.74	5 (15%)	48,52,52	2.53	6 (12%)
6	ATP	K	111	-	32,33,33	1.74	5 (15%)	48,52,52	2.50	6 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	E	111	-	-	4/22/38/38	0/3/3/3
6	ATP	K	111	-	-	4/22/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	111	ATP	C2'-C3'	7.03	1.72	1.53
6	K	111	ATP	C2'-C3'	6.92	1.72	1.53
6	E	111	ATP	C2'-C1'	-3.54	1.42	1.53
6	K	111	ATP	C2'-C1'	-3.41	1.42	1.53
6	K	111	ATP	PB-O3B	3.00	1.62	1.59
6	E	111	ATP	C5'-C4'	2.36	1.58	1.51
6	E	111	ATP	C3'-C4'	-2.31	1.47	1.53
6	K	111	ATP	C5'-C4'	2.25	1.58	1.51
6	E	111	ATP	PB-O3B	2.24	1.61	1.59
6	K	111	ATP	C3'-C4'	-2.09	1.47	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	111	ATP	C3'-C2'-C1'	-11.37	79.96	101.46
6	K	111	ATP	C3'-C2'-C1'	-11.29	80.11	101.46
6	E	111	ATP	C4'-O4'-C1'	-7.74	92.38	109.47
6	K	111	ATP	C4'-O4'-C1'	-7.59	92.72	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	111	ATP	C2'-C3'-C4'	-7.11	88.87	102.61
6	K	111	ATP	C2'-C3'-C4'	-6.85	89.37	102.61
6	E	111	ATP	O4'-C1'-C2'	5.09	117.52	106.62
6	K	111	ATP	O4'-C1'-C2'	5.01	117.35	106.62
6	K	111	ATP	O5'-C5'-C4'	2.60	117.83	108.99
6	E	111	ATP	O5'-C5'-C4'	2.55	117.67	108.99
6	E	111	ATP	C2'-C1'-N9	-2.20	107.83	113.30
6	K	111	ATP	C2'-C1'-N9	-2.04	108.22	113.30

There are no chirality outliers.

All (8) torsion outliers are listed below:

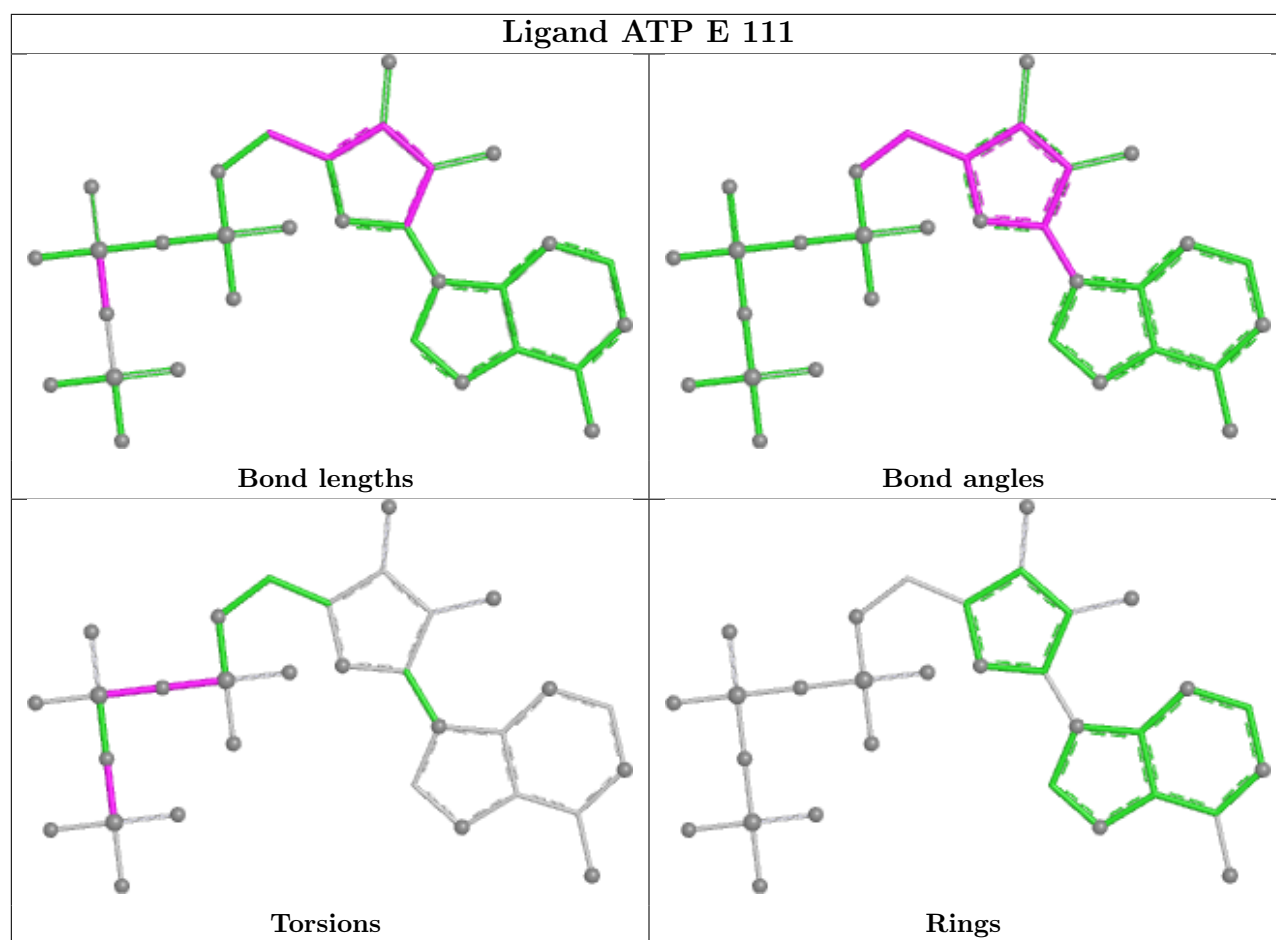
Mol	Chain	Res	Type	Atoms
6	E	111	ATP	PB-O3B-PG-O3G
6	K	111	ATP	PB-O3B-PG-O3G
6	K	111	ATP	PB-O3A-PA-O5'
6	K	111	ATP	PA-O3A-PB-O1B
6	E	111	ATP	PB-O3A-PA-O5'
6	E	111	ATP	PA-O3A-PB-O1B
6	E	111	ATP	PA-O3A-PB-O2B
6	K	111	ATP	PA-O3A-PB-O2B

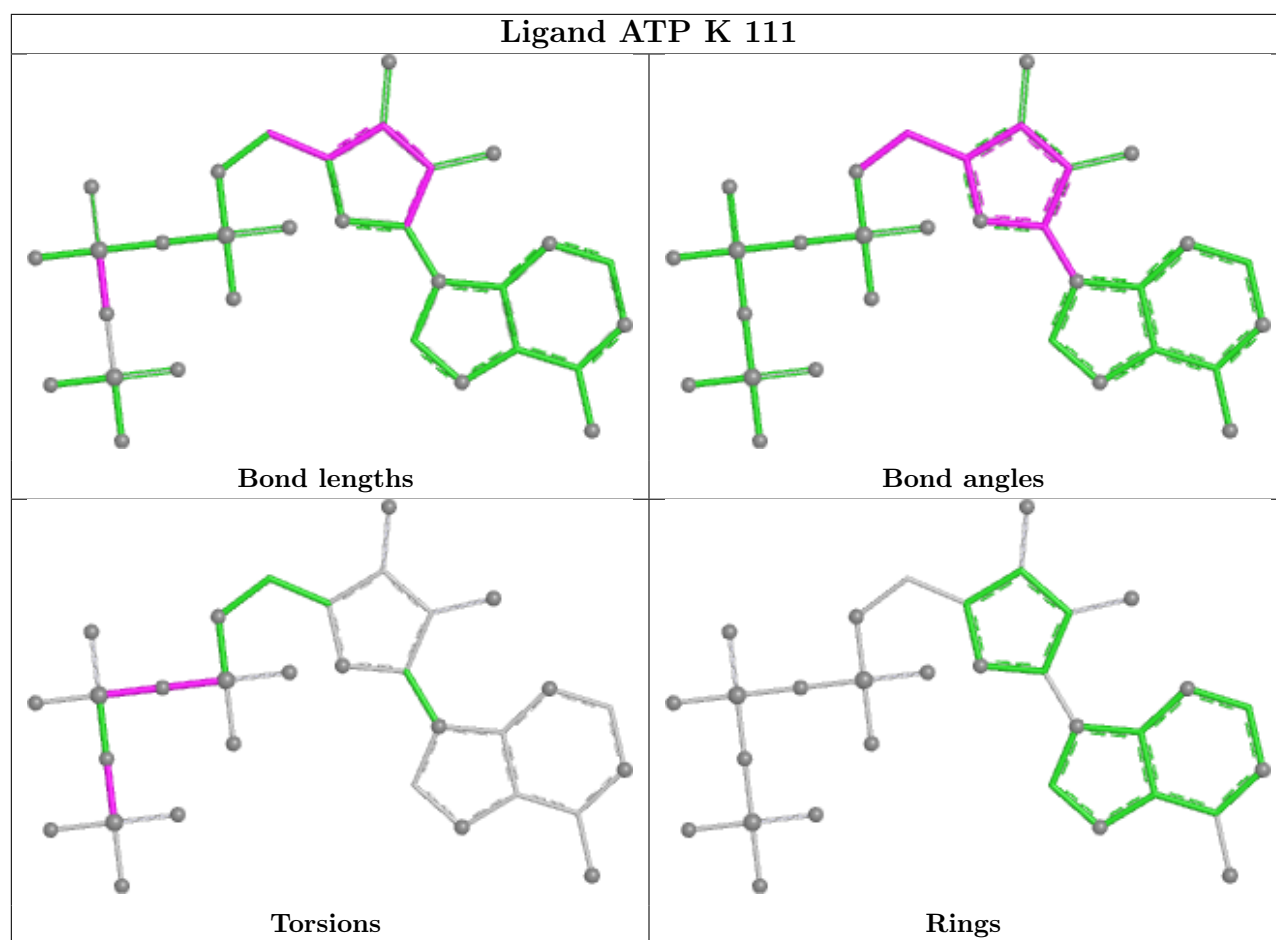
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	111	ATP	5	0
6	K	111	ATP	5	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	224/235 (95%)	-0.20	3 (1%) 75 73	3, 13, 24, 33	0
1	G	224/235 (95%)	0.46	11 (4%) 35 31	33, 47, 56, 65	0
2	B	197/199 (98%)	-0.42	2 (1%) 79 78	2, 13, 26, 37	0
2	H	197/199 (98%)	-0.28	1 (0%) 87 86	7, 19, 30, 36	0
3	C	196/199 (98%)	-0.24	6 (3%) 51 48	2, 13, 31, 38	0
3	I	196/199 (98%)	-0.08	4 (2%) 65 62	11, 23, 38, 46	0
4	D	110/110 (100%)	-0.50	0 100 100	2, 9, 26, 30	0
4	E	110/110 (100%)	-0.31	3 (2%) 56 53	2, 7, 24, 31	0
4	J	110/110 (100%)	-0.29	2 (1%) 67 65	4, 14, 30, 40	0
4	K	110/110 (100%)	-0.02	3 (2%) 56 53	12, 29, 43, 51	0
5	F	98/99 (98%)	-0.03	8 (8%) 17 15	2, 11, 39, 45	0
5	L	98/99 (98%)	0.62	9 (9%) 14 12	29, 41, 54, 63	0
All	All	1870/1904 (98%)	-0.11	52 (2%) 55 51	2, 18, 51, 65	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	208	SER	6.7
5	L	46	GLY	6.2
4	K	24	THR	4.7
5	F	46	GLY	4.5
5	L	77	SER	4.4
3	C	66	ALA	4.0
5	F	77	SER	3.9
4	E	24	THR	3.8
3	I	52	TRP	3.7
5	L	47	HIS	3.7
5	F	78	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
5	L	45	ALA	3.5
2	B	3	PRO	3.1
3	C	68	GLY	3.0
4	J	42	SER	3.0
5	F	47	HIS	3.0
5	F	79	TYR	3.0
3	I	68	GLY	3.0
3	C	15	GLN	2.9
1	A	95	ASN	2.9
1	G	206	ALA	2.9
2	B	4	GLY	2.8
5	L	3	PRO	2.8
5	F	45	ALA	2.8
1	A	96	ASN	2.7
3	C	128	GLN	2.7
3	I	128	GLN	2.7
4	E	2	VAL	2.6
1	G	22	GLY	2.6
5	F	3	PRO	2.6
1	G	170	GLN	2.5
5	L	43	SER	2.5
3	I	65	GLN	2.5
1	G	27	GLY	2.3
1	A	24	THR	2.3
5	L	29	THR	2.3
5	L	49	HIS	2.3
1	G	210	GLU	2.3
5	F	81	GLY	2.3
1	G	159	THR	2.3
1	G	137	PRO	2.2
4	K	107	GLN	2.2
4	E	23	VAL	2.2
4	J	22	GLU	2.2
1	G	47	ASN	2.2
5	L	5	HIS	2.2
3	C	63	LEU	2.1
2	H	16	HIS	2.1
1	G	203	ALA	2.0
4	K	25	PRO	2.0
1	G	179	THR	2.0
3	C	65	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

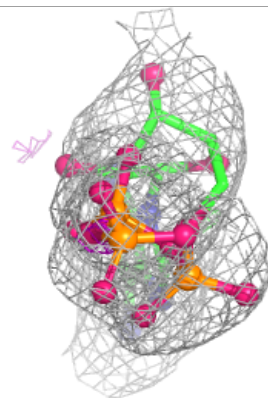
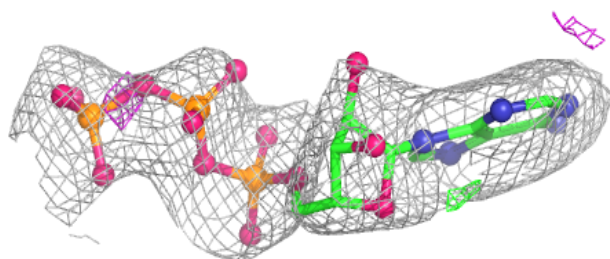
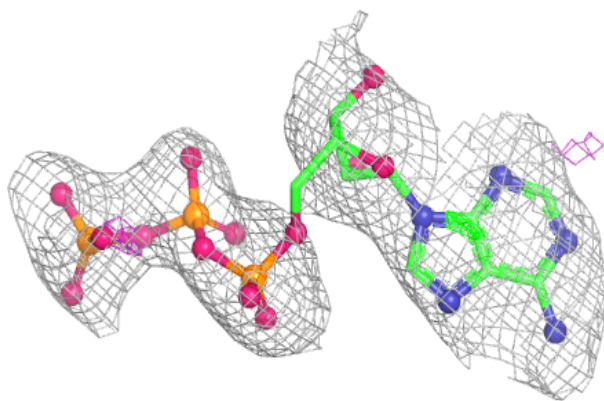
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ATP	K	111	31/31	0.95	0.07	20,24,32,33	0
6	ATP	E	111	31/31	0.96	0.08	11,15,24,25	0

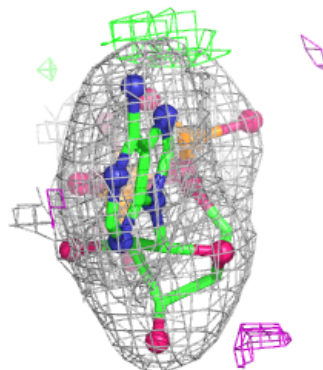
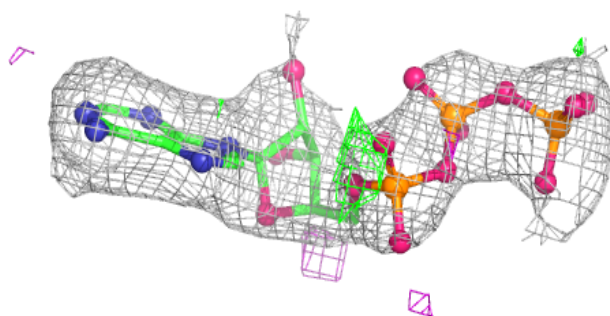
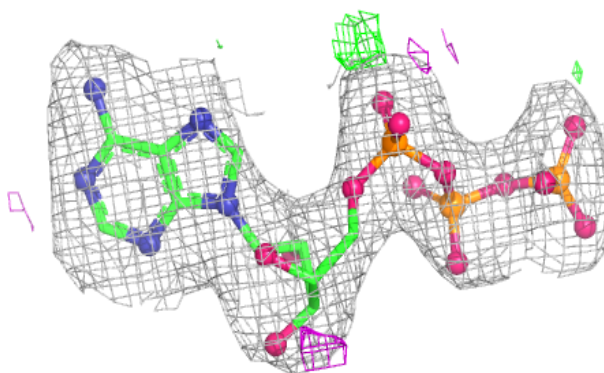
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP K 111:

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

**Electron density around ATP E 111:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.