



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:41 AM UTC

PDB ID : 1E1Q / pdb_00001e1q
Title : BOVINE MITOCHONDRIAL F1-ATPASE AT 100K
Authors : Braig, K.; Menz, R.I.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2000-05-10
Resolution : 2.61 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

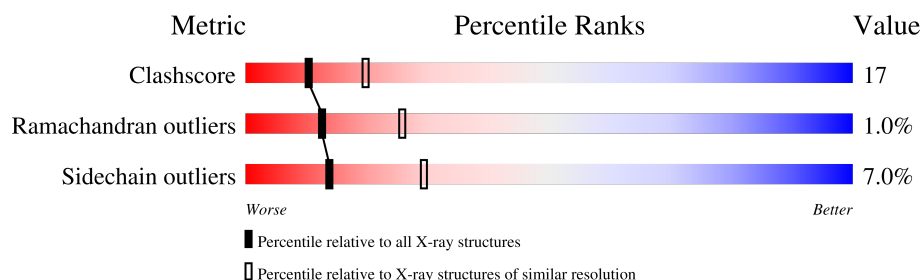
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)

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	510	
1	B	510	
1	C	510	
2	D	482	
2	E	482	
2	F	482	
3	G	272	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23366 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 BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	479	Total	C	N	O	S	0	0	0
			3656	2303	647	694	12			
1	C	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	conflict	UNP P19483
B	481	GLY	SER	conflict	UNP P19483
C	481	GLY	SER	conflict	UNP P19483

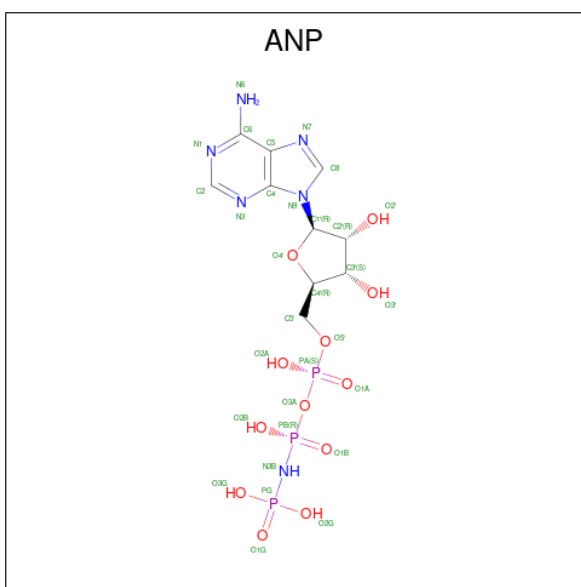
- Molecule 2 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	122	Total	C	N	O	S	0	0	0
			945	591	171	176	7			

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

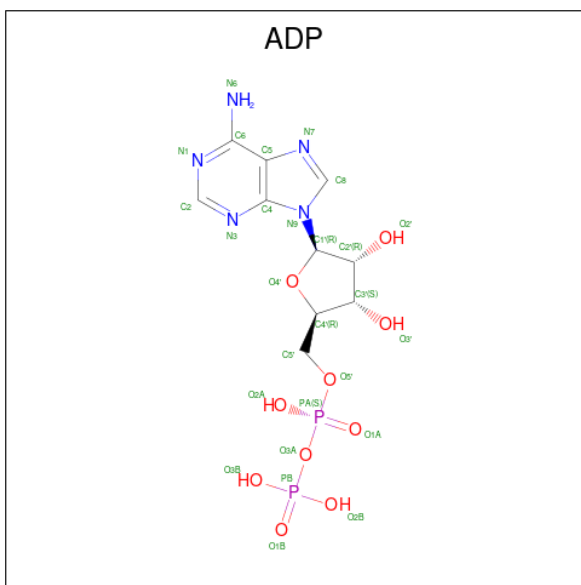


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

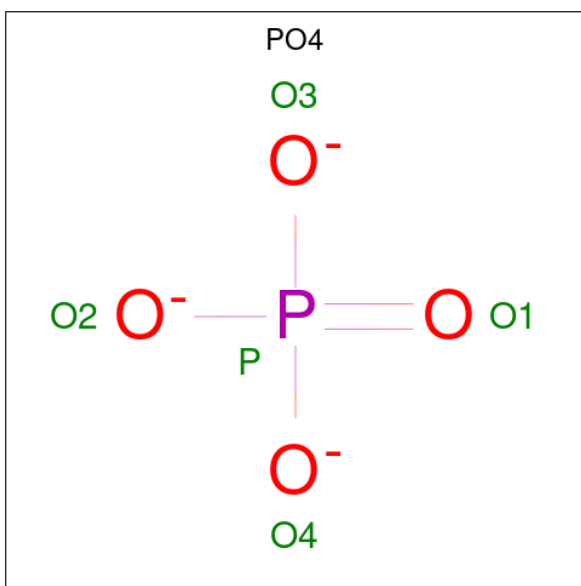
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total	O P	0	0
			5	4 1		

- Molecule 8 is water.

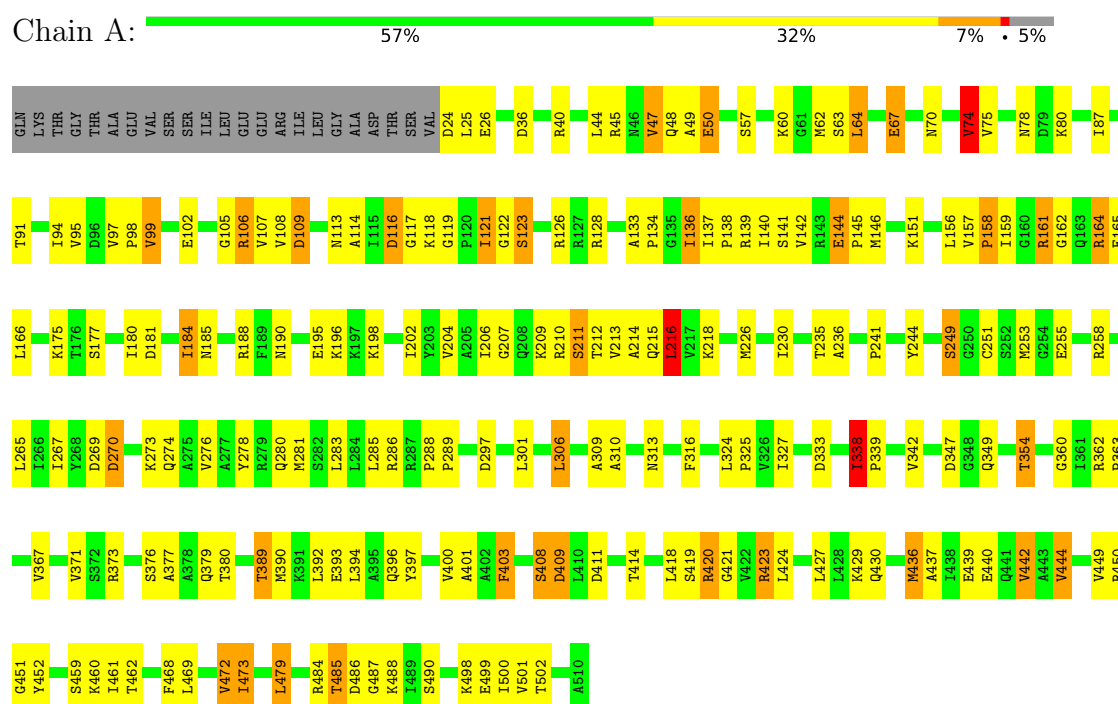
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	100	Total 100	O 100	0	0
8	B	83	Total 83	O 83	0	0
8	C	109	Total 109	O 109	0	0
8	D	92	Total 92	O 92	0	0
8	E	44	Total 44	O 44	0	0
8	F	107	Total 107	O 107	0	0
8	G	7	Total 7	O 7	0	0

3 Residue-property plots

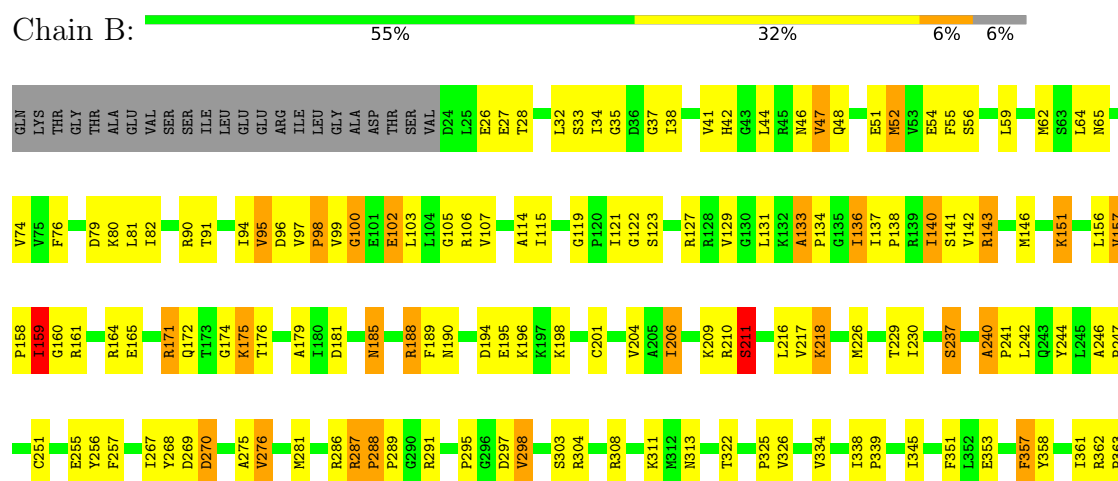
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

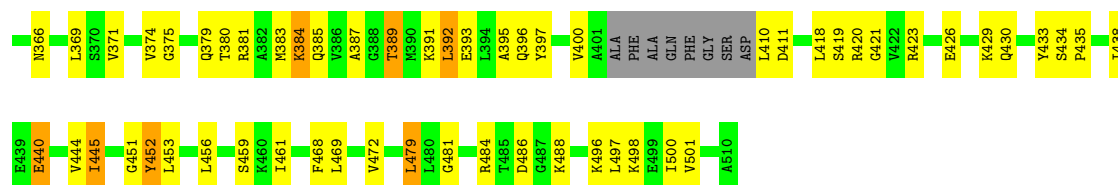
Note EDS was not executed.

• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE



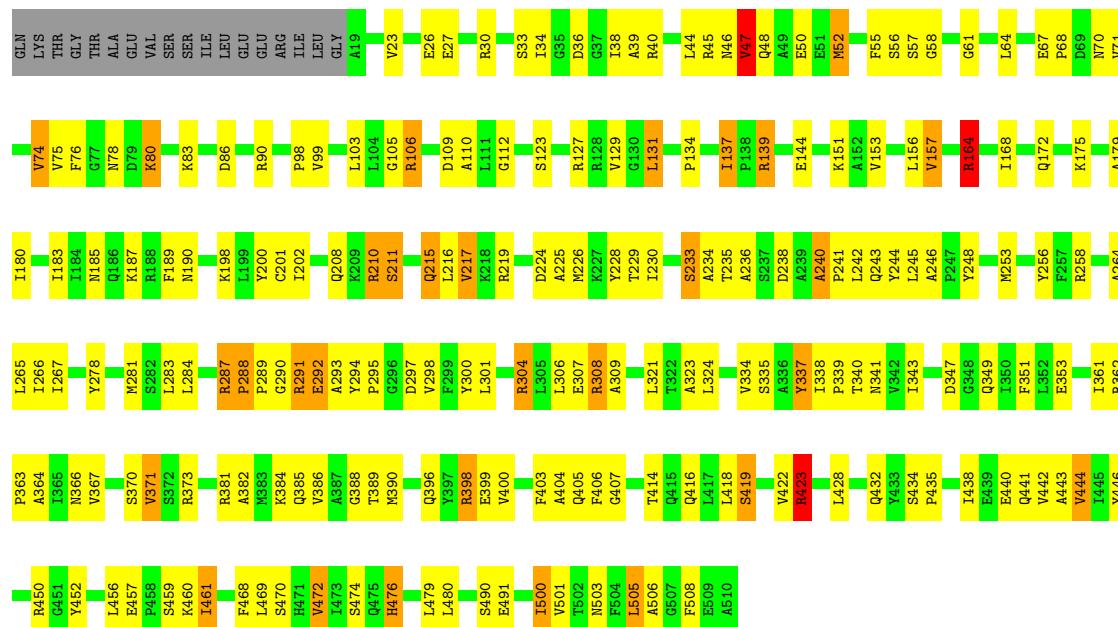
• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE





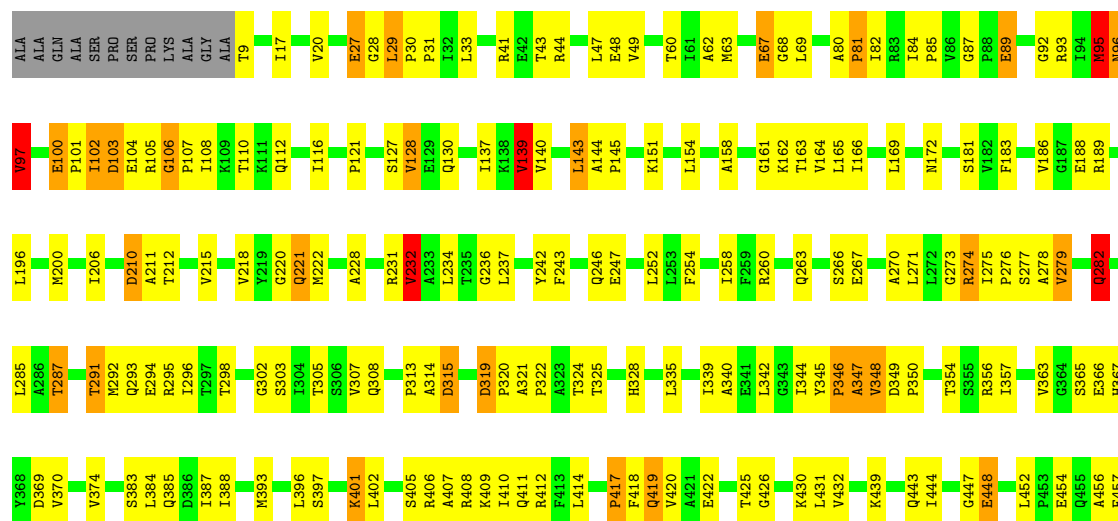
• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

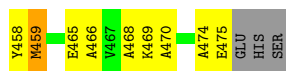
Chain C: 56% 34% 6% . .



• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

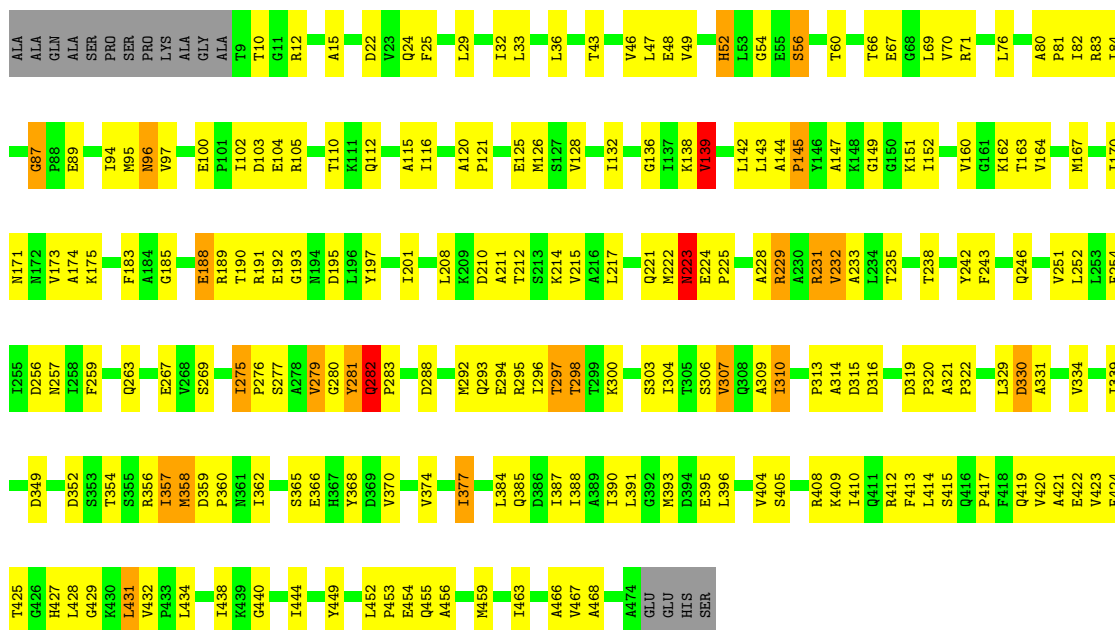
Chain D: 55% 35% 6% . .





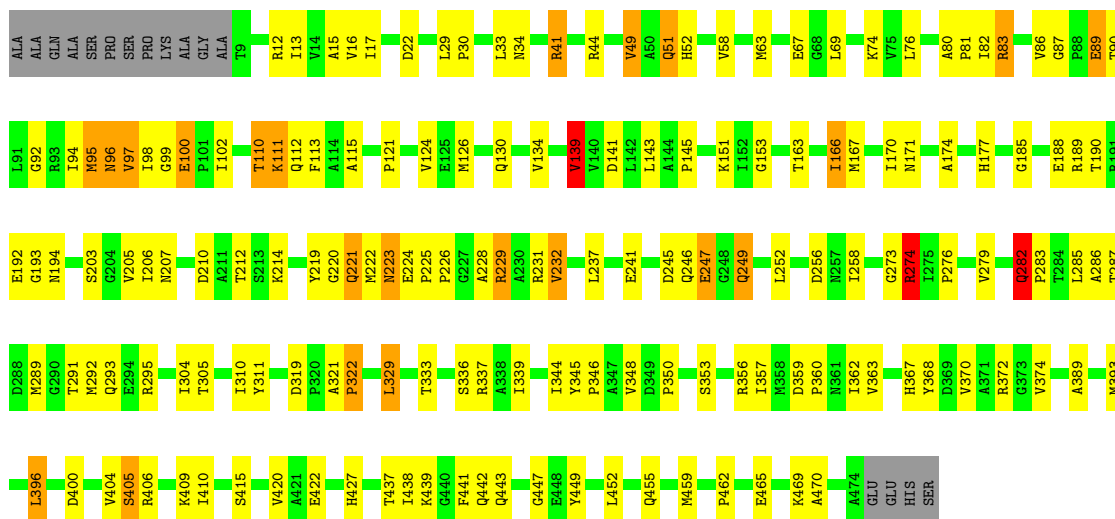
- Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

Chain E:



- Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

Chain F:



- Molecule 3: BOVINE MITOCHONDRIAL F1-ATPASE

Chain G:



TYR	GLN	GLU	TYR	SER	L209	A210	N211	S220	T221	T222	S223	E224	Q225	S226	A227	R228	M229	M232	S236	K237	N238	A239	S240	E241	M242	I243	L246	F250	R254	Q255	T259	L262	I263	L266	L272															
ILE	ALA	LEU	GLU	LEU	LEU	ASN	SER	SER	GLY	TYR	PHE	ASP	GLU	GLY	SER	ILE	PHE	ASN	ARG	PHE	ARG	SER	VAL	ILE	SER	TYR	LYS	PRO	ILE	PHE	SER	SER	ALA	SER	ASN															
C78	I81	H82	S83	K90	SER	GLU	ALA	ALA	GLY	TYR	PHE	ASP	GLU	GLY	SER	ILE	PHE	ASN	ARG	PHE	ARG	SER	VAL	ILE	SER	TYR	LYS	PRO	ILE	PHE	SER	SER	ALA	SER	ASN															
A1	I6	L10	I13	K14	T20	K21	S22	M23	A28	A32	R36	E37	L38	K39	P40	A41	R42	Y43	Y44	GLY	VAL	GLY	SER	LEU	ALA	LEU	TYR	GLU	LYS	ALA	ASP	ILE	LYS	THR	PRO	GLU	ASP	LYS	LYS	HIS	LEU	ILE	ILE	GLY	VAL	SER	SER	ASP	ARG	L77

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	280.80Å 107.40Å 139.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.61	Depositor
% Data completeness (in resolution range)	95.0 (20.00-2.61)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.232 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23366	wwPDB-VP
Average B, all atoms (Å ²)	63.0	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: ANP, MG, ADP, PO4

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	0.76	0/3766	1.59	44/5080 (0.9%)
1	B	0.78	0/3704	1.62	43/4995 (0.9%)
1	C	0.81	0/3799	1.70	54/5126 (1.1%)
2	D	0.78	0/3596	1.67	64/4879 (1.3%)
2	E	0.70	0/3587	1.58	42/4867 (0.9%)
2	F	0.82	0/3587	1.66	55/4867 (1.1%)
3	G	0.61	0/949	1.36	5/1266 (0.4%)
All	All	0.77	0/22988	1.63	307/31080 (1.0%)

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
2	D	0	1
2	E	0	1
All	All	0	2

There are no bond length outliers.

All (307) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	ASP	CA-CB-CG	15.92	128.52	112.60
1	B	185	ASN	CA-CB-CG	14.48	127.08	112.60
2	D	97	VAL	CB-CA-C	-12.81	95.79	111.81
1	A	210	ARG	CD-NE-CZ	11.07	139.89	124.40
1	B	270	ASP	CA-CB-CG	10.82	123.42	112.60
2	F	96	ASN	CA-CB-CG	10.57	123.17	112.60
2	E	282	GLN	CA-C-N	9.93	130.64	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	282	GLN	C-N-CA	9.93	130.64	119.32
1	B	159	ILE	CA-C-N	9.82	129.17	121.61
1	B	159	ILE	C-N-CA	9.82	129.17	121.61
2	F	274	ARG	CD-NE-CZ	9.58	137.82	124.40
1	C	144	GLU	CA-C-O	9.31	126.63	119.46
1	B	185	ASN	OD1-CG-ND2	-9.04	113.56	122.60
1	C	423	ARG	CD-NE-CZ	8.98	136.97	124.40
2	E	96	ASN	CA-CB-CG	8.75	121.35	112.60
2	F	41	ARG	CG-CD-NE	8.70	131.14	112.00
2	E	232	VAL	N-CA-CB	8.57	121.19	110.47
2	F	139	VAL	CB-CA-C	-8.56	100.75	111.70
1	C	47	VAL	CB-CA-C	-8.48	98.61	111.08
1	C	304	ARG	NE-CZ-NH2	8.45	126.80	119.20
2	E	330	ASP	CA-C-O	8.40	128.09	118.77
2	D	432	VAL	CA-C-O	8.09	124.53	119.51
1	B	136	ILE	CA-C-N	8.06	125.32	120.24
1	B	136	ILE	C-N-CA	8.06	125.32	120.24
2	F	225	PRO	CA-C-N	7.79	127.34	119.24
2	F	225	PRO	C-N-CA	7.79	127.34	119.24
2	D	139	VAL	CB-CA-C	-7.77	101.94	111.88
2	F	256	ASP	CA-CB-CG	7.52	120.12	112.60
2	E	232	VAL	CB-CA-C	-7.50	102.22	112.04
1	A	258	ARG	CD-NE-CZ	7.45	134.82	124.40
1	A	338	ILE	CA-C-O	7.26	123.56	118.69
2	F	171	ASN	CA-CB-CG	7.25	119.85	112.60
2	D	96	ASN	OD1-CG-ND2	7.20	129.80	122.60
1	A	338	ILE	O-C-N	-7.12	115.86	120.42
2	D	298	THR	N-CA-C	-7.07	101.20	110.53
1	B	181	ASP	CA-CB-CG	7.03	119.63	112.60
2	D	263	GLN	OE1-CD-NE2	-7.01	115.59	122.60
2	E	359	ASP	CA-CB-CG	6.98	119.58	112.60
1	C	215	GLN	CA-C-N	6.95	129.48	120.44
1	C	215	GLN	C-N-CA	6.95	129.48	120.44
1	B	211	SER	CA-CB-OG	6.91	124.93	111.10
2	F	143	LEU	CA-C-N	-6.83	115.33	122.85
2	F	143	LEU	C-N-CA	-6.83	115.33	122.85
1	B	47	VAL	CB-CA-C	-6.78	101.11	111.08
2	E	83	ARG	CD-NE-CZ	6.75	133.85	124.40
2	E	349	ASP	CA-C-N	6.71	126.34	119.56
2	E	349	ASP	C-N-CA	6.71	126.34	119.56
2	D	106	GLY	CA-C-N	6.64	126.62	119.78
2	D	106	GLY	C-N-CA	6.64	126.62	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	291	ARG	CD-NE-CZ	6.59	133.63	124.40
1	A	40	ARG	CD-NE-CZ	6.58	133.61	124.40
1	B	257	PHE	CA-C-N	6.47	129.28	120.54
1	B	257	PHE	C-N-CA	6.47	129.28	120.54
1	A	74	VAL	N-CA-CB	-6.46	103.64	111.00
2	E	222	MET	CA-C-O	-6.45	113.67	120.63
2	D	97	VAL	N-CA-CB	6.44	117.64	110.62
2	D	139	VAL	N-CA-CB	6.44	117.66	110.51
1	C	47	VAL	N-CA-CB	6.44	124.22	110.64
1	A	184	ILE	N-CA-CB	6.42	117.62	110.62
1	C	340	THR	N-CA-CB	6.42	120.23	110.28
2	E	229	ARG	NH1-CZ-NH2	6.42	127.64	119.30
1	B	52	MET	CA-CB-CG	6.39	126.88	114.10
2	E	87	GLY	CA-C-N	6.37	126.86	119.47
2	E	87	GLY	C-N-CA	6.37	126.86	119.47
2	D	144	ALA	CA-C-N	6.35	126.37	119.90
2	D	144	ALA	C-N-CA	6.35	126.37	119.90
2	F	256	ASP	CA-C-N	6.34	133.11	121.70
2	F	256	ASP	C-N-CA	6.34	133.11	121.70
1	C	386	VAL	N-CA-C	6.33	116.48	110.53
2	F	90	THR	N-CA-CB	6.31	119.44	110.67
2	D	349	ASP	CA-C-N	6.29	125.91	119.56
2	D	349	ASP	C-N-CA	6.29	125.91	119.56
2	F	274	ARG	NE-CZ-NH1	6.27	127.77	121.50
2	F	87	GLY	CA-C-N	6.25	126.16	119.28
2	F	87	GLY	C-N-CA	6.25	126.16	119.28
1	C	233	SER	N-CA-C	6.22	118.66	108.52
3	G	262	LEU	CA-C-O	6.21	127.34	120.82
1	C	71	VAL	CA-C-O	-6.21	114.00	120.27
1	C	476	HIS	CA-CB-CG	-6.19	107.61	113.80
1	B	136	ILE	N-CA-C	6.19	116.35	110.53
2	E	432	VAL	CA-C-N	6.19	126.10	119.85
2	E	432	VAL	C-N-CA	6.19	126.10	119.85
2	D	221	GLN	CA-C-N	6.18	130.49	120.60
2	D	221	GLN	C-N-CA	6.18	130.49	120.60
1	B	96	ASP	O-C-N	6.17	130.20	123.10
2	F	145	PRO	N-CA-CB	6.16	108.50	103.32
2	F	329	LEU	CA-C-O	6.16	128.67	121.46
2	D	100	GLU	CA-C-N	6.15	127.12	119.98
2	D	100	GLU	C-N-CA	6.15	127.12	119.98
1	C	308	ARG	NE-CZ-NH2	6.15	124.74	119.20
2	D	365	SER	N-CA-C	6.15	117.65	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	255	GLN	OE1-CD-NE2	-6.15	116.45	122.60
1	C	74	VAL	N-CA-CB	-6.14	104.02	111.21
2	E	269	SER	CA-CB-OG	6.13	123.35	111.10
1	A	164	ARG	CA-C-O	-6.11	113.76	120.30
1	A	265	LEU	CA-C-O	-6.11	113.76	120.36
1	B	433	TYR	CA-C-N	-6.10	116.14	122.85
1	B	433	TYR	C-N-CA	-6.10	116.14	122.85
2	E	295	ARG	CG-CD-NE	6.08	125.37	112.00
1	A	423	ARG	NE-CZ-NH2	6.07	124.66	119.20
1	A	78	ASN	CA-CB-CG	6.06	118.66	112.60
1	C	500	ILE	N-CA-C	6.06	116.80	110.62
1	B	276	VAL	CA-CB-CG2	6.05	120.69	110.40
2	E	171	ASN	OD1-CG-ND2	6.04	128.64	122.60
1	C	491	GLU	CA-C-O	6.03	126.78	119.49
1	C	144	GLU	CA-C-N	6.03	125.99	119.78
1	C	144	GLU	C-N-CA	6.03	125.99	119.78
1	C	236	ALA	N-CA-C	6.02	118.64	111.71
2	D	87	GLY	CA-C-N	5.99	125.87	119.28
2	D	87	GLY	C-N-CA	5.99	125.87	119.28
1	C	240	ALA	CA-C-O	5.99	124.07	118.44
2	D	101	PRO	N-CA-CB	5.99	108.50	103.17
1	C	287	ARG	CD-NE-CZ	-5.98	116.03	124.40
2	D	432	VAL	N-CA-C	5.98	114.73	107.61
1	B	100	GLY	N-CA-C	5.95	118.47	111.63
1	C	243	GLN	CA-C-O	5.95	126.82	120.10
2	F	121	PRO	N-CA-CB	5.93	108.47	103.25
1	B	189	PHE	CA-CB-CG	5.92	119.72	113.80
1	B	276	VAL	N-CA-CB	5.92	119.46	110.58
1	A	280	GLN	O-C-N	5.90	128.15	122.07
1	A	338	ILE	CB-CG1-CD1	5.90	126.19	113.80
2	F	282	GLN	CA-C-N	5.90	125.58	119.56
2	F	282	GLN	C-N-CA	5.90	125.58	119.56
1	C	47	VAL	O-C-N	5.90	128.70	122.62
1	A	106	ARG	CD-NE-CZ	5.90	132.66	124.40
1	C	434	SER	N-CA-CB	5.88	117.36	110.71
2	F	353	SER	CA-C-O	-5.88	114.02	120.43
2	E	139	VAL	CB-CA-C	-5.88	101.65	111.29
1	C	106	ARG	N-CA-C	5.88	119.12	109.72
1	A	158	PRO	N-CA-CB	5.87	108.42	103.25
2	F	139	VAL	N-CA-CB	5.86	116.77	110.62
1	C	46	ASN	CA-CB-CG	5.85	118.45	112.60
1	A	338	ILE	CA-C-N	5.83	125.31	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	ILE	C-N-CA	5.83	125.31	119.24
1	B	291	ARG	CA-C-O	5.83	127.31	120.96
1	B	240	ALA	CA-C-N	5.82	125.68	119.28
1	B	240	ALA	C-N-CA	5.82	125.68	119.28
2	E	307	VAL	CA-C-N	-5.80	114.59	122.77
2	E	307	VAL	C-N-CA	-5.80	114.59	122.77
1	A	274	GLN	N-CA-C	-5.80	104.92	112.23
2	F	193	GLY	N-CA-C	-5.80	105.77	112.50
1	C	423	ARG	NE-CZ-NH2	-5.80	113.98	119.20
2	F	90	THR	N-CA-C	-5.80	106.55	113.97
2	F	310	ILE	CA-C-N	5.79	128.94	120.71
2	F	310	ILE	C-N-CA	5.79	128.94	120.71
2	F	51	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	A	67	GLU	CA-C-N	5.78	125.47	119.05
1	A	67	GLU	C-N-CA	5.78	125.47	119.05
2	E	298	THR	CB-CA-C	-5.77	101.29	110.81
2	D	103	ASP	CA-CB-CG	5.77	118.37	112.60
2	D	407	ALA	CA-C-N	5.77	128.28	120.38
2	D	407	ALA	C-N-CA	5.77	128.28	120.38
2	D	315	ASP	N-CA-CB	-5.74	105.21	113.65
1	A	162	GLY	N-CA-C	-5.74	107.10	114.85
2	F	372	ARG	CD-NE-CZ	5.74	132.43	124.40
1	A	442	VAL	N-CA-CB	5.74	117.26	110.55
2	D	344	ILE	CB-CA-C	-5.72	104.38	111.08
2	D	287	THR	N-CA-CB	5.71	118.71	110.20
2	D	348	VAL	N-CA-C	5.70	116.94	109.58
2	E	275	ILE	CA-C-N	5.70	125.67	120.03
2	E	275	ILE	C-N-CA	5.70	125.67	120.03
2	E	316	ASP	CA-CB-CG	5.70	118.30	112.60
3	G	254	ARG	NH1-CZ-NH2	5.69	126.70	119.30
2	F	111	LYS	N-CA-C	-5.67	103.92	111.24
2	D	417	PRO	N-CA-CB	5.66	107.83	103.30
1	C	75	VAL	N-CA-C	5.66	116.92	108.54
2	D	426	GLY	N-CA-C	-5.65	105.15	114.76
2	D	95	MET	CA-C-N	5.63	132.60	122.64
2	D	95	MET	C-N-CA	5.63	132.60	122.64
2	F	49	VAL	CA-C-O	-5.62	114.64	121.04
1	C	58	GLY	N-CA-C	-5.61	108.01	114.69
1	A	288	PRO	N-CA-CB	5.60	108.51	103.08
2	E	288	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	67	GLU	CA-C-N	5.58	125.25	119.05
1	C	67	GLU	C-N-CA	5.58	125.25	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	417	PRO	N-CA-CB	5.58	107.77	103.30
1	C	210	ARG	CA-C-N	-5.57	112.25	120.28
1	C	210	ARG	C-N-CA	-5.57	112.25	120.28
1	A	325	PRO	CA-C-N	-5.57	115.91	123.10
1	A	325	PRO	C-N-CA	-5.57	115.91	123.10
1	B	357	PHE	CA-CB-CG	5.57	119.37	113.80
1	B	211	SER	N-CA-CB	5.57	118.86	109.78
2	F	322	PRO	N-CA-CB	5.57	109.19	103.23
2	F	304	ILE	CB-CA-C	-5.57	104.07	110.41
1	A	310	ALA	N-CA-C	5.56	116.97	108.52
2	D	121	PRO	N-CA-CB	5.56	108.14	103.25
1	A	269	ASP	CA-C-O	-5.56	114.36	120.70
1	B	140	ILE	CA-C-O	-5.56	115.46	121.19
2	D	346	PRO	N-CA-CB	5.56	108.71	102.60
2	E	231	ARG	CD-NE-CZ	-5.54	116.65	124.40
2	F	100	GLU	CA-C-N	5.53	125.45	119.76
2	F	100	GLU	C-N-CA	5.53	125.45	119.76
1	C	134	PRO	N-CA-CB	5.52	108.22	103.31
1	A	116	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	142	VAL	CA-C-O	-5.52	114.23	120.74
2	D	319	ASP	CA-C-O	5.52	125.37	120.02
1	C	106	ARG	CA-CB-CG	-5.51	103.09	114.10
1	B	119	GLY	CA-C-N	5.50	125.48	120.03
1	B	119	GLY	C-N-CA	5.50	125.48	120.03
1	A	161	ARG	CD-NE-CZ	-5.49	116.71	124.40
1	C	461	ILE	N-CA-C	5.49	115.69	110.42
2	D	105	ARG	CD-NE-CZ	5.48	132.07	124.40
2	D	222	MET	N-CA-C	5.47	119.05	112.38
1	C	219	ARG	NE-CZ-NH2	-5.47	114.28	119.20
1	B	288	PRO	CA-C-N	5.47	125.37	119.85
1	B	288	PRO	C-N-CA	5.47	125.37	119.85
1	C	139	ARG	NE-CZ-NH1	-5.46	116.04	121.50
2	D	419	GLN	CA-C-O	5.44	126.53	120.82
2	E	145	PRO	N-CA-CB	5.43	108.16	103.27
1	C	490	SER	CA-C-O	-5.43	115.40	121.81
2	F	83	ARG	CA-C-O	-5.43	114.96	120.71
2	E	233	ALA	N-CA-C	-5.42	105.92	112.54
1	B	140	ILE	CA-CB-CG1	5.42	119.62	110.40
2	E	56	SER	N-CA-CB	-5.42	104.06	112.30
1	B	98	PRO	CA-C-O	-5.41	115.18	121.34
1	C	137	ILE	CA-C-N	5.41	125.07	119.56
1	C	137	ILE	C-N-CA	5.41	125.07	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	52	HIS	CA-CB-CG	5.40	119.20	113.80
1	B	287	ARG	CA-C-N	5.40	125.94	120.38
1	B	287	ARG	C-N-CA	5.40	125.94	120.38
1	B	157	VAL	CA-C-N	5.39	126.23	119.98
1	B	157	VAL	C-N-CA	5.39	126.23	119.98
1	C	164	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	A	306	LEU	N-CA-C	5.38	117.14	111.28
2	D	419	GLN	CA-C-N	5.37	129.82	120.86
2	D	419	GLN	C-N-CA	5.37	129.82	120.86
1	C	287	ARG	NE-CZ-NH1	-5.36	116.14	121.50
2	F	44	ARG	CD-NE-CZ	-5.36	116.90	124.40
2	D	232	VAL	N-CA-C	5.35	115.98	110.36
2	E	54	GLY	CA-C-O	-5.35	118.54	122.23
2	E	232	VAL	CA-C-O	-5.35	115.49	121.05
2	E	310	ILE	N-CA-C	5.35	115.56	107.75
1	B	326	VAL	O-C-N	5.33	128.81	123.10
1	B	304	ARG	NE-CZ-NH2	5.33	123.99	119.20
2	F	229	ARG	NE-CZ-NH1	-5.33	116.17	121.50
2	E	225	PRO	CA-C-N	5.32	125.14	119.28
2	E	225	PRO	C-N-CA	5.32	125.14	119.28
1	A	403	PHE	CA-CB-CG	5.32	119.12	113.80
1	C	288	PRO	CA-C-N	5.32	125.22	119.85
1	C	288	PRO	C-N-CA	5.32	125.22	119.85
2	D	282	GLN	CA-C-N	5.32	124.93	119.56
2	D	282	GLN	C-N-CA	5.32	124.93	119.56
2	D	107	PRO	CB-CA-C	-5.30	104.45	111.23
2	E	195	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	67	GLU	CB-CG-CD	5.30	121.61	112.60
2	D	143	LEU	N-CA-C	5.27	118.18	111.69
2	D	96	ASN	CB-CA-C	-5.27	101.06	111.60
2	D	369	ASP	CA-CB-CG	5.27	117.87	112.60
1	C	144	GLU	O-C-N	-5.27	116.83	121.31
2	D	432	VAL	CA-C-N	5.25	125.16	119.85
2	D	432	VAL	C-N-CA	5.25	125.16	119.85
1	C	217	VAL	N-CA-CB	5.25	120.27	110.77
2	D	107	PRO	N-CA-CB	5.24	107.91	103.35
2	F	51	GLN	CB-CG-CD	5.23	121.49	112.60
2	D	67	GLU	CB-CG-CD	5.23	121.48	112.60
1	A	371	VAL	CA-C-O	5.22	126.67	121.45
1	B	47	VAL	N-CA-CB	5.22	121.65	110.64
1	A	285	LEU	N-CA-C	-5.20	106.72	113.16
2	D	41	ARG	CD-NE-CZ	5.20	131.68	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	71	ARG	NE-CZ-NH1	-5.19	116.31	121.50
2	E	281	TYR	CA-C-O	5.18	127.88	121.87
2	F	224	GLU	CA-C-N	5.18	125.72	120.38
2	F	224	GLU	C-N-CA	5.18	125.72	120.38
2	D	101	PRO	CB-CA-C	-5.17	104.99	111.71
3	G	228	ARG	NE-CZ-NH2	5.17	123.85	119.20
2	F	221	GLN	O-C-N	5.16	128.44	121.83
2	D	319	ASP	CA-CB-CG	5.16	117.76	112.60
3	G	243	ILE	N-CA-C	-5.16	105.68	110.53
2	F	86	VAL	CA-C-O	-5.15	116.53	121.63
2	F	249	GLN	CA-C-N	-5.14	115.36	122.30
2	F	249	GLN	C-N-CA	-5.14	115.36	122.30
2	F	311	TYR	CA-C-O	-5.13	115.54	121.19
1	C	106	ARG	CD-NE-CZ	-5.13	117.22	124.40
1	C	240	ALA	CA-C-N	5.12	124.92	119.28
1	C	240	ALA	C-N-CA	5.12	124.92	119.28
1	A	216	LEU	CA-CB-CG	5.12	134.22	116.30
2	F	359	ASP	CA-C-N	5.12	125.41	119.47
2	F	359	ASP	C-N-CA	5.12	125.41	119.47
2	F	286	ALA	CA-C-N	-5.11	111.99	120.68
2	F	286	ALA	C-N-CA	-5.11	111.99	120.68
1	C	109	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	75	VAL	N-CA-C	5.10	116.03	108.23
1	A	109	ASP	CA-C-O	-5.08	115.27	121.67
1	C	139	ARG	NH1-CZ-NH2	5.08	125.91	119.30
1	A	91	THR	CA-C-O	5.08	125.55	119.60
1	C	46	ASN	OD1-CG-ND2	-5.08	117.52	122.60
2	E	281	TYR	O-C-N	-5.08	117.00	122.79
2	D	274	ARG	CD-NE-CZ	-5.07	117.30	124.40
2	D	302	GLY	CA-C-O	-5.07	115.75	121.68
1	A	74	VAL	CB-CA-C	5.07	117.09	110.96
1	A	113	ASN	CA-CB-CG	5.07	117.67	112.60
1	B	275	ALA	CA-C-O	-5.07	114.53	120.20
2	D	102	ILE	N-CA-C	-5.06	106.51	111.88
2	F	100	GLU	CB-CG-CD	-5.06	104.00	112.60
2	F	51	GLN	CG-CD-NE2	5.05	123.97	116.40
2	D	270	ALA	O-C-N	-5.04	116.77	122.12
1	B	133	ALA	N-CA-C	5.03	115.39	109.60
2	F	333	THR	CA-CB-OG1	5.03	117.14	109.60
1	A	144	GLU	CA-C-N	5.01	125.25	119.83
1	A	144	GLU	C-N-CA	5.01	125.25	119.83
2	D	31	PRO	N-CA-CB	5.01	107.99	103.33

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	188	ARG	NE-CZ-NH1	-5.01	116.49	121.50
2	D	354	THR	CA-C-O	-5.01	115.89	121.51
2	D	29	LEU	CA-C-N	5.00	125.53	120.38
2	D	29	LEU	C-N-CA	5.00	125.53	120.38
2	F	273	GLY	CA-C-N	5.00	130.18	122.93
2	F	273	GLY	C-N-CA	5.00	130.18	122.93

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	97	VAL	Mainchain
2	E	223	ASN	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	3715	0	3814	141	0
1	B	3656	0	3765	152	0
1	C	3748	0	3845	130	0
2	D	3539	0	3592	126	0
2	E	3530	0	3587	154	0
2	F	3530	0	3586	101	0
3	G	945	0	1019	32	0
4	A	31	0	13	1	0
4	B	31	0	13	2	0
4	C	31	0	13	2	0
4	F	31	0	13	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	D	27	0	12	1	0
7	E	5	0	0	1	0
8	A	100	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	83	0	0	6	0
8	C	109	0	0	3	0
8	D	92	0	0	4	0
8	E	44	0	0	4	0
8	F	107	0	0	4	0
8	G	7	0	0	0	0
All	All	23366	0	23272	783	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 17.

All (783) 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:A:390:MET:HE3	1:A:424:LEU:HD22	1.44	0.98
2:D:282:GLN:H	2:D:282:GLN:HE21	0.96	0.96
1:C:294:TYR:HB3	1:C:298:VAL:HG21	1.52	0.91
2:D:139:VAL:HB	8:D:2027:HOH:O	1.72	0.90
1:C:187:LYS:HE3	1:C:224:ASP:HB3	1.54	0.89
2:D:145:PRO:HB2	2:D:357:ILE:HD11	1.56	0.88
2:F:282:GLN:H	2:F:282:GLN:HE21	0.89	0.88
2:E:449:TYR:HB3	2:E:452:LEU:HD12	1.56	0.87
2:F:282:GLN:H	2:F:282:GLN:NE2	1.71	0.87
2:F:16:VAL:C	2:F:17:ILE:HD12	2.00	0.87
1:A:389:THR:HB	1:A:449:VAL:HG21	1.58	0.84
2:F:282:GLN:HE21	2:F:282:GLN:N	1.74	0.83
2:D:282:GLN:H	2:D:282:GLN:NE2	1.77	0.82
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.61	0.82
2:E:388:ILE:HG23	2:E:393:MET:HB2	1.61	0.82
2:F:12:ARG:HE	2:F:74:LYS:HE3	1.44	0.82
1:A:218:LYS:HD2	2:D:128:VAL:HG21	1.62	0.81
1:C:295:PRO:O	1:C:298:VAL:HG23	1.82	0.80
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.61	0.80
2:D:393:MET:HG3	2:D:396:LEU:HD12	1.64	0.80
1:C:52:MET:HE1	1:C:76:PHE:HE2	1.47	0.80
1:B:209:LYS:HG3	8:B:2030:HOH:O	1.82	0.79
2:E:419:GLN:HA	2:E:429:GLY:HA3	1.65	0.78
2:D:196:LEU:HG	2:D:200:MET:HE2	1.66	0.77
1:B:440:GLU:HB3	1:B:469:LEU:HD11	1.66	0.76
2:F:98:ILE:HG13	2:F:100:GLU:HG3	1.68	0.76
1:A:144:GLU:HB2	1:A:161:ARG:HG3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ILE:HG12	1:A:230:ILE:HD12	1.68	0.76
2:E:170:ILE:HD13	2:E:215:VAL:HG21	1.66	0.75
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.67	0.75
1:C:404:ALA:C	1:C:406:PHE:H	1.95	0.75
2:D:242:TYR:CE1	2:D:246:GLN:HG3	2.22	0.75
1:C:472:VAL:HG23	1:C:480:LEU:HD11	1.70	0.74
1:B:444:VAL:HG23	1:B:445:ILE:HD13	1.69	0.73
1:C:240:ALA:HB3	1:C:241:PRO:HD3	1.68	0.73
1:C:52:MET:HE1	1:C:76:PHE:CE2	2.22	0.73
2:F:223:ASN:HD22	2:F:223:ASN:H	1.37	0.72
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.71	0.72
1:C:210:ARG:HG2	1:C:235:THR:HG21	1.71	0.72
1:A:94:ILE:HG12	1:A:95:VAL:H	1.54	0.72
2:E:259:PHE:CE1	2:E:313:PRO:HG3	2.25	0.72
2:F:287:THR:O	2:F:291:THR:HG23	1.90	0.71
1:B:171:ARG:HB2	1:B:171:ARG:HH11	1.55	0.71
1:C:292:GLU:O	1:C:293:ALA:HB3	1.88	0.71
1:B:453:LEU:HD13	1:B:461:ILE:HD12	1.73	0.71
1:B:374:VAL:HG23	1:B:374:VAL:O	1.89	0.71
1:A:400:VAL:HG12	1:A:418:LEU:HD21	1.73	0.71
1:B:34:ILE:HD11	1:B:79:ASP:HB2	1.72	0.71
1:C:211:SER:HB3	2:F:126:MET:HE2	1.71	0.71
2:E:404:VAL:O	2:E:408:ARG:HG3	1.91	0.70
2:F:252:LEU:HD23	2:F:305:THR:HB	1.73	0.70
1:B:366:ASN:ND2	1:B:369:LEU:HD12	2.05	0.70
1:B:334:VAL:HG11	1:B:351:PHE:HE2	1.56	0.70
2:D:388:ILE:HG21	2:D:396:LEU:HD11	1.72	0.70
2:F:396:LEU:HD13	2:F:400:ASP:HB3	1.73	0.70
2:E:223:ASN:HD22	2:E:223:ASN:H	1.40	0.70
2:E:223:ASN:H	2:E:223:ASN:ND2	1.88	0.69
1:A:196:LYS:H	1:A:196:LYS:HD2	1.57	0.69
2:F:13:ILE:HD13	2:F:69:LEU:HD13	1.75	0.69
1:A:151:LYS:HE2	1:A:427:LEU:O	1.93	0.68
1:B:171:ARG:HB2	1:B:171:ARG:NH1	2.08	0.68
1:C:400:VAL:HG12	1:C:418:LEU:HD21	1.76	0.68
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.23	0.68
2:E:201:ILE:HD13	2:E:208:LEU:HD11	1.76	0.68
2:E:183:PHE:HB3	2:E:217:LEU:HD23	1.74	0.68
1:B:114:ALA:HB2	1:B:121:ILE:HD11	1.75	0.68
1:B:156:LEU:HD22	1:B:391:LYS:HD2	1.75	0.67
2:E:280:GLY:HA2	3:G:262:LEU:HD21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:228:ALA:O	2:F:232:VAL:HG22	1.95	0.67
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.75	0.67
1:A:97:VAL:HG11	1:A:249:SER:HB3	1.76	0.67
1:B:497:LEU:HA	1:B:500:ILE:HD12	1.75	0.67
2:D:282:GLN:HE21	2:D:282:GLN:N	1.82	0.67
3:G:20:THR:HG22	3:G:236:SER:HB3	1.76	0.67
2:F:92:GLY:HA2	2:F:206:ILE:HD12	1.77	0.66
1:B:361:ILE:CD1	1:B:429:LYS:HE2	2.26	0.66
1:A:44:LEU:O	1:A:47:VAL:HG22	1.96	0.66
1:C:157:VAL:HG12	1:C:371:VAL:C	2.21	0.65
1:C:338:ILE:HD12	1:C:338:ILE:H	1.61	0.65
2:E:126:MET:HE1	2:E:297:THR:HG21	1.79	0.65
2:D:63:MET:HE1	2:D:231:ARG:HB2	1.79	0.65
2:E:139:VAL:HG13	2:E:414:LEU:HB3	1.78	0.65
2:E:163:THR:HG23	7:E:602:PO4:O2	1.96	0.65
1:C:202:ILE:HB	1:C:266:ILE:HG13	1.79	0.65
2:E:276:PRO:HD2	3:G:266:ILE:HD11	1.78	0.65
1:C:468:PHE:CE1	1:C:501:VAL:HG12	2.31	0.65
1:B:211:SER:HA	2:E:126:MET:HE2	1.79	0.65
3:G:81:ILE:HG22	3:G:82:HIS:HD2	1.62	0.65
2:F:80:ALA:HB1	2:F:81:PRO:CD	2.26	0.64
1:A:146:MET:HE3	1:A:146:MET:O	1.97	0.64
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.62	0.64
2:F:188:GLU:O	2:F:221:GLN:HB3	1.98	0.64
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.79	0.64
2:F:336:SER:HB3	2:F:339:ILE:HG13	1.79	0.64
1:A:469:LEU:O	1:A:473:ILE:HG13	1.98	0.64
1:B:151:LYS:NZ	1:B:430:GLN:HB2	2.13	0.64
2:D:220:GLY:HA3	2:D:232:VAL:HG11	1.80	0.64
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.78	0.64
2:D:143:LEU:CD1	2:D:350:PRO:HB3	2.28	0.63
2:E:282:GLN:H	2:E:282:GLN:NE2	1.96	0.63
2:E:390:ILE:HG21	3:G:28:ALA:HB3	1.80	0.63
1:A:333:ASP:HB3	8:A:2073:HOH:O	1.98	0.63
1:A:360:GLY:O	1:A:429:LYS:HE2	1.98	0.63
2:F:188:GLU:O	2:F:222:MET:HG2	1.99	0.63
1:A:87:ILE:H	1:A:87:ILE:HD12	1.64	0.62
1:B:456:LEU:HD23	1:B:461:ILE:HD13	1.81	0.62
2:D:258:ILE:HD11	2:D:292:MET:SD	2.39	0.62
2:D:408:ARG:NH1	2:D:454:GLU:OE1	2.30	0.62
1:C:423:ARG:HD3	1:C:461:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:282:GLN:H	2:E:282:GLN:HE21	1.45	0.62
1:A:408:SER:O	1:A:409:ASP:HB2	1.98	0.62
2:F:339:ILE:HG22	2:F:344:ILE:HB	1.82	0.62
1:B:65:ASN:ND2	2:F:17:ILE:HG23	2.15	0.62
1:B:201:CYS:O	1:B:229:THR:HA	1.99	0.62
2:D:93:ARG:NH2	2:D:106:GLY:O	2.24	0.62
1:B:286:ARG:HA	2:E:275:ILE:HD12	1.83	0.61
1:B:171:ARG:HH22	2:E:356:ARG:HH21	1.47	0.61
1:A:151:LYS:NZ	1:A:430:GLN:HB2	2.15	0.61
2:E:89:GLU:OE2	2:E:110:THR:HG22	2.01	0.61
1:A:158:PRO:HG3	1:A:379:GLN:NE2	2.16	0.61
2:E:149:GLY:HA2	2:E:304:ILE:O	2.00	0.61
1:B:185:ASN:HB2	1:B:435:PRO:HB2	1.83	0.61
1:B:453:LEU:HD13	1:B:461:ILE:HG23	1.83	0.60
1:B:141:SER:O	1:B:143:ARG:NH1	2.33	0.60
2:D:345:TYR:HA	2:D:346:PRO:C	2.25	0.60
2:E:29:LEU:HD23	2:E:52:HIS:ND1	2.15	0.60
1:A:392:LEU:O	1:A:396:GLN:HG3	2.02	0.60
2:E:167:MET:HE3	2:E:420:VAL:HG11	1.83	0.60
1:A:62:MET:HE3	1:A:64:LEU:HD21	1.84	0.60
1:A:121:ILE:HD11	8:A:2011:HOH:O	2.01	0.60
1:B:381:ARG:O	1:B:385:GLN:HG3	2.02	0.60
1:B:62:MET:HG3	1:B:95:VAL:HG21	1.83	0.60
2:F:111:LYS:HB2	2:F:112:GLN:OE1	2.01	0.60
1:B:400:VAL:HG12	1:B:418:LEU:HD21	1.83	0.60
2:F:405:SER:O	2:F:409:LYS:HG3	2.02	0.60
2:D:314:ALA:O	2:D:315:ASP:HB2	2.02	0.60
1:C:99:VAL:HG13	1:C:253:MET:HA	1.83	0.60
1:B:303:SER:HB2	2:F:222:MET:HB2	1.83	0.59
1:C:110:ALA:HB2	1:C:246:ALA:HB2	1.84	0.59
3:G:23:MET:SD	3:G:232:MET:HE2	2.42	0.59
2:F:406:ARG:HH21	2:F:447:GLY:HA3	1.68	0.59
1:A:157:VAL:N	1:A:158:PRO:HD3	2.17	0.59
1:C:23:VAL:HG12	1:C:23:VAL:O	2.02	0.59
1:B:102:GLU:HG3	1:B:122:GLY:C	2.27	0.59
1:B:140:ILE:HB	1:B:313:ASN:HB3	1.83	0.59
1:C:323:ALA:O	1:C:324:LEU:HD23	2.03	0.59
1:C:338:ILE:HB	1:C:339:PRO:HD3	1.85	0.59
2:F:357:ILE:HG23	2:F:362:ILE:HG21	1.84	0.59
2:D:388:ILE:HD13	2:D:396:LEU:HD11	1.83	0.59
2:E:221:GLN:N	2:E:224:GLU:OE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ASN:HB2	1:B:435:PRO:CB	2.33	0.59
1:A:44:LEU:HB3	1:A:47:VAL:HG22	1.85	0.59
1:C:404:ALA:C	1:C:406:PHE:N	2.61	0.59
2:D:234:LEU:CD2	2:D:292:MET:HG3	2.32	0.59
2:E:422:GLU:HG2	2:E:427:HIS:O	2.02	0.59
2:F:345:TYR:HA	2:F:346:PRO:C	2.26	0.59
1:C:278:TYR:CE2	1:C:295:PRO:HG2	2.38	0.59
2:D:366:GLU:O	2:D:370:VAL:HG23	2.03	0.58
2:E:321:ALA:HB3	2:E:322:PRO:HD3	1.85	0.58
1:A:151:LYS:HZ1	1:A:430:GLN:HB2	1.68	0.58
1:B:361:ILE:HD12	1:B:429:LYS:HE2	1.85	0.58
3:G:81:ILE:HG13	3:G:224:GLU:HA	1.85	0.58
2:F:223:ASN:HD22	2:F:223:ASN:N	2.00	0.58
1:A:106:ARG:NH2	1:A:119:GLY:O	2.30	0.58
1:A:362:ARG:HA	1:A:363:PRO:C	2.28	0.58
1:C:423:ARG:CD	1:C:461:ILE:HD11	2.34	0.58
1:A:440:GLU:HB3	1:A:469:LEU:HD11	1.85	0.58
1:C:187:LYS:CE	1:C:224:ASP:HB3	2.31	0.58
2:F:207:ASN:ND2	2:F:210:ASP:HB2	2.19	0.58
2:E:224:GLU:O	2:E:229:ARG:NH1	2.37	0.57
1:A:218:LYS:CD	2:D:128:VAL:HG21	2.34	0.57
1:B:44:LEU:HB3	1:B:47:VAL:HG13	1.87	0.57
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.85	0.57
1:C:418:LEU:O	1:C:422:VAL:HG23	2.03	0.57
1:C:26:GLU:HA	1:C:45:ARG:HB2	1.87	0.57
1:C:127:ARG:HH21	1:C:131:LEU:HD12	1.70	0.57
1:C:291:ARG:HD3	1:C:337:TYR:CE1	2.39	0.57
2:F:130:GLN:HB3	2:F:357:ILE:CD1	2.33	0.57
2:D:308:GLN:HG3	8:D:2031:HOH:O	2.03	0.57
2:E:415:SER:HB2	2:E:459:MET:SD	2.45	0.57
1:B:103:LEU:HB2	1:B:230:ILE:HD13	1.87	0.57
1:C:105:GLY:HA2	1:C:226:MET:O	2.04	0.57
2:E:10:THR:HG23	2:E:76:LEU:HD23	1.87	0.57
1:A:144:GLU:CB	1:A:161:ARG:HG3	2.35	0.57
2:E:387:ILE:H	2:E:387:ILE:HD12	1.70	0.57
1:B:451:GLY:C	1:B:453:LEU:H	2.13	0.56
2:D:89:GLU:CD	2:D:89:GLU:H	2.11	0.56
1:A:48:GLN:HG2	2:E:70:VAL:CG2	2.35	0.56
1:A:138:PRO:HB3	1:A:316:PHE:CZ	2.40	0.56
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.87	0.56
2:D:80:ALA:HB1	2:D:81:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:96:ASN:HB2	2:D:100:GLU:O	2.05	0.56
2:E:434:LEU:O	2:E:438:ILE:HG12	2.06	0.56
1:A:49:ALA:O	1:A:50:GLU:HB2	2.06	0.56
2:F:245:ASP:C	2:F:247:GLU:H	2.13	0.56
1:C:438:ILE:O	1:C:442:VAL:HG23	2.06	0.56
1:A:157:VAL:N	1:A:158:PRO:CD	2.69	0.56
1:B:287:ARG:NE	8:B:2051:HOH:O	2.38	0.56
1:C:175:LYS:HE2	4:C:600:ANP:O1B	2.06	0.56
2:F:130:GLN:HB3	2:F:357:ILE:HD12	1.88	0.56
1:A:390:MET:CE	1:A:424:LEU:HD22	2.27	0.55
1:B:246:ALA:HB3	1:B:247:PRO:HD3	1.88	0.55
2:D:439:LYS:O	2:D:443:GLN:HG3	2.05	0.55
2:E:263:GLN:O	2:E:267:GLU:HG3	2.06	0.55
2:F:174:ALA:O	2:F:177:HIS:HB3	2.06	0.55
1:B:127:ARG:HE	1:B:131:LEU:HD12	1.71	0.55
2:E:319:ASP:O	2:E:322:PRO:HD2	2.07	0.55
1:A:376:SER:O	1:A:377:ALA:C	2.50	0.55
1:C:335:SER:O	2:D:314:ALA:HB1	2.07	0.55
2:E:360:PRO:HG3	2:E:368:TYR:CD2	2.41	0.55
1:B:334:VAL:HG11	1:B:351:PHE:CE2	2.40	0.55
2:E:257:ASN:HB2	2:E:309:ALA:O	2.07	0.55
2:E:384:LEU:O	2:E:388:ILE:HG12	2.07	0.55
2:F:455:GLN:O	2:F:469:LYS:HE2	2.06	0.55
2:D:277:SER:OG	2:D:278:ALA:N	2.36	0.54
1:B:146:MET:HG3	1:B:322:THR:HG21	1.90	0.54
2:D:397:SER:O	2:D:401:LYS:HG2	2.08	0.54
1:C:347:ASP:C	1:C:373:ARG:HG3	2.32	0.54
1:B:452:TYR:OH	1:B:498:LYS:HG3	2.08	0.54
1:C:44:LEU:HB3	1:C:47:VAL:HG22	1.88	0.54
2:D:63:MET:CE	2:D:97:VAL:HG11	2.37	0.54
1:A:313:ASN:OD1	1:A:316:PHE:HD1	1.91	0.54
1:A:439:GLU:CD	1:A:439:GLU:H	2.16	0.54
1:C:172:GLN:HE21	4:C:600:ANP:HNB1	1.56	0.54
1:B:97:VAL:HB	1:B:98:PRO:HD2	1.88	0.54
1:B:158:PRO:O	1:B:375:GLY:HA3	2.07	0.54
1:A:190:ASN:HA	1:A:198:LYS:HG2	1.90	0.54
1:A:278:TYR:HA	1:A:281:MET:CE	2.38	0.54
1:B:210:ARG:O	1:B:211:SER:C	2.51	0.53
1:B:419:SER:O	1:B:423:ARG:HG2	2.08	0.53
1:B:62:MET:HG3	1:B:95:VAL:CG2	2.39	0.53
2:E:105:ARG:HD3	8:E:2014:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:174:ALA:CB	2:E:214:LYS:HD3	2.39	0.53
1:A:440:GLU:O	1:A:444:VAL:HG13	2.07	0.53
3:G:210:ALA:O	3:G:211:ASN:C	2.51	0.53
1:B:32:LEU:CG	1:B:42:HIS:HB2	2.39	0.53
1:B:468:PHE:CE1	1:B:501:VAL:HG12	2.43	0.53
2:D:181:SER:O	2:D:215:VAL:HA	2.08	0.53
2:F:443:GLN:HE21	2:F:449:TYR:HE2	1.56	0.53
3:G:239:ALA:O	3:G:243:ILE:HG13	2.09	0.53
1:B:164:ARG:HD3	1:B:164:ARG:N	2.24	0.53
1:B:251:CYS:HB2	1:B:268:TYR:OH	2.09	0.53
2:E:84:ILE:HG21	2:E:235:THR:HG23	1.90	0.53
2:E:29:LEU:HD23	2:E:52:HIS:CE1	2.43	0.53
1:B:383:MET:SD	1:B:387:ALA:HB2	2.49	0.53
1:C:45:ARG:NH2	1:C:68:PRO:O	2.42	0.53
2:E:12:ARG:NH2	2:E:24:GLN:OE1	2.41	0.52
2:E:243:PHE:HB2	2:E:251:VAL:HG21	1.91	0.52
2:E:275:ILE:HG23	3:G:266:ILE:HD13	1.90	0.52
1:A:215:GLN:O	1:A:218:LYS:HB3	2.09	0.52
2:D:405:SER:O	2:D:409:LYS:HG3	2.10	0.52
2:D:417:PRO:CA	2:D:459:MET:HE1	2.40	0.52
2:D:419:GLN:O	2:D:422:GLU:HG3	2.09	0.52
2:E:48:GLU:OE2	2:E:231:ARG:NH2	2.42	0.52
2:E:243:PHE:HB2	2:E:251:VAL:CG2	2.40	0.52
1:A:468:PHE:O	1:A:472:VAL:HG13	2.09	0.52
1:A:498:LYS:O	1:A:502:THR:HG23	2.10	0.52
1:C:34:ILE:HD13	1:C:39:ALA:HB2	1.90	0.52
1:C:460:LYS:HE2	8:C:2103:HOH:O	2.08	0.52
2:E:170:ILE:HG21	2:E:215:VAL:CG2	2.39	0.52
3:G:228:ARG:O	3:G:232:MET:HG2	2.10	0.52
1:A:62:MET:CE	1:A:64:LEU:HD21	2.39	0.52
1:B:240:ALA:HB3	1:B:241:PRO:HD3	1.92	0.52
2:D:243:PHE:O	2:D:247:GLU:HB2	2.09	0.52
2:E:388:ILE:HD12	2:E:396:LEU:HD11	1.92	0.52
1:C:153:VAL:HA	1:C:157:VAL:HG23	1.91	0.52
2:E:314:ALA:O	2:E:315:ASP:HB2	2.08	0.52
1:A:347:ASP:OD1	2:E:191:ARG:NH1	2.43	0.52
1:B:48:GLN:HG3	1:B:51:GLU:OE1	2.09	0.52
1:C:129:VAL:HG21	1:C:245:LEU:HD11	1.91	0.52
2:E:282:GLN:HE21	2:E:282:GLN:N	2.07	0.52
2:F:89:GLU:CD	2:F:89:GLU:H	2.16	0.52
2:D:285:LEU:C	2:D:285:LEU:HD23	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLU:HB3	1:B:46:ASN:ND2	2.24	0.52
2:D:456:ALA:HB1	2:D:466:ALA:O	2.09	0.52
3:G:38:LEU:HD11	3:G:42:ARG:NH2	2.25	0.52
1:B:129:VAL:O	1:B:308:ARG:NH1	2.39	0.52
1:B:486:ASP:C	1:B:488:LYS:H	2.18	0.52
1:A:156:LEU:HD13	1:A:367:VAL:HG11	1.92	0.51
1:B:161:ARG:HA	1:B:322:THR:OG1	2.10	0.51
2:D:417:PRO:HA	2:D:459:MET:HE1	1.92	0.51
2:E:334:VAL:HG21	2:E:352:ASP:HB3	1.92	0.51
2:F:185:GLY:HA3	2:F:219:TYR:CD1	2.44	0.51
2:D:9:THR:HG22	2:D:27:GLU:OE1	2.10	0.51
1:A:479:LEU:O	1:A:479:LEU:HD22	2.10	0.51
1:A:204:VAL:HG12	1:A:206:ILE:HD11	1.90	0.51
2:E:276:PRO:HD2	3:G:266:ILE:CD1	2.40	0.51
1:A:137:ILE:N	1:A:138:PRO:CD	2.73	0.51
2:D:340:ALA:HB2	2:D:347:ALA:HB2	1.91	0.51
2:F:126:MET:HE3	8:F:2035:HOH:O	2.10	0.51
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.46	0.51
1:B:94:ILE:O	1:B:95:VAL:C	2.54	0.51
2:F:189:ARG:HB2	2:F:192:GLU:HG3	1.92	0.51
1:B:174:GLY:HA2	4:B:600:ANP:PA	2.51	0.51
1:C:292:GLU:O	1:C:293:ALA:CB	2.54	0.51
1:A:99:VAL:CG2	1:A:253:MET:HA	2.40	0.51
1:C:501:VAL:O	1:C:505:LEU:HB2	2.10	0.51
2:F:166:ILE:HG22	2:F:167:MET:HE2	1.93	0.51
1:B:141:SER:OG	1:B:143:ARG:NH1	2.44	0.51
1:B:423:ARG:O	1:B:426:GLU:N	2.43	0.51
2:E:374:VAL:O	2:E:377:ILE:HG22	2.11	0.50
1:C:183:ILE:HD11	1:C:267:ILE:CD1	2.41	0.50
1:B:468:PHE:O	1:B:472:VAL:HG22	2.11	0.50
2:E:138:LYS:NZ	2:E:413:PHE:O	2.43	0.50
3:G:39:LYS:N	3:G:40:PRO:HD2	2.26	0.50
1:C:50:GLU:OE2	2:D:67:GLU:HG2	2.10	0.50
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.94	0.50
2:F:151:LYS:HZ1	2:F:293:GLN:HB3	1.77	0.50
1:A:133:ALA:HB1	1:A:134:PRO:HD2	1.92	0.50
2:D:313:PRO:O	2:D:314:ALA:C	2.54	0.50
1:B:479:LEU:CD1	1:B:497:LEU:HD13	2.42	0.50
1:C:27:GLU:O	1:C:90:ARG:HG3	2.11	0.50
1:A:389:THR:HG22	1:A:393:GLU:OE2	2.11	0.50
1:B:479:LEU:HD11	1:B:497:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:ALA:HA	1:C:385:GLN:OE1	2.11	0.50
2:D:402:LEU:HD21	2:D:406:ARG:NH2	2.27	0.50
1:A:196:LYS:HD2	1:A:196:LYS:N	2.25	0.49
1:C:30:ARG:HG2	1:C:30:ARG:HH11	1.77	0.49
2:D:218:VAL:HG21	2:D:236:GLY:HA2	1.94	0.49
2:E:210:ASP:O	2:E:212:THR:N	2.39	0.49
2:E:281:TYR:HB3	2:E:282:GLN:HE21	1.77	0.49
1:B:486:ASP:C	1:B:488:LYS:N	2.67	0.49
2:E:393:MET:HG3	2:E:396:LEU:HD11	1.93	0.49
2:F:241:GLU:CD	2:F:295:ARG:HH21	2.21	0.49
2:F:336:SER:CB	2:F:339:ILE:HG13	2.42	0.49
1:B:32:LEU:HG	1:B:42:HIS:HB2	1.94	0.49
1:C:40:ARG:NH1	1:C:70:ASN:OD1	2.45	0.49
2:E:319:ASP:O	2:E:320:PRO:C	2.54	0.49
2:E:357:ILE:HB	2:E:362:ILE:HG21	1.93	0.49
2:F:462:PRO:HD2	2:F:465:GLU:CD	2.37	0.49
1:C:30:ARG:HA	1:C:86:ASP:O	2.12	0.49
1:C:440:GLU:O	1:C:444:VAL:HG13	2.11	0.49
2:E:52:HIS:HB3	8:E:2006:HOH:O	2.12	0.49
1:A:180:ILE:O	1:A:184:ILE:HG12	2.13	0.49
1:B:393:GLU:HA	1:B:396:GLN:OE1	2.11	0.49
1:C:399:GLU:CG	2:D:342:LEU:HD22	2.43	0.49
1:C:443:ALA:O	1:C:446:TYR:HB3	2.12	0.49
2:E:366:GLU:O	2:E:370:VAL:HG23	2.12	0.49
1:B:240:ALA:N	1:B:241:PRO:CD	2.75	0.49
2:D:172:ASN:ND2	2:D:431:LEU:HD11	2.27	0.49
2:E:82:ILE:CG2	2:E:116:ILE:HD13	2.42	0.49
2:E:387:ILE:HD12	2:E:387:ILE:N	2.28	0.49
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.93	0.49
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.95	0.49
1:A:159:ILE:HD12	1:A:165:GLU:HG2	1.92	0.49
1:A:213:VAL:O	1:A:216:LEU:HB3	2.13	0.49
1:B:151:LYS:HG3	1:B:430:GLN:OE1	2.13	0.49
2:E:144:ALA:N	2:E:145:PRO:HD3	2.27	0.49
2:F:134:VAL:HA	2:F:141:ASP:OD1	2.12	0.49
1:B:209:LYS:HB3	2:E:294:GLU:OE2	2.12	0.49
1:B:211:SER:N	2:E:126:MET:HE2	2.28	0.49
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.94	0.49
2:E:66:THR:HB	2:E:69:LEU:HD12	1.94	0.49
2:F:153:GLY:HA3	2:F:329:LEU:HD13	1.95	0.49
1:B:41:VAL:HG11	1:B:44:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:PRO:HD2	1:C:298:VAL:CG2	2.42	0.49
2:E:440:GLY:O	2:E:444:ILE:HG12	2.13	0.49
2:F:63:MET:HE1	2:F:231:ARG:HB2	1.94	0.49
1:B:136:ILE:HG23	2:F:194:ASN:HA	1.94	0.48
2:D:108:ILE:HG22	2:D:110:THR:HG23	1.95	0.48
1:C:300:TYR:CZ	1:C:304:ARG:HD3	2.49	0.48
2:F:363:VAL:HG23	2:F:367:HIS:HB3	1.95	0.48
1:A:67:GLU:HB2	1:A:70:ASN:O	2.12	0.48
1:B:338:ILE:HB	1:B:339:PRO:HD3	1.95	0.48
1:A:338:ILE:N	1:A:339:PRO:CD	2.75	0.48
1:A:485:THR:C	1:A:487:GLY:H	2.21	0.48
1:B:159:ILE:HG22	1:B:160:GLY:N	2.27	0.48
1:C:367:VAL:HG21	1:C:398:ARG:NH2	2.27	0.48
2:D:20:VAL:HG21	2:D:271:LEU:HB2	1.95	0.48
2:D:166:ILE:HG13	2:D:307:VAL:HG11	1.96	0.48
2:F:452:LEU:HD22	2:F:470:ALA:CB	2.43	0.48
1:B:188:ARG:HG2	1:B:188:ARG:HH11	1.78	0.48
2:D:474:ALA:O	2:D:475:GLU:HB2	2.12	0.48
3:G:13:ILE:HD13	3:G:242:MET:SD	2.53	0.48
1:A:74:VAL:HG13	1:A:241:PRO:HG3	1.96	0.48
1:C:258:ARG:NH1	1:C:308:ARG:O	2.46	0.48
2:E:103:ASP:O	2:E:104:GLU:HB2	2.12	0.48
2:F:52:HIS:CD2	2:F:58:VAL:HG12	2.49	0.48
1:A:420:ARG:HH21	1:A:451:GLY:CA	2.26	0.48
1:B:27:GLU:OE1	1:B:90:ARG:NH1	2.47	0.48
1:B:41:VAL:HG11	1:B:44:LEU:CD1	2.43	0.48
1:B:100:GLY:O	1:B:103:LEU:HD13	2.14	0.48
2:D:324:THR:HG22	2:D:324:THR:O	2.14	0.48
2:E:387:ILE:HG23	2:E:391:LEU:HD12	1.95	0.48
2:F:97:VAL:HG21	2:F:228:ALA:HB1	1.96	0.48
2:F:139:VAL:HG23	8:F:2100:HOH:O	2.13	0.48
2:F:422:GLU:HG2	2:F:427:HIS:O	2.14	0.48
1:C:168:ILE:HG23	1:C:351:PHE:HD1	1.78	0.48
2:D:161:GLY:O	2:D:162:LYS:C	2.55	0.48
2:E:89:GLU:CD	2:E:89:GLU:H	2.22	0.48
2:F:406:ARG:HH21	2:F:447:GLY:CA	2.27	0.48
1:B:410:LEU:O	1:B:411:ASP:HB3	2.12	0.48
1:C:290:GLY:O	1:C:291:ARG:C	2.57	0.48
2:D:186:VAL:HG13	2:D:232:VAL:HG23	1.94	0.48
1:A:48:GLN:HG2	2:E:70:VAL:HG22	1.95	0.47
1:A:87:ILE:HD12	1:A:87:ILE:N	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ASP:C	1:A:488:LYS:H	2.22	0.47
1:B:218:LYS:HG3	2:E:128:VAL:HB	1.96	0.47
1:C:52:MET:HE2	1:C:61:GLY:O	2.14	0.47
1:C:452:TYR:CD2	1:C:501:VAL:HG21	2.48	0.47
2:D:408:ARG:HD3	2:D:454:GLU:OE2	2.14	0.47
2:E:183:PHE:HB3	2:E:217:LEU:CD2	2.42	0.47
2:D:84:ILE:HB	2:D:85:PRO:HD2	1.95	0.47
2:D:252:LEU:HD23	2:D:305:THR:HB	1.96	0.47
2:D:430:LYS:HD2	2:D:465:GLU:OE2	2.14	0.47
2:E:370:VAL:HG21	2:E:438:ILE:CG2	2.44	0.47
2:F:374:VAL:HG13	2:F:410:ILE:HG21	1.97	0.47
2:F:415:SER:HB2	2:F:459:MET:HE2	1.95	0.47
1:A:94:ILE:HG21	1:A:128:ARG:NH1	2.29	0.47
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.96	0.47
1:A:286:ARG:NH2	2:D:273:GLY:O	2.48	0.47
1:B:194:ASP:C	1:B:196:LYS:H	2.22	0.47
2:D:410:ILE:O	2:D:414:LEU:HG	2.14	0.47
2:E:405:SER:O	2:E:409:LYS:HG3	2.14	0.47
2:F:151:LYS:NZ	2:F:293:GLN:HB3	2.29	0.47
3:G:28:ALA:HA	3:G:229:MET:SD	2.54	0.47
1:B:102:GLU:HG3	1:B:122:GLY:O	2.15	0.47
2:F:389:ALA:HB1	3:G:242:MET:HE1	1.95	0.47
2:F:389:ALA:HB1	3:G:242:MET:CE	2.44	0.47
1:A:195:GLU:HA	1:A:198:LYS:HD2	1.95	0.47
1:A:420:ARG:HH21	1:A:451:GLY:HA3	1.79	0.47
1:C:99:VAL:CG1	1:C:256:TYR:HB2	2.45	0.47
1:C:137:ILE:HG21	2:D:104:GLU:OE1	2.14	0.47
1:C:362:ARG:HA	1:C:363:PRO:C	2.39	0.47
2:E:456:ALA:HB1	2:E:466:ALA:O	2.14	0.47
1:B:165:GLU:O	1:B:325:PRO:HD2	2.14	0.47
1:B:357:PHE:HD1	1:B:358:TYR:HD1	1.63	0.47
1:B:451:GLY:O	1:B:453:LEU:N	2.48	0.47
1:C:103:LEU:O	1:C:106:ARG:HB2	2.15	0.47
1:C:297:ASP:HA	2:D:267:GLU:HG2	1.96	0.47
2:E:185:GLY:HA3	2:E:188:GLU:HG2	1.97	0.47
1:A:185:ASN:OD1	1:A:188:ARG:NH1	2.48	0.47
1:A:354:THR:HG23	8:A:2028:HOH:O	2.15	0.47
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.79	0.47
2:D:279:VAL:HG12	2:D:279:VAL:O	2.15	0.47
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.44	0.47
3:G:81:ILE:HG22	3:G:82:HIS:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:HD2	1:A:309:ALA:HB3	1.97	0.47
1:A:373:ARG:NH2	2:E:189:ARG:NH2	2.62	0.47
1:A:380:THR:HG23	8:A:2021:HOH:O	2.15	0.47
1:C:55:PHE:O	1:C:56:SER:C	2.58	0.47
1:C:456:LEU:HG	1:C:457:GLU:N	2.30	0.47
2:E:374:VAL:HG13	2:E:410:ILE:HG21	1.97	0.47
1:A:244:TYR:HE1	1:A:301:LEU:HD11	1.80	0.46
1:B:175:LYS:NZ	8:B:2024:HOH:O	2.47	0.46
1:C:74:VAL:HG11	1:C:281:MET:SD	2.56	0.46
2:F:95:MET:HG3	2:F:99:GLY:HA2	1.96	0.46
1:A:99:VAL:HG22	1:A:253:MET:HA	1.97	0.46
1:A:286:ARG:NH2	3:G:272:LEU:HD13	2.31	0.46
1:B:420:ARG:HH21	1:B:451:GLY:CA	2.28	0.46
1:C:404:ALA:O	1:C:406:PHE:N	2.48	0.46
1:A:144:GLU:HA	1:A:145:PRO:HD3	1.80	0.46
1:C:309:ALA:HB1	1:C:321:LEU:O	2.14	0.46
2:D:228:ALA:O	2:D:232:VAL:HG22	2.15	0.46
2:D:321:ALA:HB3	2:D:322:PRO:HD3	1.96	0.46
2:E:97:VAL:HG21	2:E:228:ALA:HB1	1.96	0.46
2:E:254:PHE:HA	2:E:307:VAL:O	2.15	0.46
1:A:48:GLN:HA	2:E:69:LEU:O	2.16	0.46
2:F:190:THR:HA	2:F:221:GLN:HG3	1.96	0.46
1:B:385:GLN:OE1	1:B:488:LYS:HG3	2.15	0.46
1:B:438:ILE:HG22	8:B:2080:HOH:O	2.16	0.46
2:D:383:SER:O	2:D:387:ILE:HD12	2.15	0.46
2:E:49:VAL:HA	2:E:60:THR:HG22	1.98	0.46
1:A:207:GLY:HA3	1:A:273:LYS:HD3	1.96	0.46
1:A:452:TYR:CD2	1:A:501:VAL:HG21	2.50	0.46
1:B:137:ILE:N	1:B:138:PRO:CD	2.78	0.46
1:B:389:THR:O	1:B:393:GLU:HG3	2.15	0.46
2:F:289:MET:HE3	2:F:289:MET:HB2	1.86	0.46
1:A:207:GLY:O	1:A:236:ALA:HB2	2.14	0.46
2:E:370:VAL:HG21	2:E:438:ILE:HG23	1.96	0.46
2:E:422:GLU:OE1	2:E:428:LEU:HA	2.16	0.46
2:E:449:TYR:CE2	2:E:463:ILE:HG12	2.50	0.46
2:F:360:PRO:HD3	2:F:368:TYR:CD1	2.51	0.46
1:A:297:ASP:HA	8:E:2026:HOH:O	2.15	0.46
1:A:338:ILE:N	1:A:339:PRO:HD2	2.31	0.46
2:E:80:ALA:HB1	2:E:81:PRO:CD	2.39	0.46
2:F:80:ALA:HB1	2:F:81:PRO:HD3	1.97	0.46
2:F:212:THR:O	2:F:214:LYS:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LEU:HD12	1:B:103:LEU:N	2.30	0.46
1:B:171:ARG:HH11	1:B:171:ARG:CB	2.24	0.46
2:E:421:ALA:HB1	2:E:425:THR:HG21	1.97	0.46
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.46	0.46
1:A:188:ARG:NH2	1:A:436:MET:HA	2.31	0.45
1:A:267:ILE:HG13	1:A:324:LEU:HB2	1.97	0.45
1:B:353:GLU:HG3	1:B:366:ASN:HB2	1.98	0.45
2:D:410:ILE:HG13	2:D:444:ILE:HG21	1.98	0.45
3:G:38:LEU:HD11	3:G:42:ARG:CZ	2.46	0.45
1:A:180:ILE:O	1:A:181:ASP:C	2.59	0.45
1:B:286:ARG:HA	2:E:275:ILE:CD1	2.47	0.45
1:C:361:ILE:O	1:C:364:ALA:HA	2.16	0.45
2:E:36:LEU:O	2:E:46:VAL:HA	2.16	0.45
2:E:152:ILE:HA	2:E:331:ALA:O	2.17	0.45
2:F:393:MET:SD	2:F:404:VAL:HG11	2.56	0.45
1:A:157:VAL:O	1:A:159:ILE:HD13	2.15	0.45
1:A:450:ARG:HD2	8:A:2095:HOH:O	2.16	0.45
2:D:95:MET:HG3	2:D:108:ILE:CD1	2.45	0.45
2:F:282:GLN:HA	2:F:283:PRO:HD3	1.87	0.45
2:F:348:VAL:O	2:F:350:PRO:HD3	2.16	0.45
1:A:180:ILE:HD11	1:A:216:LEU:CD2	2.46	0.45
1:A:397:TYR:CG	1:A:421:GLY:HA3	2.51	0.45
1:B:99:VAL:CG1	1:B:256:TYR:HB2	2.47	0.45
1:B:127:ARG:NE	1:B:131:LEU:HD12	2.31	0.45
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.98	0.45
1:A:403:PHE:CD1	3:G:22:SER:HB2	2.52	0.45
1:C:48:GLN:HA	2:D:69:LEU:O	2.17	0.45
2:E:467:VAL:O	2:E:468:ALA:C	2.60	0.45
2:F:17:ILE:HD12	2:F:17:ILE:N	2.31	0.45
2:F:229:ARG:HA	2:F:232:VAL:CG2	2.47	0.45
1:A:204:VAL:CG1	1:A:206:ILE:HD11	2.46	0.45
1:B:107:VAL:HG12	1:B:115:ILE:HD11	1.99	0.45
2:E:95:MET:HE3	8:E:2012:HOH:O	2.15	0.45
1:A:400:VAL:HG12	1:A:418:LEU:CD2	2.44	0.45
1:B:392:LEU:O	1:B:395:ALA:HB3	2.17	0.45
1:C:76:PHE:HB3	1:C:242:LEU:HD21	1.99	0.45
2:E:170:ILE:HD13	2:E:215:VAL:CG2	2.41	0.45
2:F:337:ARG:HG3	2:F:337:ARG:HH11	1.81	0.45
1:A:249:SER:O	1:A:253:MET:HG3	2.15	0.45
1:C:234:ALA:HA	1:C:238:ASP:OD2	2.17	0.45
2:D:140:VAL:HG23	8:D:2027:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:SER:O	1:A:423:ARG:HD3	2.17	0.45
1:B:451:GLY:C	1:B:453:LEU:N	2.72	0.45
1:C:353:GLU:CD	1:C:366:ASN:HD22	2.24	0.45
2:D:363:VAL:HB	2:D:367:HIS:ND1	2.32	0.45
2:E:453:PRO:O	2:E:454:GLU:C	2.60	0.45
1:A:204:VAL:HG12	1:A:206:ILE:CD1	2.47	0.44
1:C:384:LYS:HE3	8:C:2089:HOH:O	2.17	0.44
2:E:116:ILE:HA	2:E:238:THR:OG1	2.16	0.44
2:E:292:MET:SD	2:E:293:GLN:NE2	2.90	0.44
3:G:237:LYS:O	3:G:241:GLU:HG3	2.16	0.44
3:G:259:THR:HG22	3:G:263:ILE:HD12	1.99	0.44
1:A:164:ARG:HD3	1:A:164:ARG:N	2.32	0.44
1:A:486:ASP:OD2	1:A:490:SER:HB3	2.17	0.44
1:B:54:GLU:HG3	1:B:91:THR:HG22	1.99	0.44
2:D:103:ASP:O	2:D:104:GLU:HB2	2.17	0.44
2:D:319:ASP:O	2:D:320:PRO:C	2.60	0.44
2:E:94:ILE:HD11	2:E:197:TYR:CG	2.52	0.44
2:F:94:ILE:HG22	2:F:102:ILE:HD11	1.98	0.44
1:B:99:VAL:O	1:B:123:SER:OG	2.36	0.44
1:C:33:SER:OG	1:C:40:ARG:HB2	2.18	0.44
1:C:414:THR:O	1:C:418:LEU:HG	2.17	0.44
2:E:189:ARG:NH1	2:E:192:GLU:OE1	2.51	0.44
1:B:55:PHE:O	1:B:56:SER:C	2.60	0.44
1:B:190:ASN:HA	1:B:198:LYS:HG2	1.99	0.44
2:E:377:ILE:HG21	2:E:410:ILE:CD1	2.47	0.44
2:F:34:ASN:O	2:F:49:VAL:HG23	2.18	0.44
1:A:209:LYS:HB2	2:D:294:GLU:OE1	2.18	0.44
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.52	0.44
2:E:96:ASN:HB2	2:E:102:ILE:CG2	2.47	0.44
2:E:96:ASN:HB2	2:E:102:ILE:HG23	1.99	0.44
1:B:32:LEU:HD21	1:B:42:HIS:HB2	2.00	0.44
1:C:215:GLN:HG3	2:F:356:ARG:HH12	1.83	0.44
2:E:256:ASP:HA	2:E:257:ASN:HA	1.63	0.44
2:F:29:LEU:HA	2:F:30:PRO:HD3	1.78	0.44
2:F:203:SER:OG	2:F:205:VAL:HG13	2.16	0.44
2:F:357:ILE:HG23	2:F:362:ILE:CG2	2.47	0.44
2:F:437:THR:O	2:F:441:PHE:HD2	2.00	0.44
1:A:156:LEU:HD13	1:A:367:VAL:CG1	2.48	0.44
1:B:55:PHE:CE2	1:B:82:ILE:HD13	2.53	0.44
1:B:142:VAL:HG13	8:B:2021:HOH:O	2.17	0.44
1:B:251:CYS:O	1:B:255:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:319:ASP:O	2:F:322:PRO:HD2	2.17	0.44
1:A:105:GLY:HA2	1:A:226:MET:O	2.17	0.44
1:C:419:SER:O	1:C:423:ARG:HG2	2.17	0.44
1:C:503:ASN:O	1:C:506:ALA:HB3	2.18	0.44
2:D:48:GLU:OE2	2:D:231:ARG:NE	2.32	0.44
2:E:310:ILE:CD1	2:E:329:LEU:HD11	2.48	0.44
1:A:136:ILE:HD11	2:E:193:GLY:HA3	1.99	0.44
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.45	0.44
1:C:185:ASN:OD1	1:C:435:PRO:HB2	2.18	0.44
2:D:151:LYS:HE2	2:D:328:HIS:O	2.18	0.44
1:A:166:LEU:HB3	1:A:349:GLN:HG3	2.00	0.43
1:C:151:LYS:HG2	1:C:441:GLN:HG2	1.99	0.43
2:D:266:SER:HB3	2:D:282:GLN:NE2	2.33	0.43
2:D:411:GLN:O	2:D:414:LEU:HB2	2.18	0.43
2:E:120:ALA:O	2:E:121:PRO:C	2.58	0.43
2:E:356:ARG:C	2:E:358:MET:H	2.26	0.43
1:A:211:SER:O	1:A:214:ALA:HB3	2.17	0.43
1:B:237:SER:HB3	8:B:2033:HOH:O	2.18	0.43
1:B:379:GLN:HB3	1:B:384:LYS:HE2	2.00	0.43
2:D:374:VAL:HG13	2:D:410:ILE:HG21	2.00	0.43
2:D:412:ARG:C	2:D:414:LEU:N	2.76	0.43
2:D:452:LEU:HD22	2:D:470:ALA:CB	2.48	0.43
2:E:81:PRO:HG2	2:E:115:ALA:HB1	2.00	0.43
2:E:421:ALA:HB1	2:E:425:THR:CG2	2.48	0.43
1:A:36:ASP:OD1	2:D:274:ARG:NH2	2.51	0.43
1:C:78:ASN:OD1	1:C:80:LYS:HB3	2.17	0.43
1:C:98:PRO:CG	1:C:112:GLY:HA3	2.49	0.43
1:C:225:ALA:HA	1:C:228:TYR:CE2	2.53	0.43
1:C:476:HIS:CD2	1:C:500:ILE:HD11	2.53	0.43
2:F:33:LEU:O	2:F:81:PRO:HB3	2.18	0.43
2:F:226:PRO:HA	2:F:229:ARG:HH21	1.82	0.43
1:A:108:VAL:HG12	1:A:114:ALA:HA	1.99	0.43
1:B:140:ILE:HG22	1:B:311:LYS:HG3	2.00	0.43
1:B:295:PRO:O	1:B:298:VAL:HG22	2.19	0.43
1:C:338:ILE:O	1:C:339:PRO:C	2.61	0.43
1:C:389:THR:HG22	2:D:425:THR:O	2.18	0.43
2:E:449:TYR:HB3	2:E:452:LEU:CD1	2.37	0.43
1:A:117:GLY:C	1:A:119:GLY:H	2.26	0.43
1:A:327:ILE:HD11	1:A:342:VAL:HG21	2.01	0.43
1:B:211:SER:CA	2:E:126:MET:HE2	2.45	0.43
1:B:366:ASN:HD21	1:B:369:LEU:HD12	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:151:LYS:HE3	2:E:296:ILE:HG22	2.01	0.43
2:E:388:ILE:CD1	2:E:396:LEU:HD11	2.48	0.43
3:G:78:CYS:SG	3:G:228:ARG:NH2	2.90	0.43
1:A:286:ARG:HG2	1:A:286:ARG:HH11	1.83	0.43
1:B:33:SER:HB2	2:E:52:HIS:O	2.18	0.43
1:B:106:ARG:NH1	1:B:121:ILE:HD13	2.33	0.43
1:C:240:ALA:N	1:C:241:PRO:CD	2.81	0.43
2:D:447:GLY:O	2:D:448:GLU:C	2.62	0.43
2:E:352:ASP:O	2:E:354:THR:HG23	2.19	0.43
3:G:14:LYS:HG2	3:G:243:ILE:HD13	2.00	0.43
1:C:248:TYR:OH	1:C:301:LEU:HD12	2.19	0.43
2:F:220:GLY:HA3	2:F:232:VAL:HG11	2.00	0.43
1:B:244:TYR:CD2	1:B:281:MET:HE1	2.54	0.43
1:B:269:ASP:HA	1:B:270:ASP:HA	1.74	0.43
1:B:297:ASP:HA	8:F:2061:HOH:O	2.19	0.43
1:C:36:ASP:HB3	1:C:284:LEU:HD13	2.01	0.43
2:D:27:GLU:HB2	2:D:28:GLY:H	1.68	0.43
2:D:468:ALA:O	2:D:469:LYS:C	2.62	0.43
2:E:82:ILE:HB	2:E:116:ILE:CD1	2.49	0.43
1:A:102:GLU:HG3	1:A:122:GLY:C	2.44	0.43
1:A:188:ARG:NH2	1:A:436:MET:C	2.77	0.43
1:C:164:ARG:HD2	1:C:306:LEU:O	2.18	0.43
1:C:381:ARG:HD2	1:C:381:ARG:N	2.33	0.43
1:A:97:VAL:HA	1:A:126:ARG:HH21	1.84	0.43
1:B:176:THR:O	1:B:179:ALA:N	2.49	0.43
2:D:292:MET:HE2	2:D:293:GLN:HG2	1.99	0.43
2:F:163:THR:HG21	2:F:192:GLU:OE1	2.19	0.43
1:A:306:LEU:HD23	1:A:306:LEU:HA	1.74	0.42
1:B:288:PRO:HA	1:B:289:PRO:HD3	1.88	0.42
1:C:201:CYS:O	1:C:229:THR:HA	2.18	0.42
1:C:338:ILE:HD12	1:C:338:ILE:N	2.32	0.42
2:D:17:ILE:HD13	2:D:17:ILE:HG21	1.75	0.42
2:D:49:VAL:HA	2:D:60:THR:HG22	2.01	0.42
2:E:142:LEU:HG	2:E:143:LEU:CD2	2.49	0.42
2:F:83:ARG:NH2	2:F:113:PHE:HB2	2.34	0.42
3:G:10:LEU:HD21	3:G:246:LEU:HB2	2.01	0.42
1:B:204:VAL:HG12	1:B:206:ILE:HG13	2.00	0.42
1:C:200:TYR:O	1:C:264:ALA:HA	2.19	0.42
2:D:165:LEU:O	2:D:169:LEU:HG	2.18	0.42
2:E:298:THR:HA	2:E:303:SER:HB2	2.01	0.42
1:A:244:TYR:CE1	1:A:301:LEU:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ARG:HH22	2:E:356:ARG:NH2	2.13	0.42
2:E:384:LEU:O	2:E:385:GLN:C	2.62	0.42
2:F:170:ILE:O	2:F:174:ALA:HB3	2.18	0.42
3:G:6:ILE:HG21	3:G:250:PHE:HB2	2.02	0.42
1:B:76:PHE:O	1:B:242:LEU:HD21	2.19	0.42
1:B:146:MET:SD	1:B:146:MET:C	3.02	0.42
1:C:233:SER:OG	1:C:235:THR:HG23	2.19	0.42
1:C:287:ARG:HA	1:C:288:PRO:HD3	1.78	0.42
1:C:444:VAL:CG1	1:C:469:LEU:HD13	2.49	0.42
2:F:370:VAL:HG22	2:F:442:GLN:HG2	2.01	0.42
1:A:485:THR:C	1:A:487:GLY:N	2.75	0.42
1:B:288:PRO:HB3	2:F:276:PRO:HG3	2.02	0.42
1:C:338:ILE:O	1:C:341:ASN:HB2	2.20	0.42
2:D:237:LEU:HD21	2:D:295:ARG:HB2	2.01	0.42
3:G:222:THR:O	3:G:226:SER:OG	2.37	0.42
1:A:484:ARG:O	1:A:485:THR:C	2.61	0.42
2:E:246:GLN:HA	2:E:246:GLN:HE21	1.85	0.42
1:A:138:PRO:HB3	1:A:316:PHE:CE1	2.55	0.42
1:A:159:ILE:CD1	1:A:165:GLU:HG2	2.49	0.42
1:A:468:PHE:CE1	1:A:501:VAL:HG12	2.54	0.42
1:B:481:GLY:HA2	1:B:484:ARG:NH1	2.35	0.42
1:C:244:TYR:CD2	1:C:281:MET:HE1	2.54	0.42
1:C:343:ILE:HG22	2:D:158:ALA:HB1	2.02	0.42
2:D:188:GLU:O	2:D:221:GLN:HB3	2.20	0.42
2:E:125:GLU:HA	2:E:300:LYS:HE3	2.02	0.42
1:A:175:LYS:HE3	1:A:175:LYS:HB2	1.77	0.42
1:A:389:THR:CB	1:A:449:VAL:HG21	2.38	0.42
1:C:127:ARG:NH2	1:C:131:LEU:HD12	2.35	0.42
1:C:179:ALA:HB1	1:C:267:ILE:HG12	2.01	0.42
2:E:189:ARG:O	2:E:190:THR:C	2.62	0.42
1:A:109:ASP:C	1:A:109:ASP:OD1	2.62	0.42
1:B:35:GLY:C	1:B:37:GLY:N	2.76	0.42
1:C:156:LEU:HD11	1:C:428:LEU:HD11	2.02	0.42
1:C:370:SER:O	1:C:371:VAL:HG12	2.20	0.42
2:D:181:SER:HB2	2:D:215:VAL:HG22	2.02	0.42
2:D:384:LEU:O	2:D:385:GLN:C	2.63	0.42
1:A:177:SER:OG	4:A:600:ANP:H8	2.20	0.42
1:B:105:GLY:HA2	1:B:226:MET:O	2.20	0.42
1:C:99:VAL:HG11	1:C:256:TYR:HB2	2.02	0.42
1:C:244:TYR:CE2	1:C:281:MET:HE1	2.55	0.42
2:D:29:LEU:HA	2:D:30:PRO:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:313:PRO:O	2:D:315:ASP:N	2.53	0.42
2:E:25:PHE:HB2	2:E:29:LEU:HD12	2.02	0.42
2:E:393:MET:HG3	2:E:396:LEU:CD1	2.50	0.42
2:F:82:ILE:O	2:F:115:ALA:HA	2.20	0.42
1:A:411:ASP:OD2	1:A:414:THR:HG23	2.20	0.41
1:B:137:ILE:HB	1:B:138:PRO:HD3	2.01	0.41
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.55	0.41
1:C:103:LEU:HB2	1:C:230:ILE:HD13	2.01	0.41
1:B:62:MET:HB2	1:B:76:PHE:CE2	2.54	0.41
1:B:80:LYS:HG3	1:B:81:LEU:N	2.34	0.41
2:D:163:THR:O	2:D:166:ILE:HG22	2.20	0.41
2:D:163:THR:O	2:D:164:VAL:C	2.63	0.41
2:D:370:VAL:O	2:D:374:VAL:HG23	2.20	0.41
2:F:247:GLU:HB3	2:F:249:GLN:HG2	2.02	0.41
2:F:439:LYS:HE3	2:F:443:GLN:OE1	2.20	0.41
1:A:24:ASP:C	1:A:26:GLU:H	2.28	0.41
1:B:102:GLU:CD	1:B:102:GLU:H	2.28	0.41
1:B:157:VAL:N	1:B:158:PRO:CD	2.84	0.41
2:E:94:ILE:HD11	2:E:197:TYR:CD1	2.55	0.41
2:E:330:ASP:O	2:E:356:ARG:HG3	2.19	0.41
2:D:287:THR:O	2:D:291:THR:HG23	2.21	0.41
2:D:409:LYS:HD3	2:D:457:PHE:CE1	2.55	0.41
2:E:32:ILE:O	2:E:33:LEU:HB2	2.20	0.41
1:A:188:ARG:HH21	1:A:437:ALA:N	2.18	0.41
1:B:151:LYS:HZ2	1:B:430:GLN:HB2	1.83	0.41
1:B:362:ARG:HA	1:B:363:PRO:C	2.44	0.41
1:C:295:PRO:HD2	1:C:298:VAL:HG22	2.01	0.41
2:E:126:MET:HB3	2:E:126:MET:HE3	1.82	0.41
2:E:147:ALA:HB2	2:E:357:ILE:HD13	2.02	0.41
2:E:422:GLU:O	2:E:424:PHE:N	2.53	0.41
1:C:265:LEU:HD11	1:C:324:LEU:HG	2.03	0.41
1:C:367:VAL:HG21	1:C:398:ARG:HH21	1.85	0.41
2:D:82:ILE:HB	2:D:116:ILE:HG12	2.03	0.41
2:E:421:ALA:O	2:E:422:GLU:C	2.63	0.41
2:F:139:VAL:HG11	2:F:348:VAL:HB	2.03	0.41
2:F:229:ARG:HA	2:F:232:VAL:HG22	2.03	0.41
1:B:211:SER:HA	2:E:126:MET:CE	2.47	0.41
1:C:505:LEU:O	1:C:508:PHE:HB3	2.20	0.41
2:D:346:PRO:HG3	2:D:418:PHE:CZ	2.56	0.41
2:E:36:LEU:HB2	2:E:47:LEU:HB2	2.03	0.41
3:G:209:LEU:O	3:G:210:ALA:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ILE:O	2:F:189:ARG:NE	2.53	0.41
1:C:396:GLN:HG3	2:D:458:TYR:CE2	2.55	0.41
2:D:339:ILE:O	2:D:340:ALA:C	2.63	0.41
2:D:340:ALA:HB2	2:D:347:ALA:CB	2.51	0.41
2:E:25:PHE:O	2:E:56:SER:HB3	2.21	0.41
2:E:292:MET:HE1	2:E:293:GLN:NE2	2.36	0.41
2:E:298:THR:HA	2:E:303:SER:CB	2.51	0.41
2:F:274:ARG:HA	8:F:2064:HOH:O	2.20	0.41
3:G:32:ALA:O	3:G:36:ARG:HG3	2.20	0.41
1:A:134:PRO:HG2	1:A:139:ARG:NH2	2.36	0.41
1:A:235:THR:HB	8:A:2038:HOH:O	2.21	0.41
1:A:251:CYS:O	1:A:255:GLU:HG3	2.21	0.41
1:A:283:LEU:CD2	1:A:289:PRO:HB3	2.50	0.41
1:A:394:LEU:HD23	1:A:394:LEU:HA	1.89	0.41
1:B:64:LEU:HG	1:B:65:ASN:ND2	2.34	0.41
1:B:172:GLN:HA	4:B:600:ANP:HNB1	1.85	0.41
1:B:423:ARG:HD2	1:B:461:ILE:HD11	2.02	0.41
1:C:432:GLN:NE2	8:C:2097:HOH:O	2.53	0.41
2:D:186:VAL:HG12	2:D:260:ARG:HB2	2.03	0.41
2:D:188:GLU:OE1	2:D:188:GLU:HA	2.21	0.41
2:D:275:ILE:HG23	2:D:276:PRO:HD2	2.02	0.41
2:F:285:LEU:C	2:F:285:LEU:HD23	2.46	0.41
2:F:438:ILE:O	2:F:442:GLN:HG3	2.21	0.41
2:D:92:GLY:HA2	2:D:206:ILE:HG12	2.02	0.41
2:D:189:ARG:O	2:D:221:GLN:OE1	2.38	0.41
2:D:210:ASP:HB2	2:D:211:ALA:H	1.69	0.41
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.56	0.41
2:E:254:PHE:CD1	2:E:307:VAL:HB	2.55	0.41
1:A:97:VAL:HB	1:A:98:PRO:CD	2.47	0.40
1:B:38:ILE:HD11	1:B:74:VAL:HG22	2.02	0.40
1:C:36:ASP:OD2	2:F:274:ARG:HD2	2.20	0.40
1:C:419:SER:HB3	1:C:423:ARG:HH12	1.85	0.40
2:D:47:LEU:HD23	2:D:62:ALA:HA	2.03	0.40
2:E:96:ASN:HD22	2:E:100:GLU:HB2	1.85	0.40
2:E:282:GLN:HA	2:E:283:PRO:HD3	1.80	0.40
2:F:89:GLU:OE2	2:F:110:THR:HG22	2.21	0.40
2:F:245:ASP:C	2:F:247:GLU:N	2.78	0.40
1:B:374:VAL:O	1:B:374:VAL:CG2	2.61	0.40
2:D:9:THR:HA	2:D:27:GLU:OE1	2.20	0.40
2:D:183:PHE:CD2	2:D:254:PHE:HB2	2.56	0.40
2:E:144:ALA:N	2:E:145:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:162:LYS:NZ	2:E:256:ASP:OD2	2.40	0.40
1:A:212:THR:HG23	2:D:356:ARG:HH12	1.86	0.40
1:B:133:ALA:O	1:B:134:PRO:C	2.64	0.40
1:B:140:ILE:CG2	1:B:311:LYS:HG3	2.51	0.40
1:C:74:VAL:CG1	1:C:241:PRO:CG	2.99	0.40
1:C:406:PHE:HE2	2:D:393:MET:HB2	1.86	0.40
1:C:450:ARG:HA	1:C:450:ARG:HD3	1.76	0.40
2:D:348:VAL:HG21	8:D:2027:HOH:O	2.22	0.40
2:E:321:ALA:N	2:E:322:PRO:HD2	2.36	0.40
2:E:412:ARG:O	2:E:415:SER:OG	2.36	0.40
1:A:327:ILE:HD12	1:A:338:ILE:HG22	2.03	0.40
1:C:139:ARG:HH11	1:C:139:ARG:HD3	1.59	0.40
1:A:80:LYS:HE3	2:D:33:LEU:HD12	2.02	0.40
1:B:194:ASP:OD2	1:B:196:LYS:HB2	2.21	0.40
1:B:496:LYS:HG2	1:B:500:ILE:HD11	2.02	0.40
1:C:373:ARG:HA	6:D:600:ADP:O3'	2.22	0.40
1:C:403:PHE:CG	2:D:408:ARG:NH2	2.89	0.40
3:G:39:LYS:HB2	3:G:40:PRO:HD3	2.02	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	485/510 (95%)	452 (93%)	25 (5%)	8 (2%)	7	15
1	B	475/510 (93%)	434 (91%)	38 (8%)	3 (1%)	21	39
1	C	490/510 (96%)	457 (93%)	28 (6%)	5 (1%)	12	26
2	D	465/482 (96%)	429 (92%)	32 (7%)	4 (1%)	14	28
2	E	464/482 (96%)	419 (90%)	40 (9%)	5 (1%)	11	23
2	F	464/482 (96%)	431 (93%)	31 (7%)	2 (0%)	30	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	116/272 (43%)	107 (92%)	6 (5%)	3 (3%)	4	6
All	All	2959/3248 (91%)	2729 (92%)	200 (7%)	30 (1%)	12	26

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	409	ASP
2	E	211	ALA
1	B	452	TYR
1	C	337	TYR
1	C	388	GLY
2	E	357	ILE
2	F	247	GLU
3	G	210	ALA
1	A	25	LEU
1	B	195	GLU
1	C	405	GLN
1	C	407	GLY
2	E	423	VAL
1	A	118	LYS
1	A	123	SER
1	A	141	SER
1	C	292	GLU
2	D	347	ALA
2	D	448	GLU
2	E	455	GLN
2	F	246	GLN
1	A	401	ALA
1	A	485	THR
3	G	211	ASN
1	B	95	VAL
1	A	500	ILE
3	G	81	ILE
2	D	81	PRO
2	E	279	VAL
2	D	279	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	393/412 (95%)	359 (91%)	34 (9%)	9	20
1	B	388/412 (94%)	361 (93%)	27 (7%)	14	29
1	C	397/412 (96%)	366 (92%)	31 (8%)	11	25
2	D	377/386 (98%)	352 (93%)	25 (7%)	15	32
2	E	376/386 (97%)	352 (94%)	24 (6%)	16	33
2	F	376/386 (97%)	353 (94%)	23 (6%)	17	35
3	G	102/230 (44%)	97 (95%)	5 (5%)	22	44
All	All	2409/2624 (92%)	2240 (93%)	169 (7%)	14	29

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	47	VAL
1	A	50	GLU
1	A	57	SER
1	A	60	LYS
1	A	63	SER
1	A	64	LEU
1	A	74	VAL
1	A	99	VAL
1	A	121	ILE
1	A	123	SER
1	A	136	ILE
1	A	140	ILE
1	A	211	SER
1	A	216	LEU
1	A	249	SER
1	A	270	ASP
1	A	276	VAL
1	A	338	ILE
1	A	354	THR
1	A	389	THR
1	A	408	SER
1	A	420	ARG
1	A	436	MET

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Mol	Chain	Res	Type
1	A	442	VAL
1	A	444	VAL
1	A	459	SER
1	A	460	LYS
1	A	461	ILE
1	A	462	THR
1	A	472	VAL
1	A	473	ILE
1	A	479	LEU
1	A	499	GLU
1	B	28	THR
1	B	52	MET
1	B	59	LEU
1	B	102	GLU
1	B	143	ARG
1	B	151	LYS
1	B	159	ILE
1	B	171	ARG
1	B	175	LYS
1	B	206	ILE
1	B	211	SER
1	B	216	LEU
1	B	217	VAL
1	B	218	LYS
1	B	237	SER
1	B	276	VAL
1	B	298	VAL
1	B	371	VAL
1	B	380	THR
1	B	384	LYS
1	B	389	THR
1	B	392	LEU
1	B	434	SER
1	B	440	GLU
1	B	445	ILE
1	B	459	SER
1	B	479	LEU
1	C	38	ILE
1	C	47	VAL
1	C	52	MET
1	C	57	SER
1	C	64	LEU

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Mol	Chain	Res	Type
1	C	80	LYS
1	C	83	LYS
1	C	123	SER
1	C	131	LEU
1	C	157	VAL
1	C	164	ARG
1	C	189	PHE
1	C	208	GLN
1	C	211	SER
1	C	217	VAL
1	C	307	GLU
1	C	334	VAL
1	C	349	GLN
1	C	371	VAL
1	C	390	MET
1	C	398	ARG
1	C	416	GLN
1	C	419	SER
1	C	423	ARG
1	C	444	VAL
1	C	459	SER
1	C	470	SER
1	C	472	VAL
1	C	474	SER
1	C	479	LEU
1	C	505	LEU
2	D	27	GLU
2	D	43	THR
2	D	44	ARG
2	D	89	GLU
2	D	95	MET
2	D	97	VAL
2	D	102	ILE
2	D	112	GLN
2	D	127	SER
2	D	128	VAL
2	D	130	GLN
2	D	137	ILE
2	D	139	VAL
2	D	154	LEU
2	D	210	ASP
2	D	212	THR

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Mol	Chain	Res	Type
2	D	232	VAL
2	D	282	GLN
2	D	291	THR
2	D	303	SER
2	D	325	THR
2	D	335	LEU
2	D	401	LYS
2	D	420	VAL
2	D	459	MET
2	E	43	THR
2	E	67	GLU
2	E	112	GLN
2	E	132	ILE
2	E	139	VAL
2	E	160	VAL
2	E	164	VAL
2	E	173	VAL
2	E	175	LYS
2	E	188	GLU
2	E	223	ASN
2	E	232	VAL
2	E	252	LEU
2	E	277	SER
2	E	279	VAL
2	E	282	GLN
2	E	297	THR
2	E	306	SER
2	E	339	ILE
2	E	358	MET
2	E	365	SER
2	E	377	ILE
2	E	395	GLU
2	E	431	LEU
2	F	41	ARG
2	F	51	GLN
2	F	67	GLU
2	F	76	LEU
2	F	89	GLU
2	F	95	MET
2	F	96	ASN
2	F	97	VAL
2	F	110	THR

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Mol	Chain	Res	Type
2	F	124	VAL
2	F	139	VAL
2	F	166	ILE
2	F	223	ASN
2	F	232	VAL
2	F	237	LEU
2	F	258	ILE
2	F	274	ARG
2	F	279	VAL
2	F	282	GLN
2	F	292	MET
2	F	396	LEU
2	F	405	SER
2	F	420	VAL
3	G	77	LEU
3	G	83	SER
3	G	220	SER
3	G	236	SER
3	G	262	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	330	GLN
1	A	379	GLN
1	A	405	GLN
1	A	471	HIS
1	A	475	GLN
1	B	65	ASN
1	B	186	GLN
1	B	243	GLN
1	B	366	ASN
1	B	432	GLN
1	B	503	ASN
1	C	46	ASN
1	C	172	GLN
1	C	215	GLN
1	C	263	HIS
1	C	405	GLN
1	C	415	GLN
1	C	476	HIS

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Mol	Chain	Res	Type
2	D	171	ASN
2	D	172	ASN
2	D	198	HIS
2	D	221	GLN
2	D	282	GLN
2	D	419	GLN
2	E	223	ASN
2	E	246	GLN
2	E	282	GLN
2	E	293	GLN
2	E	308	GLN
2	E	419	GLN
2	E	442	GLN
2	E	455	GLN
2	F	223	ASN
2	F	249	GLN
2	F	282	GLN
2	F	375	GLN
2	F	411	GLN
2	F	443	GLN
3	G	82	HIS
3	G	211	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](#)

Of 11 ligands modelled in this entry, 5 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
4	ANP	A	600	5	33,33,33	1.47	5 (15%)	45,52,52	1.29	5 (11%)
7	PO4	E	602	-	4,4,4	0.81	0	6,6,6	0.55	0
4	ANP	C	600	5	33,33,33	1.66	8 (24%)	45,52,52	1.34	6 (13%)
4	ANP	B	600	5	33,33,33	1.65	7 (21%)	45,52,52	2.28	6 (13%)
4	ANP	F	600	5	33,33,33	1.55	7 (21%)	45,52,52	1.34	6 (13%)
6	ADP	D	600	5	28,29,29	1.25	3 (10%)	43,45,45	1.08	4 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	A	600	5	-	3/18/38/38	0/3/3/3
4	ANP	C	600	5	-	3/18/38/38	0/3/3/3
4	ANP	B	600	5	-	3/18/38/38	0/3/3/3
4	ANP	F	600	5	-	4/18/38/38	0/3/3/3
6	ADP	D	600	5	-	5/16/32/32	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	ANP	PG-O3G	-4.40	1.45	1.56
4	C	600	ANP	PG-O3G	-4.06	1.46	1.56
6	D	600	ADP	PA-O3A	3.79	1.63	1.59
4	F	600	ANP	PG-O3G	-3.74	1.46	1.56
4	C	600	ANP	PB-O3A	-3.67	1.54	1.59
4	A	600	ANP	PG-O3G	-3.50	1.47	1.56
4	B	600	ANP	PG-O1G	3.49	1.51	1.46
4	F	600	ANP	PB-O1B	3.43	1.51	1.46
4	B	600	ANP	PA-O3A	3.43	1.63	1.59
4	A	600	ANP	PB-O2B	-3.42	1.47	1.56
4	C	600	ANP	PG-O2G	-3.38	1.47	1.56
4	A	600	ANP	PG-O2G	-3.34	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	600	ANP	PA-O3A	3.29	1.63	1.59
4	C	600	ANP	PB-O2B	-3.21	1.48	1.56
4	F	600	ANP	PB-O2B	-3.08	1.48	1.56
4	A	600	ANP	PB-O3A	3.06	1.62	1.59
4	A	600	ANP	C2-N1	2.92	1.39	1.33
4	F	600	ANP	PG-O2G	-2.86	1.49	1.56
4	B	600	ANP	PG-O2G	-2.64	1.49	1.56
4	F	600	ANP	C2-N1	2.48	1.38	1.33
4	B	600	ANP	PB-O3A	2.45	1.62	1.59
4	C	600	ANP	C2-N1	2.42	1.38	1.33
4	F	600	ANP	PA-O3A	-2.39	1.56	1.59
4	B	600	ANP	PG-N3B	-2.37	1.57	1.63
4	C	600	ANP	PB-N3B	2.25	1.69	1.63
4	B	600	ANP	C2-N1	2.25	1.37	1.33
4	C	600	ANP	C2-N3	-2.18	1.30	1.33
6	D	600	ADP	PB-O2B	-2.16	1.46	1.54
4	F	600	ANP	C2-N3	-2.14	1.30	1.33
6	D	600	ADP	PB-O3B	-2.13	1.46	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	ANP	O1B-PB-N3B	12.61	130.33	111.77
4	A	600	ANP	O2B-PB-O1B	4.50	119.52	109.87
4	B	600	ANP	O2G-PG-O1G	-4.18	102.97	113.45
4	C	600	ANP	O2B-PB-O3A	3.35	115.81	104.64
4	C	600	ANP	O2G-PG-O3G	3.30	116.45	107.59
4	F	600	ANP	O3A-PA-O1A	3.26	120.51	110.70
4	F	600	ANP	O2G-PG-O3G	3.19	116.17	107.59
4	F	600	ANP	O1G-PG-N3B	-3.11	107.19	111.77
4	F	600	ANP	N6-C6-N1	-2.91	111.89	118.38
4	B	600	ANP	O2G-PG-O3G	2.85	115.25	107.59
4	C	600	ANP	O2G-PG-O1G	-2.77	106.50	113.45
4	F	600	ANP	C5-C6-N6	2.77	130.15	123.29
4	A	600	ANP	O1B-PB-N3B	2.69	115.73	111.77
4	A	600	ANP	O2G-PG-O3G	2.55	114.44	107.59
4	B	600	ANP	C2'-C3'-C4'	2.52	107.48	102.61
6	D	600	ADP	O2B-PB-O3A	2.48	112.96	104.64
4	C	600	ANP	O3A-PB-N3B	-2.33	100.13	106.59
4	C	600	ANP	C2'-C3'-C4'	2.33	107.10	102.61
6	D	600	ADP	C1'-N9-C8	2.26	132.10	127.09
4	F	600	ANP	O2B-PB-O3A	2.26	112.17	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	600	ADP	O3B-PB-O2B	2.21	116.07	107.80
4	A	600	ANP	O2G-PG-O1G	-2.18	107.99	113.45
6	D	600	ADP	C4-N9-C1'	-2.14	121.64	126.63
4	C	600	ANP	O1G-PG-N3B	-2.11	108.66	111.77
4	B	600	ANP	O3A-PB-N3B	-2.09	100.80	106.59
4	A	600	ANP	C2'-C1'-N9	-2.04	108.24	113.30
4	B	600	ANP	C4'-O4'-C1'	2.01	113.91	109.47

There are no chirality outliers.

All (18) torsion outliers are listed below:

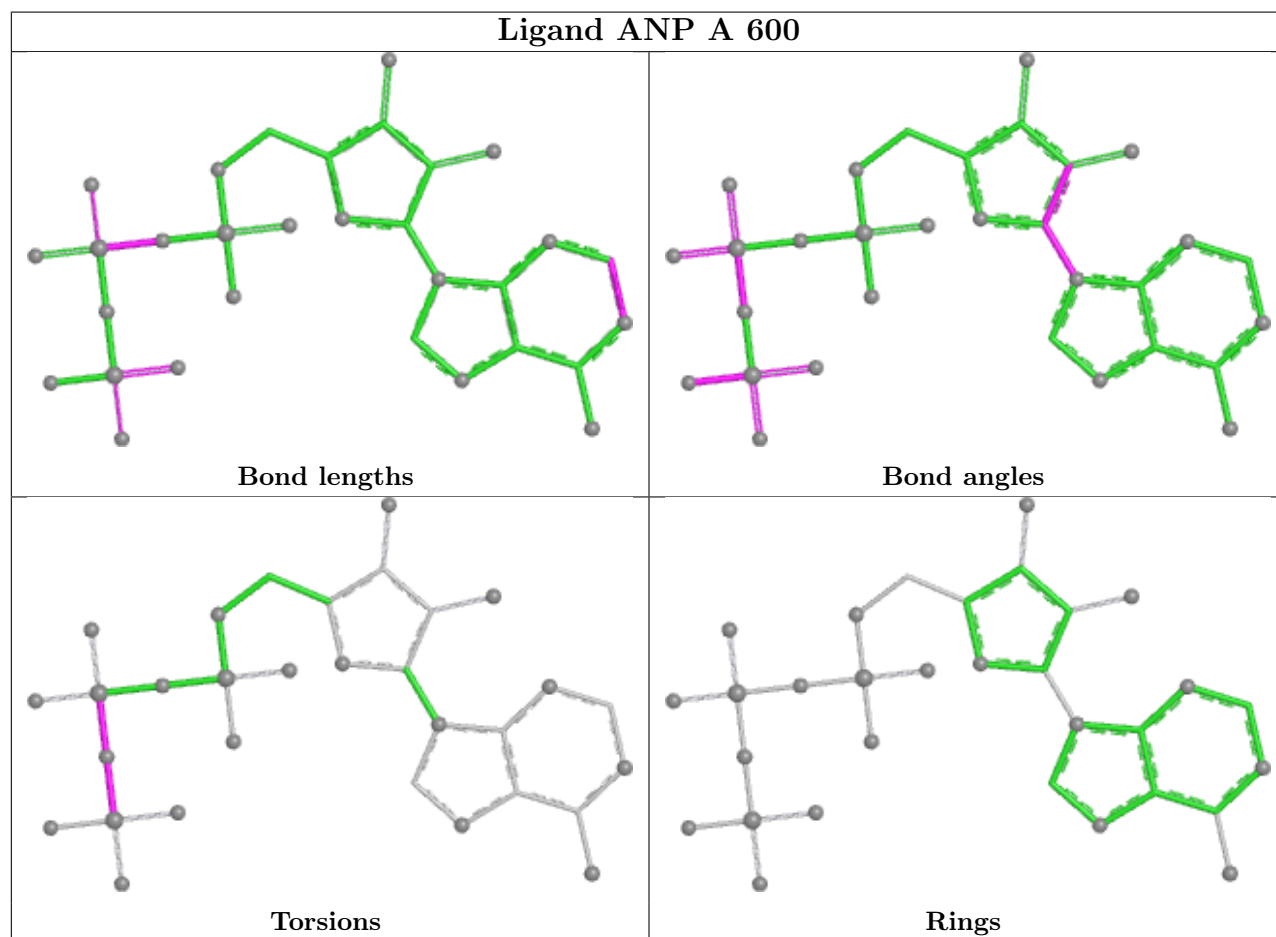
Mol	Chain	Res	Type	Atoms
4	A	600	ANP	PB-N3B-PG-O1G
4	A	600	ANP	PG-N3B-PB-O1B
4	B	600	ANP	PB-N3B-PG-O1G
4	B	600	ANP	PG-N3B-PB-O1B
4	C	600	ANP	PB-N3B-PG-O1G
4	C	600	ANP	PG-N3B-PB-O1B
4	C	600	ANP	PG-N3B-PB-O3A
4	F	600	ANP	PB-N3B-PG-O1G
4	F	600	ANP	PG-N3B-PB-O1B
4	F	600	ANP	PA-O3A-PB-O2B
6	D	600	ADP	PA-O3A-PB-O2B
6	D	600	ADP	C5'-O5'-PA-O3A
6	D	600	ADP	C3'-C4'-C5'-O5'
6	D	600	ADP	O4'-C4'-C5'-O5'
6	D	600	ADP	PA-O3A-PB-O3B
4	B	600	ANP	PA-O3A-PB-O1B
4	F	600	ANP	PA-O3A-PB-O1B
4	A	600	ANP	PG-N3B-PB-O3A

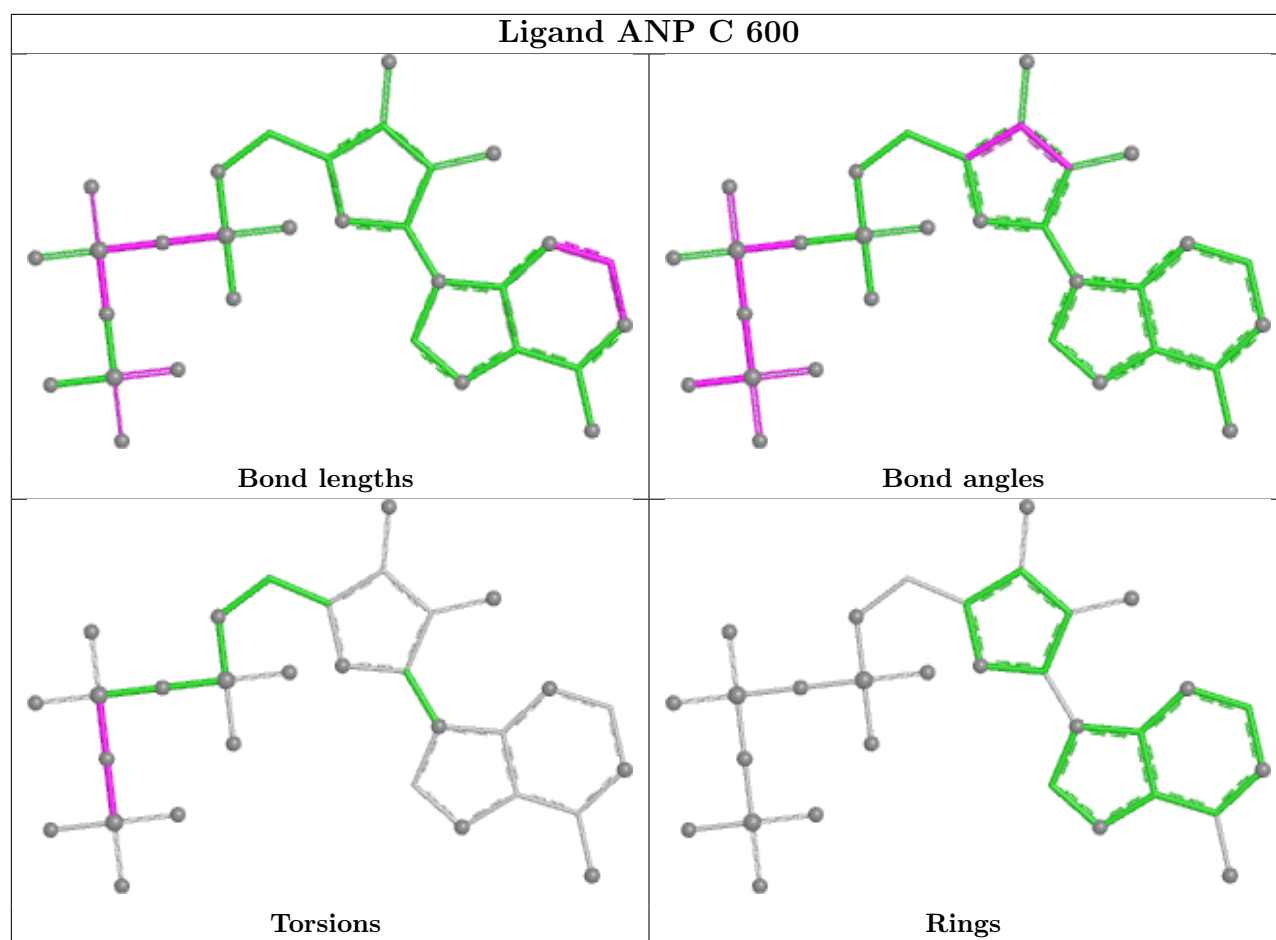
There are no ring outliers.

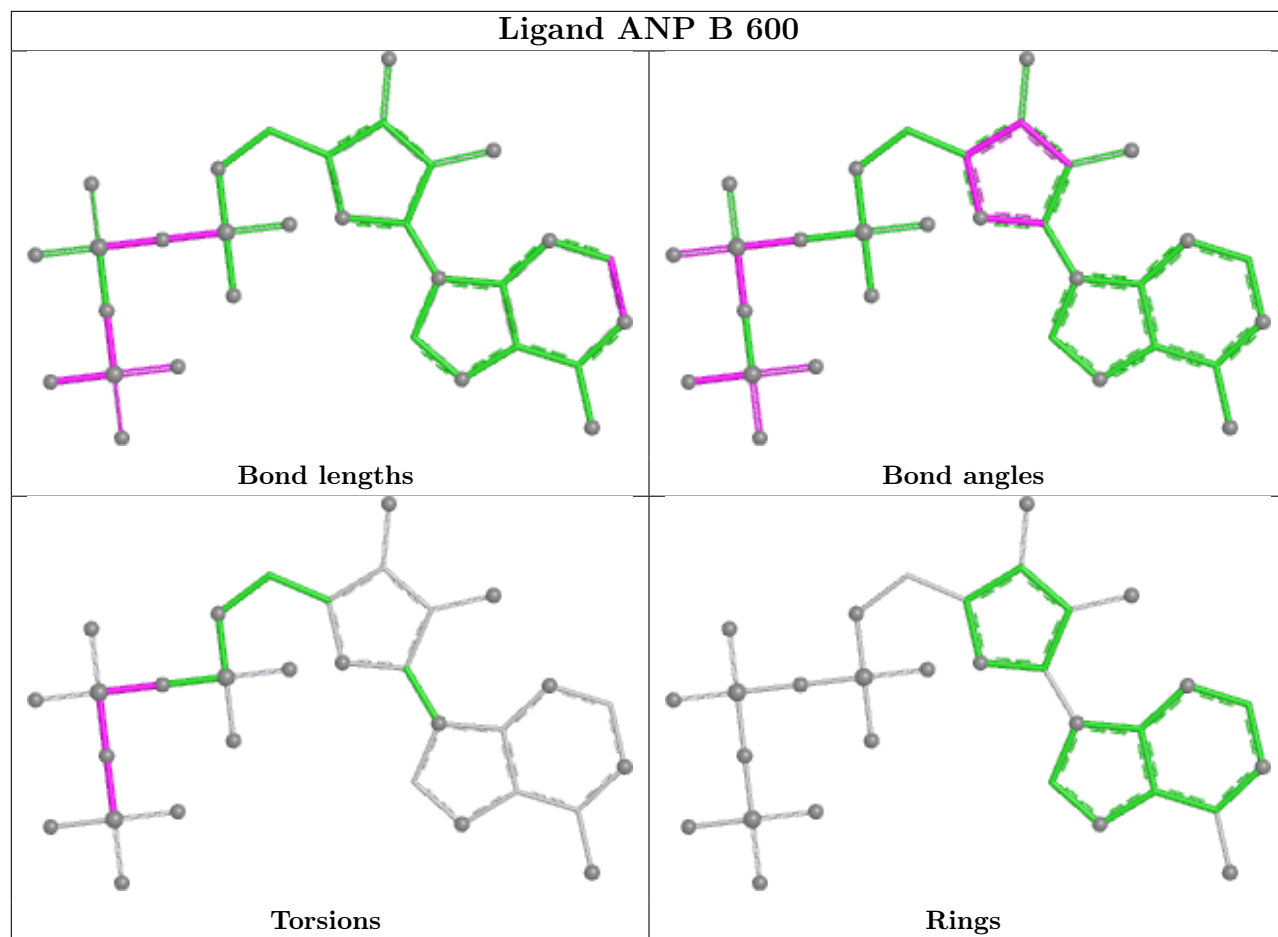
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	ANP	1	0
7	E	602	PO4	1	0
4	C	600	ANP	2	0
4	B	600	ANP	2	0
6	D	600	ADP	1	0

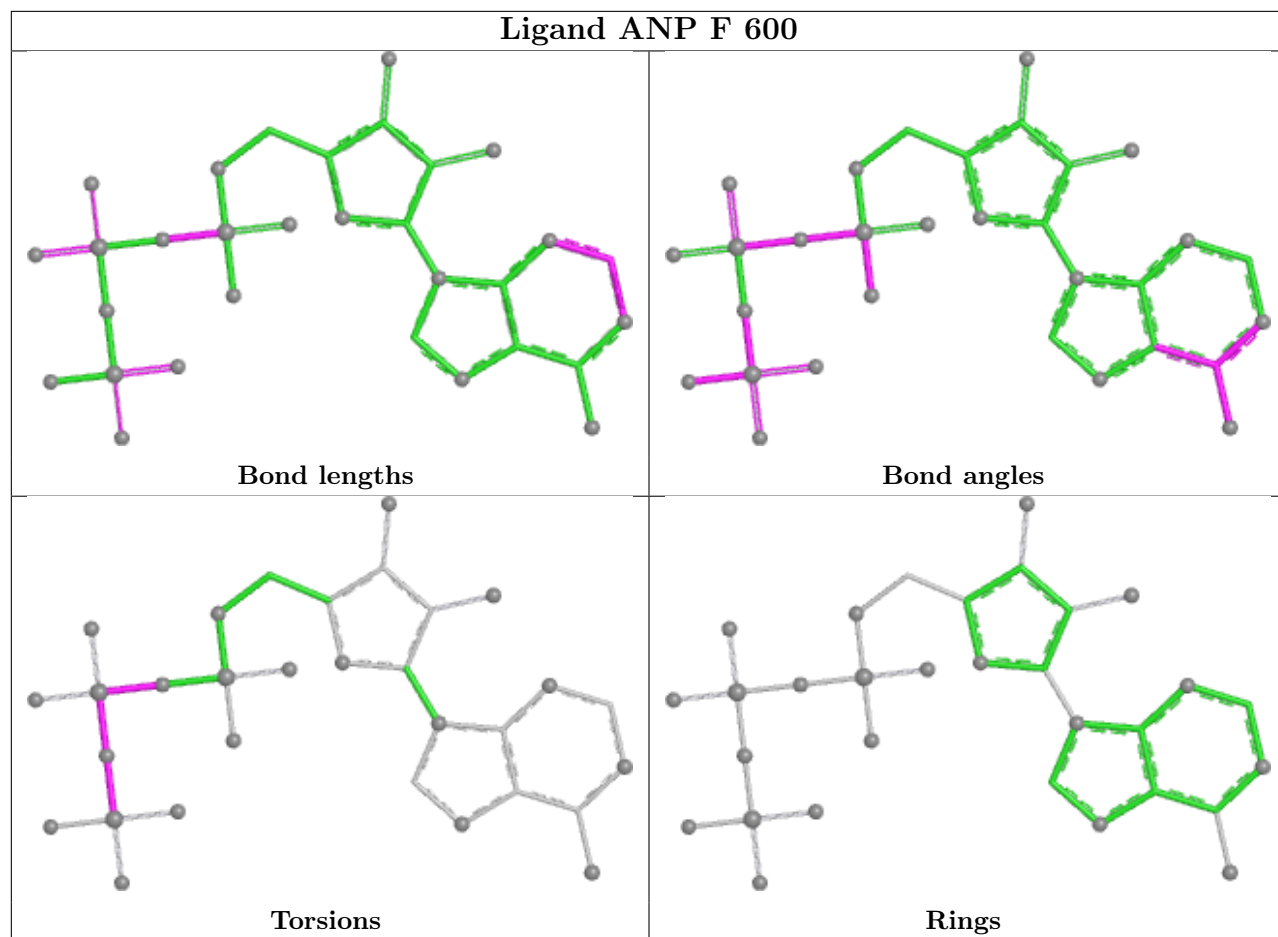
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



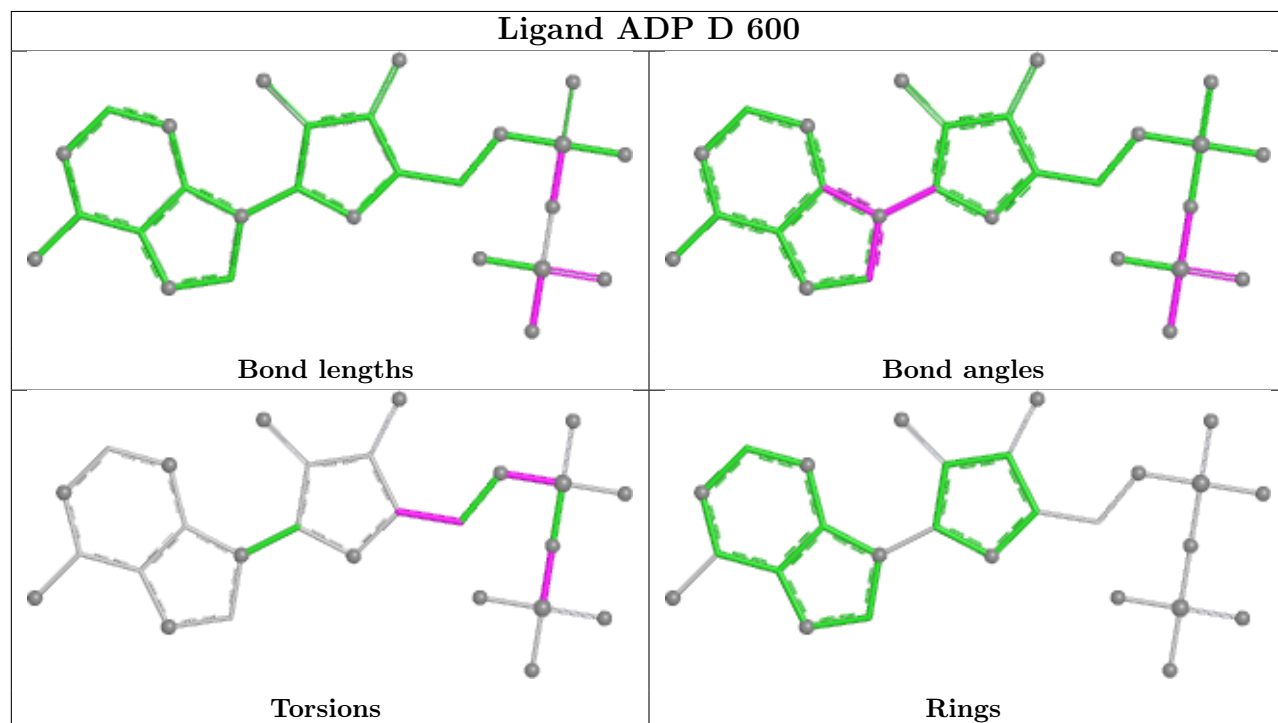




Ligand ANP F 600



Ligand ADP D 600



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.