



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:02 PM UTC

PDB ID : 1F9A / pdb_00001f9a
Title : CRYSTAL STRUCTURE ANALYSIS OF NMN ADENYLYLTRANSFERASE FROM METHANOCOCCUS JANNASCHII
Authors : D'Angelo, I.; Raffaelli, N.; Dabusti, V.; Lorenzi, T.; Magni, G.; Rizzi, M.
Deposited on : 2000-07-09
Resolution : 2.00 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

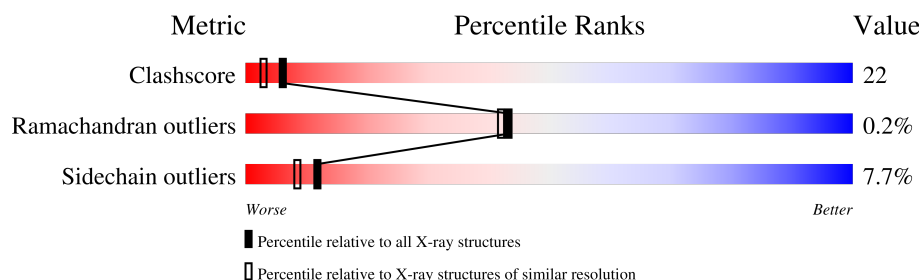
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	168	
1	B	168	
1	C	168	
1	D	168	
1	E	168	
1	F	168	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	E	704	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8923 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 HYPOTHETICAL PROTEIN MJ0541.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1341	869	231	238	3			
1	B	164	Total	C	N	O	S	0	0	0
			1341	869	231	238	3			
1	C	164	Total	C	N	O	S	0	0	0
			1338	866	231	238	3			
1	D	164	Total	C	N	O	S	0	0	0
			1348	875	231	239	3			
1	E	164	Total	C	N	O	S	0	0	0
			1348	875	231	239	3			
1	F	164	Total	C	N	O	S	0	0	0
			1351	876	231	241	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	LEU	MET	conflict	UNP Q57961
B	1	LEU	MET	conflict	UNP Q57961
C	1	LEU	MET	conflict	UNP Q57961
D	1	LEU	MET	conflict	UNP Q57961
E	1	LEU	MET	conflict	UNP Q57961
F	1	LEU	MET	conflict	UNP Q57961

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

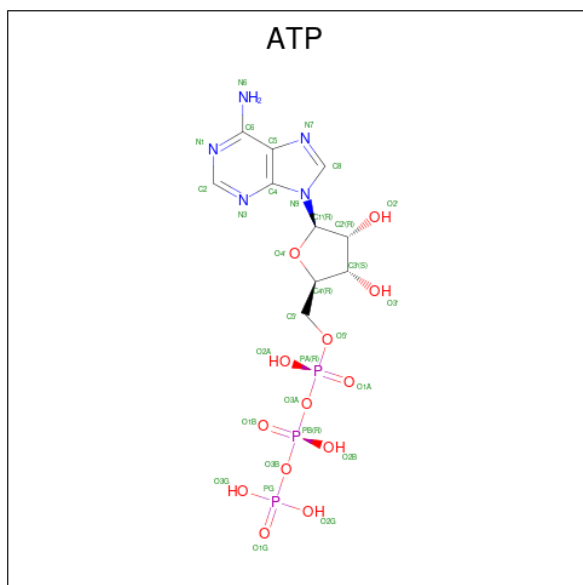
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is water.

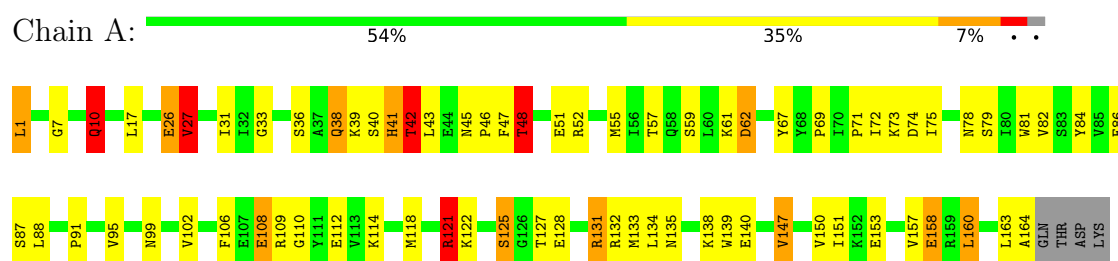
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total 105	O 105	0	0
4	B	100	Total 100	O 100	0	0
4	C	103	Total 103	O 103	0	0
4	D	93	Total 93	O 93	0	0
4	E	122	Total 122	O 122	0	0
4	F	141	Total 141	O 141	0	0

3 Residue-property plots

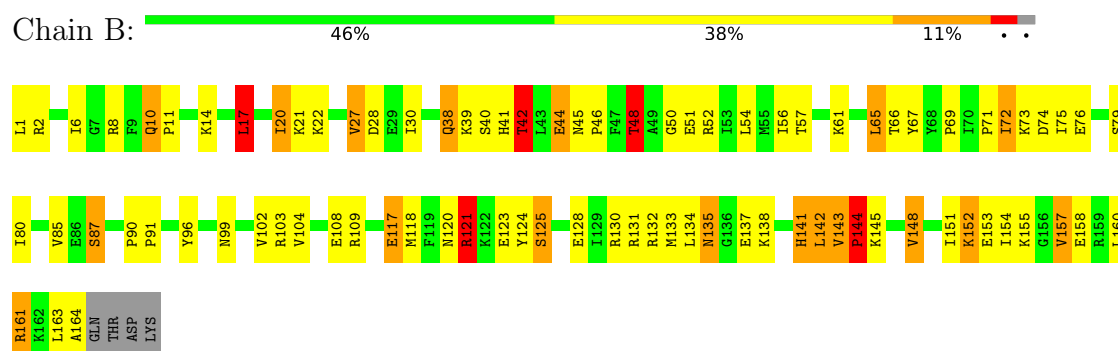
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

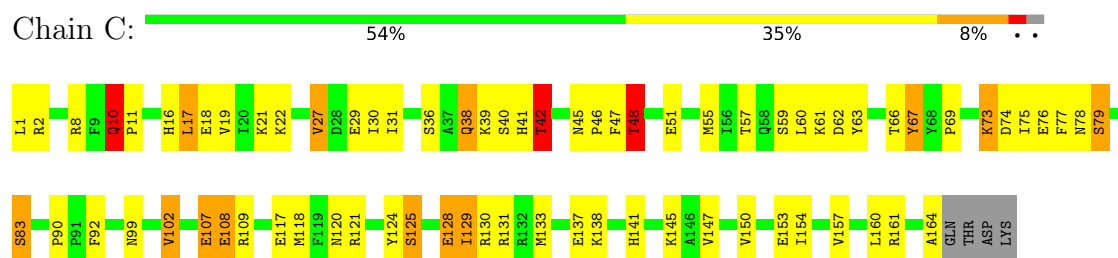
• Molecule 1: HYPOTHETICAL PROTEIN MJ0541



• Molecule 1: HYPOTHETICAL PROTEIN MJ0541

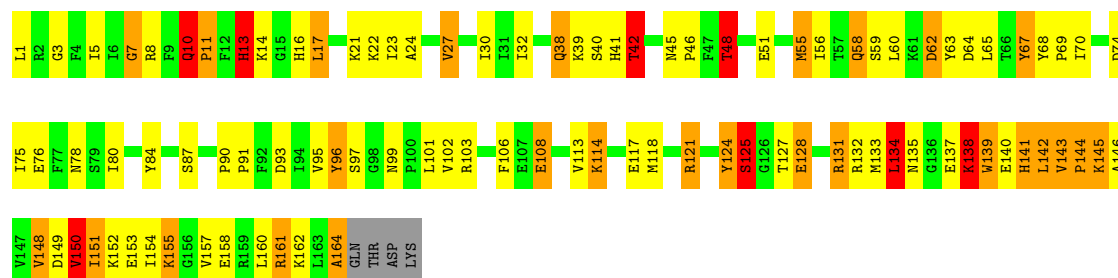


• Molecule 1: HYPOTHETICAL PROTEIN MJ0541



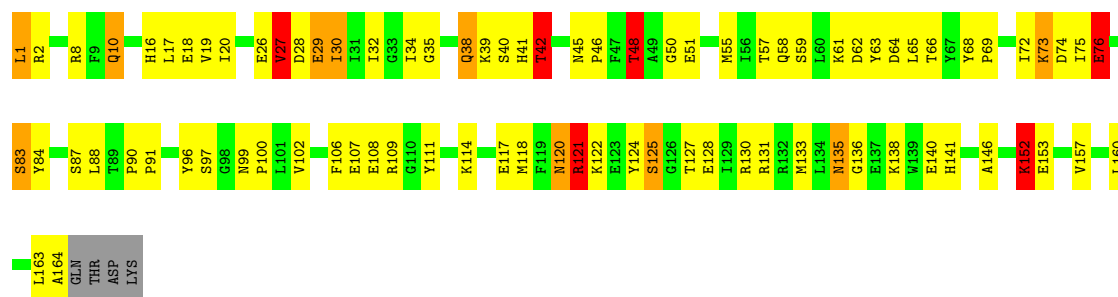
• Molecule 1: HYPOTHETICAL PROTEIN MJ0541





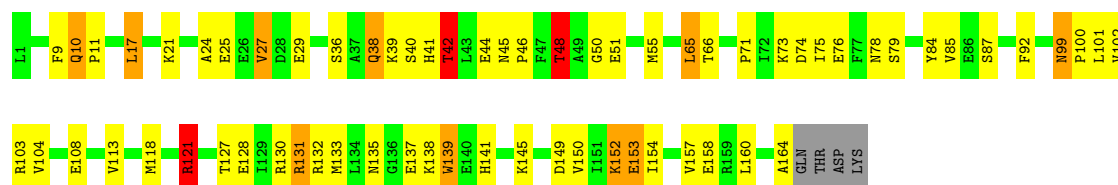
• Molecule 1: HYPOTHETICAL PROTEIN MJ0541

Chain E: 47% 41% 6% . .



• Molecule 1: HYPOTHETICAL PROTEIN MJ0541

Chain F: 58% 32% 6% . .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.77Å 112.64Å 79.87Å 90.00° 116.94° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	96.0 (20.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.215 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8923	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.99	1/1371 (0.1%)	2.14	60/1849 (3.2%)
1	B	0.94	0/1371	2.19	69/1849 (3.7%)
1	C	0.99	0/1368	2.01	45/1845 (2.4%)
1	D	1.00	1/1379 (0.1%)	2.22	77/1860 (4.1%)
1	E	1.02	2/1379 (0.1%)	2.07	54/1860 (2.9%)
1	F	1.07	2/1382 (0.1%)	1.94	35/1864 (1.9%)
All	All	1.00	6/8250 (0.1%)	2.10	340/11127 (3.1%)

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	5
1	B	1	4
1	C	1	3
1	D	0	14
1	E	1	9
1	F	1	2
All	All	4	37

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	70	ILE	N-CA	6.10	1.50	1.45
1	E	87	SER	CA-CB	5.63	1.62	1.53
1	E	72	ILE	C-O	5.62	1.30	1.24
1	F	85	VAL	N-CA	5.49	1.52	1.46
1	A	87	SER	CA-CB	5.42	1.61	1.53
1	F	36	SER	C-N	5.20	1.41	1.33

All (340) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ARG	NE-CZ-NH2	19.42	136.68	119.20
1	E	75	ILE	O-C-N	-12.38	109.97	122.97
1	F	75	ILE	O-C-N	-12.35	109.75	122.97
1	A	48	THR	N-CA-CB	-12.31	93.52	110.38
1	D	68	TYR	O-C-N	11.97	128.45	121.27
1	C	48	THR	N-CA-CB	-11.81	93.55	110.44
1	B	8	ARG	NE-CZ-NH1	-11.62	109.88	121.50
1	B	152	LYS	CA-C-O	-11.46	108.79	120.82
1	A	109	ARG	NH1-CZ-NH2	-10.70	105.39	119.30
1	D	48	THR	N-CA-CB	-10.53	95.95	110.38
1	F	75	ILE	N-CA-C	-9.90	93.54	108.99
1	F	149	ASP	CA-CB-CG	9.84	122.44	112.60
1	B	75	ILE	O-C-N	-9.82	112.99	122.12
1	F	48	THR	N-CA-CB	-9.82	96.90	110.25
1	E	48	THR	N-CA-CB	-9.73	96.34	110.26
1	E	8	ARG	NE-CZ-NH1	-9.69	111.81	121.50
1	C	130	ARG	CD-NE-CZ	9.48	137.67	124.40
1	D	150	VAL	O-C-N	-9.47	112.05	121.90
1	A	75	ILE	O-C-N	-9.45	113.11	123.03
1	D	141	HIS	CA-C-O	9.43	130.39	119.35
1	F	130	ARG	CD-NE-CZ	9.33	137.46	124.40
1	A	61	LYS	CA-C-N	9.28	133.07	120.54
1	A	61	LYS	C-N-CA	9.28	133.07	120.54
1	E	109	ARG	NE-CZ-NH2	9.23	127.51	119.20
1	F	48	THR	CA-CB-OG1	9.06	123.19	109.60
1	F	121	ARG	CD-NE-CZ	9.03	137.04	124.40
1	B	48	THR	N-CA-CB	-8.94	97.58	110.36
1	E	75	ILE	N-CA-C	-8.94	96.27	108.96
1	C	10	GLN	OE1-CD-NE2	-8.92	113.68	122.60
1	D	42	THR	N-CA-CB	-8.89	97.29	111.43
1	B	42	THR	N-CA-CB	-8.88	97.31	111.43
1	D	10	GLN	OE1-CD-NE2	-8.88	113.72	122.60
1	C	102	VAL	CA-C-O	8.87	130.18	120.95
1	F	152	LYS	N-CA-C	8.85	120.54	111.07
1	F	10	GLN	OE1-CD-NE2	-8.82	113.78	122.60
1	D	78	ASN	CA-C-N	8.81	133.24	120.38
1	D	78	ASN	C-N-CA	8.81	133.24	120.38
1	E	76	GLU	CA-C-O	-8.77	107.97	120.51
1	B	10	GLN	OE1-CD-NE2	-8.76	113.84	122.60
1	F	92	PHE	CA-CB-CG	8.76	122.56	113.80
1	B	154	ILE	CA-C-O	8.69	129.36	119.89
1	A	61	LYS	O-C-N	8.63	134.37	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ILE	N-CA-C	-8.63	95.56	108.85
1	E	10	GLN	OE1-CD-NE2	-8.55	114.05	122.60
1	D	128	GLU	CA-C-O	-8.55	111.36	120.42
1	A	61	LYS	N-CA-C	-8.39	102.49	112.89
1	E	121	ARG	CA-C-O	-8.36	109.37	119.49
1	B	2	ARG	NE-CZ-NH1	8.32	129.82	121.50
1	D	48	THR	OG1-CB-CG2	8.29	125.89	109.30
1	E	73	LYS	N-CA-CB	-8.25	98.57	110.36
1	D	69	PRO	N-CA-CB	8.24	107.54	102.92
1	C	42	THR	N-CA-CB	-8.23	97.23	111.55
1	F	99	ASN	CA-C-O	8.10	125.70	119.46
1	F	75	ILE	CA-C-N	-8.06	111.98	122.79
1	F	75	ILE	C-N-CA	-8.06	111.98	122.79
1	B	143	VAL	O-C-N	8.06	128.74	121.57
1	D	87	SER	CA-CB-OG	-8.03	95.03	111.10
1	E	48	THR	OG1-CB-CG2	8.03	125.35	109.30
1	D	78	ASN	OD1-CG-ND2	-7.97	114.63	122.60
1	D	69	PRO	CA-C-N	-7.95	115.94	122.85
1	D	69	PRO	C-N-CA	-7.95	115.94	122.85
1	A	48	THR	OG1-CB-CG2	7.93	125.17	109.30
1	A	10	GLN	OE1-CD-NE2	-7.80	114.80	122.60
1	E	152	LYS	CA-C-O	-7.78	112.83	121.00
1	E	42	THR	N-CA-CB	-7.78	98.02	111.55
1	D	124	TYR	N-CA-CB	-7.76	101.07	110.53
1	E	8	ARG	CD-NE-CZ	-7.76	113.54	124.40
1	F	42	THR	N-CA-CB	-7.73	99.14	111.43
1	E	107	GLU	N-CA-C	7.71	120.65	111.33
1	B	48	THR	OG1-CB-CG2	7.69	124.68	109.30
1	B	104	VAL	CA-C-O	-7.69	113.28	121.27
1	B	109	ARG	NE-CZ-NH2	-7.68	112.29	119.20
1	D	14	LYS	CA-C-O	7.65	128.23	119.27
1	A	10	GLN	CG-CD-NE2	7.63	127.84	116.40
1	B	48	THR	CA-CB-OG1	7.61	121.02	109.60
1	B	8	ARG	NH1-CZ-NH2	7.59	129.16	119.30
1	D	69	PRO	CB-CA-C	-7.55	105.53	111.87
1	D	142	LEU	N-CA-C	7.54	122.51	113.16
1	F	50	GLY	N-CA-C	-7.42	103.51	112.49
1	B	42	THR	OG1-CB-CG2	7.41	124.13	109.30
1	E	18	GLU	CA-C-O	-7.39	113.06	120.82
1	B	87	SER	CA-C-O	-7.34	112.77	120.55
1	D	146	ALA	CA-C-O	7.30	128.36	119.97
1	F	164	ALA	CA-C-O	-7.29	108.41	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	97	SER	CA-C-O	-7.28	112.88	120.89
1	B	75	ILE	CA-C-N	-7.25	113.20	123.20
1	B	75	ILE	C-N-CA	-7.25	113.20	123.20
1	B	65	LEU	N-CA-C	7.23	121.62	110.20
1	B	28	ASP	N-CA-C	7.22	120.19	111.82
1	C	48	THR	CA-CB-OG1	7.18	120.38	109.60
1	C	61	LYS	O-C-N	7.17	130.37	122.20
1	A	10	GLN	N-CA-CB	7.12	121.68	111.21
1	D	75	ILE	O-C-N	-7.12	113.82	122.36
1	C	75	ILE	O-C-N	-7.07	114.63	122.69
1	F	153	GLU	CB-CG-CD	7.06	124.60	112.60
1	A	91	PRO	O-C-N	-7.05	114.25	122.85
1	C	10	GLN	CG-CD-NE2	7.03	126.95	116.40
1	F	87	SER	CB-CA-C	-7.03	98.91	110.85
1	C	78	ASN	OD1-CG-ND2	7.02	129.62	122.60
1	E	27	VAL	CA-C-O	-6.98	113.88	121.28
1	B	66	THR	CA-CB-OG1	-6.97	99.14	109.60
1	D	16	HIS	N-CA-CB	6.97	120.11	110.01
1	D	137	GLU	CA-C-O	-6.96	114.22	121.87
1	B	8	ARG	N-CA-C	-6.92	104.98	113.50
1	C	154	ILE	O-C-N	6.92	128.32	122.09
1	C	48	THR	CA-CB-CG2	6.91	122.25	110.50
1	A	43	LEU	O-C-N	-6.89	114.81	122.12
1	B	10	GLN	CG-CD-NE2	6.89	126.73	116.40
1	D	138	LYS	CA-C-O	-6.88	113.60	121.72
1	D	148	VAL	CA-C-O	-6.88	114.25	121.41
1	E	96	TYR	CA-C-O	-6.88	113.38	120.54
1	E	87	SER	CA-CB-OG	-6.87	97.36	111.10
1	B	155	LYS	CA-C-N	6.85	127.55	119.94
1	B	155	LYS	C-N-CA	6.85	127.55	119.94
1	E	10	GLN	CG-CD-NE2	6.82	126.64	116.40
1	C	10	GLN	O-C-N	6.81	127.71	121.04
1	D	10	GLN	CG-CD-NE2	6.81	126.61	116.40
1	B	123	GLU	N-CA-C	-6.79	104.63	113.12
1	B	148	VAL	CA-C-O	-6.78	112.30	120.78
1	D	68	TYR	CA-C-O	-6.74	113.55	120.63
1	C	47	PHE	CA-CB-CG	-6.72	107.08	113.80
1	D	27	VAL	CA-C-N	6.72	129.83	120.29
1	D	27	VAL	C-N-CA	6.72	129.83	120.29
1	D	146	ALA	N-CA-C	-6.69	104.06	111.82
1	E	117	GLU	CA-C-O	-6.65	113.72	121.16
1	F	10	GLN	CG-CD-NE2	6.62	126.33	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	LEU	N-CA-C	6.62	118.49	111.28
1	F	139	TRP	N-CA-C	6.61	121.34	113.28
1	B	69	PRO	CA-C-N	-6.58	117.60	123.33
1	B	69	PRO	C-N-CA	-6.58	117.60	123.33
1	A	147	VAL	N-CA-C	6.58	117.33	110.62
1	D	155	LYS	O-C-N	-6.57	114.78	122.86
1	B	157	VAL	N-CA-C	6.57	117.32	110.62
1	E	28	ASP	CA-CB-CG	-6.55	106.05	112.60
1	D	131	ARG	CA-C-O	-6.54	112.45	119.97
1	A	132	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	E	107	GLU	O-C-N	-6.50	115.23	122.12
1	C	8	ARG	NE-CZ-NH1	-6.48	115.02	121.50
1	D	146	ALA	O-C-N	-6.48	114.31	122.27
1	A	78	ASN	CA-C-O	6.44	127.38	120.10
1	E	135	ASN	CB-CG-ND2	6.44	126.06	116.40
1	A	52	ARG	NE-CZ-NH2	-6.43	113.41	119.20
1	F	42	THR	OG1-CB-CG2	6.40	122.09	109.30
1	B	152	LYS	N-CA-C	6.38	117.90	111.07
1	D	141	HIS	N-CA-C	-6.37	105.14	113.17
1	A	72	ILE	N-CA-CB	-6.32	102.69	111.41
1	B	44	GLU	CB-CA-C	6.31	120.29	109.24
1	D	75	ILE	CA-C-N	-6.30	114.35	122.79
1	D	75	ILE	C-N-CA	-6.30	114.35	122.79
1	E	75	ILE	CA-C-N	-6.30	109.51	121.54
1	E	75	ILE	C-N-CA	-6.30	109.51	121.54
1	B	153	GLU	CA-CB-CG	6.27	126.64	114.10
1	D	87	SER	CA-C-O	-6.26	113.92	120.55
1	A	75	ILE	CA-C-N	-6.25	113.63	123.12
1	A	75	ILE	C-N-CA	-6.25	113.63	123.12
1	F	99	ASN	O-C-N	-6.24	116.01	121.31
1	D	161	ARG	NE-CZ-NH2	-6.21	113.61	119.20
1	E	135	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	D	150	VAL	CA-C-O	6.20	127.93	121.05
1	B	72	ILE	N-CA-CB	-6.18	103.67	111.46
1	D	128	GLU	O-C-N	6.16	129.17	122.15
1	B	79	SER	CA-C-N	-6.15	113.53	122.69
1	B	79	SER	C-N-CA	-6.15	113.53	122.69
1	F	104	VAL	CA-C-O	-6.10	114.60	120.95
1	F	101	LEU	CA-C-O	-6.06	114.46	120.82
1	B	96	TYR	CA-C-O	-6.05	113.80	120.70
1	A	79	SER	CA-CB-OG	-6.04	99.01	111.10
1	A	131	ARG	NE-CZ-NH1	-6.04	115.46	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	VAL	CA-C-O	-5.98	112.81	120.95
1	A	135	ASN	CB-CA-C	5.96	120.01	109.65
1	D	69	PRO	O-C-N	5.94	126.95	122.73
1	B	161	ARG	CA-C-O	-5.93	113.16	119.97
1	C	108	GLU	N-CA-C	-5.93	105.54	112.89
1	B	121	ARG	CD-NE-CZ	5.91	132.68	124.40
1	E	127	THR	CA-CB-CG2	5.90	120.53	110.50
1	F	84	TYR	CA-C-N	-5.90	113.13	120.56
1	F	84	TYR	C-N-CA	-5.90	113.13	120.56
1	D	58	GLN	N-CA-C	-5.89	104.98	111.82
1	D	153	GLU	CA-CB-CG	5.89	125.88	114.10
1	C	31	ILE	CA-C-N	-5.89	115.22	122.93
1	C	31	ILE	C-N-CA	-5.89	115.22	122.93
1	C	153	GLU	CB-CG-CD	5.86	122.57	112.60
1	B	48	THR	N-CA-C	5.83	118.22	110.53
1	D	87	SER	CB-CA-C	-5.82	101.12	110.79
1	A	62	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	72	ILE	CA-C-O	5.80	126.48	120.39
1	E	87	SER	CB-CA-C	-5.80	99.53	110.67
1	E	8	ARG	NH1-CZ-NH2	5.80	126.84	119.30
1	E	97	SER	O-C-N	5.77	129.94	123.48
1	A	62	ASP	N-CA-CB	-5.76	101.35	109.94
1	A	72	ILE	CA-C-N	5.76	129.66	121.42
1	A	72	ILE	C-N-CA	5.76	129.66	121.42
1	E	61	LYS	CA-C-O	-5.76	113.59	120.10
1	D	93	ASP	CB-CG-OD2	5.76	131.65	118.40
1	B	87	SER	CA-CB-OG	-5.74	99.62	111.10
1	B	17	LEU	N-CA-C	5.73	118.01	111.02
1	C	57	THR	CA-C-O	-5.73	114.80	120.70
1	A	71	PRO	CB-CA-C	-5.72	105.32	111.56
1	F	27	VAL	CA-CB-CG1	5.72	120.12	110.40
1	F	153	GLU	CA-CB-CG	5.71	125.53	114.10
1	A	164	ALA	CA-C-O	-5.70	111.11	120.80
1	B	71	PRO	N-CA-CB	5.67	107.83	103.30
1	E	83	SER	CA-CB-OG	-5.66	99.77	111.10
1	E	42	THR	CA-C-O	-5.66	114.82	121.44
1	D	108	GLU	N-CA-C	-5.65	105.64	112.54
1	E	153	GLU	CB-CG-CD	5.62	122.16	112.60
1	E	130	ARG	CA-C-O	5.62	126.43	119.97
1	D	58	GLN	CG-CD-OE1	-5.60	109.60	120.80
1	F	79	SER	CA-CB-OG	-5.60	99.91	111.10
1	A	36	SER	CA-CB-OG	-5.59	99.91	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	ALA	CA-C-O	-5.59	111.30	120.80
1	E	27	VAL	N-CA-CB	-5.58	101.48	111.92
1	E	138	LYS	CA-C-O	-5.58	114.69	121.05
1	C	73	LYS	CA-C-O	-5.57	115.41	121.87
1	E	48	THR	CA-CB-OG1	5.56	117.94	109.60
1	D	58	GLN	CG-CD-NE2	5.54	124.71	116.40
1	C	83	SER	O-C-N	-5.53	116.38	122.07
1	D	59	SER	CA-CB-OG	-5.52	100.06	111.10
1	E	120	ASN	CA-C-O	-5.52	115.44	121.84
1	C	67	TYR	CA-CB-CG	-5.51	103.97	113.90
1	B	151	ILE	CA-C-N	5.51	127.60	120.44
1	B	151	ILE	C-N-CA	5.51	127.60	120.44
1	A	86	GLU	CA-C-N	5.50	128.11	120.29
1	A	86	GLU	C-N-CA	5.50	128.11	120.29
1	C	153	GLU	CG-CD-OE1	5.50	131.06	118.40
1	E	29	GLU	CB-CG-CD	5.49	121.93	112.60
1	B	152	LYS	N-CA-CB	-5.48	102.06	110.01
1	E	57	THR	O-C-N	-5.48	116.31	122.12
1	A	150	VAL	N-CA-C	5.48	116.11	110.36
1	E	76	GLU	CB-CA-C	5.48	121.32	110.42
1	D	139	TRP	CA-C-O	-5.47	112.68	120.51
1	E	140	GLU	CG-CD-OE2	5.47	130.99	118.40
1	D	24	ALA	N-CA-CB	-5.47	101.31	110.39
1	A	87	SER	CA-CB-OG	-5.46	100.17	111.10
1	A	108	GLU	N-CA-C	-5.46	106.12	112.89
1	C	42	THR	OG1-CB-CG2	5.45	120.20	109.30
1	D	13	HIS	CA-C-O	-5.45	113.97	121.98
1	D	42	THR	CA-CB-CG2	5.45	119.76	110.50
1	C	36	SER	CA-CB-OG	-5.44	100.22	111.10
1	B	145	LYS	CA-C-O	-5.41	114.68	120.42
1	B	27	VAL	CA-C-N	5.41	128.53	120.31
1	B	27	VAL	C-N-CA	5.41	128.53	120.31
1	F	152	LYS	CA-C-O	-5.40	115.14	120.82
1	E	32	ILE	N-CA-CB	-5.39	106.08	111.90
1	E	153	GLU	CA-CB-CG	5.39	124.88	114.10
1	D	127	THR	N-CA-C	5.38	117.15	111.28
1	C	128	GLU	N-CA-C	-5.36	105.10	111.69
1	D	8	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	B	151	ILE	N-CA-C	5.34	116.07	110.62
1	C	102	VAL	O-C-N	-5.34	116.69	121.87
1	E	32	ILE	N-CA-C	5.34	114.95	107.37
1	A	69	PRO	N-CD-CG	-5.33	95.20	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	164	ALA	CA-C-O	-5.33	111.75	120.80
1	D	154	ILE	N-CA-C	-5.32	107.56	112.83
1	A	158	GLU	N-CA-C	5.32	117.49	111.11
1	D	69	PRO	CA-C-O	-5.31	115.38	121.11
1	B	148	VAL	CA-CB-CG1	5.31	119.42	110.40
1	C	161	ARG	N-CA-C	5.30	117.06	111.28
1	B	137	GLU	CA-C-O	-5.30	115.40	121.82
1	E	121	ARG	N-CA-C	5.29	118.83	112.38
1	C	129	ILE	N-CA-C	5.28	116.01	110.62
1	A	135	ASN	CA-CB-CG	-5.28	107.32	112.60
1	C	30	ILE	O-C-N	5.28	128.47	123.03
1	A	163	LEU	CA-C-O	5.26	125.84	119.31
1	B	66	THR	CA-C-O	-5.26	114.54	120.43
1	F	42	THR	CA-C-O	-5.26	115.48	121.58
1	D	67	TYR	CA-C-N	-5.25	116.49	122.26
1	D	67	TYR	C-N-CA	-5.25	116.49	122.26
1	C	92	PHE	CA-CB-CG	5.24	119.04	113.80
1	D	140	GLU	CA-CB-CG	-5.23	103.64	114.10
1	D	27	VAL	O-C-N	-5.22	117.25	123.00
1	B	142	LEU	N-CA-C	5.22	119.71	113.23
1	E	42	THR	OG1-CB-CG2	5.22	119.74	109.30
1	A	127	THR	CA-C-O	5.20	126.06	120.55
1	C	137	GLU	N-CA-C	5.20	117.39	110.53
1	A	27	VAL	CA-C-N	5.19	127.66	120.29
1	A	27	VAL	C-N-CA	5.19	127.66	120.29
1	B	79	SER	CA-C-O	-5.19	113.21	119.49
1	C	107	GLU	N-CA-CB	5.19	118.32	110.28
1	B	54	LEU	O-C-N	-5.18	116.73	122.07
1	C	27	VAL	CA-C-O	-5.18	116.27	121.45
1	E	59	SER	N-CA-C	5.18	117.01	111.36
1	E	152	LYS	O-C-N	5.18	127.41	122.03
1	D	106	PHE	CA-CB-CG	5.17	118.97	113.80
1	D	143	VAL	O-C-N	5.17	125.34	121.72
1	D	146	ALA	CB-CA-C	5.17	120.60	110.67
1	A	78	ASN	O-C-N	-5.16	116.18	122.22
1	A	82	VAL	O-C-N	-5.16	116.85	121.91
1	B	161	ARG	NH1-CZ-NH2	5.16	126.01	119.30
1	B	117	GLU	CA-C-O	-5.15	114.82	120.69
1	C	108	GLU	CA-C-O	5.15	125.70	119.31
1	D	142	LEU	CA-C-O	-5.15	113.05	119.28
1	A	27	VAL	CA-CB-CG1	5.15	119.16	110.40
1	E	140	GLU	OE1-CD-OE2	-5.15	110.54	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	ARG	N-CA-CB	-5.14	103.01	110.47
1	B	30	ILE	CA-C-N	-5.13	115.95	122.37
1	B	30	ILE	C-N-CA	-5.13	115.95	122.37
1	A	139	TRP	N-CA-C	-5.13	106.95	114.39
1	A	42	THR	OG1-CB-CG2	5.13	119.56	109.30
1	D	80	ILE	N-CA-CB	-5.13	105.69	112.36
1	C	107	GLU	CA-C-O	-5.13	114.07	119.97
1	D	114	LYS	CA-C-O	-5.13	114.76	120.66
1	B	20	ILE	N-CA-C	5.13	115.90	110.72
1	D	125	SER	CA-C-O	-5.12	114.24	120.54
1	A	153	GLU	CB-CG-CD	5.12	121.31	112.60
1	D	143	VAL	CA-C-O	-5.12	114.83	121.13
1	C	109	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	D	96	TYR	CA-C-O	-5.12	114.88	120.36
1	D	3	GLY	CA-C-N	-5.11	115.78	122.99
1	D	3	GLY	C-N-CA	-5.11	115.78	122.99
1	E	106	PHE	N-CA-C	5.11	116.54	111.07
1	A	121	ARG	CD-NE-CZ	5.11	131.55	124.40
1	A	10	GLN	CA-C-O	5.10	127.71	120.83
1	D	27	VAL	CA-CB-CG2	5.09	119.06	110.40
1	C	2	ARG	CA-C-O	5.09	126.19	120.70
1	B	141	HIS	CA-CB-CG	-5.07	108.73	113.80
1	D	141	HIS	O-C-N	-5.07	116.00	122.34
1	C	63	TYR	N-CA-C	5.07	117.39	110.55
1	B	132	ARG	CA-C-O	-5.07	115.05	120.42
1	F	127	THR	CA-CB-OG1	-5.07	102.00	109.60
1	A	41	HIS	O-C-N	-5.06	115.77	122.40
1	A	33	GLY	CA-C-O	5.06	124.50	120.30
1	C	75	ILE	CA-C-N	-5.06	115.03	122.06
1	C	75	ILE	C-N-CA	-5.06	115.03	122.06
1	B	144	PRO	CA-C-O	-5.06	115.63	121.95
1	D	80	ILE	N-CA-C	-5.05	108.20	113.10
1	F	154	ILE	CA-C-O	5.04	125.59	119.54
1	B	130	ARG	CA-C-O	5.04	125.89	120.55
1	C	147	VAL	CA-C-O	5.04	127.03	121.18
1	E	164	ALA	CA-C-O	-5.04	112.23	120.80
1	A	10	GLN	O-C-N	-5.04	116.83	121.37
1	A	106	PHE	CA-C-O	-5.04	115.53	120.82
1	F	87	SER	N-CA-C	-5.04	105.87	111.36
1	B	138	LYS	CA-C-O	-5.03	115.69	121.47
1	F	78	ASN	CA-C-O	5.03	125.75	119.97
1	C	79	SER	CA-CB-OG	-5.02	101.06	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	16	HIS	CA-CB-CG	-5.02	108.78	113.80
1	B	161	ARG	NE-CZ-NH2	-5.02	114.68	119.20
1	A	57	THR	N-CA-C	5.01	116.74	111.28
1	A	59	SER	CA-C-O	-5.01	115.24	120.55

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	48	THR	CB
1	C	48	THR	CB
1	E	48	THR	CB
1	F	48	THR	CB

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	GLY	Mainchain
1	A	125	SER	Mainchain
1	A	7	GLY	Mainchain
1	A	81	TRP	Mainchain
1	A	95	VAL	Mainchain
1	B	103	ARG	Mainchain
1	B	135	ASN	Mainchain
1	B	80	ILE	Mainchain
1	B	87	SER	Mainchain
1	C	107	GLU	Mainchain
1	C	77	PHE	Mainchain
1	C	83	SER	Mainchain
1	D	11	PRO	Mainchain
1	D	125	SER	Mainchain
1	D	13	HIS	Mainchain
1	D	134	LEU	Mainchain
1	D	144	PRO	Mainchain
1	D	145	LYS	Mainchain
1	D	150	VAL	Mainchain
1	D	151	ILE	Mainchain
1	D	155	LYS	Mainchain
1	D	32	ILE	Mainchain
1	D	55	MET	Mainchain
1	D	56	ILE	Mainchain
1	D	7	GLY	Mainchain
1	D	84	TYR	Mainchain

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Mol	Chain	Res	Type	Group
1	E	111	TYR	Mainchain
1	E	163	LEU	Mainchain
1	E	2	ARG	Mainchain
1	E	26	GLU	Mainchain
1	E	34	ILE	Mainchain
1	E	50	GLY	Mainchain
1	E	69	PRO	Mainchain
1	E	76	GLU	Mainchain
1	E	90	PRO	Mainchain
1	F	153	GLU	Mainchain
1	F	71	PRO	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1341	0	1375	53	0
1	B	1341	0	1375	67	0
1	C	1338	0	1366	60	0
1	D	1348	0	1382	77	0
1	E	1348	0	1382	60	0
1	F	1351	0	1384	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	31	0	11	1	0
3	B	31	0	12	0	0
3	C	31	0	12	1	0
3	D	31	0	12	6	0
3	E	31	0	11	0	0
3	F	31	0	12	0	0
4	A	105	0	0	16	0
4	B	100	0	0	16	0
4	C	103	0	0	9	0
4	D	93	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	122	0	0	17	0
4	F	141	0	0	19	0
All	All	8923	0	8334	373	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 22.

All (373) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:MET:HE3	1:E:121:ARG:HD2	1.16	1.16
1:A:55:MET:SD	4:A:791:HOH:O	2.07	1.13
1:A:118:MET:HE3	1:A:121:ARG:HD2	1.19	1.11
1:C:118:MET:HE3	1:C:121:ARG:HD2	1.27	1.11
1:B:134:LEU:HD21	1:B:161:ARG:HA	1.18	1.10
1:D:42:THR:HG21	4:D:728:HOH:O	1.52	1.10
1:A:131:ARG:HG2	1:A:131:ARG:HH11	1.12	1.07
1:D:42:THR:HG22	1:D:45:ASN:H	1.13	1.07
1:F:118:MET:HE3	1:F:121:ARG:HD2	1.37	1.05
1:E:121:ARG:HH21	1:E:125:SER:HB2	1.19	1.04
1:D:121:ARG:HH21	1:D:125:SER:HB2	1.21	1.04
1:B:118:MET:HE3	1:B:121:ARG:HD2	1.05	1.04
1:B:118:MET:CE	1:B:121:ARG:HD2	1.87	1.02
1:A:48:THR:HG21	4:F:814:HOH:O	1.59	1.02
1:B:134:LEU:HD22	4:B:785:HOH:O	1.58	1.01
1:A:42:THR:HG22	1:A:45:ASN:H	1.24	1.00
1:B:118:MET:HE3	1:B:121:ARG:CD	1.91	1.00
1:E:118:MET:CE	1:E:121:ARG:HD2	1.91	1.00
1:A:42:THR:HG21	4:A:733:HOH:O	1.62	0.99
1:C:42:THR:HG21	4:C:714:HOH:O	1.60	0.99
1:C:42:THR:HG22	1:C:45:ASN:H	1.23	0.99
1:C:38:GLN:H	1:C:38:GLN:HE21	1.06	0.97
1:B:61:LYS:HE3	4:B:783:HOH:O	1.63	0.97
1:D:158:GLU:HG3	4:D:743:HOH:O	1.62	0.96
1:B:163:LEU:HD11	4:B:767:HOH:O	1.66	0.95
1:D:118:MET:HE3	1:D:121:ARG:HD2	1.48	0.94
1:B:42:THR:HG22	1:B:45:ASN:H	1.29	0.94
1:E:133:MET:HE3	1:E:157:VAL:HG22	1.50	0.94
1:C:131:ARG:HH11	1:C:131:ARG:HG2	1.31	0.94
1:B:133:MET:HE2	1:B:160:LEU:HD23	1.50	0.94
1:F:42:THR:HG22	1:F:45:ASN:H	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:MET:HE3	1:A:157:VAL:HG22	1.47	0.92
1:D:38:GLN:H	1:D:38:GLN:HE21	1.01	0.92
1:A:121:ARG:HH21	1:A:125:SER:HB2	1.33	0.91
1:F:131:ARG:HG2	1:F:131:ARG:HH11	1.34	0.91
1:C:118:MET:CE	1:C:121:ARG:HD2	2.01	0.90
1:F:42:THR:HG21	4:F:817:HOH:O	1.69	0.90
1:B:38:GLN:H	1:B:38:GLN:HE21	1.20	0.90
1:E:152:LYS:HD2	4:E:842:HOH:O	1.69	0.90
1:F:38:GLN:H	1:F:38:GLN:HE21	1.20	0.90
1:B:133:MET:HE3	1:B:157:VAL:HG22	1.53	0.89
1:E:42:THR:HG22	1:E:45:ASN:H	1.37	0.89
1:E:131:ARG:HH11	1:E:131:ARG:HG2	1.38	0.89
1:E:118:MET:HE3	1:E:121:ARG:CD	2.01	0.88
1:A:73:LYS:HE3	4:A:780:HOH:O	1.73	0.87
1:C:73:LYS:HE3	4:C:778:HOH:O	1.73	0.87
1:A:131:ARG:HG2	1:A:131:ARG:NH1	1.89	0.87
1:C:38:GLN:HE22	1:C:74:ASP:H	1.19	0.86
1:A:131:ARG:HH11	1:A:131:ARG:CG	1.88	0.85
1:E:38:GLN:H	1:E:38:GLN:HE21	1.19	0.85
3:D:703:ATP:H5'1	4:D:786:HOH:O	1.76	0.84
1:B:131:ARG:HG2	1:B:131:ARG:HH11	1.43	0.83
1:E:39:LYS:HE3	1:E:74:ASP:OD2	1.78	0.83
1:A:38:GLN:HE22	1:A:74:ASP:H	1.26	0.83
1:D:48:THR:HG22	1:D:51:GLU:H	1.40	0.83
1:B:134:LEU:HD23	1:B:161:ARG:HG2	1.61	0.83
1:C:48:THR:HG21	4:E:811:HOH:O	1.79	0.82
1:C:118:MET:HE3	1:C:121:ARG:CD	2.08	0.82
4:C:723:HOH:O	1:E:48:THR:HG21	1.79	0.82
1:E:38:GLN:HE22	1:E:74:ASP:H	1.25	0.82
1:C:39:LYS:NZ	1:C:74:ASP:OD2	2.12	0.81
1:B:42:THR:HG21	4:B:711:HOH:O	1.80	0.81
1:E:63:TYR:O	1:E:64:ASP:CB	2.26	0.81
1:D:42:THR:HG22	1:D:45:ASN:N	1.95	0.81
1:B:48:THR:HG21	4:D:726:HOH:O	1.79	0.81
1:B:134:LEU:CD2	1:B:161:ARG:HA	2.08	0.81
1:D:103:ARG:HG3	1:D:113:VAL:HG11	1.63	0.81
1:D:38:GLN:HE22	1:D:74:ASP:H	1.26	0.81
1:D:7:GLY:HA2	4:D:786:HOH:O	1.81	0.80
1:B:121:ARG:HH21	1:B:125:SER:HB2	1.46	0.80
1:E:128:GLU:OE1	1:E:131:ARG:NH2	2.15	0.80
1:C:42:THR:HG22	1:C:45:ASN:N	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:THR:HG22	1:B:51:GLU:H	1.48	0.79
1:E:42:THR:HG21	4:E:826:HOH:O	1.83	0.79
1:F:135:ASN:ND2	1:F:137:GLU:OE2	2.16	0.79
4:A:710:HOH:O	1:F:48:THR:HG21	1.81	0.79
1:A:38:GLN:H	1:A:38:GLN:HE21	1.27	0.78
1:F:42:THR:CG2	1:F:45:ASN:H	1.96	0.78
1:B:158:GLU:HG3	4:B:725:HOH:O	1.84	0.78
1:C:40:SER:OG	1:C:41:HIS:HD2	1.67	0.78
1:A:147:VAL:HG12	1:A:151:ILE:HD12	1.65	0.78
3:D:703:ATP:C5'	4:D:786:HOH:O	2.30	0.78
1:F:158:GLU:HG3	4:F:895:HOH:O	1.84	0.77
1:F:131:ARG:NH1	4:F:939:HOH:O	2.18	0.77
1:A:41:HIS:HE1	1:C:108:GLU:OE1	1.68	0.77
1:D:17:LEU:HD22	1:D:21:LYS:HE3	1.67	0.77
1:F:131:ARG:HG2	1:F:131:ARG:NH1	1.99	0.76
1:C:76:GLU:HB2	4:C:750:HOH:O	1.85	0.76
1:F:25:GLU:CD	4:F:937:HOH:O	2.28	0.76
1:B:133:MET:CE	1:B:160:LEU:HD23	2.15	0.76
1:C:133:MET:HE3	1:C:157:VAL:HG22	1.67	0.75
1:B:38:GLN:HE22	1:B:74:ASP:H	1.33	0.75
4:B:733:HOH:O	1:D:48:THR:HG21	1.87	0.75
1:D:38:GLN:HE21	1:D:38:GLN:N	1.82	0.75
1:F:42:THR:HG22	1:F:45:ASN:N	2.02	0.75
1:F:133:MET:HE3	1:F:157:VAL:HG22	1.69	0.74
1:D:128:GLU:OE1	1:D:131:ARG:NH2	2.20	0.74
1:D:22:LYS:HE2	1:D:117:GLU:OE2	1.87	0.74
1:C:42:THR:CG2	1:C:45:ASN:H	1.99	0.74
1:C:131:ARG:HG2	1:C:131:ARG:NH1	2.03	0.74
1:F:40:SER:OG	1:F:41:HIS:HD2	1.70	0.74
1:D:121:ARG:HG2	3:D:703:ATP:N6	2.03	0.73
1:C:128:GLU:OE1	1:C:131:ARG:NH2	2.22	0.73
1:F:158:GLU:CD	4:F:926:HOH:O	2.32	0.72
1:A:128:GLU:OE1	1:A:131:ARG:NH2	2.24	0.71
1:E:99:ASN:HD22	1:E:102:VAL:H	1.36	0.71
1:B:128:GLU:OE1	1:B:131:ARG:NH2	2.24	0.71
1:B:48:THR:CG2	1:B:51:GLU:H	2.04	0.70
1:E:1:LEU:N	4:E:880:HOH:O	2.24	0.70
4:A:720:HOH:O	1:C:79:SER:HB2	1.91	0.69
1:C:133:MET:HE2	1:C:160:LEU:HD23	1.73	0.69
1:A:48:THR:HG22	1:A:51:GLU:H	1.57	0.69
1:A:138:LYS:HE3	4:A:782:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:GLU:HB2	4:B:788:HOH:O	1.92	0.68
1:E:41:HIS:HE1	1:F:108:GLU:OE1	1.75	0.68
1:F:145:LYS:HG2	4:F:858:HOH:O	1.93	0.68
1:D:40:SER:OG	1:D:41:HIS:HD2	1.75	0.67
1:E:42:THR:HG22	1:E:45:ASN:N	2.09	0.67
1:F:38:GLN:HE22	1:F:74:ASP:H	1.40	0.67
1:E:48:THR:HG22	1:E:51:GLU:H	1.59	0.67
1:A:118:MET:CE	1:A:121:ARG:HD2	2.12	0.67
1:A:26:GLU:HG2	4:A:774:HOH:O	1.94	0.66
1:A:99:ASN:HD22	1:A:102:VAL:H	1.44	0.66
1:E:76:GLU:HB2	4:E:848:HOH:O	1.94	0.66
1:A:48:THR:CG2	1:A:51:GLU:H	2.07	0.66
1:E:30:ILE:HG13	1:E:65:LEU:HD11	1.77	0.66
1:F:132:ARG:HD3	4:F:876:HOH:O	1.95	0.66
1:A:1:LEU:HB2	4:A:755:HOH:O	1.96	0.65
1:A:1:LEU:HB3	1:A:27:VAL:HG22	1.79	0.65
1:E:42:THR:CG2	1:E:45:ASN:H	2.08	0.65
1:C:99:ASN:HD22	1:C:102:VAL:H	1.42	0.65
1:A:39:LYS:HE3	1:A:74:ASP:OD2	1.97	0.65
1:C:51:GLU:O	1:C:55:MET:HG3	1.97	0.65
1:D:21:LYS:HE2	1:D:63:TYR:CE2	2.32	0.65
1:B:131:ARG:HG2	1:B:131:ARG:NH1	2.12	0.65
1:A:133:MET:HE2	1:A:160:LEU:HD23	1.79	0.64
1:D:76:GLU:HB2	4:D:771:HOH:O	1.97	0.64
1:D:121:ARG:NH2	1:D:125:SER:HB2	2.04	0.64
1:F:133:MET:HE2	1:F:160:LEU:HD23	1.80	0.64
1:E:122:LYS:NZ	4:E:850:HOH:O	2.17	0.63
1:A:42:THR:HG22	1:A:45:ASN:N	2.06	0.63
1:B:42:THR:HG22	1:B:45:ASN:N	2.09	0.63
1:C:59:SER:O	1:C:62:ASP:OD2	2.17	0.63
1:B:108:GLU:OE1	1:C:41:HIS:HE1	1.81	0.63
1:E:131:ARG:HG2	1:E:131:ARG:NH1	2.01	0.63
1:D:162:LYS:HE2	4:E:876:HOH:O	1.97	0.63
1:F:139:TRP:HA	4:F:876:HOH:O	1.97	0.63
1:E:38:GLN:HE21	1:E:38:GLN:N	1.96	0.62
1:E:20:ILE:HG23	1:E:30:ILE:HD12	1.81	0.62
1:A:131:ARG:NH2	4:A:740:HOH:O	2.33	0.61
1:D:42:THR:CG2	1:D:45:ASN:H	2.01	0.61
1:E:91:PRO:HD3	4:E:855:HOH:O	2.00	0.61
1:A:62:ASP:HA	4:A:750:HOH:O	2.00	0.61
1:F:46:PRO:HB3	1:F:160:LEU:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:GLU:HG2	1:C:66:THR:HB	1.82	0.61
1:F:128:GLU:OE1	1:F:131:ARG:NH2	2.34	0.61
1:F:138:LYS:HG2	4:F:897:HOH:O	2.00	0.61
1:A:140:GLU:HG3	4:A:731:HOH:O	2.00	0.60
1:A:121:ARG:NH2	3:A:700:ATP:O2B	2.34	0.60
1:B:133:MET:CE	1:B:160:LEU:CD2	2.80	0.60
1:D:62:ASP:CG	1:D:62:ASP:O	2.45	0.60
1:F:76:GLU:HB2	4:F:836:HOH:O	2.01	0.60
1:C:48:THR:HG22	1:C:51:GLU:CG	2.32	0.60
1:F:99:ASN:HD22	1:F:102:VAL:H	1.50	0.59
1:C:40:SER:OG	1:C:41:HIS:CD2	2.53	0.58
1:B:57:THR:HG23	1:B:67:TYR:OH	2.03	0.58
1:A:38:GLN:HE22	1:A:74:ASP:N	1.99	0.58
1:D:108:GLU:OE1	1:F:41:HIS:HE1	1.85	0.58
1:D:51:GLU:O	1:D:55:MET:HG3	2.03	0.58
1:D:7:GLY:CA	4:D:786:HOH:O	2.47	0.58
1:D:124:TYR:O	3:D:703:ATP:N6	2.37	0.58
1:D:64:ASP:C	4:D:762:HOH:O	2.47	0.58
1:D:99:ASN:HD22	1:D:102:VAL:H	1.50	0.58
1:A:133:MET:HE3	1:A:157:VAL:CG2	2.28	0.57
1:C:48:THR:HG22	1:C:51:GLU:H	1.68	0.57
1:D:103:ARG:HD2	4:D:753:HOH:O	2.04	0.57
1:C:48:THR:HG22	1:C:51:GLU:HG3	1.86	0.57
1:D:133:MET:HE2	1:D:160:LEU:HD23	1.85	0.57
1:D:150:VAL:O	1:D:152:LYS:N	2.37	0.57
1:D:99:ASN:ND2	1:D:101:LEU:H	2.03	0.57
1:E:48:THR:CG2	1:E:51:GLU:H	2.17	0.57
1:B:39:LYS:HE3	1:B:74:ASP:OD2	2.05	0.57
1:F:51:GLU:O	1:F:55:MET:HG3	2.04	0.56
1:B:120:ASN:HB3	1:B:124:TYR:CD1	2.40	0.56
1:B:17:LEU:HD22	1:B:21:LYS:HE3	1.88	0.56
1:C:90:PRO:HA	4:E:871:HOH:O	2.04	0.56
1:E:121:ARG:NH2	1:E:125:SER:HB2	2.04	0.56
1:F:29:GLU:HG2	1:F:66:THR:HB	1.87	0.56
1:E:38:GLN:H	1:E:38:GLN:NE2	1.97	0.56
1:A:131:ARG:NH1	1:A:131:ARG:CG	2.54	0.55
1:B:134:LEU:CD2	4:B:785:HOH:O	2.35	0.55
1:C:38:GLN:H	1:C:38:GLN:NE2	1.90	0.55
1:D:148:VAL:O	1:D:149:ASP:C	2.49	0.55
1:B:133:MET:HE2	1:B:160:LEU:CD2	2.32	0.55
1:C:121:ARG:HG2	3:C:702:ATP:N6	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:LYS:HD2	1:E:73:LYS:HZ3	1.70	0.55
1:D:144:PRO:O	1:D:145:LYS:C	2.50	0.55
1:B:41:HIS:HB3	4:B:767:HOH:O	2.06	0.55
1:E:131:ARG:HG3	1:E:135:ASN:HD22	1.71	0.55
1:A:122:LYS:HD3	4:A:748:HOH:O	2.06	0.54
1:D:118:MET:HA	3:D:703:ATP:C2	2.42	0.54
1:D:39:LYS:HE3	1:D:74:ASP:OD2	2.07	0.54
1:B:44:GLU:HG3	4:B:787:HOH:O	2.08	0.54
1:C:131:ARG:NH1	4:C:779:HOH:O	2.38	0.54
1:E:133:MET:HE2	1:E:160:LEU:HD23	1.90	0.54
1:D:41:HIS:HE1	1:E:108:GLU:OE1	1.91	0.54
1:A:131:ARG:NE	4:A:811:HOH:O	2.22	0.53
1:A:42:THR:CG2	1:A:45:ASN:H	2.09	0.53
1:E:29:GLU:HG2	1:E:66:THR:HB	1.90	0.53
1:F:25:GLU:OE1	4:F:937:HOH:O	2.18	0.53
1:B:40:SER:OG	1:B:41:HIS:HD2	1.91	0.53
1:F:17:LEU:HD22	1:F:21:LYS:HE3	1.90	0.53
1:D:48:THR:CG2	1:D:51:GLU:H	2.15	0.53
1:B:73:LYS:HE3	4:B:793:HOH:O	2.08	0.53
1:B:42:THR:HG23	1:B:44:GLU:H	1.73	0.53
1:F:132:ARG:CD	4:F:876:HOH:O	2.53	0.52
1:B:134:LEU:CD2	1:B:161:ARG:HG2	2.37	0.52
1:A:48:THR:HG22	1:A:51:GLU:CB	2.39	0.52
1:C:69:PRO:HG2	4:C:804:HOH:O	2.10	0.52
1:E:120:ASN:HB3	1:E:124:TYR:CD1	2.45	0.52
1:B:152:LYS:HD3	4:B:776:HOH:O	2.09	0.52
1:E:46:PRO:HB3	1:E:160:LEU:HD13	1.91	0.52
1:D:63:TYR:HB3	1:D:65:LEU:HG	1.91	0.51
1:F:38:GLN:H	1:F:38:GLN:NE2	1.99	0.51
1:B:38:GLN:HE22	1:B:74:ASP:N	2.04	0.51
1:F:103:ARG:HD3	4:F:846:HOH:O	2.10	0.51
1:B:152:LYS:HB3	4:B:776:HOH:O	2.10	0.51
1:C:17:LEU:HD22	1:C:21:LYS:HE3	1.92	0.51
1:C:18:GLU:HG2	4:C:781:HOH:O	2.10	0.51
1:E:133:MET:HE3	1:E:157:VAL:CG2	2.33	0.51
1:B:42:THR:CG2	1:B:45:ASN:H	2.13	0.51
1:F:103:ARG:NH1	4:F:846:HOH:O	2.43	0.51
1:A:48:THR:HG22	1:A:51:GLU:HB2	1.93	0.50
1:B:118:MET:HE3	1:B:121:ARG:CG	2.39	0.50
1:E:114:LYS:NZ	4:E:892:HOH:O	2.39	0.50
1:D:17:LEU:CD2	1:D:21:LYS:HE3	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:LYS:CE	1:B:74:ASP:OD2	2.59	0.50
1:D:21:LYS:HE2	1:D:63:TYR:CZ	2.46	0.50
1:D:128:GLU:O	1:D:132:ARG:HG3	2.12	0.50
1:E:141:HIS:HE1	4:E:803:HOH:O	1.95	0.50
1:F:39:LYS:HE3	1:F:74:ASP:OD2	2.11	0.50
4:B:746:HOH:O	1:D:58:GLN:NE2	2.45	0.50
1:C:17:LEU:CD2	1:C:21:LYS:HE3	2.43	0.49
1:D:157:VAL:O	1:D:161:ARG:HG3	2.12	0.49
1:F:42:THR:HG22	1:F:45:ASN:HB2	1.95	0.49
1:B:46:PRO:HB3	1:B:160:LEU:HD13	1.93	0.49
1:F:48:THR:CG2	1:F:51:GLU:H	2.26	0.49
1:D:60:LEU:HB3	1:D:65:LEU:HD12	1.95	0.49
1:C:118:MET:HE2	4:C:798:HOH:O	2.12	0.49
1:B:17:LEU:CD2	1:B:21:LYS:HE3	2.42	0.49
1:C:48:THR:CG2	1:C:51:GLU:H	2.26	0.49
1:B:65:LEU:N	1:B:65:LEU:HD23	2.27	0.48
1:E:38:GLN:HE22	1:E:74:ASP:N	2.01	0.48
1:D:97:SER:HB2	4:D:768:HOH:O	2.12	0.48
1:B:22:LYS:HE2	1:B:117:GLU:OE2	2.13	0.48
1:D:118:MET:CE	1:D:121:ARG:HD2	2.33	0.48
1:D:38:GLN:H	1:D:38:GLN:NE2	1.86	0.48
1:D:135:ASN:OD1	1:D:135:ASN:O	2.31	0.48
1:A:46:PRO:HB3	1:A:160:LEU:HD13	1.95	0.48
1:B:14:LYS:NZ	1:B:141:HIS:O	2.35	0.48
1:B:143:VAL:HG23	1:B:144:PRO:O	2.13	0.48
1:F:24:ALA:CB	1:F:65:LEU:HD21	2.44	0.48
1:F:48:THR:HG22	1:F:51:GLU:H	1.78	0.47
1:B:41:HIS:CB	4:B:767:HOH:O	2.62	0.47
1:D:13:HIS:HA	1:D:143:VAL:HG12	1.95	0.47
1:D:138:LYS:HG3	1:D:139:TRP:N	2.28	0.47
1:A:48:THR:HG22	1:A:51:GLU:CG	2.44	0.47
1:A:138:LYS:CE	4:A:782:HOH:O	2.56	0.47
1:C:138:LYS:NZ	1:C:141:HIS:CG	2.83	0.47
1:C:60:LEU:C	1:C:62:ASP:N	2.71	0.47
1:E:62:ASP:HB2	4:E:883:HOH:O	2.14	0.47
1:E:131:ARG:HD2	4:E:885:HOH:O	2.14	0.47
1:F:135:ASN:ND2	4:F:939:HOH:O	2.47	0.47
1:C:121:ARG:HH21	1:C:125:SER:HB2	1.80	0.46
1:A:40:SER:OG	1:A:41:HIS:HD2	1.98	0.46
1:B:135:ASN:C	1:B:135:ASN:OD1	2.58	0.46
1:F:48:THR:HG22	1:F:51:GLU:CG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:ILE:HG22	1:D:30:ILE:HD11	1.96	0.46
1:A:84:TYR:CZ	1:A:88:LEU:HD11	2.50	0.46
1:B:133:MET:HE3	1:B:157:VAL:CG2	2.35	0.46
1:B:141:HIS:CE1	1:B:142:LEU:HD21	2.51	0.46
1:B:72:ILE:HD13	1:B:85:VAL:HG22	1.99	0.45
1:C:46:PRO:HB3	1:C:160:LEU:HD13	1.98	0.45
1:F:131:ARG:HH11	1:F:131:ARG:CG	2.14	0.45
1:E:51:GLU:O	1:E:55:MET:HG3	2.16	0.45
1:F:38:GLN:HE21	1:F:38:GLN:N	2.01	0.45
1:C:120:ASN:HB3	1:C:124:TYR:CD1	2.51	0.45
1:B:99:ASN:HD22	1:B:102:VAL:H	1.64	0.45
1:D:10:GLN:HG2	1:D:46:PRO:CD	2.46	0.45
1:E:40:SER:OG	1:E:41:HIS:HD2	1.99	0.45
1:D:40:SER:OG	1:D:41:HIS:CD2	2.64	0.45
1:D:158:GLU:N	4:D:743:HOH:O	2.39	0.45
1:A:108:GLU:OE1	1:B:41:HIS:HE1	2.00	0.44
1:A:38:GLN:H	1:A:38:GLN:NE2	2.07	0.44
1:E:131:ARG:NH1	4:E:828:HOH:O	2.25	0.44
1:D:10:GLN:HG2	1:D:46:PRO:HG2	2.00	0.44
1:A:147:VAL:CG1	1:A:151:ILE:HD12	2.42	0.44
1:D:96:TYR:HA	1:D:114:LYS:O	2.18	0.44
1:E:131:ARG:NH1	1:E:131:ARG:CG	2.73	0.44
1:D:150:VAL:O	1:D:151:ILE:C	2.61	0.44
1:A:41:HIS:CE1	1:C:108:GLU:OE1	2.59	0.44
1:C:10:GLN:HA	1:C:11:PRO:HA	1.77	0.44
1:D:95:VAL:HB	1:D:113:VAL:HG22	2.00	0.44
1:F:141:HIS:H	1:F:141:HIS:CD2	2.36	0.44
1:B:1:LEU:HD12	1:B:1:LEU:HA	1.80	0.43
1:E:58:GLN:HB3	1:E:146:ALA:HB1	2.00	0.43
1:F:158:GLU:CG	4:F:895:HOH:O	2.54	0.43
1:F:99:ASN:HA	1:F:100:PRO:HD3	1.87	0.43
1:A:147:VAL:HG12	1:A:151:ILE:CD1	2.42	0.43
1:D:30:ILE:O	1:D:67:TYR:HA	2.18	0.43
1:D:90:PRO:HA	1:D:91:PRO:HD3	1.83	0.43
1:D:138:LYS:HG3	1:D:139:TRP:H	1.83	0.43
1:D:23:ILE:HG22	1:D:30:ILE:CD1	2.48	0.43
1:E:122:LYS:CE	4:E:850:HOH:O	2.65	0.43
1:E:133:MET:HE2	1:E:160:LEU:CD2	2.49	0.43
1:E:68:TYR:CD1	1:E:68:TYR:N	2.87	0.43
1:F:55:MET:HG2	1:F:150:VAL:HG11	2.00	0.43
1:D:131:ARG:HG2	1:D:131:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:MET:HE3	1:C:157:VAL:HA	2.01	0.43
1:D:125:SER:O	1:D:125:SER:OG	2.36	0.43
1:C:129:ILE:HG21	1:C:129:ILE:HD13	1.81	0.42
1:C:138:LYS:HZ1	1:C:141:HIS:HB3	1.82	0.42
1:E:84:TYR:CZ	1:E:88:LEU:HD11	2.54	0.42
1:F:48:THR:HG22	1:F:51:GLU:HG3	2.01	0.42
1:E:16:HIS:O	1:E:19:VAL:HG12	2.19	0.42
1:E:42:THR:HG22	1:E:45:ASN:HB2	2.01	0.42
1:E:1:LEU:HB3	1:E:27:VAL:HG22	2.01	0.42
1:F:145:LYS:HE2	4:F:858:HOH:O	2.20	0.42
3:D:703:ATP:O2G	4:D:745:HOH:O	2.21	0.42
1:B:134:LEU:HD13	1:B:164:ALA:HB2	2.00	0.42
1:F:103:ARG:HG3	1:F:113:VAL:HG11	2.01	0.42
1:F:42:THR:HG22	1:F:45:ASN:CA	2.51	0.41
1:D:103:ARG:HG3	1:D:113:VAL:CG1	2.44	0.41
1:A:67:TYR:HE2	4:A:714:HOH:O	2.03	0.41
1:C:11:PRO:HA	1:C:55:MET:HE1	2.02	0.41
1:C:22:LYS:HE2	1:C:117:GLU:OE2	2.20	0.41
1:D:132:ARG:HD3	1:D:138:LYS:O	2.20	0.41
1:F:42:THR:CG2	1:F:45:ASN:N	2.73	0.41
1:B:52:ARG:O	1:B:56:ILE:HG13	2.21	0.41
1:D:133:MET:HE3	1:D:157:VAL:HG22	2.02	0.41
1:D:134:LEU:HD11	1:D:164:ALA:HB2	2.02	0.41
1:E:131:ARG:NH2	4:E:849:HOH:O	2.51	0.41
1:B:90:PRO:HA	1:B:91:PRO:HD3	1.94	0.41
1:F:42:THR:CG2	1:F:45:ASN:HB2	2.51	0.41
1:E:141:HIS:CD2	1:E:141:HIS:H	2.39	0.41
1:F:133:MET:CE	1:F:157:VAL:HA	2.51	0.41
1:D:60:LEU:HD22	1:D:65:LEU:CD1	2.51	0.41
1:E:38:GLN:NE2	1:E:74:ASP:H	2.04	0.41
1:E:136:GLY:HA2	4:E:831:HOH:O	2.20	0.41
1:F:40:SER:OG	1:F:41:HIS:CD2	2.61	0.41
1:F:73:LYS:HE3	4:F:863:HOH:O	2.20	0.41
1:B:41:HIS:HA	4:B:767:HOH:O	2.21	0.41
1:C:16:HIS:HA	1:C:19:VAL:HG12	2.02	0.41
1:D:99:ASN:HD21	1:D:101:LEU:HB3	1.86	0.41
1:F:9:PHE:O	1:F:11:PRO:HA	2.21	0.41
1:F:42:THR:HG23	1:F:44:GLU:H	1.86	0.41
1:C:55:MET:HG2	1:C:150:VAL:HG11	2.03	0.40
1:C:131:ARG:NH1	1:C:131:ARG:CG	2.71	0.40
1:C:131:ARG:NH1	4:C:790:HOH:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:MET:CE	1:C:157:VAL:HA	2.51	0.40
1:D:5:ILE:HG21	1:D:5:ILE:HD13	1.74	0.40
1:D:23:ILE:CG2	1:D:30:ILE:CD1	2.99	0.40
1:F:10:GLN:OE1	1:F:45:ASN:OD1	2.39	0.40
1:A:158:GLU:HG3	4:A:743:HOH:O	2.21	0.40
1:C:67:TYR:CD2	1:C:67:TYR:N	2.87	0.40
1:B:48:THR:HG23	1:B:50:GLY:N	2.36	0.40
1:C:138:LYS:HZ1	1:C:141:HIS:CG	2.39	0.40
1:D:38:GLN:HE22	1:D:74:ASP:N	2.05	0.40
1:A:10:GLN:HG2	1:A:47:PHE:H	1.86	0.40
1:A:112:GLU:OE2	1:A:114:LYS:HE3	2.21	0.40
1:B:40:SER:OG	1:B:41:HIS:CD2	2.72	0.40
1:B:134:LEU:HD23	1:B:134:LEU:HA	1.89	0.40
1:D:141:HIS:CE1	1:D:142:LEU:HD21	2.56	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	162/168 (96%)	157 (97%)	5 (3%)	0	100	100
1	B	162/168 (96%)	154 (95%)	7 (4%)	1 (1%)	21	17
1	C	162/168 (96%)	155 (96%)	7 (4%)	0	100	100
1	D	162/168 (96%)	152 (94%)	10 (6%)	0	100	100
1	E	162/168 (96%)	153 (94%)	8 (5%)	1 (1%)	21	17
1	F	162/168 (96%)	155 (96%)	7 (4%)	0	100	100
All	All	972/1008 (96%)	926 (95%)	44 (4%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	35	GLY
1	B	148	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	146/152 (96%)	134 (92%)	12 (8%)	10	7
1	B	146/152 (96%)	134 (92%)	12 (8%)	10	7
1	C	145/152 (95%)	136 (94%)	9 (6%)	16	13
1	D	147/152 (97%)	134 (91%)	13 (9%)	9	6
1	E	147/152 (97%)	134 (91%)	13 (9%)	9	6
1	F	148/152 (97%)	139 (94%)	9 (6%)	17	14
All	All	879/912 (96%)	811 (92%)	68 (8%)	12	8

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	10	GLN
1	A	17	LEU
1	A	26	GLU
1	A	27	VAL
1	A	31	ILE
1	A	38	GLN
1	A	42	THR
1	A	48	THR
1	A	121	ARG
1	A	134	LEU
1	A	160	LEU
1	B	6	ILE
1	B	10	GLN
1	B	11	PRO
1	B	17	LEU
1	B	20	ILE

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Mol	Chain	Res	Type
1	B	27	VAL
1	B	38	GLN
1	B	42	THR
1	B	48	THR
1	B	121	ARG
1	B	125	SER
1	B	144	PRO
1	C	1	LEU
1	C	10	GLN
1	C	17	LEU
1	C	27	VAL
1	C	38	GLN
1	C	42	THR
1	C	48	THR
1	C	125	SER
1	C	145	LYS
1	D	1	LEU
1	D	10	GLN
1	D	11	PRO
1	D	17	LEU
1	D	27	VAL
1	D	38	GLN
1	D	42	THR
1	D	48	THR
1	D	62	ASP
1	D	121	ARG
1	D	125	SER
1	D	134	LEU
1	D	138	LYS
1	E	1	LEU
1	E	10	GLN
1	E	17	LEU
1	E	27	VAL
1	E	30	ILE
1	E	38	GLN
1	E	42	THR
1	E	48	THR
1	E	83	SER
1	E	100	PRO
1	E	121	ARG
1	E	125	SER
1	E	152	LYS

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Mol	Chain	Res	Type
1	F	17	LEU
1	F	27	VAL
1	F	38	GLN
1	F	42	THR
1	F	48	THR
1	F	65	LEU
1	F	121	ARG
1	F	131	ARG
1	F	152	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	41	HIS
1	A	99	ASN
1	A	141	HIS
1	B	38	GLN
1	B	41	HIS
1	B	99	ASN
1	B	141	HIS
1	C	38	GLN
1	C	41	HIS
1	C	99	ASN
1	C	141	HIS
1	D	38	GLN
1	D	41	HIS
1	D	78	ASN
1	D	99	ASN
1	D	141	HIS
1	E	38	GLN
1	E	41	HIS
1	E	78	ASN
1	E	99	ASN
1	E	135	ASN
1	E	141	HIS
1	F	38	GLN
1	F	41	HIS
1	F	99	ASN
1	F	141	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ATP	F	705	2	32,33,33	1.52	4 (12%)	48,52,52	1.48	7 (14%)
3	ATP	B	701	-	32,33,33	1.36	4 (12%)	48,52,52	1.45	6 (12%)
3	ATP	D	703	2	32,33,33	1.31	2 (6%)	48,52,52	1.84	9 (18%)
3	ATP	E	704	2	32,33,33	1.55	5 (15%)	48,52,52	2.56	18 (37%)
3	ATP	A	700	2	32,33,33	1.45	5 (15%)	48,52,52	1.81	11 (22%)
3	ATP	C	702	2	32,33,33	1.38	3 (9%)	48,52,52	1.36	7 (14%)

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
3	ATP	F	705	2	-	2/22/38/38	0/3/3/3
3	ATP	B	701	-	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	D	703	2	-	3/22/38/38	0/3/3/3
3	ATP	E	704	2	1/1/7/7	5/22/38/38	0/3/3/3
3	ATP	A	700	2	-	2/22/38/38	0/3/3/3
3	ATP	C	702	2	-	0/22/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	704	ATP	C5-N7	-4.43	1.31	1.39
3	C	702	ATP	C5-N7	-4.17	1.31	1.39
3	D	703	ATP	C5-N7	-4.08	1.31	1.39
3	A	700	ATP	C5-N7	-3.77	1.32	1.39
3	F	705	ATP	C5-N7	-3.73	1.32	1.39
3	B	701	ATP	C5-N7	-3.62	1.32	1.39
3	F	705	ATP	PG-O2G	-3.39	1.42	1.54
3	E	704	ATP	C2-N1	3.37	1.39	1.33
3	B	701	ATP	PB-O3A	-3.29	1.55	1.59
3	F	705	ATP	C2-N1	3.15	1.39	1.33
3	C	702	ATP	C2-N1	2.95	1.39	1.33
3	A	700	ATP	C2'-C3'	2.83	1.61	1.53
3	B	701	ATP	PG-O2G	-2.63	1.45	1.54
3	E	704	ATP	PG-O2G	-2.39	1.45	1.54
3	E	704	ATP	O2'-C2'	2.39	1.48	1.43
3	A	700	ATP	PG-O2G	-2.31	1.46	1.54
3	C	702	ATP	PG-O2G	-2.29	1.46	1.54
3	F	705	ATP	PB-O1B	-2.24	1.43	1.50
3	A	700	ATP	PA-O2A	-2.17	1.45	1.55
3	D	703	ATP	C2-N1	2.11	1.37	1.33
3	B	701	ATP	PB-O2B	-2.06	1.45	1.55
3	E	704	ATP	C2-N3	-2.04	1.30	1.33
3	A	700	ATP	O4'-C1'	-2.03	1.37	1.42

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	704	ATP	C2'-C1'-N9	7.80	132.67	113.30
3	E	704	ATP	C4-N9-C8	-6.31	99.12	105.74
3	D	703	ATP	C4-N9-C8	-5.99	99.45	105.74
3	A	700	ATP	C2'-C1'-N9	5.86	127.87	113.30
3	D	703	ATP	O4'-C1'-N9	5.68	119.00	108.09
3	E	704	ATP	O4'-C1'-N9	5.11	117.91	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	ATP	C4-N9-C8	-5.10	100.38	105.74
3	E	704	ATP	C6-C5-N7	-4.66	123.10	132.09
3	E	704	ATP	N9-C8-N7	4.44	120.24	113.94
3	D	703	ATP	N9-C8-N7	4.18	119.87	113.94
3	C	702	ATP	C4-N9-C8	-4.12	101.42	105.74
3	C	702	ATP	O4'-C1'-N9	3.88	115.55	108.09
3	F	705	ATP	C4-N9-C8	-3.80	101.75	105.74
3	E	704	ATP	C4-N9-C1'	3.72	135.33	126.63
3	A	700	ATP	O4'-C1'-N9	3.70	115.19	108.09
3	A	700	ATP	O2B-PB-O3B	3.62	117.05	107.27
3	E	704	ATP	C4-C5-N7	3.58	114.68	110.58
3	A	700	ATP	C2'-C3'-C4'	-3.56	95.73	102.61
3	E	704	ATP	C6-C5-C4	3.52	121.99	117.18
3	E	704	ATP	O2'-C2'-C3'	-3.46	100.74	111.82
3	D	703	ATP	O2G-PG-O3B	3.40	116.05	104.64
3	E	704	ATP	O2G-PG-O3B	3.38	115.98	104.64
3	A	700	ATP	C4-N9-C8	-3.32	102.25	105.74
3	A	700	ATP	O2'-C2'-C3'	-3.24	101.42	111.82
3	A	700	ATP	O2B-PB-O3A	-3.24	98.51	107.27
3	E	704	ATP	C5-C4-N3	-3.24	122.26	126.72
3	C	702	ATP	O2G-PG-O3B	3.23	115.48	104.64
3	B	701	ATP	N9-C8-N7	3.08	118.30	113.94
3	F	705	ATP	O2'-C2'-C3'	-3.04	102.08	111.82
3	F	705	ATP	O2G-PG-O3B	3.03	114.81	104.64
3	F	705	ATP	C5'-C4'-C3'	-2.98	104.48	115.21
3	B	701	ATP	O4'-C1'-N9	2.94	113.74	108.09
3	D	703	ATP	C6-C5-C4	2.93	121.18	117.18
3	D	703	ATP	C6-C5-N7	-2.85	126.59	132.09
3	E	704	ATP	O2B-PB-O3A	-2.84	99.60	107.27
3	C	702	ATP	O3G-PG-O1G	-2.75	100.13	110.83
3	E	704	ATP	N3-C4-N9	2.73	131.81	127.17
3	F	705	ATP	O4'-C1'-N9	2.72	113.31	108.09
3	E	704	ATP	O2B-PB-O3B	2.69	114.55	107.27
3	C	702	ATP	C1'-N9-C8	2.65	132.98	127.09
3	B	701	ATP	C2'-C1'-N9	2.65	119.89	113.30
3	F	705	ATP	O3G-PG-O2G	2.50	117.17	107.80
3	A	700	ATP	C4'-O4'-C1'	-2.41	104.14	109.47
3	B	701	ATP	C5-C6-N6	2.40	129.24	123.29
3	D	703	ATP	C2'-C1'-N9	2.33	119.10	113.30
3	E	704	ATP	N6-C6-N1	2.29	123.48	118.38
3	A	700	ATP	O3A-PB-O1B	2.29	117.59	110.70
3	E	704	ATP	C5-N7-C8	-2.28	99.86	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	703	ATP	O3G-PG-O3B	2.25	112.17	104.64
3	A	700	ATP	C1'-N9-C8	2.23	132.04	127.09
3	B	701	ATP	C1'-N9-C8	2.18	131.94	127.09
3	F	705	ATP	O3'-C3'-C4'	-2.17	104.85	111.08
3	C	702	ATP	C2'-C3'-C4'	-2.13	98.50	102.61
3	E	704	ATP	O3A-PA-O1A	2.12	117.09	110.70
3	E	704	ATP	O5'-PA-O1A	2.10	117.24	108.94
3	D	703	ATP	O2A-PA-O3A	2.09	112.92	107.27
3	C	702	ATP	N9-C8-N7	2.05	116.85	113.94
3	A	700	ATP	O4'-C1'-C2'	2.03	110.95	106.62

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	704	ATP	C1'

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	700	ATP	C5'-O5'-PA-O1A
3	E	704	ATP	C3'-C4'-C5'-O5'
3	D	703	ATP	PA-O3A-PB-O3B
3	D	703	ATP	PG-O3B-PB-O2B
3	F	705	ATP	PG-O3B-PB-O2B
3	B	701	ATP	PA-O3A-PB-O3B
3	B	701	ATP	PG-O3B-PB-O2B
3	A	700	ATP	C3'-C4'-C5'-O5'
3	E	704	ATP	O4'-C4'-C5'-O5'
3	E	704	ATP	PA-O3A-PB-O3B
3	B	701	ATP	PG-O3B-PB-O1B
3	B	701	ATP	PA-O3A-PB-O1B
3	E	704	ATP	PA-O3A-PB-O1B
3	F	705	ATP	PG-O3B-PB-O1B
3	D	703	ATP	O4'-C4'-C5'-O5'
3	E	704	ATP	PG-O3B-PB-O1B

There are no ring outliers.

3 monomers are involved in 8 short contacts:

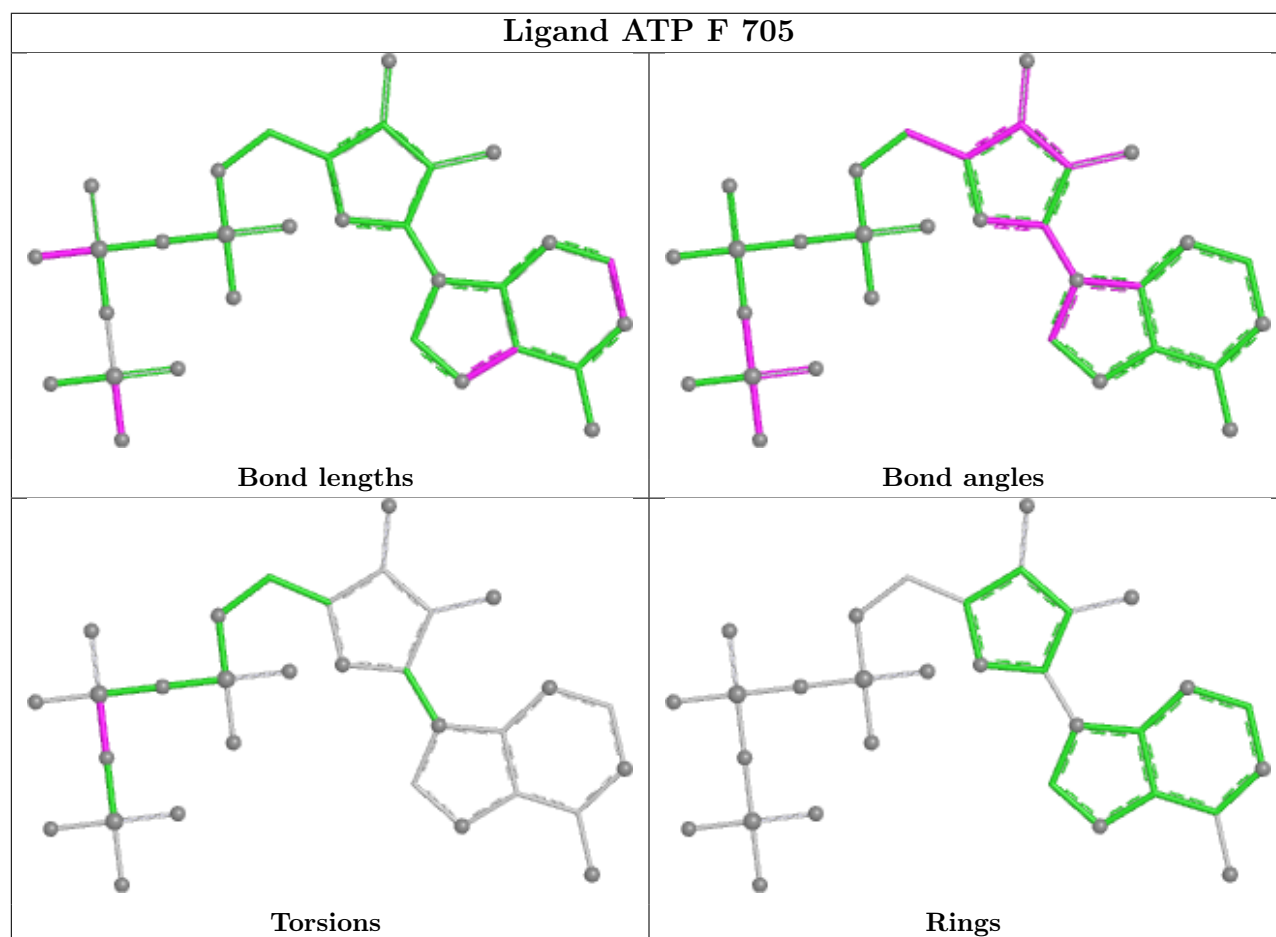
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	703	ATP	6	0

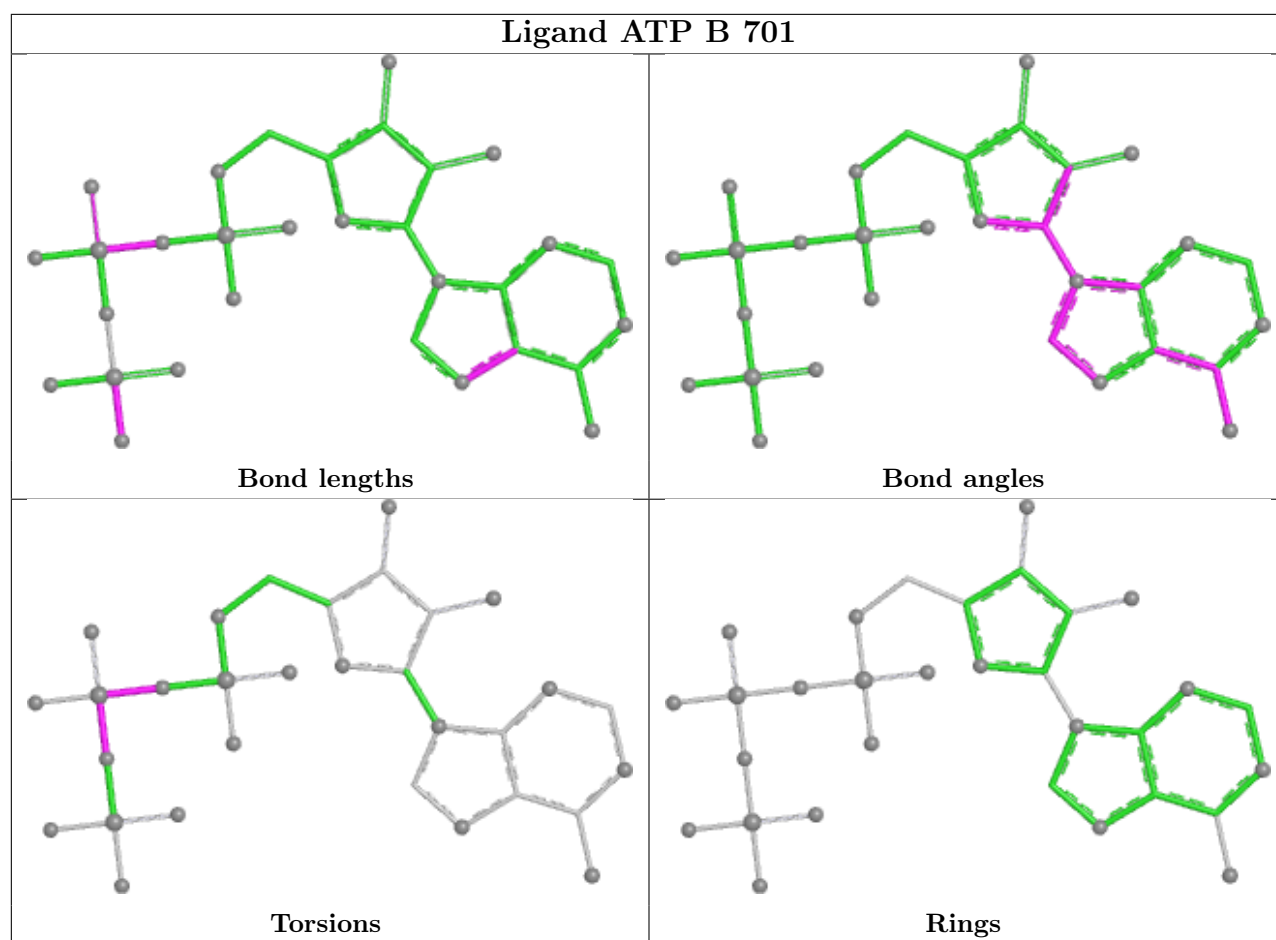
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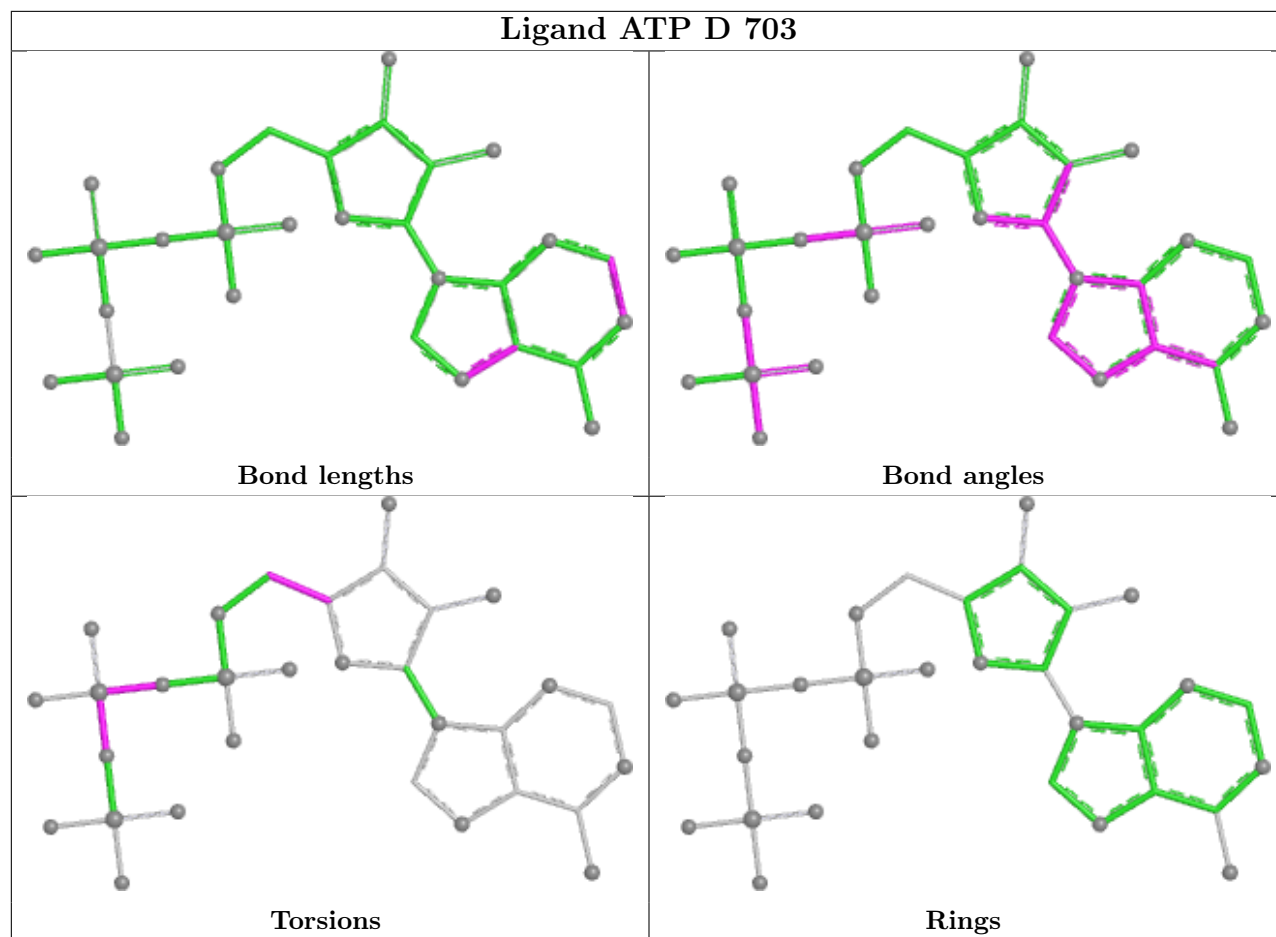
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	700	ATP	1	0
3	C	702	ATP	1	0

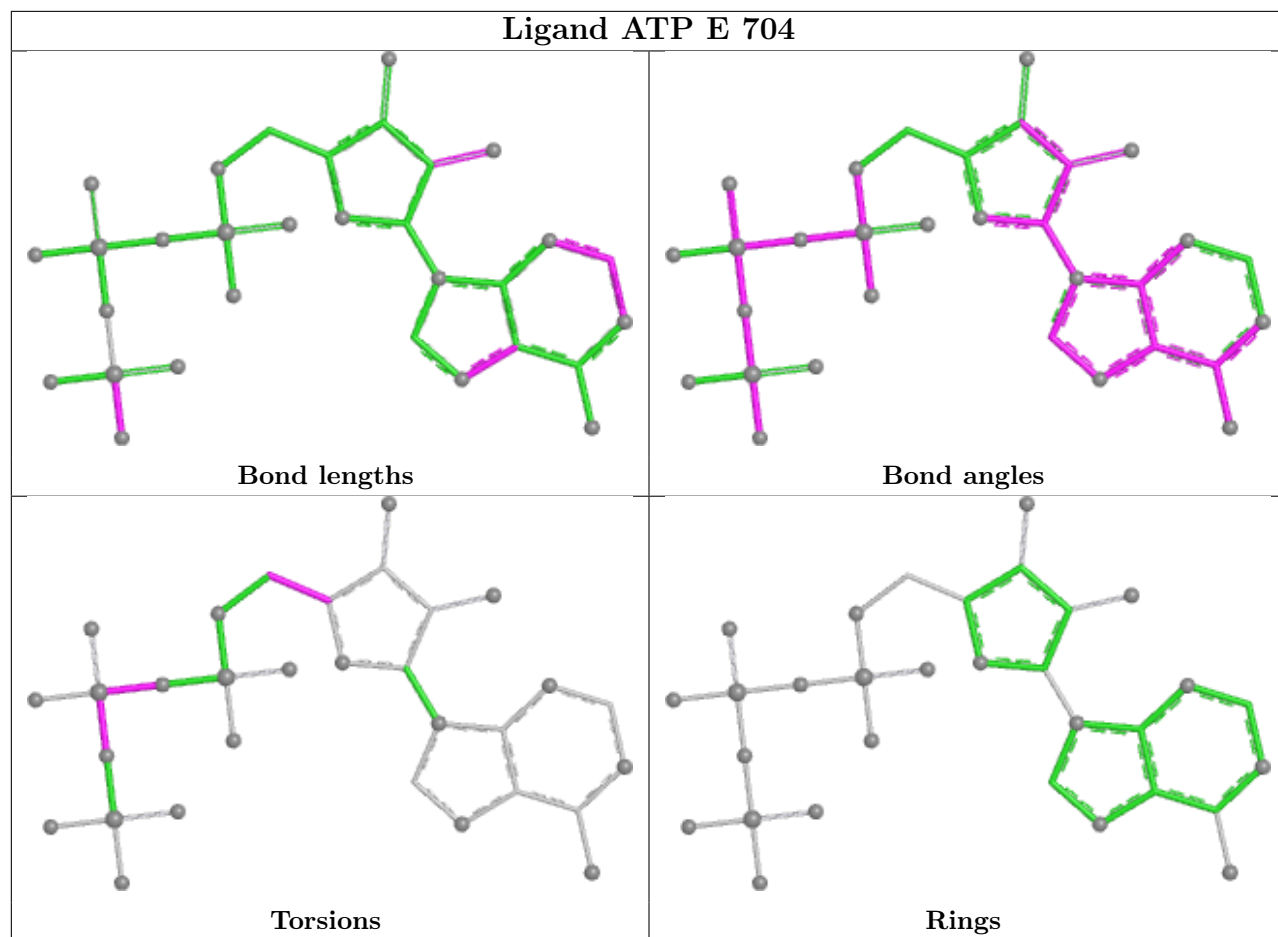
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

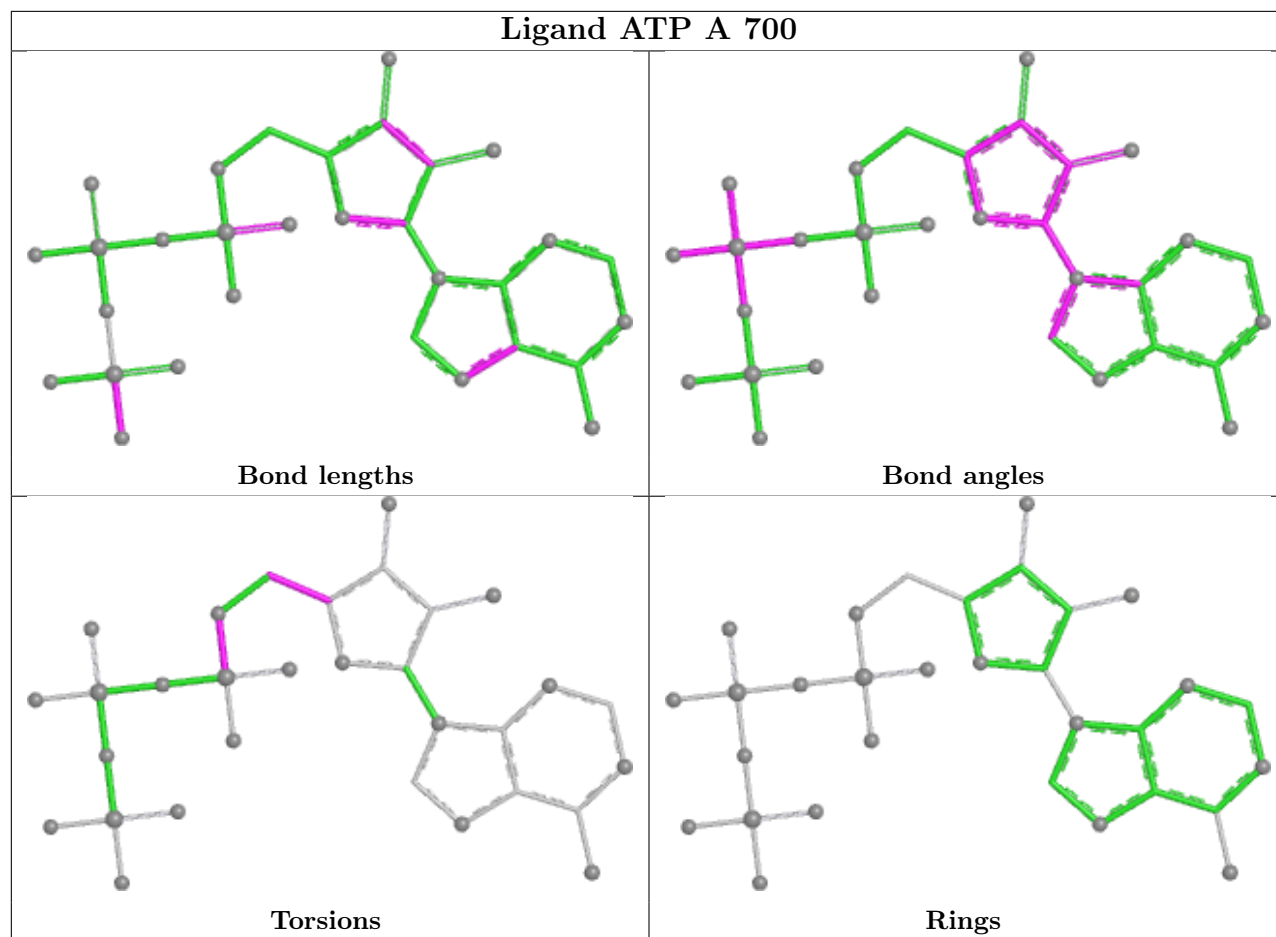


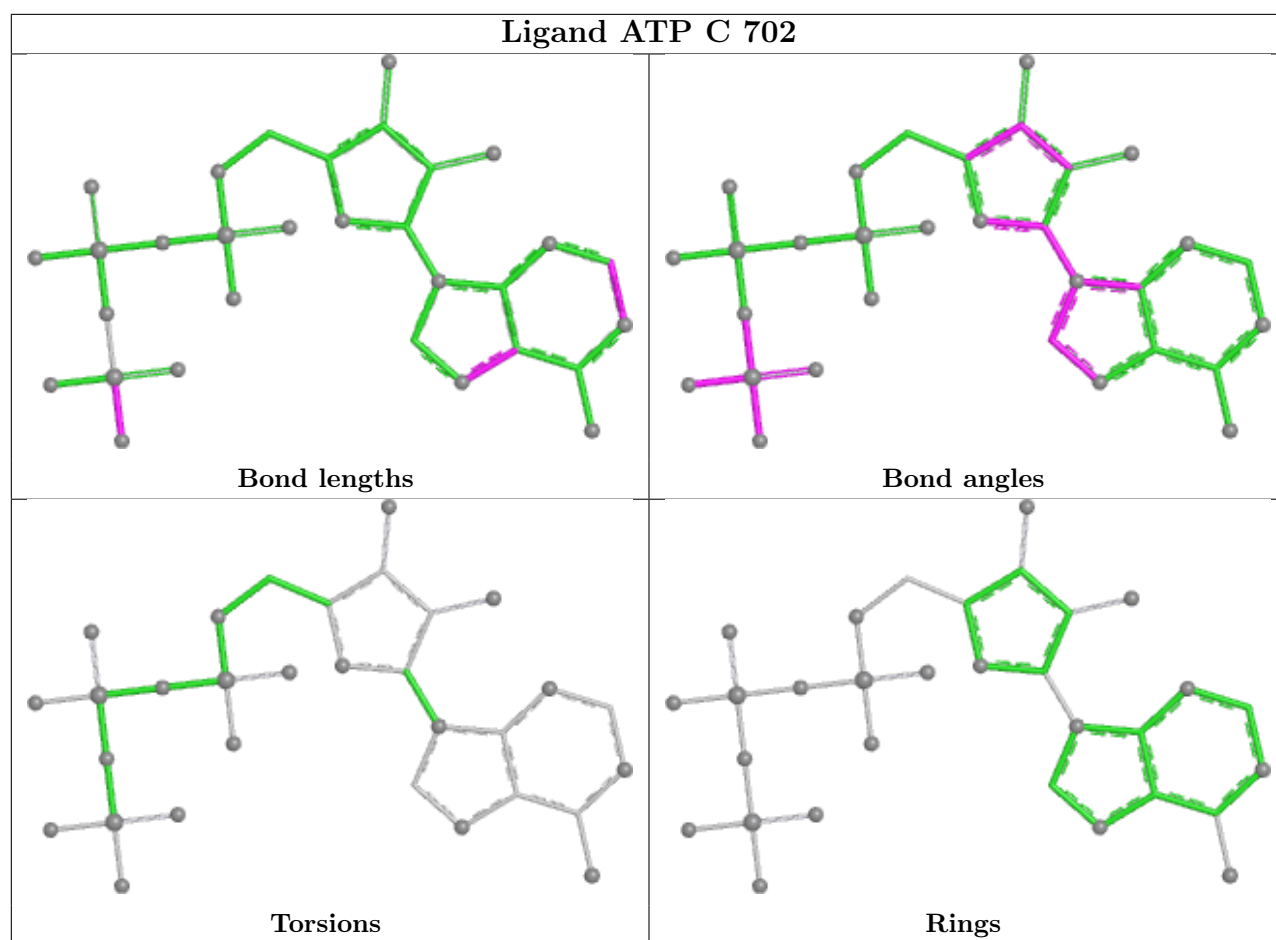




Ligand ATP E 704







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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.